Publication Series of the John von Neumann Institute for Computing (NIC)
NIC Series Volume 8

John von Neumann Institute for Computing (NIC)

Friedel Hossfeld, Kurt Binder (Editors)

Europhysics Conference on Computational Physics 2001

5 - 8 September 2001, Aachen, Germany

Book of Abstracts

organized by
John von Neumann Institute for Computing

NIC Series Volume 8

ISBN 3-00-008236-0

Die Deutsche Bibliothek – CIP-Cataloguing-in-Publication-Data
A catalogue record for this publication is available from Die Deutsche Bibliothek.

Publisher: NIC-Directors

Distributor: NIC-Secretariat
Research Centre Jülich
52425 Jülich
Germany

Internet: www.fz-juelich.de/nic

Printer: Graphische Betriebe, Forschungszentrum Jülich

NIC Series Volume 8
ISBN 3-00-008236-0

Preface

Computational Physics is today well-established as the third branch of physics in addition to experiment and theory. Research investigations range from small computer experiments on laptops to extended simulations which can only be performed by high-end supercomputers. Applications are found in almost every area of modern physics.

The Conference on Computational Physics 2001 (CCP 2001) is already the 13th in an international series of conferences which has served as a lively forum for computational physicists from around the world. The previous conferences were held in Boston (1989), Amsterdam (1990), San Jose (1991), Prague (1992), Albuquerque (1993), Lugano (1994), Pittsburgh (1995), Cracow (1996), Santa Cruz (1997), Granada (1998), Atlanta (1999), and Brisbane (2000). The CCP series is held jointly under the auspices of the Commission on Computational Physics (C20) of the International Union of Pure and Applied Physics (IUPAP), the Computational Physics Group of the European Physical Society (EPS), and the Division of Computational Physics of the American Physical Society (APS). Since 1997, the conferences have been part of the CCP series which succeeded the EPS-APS Joint Conferences "Physics Computing" (PC) organized annually since 1989.

CCP 2001 is organized by the John von Neumann Institute for Computing (NIC), which was founded jointly by Forschungszentrum Jülich and Deutsches Elektronen-Synchrotron DESY in order to support supercomputer-aided scienti£c research and development in Germany. Its major objectives are the nationwide provision of supercomputer capacity for research projects in the £elds of modeling and computer simulation, the supercomputer-oriented research and development in selected £elds of physics and other natural sciences by research groups in supercomputing applications, and education and training in scienti£c computing by organizing conferences, workshops, schools and courses. The latter objective in particular motivated the NIC's application to the Computational Physics Group of EPS to organize this year's Conference on Computational Physics.

The CCP series covers all £elds of computational physics, this year summarized by the motto

Computational Modeling and Simulation of Complex Systems

The following topics are treated in 16 invited plenary presentations, 48 invited talks, 72 oral contributions and nearly 300 posters:

- Materials Science
  (Electronic Structure, Ab-Initio Molecular Dynamics, Nanostructures, etc.)
- Soft Matter (Polymers, Membranes, Proteins, etc.)
- Common Themes in Computational Statistical Physics and Lattice Gauge Theory
- Particle Beams and Accelerator Physics
- Astrophysics
- Turbulence and Reactive Flows
- Interdisciplinary Applications (Econophysics, Traf£c Flow, etc.)
- Frontiers in Large Scale Computing
- Methodological Developments in Computer Simulation

The programme was compiled by the Local Programme Committee, which selected the plenary and invited speakers from suggestions given by the International Advisory Committee, and organized a refereeing process for the submitted oral and poster contributions. We wish to heartily thank all members of these various committees for their invaluable help.

Many organizations and individuals have contributed signi£cantly to the success of the conference. We are grateful for the generous £nancial support provided by Deutsche Forschungsgemeinschaft (DFG) and the Federal Ministry for Education and Research (BMBF), by the Deutsche Physikalische Gesellschaft

(DPG) and the Wilhelm und Else Heraeus-Stiftung, by the International Union of Pure and Applied Physics (IUPAP), the European Physical Society (EPS) and its East-West Task Force (EWTF), and last but not least by the Forschungszentrum Jülich. The American Physical Society (APS) formally endorsed the conference.

The £nancial support of Wilhelm und Else Heraeus-Stiftung, BMBF, IUPAP, and Forschungszentrum Jülich enabled us to give more than 70 travel grants to conference attendees from developing and former east-block countries. This allowed the conference continue the tradition of the CCP series to be a place of intense exchange of scienti£c ideas and results between East and West, North and South.

Special thanks are due to Cray Inc. and the Verein der Freunde und Förderer der KFA for additional support.

For their most valuable help with the local arrangements we are greatly indebted to the Local Organization Committee of the Forschungszentrum Jülich who performed the lion's share of the work, namely Rüdiger Esser, Bernhard Krahl-Urban, Manfred Kremer, and Jörg Striegnitz, and last but not least the conference secretaries Elke Bielitza, Erika Wittig, and Yasmin Abdel-Fattah. Furthermore, we appreciate the work of Karolin Laukamp and Petra Thelen from the Aachen Tourist Service, who processed the registration and accomodation requests. Special thanks go to Anke Häming for her commitment concerning the composition and realization of this Book of Abstracts.

Jülich, September 2001

Friedel Hossfeld Kurt Binder Norbert Attig

Sponsoring Organizations

International Union of Pure and Applied Physics (IUPAP)
European Physical Society (EPS)
American Physical Society (APS)

Conference Chairmen

Friedel Hoßfeld (Chairman), NIC/ZAM, Forschungszentrum Jülich, Germany
Kurt Binder (Vice-Chairman), University of Mainz, Germany
Norbert Attig (Scienti£c Secretary), NIC/ZAM, Forschungszentrum Jülich, Germany

International Advisory Committee

Joan Adler, Israel Institute of Technology, Haifa, Israel
Ezequiel V. Albano, University of La Plata, Argentina
M.P. Allen, University of Bristol, UK
Per Bak, Imperial College, London, UK
Peter H. Borcherds, University of Birmingham, UK
Marian Bubak, Institute of Computer Science and ACC CYFRONET, AGH, Cracow, Poland
William J. Camp, Sandia National Laboratories, Albuquerque, USA
Bikas K. Chakrabarti, Saha Institute of Nuclear Physics, India
Rashmi C. Desai, University of Toronto, Canada
Masao Doi, Nagoya University, Japan
Peter D. Drummond, University of Queensland, Brisbane, Australia
Daan Frenkel, FOM-AMOLF, Amsterdam, The Netherlands
Lucio Grandinetti, University of Calabria, Rende, Italy
Ralf Gruber, École Polytechnique Fédérale de Lausanne, Switzerland
Alex Hansen, University of Trondheim, Norway
Richard D. Kenway, University of Edinburgh, UK
Janos Kertesz, Technical University of Budapest, Hungary
David P. Landau, University of Georgia, Athens, USA
Michel Marechal, CECAM, Lyon, France
Joaquin Marro, University of Granada, Spain
Ole G. Mouritsen, Technical University of Denmark, Lyngby, Denmark
Jaroslav Nadrchal, Institute of Physics - AVCR, Prague, Czech Republic
Risto Nieminen, Helsinki University of Technology, Finland
Michele Parrinello, MPI for Solid State Physics, Stuttgart, Germany
Charles H. Patterson, Trinity College, Dublin, Ireland
Sanjay Puri, Jawaharlal Nehru University, New Dehli, India
Claudio Rebbi, Boston University, USA
Dongsu Ryu, Chungnam National University, South Korea
Helmut Satz, University of Bielefeld, Germany
Klaus Schulten, University of Illinois, Urbana, USA
Lev N. Shchur, Landau Institute, Chernogolovka, Russia
Chandra V. Sheth, University of Zambia, Zambia
Horst D. Simon, Lawrence Berkeley National Laboratory, Berkeley, USA
Peter M.A. Sloot, University of Amsterdam, The Netherlands
Constantino Tsallis, National Academy of Sciences of Brazil
Pavel N. Vorontsov-Velyaminov, Saint Petersburg State University, Russia
Jian-Sheng Wang, National University of Singapore, Republic of Singapore
Jürgen Warnatz, University of Heidelberg, Germany
A. Peter Young, University of California, Santa Cruz, USA

Local Programme Committee

Norbert Attig, NIC/ZAM, Forschungszentrum Jülich
Peter L. Biermann, Max Planck Institute for Radio Astronomy, Bonn
Kurt Binder, University of Mainz
Peter Grassberger, NIC, Forschungszentrum Jülich
Siegfried Großmann, University of Marburg
Friedel Hoßfeld, NIC/ZAM, Forschungszentrum Jülich
Heiner Müller-Krumbhaar, IFF, Forschungszentrum Jülich
Michael Müller-Preußker, Humboldt University of Berlin
Horst Rollnik, University of Bonn
Walter Selke, University of Technology Aachen
Dietrich Stauffer, University of Cologne
Dietrich Wolf, University of Duisburg

Local Organizing Committee

Friedel Hoßfeld, Conference Chairman
Norbert Attig, Scienti£c Secretary
Bernd Krahl-Urban, Conference Arrangements
Rüdiger Esser, Finance and Grants
Manfred Kremer, Proceedings
Jörg Striegnitz, Public Relations
Anke Häming, Contribution Management
Elke Bielitza, Conference Secretary and Grants
Erika Wittig, Conference Secretary
Yasmin Abdel-Fattah, Conference Secretary

all from Forschungszentrum Jülich

Structure of the Conference

Wednesday 5th	**Thursday 6th**	**Friday 7th**	**Saturday 8th**
09:00 P1 D. Frenkel	09:00 P5 D. Ceperley	09:00 P9 H.D. Simon	09:00 P13 H. Satz
09:45 P2 M. Klein	09:45 P6 M. Schef¤er	09:45 P10 C.S. Frenk	09:45 P14 B. Berg
Coffee break	10:30 P7 D. Sornette	Coffee break	
11:00 P3 J. Yeomans	Coffee break	11:00 P11 G. Wittum	11:00 P15 H. Blöte
11:45 P4 F. Esquembre	11:45 P8 K. Binder	11:45 P12 M. Newman	11:45 P16 P. Grassberger
12.30 Lunch break			12:45 End of Conference
14:00 Parallel sessions Invited Talks and Oral Contributions			
Coffee break			
16:30 Parallel Sessions Invited Talks and Oral Contributions			
18:30 Poster Session A		18:30 Poster Session B	

Wednesday, 5 September 2001

8:45 - **Registration** (continued) and Mounting of Posters

Plenary Sessions *Lecture Hall Brüssel*

8:45 - 9:00 Opening

9:00 - 10:30 **Session 1: Plenary Session I**

9:00 D. Frenkel; FOM-Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands
P 1 Simulating crystal nucleation rates
9:45 M. Klein; University of Pennsylvania, Philadelphia, USA
P 2 Computer simulations studies of biomolecules at soft interfaces

10:30 - 11:00 Coffee Break

11:00 - 11:45 **Session 2: Plenary Session II**

11:00 J. Yeomans; University of Oxford, U.K.
P 3 Simulations of liquid crystal hydrodynamics
11:45 F. Esquembre; University of Murcia, Spain
P 4 Computers in physics education

12:30 - 14:00 Lunch Break

Parallel Sessions *Lecture Hall Brüssel, Rooms K3 – K5*

14:00 - 16:00 Parallel Sessions 3,5,7,9

16:00 - 16:30 Coffee Break

16:30 - 18:30 Parallel Sessions 4,6,8,10

Poster Session A *Rooms K1 / K2*

18:30 - 20:00 Poster Session A and Reception

Wednesday, 5 September 2001

Sessions 3 and 4 *Lecture Hall Brüssel*

14:00 - 16:00 **Session 3: Material Science: Many-Body Quantum Mechanics and Methodical Developments**

14:00 K. Schwarz; Technical University of Vienna, Austria
I 1 Electronic structure calculations of solids using the WIEN2k package for materials science
14:30 K. Hukushima; University of Tokyo, Kashiwa, Japan
I 2 Extended ensemble Monte Carlo approach to hardly-relaxing problems
15:00 M.H. Müser and F. Krajewski; University of Mainz, Germany
O 1 On new ef£cient algorithms for PIMC and PIMD
15:20 T. Sakai and Y. Takahashi*; Tokyo Metropolitan Institute of Technology, Japan, *Himeji Institute of Technology, Hyogo, Japan
O 2 Finite-temperature Lanczos algorithm study on pseudogap in high-T_c superconductors
15:40 P.H. Borcherds; University of Birmingham, U.K.
O 3 A computational study of some Josephson junction circuits

16:00 Coffee break

16:30 - 18:30 **Session 4: Materials Science: Structure and Magnetism**

16:30 K. Kaski; Helsinki University of Technology, Espoo, Finland
I 3 Computational studies of carbon nanotube structures
17:00 A.P. Lyubartsev; Stockholm University, Sweden
I 4 Inverse Monte Carlo method and its application to compute effective potentials
17:30 G. Bihlmayer, Ph. Kurz et al.; Forschungszentrum Jülich, Germany
O 4 Ab-initio prediction of complex magnetic structures in low dimensions
17:50 V.S. Stepanyuk[1,2], D.I. Bazhanov[1,3] et al.; [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany, [2]University of Halle-Wittenberg, Germany, [3]Moscow State University, Russia
O 5 Quasi-ab initio molecular dynamics simulations of atomic scale structures on metal surfaces
18:10 S.-H. Tsai, A. Bunker, D.P. Landau; University of Georgia, Athens, USA
O 6 Dynamic critical behavior of the classical anisotropic BCC Heisenberg antiferromagnet

Wednesday, 5 September 2001

Sessions 5 and 6 ***Room K3***

14:00 - 16:00 **Session 5: Soft Matter: Polymers; Colloids**

14:00 F. Schmid; University of Bielefeld, Germany
I 5 Surface anchoring on liquid crystalline polymer brushes
14:30 B. Jönsson; University of Lund, Sweden
I 6 Ion-ion correlations in charged colloidal systems
15:00 R. Messina, Ch. Holm, K. Kremer; Max-Planck-Institute for Polymer Research, Mainz, Germany
O 7 Strong electrostatic interactions in colloidal systems
15:20 C. Micheletti, A. Maritan et al.; International School for Advanced Studies, Trieste, Italy
O 8 Optimal shapes of compact strings
15:40 Ch. Seidel; Max-Planck-Institut für Kolloid- und Grenz¤ächenforschung, Golm, Germany
O 9 Molecular dynamics study of polyelectrolyte brushes

16:00 Coffee break

16:30 - 18:30 **Session 6: Soft Matter: Wetting Phenomena; Polymers**

16:30 S. Puri; Jawaharlal Nehru University, New Dehli, India
I 7 Kinetics of wetting and phase separation at surfaces
17:00 M. Müller; University of Mainz, Germany
I 8 Interplay between wetting and miscibility in thin binary polymer £lms
17:30 A.V. Lyulin and M.A.J. Michels; Eindhoven University of Technology and Dutch Polymer Institute, The Netherlands
O 10 Large-scale computer simulation of local segmental dynamics in amorphous atactic polystyrene
17:50 A. Milchev[1,2] and K. Binder[2]; [1]Bulgarian Academy of Sciences, So£a, Bulgaria, [2]University of Mainz, Germany
O 11 Dynamics of droplet spreading
18:10 A.A. Rzepiela; Wageningen University, The Netherlands
O 12 Large shear deformation of particle gels studied by Brownian dynamics simulations

Wednesday, 5 September 2001

Sessions 7 and 8 *Room K4*

14:00 - 16:00 **Session 7: Common Themes in Computational Statistical Physics and Lattice Gauge Theory I**

14:00 W. Janke; University of Leipzig, Germany
I 9 Numerical tests of CFT conjectures for 3D systems
14:30 U.-J. Wiese; University of Bern, Switzerland
I 10 Meron-cluster solution of fermion and other sign problems
15:00 A. Krug[1,2] and A. Buchleitner[1]; [1]Max-Planck-Institute for Physics and Complex Systems, Dresden, Germany, [2]Max-Planck-Institute for Quantum Optics, Garching, Germany
O 13 Chaotic ionization of non-classical alkali Rydberg states – Computational physics beats experiment
15:20 Ch. Gattringer and C.B. Lang*; University of Regensburg, Germany, *University of Graz, Austria
O 14 Improving the Dirac operator in lattice QCD
15:40 S.H. Meyer; University of Kaiserslautern, Germany
O 15 Universal ¤uctuations of Dirac spectra in QCD

16:00 Coffee break

16:30 - 18:30 **Session 8: Common Themes in Computational Statistical Physics and Lattice Gauge Theory II**

16:30 P.M.C. de Oliveira; Universidade Federal Fluminense, Niteroi RJ, Brasil
I 11 A simple dynamics for broad histogram method
17:00 N. Hatano; Aoyama Gakuin University, Tokyo, Japan
I 12 Double degeneracy in the ground state of the 3D $\pm$ J spin glass
17:30 M. Henkel[1] and M. Pleimling[1,2]; [1]University of Nancy, France, [2]University of Erlangen-Nürnberg, Germany
O 16 Anisotropic scaling and generalized conformal invariance at Lifshitz points
17:50 G. Münster and Ch. Kamp; University of Münster, Germany
O 17 Distribution of instanton sizes in a simpli£ed instanton gas model
18:10 J. Hove, S. Mo and A. Sudbø; Norwegian University of Science and Technology, Trondheim, Norway
O 18 The fractal dimension of the critical ¤uctuations in Abelian gauge theories

Wednesday, 5 September 2001

Sessions 9 and 10 *Room K5*

14:00 - 16:00 **Session 9: Methodical Aspects of Monte Carlo and Molecular Dynamics Simulations**

14:00 M.A. Novotny; Florida State University, Tallahassee, USA
I 13 Magnetization reversal using novel new event-driven Monte Carlo algorithms
14:30 J. Adler; Technion - Israel Institute of Technology, Haifa, Israel
I 14 Visualization of MD and MC simulations for atomistic modeling
15:00 G. Wagner[1,2], E.G. Flekkøy[2,3] et al.; [1]Technion Institute of Technology, Haifa, Israel, [2]Fracton as, Oslo, Norway, [3]University of Oslo, Norway
O 19 Coupling molecular dynamics and continuum dynamics
15:20 D.P. Landau and F. Wang; University of Georgia, Athens, USA
O 20 Determining the density of states for classical statistical models: A random walk algorithm to produce a ¤at histogram
15:40 J. Houdayer; University of Mainz, Germany
O 21 A cluster Monte Carlo algorithm for 2-dimensional spin glasses

16:00 Coffee break

16:30 - 18:10 **Session 10: Methodical Developments in High Energy and Plasma Physics Simulations**

16:30 G.E. Norman; Moscow State University, Russia
I 15 Stochastic and dynamic properties of MD systems: Simple liquids, plasma and electrolytes, polymers, etc.
17:00 D. Perret-Gallix; LAPP, Annecy-le-Vieux, France
I 16 Simulation and event generation in high-energy physics
17:30 A.N. Fedorova and M.G. Zeitlin; Russian Academy of Sciences, St. Petersburg, Russia
O 22 Pattern formation and coherent structures in collective models from accelerator physics
17:50 C. Heerlein and C. Toepffer; University of Erlangen, Germany
O 23 Vlasov Poisson solver for density enhancement near ions at rest in magnetized electron plasmas

Thursday, 6 September 2001

Plenary Sessions *Lecture Hall Brüssel*

9:00 - 11:15 **Session 11: Plenary Session III**

9:00	D.M. Ceperley; University of Illinois, Urbana, USA
P 5	**Methods for coupled quantum-classical Monte Carlo**
9:45	M. Schef¤er; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
P 6	**Predictive modeling of materials by ab initio thermodynamics and statistical mechanics**
10:30	D. Sornette; University of California, Los Angeles, USA and University of Nice, France
P 7	**Pushing the limits: extremes and crashes in £nance and economics**

11:15 Coffee break

11:45 - 12:30 **Session 12: Plenary Session IV**

11:45	M. Marechal; CECAM, Lyon, France
	Berni J. Alder CECAM Prize Ceremony
12:00	K. Binder; University of Mainz, Germany (Berni J. Alder CECAM Prize Awardee 2001)
P 8	**Simulations of phase transitions in macromolecular systems**

12:30 - 14:00 Lunch Break

Parallel Sessions *Lecture Hall Brüssel, Rooms K3 – K5*

14:00 - 16:00 Parallel Sessions 13,15,17,19

16:00 - 16:30 Coffee Break

16:30 - 18:30 Parallel Sessions 14,16,18,20

19:00 Organ Recital ***Aachen Cathedral***

20:30 Conference Dinner ***Coronation Hall in the Aachen Town Hall***

Thursday, 6 September 2001

Sessions 13 and 14 *Lecture Hall Brüssel*

14:00 - 16:00 **Session 13: Materials and Surface Science**

14:00 M. Pleimling; University of Erlangen-Nürnberg, Germany
I 17 Phase transitions at surfaces, edges, and corners
14:30 A. Alavi; University of Cambridge, U.K.
I 18 Ab-initio surface energy calculations and the oxidation of NiAl(110): Can we predict growth modes of the oxide layer?
15:00 M. Ahr and M. Biehl; University of Würzburg, Germany
O 25 Modelling (001) surfaces of II-VI semiconductors
15:20 Ph. Sonnet[1] and P.C. Kelires[1,2]; [1]Foundation for Research and Technology - Hellas (FORTH), Heraclion, Crete, Greece, [2]University of Crete, Heraclion, Crete, Greece
O 26 Monte Carlo simulations of Ge quantum dots on Si(100): Stress £elds and intermixing
15:40 L. Brendel[1], B. Hinnemann[1,2] et al.; [1]University of Duisburg, Germany, [2]Technical University of Denmark, Lyngby, Denmark
O 27 Different types of scaling in epitaxial growth

16:00 Coffee break

16:30 - 18:30 **Session 14: Nonequilibrium Transitions and Related Topics in Materials Science**

16:30 J. Marro; University of Granada, Spain
I 19 Modeling nonequilibrium phase transitions and critical behavior in complex systems
17:00 B.K. Chakrabarti; Saha Institute of Nuclear Physics, Calcutta, India
I 20 Dynamic transitions in pure Ising magnets under pulsed and oscillating £elds
17:30 K. Kadau and P. Entel; University of Duisburg, Germany
O 28 Molecular dynamics study of martensitic transformations in sintered Fe-Ni nanoparticles
17:50 M.-H. Tsai; National Sun Yat-sen University, Kaohsiung, Taiwan
O 30 First-principles molecular-dynamics simulations of the sticking of Ga and N gas-phase atoms on wurtzite GaN surfaces

Thursday, 6 September 2001

Sessions 15 and 16 ***Room K3***

14:00 - 16:10 **Session 15: Soft Matter: Biological Systems, Polymers**

14:00 A. Hansen; University of Trondheim, Norway
I 21 **Thermodynamics of proteins: Fast folders versus tight transitions**
14:30 H. Grubmüller; Max-Planck-Institut für biophysikalische Chemie, Göttingen, Germany
I 22 **Protein dynamics simulations: Grasping molecular nano-machines**
15:00 O.G. Mouritsen; Technical University of Denmark, Lyngby, Denmark
I 23 **Nano-scale structure in membranes in relation to enzyme action - computer simulation vs experiment**
15:30 Ch. Holm and H.-J. Limbach; Max-Planck-Institute for Polymer Research, Mainz, Germany
O 31 **How pearl-necklaces unwind**
15:50 V.A. Ivanov, P.G. Khalatur*, and A.R. Khoklov; Moscow State University, Russia, *Tver State University, Russia
O 32 **Sequence design of AB-copolymers: Conformation-dependent scheme**

16:10 Coffee break

17:00 - 18:30 **Session 16: More on Soft Matter; Electronic Structure**

17:00 R.O. Jones and P. Ballone*; Forschungszentrum Jülich, Germany, *University of Messina, Italy
I 24 **Equilibrium polymerization of polycarbonates**
17:30 J.-W. van der Horst, P.A. Bobbert et al.; COBRA Research School and Dutch Polymer Institute, Eindhoven, The Netherlands
O 34 **Excitons in conjugated polymers from £rst principles**
17:50 A. Canning, W. Mannstadt*, A.J. Freeman**; NERSC, Lawrence Berkeley National Laboratory, Berkeley, USA, *University of Marburg, Germany, **Northwestern University, Evanston, USA
O 35 **The all electron FLAPW method and its implementation on massively parallel computers**
18:10 W. Mannstadt, A. Canning*, and A.J. Freeman**; University of Marburg, Germany, *NERSC, Lawrence Berkeley National Laboratory, Berkeley, USA, **Northwestern University, Evanston, USA
O 36 **Application of the newly developed parallel FLAPW method to complex materials**

Thursday, 6 September 2001

Sessions 17 and 18 ***Room K4***

14:00 - 16:00 **Session 17: Quantum Physics**

14:00 R.N. Bhatt; Princeton University, New Jersey, USA
I 25 Numerical simulations of random spin (and fermionic) models with wide distribution of energy scales
14:30 A. Muramatsu; University of Stuttgart, Germany
I 26 Simulation of in£nitely strongly interacting fermions from one to two dimensions
15:00 K.A. Gernoth; University of Manchester, U.K.
O 37 Monte Carlo calculations of the microstructure of solids and liquids
15:20 Y. Li, T.-S. Chao*, and S.M. Sze; National Chiao Tung University, Hsinchu, Taiwan, *National Nano Device Laboratories, Hsinchu, Taiwan
O 38 A domain partition approach to parallel adaptive simulation of dynamic threshold voltage MOSFET
15:40 Yu.I. Prylutskyy and M.V. Makarets; Kiev National Shevchenko University, Ukraine
O 39 Computer simulation of radiation effect on the electronic properties of carbon nanotubes

16:00 Coffee break

16:00 - 18:30 **Session 18: Methodical Developments in Simulations**

16:30 E. Marinari; University of Rome, Italy
I 27 Dynamical properties of ”sequence alignment”: Aging and more
17:00 H. Rieger; University of Saarbrücken, Germany
I 28 Application of exact combinatorial optimization algorithms to the physics of disordered systems
17:30 D. Sebastiani and M. Parrinello*; Max-Planck-Institute for Polymer Research, Mainz, Germany, *ETH Zürich and Swiss Center for Scienti£c Computing, Manno, Switzerland
O 40 A new ab-initio approach for the calculation of NMR chemical shifts in periodic systems
17:50 G.P. Trabado, O. Plata, E.L. Zapata; University of Málaga, Spain
O 41 On the parallelization of molecular dynamics codes
18:10 P.N. Vorontsov-Velyaminov and A.P. Lyubartsev*; St. Petersburg State University, Russia, *University of Stockholm, Sweden
O 42 Expanded ensemble Monte Carlo method for free energy calculations

Thursday, 6 September 2001

Sessions 19 and 20 ***Room K5***

14:00 - 16:00 **Session 19: Lattice Boltzmann Methods and Fluid Dynamics**

14:00	B. Chopard; University of Geneva, Switzerland
I 29	**Lattice Boltzmann models: an ef£cient and simple approach to complex ¤ow problems**
14:30	S. Succi; C.N.R., Rome, Italy
I 30	**Computational multiphysics with the lattice Boltzmann method**
15:00	W. Rehm, W. Jahn et al.; Forschungszentrum Jülich, Germany
O 43	**CFD simulations of turbulent reactive ¤ows with supercomputing for hydrogen safety**
15:20	D.C. Kim; Technical Design Institute of Applied Microelectronics, Novosibirsk, Russia
O 44	**A nonlinear wave dynamical model for two-phase ¤ows and its numerical solutions**
15:40	T. Gotoh; Nagoya Institute of Technology, Japan
O 45	**Small scale statistics of turbulence at high Reynolds numbers by massive computation**

16:00 Coffee break

16:00 - 18:30 **Session 20: Applications of Computational Physics to Engineering, Traf£c Flow, and Economic Science**

16:30	W.P. Jones; Imperial College, London, U.K.
I 31	**Large eddy simulation of turbulent combustion processes**
17:00	K. Nagel; ETH Zürich, Switzerland
I 32	**Large scale transportation simulations**
17:30	A. Chakraborti, S. Pradhan, B.K. Chakrabarti; Saha Institute of Nuclear Physics, Calcutta, India
O 46	**Study of the distribution functions in minimal model market**
17:50	R. Kutner; University of Warsaw, Poland
O 47	**Are hierarchical Weierstrass walks present on a stock market?**
18:10	R. Wang and H.J. Ruskin; Dublin City University, Ireland
O 48	**Modelling traf£c ¤ow for a single-lane urban roundabout**

Friday, 7 September 2001

Plenary Sessions *Lecture Hall Brüssel*

9:00 - 10:30 **Session 21: Plenary Session V**

9:00 H.D. Simon; NERSC, Lawrence Berkeley National Laboratory, Berkeley, California, USA
P 9 Future directions in scienti£c supercomputing for computational physics
9:45 C.S. Frenk; University of Durham, U.K.
P 10 Cosmic architecture: Simulating the origin structure of the Universe

10:30 Coffee break

11:00 - 12:30 **Session 22: Plenary Session VI**

11:00 G. Wittum; IWR Heidelberg, Germany
P 11 Parallel adaptive simulation of large scale systems on unstructured grids
11:45 M. Newman; Santa Fe Institute, New Mexico, USA
P 12 The structure and function of networks

12:30 Lunch break

Parallel Sessions *Lecture Hall Brüssel, Rooms K3 – K5*

14:00 - 16:00 Parallel Sessions 23,25,27,29

16:00 - 16:30 Coffee Break

16:30 - 18:30 Parallel Sessions 24,26,28,30

Poster Session B *Rooms K1 / K2*

18:30 - 20:00 Poster Session B

Friday, 7 September 2001

Session 23 and 24 *Lecture Hall Brüssel*

14:00 - 16:00 **Session 23: Materials Science: Granular Matter and Friction**

14:00 S. Luding; University of Stuttgart, Germany
I 33 From microscopic simulations to macroscopic behaviour
14:30 J. Kertesz; Budapest University of Technology, Hungary
I 34 Simulation of shear processes in granular systems
15:00 V.Ya. Rudyak, A.A. Belkin, G.V. Kharlamov; Novosibirsk State University of Civil Engineering, Russia
O 49 Molecular dynamics simulation of the nanoparticles transfer in gases and liquids
15:20 D.C. Rapaport; Bar-Ilan University, Ramat-Gan, Israel
O 50 The wonderful world of granular ratchets
15:40 C. Jun[1,2] and J.-S. Wang[2]; [1]National University of Singapore, Republic of Singapore, [2]Beijing Normal University, Beijing, China
O 51 Friction between Si tip and (001)-2 x 1 surface: a molecular dynamics simulation

16:00 Coffee break

16:30 - 18:10 **Session 24: Materials Science: Phase Transitions and Multiscale Aspects**

16:30 N.B. Wilding; University of Liverpool, U.K.
I 35 Wetting of a symmetrical binary ¤uid mixture on a wall
17:00 W. Kob; University of Montpellier II, France
I 36 Parallel tempering algorithm to equilibrate glassy systems
17:30 C. Brangian, W. Kob*, K. Binder; University of Mainz, Germany, * University of Montpellier II, France
O 52 A numerical study of the 10 states Potts glass
17:50 J. Jakumeit; GMD - German National Research Center for Information Technology, Sankt Augustin, Germany
O 53 Simulation of electron-electron scattering in semiconductor devices by the local iterative Monte Carlo technique

Friday, 7 September 2001

Session 25 and 26 ***Room K3***

14:00 - 16:00 **Session 25: Statistical Properties of Turbulent Flows**

14:00 B. Eckhardt; University of Marburg, Germany
I 37 Turbulence in dilute polymer solutions: A phase diagram
14:30 M.H. Jensen; Niels Bohr Institute, Copenhagen, Denmark
I 38 Intermittency and multiscaling in turbulence
15:00 W.-Ch. Müller, B. Knaeppen et al.; Euratom-Belgian State Association, Université Libre de Bruxelles, Belgium
O 55 Dynamic subgrid-modeling in large-eddy simulations of magnetohydrodynamic turbulence
15:20 Z.A. Walenta, A. Kucaba-Pietal*, and Z. Peradzynski**; Polish Academy of Sciences, Warsaw, Poland, *University of Technology, Rzeszow, Poland, **University of Warsaw, Poland
O 56 Fluid ¤ows in narrow channels
15:40 W. Alda, W. Dzwinel, and J. Kitowski; Institute of Computer Science AGH, Cracow, Poland
O 57 Simulation of ¤uid ¤ow in the presence of particles

16:00 Coffee break

16:30 - 18:10 **Session 26: Frontiers in High Energy Physics Computing**

16:30 I. Augustin; CERN, Geneva, Switzerland
I 39 The DataGrid as tool for global high energy physics computing
17:00 K. Jansen, N. Paschedag et al.; John von Neumann Institute for Computing (NIC) and Deutsches Elektronen-Synchrotron (DESY), Zeuthen, Germany
O 58 APE – T¤ops computers for theoretical particle physics
17:30 R. Tripiccione; INFN, Pisa, Italy
I 40 Dedicated computing for lattice gauge theories: The APE(s) projects
17:50 G. Allen[1], W. Benger[1,2] et al.; [1]Max-Planck-Institut für Gravitationsphysik, Golm, Germany, [2]Konrad-Zuse-Zentrum für Informationstechnik (ZIB), Berlin, Germany
O 59 Large scale & grid computing with Cactus

Friday, 7 September 2001

Session 27 and 28 ***Room K4***

14:00 - 16:00 **Session 27: Applications of Computational Physics to Economy and Social Science**

14:00 A.Z. Maksymowicz; University of Mining and Metallurgy, Cracow, Poland
I 41 Simulation of population growth and structure of the population
14:30 M. Ausloos; University of LiÁege, Belgium
I 42 Multi-fractal nature of stock exchange
15:00 B. Tadic; J. Stefan Institute, Ljubljana, Slovenia
O 61 Growth & structure of the world-wide web: Towards realistic modeling
15:20 A.T. Bernardes; Universidade Federal de Ouro Preto, Brazil
O 62 A model for proportional voting process
15:40 C.V. Sheth; University of Zambia, Lusaka, Zambia
O 63 Computational physics programme in research and teaching – An African experience

16:00 Coffee break

16:30 - 18:30 **Session 28: Complex Systems**

16:30 L.N. Shchur; Landau Institute for Theoretical Physics, Chernogolovka, Russia
I 43 On the distribution function of the information speed in computer network
17:00 A.-L. Bárabasi; University of Notre Dame, Indiana, USA
I 44 Emergence of scaling in complex networks: From the topology of the www to the structure of the cell
17:30 H.A. Knudsen, A. Hansen; University of Trondheim, Norway
O 64 Steady state two-phase bulk ¤ow in 2D porous media by network models
17:50 H. Arkin, F. Yaçar et al.; Hacettepe University, Ankara, Turkey
O 65 Multicanonical simulations of some peptides
18:10 U.H.E. Hansmann; Michigan Technological University, Houghton, USA
O 66 New algorithms and the statistical physics of protein folding

Friday, 7 September 2001

Session 29 and 30 ***Room K5***

14:00 - 16:00 **Session 29: Cosmology**

14:00 B. Leibundgut; ESO Garching, Germany
I 45 Cosmological implications from observations of type Ia supernovae
14:30 R. Engel; Bartol Research Institute, University of Delaware, Newark, USA
I 46 Simulation of hadronic particle production in astrophysical environments
15:00 S. Moiseenko, N.V. Ardeljan*, G.S. Bisnovatyi-Kogan; Space Research Institute, Moscow, Russia; *Moscow State University, Russia
O 67 Magnetorotational supernova explosion. Simulation Lagrangian implicit numercial method on triangular grid with grid reconstruction
15:20 D. Ryu, H. Kang*, and P. Biermann**; Chungnam National University, Daejeon, Korea, *Pusan National University, Korea, **Max-Planck-Institute for Radioastronomy, Bonn, Germany
O 68 The effects of cosmic rays on the large scale structure formation in the Universe
15:40 V. Antonuccio-Delogu, U. Becciani et al.; Osservatorio Astro£sico di Catania, Italy
O 69 Performing and analysing cosmological simulations with FLY and AstroMD

16:00 Coffee break

16:30 - 18:30 **Session 30: High Energy Physics and Magnetic Fields**

16:30 Th. Lippert; University of Wuppertal, Germany
I 47 Computional particle physics with the cluster computer ALiCE
17:00 A. Brandenburg; Nordita, Copenhagen, Denmark
I 48 Hydromagnetic turbulence in computer simulations
17:30 T.W. Jones,I.L. Tregillis, and D. Ryu*; University of Minnesota, Minneapolis, USA, *Chungnam National University, Daejeon, Korea
O 70 Computation of relativistic electron acceleration, transport and emissions in complex astrophysical ¤ows
17:50 E.E. Antonov, I.L. Buylova et al.; Moscow State University, Russia
O 71 Estimates of arrival directions of giant air showers
18:10 E.E. Antonov, L.G. Dedenko et al.; Moscow State University, Russia
O 72 Estimation of the attenuation length of the charged particle density at 600 metres from the shower axis

Saturday, 8 September 2001

Plenary Sessions *Lecture Hall Brüssel*

9:00 - 10:30 **Session 31: Plenary Session VII**

9:00 H. Satz; University of Bielefeld, Germany
P 13 Cluster percolation and thermal critical behaviour
9:45 B.A. Berg; Florida State University, Tallahassee, USA
P 14 Generalized ensemble simulations of complex systems

10:30 Coffee break

11:00 - 12:30 **Session 32: Plenary Session VIII**

11:00 H. Blöte; Delft University of Technology, The Netherlands
P 15 Cluster Monte Carlo: Extending the range
11:45 P. Grassberger; John von Neumann Institute for Computing (NIC), Jülich, Germany
P 16 Go-with-the-winners simulations

12:30 **Closing**

12:45 End of Conference

CONTENTS

I Invited Plenary Contributions

II Invited Contributions

I1 Electronic structure calculations of solids using the WIEN2k package for materials science
Schwarz, K.

I2 Extended ensemble Monte Carlo approach to hardly-relaxing problems
Hukushima, K., Iba, Y.

I3 Computational studies of carbon nanotube structures
Huhtala, M., Kuronen, A., Kaski, K.

I4 Inverse Monte Carlo method and its application to compute effective potentials
Lyubartsev, A. P.

I5 Surface anchoring on liquid crystalline polymer brushes
Lange, H., Schmid, F.

I6 Ion-ion correlations in charged colloidal systems
Jönsson, Bo

I7 Kinetics of wetting at surfaces
Puri, S.

I8 Interplay between wetting and miscibility in thin binary polymer £lms
Müller, M.

I9 Numerical tests of CFT conjectures for 3D systems
Janke, W., Weigel, M.

I10 Meron-cluster solution of fermion and other sign problems
Wiese, U.

I11 Simple dynamics for broad histogram method
Oliveira, P. M. C. de

I12 Double degeneracy in the ground-state of the 3D $\pm J$ spin glass
Hatano, N., Gubernatis, J. E.

I13 Magnetization reversal using novel new event-driven Monte Carlo algorithms
Novotny, M. A.

I14 Visualization of MD and MC simulations for atomistic modeling
Adler, J., Hashibon, A., Schreiber, N., Sorkin, A., Sorkin, S., Wagner, G.

I15 Stochastic and dynamic properties of molecular dynamics systems: Simple liquids, plasma and electrolytes, polymers, etc.
Norman, G. E.

I16 Simulation and event generation in high-energy physics
Perret-Gallix, D.

I17 Phase transitions at surfaces, edges, and corners
Pleimling, M.

I18 Ab initio surface energies and the oxidation of NiAl(110): Can we predict growth modes of the oxide layer?
Alavi, A., Lozovoi, A. Y.

I19 Modeling nonequilibrium phase transitions and critical behavior in complex systems
Marro, J.

I20 Dynamic transitions in pure ising magnets under pulsed & oscillating £elds
Chakrabarti, B. K., Misra, A.

I21 Proteins top-down
Hansen, A., Bakk, A., Dommersnes, P. G., Jensen, M. H., Høye, J. S., Sneppen, K.

I22 Protein dynamics simulations: Grasping molecular nano-machines
Heymann, B., Böckmann, R., Grubmüller, H.

I23 Nano-scale structure in membranes in relation to enzyme action – computer simulation vs experiment
Mouritsen, O. G., Hoyrup, P., Kaasgaard, T., Kildemark, L., Jorgensen, K.

I24 Equilibrium polymerization of polycarbonates
Jones, R. O., Ballone, P.

I25 Numerical simulations of random spin (and fermionic) models with wide distribution of energy scales
Bhatt, R. N.

I26 Simulation of in£nitely strongly interacting fermions from one to two dimensions
Brunner, M., Lavalle, C., Assaad, F. F., Muramatsu, A.

I27 Dynamical properties of ”sequence alignment”: Aging and more
Marinari, E.

I28 Application of exact combinatorial optimization algorithms to the physics of disordered systems
Rieger, H.

I29 Lattice Boltzmann models: an ef£cient and simple approach to complex ¤ow problems
Chopard, B., Dupuis, A.

I30 Multiscale lattice Boltzmann methods
Succi, S., Filippova, O.

I31 Large eddy simulation of turbulent combustion processes
Jones, W. P.

I32 Large scale multi-agent transportation simulations
Nagel, K.

I33 From microscopic simulations to macroscopic material behavior
Luding, S.

I34 Instabilities in sheared loosed granular matter
Kertész, J., Török, J., Sasvári, M., Wolf, D. E., Krishnamurthy, S., Roux, S.

I35 Wetting of a symmetrical binary ¤uid mixture on a wall
Wilding, N. B., Schmid, F.

I36 Parallel tempering algorithm to equilibrate glassy systems
Kob, W., Binder, K., Michele, C. De, Sciortino, F., Stühn, T., Yamamoto, R.

I37 Turbulence in dilute polymer solutions: A phase diagram
Eckhardt, B., Kronjäger, J., Schumacher, J.

I38 Intermittency and multiscaling in turbulence
Jensen, M. H.

I39 The DataGrid as tool for global high energy physics computing
Augustin, I.

I40 Dedicated computing for lattice Gauge theories: The APE(s) projects
Tripiccione, R.

I41 Simulation of population growth and structure of the population
Maksymowicz, A. Z.

I42 Multi-fractal nature of stock exchange prices
Ausloos, M., Ivanova, K.

I43 On the distribution function of the information speed in computer network
Shchur, L. N.

I44 Emergence of scaling in complex networks: from the topology of the www to the structure of the cell
Barabási, A.-L.

I45 Cosmological implications from observations of type Ia supernovae
Leibundgut, B.

I46 Simulation of hadronic particle production in astrophysical environments
Engel, R.

I47 Computational particle physics with the cluster computer ALiCE
Eicker, N., Neff, H., Lippert, Th., Orth, B., Schilling, K.

I48 Hydromagnetic turbulence in computer simulations
Brandenburg, A., Dobler, W.

III Oral Contributions

O1 On new ef£cient algorithms for PIMC and PIMD
Müser, M. H., Krajewski, F.

O2 Finite-temperature Lanczos algorithm study on pseudogap in high-T_c superconductors
Sakai, T., Takahashi, Y.

O3 A computational study of some Josephson junction circuits
Borcherds, P. H.

O4 Ab-initio prediction of complex magnetic structures in low dimensions
Bihlmayer, G., Kurz, Ph., Förster, F., Blügel, S.

O5 Quasi-ab initio molecular dynamics simulations of atomic scale structures on metal surfaces
Stepanyuk, V. S., Bazhanov, D. I., Baranov, A. N., Hergert, W.

O6 Dynamic critical behavior of the classical anisotropic BCC Heisenberg antiferromagnet
Tsai, S., Bunker, A., Landau, D. P.

O7 Strong electrostatic interactions in colloidal systems
Messina, R., Holm, C., Kremer, K.

O8 Optimal shapes of compact strings
Micheletti, C., Maritan, A., Trovato, A., Banavar, J.

O9 Molecular dynamics study of polyelectrolyte brushes
Seidel, C.

O10 Large-scale computer simulation of local segmental dynamics in amorphous atactic polystyrene
Lyulin, A. V., Michels, M. A. J.

O11 Dynamics of droplet spreading
Milchev, A., Binder, K.

O12 Large shear deformation of particle gels studied by Brownian dynamics simulations
Rzepiela, A. A.

O13 Chaotic ionization of non-classical alkali Rydberg states – computational physics beats experiment
Krug, A., Buchleitner, A.

O14 Improving the Dirac operator in lattice QCD
Gattringer, C., Lang, C. B.

O15 Universal ¤uctuations of Dirac spectra in QCD
Meyer, S. H.

O16 Anisotropic scaling and generalized conformal invariance at Lifshitz points
Henkel, M., Pleimling, M.

O17 Distribution of instanton sizes in a simpli£ed instanton gas model
Münster, G., Kamp, C.

O18 The fractal dimension of the critical ¤uctuations in Abelian gauge theories
Hove, J., Mo, S., Sudbø, A.

O19 Coupling molecular dynamics and continuum dynamics
Wagner, G., Flekkøy, E.G., Feder, J., Jøssang, T.

O20 Determining the density of states for classical statistical models: A random walk algorithm to produce a ¤at histogram
Landau, D. P., Wang, F.

O21 A cluster Monte Carlo algorithm for 2-dimensional spin glasses
Houdayer, J.

O22 Pattern formation and coherent structures in collective models from accelerator physics
Fedorova, A. N., Zeitlin, M. G.

O23 Vlasov Poisson solver for density enhancement near ions at rest in magnetized electron plasmas
Heerlein, C., Toepffer, C.

O25 Modelling (001) surfaces of II-VI semiconductors
Ahr, M., Biehl, M.

O26 Monte Carlo simulations of Ge quantum dots on Si(100): stress £elds and intermixing
Sonnet, Ph., Kelires, P. C.

O27 Different types of scaling in epitaxial growth
Brendel, L., Hinnemann, B., Hinrichsen, H., Schindler, A., Driesch, M. von den, Westerhoff, F., Wolf, D. E.

O28 Molecular dynamics study of martensitic transformations in sintered Fe-Ni nano-particles
Kadau, K., Entel, P.

O30 First-principles molecular-dynamics simulations of the sticking of Ga and N gas-phase atoms on wurtzite GaN surfaces
Tsai, M.

O31 How pearl-necklaces unwind
Holm, C., Limbach, H.

O32 Sequence design of AB-copolymers: Conformation-dependent scheme
Ivanov, V. A., Khalatur, P. G., Khokhlov, A. R.

O34 Excitons in conjugated polymers from £rst principles
Horst, J.-W. van der, Bobbert, P. A., Pasveer, W. F., Michels, M. A. J., Brocks, G., Kelly, P. J.

O35 Electronic structure at a new level of complexity with parallel FLAPW
Mannstadt, W., Canning, A., Freeman, A. J.

O36 P-FLAPW: A large scale parallel all electron £rst principles code
Canning, A., Mannstadt, W., Freeman, A. J.

O37 Monte Carlo calculations of the microstructure of solids and liquids
Gernoth, K. A.

O38 A domain partition approach to parallel adaptive simulation of dynamic threshold voltage MOSFET
Li, Y., Chao, T., Sze, S. M.

O39 Computer simulation of radiation effect on the electronic properties of carbon nanotubes
Prylutskyy, Yu. I., Makarets, M. V.

O40 A new ab-initio approach for the calculation of NMR chemical shifts in periodic systems
Sebastiani, D., Parrinello, M.

O41 On the parallelization of molecular dynamics codes
Trabado, G. P., Plata, O., Zapata, E. L.

O42 Expanded ensemble Monte Carlo method for free energy calculations
Vorontsov-Velyaminov, P. N., Lyubartsev, A. P.

O43 CFD simulations of turbulent reactive ¤ows with supercomputing for hydrogen safety
Rehm, W., Jahn, W., Vogelsang, R., Wang, B. L.

O44 A nonlinear wave dynamical model for two-phase ¤ows and its numerical solutions
Kim, D. C.

O45 Small scale statistics of turbulence at high Reynolds numbers by massive computation
Gotoh, T.

O46 Study of the distribution functions in minimal model market
Chakraborti, A., Pradhan, S., Chakrabarti, B. K.

O47 Are hierarchical Weierstrass walks present on a stock market?
Kutner, R.

O48 Modelling traf£c ¤ow for a single-lane urban roundabout
Wang, R., Ruskin, H. J.

O49 Molecular dynamics simulation of the nanoparticles transfer in gases and liquids
Rudyak, Ya., Belkin, A., Kharlamov, V.

O50 The wonderful world of granular ratchets
Rapaport, D. C.

O51 Friction between Si tip and (001)-2×1 surface: a molecular dynamics simulation
Jun, C., Wang, J.-S.

O52 A numerical study of the 10 states Potts glass
Brangian, C., Kob, W., Binder, K.

O53 Simulation of electron-electron scattering in semiconductor devices by the local iterative Monte Carlo technique
Jakumeit, J.

O55 Dynamic subgrid-modeling in large-eddy simulations of magnetohydrodynamic turbulence
Müller, W., Knaepen, B., Debliquy, O., Carati, D.

O56 Fluid ¤ows in narrow channels
Walenta, Z. A., Kucaba-Pietal, A., Peradzynski, Z.

O57 Simulation of ¤uid ¤ow in the presence of particles
Alda, W., Dzwinel, W., Kitowski, J.

O58 APE – T¤ops computers for theoretical particle physics
Jansen, K., Paschedag, N., Pleiter, D., Simma, H., Wegner, P.

O59 Large scale & grid computing with Cactus
Allen, G., Benger, W., Dramlitsch, T., Goodale, T., Hege, H., Lanfermann, G., Merzky, A., Radke, T., Seidel, E., Shalf, J.

O61 Growth & structure of the world-wide web: Towards realistic modeling
Tadić, B.

O62 A model for proportional voting process
Bernardes, A. T.

O63 Computational physics programme in research and teaching - An african experience
Sheth, C. V.

O64 Steady state two-phase bulk ¤ow in 2D porous media by network models
Knudsen, H. A., Hansen, A.

O65 Multicanonical simulations of some peptides
Arkın, H., Yaşar, F., Çelik, T., Berg, B. A., Meirovitch, H.

O66 New algorithms and the statistical physics of protein folding
Hansmann, U. H. E.

O67 Magnetorotational supernova explosion. Simulation Lagrangian implicit numerical method on triangular grid with grid reconstruction
Moiseenko, S. G., Ardeljan, N. V., Bisnovatyi-Kogan, G. S.

O68 The effects of cosmic rays on the large scale structure formation in the universe
Ryu, D., Kang, H., Biermann, P. L.

O69 Performing and analysing cosmological simulations with FLY and AstroMD
Antonuccio-Delogu, V., Becciani, U., Ferro, D., Germaná, A., Pagliaro, A., Buonomo, F., Gheller, C.

O70 Computation of relativistic electron acceleration, transport and emissions in complex astrophysical ¤ows
Jones, T. W., Tregillis, I. L., Ryu, D.

O71 Estimates of arrival directions of giant air showers
Antonov, E. E., Buylova, I. L., Dedenko, L. G., Fedorova, G. F., Glushkov, A. V., Kolosov, V. A., Komissarova, T. M., Pravdin, M. I., Pyt'ev, Yu. P., Roganova, T. M., Sleptsov, I. E.

O72 Estimation of the attenuation length of the charged particle density at 600 metres from the shower axis
Antonov, E. E., Dedenko, L. G., Fedorova, G. F., Fedunin, E.Yu., Glushkov, A. V., Kolosov, V. A., Pravdin, M. I., Roganova, T. M., Sleptsov, I. E.

IV Poster Session A

A1 Magnetic quantum tunneling in systems of dipolar Ising spins
Alonso, J. J., Fernández, J. F.

A2 Target heating during ion-solid interactions
Angelov, C., Kirov, N.

A3 Diffusion in Cayley tree structures
Argyrakis, P.

A4 Molecular dynamics analysis of coalescence behavior in the nanorods formation
Ascencio, J. A., Liu., H. B.

A5 Molecular dynamics study of cluster formation via vaporized media condensation
Assatourova, I. M.

A6 Fully solvated molecular dynamics simulations of duplexes formed by modi£ed oligonucletides with nonisosteric phosphonate and xylo internucleoside linkages and their natural counterpart
Barvík Jr., I., Štěpánek, J., Bok, J.

A7 Toughness dependence on failure regimes
Menezes-Sobrinho, I. L., Bernardes, A. T., Moreira, J. G.

A8 Terrace sizes, slope selection and the role of desorption in unstable epitaxial growth
Biehl, M., Ahr, M., Kinne, M., Kinzel, W., Schinzer, S.

A9 Propagation of nonlinear surface polaritons in 2D electron system
Beletskii, N. N., Bludov, Y. V.

A10 Melting of metallic clusters studied by *ab initio* electronic structure methods
Blundell, S. A., Zope, R. R.

A11 Optical spectra of indium bromide: Theory and experiment
Kolinko, M. I., Bovgyra, O. V.

A12 Estimation of electrical durability of dielectrics
Brigadnov, I. A.

A13 Phase constitution of Ni-based quaternary alloys studied by Monte Carlo simulation
Buršík, J.

A14 First principle investigation of the intermediate range order in disordered materials: the case of $SiSe_2$
Celino, M., Massobrio, C.

A15 Calculation of linear and nonlinear optical properties of granulated multilayers
Barskii, D.R., Cherichihin, I. N., Mishina, E.D.

A16 On short life energy ¤uctuations in low dimensional systems
Chicea, D., Stoicescu, D. Gh.

A17 The ampere force computation
Chicea, D.

A18 Simulation of peculiarities of lowtemperature luminescence of cadmium tungstate crystals doped with Dy^{3+} ions
Chukova, V., Nedilko, G., Scherbatskiy, P., Sheludko, I.

A19 Visualization of Coulomb correlations in £nite metallic systems
Berry, F. D. R. S.

A20 SiC(0001) surfaces: Stacking defects and the implications for the epitaxial growth of silicon carbide
Borghi, G., Felice, R. Di, Bertoni, C. M., Catellani, A.

A21 Examination of the Li^+-water potential derived from $ab\ initio$ MD in a wide temperature range
Egorov, A. V., Komolkin, A. V., Chizhik, V. I., Yushmanov, P. V., Lyubartsev, A. P., Laaksonen, A.

A22 Three body bound state calculations with three body forces without angular momentum decomposition
Elster, Ch., Liu, H., Glöckle, W.

A23 Six-state model of glassy crystal cyanoadamantane. Monte Carlo simulations
Fabanski, R., Kuchta, B., Firlej, L., Descamps, M.

A24 Monte Carlo simulations of carbon-based structures based on an extended Brenner potential.
Fasolino, A., Los, J.

A25 Computer simulation of femsosecond pulse propagation in bulk dielectric samples
Smirnova, T. V., Fedotova, O. M., Khasanov, O. K.

A26 *ab initio* Density functional study of GaAs clusters
Boo, T. B., Feng, Y. P.

A27 Computer aided estimation of the lifetime of a material by the thermo-gravimetric analysis
Georgescu, M., Ghelmez, M., Dumitru, B., Georgescu, M., Serban, S.

A28 Explicit kinetic functionals for diatomic molecules
García-Aldea, D., Alvarellos, J. E.

A29 Chaos of two particles in the ding-a-ling model
Gawronski, P., Kulakowski, K.

A30 Numerical simulation of the modi£ed Ginzburg-Landau type equations for a Josephson junction
Genchev, Z. D., Boyadjiev, T. L.

A31 Electronic and magnetic structure of NiO(001) and NiO/Ag(001)
Ködderitzsch, D., Hergert, W., Temmerman, W., Szotek, Z.

A32 Energy relaxation and transfer in trimer
Heřman, P., Barvík, I., Urbanec, M.

A33 Boundaries in collaborative virtual environments: How to classify them to introduce in a new awareness model
Herrero, P., Antonio, A. de

A34 Computation of optical properties of Si-based photonic crystals
Hillebrand, R., Hergert, W.

A35 Cluster approach in calculations of electronic structure of defects in $PbWO_4$
Hizhnyi, Yu. A., Nedilko, S. G., Bilyi, M. U.

A36 A Lattice–Boltzmann method for the simulation of transport phenomena in charged colloids
Horbach, J., Frenkel, D.

A37 Study of thin £lm growth by means of computer simulation and image analysis
Hrach, R., Šimek, J., Kostern, M.

A38 Sheath evolution in electronegative plasmas
Hrach, R., Hrachová, V., Vicher, M.

A39 Variation effect on the insecticide activity of DDT analogs - A chemometoric approach
Itoh, S., Arai, M., Kobayashi, K., Nagashima, U.

A40 Quanti£cation of channels of plasma polymerisation using a chemical model based on mass spectrometry
Ihrig, D. F., Stockhaus, J., Scheide, F., Winkelhake, O., Streuber, O.

A41 Modelling of the phase separation in a supersaturated solid solution
Ischenko, T., Demishev, S. V., Gust, W.

A42 Contact dynamics simulations of compacting cohesive granular systems
Kadau, D., Bartels, G., Brendel, L., Wolf, D. E.

A43 Large-scale simulations of the £nite-temperature properties of the molecular assemblies Mn_6 and Ni_{12}
Kamieniarz, G., Matysiak, R., D'Auria, A. C., Esposito, F., Benelli, C.

A44 Finite-temperature quantum transfer-matrix simulations of the frustrated spin 1/2 chains
Kamieniarz, G., Bieliński, M., Szymczak, H., Renard, J.-P.

A45 Temperature dependence of vibrational properties of a Σ 5(310)[001] NiO grain boundary: A molecular dynamics study
Karakasidis, T. E.

A46 Performance analysis of parallel molecular dynamics simulation of Lennard-Jones liquids on a small Beowulf cluster
Karakasidis, T. E., Cholevas, N., Liakopoulos, A.

A47 Perturbation theory and numerical calculations for the effective conductivity of two-dimensional structures
Khalatnikov, I. M.

A48 Computer modeling of interface structure in Al-Be system
Abramov, E., Kiv, A., Zamir, G.

A49 Wave packet molecular dynamics simulations of hydrogen at Mbar pressures
Knaup, M., Reinhard, P.-G., Toepffer, C., Zwicknagel, G.

A50 Justi£cation of the "net" model for a high-contrast structure and its application to randomly £lled composite
Berlyand, V., Kolpakov, G.

A51 Theoretical modeling of the erosion coef£cient and temperature £elds under action of plasma ¤ows of various energies and intensities
Kostyuk, G. I.

A52 Research of growth of crystall from melt by method molecular dynamics
Vladimirovich, K. S., Pavlovich, K. Y.

A53 The spinodal of the overheated solid
Krivoguz, M. N.

A54 Constructing isotropic polycrystal materials via molecular dynamics
Krivtsov, A. M.

A55 Density-functional study of multielectron ionization of sodium clusters by strong femtosecond laser pulses
Kurkina, L. I.

A56 Stability of sodium nanoclusters and phase transition
Liu, H. B., Ascencio, J. A., Yacaman, M. J.

A57 Percolation in a $1+1$ ballistic deposition model
Lebovka, N. I., Vygornitskii, N. V.

A58 Numerical simulation of thin £lm growth
Levchenko, I. G.

A59 Atomistic study of structural correlations at a model liquid-solid interface
Hashibon, A., Adler, J., Finnis, M. W., Kaplan, W. D.

A60 Computational study of structures of amorphous carbon
Sorkin, A., Adler, J.

A61 In¤uence of point defects on the shear elastic coef£cients and on the melting temperature of vanadium
Sorkin, V., Adler, J., Polturak, E.

A62 Sequence design of protein-like copolymers using time evolution of the system
Chertovich, A. V., Ivanov, V. A., Khokhlov, A. R.

A63 A simple model for the DNA denaturation transition
Causo, M. S., Coluzzi, B., Grassberger, P.

A64 Solvation of molecular complexes. A combined self-consistent-£eld and integral equation study
Chuev, N., Tikhonov, A.

A65 A diffusion-collision model uses the thermodynamic information extracted by a neural network to predict the folding times of all-α proteins
Compiani, M., Capriotti, E., Casadio, R.

A66 Adaptive numerical method for Poisson-Boltzmann equation and its applications
Dyshlovenko, P.

A67 Rigid-body formalism for simulating the macromolecules
Ejtehadi, M. R., Everaers, R., Site, L. D., Kremer, K.

A68 Computer simulation study of irreversible adsorption: coverage ¤uctuations
Faraudo, J., Bafaluy, J.

A69 Molecular dynamics study of structure formation of a polymer chain in solution
Fujiwara, S., Sato, T.

A70 Dynamics of orientationally ordered domains in a short chain-molecule system: size dependence of domain oscillation
Nakamura, H., Fujiwara, S., Sato, T.

A71 Molecular process of slippage of macromolecular chain in highoriented linear polyethylene
Gafurov, U.

A72 Simulation of diffusion in multi-protein-systems
Gorba, C., Helms, V.

A73 Binding isotherms calculated for Cu2+ and Ca2+ ions interaction with DNA on its condensation in solution
Hackl, E., Galkin, V. L., Blagoi, Yu.

A74 Ground state structures of polymers
Hauck, J., Mika, K.

A75 Direct pair correlation functions and elastic constants in liquid crystals: A computer simulation study
Phuong, N. H., Germano, G., Schmid, F.

A76 New cellular automaton designed to simulate geometration in gel electrophoresis
Krawczyk, M. J., Kulakowski, K., Maksymowicz, A. Z.

A77 AB-copolymers mimicking some properties of membrane proteins: MC computer simulation
Lazutin, A., Ivanov, A., Khokhlov, R.

A78 Orientational instability induced by light wave in waveguide with liquid crystal core
Lednei, M. F., Pinkevich, I. P.

A79 A novel parallel £nite volume solution of 3D nonlinear Poisson-Boltzmann equation in biophysics
Li, Y., Lu, H., Sze, S. M.

A80 Phase transitions in highly charged colloidal suspensions
Lobaskin, V., Linse, P.

A81 Interface properties and the wetting transition of polymers at a wall
MacDowell, L. G., Müller, M.

A82 Critical properties of the bond-diluted Ising model in three dimensions
Berche, P. E., Chatelain, C., Berche, B., Janke, W.

A83 New results in the computation of large-order high-temperature expansions for observables of the Ising model
Paolo, B., Comi, M.

A84 In¤uence of dilution on the strong £rst-order phase-transition of the 3D 4-state Potts model
Chatelain, C., Berche, P-E., Berche, B., Janke, W.

A85 Critical behaviour of fully-frustrated Potts models
Foster, D. P., Gérard, C., Puha, I.

A86 Monte Carlo study of the critical phenomena in the double exchange systems using massive parallel computers
Furukawa, N., Motome, Y.

A87 Finite size critical behaviour of the driven lattice gas in two and three dimensions
Caracciolo, S., Gambassi, A., Gubinelli, M., Pelissetto, A.

A88 High temperature series expansions for d-dimensional disordered Potts models
Hellmund, M., Janke, W.

A89 Critical behavior of the two-dimensional dipolar in-plane Ising model
Hucht, A.

A90 Collective pattern of random expansion by pairs in moderate number of £nite systems
Kozlowski, W.

A91 Monte Carlo simulations of vector spin glasses at low temperatures
Katzgraber, H. G., Young, A. P.

A92 Density of partition function zeroes and phase transition strength
Janke, W., Kenna, R.

A93 The program for calculation of pulsed magnetic £elds in the experimental device with a complex electrode structure
Chorniy, A., Nemchenko, K.

A94 Orbital dynamics via multiresolution
Fedorova, A. N., Zeitlin, M. G.

A95 Simulation of Coulomb interacting particles in a potential well
Bassi, G., Bazzani, A., Turchetti, G.

A96 New numerical tools to study waves and instabilities of ¤owing plasmas
Belien, A. J. C., Botchev, M. A., Goedbloed, J. P., Holst, B. van der

A97 Modelling of black holes in the string Einstein-Born-Infeld gravity with massive dilaton
Boyadjiev, T. L., Yazadjiev, S.

A98 ASTROMD. A data analysis and visualization tool for astrophysics
Buonomo, F., Gheller, C., Becciani, U.

A99 Jet ¤ows in the astrophysical environment
Camenzind, M., Krause, M., Thiele, M.

A100 Automatization of calculations for analysis and visualization of magnetic £eld and space plasma data (ADO)
Pérez, G. C., Cano, X. B.

A101 Separation of muons in the giant air showers by the geomagnetic £eld
Antonov, E. E., Dedenko, L. G., Fedorova, G. F., Glushkov, A. V., Kolosov, V. A., Pravdin, M. I., Pyt'ev, Yu. P., Roganova, T. M., Sleptsov, I. E.

A102 Numerical simulations of the global baroclinic instability in accretion disks
Klahr, H., Bodenheimer, P.

A103 *Maartje*: Three–dimensional astrophysical gasdynamics and radiative transfer
Mellema, G., Lim, A.

A104 Non charge symmetry violation in the D(d,p) T and D(d,n)3He reactions at stellar energies
Nebia, F., Beaumevieille, H., Ouichaoui., S.

A105 Direct n-body integration with variational equations and close encounters multi-regularization: The *NNEWTON* package
Nunes, A., Pereira, N.

A106 Spiral arms in astrophysical discs
Pfalzner, S.

A107 Jump processes in option pricing theory
Albanese, C., Campolieti, J., Jaimungal, S., Rubisov, D.

A108 Learning from examples by PCA
Bunzmann, C., Biehl, M., Urbanczik, R.

A109 A computational ef£cient solution technique for traf£c netwok O/D matrix estimation
Cho, H., Chen, C., Lin, P., Ng, I.

A110 Series solutions of the anharmonic motion equations
Chouikha, A. R.

A111 Quantifying coexistence of collectivity and noise in complex systems
Drożdż, S., Grümmer, F., Kwapień, J., Sawa, M., Speth, J., Wójcik, M.

A112 Fast and reliable techniques for using Racah's algebra in many–particle physics
Fritzsche, S., Fricke, B., Gaigalas, G., Jacob, T., Tomaselli, M.

A113 Numerical calculation of space charge distribution for dust grains in a plasma sheath equilibrium
Garcia, L. G., Goedert, J.

A114 Universal scaling functions for bond percolation on planar random and square lattices with multiple percolating clusters
Hsu, H., Lin, S. C., Hu, C.

A115 The evolution of nonlinear spatial economic models
Bulanov, S. V., Echkina, E. Yu., Inovenkov, I. N.

A116 Monte Carlo simulation of biomolecular systems with BIOMCSIM
Kamberaj, H., Helms, V.

A117 Phase dynamics in current driven Josephson junction networks
Kawaguchi, T.

A118 Nonlinear plastic behavior of phase-phase correlations in Josephson junction systems
Kawaguchi, T.

A119 Statistical mechanics of the three-state neural network: From the mutual information to the hamiltonian
Korutcheva, E., Dominguez, D.

A120 Friction mechanisms between polymer bearing surfaces
Kreer, T., Müser, M. H., Binder, K.

A121 A Monte Carlo simulation for multi-dimensional traf£c dispersion model
Cho, H., Lai, F., Lu, H.

A122 Parallel traf£c ¤ow simulation using semi-viscous model
Lai, F., Lu, H., Lin, S. S., Cho, H.

A123 Numerical methods for multilane traf£c ¤ow simulation
Cho, H., Lin, C.

A124 Numerical analysis of a self-consistent dynamic traf£c ¤ow model
Cho, H., Lo, S.

A125 Modeling and comparison of different vehicular ¤ow processes
Cho, H., Lo, S.

A126 Effect of time slowing in biological ageing
Magdoń-Maksymowicz, M. S., Sitarz, M., Bubak, M., Maksymowicz, A. Z., Szewczyk, J.

A127 Shear stress in lattice Boltzmann simulations
Artoli, A. M., Kandhai, D., Hoefsloot, H. G., Hoekstra, A. G., Sloot, P. M. A.

A128 Computing sensitivities of the electrostatic potential by automatic differentiation
Bischof, C. H., Bücker, H. M., Rasch, A., Risch, J. W.

A129 Mapping cellular automata applications into cellular automata networks ones
Calidonna, C. R., Gregorio, S. di, Furnari, M. M.

A130 An ef£cient data compression method for the Davidson subspace diagonalization scheme - New possibilities in computational science
Dachsel, H.

A131 Analytical Hartree-Fock gradients for periodic systems
Doll, K.

A132 New representation of the Ising model and new cluster method [1ex] for £nite and in£nite size systems
Evertz, H. G., Erkinger, H. M., Linden, W. von der

A133 Variable high order £nite difference algorithms and important domain sampling for solving the Schrödinger equation in molecular dynamics
Farantos, S. C.

A134 Numerical solution of an inverse problem for the hydraulic properties of porous media
Fatullayev, A. G.

A135 A new lattice Boltzmann approach to the mechanical properties and microstructure of the pattern formation in magnetic ¤uids
Hirabayashi, M., Chen, Yu, Ohashi, H.

A136 Generalized evolutionary programming with Lévy-type mutation
Iwamatsu, M.

A137 Rapid transit system origin-destination pattern calculation with statistical Gibbs sampling and Kalman £lter techniques
Jou, Y.

A138 New integrator for molecular dynamics simulations
Khakimov, Z. M.

A139 Feature extraction and classi£cation with cellular spaces
Kuhn, C.

A140 Validation of the Lowe-Frenkel tracer dispersion method in the lattice Boltzmann method
Merks, R. M. H., Hoeksta, A. G., Sloot, P. M. A.

A141 Dynamical memory time in molecular dynamic simulations
Morozov, I. V., Norman, G. E., Valuev, A. A.

V Poster Session B

B1 Calculation of induced electron states in three dimensional semiconductor arti£cial molecules
Li, Y., Voskoboynikov, O., Lee, C. P., Sze, S. M.

B2 Numerical simulation of quantum effects in high-k gate dielectrics MOS structures using quantum mechanical models
Li, Y., Lee, J., Tang, T., Chao, T., Lei, T., Sze, S. M.

B3 A novel simulation approach for the numerical solution of heterojunction bipolar transistors
Li, Y., Huang, K., Lee, C. P., Sze, S. M.

B4 Calculation of the electronic structure and disordering effects in $La_{0.5}Li_{0.5}TiO_3$ compound
Tymoshevska, L. V., Yanchitskii, B. Z., Belous, A. G.

B5 Simulation of liquid solution doping from gas phase by the method of molecular dynamics
Lyutikov, A. R., Khukhryansky, Yu. P.

B6 Dynamic structure of liquid germanium studied by a £rst-principles and a classical molecular-dynamics simulations
Munejiri, S., Shimojo, F., Hoshino, K., Itami, T.

B7 Computation of the thermodynamic criterion for migrating grain boundary pinning during recrystallization processes in the dispersion-hardened alloys
Marvina, L. A., Marvin, V. B., Karibyants, V. R., Neupokoeva, I. V.

B8 Simulating stochastic geometries: Topological and morphological phase transitions of overlapping grains
Brodatzki, U., Mecke, K. R.

B9 Classical and ab initio molecular dynamic simulation of a silica surface
Mischler, C., Kob, W., Binder, K.

B10 A kinetic Monte Carlo method for the simulation of heteroepitaxial growth
Much, F., Ahr, M., Biehl, M., Kinzel, W.

B11 Electronic structure of oxidized and oxygen de£cient $SnO_2(110)$ surfaces
Mäki-Jaskari, M. A., Rantala, T. T.

B12 Theoretical calculations of the energy dissipation in complex luminescence centers in ion-covalent oxide crystals
Nedilko, G.

B13 Phase-£eld modelling of multi-phase solidi£cation
Nestler, B.

B14 Band structure of the orthorhombic indium chloride
Kolinko, M. I., Nevidomskyy, A. H.

B15 Kinetics of ordering during codeposition
Ni, J., Gu, B.

B16 Stochastic dynamics for switching between the metastable state and the ground state in photoinduced phase transition
Nishino, M., Miyashita, S.

B17 Image analysis of composite £lms
Novák, S., Hrach, R., Sobotka, M.

B18 Incommensurate phases in adsorbed monolayers: structure and energy of domain-walls
Patrykiejew, A., Sokołowski, S., Binder, K.

B19 Hybrid computer modelling of plasma oxidation process
Hrach, R., Vicher, M., Pavlík, J.

B20 Surface effects in GaN growth
Pignedoli, C. A., Felice, R. Di, Bertoni, C. M.

B21 Charge dependence of temperature-driven phase transitions of molecular nanoclusters: molecular dynamics simulation
Pisov, S., Proykova, A.

B22 Parallel J-W Monte Carlo simulations of thermal phase changes in £nite-size systems
Radev, R., Proykova, A.

B23 Computer modeling of processes of second harmonic generation and methods of their optimization in one-dimensional photonic bandgap structures
Pryamikov, A. D., Bushuev, V. A.

B24 Simulation of thermodynamic variables ¤uctuations in ¤uids by the molecular dynamics method
Rudyak, Ya., Kharlamov, V.

B25 Applications of cluster computing for the Anderson model of localization
Cain, P., Milde, F., Römer, R. A., Schreiber, M.

B26 The dynamics of supercooled liquids in con£nement
Scheidler, P., Kob, W., Binder, K.

B27 Structure of steps and small islands on Si(111):As
Antons, A., Berger, R., Blügel, S., Schroeder, K.

B28 Fluctuations of steps on crystal surfaces
Selke, W., Szalma, F., Hager, J.

B29 Non-unique universal distributions of largest cluster size at the percolation threshold
Sen, P.

B30 Interlayer atomic diffusion as the reason for self-assembled quantum dots formation
Brunev, D. V., Neizvestny, I. G., Shwartz, N. L., Yanovitskaya, Z. Sh.

B31 Usage of adaptive grids for Fokker-Planck model of rari£ed gas ionization in ECR plasma source
Smirnov, A. P., Shmelev, A. B.

B32 Numerical solution of three-dimensional Poisson equation for electric £eld potential in the presence of set of conductors
Smirnov, A. P., Oh, J. J., Sheina, E. A., Shin, J. K., Shmelev, A. B.

B33 Numerical modelling of soliton formation and transients in dense resonant media
Afanas'ev, A. A., Vlasov, R. A., Khasanov, O. K., Smirnova, T. V., Fedotova, O. M.

B34 Structure and surface tension of interfaces between demixing liquids con£ned in porous materials
Patrykiejew, A., Rżysko, W., Sokołowski, S.

B35 Decomposition of multicomponent experimental ESEEM signals measured at low temperatures
Stanislavsky, A. A., Hilczer, W., Weron, K.

B36 Dynamical memory time in molecular systems
Stegailov, V. V.

B37 Parallel computing in superradiation spin dynamics
Davis, C. L., Henner, V. K., Tchernatinsky, A. V.

B38 Short-range order and hyper£ne interactions in the fcc Fe-N alloys
Timoshevskii, A. N., Yanchitskii, B. Z., Timoshevskii, V. A.

B39 Molecular polarizability of semiconductor clusters and nanostructures
Torrens, F.

B40 Mathematical simulation of photoacoustic microscopy with piezoelectric registration
Vertsanova, O.

B41 The computer investigation of the super¤uid Bose-liquid with paired interaction and with coherent condensate of the boson pair as model quantum liquid ^4He.
Pashytskiy, E. A., Vilchynskyy, S. I.

B42 Monte-Carlo simulations of the quantum phase transition in disordered itinerant antiferromagnets
Vojta, T., Bekhechi, S., Schreiber, M.

B43 Effects of anisotropy at semiconductor surfaces
Volkmann, T., Ahr, M., Biehl, M., Kinzel, W.

B44 Finite temperature properties of small quantum systems: Analytical and computer treatment
Vorontsov-Velyaminov, P. N., Gorbunov, R. I.

B45 Agglomeration in charged suspensions
Werth, J., Farkas, Z., Dammer, S., Hinrichsen, H., Wolf, D. E.

B46 Molecular dynamics study of heavy metal atoms (Pb, Bi, Sb) clustering in hydrogen reduced silicate glasses
Witkowska, A., Rybicki, J., Mancini, G., Feliziani, S.

B47 Auxetics and their microscopic mechanisms
Wojciechowski, K. W.

B48 A new algorithm of analyzing the metal-insulator transition of the Anderson model
Yamasaki, J., Hatano, N.

B49 Mesoscopic phase transitions and their critical behavior of nano structured materials
Yamazaki, Y., Gleiter, H., Abe, Y., Nakamura, K., Mizoguchi, H., Irie, T., Ito, D., Watanabe, M.

B50 Adenine tautomer complexes with closed- and open-shell copper ions. *Ab initio* examination
Rubina, Yu., Rubin, V., Sorokin, V.A., Shukla, K., Leszczynski, J.

B51 FTBF: A new software package for the analysis of extended X-ray absorption £ne structure (EXAFS) spectra
Zhuchkov, N., Gnezdilov, V.

B52 Epitaxial growth on porous $\{111\}$ and $\{100\}$ Si surfaces
Chemakin, A. V., Shwartz, N. L., Yanovitskaya, Z. Sh., Zverev, A. V.

B53 Tight binding modeling of bonding and electronic properties of heterostructures
Ünlü, H.

B54 Folding in lattice models with sidechains
Li, M. S.

B55 Effects of geometric anisotropy on local £eld in composite media
Lo, C. K., Wan, J. T. K., Yu, K. W.

B56 Computer modelling of light scattering in £lled liquid crystals
Lednei, M. F., Pinkevich, I. P., Reshetnyak, V. Yu., Sluckin, T. J.

B57 First-order scaling near a second-order phase transition: Tricritical polymer collapse
Prellberg, T., Owczarek, A. L.

B58 Mathematical model of biosensor with multilayer charged membrane
Rossokhaty, V., Rossokhata, N.

B59 Calculation of the condensate fraction in liquid Helium-4
Rovenchak, A. A., Vakarchuk, I. O.

B60 Non-equilibrium molecular dynamics simulation of block copolymers in selective solvents
Rychkov, I., Yoshikawa, K.

B61 Kinetic theory of mechanical strength of carbon nanotubes
Samsonidze, Guram G., Samsonidze, Georgii G.

B62 Representation of a network of £ller particles in polymeric composites as a mass multifractal
Kozlov, G. V., Shustov, G. B., Dolbin, I. V.

B63 Adsorption of polymer chains with variable stiffness onto a surface: Molecular dynamics simulations
Sorkin, V. A., Kramarenko, E. Yu., Khalatur, P. G., Khokhlov, A. R.

B64 One-particle diffusional model to mimic some properties of glass transition
Sorkin, V., Ivanov, A.

B65 Phase transitions of hard- and soft- disks in external periodic potentials: A Monte Carlo study
Strepp, W., Sengupta, S., Lohrer, M., Nielaba, P.

B66 Different structures of stiff-chain macromolecules: A Monte Carlo simulation
Stukan, M. R., Ivanov, V. A., Paul, W., Binder, K.

B67 Friction in atomistic Brownian systems
Sutmann, G., Steffen, B.

B68 Electrostatic effects in colloidal systems : Monte Carlo simulations
Terao, T., Nakayama, T.

B69 Glass transition in polymer £lms: A molecular dynamics study
Varnik, F., Baschnagel, J., Binder, K.

B70 Monte Carlo approach to double-stranded polymers
Velichko, Y. S., Yoshikawa, K., Khokhlov, A. R.

B71 Phase diagrams of compressible polymer-solvent mixtures - A Monte Carlo investigation
Virnau, P., Müller, M., McDowell, L.

B72 Constraints on clusters of colloidal particles by interactive molecular dynamics
Vormoor, O.

B73 Effect of binary mixtures on the isotropic-nematic transition: A lattice model simulation study
Yarmolenko, V. V., Cleaver, D. J.

B74 Field-induced structure transformation in ER solids: Beyond the point-dipole approximation
Yu, K. W., Lo, C. K., Wan, J. T. K., Siu, Y. L.

B75 Monte Carlo simulations of continuous phase transitions in the 3D Ashkin-Teller model
Musiał, G., Kamieniarz, G., Dębski, L.

B76 Statistical synchronization in Bose-Einstein condensation
Kutner, R., Regulski, M.

B77 On non-Markovian quantum master equations
Lendi, K., Aissani, A.

B78 Numerical study of complex quantum systems by a method of approximate integration in metric spaces
Lobanov, Yu. Yu.

B79 Monte Carlo investigation of critical phenomena in models of real magnetics with crossovers
Murtazaev, A. K., Kamilov, I. K., Magomedov, M. A.

B80 The coordinated valence - force £eld and thermodynamic properties of organic sulphur molecules and radicals
Orlov, Yu., Turovtsev, V.

B81 High-precision estimates of critical parameters by means of improved hamiltonians
Campostrini, M., Hasenbusch, M., Pelissetto, A., Rossi, P., Vicari, E.

B82 Microcanonical analysis of continuous phase transitions: ef£cient algorithm and critical exponents
Pleimling, M., Hüller, A.

B83 Quantum chaos and its testing
Prykarpatsky, A. K., Basiura, R., Prykarpatska, K.

B84 Nucleation in the two-dimensional Ising model
Rutkevich, S. B.

B85 Molecular dynamics simulation study of N,N-dimethylformamide – water solutions
Koufou, A., Chalaris, M., Samios, J.

B86 Solute-solvent interactions in in£nitely dilute supercritical mixtures: A molecular dynamics investigation
Cournia, Z., Dellis, D., Samios, J.

B87 Ultrametric £eld theory and Random Energy Model (REM) statistical mechanics
Saakian, D. B.

B88 Common features of decon£ning and chiral critical points in QCD and the three state Potts model in an external £eld
Karsch, F., Schmidt, Ch., Stickan, S.

B89 Study of plasma-solid interaction in low-temperature plasma
Vicher, M., Hrach, R., Entlicher, M., Mareš, R.

B90 Avalanches in the ground state of the 3d gaussian random £eld ising model driven by an external £eld
Frontera, C., Vives, E.

B91 A model of internal waves mixing via numerical solution of Korteweg-de Vries system
Halim, A. A., Kshevetskii, S. P., Leble, S. B.

B92 Computational method for transition to chaos prediction of the forced oscillations
Bashkirtseva, I. A., Ryashko, L. B.

B93 Localization and coherent structures in wave dynamics via multiscales
Fedorova, A. N., Zeitlin, M. G.

B94 Numerical simulation ¤uid ¤ow with a obstacle on a channel wall: Quasi - oscillation regime
Gorbatchevski, A. Ya., Churbanov, A. G.

B95 Convection instability in a small Rayleigh-Bénard system
Hasegawa, M.

B96 Interaction of dissipative quasi-particles: Scattering, formation of bound states, generation and annihilation
Liehr, A. W., Bode, M., Purwins, H.

B97 Computation of a diverging LX-17 detonation
Eryan, L., Bangdi, L., Yuanshu, W.

B98 Computational analysis of the evolution of steep gravity waves on ¤uid of an arbitrary depth
Lukomsky, P., Gandzha, S., Lukomsky, V., Tsekhmister, V.

B99 Analysis of vortex structures in a compressible isotropic turbulence
Miura, H.

B100 Numerical modeling of turbulent wakes dynamics in strati£ed medium
Chernykh, G. G., Moshkin, N. P., Voropayeva, O. F.

B101 Generalized thermostatistics description of turbulent temperature ¤uctuations
Ramos, F. M., Rosa, R. R., Neto, C. R., Bolzan, M. J. A., Sá, L. D. A.

B102 Gastrulation as a self-organized symmetry breaking process
Castro-e-Silva, A., Bernardes, A. T.

B103 Uni£ed information sharing system and computational physics
Itoh, S., Saito, T., Ohnishi, S., Takaki, R., Ogawa, S.

B104 Multifractality of cloud base height pro£les
Ivanova, K., Gospodinova, N., Shirer, H. N., Ackerman, T. P., Michalev, M. A., Ausloos, M.

B105 Study of some laser signals emergent from nonlinear optical media
Ghelmez, M., Toma, C., Sterian, P. E.

B106 Fluctuations of WIG- the index of Warsaw stock exchange
Makowiec, D., Gnaciński, P.

B107 Neural networks in image analysis of complex systems
Malý, M., Hrach, R., Novotný, D.

B108 Pressure measurements in NVE simulations: The case of lipid bilayers
Penna, G. La, Minicozzi, V., Morante, S., Rossi, G. C.

B109 Dynamical system's approach to the busy beaver problem
Nameda, E., Ohira, T., Ikegami, T.

B110 Characterisation of degree of arrangement in image analysis of complex systems
Hrach, R., Novotný, D., Sobotka, M., Vicher, M., Kostern, M.

B111 Stochastic three state model with delay
Sazuka, N., Ohira, T.

B112 Synaptic polarities studied by the recurrent back-propagation
Omata, K., Osana, Y., Kawamura, K.

B113 On a £nite-dimensional reduction for a class of conservative dynamical systems and its applications
Prykarpatska, N. K., Prykarpatsky, A. K.

B114 Finite dimensional reductions of conservative dynamical systems and numerical analysis
Prykarpatsky, A. K., Prykarpatsky, N. K.

B115 A study on the form factors kernel function
Zéghers, E., Christophe, Renaud.

B116 Least squares £tting of a polynomial of degree two to a set of data points
Sheth, C. V.

B117 Pattern analysis for packing cells of wings of Pterygota
Seino, M., Kakazu, Y., Aoki, D.

B118 A model of urban mobility
Bazzani, A., Giorgini, B., Servizi, G., Turchetti, G.

B119 Application of parallel computations for the modelling of electromagnetic waves propagation in an anisotropic layer
Sharkova, N. M., Andronov, I. V.

B120 Energetics ef£ciency in homogeneous forced ratchets
Sintes, T., Sumithra, K.

B121 Networked virtual reality space for analyzing numerical simulation result
Tamura, Y., Kageyama, A., Sato, T.

B122 Dynamical behavior of individual agents in Hogg-Huberman model
Inoue, M., Tanaka, T., Shibata, J.

B123 Quantum spectral properties of a spin-1/2 particle in coupled quartic oscillator potential
Tomiya, M., Yoshinaga, N.

B124 Optical soliton propagation in coupled systems with random perturbations
Umarov, B. A.

B125 Modi£ed oscillator J-matrix method for scattering
Vanroose, W., Broeckhove, J., Arickx, F.

B126 A numeric investigation of a vehicular traf£c ¤ow model based on a stochastic acceleration process
Waldeer, K. T.

B127 Rotating dielectric sphere near a substrate interface
Wan, J. T. K., Gu, G. Q., Yu, K. W.

B128 Quasiclassical calculations of Wigner functions in nonlinear dynamics via multiresolution
Fedorova, A. N., Zeitlin, M. G.

B129 Shifted contour auxiliary £eld Monte Carlo: Accurate electronic structure of molecules and extended model systems
Baer, R., Neuhauser, D.

B130 A parallel Moore-Penrose generalized inverse algorithm for equilibrium network ¤ow sensitivity simulation
Cho, H., Fan, C.

B131 A fast way to optimize the design of an asymmetric dc–SQUID
Calidonna, C. R., Furnari, M. M., Pagano, S., Sarnelli, E., Testa, G.

B132 Non-relativistic electron transport in metals: A Monte Carlo approach
Rahimi, M. F., Ghal-eh, N.

B133 New cluster algorithm and its application to the $S = 1/2$ XXZ chain
Otsuka, H.

B134 Contrasting models for the simulation of multi-particle collisions and dynamics in a one-dimensional space
Oyedele, J. A.

B135 Dynamic Monte Carlo simulations with a phonon heat bath for a square-lattice ising ferromagnet
Park, K., Novotny, M. A.

B136 Path integral Monte Carlo study of a two dimensional polaron gas
Titantah, J. T., Pierleoni, C., Ciuchi, S.

B137 Study of bifurcations and stability in Rayleigh-Bénard convection
Puigjaner, D., Simó, C., Giralt, F.

B138 Kinetic theory for a ¤uctuating heat conduction equation
Ripoll, M., Espa nol, P.

B139 An alternative approach to the computation of critical properties with the renormalization group
Ron, D., Swendsen, R. H.

B140 Local sensitivity computational analysis of stochastic 3D-cycles
Ryashko, L. B., Bashkirtseva, I. A.

B141 Load-balancing of plasma particle-in-cell simulations
Schüle, J., Othmer, C.

B142 Semi-quantal simulations of hydrogen under extreme conditions
Knaup, M., Reinhard, P.-G., Toepffer, C., Zwicknagel, G.

B143 Non-Boltzmann sampling for percolation and the q-states Potts models
Weigel, M.

B144 A dynamic Monte Carlo study of random-bond Potts ferromagnet with trinary disorder distributions
Ying, H. P., Ji, D. R., Schülke, L.

Invited Plenary Contributions

Simulating crystal nucleation rates

Daan Frenkel

Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands

Classical Nucleation Theory dates back to the 1920's and has been the standard tool to predict and interpret experiments on (crystal) nucleation. It is now becoming possible to compute absolute nucleation rates directly by computer simulation, even when the actual rates are as low as one nucleus per cubic centimeter per month! However, simulations of crystal nucleation in colloidal suspensions yield rather large discrepancies with experiment. In my talk, I shall review what simulation tells us about the pathway for colloidal crystallization and I shall discuss some of the factors that may be responsible for the discrepancy between simulation and experiment. In particular, I shall discuss recent simulation results that shed a new light on crystallization in amorphous materials.

Computer simulation of biomolecules at soft interfaces

Michael L. Klein
Center for Molecular Modeling, Department of Chemistry
University of Pennsylvania
klein@lrsm.upenn.edu

Abstract not available at time of printing

Modelling liquid crystal hydrodynamics

Julia Yeomans

University of Oxford, Theoretical Physics, 1 Keble Road,
Oxford, OX1 3NP, England

Tel: 44 1865 273992, Fax: 44 1865 273947,
E-mail: J.Yeomans1@physics.ox.ac.uk

There is great interest in obtaining a fundamental physical understanding of the ¤ow properties of liquid crystals, polymer melts and droplet suspensions. The hydrodynamics of such complex ¤uids can be complicated and very different from that of simple liquids because of the coupling between the microscopic structure and the velocity £eld. Examples include shear thinning and non-equilibrium phase transitions such as banding under shear.

Developing modelling approaches is challenging because of the diverse length and time scales involved. One attempt to overcome the problems has been the development of mesoscale modelling methods such as lattice Boltzmann simulations[1]. These solve the hydrodynamic equations of motion while inputting suf£cient, albeit generic, molecular information to model the important microscopic physics of the ¤uid. This is often done by imposing a Landau free energy functional which is minimised in equilibrium.

Looking to extend mesoscale approaches to non-Newtonian ¤uids we have developed a lattice Boltzmann model of liquid crystal hydrodynamics[2]. The approach is based on the hydrodynamic equations of motion written in terms of a tensor order parameter[3] and is able to model the isotropic, uniaxial nematic, and biaxial nematic liquid crystal phases. Back-¤ow, the coupling of the order parameter to the ¤ow £eld, and variations in the magnitude of the order parameter appear naturally within the simulations. Hence we are able to investigate, inter alia, the role of hydrodynamics in the movement of topological defects, domain wall movement in liquid crystal switching, phase ordering in liquid crystals following a quench and director con£gurations in a ¤ow £eld.

We show that the velocity of topological defects can be strongly affected by hydrodynamics. Defects of different topological charge couple to the ¤ow £eld in different ways and hence have different velocities for a given driving force. As liquid crystal devices switch domains of the new phase have been observed to grow anisotropically[4] and we demonstrate that this can be explained by invoking hydrodynamic coupling to defects which form at the domain walls.

A current aim of the electronics industry is to develop bistable devices which can retain a memory of two distinct director con£gurations even when the external £eld is switched off. Such devices would lead to enormous power savings for infrequently updated displays. We describe switching in one such device, the zenithal bistable nematic, and show that the switching can be driving by a surface ¤exoelectric effect.

References

1. S. Chen and G.D. Doolen, Annual Rev. Fluid Mech. **30** 329 (1998).
2. C. Denniston, E. Orlandini and J.M. Yeomans, Europhys. Lett. **52** 481 (2000).
3. A.N. Beris and B.J. Edwards, *Thermodynamics of Flowing Systems*, Oxford University Press, (1994).
4. E.J. Acosta, M.J. Towler and H.G. Walton, Liquid Crystals, **27** 977 (2000).

Computers in physics education

Francisco Esquembre

Departamento de Matemáticas, Universidad de Murcia, 30071 Murcia, Spain

phone:+34 968363534, fax:+34 968264182, e-mail: fem@um.es

Although the question of whether students really learn the fundamental concepts of Physics after succeeding introductory courses, has (or at least should have) always worried faculty, greater concern has arisen as the £gures of enrolments of students have started a long-lasting decline. Of course, this problem can be due to several causes, not all of them academic [1]. But certainly, increasing the degree of satisfaction of the students and their ultimate understanding of what Physics is and how exciting working with Physics is for all of us, would help maintain or even increase the attraction of Physic courses to both future professionals and students from other disciplines.

As part of the reaction to this concern, many faculty have turned their eyes to computers as a tool to improve their day-to-day task of lecturing. However, it is not clear that just using a new media actually improves the learning [2]. The correct approach (and this is the one that we will defend in our exposition) seems to be to learn about all the work conducted in the past two decades in the £eld of Physics Education Research (PER), and use their already widely accepted core of results to design and implement new successful teaching strategies [3].

Fortunately for those interested and keen on computers, it turns out that many of the features and 'best practices' that PER recommends [4] are not only possible with computers, but in some cases, they are very dif£cult to implement (in the reasonable limited time that we are usually given to teach) without a computer.

We will revise the recommendations of PER in this talk as well as discuss how these can be correctly implemented using computers. We will also expend some time taking a brief glance (with de£nitely no attempt for comprehensiveness) at some of the successful or interesting experiences and software that is currently being developed and used in Physics classrooms.

We will end this talk with a discussion of the opportunities and threats that the use of Computers in Physics Education (and sometimes not only in Education!) face in our days. Certainly, this will be the most subjective, (and perhaps controversial) part of the talk.

References

1. Ruth H. Howes. "Undergraduate Physics in the Age of Compassionate Conservatism". Talk at James Madison University. (March 2001).
2. A. Szabo, N. Hastings. "Using IT in the undergraduate classroom". Computers and Education 35 (2000) 175-187.
3. Edward F. Redish. "Millikan Award Lecture (1998): Building a Science of Teaching Physics". Am. J. Phys. 65(1), 45-54.
4. Leon M. Lederman "ARISE: white paper". FERMILAB-TM-2051 (1998)

Methods for coupled quantum-classical Monte Carlo

D. M. Ceperley[1] **and M. Dewing**[2]

[1]*University of Illinois, 1110 W Green St., Urbana, IL 61801, USA*
[2]*INTEL, Fox Dr., Champaign, IL 61821, USA*
ceperley@uiuc.edu

Quantum Monte Carlo (QMC) methods such as Variational Monte Carlo, Diffusion Monte Carlo or Path Integral Monte Carlo are the most accurate and general methods for computing total electronic energies. Taking many-body hydrogen at high pressure as an example, each method has a limited range of applicability, particularly at £nite temperature.

We have introduced a method[1] to perform a coupled QMC for the electrons and another MC simulation for the ions (CEIMC). Using quantum Monte Carlo, one estimates the Born-Oppenheimer energy which is then used in a Metropolis simulation of the ionic degrees of freedom. We have shown that one can modify the usual Metropolis acceptance probability to eliminate the bias caused by noise in this energy difference, thus allowing more noisy estimates of the energy difference and thereby drastically reducing the sampling time of the electronic degrees of freedom. We have implemented[2] several different QMC methods for estimating the energy change including Diffusion Monte Carlo and Variational Monte Carlo. We have also developed a correlated sampling technique so that the variance of the difference is smaller than of each energy individually.

Using these methods, we have performed simulations of liquid H_2 on a parallel computer. We have developed novel methods to move the H_2molecules (separate translations, rotations and vibrations) and ways to pre-reject the moves using an empirical potential in an effort to speed up the simulation. We discuss some possible advantages of the CEIMC method relative to Car-Parinello simulations concerning how the quantum effects of the ionic degrees of freedom can be included and how the boundary conditions on the phase of the wavefunction can be integrated over[3].

References

1. Ceperley, D. M. and M. Dewing, ”The Penalty Method for Random Walks with Uncertain Energies”, J. Chem. Phys., 110, 9812-9820 (1999).
2. Dewing, M and D. M. Ceperley, ”Methods for Coupled Electronic-Ionic Monte Carlo”, Recent Advances in Quantum Monte Carlo Methods, II, ed. S. Rothstein, World Scient£c, in press (2001).
3. C. Lin, F.-H. Zong and D. M. Ceperley, ”Twist-averaged boundary conditions in continuum Quantum Monte Carlo algorithms”, Phys. Rev. E 64 , 016702 (2001).

Predictive modeling of materials by *ab initio* thermodynamics and statistical mechanics

Matthias Schef¤er

Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4-6, D-14195 Berlin, Germany
http://www.fhi-berlin.mpg.de/th/th.html

In this talk I will sketch the "*ab initio* line" of "Computational Materials Science and Engineering", that at present is signi£cantly increasing in importance and impact. To predict materials properties starting from the electronic structure and going all the way to technically relevant time and length scales, is a desire that has existed for many years in particular in condensed-matter physics, materials science, surface physics, chemistry, and bio-chemistry. However, only recent, spectacular developments in methodology, and the availability of fast computers, enable us now to approach this goal.

I will emphasize how density-functional theory calculations can and should be combined with methods from statistical mechanics [1,2], meso-/macroscopic continuum mechanics [3], and thermodynamics [3,4,5], and I will demonstrate the value of such studies using selected examples. These examples include:

- phase transitions of crystals with relevance to mineralogy and geophysics,
- predictions and description of the function of materials surfaces (e.g., atomic structure, chemical activity),
- excited states, core-level spectroscopy (many-electron effects), etc.,
- crystal growth and self-assembly of nano structures,
- insights into the nature of interactions in biological molecules.

Emphasis will be placed on methodology, simple physical models, concepts, and the development of understanding.

References

1. A. Gross and M. Schef¤er, *Ab initio quantum and molecular dynamics of the dissociative adsorption of hydrogen on Pd(100)*, Phys. Rev. B **57**, 2493 (1998); http://www.fhi-berlin.mpg.de/th/paper.html
2. P. Kratzer and M. Schef¤er, *Molecular Modeling of Surfaces from First Principles*. To appear in Computing in Science and Engineering (2001); http://www.fhi-berlin.mpg.de/th/paper.html
3. Q.K.K. Liu, N. Moll, M. Schef¤er, and E. Pehlke, *Equilibrium shapes and energies of coherent strained InP islands*. Phys. Rev. B **60**, 17008(1999); L.G. Wang, P. Kratzer, N. Moll, and M. Schef¤er, *Size, shape, and stability of InAs quantum dots on the GaAs(001) substrate*. Phys. Rev. B **62**, 1897 (2000).
http://www.fhi-berlin.mpg.de/th/paper.html
4. X.-G. Wang, A. Chaka, and M. Schef¤er, *Effect of the environment on alpha-Al2O3 (0001) surface structures*. Phys. Rev. Lett. **84**, 3650 (2000).
5. C. Stamp¤, M.V. Ganduglia-Pirovano, K. Reuter, and M. Schef¤er, *Catalysis and corrosion: The theoretical surface-science context*.To appear in Surf. Sci. 500 (2001); http://www.fhi-berlin.mpg.de/th/paper.html

Pushing the limits: Extremes and crashes in £nance and economics

D. Sornette[1,2]

[1]*Institute of Geophysics and Planetary Physics*
and Department of Earth and Space Science
University of California, Los Angeles, California 90095, USA
[2]*Laboratoire de Physique de la Mati¶re Condensée CNRS UMR6622*
and Université des Sciences
B.P. 70, Parc Valrose, 06108 Nice Cedex 2, France
tel: 33-4 92 07 67 83, fax: 33-4 92 07 67 54, e-mail: sornette@unice.fr

A market crash occurring simultaneously on most of the stock markets of the world as witnessed in Oct. 1987 would amount to the quasi-instantaneous evaporation of trillions of dollars. In values of Jan. 2001, a stock market crash of 30% indeed would correspond to an absolute loss of about 13 trillion dollars! Market crashes can thus swallow years of pension and savings in an instant. Could they make us suffer even more by being the precursors or triggering factors of major recessions as in 1929-33 after the great crash of Oct. 1929? Or could they lead to a general collapse of the £nancial and banking system as seems to have being barely avoided several times in the not-so-distant past? Stock market crashes are also fascinating because they personify the class of phenomena known as "extreme events" [1].

What are crashes? How do they happen? Why do they occur? When do they occur?

The study of the frequency distribution of drawdowns, or runs of successive losses, shows that large £nancial crashes are "outliers": they form a class of their own as can be seen from their statistical signatures. If large £nancial crashes are "outliers", they are special and thus require a special explanation, a speci£c model, a theory of their own. The main mechanisms leading to positive feedbacks, i.e., self-reinforcement, such as imitative behavior and herding between investors are then described. Positive feedbacks provide the fuel for the development of speculative bubbles, preparing the instability for a major crash. We have developed rational models of speculative bubbles and crashes based on the interplay between imitation between noise traders and risk aversion by rational investors.

Our most important message is the discovery of robust and universal signatures of the approach to crashes. These precursory patterns have been documented for essentially all crashes on developed as well as emergent stock markets, on currency markets, on company stocks, etc. The analysis demonstrates the empirical evidence of the universal nature of the critical log-periodic precursory signature of crashes. We examine in details what are the forecasting skills and their limitations, in particular in terms of the horizon of visibility and expected precision. We also present the concept of an "anti-bubble", with the Japanese collapse from the beginning of 1991 to present, taken as a prominent example. A prediction issued and advertised in Jan. 1999 has been until now born out with remarkable precision, predicting correctly several changes of trends, a feat notoriously dif£cult using standard techniques of economic forecasting.

References

1. Sornette, D. (2001) Predictability of catastrophic events: material rupture, earthquakes, turbulence, £nancial crashes and human birth, Proceedings of the National Academy of Sciences USA, in press (2001) (e-print at http://arXiv.org/abs/cond-mat/0107173)
2. Sornette, D. (2001) Critical market crashes, to be published (Princeton University Press, Princeton, NJ).

Simulations of phase transitions in macromolecular systems

Kurt Binder

Institut für Physik, Johannes-Gutenberg-Universität Mainz
Staudinger Weg 7, 55099 Mainz, Germany
Tel: + 49 (06131) – 39-23348, Fax: + 49 (06131) – 39-25441
e-mail: kurt.binder@uni-mainz.de

The study of phase transitions in concentrated solutions and melts of ¤exible or stiff polymers is a computational challenge for computer simulations, since already a single polymer coil exhibits nontrivial structure from the scale of a chemical bond (1Å) to the coil radius (100Å), and for the simulation of collective phenomena huge simulation boxes containing many polymers are required. A strategy to deal with this problem is the use of highly coarse-grained models on a lattice, such as the bond ¤uctuation model. Several studies employing such models will be brie¤y reviewed, e. g: the temperature-driven - isotropic–nematic phase transition in concentrated solutions of semi¤exible polymers, unmixing of polymer blends in the bulk and in a geometry con£ned between walls which prefer one component. It is shown that the £nite size scaling techniques previously developed for Ising-type models are useful in this context, too. Simulation of unmixed polymer blends between competing walls allows a study of an interface localization-delocalization transition and to observe anomalous interfacial broadening (depending on thin £lm thickness). These simulations have also elucidated corresponding experiments.

Future directions in scienti£c supercomputing for computational physics

Horst D. Simon
NERSC, Lawrence Berkeley National Laboratory
Mail Stop 50B-4230
Berkeley, CA 94720, USA
Hdsimon@lbl.gov

NERSC, the National Energy Research Scienti£c Computing Center, is DOE's premier scienti£c computing facility for unclassi£ed research, and has had a signi£cant impact on computational physics in the US. In this presentation I will summarize the recent experience at NERSC, and present elements of our strategic plan for the next £ve years. Signi£cant changes are expected to happen in computational science during this period. Traditional supercomputer centers will have to anticipate these changes, and be ready yet again to change their model of service.

For the last £ve years the transition from a vector-parallel to a massively parallel computing environment were the most signi£cant event. This was accomplished by combining a commitment to providing *high-end systems* and with a strong effort in *comprehensive scienti£c support* for its users. Supercomputer centers evolved from the cycle-shop, mainframe oriented mentality of the 1980s to the concept of an intellectual center in the late 1990s.

In 2001 two new trends are apparent: (1) the emergence of large, multidisciplinary teams for computational physics simulations, and (2) the convergence of computation, experiment, and theory on an iterative, real-time basis. Here I will present a vision on how a center will change its activities and set new directions over the next £ve years to address these changes.

The £rst new element is support for *Scienti£c Challenge Teams*. It is envisioned that these large-scale teams will be formed to develop and deploy advanced modeling and simulation codes, as well as new mathematical models and computational methods that take full advantage of the new generation of terascale computers. These teams are representative of a shift from the single-principal-investigator model for high-end computing to a collaborative model aimed at producing "community codes" whose development is shared by entire scienti£c research communities.

A second new component of the center strategy addresses another change in the practice of scienti£c computing. In recent years rapid increases in available networking bandwidth, combined with continuing increases in computer performance, are making possible an unprecedented *simultaneous* integration of computational simulation with theory and experiment. This change will have a fundamental impact on areas of science that have not yet made much use of high-end computing. By deploying critical parts of a *Uni£ed Science Environment (USE)*, NERSC anticipates playing a key role in the emergence of a new paradigm in computational science.

Supercomputer centers worldwide must continue to enhance their successful role as a centers that bridge the gap between advanced development in computer science and mathematics on one hand, and scienti£c research in the physical, chemical, biological, and earth sciences on the other. Implementing such a strategy will position NERSC and other centers in the US to continue to enhance the scienti£c productivity of the computational physics community, and to be an indispensable tool for scienti£c discovery.

Cosmic architecture: computer simulations of structure in the Universe

C. S. Frenk

Physics Department, University of Durham, Durham DH1 3LE, England

44 191 3742165 (tel), 44 191 3747465 (fax), c.s.frenk@durham.ac.uk

Cosmology confronts some of the most fundamental questions in the whole of science. How and when did our universe begin? What is it made of? How did it acquire its current appearance? How will it end? There has been enormous progress over the past £fty years towards answering these questions. There is now incontrovertible evidence that our universe began about 13 billion years ago in a hot, dense phase – the Big Bang – and that most of its material content today consists of invisible "dark matter," very likely made up of exotic elementary particles. The radiation generated by the primordial £reball is detected today as a background of microwaves and this provides a direct window to the early universe. In the 1990s astronomers discovered tiny ripples in this radiation, the fossil records of primordial irregularities which have been ampli£ed by the gravity of the dark matter to produce the rich variety of structures seen today in large galaxy surveys. Precise measurements show that the properties of these irregularities agree remarkably well with the predictions of the "in¤ationary" theory of the early universe.

Using the laws of Physics, computer simulations recreate the evolution of the universe and provide the means for connecting objects or 'events' observed at widely different cosmic epochs. On the scales of galaxies and clusters, the evolution is complex and involves not only gravitational interactions, but also gasdynamic and radiative effects associated with the gas that ultimately ends up in the stars that make up the galaxies. Cosmological simulations present a formidable computational challenge not only because of the non-linear nature of the problem, but also because of the huge range of scales involved. The processes that lead to the formation of an individual star operate on a length scale at least one hundred million times smaller than the size of the largest galaxy structures seen in the universe. To overcome these problems, cosmologists have devised ef£cient algorithms, including novel methods for computing the evolution of N-body and ¤uid dynamical systems [1].

In spite of its apparent complexity, the cosmological problem is better posed than most computational problems in Physics or Biology: the initial conditions are known precisely, from the ripples in the microwave background radiation and from early universe Physics. Starting from such initial conditions, cosmological simulations follow the coupled evolution of dark matter and gas into the present day, recreating the major events which have shaped our Universe: the irradiation of the primordial plasma by the earliest quasars and stars, the motion of primordial hydrogen gas clouds and their accretion onto spinning dark matter clumps, the growth of dark matter halos and galaxies within them by repeated mergers of substructures, the emergence of spiral galaxies like the Milky Way and of the great aggregates of galaxies like the Coma cluster. The output of a simulation is a virtual universe. Finding the best match to the real one, reveals the model assumptions and parameter values that best describe our Universe [2].

In this talk, I will review the successes and some of the future challenges faced by computational cosmology. I will argue that although some fundamental issues remain to be settled, a coherent picture of cosmic evolution is beginning to emerge.

References

1. Frenk, C.S. etal 1999, Astrophys. J., 525, 554
2. Benson, A.J., Cole, S., Frenk, C.S., Baugh, C. & Lacey, C., 2000, Mon. Not. Royal astr. Soc, 311, 793

Parallel adaptive simulation of large systems on unstructured grids

G. Wittum
Interdisziplinäres Zentrum für Wissenschaftliches Rechnen (IWR)
Heidelberg, Germany
wittum@iwr.uni-heidelberg.de

Numerical simulation has become one of the major topics in Computational Science. To promote modelling and simulation of complex problems new strategies are needed allowing for the solution of large, complex model systems. Crucial issues for such strategies are reliability, ef£ciency, robustness, usability, and versatility. After discussing the needs of large-scale simulation we point out basic simulation strategies such as adaptivity, parallelism and multigrid solvers. These strategies are combined in the simulation system UG (*Unstructured Grids*) being presented in the following. In the second part of the seminar we show the application of these strategies to the simulation of processes from computational mechanics. In particular we will show results of 3d elasto-plastic computations as well as two-phase ¤ow computations of rising air bubbles in water and density-driven groundwater ¤ow. In these examples we will also discuss issues of reliability and validation.

The structure and function of networks

Mark Newman

Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501, U.S.A.

Tel: +1–505–984–8800, Fax: +1–505–982–0565, E-mail: mark@santafe.edu

Many different de£nitions of complex systems have been given, but one of the most common de£nes a complex system as a system composed of many interacting parts, or agents. Societies, the Internet, ecosystems, and markets are frequently cited examples of such systems. Much research has focused on the nature of the agents in these systems, and much on the nature of the interactions between agents. Until recently however little attention has been paid to the *pattern* of interaction between agents – who is connected to whom – although with hindsight it is clear that understanding this pattern is crucial to understanding the system as a whole. The interactions between agents in a complex system form a network or graph. In this talk I will discuss the structure of some real-world networks, and what that structure implies for our modeling of complex systems.

I will show a number of examples of networks for which good structural data exist, including the Internet and the World-Wide Web, collaboration networks of scientists and business-people and other social networks, and food webs. I will focus on three speci£c statistic properties of these networks:

1. the “small world” effect, in which the average distance through the network between randomly chosen pairs of agents is short – usually only logarithmic in the volume of the system;
2. “clustering” in networks, in which agents form into communities with high local connectivity, indicated by high network transitivity or a large value of the so-called clustering coef£cient;
3. right-skewed degree distributions, where there are typically a small number of agents in the network that are connected to very many others, and many that are connected to only a few. Often the degree distribution is found to follow a power law, although exponential and truncated power-law distributions are common too.

I will discuss some recently proposed models of networks that show these characteristics, and give some examples of how they are being used in the study of complex systems, particularly the Internet and social networks. I will also show results from a variety of simulations demonstrating that dynamics on complex networks is entirely unlike dynamics on regular lattices [1, 2, 3, 4]. These results make it clear that to gain a full understanding of complex systems we need to develop the mathematical and computational techniques to handle systems with network structure of the kind described here.

References

1. D. J. Watts and S. H. Strogatz, *Nature* **393**, 440–442 (1998).
2. M. E. J. Newman, *J. Stat. Phys.* **101**, 819–841 (2000).
3. D. S. Callaway, M. E. J. Newman, S. H. Strogatz and D. J. Watts, *Phys. Rev. Lett.* **85**, 5468–5471 (2000).
4. D. S. Callaway, J. E. Hopcroft, J. M. Kleinberg, M. E. J. Newman, and S. H. Strogatz, *Phys. Rev. E*, in press. Also cond-mat/0104546.

Cluster percolation and thermal critical behavior

Helmut Satz
Fakultät für Physik, Universität Bielefeld
D-33501 Bielefeld, Germany

Continuous phase transitions in simple spin systems can be formulated as percolation of suitably de£ned clusters. We review this equivalence and discuss how it can be extended to include longer range interactions, £nite external £elds and £rst order transitions. We then survey £rst attempts to treat the QCD decon£nement transition between hadronic matter and a quark-gluon plasma in terms of percolation. Finally, we speculate on a possible generalization of critical behavior based on the percolation transition.

Generalized ensemble simulations of complex systems

Bernd A. Berg

Physics Department, Florida State University, Tallahassee, FL 32306, USA

+1-850-6446246, +1-850-6446735, berg@hep.fsu.edu

Monte Carlo (MC) simulations are an indispensable tool for the investigation of physical models. The most ef£cient MC weights for the calculation of physical, canonical expectation values are not necessarily those of the canonical ensemble, but the use of suitably generalized ensembles can lead to much faster convergence. Although not realized by nature, these ensembles can be implemented on computers.

In recent years the generalized ensemble approach has in particular been studied for the simulation of complex systems. For these systems it is typical that con¤icting constraints lead to free energy barriers, which fragment the con£guration space. Examples of major interest are spin glasses and proteins. In my overview I will £rst comment on the strengths and weaknesses of a few major approaches, including parallel tempering, multicanonical and transition variable methods. Subsequently, selected examples from applications to spin glasses and proteins will be presented.

For a review of the generalized ensemble approach in the context of protein folding see Hansmann and Okamoto [1]. The multicanonical approach, to some extent along with parallel tempering and transition variable methods, is reviewed in Ref.[2]. The featured applications will include Helix-coil transitions of amino-acid homo-oligomers in an aqueous solution [3] and a new analysis of the Parisi overlap distribution from a simulation of the 3d Edwards-Anderson Ising spin glass by Billoire, Janke and the speaker [4].

References

1. U.H.E. Hansmann and Y. Okamoto, *The generalized-ensemble approach for protein folding simulations*, in *Annual Reviews of Computational Physics VI*, D. Stauffer (ed.), World Scienti£c, Singapore 1999, pp.129–157.
2. B.A. Berg, *Introduction to Multicanonical Monte Carlo Simulations*, Fields Institute Communications 20 (2000) 1–24.
3. A. Mitsutake and Y. Okamoto, *Helix-coil transitions of amino-acid homo-oligomers in aqueous solution studied by multicanonical simulations*, J. Chem. Phys. 112 (2000) 10638–10647.
4. W. Janke, B.A. Berg and A. Billoire, *Energy Barriers of Spin Glasses from Multi-Overlap Simulations*, Ann. Phys. (Leipzig) 7 (1998) 544–553.

Cluster Monte Carlo: Extending the range

H.W.J. Blöte[1,2], J.R. Heringa[1] and E. Luijten[3]

[1] *Laboratory of Applied Physics, Delft University of Technology, Lorentzweg 1, P.O. Box 5046, 2600 GA Delft, The Netherlands*
[2] *Instituut Lorentz, Leiden University, Niels Bohrweg 2, P.O. Box 9506, 2300 RA Leiden, The Netherlands*
[3] *Institute for Physical Science & Technology, University of Maryland, College Park, MD 20742-2431, USA*
£rst author: tel. (+31) (0)15 278 6156, FAX (+31) (0)15 278 6081, e-mail bloete@tnw.tudelft.nl

Monte Carlo simulations of lattice models frequently use local updates. Near criticality, such algorithms suffer from the critical-slowing-down phenomenon. Cluster algorithms, which use nonlocal updates, can suppress this phenomenon and thereby achieve much better statistical accuracies. The gain in ef£ciency with respect to local algorithms depends on the system size, and still varies from case to case. It can reach extreme proportions, for instance a factor 10^8 in the case of an investigation of an Ising model with long-range interactions [1]. However, these nonlocal algorithms are not as easy to generalize as local (Metropolis-type) algorithms and thus restricted to a limited range of applicability.

We review a number of existing cluster algorithms, and present new ones. The success of such algorithms obviously depends on two conditions: £rst one needs a proof of detailed balance, so that one can be assured to obtain an unbiased sample of the pertinent ensemble; and second, the algorithm has to be ef£cient in comparison with local algorithms.

In general a cluster algorithm can be formulated on the basis of a symmetry property of the model, i.e. the Hamiltonian should be invariant under that symmetry. Moreover the symmetry operation should be self-inverse. These two conditions are suf£cient to prove detailed balance [2]. The Swendsen-Wang algorithm [3] is thus based on the q-state permutation symmetry of the Potts model (or up-down symmetry in the Ising case). The 'geometric cluster algorithm' [2] uses instead a spatial symmetry, for instance the geometric inversion symmetry of the lattice. The Hamiltonian of the chiral Potts model is not invariant under each of these symmetry operations. But a lattice inversion combined with an inversion of the q Potts states $\sigma \to s - \sigma \bmod q$ (where s is an arbitrary integer) leaves the Hamiltonian invariant, and can thus serve as the basis of a nonlocal Monte Carlo algorithm.

For reasons of ef£ciency, the percolation threshold of the cluster-formation process should preferably coincide with the critical point. In a number of cases, such as the Swendsen-Wang algorithm and the geometric cluster algorithm applied to the Potts model, this coincidence can be proved.

However, even in the absence of this coincidence, the ef£ciency of nonlocal algorithms can far exceed that of local methods. This situation was realized in a recent application of a cluster algorithm to an Ising model with two- and three-spin interactions, investigated earlier with a special-purpose computer [4]. The new results enable a fairly accurate estimate of the speci£c-heat exponent, close to $\alpha = 2/3$ as expected for the 4-state Potts universality class.

References

1. E. Luijten and H.W.J. Blöte, Int. J. Mod. Phys. **C6** 359 (1995).
2. J.R. Heringa and H.W.J. Blöte, Phys. Rev. E **57** 4976 (1998).
3. R.H. Swendsen and J.-S. Wang, Phys. Rev. Lett. **58** 86 (1987).
4. H.W.J. Blöte, A. Compagner, P.A.M. Cornelissen, A. Hoogland, F. Mallezie and C. Vanderzande, Physica A **139** 395 (1986).

Go-with-the-winners simulations

P. Grassberger

John von Neumann Institute for Computing (NIC), Forschungszentrum Jülich, D-52425 Jülich, Germany

p.grassberger@fz-juelich.de

In many problems of statistical physics one is interested in taking random samples according to some prescribed non-uniform measure. These samples are then dominated by a priori rare events. We discuss a class of algorithms which – in contrast to Markov chain Monte Carlo – are similar in spirit to evolutionary algorithms. Like the latter, they use ”population control” to clone ‘good’ and to kill ‘bad’ instances (con£gurations, paths, ...), but such that all expectation values are obtained correctly. Such strategies have been used since long time for (diffusion type) quantum Monte Carlo and for polymer simulations, but their general usefulness was fully appreciated only recently. We present new applications to polymers, DNA melting, percolation, lattice animals, the alignment of DNA sequences, and simple population dynamics models.

Invited Contributions

Electronic structure calculations of solids using the WIEN2k package for materials science

Karlheinz Schwarz
Vienna University of Technology, A-1060 Vienna, Getreidemarkt 9, Austria
telephone number +43-1-58801-15670, fax number +43-1-58801-15698
e-mail: kschwarz@theochem.tuwien.ac.at

The quantum mechanical description of solids requires the calculation of the electronic structure which is mainly done within Density Functional Theory (DFT). The corresponding Kohn-Sham one-electron equations can be solved by several techniques. One among the most accurate schemes is based on the Linearized Augmented Plane Wave (LAPW) method, in which the unit cell is partitioned into spheres centered at all atomic sites and the remaining interstitial region. In the latter the wave functions are expanded into plane waves (PWs) each of which are augmented by atomic solutions in form of partial waves, i.e. a radial function times spherical harmonics. In LAPW the energy dependence of each radial function (for given azimuthal quantum number l) is linearized by taking a linear combination of the solution u at a £xed linearization energy and its energy derivative $\dot{u}$ computed at the same energy. Each PW is joined continuously (in value and slope) to the one-center solution de£ning the relative weight of u and $\dot{u}$.

The treatment of high-lying semi-core states with a principal quantum number which is one less than for the valence states can be ef£ciently handled by extending the LAPW basis set with local orbitals (LOs), which are completely con£ned inside the corresponding sphere.

Recently an alternative approach was proposed, namely the APW + lo (local orbital) method [1]. Here the augmentation is similar to the original APW scheme but each radial wave function is computed at a £xed linearization energy in order to avoid the non-linear eigenvalue problem that complicated the original APW scheme. Thus only the condition of continuity can be required and the basis functions may contain a kink at the sphere boundary. The missing variational freedom can be recovered by adding another type of local orbital containing the $\dot{u}$. Recent tests have shown [2] that this new scheme leads to the same result as LAPW but converges signi£cantly faster, since the new basis is less constraint. For large systems the matrix size can be nearly halved reducing the computation effort by almost an order of magnitude. The ef£cient APW+lo basis set requires - due to the discontinuity in slope at the sphere boundary - additional adaptations such as surface terms e.g. in the calculation of forces.

The APW+lo scheme has been implemented into the WIEN code [3] and will be the default option in the new WIEN2k version. For further details see www.wien2k.at [4]. New features such as a more accurate treatment of the spin orbit coupling and the implementation of LDA+U for highly correlated systems should be mentioned. In addition to the method improvements a coarse (on the k-point level) and £ne grain parallelization with optimized algorithms for the eigensolver allows to treat large systems relevant for materials science.

I am pleased to acknowledge the help of the co-authors of the WIEN2k code [4] and many persons who have contributed to the development and improvement of this code.

References

1. E.Sjöstedt, L.Nordström, D.J.Singh, Solid state commun. **114**, 15 (2000).
2. G.K.H.Madsen, P.Blaha, K.Schwarz, E.Sjöstedt, L.Nordström, Phys.Rev.B. (in press 2001).
3. P.Blaha, K.Schwarz, P.I.Sorantin, S.B.Trickey, Comput.Phys.Commun. **59** 339 (1990).
4. P.Blaha, K.Schwarz, G.K.H.Madsen, D.Kvasnicka, J.Luitz, WIEN2k (2001).

Extended ensemble Monte Carlo approach to hardly-relaxing problems

Koji Hukushima[1] **and Yukito Iba**[2]

[1]*Institute for Solid State Physics, University of Tokyo,*
5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-8581 Japan.
[2]*The Institute of Statistical Mathematics,*
4-6-7 Minami Azanu, Minato-ku, Tokyo, 106-8569 Japan.
hukusima@issp.u-tokyo.ac.jp

Monte Carlo (MC) simulations have successfully been used in studying various £elds including statistical physics, statistical sciences, optimization problems, and so on. The conventional MC algorithm based on *local* updating processes in *canonical ensemble* is, however, known to be ineff£cient for the so-called *hardly-relaxing* problems. A typical example occurs in systems with con¤icting constraint such as spin glasses (SG), optimization problems and polymers. These systems commonly have numerous local free-energy minima which are separated to each other by energy barriers. The characteristic time for escaping from one of such local minima increases rapidly as temperature decreases, and equilibration of the system is hardly realized.

An improvement has recently been developed on MC algorithm based on the idea of an extended ensemble[1]. Namely, the ensemble or the weight to be simulated is modi£ed or extended in such a way that the system visits more frequently to states which are less or hardly visited by the conventional MC algorithm. The multicanonical method, the simulated tempering (expanded ensemble) and the exchange MC method (parallel tempering)belong to this category called the extended ensemble method. These methods have been applied to various hardly-relaxing systems and turned out to be quite useful.

We brie¤y review the exchange MC method as an example of the extended ensemble method. We report numerical results of the exchange MC simulations on hardly-relaxing problems. By making use of the method, we have studied short-range Edwards-Anderson SG models, which is a typical case exhibiting the hardly-relaxing problem. It is found that a characteristic time scale for equilibration in the exchange MC method is largely reduced as compared with that of the conventional MC method. As a result, equilibrium average can be obtained within much shorter MC steps at low temperatures. We show a clear evidence of a £nite-temperature phase transition with *strong ordering* of the short-range SG models[2, 3], hardly observed in the previous works. We also present another application to a kind of optimization problem.

References

1. For review, see Y.Iba cond-mat/0012323.
2. K. Hukushima, Phys. Rev. E **60**, 3606 (1999).
3. K. Hukushima, in *Computer Simulation Studies in Condensed Matter Physics XIII*, p137(Springer Verlag, Heidelberg, Berlin, 2000).

Computational studies of carbon nanotube structures

Maria Huhtala, Antti Kuronen and Kimmo Kaski

Research Centre for Computational Science and Engineering,
Helsinki University of Technology,
P.O. Box 9400, FIN-02015 HUT, Finland

Single walled carbon nanotubes as all-carbon molecules of tubular form exemplify modern nanometre scale material structures, where the number of atoms range from less than a million up to few millions. Thus such systems can be studied quite accurately and realistically with computational methods like Molecular Dynamics simulations, rendering these studies in a way predictive. This point of view we try to explore through simulations of novel ring-like carbon nanotubes, observed experimentally. Whether these structures are toroidal or coiled is under debate. To this question we seek insight by studying the structure, the minimum energy con£guration, and the thermal stability of large toroidal nanotubes of (n,n)- and (n,0)-helicity using large scale Molecular Dynamics simulations based on the interaction potential by Brenner. Our simulations indicate that the toroidal form in¤uences strongly the structure of the tubes for small tori while for the larger tori the structural changes are extremely small. We also £nd that there exists a critical tube radius dependent buckling radius at which the torus buckles. This was also found to be helicity dependent.

Inverse Monte Carlo method and its application to compute effective potentials

Alexander P. Lyubartsev

Division of Physical Chemistry, Arrhenius Laboratory,
Stockholm University, Stockholm, S-10691, Sweden.

+46-8-161193, +46-8-152187, sasha@physc.su.se

Recently, a new method for reconstruction of atom-atom pair interaction potentials from a known set of radial distribution functions (RDF) within the Monte Carlo simulation scheme has been suggested [1]. It can be proved that for any set of RDFs, there exists a unique set of pairwise effective potentials reproducing the original RDFs. The suggested method allows one to £nd the interaction potentials in a procedure, similar to solution of a non-linear multi-dimensional equation by the Newton-Raphson method. On each iteration step, a statistical evaluation of Jacobian of transformation: interaction potential $\rightarrow$ RDF, in a grid approximation is carried out in order to "re£ne" interaction potentials.

Two applications are considered. First one is calculation of effective potentials for simpli£ed (coarse-grained) molecular models, without taking into account all molecular (e.g solvent) degrees of freedom. This set of potentials can be used for molecular simulations on a substantially larger scale. The general scheme of this approach starts from a simulation of a detailed system on the full-atomic level, which is normally carried out by molecular dynamics and yields a set of RDFs between interesting sets of atoms, for example between solute molecules in a solvent. The obtained RDF-s are then used to derive the effective potentials for simpli£ed (continuum solvent) models. Then the obtained potentials can be used for simulations of the very same system without explicit account of solvent molecules, which permits simulations of much bigger systems. The approach is illustrated by calculating the effective potentials between Na^+ and Cl^- ions in water solution and between the ions and DNA molecule. These effective potentials have been used to calculate relative binding af£nities of different alkali ions to DNA. In another work, the ion-ion effective potentials have been plugged in into the hyppernetted chain equation to calculate effective forces in electrical double layer.

The second application concerns calculations of effective atom-atom potentials from *ab-initio* RDF, obtained in Car-Parrinello MD simulations. The method is applied for calculation of the effective pairwise potential between hydrogens and oxygens atoms in a three-point water model, and between Li^+ ion and classical SPC water model. Properties of the obtained in this way molecular models are discussed.

Other possible applications of the inverse Monte Carlo method to construct effective potentials for coarse-grained models and to bridge the time- and length- scale gap in computer simulations are discussed brie¤y.

References

1. A.P.Lyubartsev and A.Laaksonen, *Phys.Rev.E, 52, 3730 (1995).*

Surface anchoring on liquid crystalline polymer brushes

Harald Lange and Friederike Schmid

Theoretical Physics, University of Bielefeld, 33501 Bielefeld, Germany

Tel. +49-521-1066191, schmid@physik.uni-bielefeld.de

The alignment of liquid crystals at surfaces plays a key role for the design of liquid crystal display devices[1]. Surfaces with grafted liquid-crystalline polymer brushes have been suggested as possible candidates for alignment layers[2, 3]. Theoretical considerations predict that the orientation of the liquid crystal in the bulk can be manipulated under certain conditions by varying the grafting density of the brush[2]. So far, there have been no computer simulations of such systems.

We have investigated the in¤uence of swollen liquid-crystalline polymer brushes on the orientation of a nematic solvent by Monte Carlo simulations. The liquid crystalline particles are modeled by soft ellipsoids, and the polymers by chains of such particles. The substrate is chosen such that it induces a planar orientation (parallel to the surface) in nearby solvent molecules. An appropriately modi£ed version of the con£gurational bias Monte Carlo algorithm[4] has been implemented, which removes and redistributes chain bonds rather than whole monomers. With this algorithm, a wide range of grafting densities could be studied.

Depending on the grafting density, we £nd three regimes: Planar, tilted, and perpendicular alignment. At low grafting densities, the alignment is mainly driven by the substrate. At high grafting densities, the substrate gradually loses its in¤uence and the alignment is instead determined by the structure of the interface between the brush and the pure solvent.

References

1. B. Bahadur (edt.) *Liquid crystals and uses*, World Scienti£c, Singapore (1990).
2. A. Halperin, D. R. M. Williams, Europhys. Lett. **21**, 575 (1993).
3. B. Peng, J. Rühe, D. Johannsmann, Adv. Mater. **12**, 821 (2000).
4. M. N. Rosenbluth and A. W. Rosenbluth, J. Chem. Phys. **23**, 356 (1955).

Ion-ion correlations in charged colloidal systems

Bo Jönsson
Department of Theoretical Chemistry
University of Lund, Chemical Center
Bo.Jonsson@teokem.lu.se

Abstract not available at time of printing

Kinetics of wetting at surfaces

Sanjay Puri

School of Physical Sciences,
Jawaharlal Nehru University,
New Delhi – 110067, India
0091-11-6189701, puri@jnuniv.ernet.in

There has been much interest in the dynamics of phase separation of binary mixtures (AB), which have been rendered thermodynamically unstable by a rapid quench below the critical temperature. Typically, the unstable mixture segregates into domains which are enriched in either of the components. These domains coarsen with time and are characterized by a time-dependent length scale $L(t)$, where t is the time after the quench. There is now a reasonable understanding of the various mechanisms which enable bulk phase separation [1].

In this talk, we will focus on the experimentally interesting situation of an unstable binary mixture in contact with a surface which has a preference for one of the components of the mixture [2]. There are two dynamical processes involved, i.e., the kinetics of wetting at the surface; and the dynamics of phase separation in the bulk. In earlier work, we have formulated phenomenological models for this physical situation [3].

The present work describes comprehensive Langevin simulations of this model in conjunction with simple analytical arguments. In particular, we focus on the kinetics of the wetting layer at the surface as a function of the mixture composition.

References

1. For reviews, see K. Binder, in *Materials Science and Technology, Vol. 5 : Phase Transformations in Materials* (ed. R.W. Cahn, P. Haasen and E.J. Kramer), p. 405, VCH, Weinheim, New York (1991); A.J. Bray, Adv. Phys. **43**, 357 (1994).
2. G. Krausch, Mat. Sci. Eng. Rep. **R14**, 1 (1995).
3. This work is reviewed in S. Puri and H.L. Frisch, J. Phys. Condensed Matter **9**, 2109 (1997).

Interplay between wetting and miscibility in thin binary polymer £lms

Marcus Müller

Institut für Physik, Johannes-Gutenberg-Universität Mainz
Staudinger Weg 7, 55099 Mainz, Germany

phone: 06131 3923642, fax: 06131 3925441, Marcus.Mueller@uni-mainz.de

Con£ning a binary mixture, one can profoundly alter its miscibility behaviour. The phase behaviour of AB mixtures in pores, slits and £lms has attracted interest from both theorists and experimentalists. The qualitative features of the miscibility in con£ned geometry are rather universal and shared by polymer mixtures as well as small molecules. Symmetric binary polymer blends are, however, particularly well suited to study the interplay between wetting and miscibility, because (i) the wetting transition temperature typically is much lower than critical temperature, where the demixing occurs in the bulk, and (ii) ¤uctuations can be controlled by the degree of interdigitation. The more extended the molecule is, the larger is the number of neighbours it interacts with, and the smaller the effect of ¤uctuations. The spatial extension of the molecules also facilitates experimental investigations.

We study the interplay between wetting and miscibility of a symmetric AB polymer mixture via large scale Monte Carlo simulations in the framework of the bond ¤uctuation model and via numerical self–consistent £eld calculations. The £lm surfaces interact with the monomers via short ranged potentials. One surface attracts the A component of the mixture and the corresponding semi–in£nite system exhibits a £rst order wetting transition. The wetting transition can be accurately located in the simulations via the Young equation[1].
The surface interaction of the opposite surface is varied as to study the crossover from capillary condensation for symmetric surface £elds to the interface localisation/delocalisation transition for antisymmetric surface £elds. In the former case the phase diagram has a single critical point close to the critical point of demixing in the bulk. In the latter case the phase diagram exhibits two critical points which correspond to the prewetting critical points of the semi–in£nite system. The crossover between these qualitatively different limiting behaviours occurs gradually; however, the critical temperature and the critical composition exhibits a non–monotonic dependence on the surface £eld[2].
We study the dependence of the phase diagram on the £lm thickness D for antisymmetric surface £elds. Upon decreasing the £lm thickness the two critical points approach the symmetry axis of the phase diagram, and below a certain thickness $D_{\rm tri}$, there remains only a single critical point at symmetric composition. This corresponds to a second order interface localisation/delocalisation transition. At $D_{\rm tri}$ tricritical behaviour is found[3].
The critical behaviour and the role of ¤uctuations is investigated by Monte Carlo simulations. In the vicinity of the tricritical point there is a rich crossover between two–dimensional Ising critical behaviour, tricritical behaviour and their mean £eld counterparts. Fluctuations are also important away from the critical points and we present evidence for a renormalisation of the effective interface potential (i.e., the interaction between the AB interface and the surface) by capillary waves of the interface[4].

References

1. M. Müller and K. Binder, Macromolecules **31**, 8323 (1999).
2. M. Müller, K. Binder, and E.V. Albano, Europhys.Lett. **50**, 724 (2000).
3. M. Müller, E.V. Albano, and K. Binder, Phys.Rev. **E 62**, 5281 (2000). M. Müller, K. Binder, and E.V. Albano, Physica **A 279**, 188 (2000).
4. M. Müller and K. Binder, Phys.Rev. **E 63**, 021602 (2001).

Numerical tests of CFT conjectures for 3D systems

Wolfhard Janke and Martin Weigel

Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11
04109 Leipzig, Germany

Wolfhard.Janke@itp.uni-leipzig.de; Martin.Weigel@itp.uni-leipzig.de

Augmenting the scale invariance of a statistical physics system at criticality by the additional symmetries of rotational, translational and inversion invariance leads to the *conformal* symmetry group. In two dimensions (2D), where this group is in£nite-dimensional, the emerging conformal £eld theory (CFT) provides a complete (continuum) solution of critical systems, in particular comprising £nite-size scaling (FSS) laws *including the amplitudes.* For an in£nitely long cylinder $S^1 \times \mathbb{R}$ with circumference L, this implies in the large-distance limit of a critical two-point correlation function of a primary operator ϕ a longitudinal correlation length of

$$\xi_{\parallel} = \frac{AL}{x}, \tag{1}$$

with x being the scaling dimension of ϕ and $A = 1/2\pi$ [1].

While the CFT argument breaks down for three-dimensional (3D) systems of geometry $S^1 \times S^1 \times \mathbb{R}$, a transfer matrix study of the Ising model [2] showed agreement with Eq. (1) for the case of *antiperiodic* boundary conditions along the torus directions. Using an elaborate set of simulational tools and statistically optimized methods of data analysis we investigate the scaling behavior of the correlation lengths of 3D classical O(n) spin models with Wolff cluster-update Monte Carlo simulations. Our results for the Ising ($n = 1$), the XY ($n = 2$), the Heisenberg ($n = 3$) and the $n = 10$ generalized Heisenberg models indicate the validity of the scaling relation (1) for the mentioned geometry and the case of antiperiodic boundary conditions at a high level of precision [3]. The amplitude A of Eq. (1), however, now depends on the model under consideration, indicating a reduction in the universality of this statement. Based on further simulations for the case of *periodic* boundary conditions we propose a generalized scaling relation involving an additional universal factor depending on the boundary conditions only [3]. A striking mismatch of the $n \to \infty$ extrapolation of our numerical results against analytical calculations is traced back to a breakdown of the identi£cation of this limit with the spherical model in the case of multi-point correlation functions of local operators [3].

For the spherical geometry $S^{d-1} \times \mathbb{R}$ some formal generalization of statement (1) is possible [1]; it is unclear, however, to which operators it should apply. Using slightly irregular discretizations of the sphere S^2 we checked with Monte Carlo simulations for the validity of this scaling relation and found it ful£lled for the Ising model and the correlation lengths of the densities of magnetization and energy [4]. The level of universality of this statement is still not completely explored though.

References

1. J.L. Cardy, J. Phys. A **17**, L385 (1984); *ibid.* A **18**, L757 (1985).
2. M. Henkel, J. Phys. A **20**, L769 (1987).
3. M. Weigel and W. Janke, Phys. Rev. Lett. **82**, 2318 (1999); Phys. Rev. B **62**, 6343 (2000).
4. M. Weigel and W. Janke, Europhys. Lett. **51**, 578 (2000).

Meron-cluster solution of fermion and other sign problems

Uwe-Jens Wiese

Institut für Theoretische Physik, Universität Bern, Switzerland

wiese@itp.unibe.ch

Negative sign and complex action problems prevent the numerical solution of numerous important problems in physics at energies ranging from meV to MeV and even up to the Planck scale. For example, a better understanding of high-temperature superconductivity is hindered by severe fermion sign problems, lattice simulations of Quantum Chromodynamics (QCD) at non-zero quark density suffer from a notorious complex action problem, and the matrix model underlying string theory (M-theory) also has a sign problem. In all these cases, the Boltzmann factors that appear in the Euclidean path integral can be negative or even complex, and can hence not be interpreted as probabilities to generate £eld con£gurations using importance sampling. As a consequence, as the system size increases, naive numerical approaches become exponentially inef£cient. A general strategy for solving these problems is to explicitly cancel all negative or complex contributions to the path integral, and to treat the remaining positive contributions with importance sampling techniques. In several cases, this strategy can be realized using the so-called meron-cluster algorithm. A meron-cluster is a conglomerat of £eld variables whose update leads to explicit cancellations. The meron-cluster algorithm has led to a complete solution of the fermion sign problem in attractive Hubbard-type models, of the complex action problem in the Potts model approximation to dense QCD, as well as of other sign problems, for example, in quantum spin ladders in an external magnetic £eld.

Simple dynamics for broad histogram method

Paulo Murilo Castro de Oliveira
Instituto de Física, Universidade Federal Fluminense, av. Litorânea s/n, Boa Viagem, Niterói RJ, Brasil 24210-340
(55)(21)2620-6735, (55)(21)2620-3881, pmco@if.uff.br

The Broad Histogram Method (BHM)[1] is based on the exact [2] equation

$$g(E) < N_{\rm up}(E) > = \ g(E+\Delta E) < N_{\rm dn}(E+\Delta E) > \ ,$$

valid for any system, completely general. $g(E)$ counts the number of states sharing the same energy E, and ΔE is a £xed energy jump. For each state, $N_{\rm up}$ counts the number of potential movements (single-spin ¤ips, for instance) which increase the current energy by the amount ΔE, while $N_{\rm dn}$ corresponds to energy decrements by the same amount. These quantities and the above equation, both introduced in [1], are also the basis for a lot of other very ef£cient methods as well. The notation $< Q(E) >$ stands for the microcanonical average of some quantity Q. Thus, BHM consists in: 1) measuring $< N_{\rm up}(E) >$ and $< N_{\rm dn}(E) >$ as functions of E; 2) using the above equation in order to determine $g(E)$.

Microcanonical averages can be obtained by Monte Carlo sampling, with **the only** constraint being to randomly choose the averaging states with **uniform probability** among all $g(E)$ states with energy E. Contrary to all reweighting or important sampling methods, one does not need to be concerned with detailed balance between different energy levels: microcanonical averages and BHM itself do not depend on the number of visits to each energy level, as compared to others. The only role the number of visits to each level plays concerns statistical accuracy. This feature provides an enormous freedom in choosing the dynamic rule to be adopted.

Here, we present numerical tests concerning a simple dynamics [3], inspired by another, older one [4] introduced within a different context. First, one needs to choose some protocol of **real** movements to be randomly performed on the current state (nothing to do with the **virtual** movements corresponding to $N_{\rm up}$ and $N_{\rm dn}$). Among them, the maximum energy jump is δE (nothing to do with ΔE), to above or to below the current energy. Then, for a £xed energy E, the dynamic rule is: 1) to accept any randomly chosen movement which keeps the system inside the energy window $[E-\delta E, E+\delta E]$, rejecting it otherwise; 2) to measure averages whenever the system returns to the £xed value E. No averages are taken in visits to other energies. This is a rejection-free dynamic rule for the energy level under averaging. This feature is supposed to avoid undesirable arti£cial biases. Moreover, random numbers are used only in order to choose the next attempted movement (to choose which is the next spin to be ¤ipped, for instance), never in order to decide whether to accept this movement. One does not need to compare random numbers with pre-de£ned accurate probabilities, thus no high-quality random number generators are necessary.

References

1. P.M.C. de Oliveira, T.J.P. Penna and H.J. Herrmann, *Braz. J. Phys.* **26**, 677 (1996) (COND-MAT 9610041).
2. P.M.C. de Oliveira, *Eur. Phys. J.* **B6**, 111 (1998) (COND-MAT 9807354).
3. P.M.C. de Oliveira, *Braz. J. Phys.* **30**, 766 (2000) (COND-MAT 0101171).
4. K.-C. Lee, *J. Phys.* **A23**, 2087 (1990).

Double degeneracy in the ground-state of the 3D $\pm J$ spin glass

Naomichi Hatano[1] **and James E. Gubernatis**[2]

[1]*Department of Physics, Aoyama Gakuin University, Chitosedai, Setagaya, Tokyo 157-8572, Japan*
[2]*Center for Nonlinear Science and Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

Phone: +81-3-5384-6582, Fax: +81-3-5384-6100, e-mail: hatano@phys.aoyama.ac.jp

We carried out a Monte Carlo simulation of the $\pm J$ spin glass in three dimensions.[1, 2] The Hamiltonian is given by

$$\mathcal{H} \equiv - \sum_{\alpha=1,2} \sum_{\langle i,j \rangle} J_{ij} \sigma_i^{(\alpha)} \sigma_j^{(\alpha)}, \tag{1}$$

where the £rst summation runs over two replicas, while the second summation runs over all nearest-neighbor pairs of the Ising spins on a cubic lattice. The frustration of the exchange interactions $\{J_{ij}\}$ generates many local minima in the free energy landscape. At low temperatures, the spins may freeze into some con£guration, and this slow dynamics is the essence of the spin-glass "order." Because of the nature of this order, equilibration of spin glasses in simulations and experiments is often very hard.

In the present study, we reduced the dif£culty of the slow dynamics signi£cantly by using a bivariate multicanonical Monte Carlo method. Multicanonical simulations are performed independent of temperature or of a range of nearby temperatures and estimate the density of states. From it we can in principle calculate expectation values at any temperature.

We discuss the nature of the ground-state degeneracy. Because of the discretized energy levels of the Hamiltonian (1), there is always multiple degeneracy in the ground state of the $\pm J$ model. Our numerical results indeed indicate the residual entropy. The question, however, is whether the multiple degeneracy is microscopic or macroscopic. We de£ne a toy model for the ground-state degeneracy, where local spin ¤ips result in the residual entropy. The toy model shows the microscopic multiple degeneracy is completely consistent with the macroscopic double degeneracy. Our numerical results suggest that the toy-model scenario of the double degeneracy is, after some generalization, realized in the $\pm J$ model in three dimensions.

Our main £ndings supporting the double degeneracy are as follows: (1) the order-parameter distribution $P(q)$ near $q \simeq 0$ decreasing at low temperatures as the system size is increased, (2) the Binder parameter approaching unity at low temperatures, and (3) the effect of the ground-state degeneracy on moments of the overlap order parameter.

References

1. N. Hatano and J.E. Gubernatis, cond-mat/0008115.
2. Preliminary results have been reported at the 8th Tohwa University International Symposium, Fukuoka, Japan, at the 12th Annual Workshop of Center for Simulational Physics, University of Georgia, and at the 5th International Conference on Computational Physics, Kanazawa, Japan. See the proceedings, N. Hatano and J. E. Gubernatis, in *Slow Dynamics in Complex Systems*, edited by M. Tokuyama and I. Oppenheim, pp. 565–566 (American Institute of Physics, Maryland, 1999); Glass in *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, edited by D. P. Landau, pp. 149–161 (Springer, Berlin, 2000); Prog. Theor. Phys. Suppl. **138** 442–447 (2000).

Magnetization reversal using novel new event-driven Monte Carlo algorithms

M. A. Novotny

CSIT, Florida State University, Tallahassee, FL 32306-4120, USA

phone: 1-850-644-7026, fax: 1-850-644-0098, email: novotny@csit.fsu.edu

One of the most dif£cult problems in simulating dynamics of physical systems is that there are often disparate time scales in the problem. For example, here we consider the study of thermal reversal of the magnetization of nanoscale ferromagnets following a £eld reversal. The attempt frequency which enters dynamic Monte Carlo simulations for such systems is about 10^{-11} sec. The time scales to be simulated in this problem corresponds to the time for data integrity in information storage (years to decades). Consequently, faster-than-real-time algorithms for simulating such systems are necessary — while the algorithms cannot modify the underlying physical dynamic.

The rejection-free method called the n-fold way [1] accomplishes this goal at low temperatures for discrete spin models. The n-fold way algorithm can be many orders of magnitude faster than standard dynamic Monte Carlo algorithms. A modi£cation of the n-fold way algorithm to discrete time allows for generalization by including the methodology of absorbing Markov chains in the Monte Carlo simulation [2]. In certain regimes of metastable decay of discrete ferromagnetic models, such as the Ising model, this MCAMC (Monte Carlo with Absorbing Markov Chains) method can increase simulation time by more that 10 *orders of magnitude* compared with the n-fold way method [2].

We have also implemented rejection-free methods on massively parallel computers [3]. This non-trivial parallelization is accomplished by introducing a 'virtual time' one each block of spins that are placed on a processor. Using a conservative technique to guard against casuality violations, we have proven that the computation phase of such algorithms is scalable. This proof has been con£rmed by using up to 480 processing elements on a Cray T3E [3].

We have recently been able to utilize ideas of the Broad Histogram Method to obtain a rejection-free algorithm that is not restricted to systems with discrete states [4].

This talk will introduce the n-fold way, parallel rejection-free, and MCAMC algorithms that allow for faster-than-real-time simulations for discrete spin models. These will be applied to dynamic Monte Carlo studies of the Ising ferromagnet. Also the rejection-free method for dynamics of continuous spin models, applied to the classical Heisenberg model, will be described.

References

1. "A New Algorithm for Monte Carlo Simulation of Ising Spin Systems", A.B. Bortz, M.H. Kalos, and J.L. Lebowitz, J. Comput. Phys. **17**, 10 (1975).
2. "Monte Carlo with Absorbing Markov Chains: Fast Local Algorithms for Slow Dynamics", M.A. Novotny, Phys. Rev. Lett. **74**, 1 (1995); erratum **75**, 1424 (1995).
3. "Parallel Simulations of Magnetization Reversal in Ising-like Systems", G. Korniss, M.A. Novotny, and P.A. Rikvold, J. Comput. Phys. **153**, 488 (1999).
4. "Rejection-free Monte Carlo Algorithms for Models with Continuous Degrees of Freedom", J.D. Muñoz, M.A. Novotny, and S.J. Mitchell, Phys. Rev. Lett., submitted.

Visualization of MD and MC simulations for atomistic modeling

Joan Adler, Adham Hashibon, Nir Schreiber, Anastasia Sorkin, Slava Sorkin and Geri Wagner

Technion - Israel Institute of Technology, Haifa 32000, Israel

97248293937, 97248221514, phr76ja@tx.technion.ac.il

We will discuss the rôle of visualization in atomistic modeling, presenting arguments in favour and discussing reasons why some might £nd this dif£cult. Arguments in favour include help in debugging, help in understanding what is happening in the simulation and resultant insights into the physics of the systems. Visualization faciltates discussion with experimental collaborators and presentation.

The MC and MD calculations made in the Computational Physics Group at the Technion will then be described. These include modeling of diamond/graphite systems and aluminium/alumina interfaces, as well as studying defects in copper and vanadium. Some examples of new physics results obtained thru our older visualizations of simulation samples will be given[1].

After discussing problems with the implementation of existing visualization systems for our purposes our new AViz[2] package will be introduced. Our selection of Mesa and the QT GUI as well as the options we have built into AViz will be explained. Examples of AViz' use such as modeling the creation of interstitial defects in diamond, and the behaviour of a 50,000 atom drop of aluminium on an alumina surface will be presented. Some tricks for 3d visualization, such as highlighting atoms with changed coordination numbers and bonds as well as their implementation in AViz will be described.

Visualization of spin systems is also possible with AViz, as is the preparation of animations and movies. A discussion of how we are trying to make our package easy for others to use and how we have solved possible problems with visualization such as cost will also be given. AViz is Open Source (GNU license) and is downloadable from our website in .rpm for LINUX[2]. Versions for other systems are in preparation, and we are happy to hear from others who wish to use AViz and help in its further development.

References

1. D. Saada, J. Adler and R.Kalish, PRB **59**,6650 (1999)
2. http://phycomp.technion.ac.il/∼ aviz

Stochastic and dynamic properties of molecular dynamics systems: Simple liquids, plasma and electrolytes, polymers, etc.

Guenri E. Norman

Department of Molecular Physics, Moscow Institute of Physics and Technology, Institutskii per. 9, 141700, Dolgoprudnyi, Russia

e-mail: henry_n@orc.ru

Molecular dynamics method (MDM) supplies to the solution of fundamental contradiction between macroscopic irreversibility and microscopic reversibility with data which help to reveal the origin of stochastization in many particle systems. Systems of neutral particles [1, 2], one- [3] and two-component [4] strongly coupled plasmas and polymers [5]are analyzed. Numerical integration serve as a coarse-graining procedure. The errors are essential due to Lyapunov exponential instability of the Newton equations. The values of K-entropy (Lyapunov exponent) for electrons and ions coincide with each other [4] at the initial stage of trajectories divergence. The same coincidence of K values for different degrees of freedom is found for polymer system [5].

The concept [2, 3, 4, 5, 6] of dynamic memory time t_m is discussed. The conservation of energy E only in average is another consequence of the numerical integration. The relation between t_m, energy ¤uctuation ΔE and K-entropy is treated. MDM is a method which retains Newtonian dynamics only at the times less than t_m and carries out a statistical averaging over initial conditions along the trajectory run.

Meaning of t_m for real systems is related to the quantum uncertainty, which might be small but always £nite for any classical system and in¤uence upon particle trajectories in a coarse-graining manner. The intrinsic irreversibility arises as a consequence of measurement procedure in quantum mechanics. The concept of quasiclassical trajectories is introduced in MDM. The value of t_m is estimated to be in picosecond range for atoms.

Experimental evidence [7] for different pathways for hydrolysis and synthesis of ATP and some other forward and reverse enzymatic reactions means violation of the microscopic reversibility principle. If there are two pathways along the hypersuface of potential energy between initial and £nal states there should be at least two bifurcation points. It is not Maxwell demon but Lyapunov instability, small quantum stochastic terms and asymmetry of potential relief (with thermal ¤uctuations) that de£ne the local choice of reaction pathway in the bifurcation point.

Systems far from equilibrium and relaxation processes are studied by MDM. K-entropy values for equilibrium and non-equilibrium cases differ from each other remarkably. Non-equilibrium K-entropy value coincides with inverse relaxation time. Systems with several relaxation times are studied. Examples are given for Lennard-Jones liquids [2] and strongly coupled plasmas.

References

1. W. G. Hoover, *Time Reversibility, Computer Simulation and Chaos* (World Scienti£c, Singapore, 1999).
2. G. E. Norman and V. V. Stegailov, Zh. Eksp. Theor. Phys. **119**, No.5, (2001).
3. D. M. Barnett, T. Tajima and Y. Ueshima, Phys. Rev. Lett.**83**, 2677 (1999).
4. I. V. Morozov, G. E. Norman, A. A. Valuev, Phys. Rev. E **63**, March 2001.
5. G. E. Norman and A. I. Yaroshchuk, Unpublished (2001).
6. Yu. A. Kravtsov, in *Limits of Predictability*, edited by Yu. A. Kravtsov (Springer, Berlin, 1993), p. 173.
7. A. D. Vinogradov, J. Exper. Biology**203**, 41 (2000).

Simulation and event generation in high-energy physics

Denis Perret-Gallix
CNRS-Japon, Maison Franco-Japonaise 6F
3-9-25, Ebisu, Shibuya-ku, Tokyo 150-0013, Japan
Tel : 81 3 3443 8551, Fax : 81 3 3443 8552
email : Denis.Perret-Gallix@www.jp.cnrs.fr

High-energy physics experiments at LHC[1] or LC are probably the most demanding sites, whatsoever, for high performance computing systems. All requirements seen in other endeavors are stressed here, only at a higher level: huge number of data channels (100 millions), high speed data recording (100KHz), gigantic databases (Terabytes per day and much more for simulated data), unprecedented high level of monitoring, safety and security. High-energy physics has always been a front-runner and a test bed for new technologies. Even if the main goal is the improvement of matter and Universe basic knowledge, remote from any short term practical applications, due to its requirements and to the strong connections with applied and technology oriented researches, it had led to the development of new analysis tools or even to new industries (i.e. synchrotron radiation, the Internet).

Simulation is the art of mimicking nature. All known experimental results are reproduced by the basic theory of fundamental forces: the Standard Model (SM). This knowledge is the core of the event generation stage which predicts event rates and differential distributions associated to a given process and provides the energy, momentum and helicity of each £nal state particle. Their subsequent interactions with the various detectors are £nely simulated leading to the same raw analog output the detector would have produced if hit by a similar real particle. Then comes the reconstruction program, blind to the data origin whether real or simulated. From all the detectors data pieces, it reconstructs the full event and rebuilds the original interaction. By comparing the original simulated event and what has been reconstructed, one estimates the accuracy and the ef£ciency of the detectors. By comparing the simulated and the real data, one can check the validity of the SM. In principle, any difference between the simulated and the experimental data is a sign for new physics, not predicted by the SM: a physics discovery. Simulation is therefore a mandatory component of any experiment from the design stage to the £nal result.

The £rst link of the ”simulation chain” is the event generation, purely based on the theoretical knowledge of particle interactions. Since a few years, several speci£c packages have been developed based on the so-called ”Feynman Diagram” procedure. They can perform most of those computations in an ”automatic way” without human intervention. However, the high experimental precision requiring higher order diagram computations and the higher energy of the initial states have led to a dramatic increase in the complexity of those computations. The new conjectured models (Supersymetry, Superstring theories, Higher dimension), embedding SM but extending its scope, has led to a ¤urry of new hypothetical particles whose production rate and interaction computations must be performed. Consequently the number and the computing time of those calculations have increased dramatically, raising numerous computing issues concerning: symbolic manipulation, parallel computation, multi-dimensional integration of singular integrants, high precision ¤oating-point calculation ef£ciency and database management.

A short description of some of the fully automated packages (like Grace[2] and CompHep[2]) will be given. Some examples of the physics output will be presented.

In conclusion we will stress the necessity to build up an open and ¤exible computing framework able to embed most of the tools which are being developed worldwide and to increase furthermore the level of automation.

References

1. CERN, LHC project http://lhc.web.cern.ch/lhc/
2. http://www-sc.kek.jp/minami/, http://theory.npi.msu.su/∼pukhov/comphep_html/comphep.html

Phase transitions at surfaces, edges, and corners

Michel Pleimling

Institut für Theoretische Physik I, Universität Erlangen-Nürnberg,
D – 91058 Erlangen, Germany

and

Laboratoire de Physique des Matériaux, Université Henri Poincaré I,
B.P. 239, F – 54506 Vandœuvre lÁs Nancy Cedex, France

phone +49-9131-85-28451, fax +49-9131-85-28444,
pleim@theorie1.physik.uni-erlangen.de

Critical phenomena may occur not only in the bulk but also at its surfaces. In the three-dimensional semi-in£nite Ising model with short-range interactions two typical scenarios may be encountered: (i) bulk and surface may order at the same temperature (**ordinary transition**), but with different power laws and (ii) the surface may order £rst (**surface transition**), due to strong surface couplings, followed by ordering of the bulk (**extraordinary transition**) at the lower bulk transition temperature.

At the surface phase transitions, edge and corner quantities also present singularities. For the ordinary transition, Cardy [1] noted the dependence of edge critical exponents on the opening angle between the surfaces forming the wedge. However, edge critical properties at the surface transition have been largely overlooked.

In this contribution, I present results of large-scale simulations, using Monte Carlo techniques, of three-dimensional Ising models with edges and corners. In particular, at the ordinary transition, the critical exponents of the edge and corner magnetizations of various geometries, computed with the one-cluster-¤ip algorithm, are compared to analytical estimates [2]. At the surface transition, edge and corner magnetizations show nonuniversal, coupling-dependent critical behaviour in the thermodynamic limit [3]. This nonuniversal behaviour of local quantities is due to the two-dimensional character of the critical ¤uctuations at this transition. Intriguing magnetization pro£les, showing the in¤uence of the disordered bulk, are discussed. The simulational results obtained at the surface transiton for three-dimensional models with edges and corners are compared to exact £ndings on critical two-dimensional Ising models with different types of defects.

Nonuniversal local critical behaviour is also observed in thin Ising £lms with additional lines of atoms on the surface [4]. The dependence of these nonuniversal features on the local couplings as well as on the £lm thickness is brie¤y discussed.

References

1. J. Cardy, J. Phys. A: Math. Gen. **16**, 3617 (1983).
2. M. Pleimling and W. Selke, Eur. Phys. J. B **5**, 805 (1998).
3. M. Pleimling and W. Selke, Phys. Rev. B **59**, 65 (1999); M. Pleimling and W. Selke, Phys. Rev. E **61**, 933 (2000).
4. M.-C. Chung, M. Kaulke, I. Peschel, M. Pleimling, and W. Selke, Eur. Phys. J. B **18**, 655 (2000).

Ab initio surface energies and the oxidation of NiAl(110): Can we predict growth modes of the oxide layer?

A. Alavi and A.Y. Lozovoi
Department of Chemistry
University of Cambridge
alavi@theor.ch.cam.ac.uk

Reactivity at metal surfaces is of widespread importance in chemistry and materials science (for example in heterogeneous catalysis, oxidation, corrosion, metal/oxide interfaces etc). Because of the strong chemical interaction between the substrate (metal surface) and adsorbate, modelling based on ab-initio electronic-structure theory (DFT) is indispensible. On the other hand, to be able to make predictions regarding the thermodynamic behaviour of the surfaces requires calculation of the surface free energies as function of external parameters such as temperature, pressure, and composition. An essential element in the calculation of surface energies is the calculation of bulk chemical potentials. These, in practice, can only be computed in conjunction with statistical mechanical models.

In this talk, we will discuss a method of calculating surface energies for oxidising surfaces of intermetallic compounds, taking NiAl as our example. In this system, the af£nity for oxygen of Al is much greater than that of Ni. As a result, the oxidation of the surface induces large-scale stiochiometric redistribution of the species close to the vicinity of the surface. The surface energies turn out to be remarkably sensitive to the surface composition (in particular the Ni content). We show that at low temperatures, when the stiochiometric redistribution cannot take place due to large kinetic barriers, the surface energy calculations indicate that oxidising surface should grow in a layer-by-layer manner. Allowing for redistribution (by annealing from a high temperature), however, should lead to change in the growth-mode, to island-growth. Very recent electron-microscopy experiments of in-situ oxidation at low and high temperatures support this idea.

We show that a fruitful interplay between ab-initio and statistical mechanical modelling can go a long way in describing surface thermodynamics which, because of the very limited time and length scales accessible to the ab-initio simulations, would be virtually impossible in a direct simulation.

Modeling nonequilibrium phase transitions and critical behavior in complex systems

J. Marro

Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, 18071-Granada, Spain

Fax: +34 958 242 353

Complex systems [1] are, in general, out of a thermodynamic equilibrium state. Their instabilities, often described as nonequilibrium phase transitions, are associated with pattern formation, morphogenesis, and self-organization, which connect the microscopic level of simple interacting units with the coherent structures observed, for example, in organisms and communities. Detailed investigation of phase transitions in simple models out of equilibrium is therefore most interesting. The simplest analysis is for lattice models which represent very varied situations including, for instance, avalanches in sand piles, driven ¤uids and traf£c models, contact processes, reactions competing with diffusion, surface catalytic reactions, branching annihilating random walks, and sequential adsorption [2]. Given the absence of both general unifying principles for this varied set of models and a general formalism, analogous to equilibrium statistical mechanics, the £eld presents a particular challenge to theoretical physics.

I shall illustrate in this talk, by means of simple, lattice examples that violate the principle of detailed balance [3,4], some of the diversity of nonequilibrium phase transitions. Note that the term ”nonequilibrium phase transition” represents not a super£cial resemblance to equilibrium phenomena, but a precise use of the terms ”phase” and ”phase transition” in their statistical mechanics sense. Even in the absence of a free energy, we can recognize a *phase* of a many-particle system from well-de£ned relations between its distribution functions and the parameters governing its dynamics. A phase transition is characterized by a singular dependence of these attributes upon the control parameters. From this vantage, equilibrium is a special case, in which the dynamics happens to be derivable from an energy function, thereby permitting an analysis with no reference to time. Out of equilibrium one must actually £nd the time-independent solution(s) of the master equation for the process. This is a formidable task and can only be carried out approximately for some lattice models. [2]

A well-known disadvantage of lattice models is that they are usually too crude to be directly comparable with experiment. In fact, if one is interested in predicting a nonequilibrium phase diagram, it is better, for cases in which ¤uctuations are of minor signi£cance, to employ a macroscopic description, i.e., a set of (deterministic) partial differential equations. However, macroscopic descriptions hold little surprise in the way of criticality; mean-£eld behavior is implicit at this level. The range of critical phenomena exhibited by our models [2,3,4], by contrast, is at least as interesting as in equilibrium.

References

1. See, for instance, special issue on complexity: *Science*, vol. 284, 2 April 1999, several authors.
2. J. Marro and R. Dickman, ”Nonequilibrium Phase Transitions in Lattice Models”, Cambridge University Press, Cambridge U.K. 1999.
3. A. Achahbar *et al.*, to be published.
4. P.I. Hurtado *et al.*, to be published.

Dynamic transitions in pure ising magnets under pulsed & oscillating £elds

B. K. Chakrabarti[1], **A. Misra**[2]

[1] *Saha Institute of Nuclear Physics, Calcutta – 700064, India*
[2] *University of Duisburg, 47048 Duisburg, Germany*

Response of pure Ising systems to time-dependent external magnetic £elds, like oscillating or pulsed £elds, will be discussed [1,2]. Because of the two time scales involved, namely the thermodynamic relaxation time of the system and the time period or pulse width of the external £eld, dynamically broken symmetric phases appear when both become comparable. A particularly simple case is that of an Ising magnet below its static critical temperature, when it is perturbed by a pulsed magnetic £eld competing with the existing order for a short duration. The magnetisation reversal transition here shows intriguing dynamic transition behaviour. Mean £eld theories and Monte Carlo studies for such dynamic transitions will be discussed. We will also discuss about the Monte Carlo observations regarding the ¤uctuation behaviour near these dynamic transitions.

References

1. B. K. Chakrabarti and M. Acharyya, Rev. Mod. Phys., vol. 71 (1999) 847
2. A. Misra and B. K. Chakrabarti, J. Phys. A, vol. 33 (2000) 4249

Proteins top-down

Alex Hansen[1]**, Audun Bakk,**[1]**, Paul G. Dommersnes,**[1]
Mogens H. Jensen,[2] **Johan S. Høye and Kim Sneppen**[1]

[1]*Institutt for fysikk, NTNU, N-7491 Trondheim, Norway*
[2]*Niels Bohr Institute Blegdamsvej 17, DK-2100 Copenhagen, Denmark*
Phone: +47 73 59 36 49, Fax: +47 73 59 33 72, email: Alex.Hansen@phys.ntnu.no

Proteins have interesting thermodynamic features. One of the more surprising is the cold unfolding transition. At high temperature, the proteins are unfolded due to thermal rattling. As the temperature is lowered, they undergo a phase transition and fold. But, if the temperature is further decreased, they may undergo a second transition and revert to the unfolded state, thus melting as the temperature is lowered.

We present a model that demonstrates the mechanism resposible for this strange behavior based on hydrophobicity [1, 2, 3].

Studying proteins numerically is a very challenging problem. We discuss how this challenge may be met using simple models [3].

In vivo, it is not the protein thermodynamics which is important, but rather their out of equillibrium properties. Some proteins act as molecular motors. These are little machines that convert chemical energy into organized motion in spite of being knocked around by the surrounding thermally agitated water. We use the model constructed to understand the thermodynamics of proteins to sketch what could be the underlying principles that make it possible for proteins to act as motors [4].

References

1. A. Hansen, M. H. Jensen, K. Sneppen and G. Zocchi, Eur. Phys. J. B **6**, 157 (1998).
2. A. Bakk, J. S. Høye and A. Hansen, Cond-mat/0102329.
3. P. G. Dommersnes, A. Hansen, M. H. Jensen and K. Sneppen, Cond-mat/0006304.
4. A. Hansen, M. H. Jensen, K. Sneppen and G. Zocchi, Europhys. Lett. **50**, 120 (2000).

Protein dynamics simulations: Grasping molecular nano-machines

Berthold Heymann, Rainer Böckmann, and Helmut Grubmüller

Theoretical Molecular Biophysics Group
Max-Planck-Institute for Biophysical Chemistry, 37077 Göttingen, Germany
Tel. ++49/551/201-1763, Fax: ++49/551/201-1089
e-mail: hgrubmu@gwdg.de

Many proteins are molecular 'nano machines'; their conformational plasticity and dynamics determines their function. Recently developed molecular dynamics based methods allow to simulate and predict such conformational motions at the atomic level and permit comparison with single molecule experiments [1]. Force probe simulations and experiments, in particular, provide a very tight interaction between theory and experiment.

Two examples shall highlight the role of conformational protein motions and their theoretical description:

(1) Force probe simulations of molecular recognition processes in antibody molecules [2] reveal an optimization of the binding kinetics through conformational ¤exibility of the binding pocket. Entropic contributions to the free energy landscape turn out to be important here [3]. Computation of binding forces allows direct comparison with experiment. The excellent agreement validates our simulations.

(2) Primary ATP synthesis steps in F_1-ATPase were studied. Remakably, the synthesis involves electro-mechano-chemical energy coupling. In the human body, this enzyme produces ca. 60 kg ATP per day. Homologs are found in plants and bacteria. By enforced rotation of the γ-'stalk', as caused by protonmotive F_o-rotation, a time-resolved atomic model for the mechanical energy transfer to the ATP synthesis sites in terms of propagating conformational motions is obtained. The simulations rationalize mutation studies and complement recently proposed models for ATP release [4].

References

1. Helmut Grubmüller, Berthold Heymann, and Paul Tavan. Ligand binding: Molecular mechanics calculation of the streptavidin-biotin rupture force. *Science*, 271(5251):997–999, 1996.
2. Berthold Heymann and Helmut Grubmüller. AN02/DNP unbinding forces studied by molecular dynamics AFM simulations. *Chem. Phys. Lett.*, 303:1–9, 1999.
3. Berthold Heymann and Helmut Grubmüller. Molecular dynamics force probe simulations of antibody/antigen unbinding: Entropic control and non-additivity of unbinding forces. *Biophys. J.*, 81, 2001. In press.
4. R. Böckmann and H. Grubmüller. First principles simulation of primary mechanical energy transfer steps in F_1-ATP synthase. 2001. Submitted.

Nano-scale structure in membranes in relation to enzyme action – computer simulation vs experiment

Ole G. Mouritsen, Pernille Hoyrup, Thomas Kaasgaard, Lars Kildemark, and Kent Jorgensen

MEMPHYS - Center for Biomembrane Physics
Department of Chemistry, Technical University of Denmark
Building 206, DK-2800 Lyngby, Denmark
e-mail: ogm@kemi.dtu.dk; http://memphys.kemi.dtu.dk

There is increasing theoretical and experimental evidence indicating that small-scale domain structure and dynamical heterogeneity develop in lipid membranes as a consequence of the many-particle character of the system [1,2]. This small-scale structure occurs in the nano-meter range and can be perceived as either density ¤uctuations, compositional ¤uctuations, or bilayer thickness ¤uctuations. Theoretical predictions are confronted with recent experimental data obtained from e.g. ¤uorescence spectroscopy and atomic-force microscopy. The nano-scale structure is shown to be important for controlling the activity of an enzyme, phospholipase A2, which acts at membranes [3]. A simple statistical mechanical model for the equilibrium phase behavior of lipid bilayers is extended to account for the non-equilibrium action of the enzyme phospholipase A2 which hydrolyses lipid-bilayer substrates, forming product molecules that lead to local variations in the bilayer interfacial pressure [4]. Computer simulation of the model shows, in quantitative agreement with experimental data, that the enzyme activity is modulated by nano-scale lipid-domain formation in the lipid bilayer leading to a characteristic lag-burst behavior.

References

1. O. G. Mouritsen and K. Jorgensen, Small scale lipid membrane structure, Curr. Opin. Struct. Biol. 7, 518-527 (1997).
2. L. K. Nielsen, T. Bjornholm, and O. G. Mouritsen, Fluctuations caught in the act, Nature 404, 352 (2000); L. K. Nielsen, A. Vishnyakov, K. Jorgensen, T. Bjornholm, and O. G. Mouritsen, J. Phys.: Condens. Matt. Phys. 12, A309-A314 (2000).
3. T. Kaasgaard, J. H. Ipsen, O. G. Mouritsen, and K. Jorgensen, J. Probe Microscopy (in press, 2001).
4. P. Hoyrup, Kent Jorgensen, and O. G. Mouritsen (submitted, 2001).

Equilibrium polymerization of polycarbonates

R. O. Jones[1] **and P. Ballone**[2]

[1]*Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany*

[2]*Department of Physics, University of Messina, 98166 Messina, Italy*

(r.jones@fz-juelich.de Tel.: (+49)2461-614202 Fax: (+49)2461-612850)

"Living polymers" contain an active site that catalyzes polymerization to an equilibrium distribution of chains of different sizes [1]. Ring-opening polymerization of polycarbonates is an example. We have simulated the equilibrium polymerization of cyclic oligomers, triggered by a catalyst that can break and form covalent bonds, using a model that mimics the reaction mechanism identi£ed by density functional (DF) computations on polycarbonate tetramers [2]. The monomers are represented by Lennard-Jones particles that form one or two harmonic bonds with their neighbors, giving rise to open chains and polymeric rings. The "catalyst" is an active particle able to interchange bonds among two pairs of neighboring monomers, leading to equilibrium with a range of chain lengths. The reactants and products have the same average potential energy, as found in the DF study, and the reaction barrier is set to zero. Starting from an assembly of oligomers (10002 particles, one active) in 2 and 3 dimensions, the system evolves by a Monte Carlo algorithm that samples different atomic positions and bonding con£gurations. We address two questions: (a) Does this simple model lead to polymerization? (b) If polymerization occurs, what is the thermodynamic driving force?

Most equilibrated samples show a high degree of polymerization that is enhanced by increasing density and temperature, and polymerization is less effective in 2D than in 3D. In 2D there appears to be a £rst-order transition in the density dependence of the degree of polymerization, which differs from the continuous transition found in previous studies of other polymerization mechanisms [3]. In 3D the results suggest the presence of a similar transition, but the data are affected by £nite-size effects and are not conclusive. All polymerized samples show a broad distribution of sizes that *does not* approach the exponential law often associated with living polymers [4]. The easy interconversion of different sizes mediated by the active particle makes polymerization highly reversible.

The similarity of potential energy and vibrational properties of reactants and products, as well as the temperature dependence of the degree of polymerization, indicate that the entropy of polydispersed samples is the driving force. The entropy provided by a wide range of sizes is offset only partially by the loss of long range mobility due to intra-molecular constraints, and the parallel to crystallization would explain the £rst order character of the transition. The difference between these results and those of previous studies underlines the importance of the underlying polymerization mechanism.

References

1. S. C. Greer, J. Phys. Chem. B **102**, 5413 (1998).
2. P. Ballone, B. Montanari, R. O. Jones, J. Phys. Chem. **104**, 2793 (2000).
3. Theoretical and computational studies of living polymers are reviewed in: J. P. Wittmer, A. Milchev, and M. E. Cates, J. Chem. Phys. **109**, 834 (1998).
4. P. J. Flory, J. Am. Chem. Soc. **58**, 1877 (1936).

Numerical simulations of random spin (and fermionic) models with wide distribution of energy scales

Ravindra N. Bhatt
School of Engineering and Applied Science, Princeton University,
Princeton, New Jersey 08544-5263, USA
ravin@ee.princeton.edu

The magnetic behavior of semiconductors doped with randomly distributed magnetic elements (such as Iron or Magnanese) and/or bound carriers (such as Phosphorus or Boron in Silicon) are described by many-body Hamiltonians with a broad distribution of coupling constants and energy scales. Such a wide distribution (covering several orders of magnitude in some cases) leads to unusual properties, such as strong suppression of magnetic phase transitions due to quantum ¤uctuations, unusual thermodynamic behavior in the magnetically ordered phase etc. The wide distribution also poses several challenges to both analytical and computational approaches used to calculate the physical properties of such systems. This talk will illustrate some of the techniques that have been applied successfully to such systems, including numerical renormalization group as well as Monte Carlo methods. Examples will be drawn from lightly doped conventional semiconductors [Si, Ge] as well as diluted magnetic semiconductors [such as (Cd,Mn)Te and (Ga,Mn)As]. Extension of these methods to diluted magnetic semiconductors in the metallic regime with itinerant carriers (fermionic degrees of freedom) will also be described.

Simulation of in£nitely strongly interacting fermions from one to two dimensions

M. Brunner[1,2], **C. Lavalle**[1], **F.F. Assaad**[1], **and A. Muramatsu**[1]

[1]*Institut für Theoretische Physik III, Universität Stuttgart*
Pfaffenwaldring 57, D-70550 Stuttgart, Germany
[2]*School of Physics, The University of New South Wales, Sidney, NSW 2052, Australia*
tel:+49-711-685-5204, fax:+49-711-685-5098, mu@theo3.physik.uni-stuttgart.de

The limit of in£nitely strong interaction is the relevant one for the understanding of the low energy sector of strongly correlated electronic systems like high temperature superconductors and new related compounds like the so-called ladder materials. Generically, those systems are well represented by the t-J model, where strong correlation is taken into account by projecting out doubly occupied sites. Such a constraint prevented until now from controlled analytical treatments such that most of the information presently available relies on exact diagonalizations, implying that only very small systems on a microscopic scale could be treated. [1].

We present spectral properties for single-hole excitations in the t-J model obtained with newly developed quantum Monte Carlo algorithms, in chains, ladders, and planes, where both the spectral function and the quasiparticle weight are obtained. Simulations of the one-dimensional case show that a simple charge-spin separation *Ansatz* is able to describe the overall features of the spectral function such as the bandwidth and the compact support of the spectral function. The quasiparticle weight Z_k is computed on lattices up to $L = 128$ sites in one dimension, and scales as $Z_k \propto L^{-1/2}$ at the supersymmetric point $J/t = 2$. [2].

Ladder systems with two and three legs show a non-monotonous behavior of the quasiparticle weight accompanying the behavior of the spin-gap. The lowest bands in two-leg ladders are related by spin-1 excitations with a wavevector $\vec{k} = (\pi, \pi)$, the antibonding band being a shadow of the bonding one, both with a large quasiparticle weight. The three-leg ladder has one antisymmetric band reminiscent of the single chain and two symmetric ones similar to the 2-leg ladder. Whereas quasiparticles do not exist in the antisymmetric channel, they have a £nite weight on the symmetric one, clearly indicating a splitting of the system in a chain and a two-leg ladder [3].

In two dimensions the single hole dynamics is studied on square lattices with up to 24×24 sites. A £nite size scaling of the quasiparticle weight Z_k leads to a £nite result in the thermodynamic limit for the considered values of J/t, resolving thus, a long standing question. Resonances above the lowest edge of the spectrum are identi£ed, revealing that quasiparticles are composed of spin and charge defects con£ned by a linear potential. [4].

Finally, recent results for doped chains are presented, where charge-spin separation properly describes both photoemission and inverse photoemission spectra obtained by our quantum Monte Carlo simulations.

References

1. E. Dagotto, Rev. Mod. Physics, **66**, 763 (1994).
2. M. Brunner, F.F. Assaad, and A. Murammatsu, Eur. Phys. J. B **16**, Rapid Note, 209 (2000).
3. M. Brunner, S. Capponi, F.F. Assaad, and A. Muramatsu, Phys. Rev. B **63**, 18051(R) (2001).
4. M. Brunner, F.F. Assaad, and A. Murammatsu, Phys. Rev. B **62**, 15480 (2000).

Dynamical properties of ”sequence alignment”: Aging and more

E. Marinari
Dipartimento di Fisica, Universitá di Roma La Sapienza,
P. A. Moro 2, 00185 Roma, Italy
Enzo.Marinari@roma1.infn.it

I discuss dynamical properties of the so called ”sequence alignment”, where one tries to £nd the best possible alignment of two or more given sequences under a given cost matrix. I introduce a local dynamical process, and use time dependent correlation functions to show, among others, that the system undergoes aging.

Application of exact combinatorial optimization algorithms to the physics of disordered systems

Heiko Rieger

Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany
+49 681 302 3969, +49 681 302 4899, rieger@lusi.uni-sb.de

The physical properties of solid materials which contain a substantial degree of quenched disorder, so called disordered systems, have been an experimental and a theoretical challenge for many decades. The different thermodynamic phases emerging in random magnets, the aging properties and memory effects of spin glasses, the disorder induced conductor-to-insulator transition in electronic or bosonic systems, the collective behavior of magnetic ¤ux lines in amorphous high temperature superconductors, and the roughening transition of a disordered charge density wave systems are only a few examples for these fascinating phenomena that occur due to the presence of quenched disorder.

Analytic studies of models for these systems are usually based on perturbation theories valid for weak disorder, on phenomenological scaling pictures or on mean-£eld approximations. Therefore the demand for ef£cient numerical techniques that allow the investigation of the model Hamiltonians of disordered systems has always been high. Three facts make life dif£cult here: 1) The regime, where disorder effects are most clearly seen, are at low temperatures – and are even best visible at zero temperature; 2) the presence of disorder slows the dynamics of theses systems down, they become *glassy*, such that for instance conventional Monte-Carlo or molecular dynamics simulations encounter enormous equilibration problems; 3) any numerical computation of disordered systems has to incorporate an extensive disorder average.

In recent years more and more model systems with quenched disorder were found that can be investigated numerically 1) at zero temperature, 2) without equilibration problems, 3) extremely fast, in polynomial time (for a review on these developments see [1, 2]). This *is* indeed progress, which became possible by the application of *exact* combinatorial optimization algorithms developed by mathematicians and computer scientists over the last few decades. This gift is not for free: £rst a mapping of the problem of £nding the *exact* ground state of the model Hamiltonian under consideration onto a standard combinatorial optimization problem has to be found. If one is lucky, this problem falls into the class of P-problems, for which polynomial algorithms exist. If not, the intellectual challenge for the theoretical physicist remains to reformulate the model Hamiltonian in such a way that its universality class is not changed but a mapping on a P-problem becomes feasible.

In this talk we review some of the recent progress that has been made in this direction. In particular we will discuss, with an emphasis on the computational point of view, the collective behavior of a ¤ux line ensemble in a disordered environment [3, 4], the disorder induced roughening transition in a periodic elastic medium and the critical properties of the random bond Potts model in the limit $q \to \infty$.

References

1. H. Rieger, Lecture Notes in Physics **501** (ed. J. Kertesz and I. Kondor), p. 122–158 (Springer Verlag, Berlin-Heidelberg-New York, 1998).
2. M. Alava, P. Duxbury, C. Moukarzel und H. Rieger, Phase Transition and Critical Phenomena, Vol. **18** (ed. C. Domb and J. L. Lebowitz), p.141–317, (Academic Press, Cambridge, 2000).
3. H. Rieger, Phys. Rev. Lett. **81**, 4488 (1998).
4. T. Knetter, G. Schröder, M. J. Alava und H. Rieger, Europhys. Lett., in press (2001).

Lattice Boltzmann models: an ef£cient and simple approach to complex ¤ow problems

Bastien Chopard and Alexandre Dupuis

Computer Science Department, University of Geneva, 1211 Geneva 4, Switzerland

phone: +41 22 705 7623, fax: +41 22 705 7780,

e-mail: Bastien.Chopard@cui.unige.ch

The lattice Boltzmann (LB) method is a technique aimed at modeling a system of particles, such as a ¤uid for instance, in terms of a mesoscopic dynamics on a discrete space-time universe. In the limit of a small lattice spacing and small time step, a LB ¤uid is shown to obey the Navier-Stokes equation.

In this contribution we consider an extension of the LB approach to simulate the erosion, transport and deposition processes in a ¤uid. Solid point-particles are added on top of the LB ¤uid and simple mechanisms are proposed to describe the interaction between the two components.

We study several applications, ranging from snowdrift formation to erosion in river beds. A good agreement between the simulations and £eld experiments is obtained. We also consider the phenomena of meandering rivers and propose an explanation for their formation.

Multiscale lattice Boltzmann methods

Sauro Succi[1] **and Olga Filippova**[2]

[1]*Istituto Applicazioni Calcolo, v.le Policlinico 137, 00161 Roma, Italy*
[2]*Institute for Combustion and Gas Dynamics, University of Duisburg, D-47048 Duisburg, Germany*

+39 06 88470 256, +39 06 4404306, succi@iac.rm.cnr.it

The Lattice Boltzmann (LB) method is a hyperstylized form of the Boltzmann equation based on a £ctitious particle dynamics in which all microscopic details are given away except those strictly needed to recover correct hydrodynamic equations at a macroscopic scale [1, 2, 3]. Due its mathematical simplicity, physical soundness and ¤exibility, as well as its outstanding amenability to parallel computing, the LB method has enjoyed considerable success in the last decade for the simulation of complex ¤ows, ranging from slow ¤ows in grossly irregular geometry to fully developed single and multiphase turbulent ¤ows [4, 5]. Owing to its peculiar Janus-bifaced nature, a telescope for Molecular Dynamics, a microscope for Fluid Dynamics, the LB is also a promising candidate for multiscale/multiphysics applications involving complex phenomena at different scales (¤ows with phase transitions, colloidal ¤ows, ¤uid-wall interactions and the like). As the LB method heads towards these new applications of increasing complexity, it becomes apparent that a signi£cant extensions of the basic scheme are called for. Among others, particularly important is the possibility of selectively clustering mesh points there where sharp physics occurr, such as two-¤uid interfaces or solid-¤uid boundaries. To this purpose, local grid re£nement and attendant multiscale capabilities have been recently developed [6, 7] and successfully applied to turbulent ¤ows [8]. In this paper we shall describe basic ideas behind the multiscale LB methods and present applications to fully turbulent ¤ows in relatively complex geometries. In addition, future extensions to exploit multiscale capabilities aimed at incorporating additional physics (say ¤uid-wall interactions) at the mesoscopic scale will be discussed and commented on.

References

1. G. McNamara and G. Zanetti, Use of the Boltzmann equation to simulate lattice–gas automata, PHYS. REV. LETT., **61**, 2332 (1988);
2. F. Higuera, S. Succi and R. Benzi, Lattice gas dynamics with enhanced collisions, EUROPHYS. LETT., **9**, 345 (1989);
3. Y.H. Qian, D. d'Humieres and P. Lallemand, Lattice BGK models for Navier-Stokes equation, EUROPHYS. LETT. **17**(6), 479 (1992);
4. R. Benzi, S. Succi and M. Vergassola, The Lattice Boltzmann equation: theory and applications, PHYSICS REPORTS, **222(3)**, 145 (1992).
5. S. Succi, The Lattice Boltzmann equation, Oxford University Press, June 2001, to appear.
6. O. Filippova and D. Hänel, Grid re£nement for lattice-BGK models, J. COMPUT. PHYS., **147**, 219 (1998).
7. O. Filippova and D. Hänel, Acceleration of Lattice-BGK schemes with grid re£nement,J. COMPUT. PHYS., **165**, 407 (2000).
8. O. Filippova S. Succi, D. Hänel, G. Bella, Multiscale lattice-BGK models with turbulence models, J. COMPUT. PHYS., submitted.

Large eddy simulation of turbulent combustion processes

W. P. Jones

Department of Mechanical Engineering,
Imperial College of Science, Technology and Medicine,
Exhibition Road, London SW7 2BX, England

Tel: +44 (0)20 7954 7037, Fax: +44 (0)20 7581 5495,
email: w.jones@ic.ac.uk

Large Eddy Simulation (LES) is increasingly viewed as a method suitable for application to practical systems where it promises a greater degree of predictive realism and generality than Reynolds averaged approaches that rely heavily on the adequacy of approximate statistical models of turbulence. Whilst computationally more demanding LES is physically much more realistic and offers the prospect of being able to represent accurately a wide range of engineering ¤ows. LES involves the direct three-dimensional time dependent computation of the large-scale turbulent motions responsible for turbulent transport whilst those with scales smaller than the computational grid, or more strictly the £lter width, are modelled. For inert ¤ows at high turbulence Reynolds numbers the details of the £ne scale motions are not rate controlling - their main role is to dissipate energy - and LES is thus likely to be relatively insensitive to modelling assumptions compared to conventional Reynolds averaged methods. The sub-grid scale model can thus be much simpler than the type of models used in Reynolds averaged methods. It is required only to represent the in¤uence of relatively small eddies which tend to have isotropic properties and usually make a negligible contribution to the turbulent mixing processes. For combusting ¤ows however the modelling requirements are much more severe as burning will inevitably occur within the £ne sub-grid scales. For this reason the problems posed in applying LES to turbulent ¤ames are very similar to those that arise in conventional Reynolds averaged modelling approaches. In LES the dif£-culty is manifest by the need to evaluate the spatially £ltered source terms (representing the net rate of formation through chemical reaction) that appear in the equations for chemical species mass fractions. Suitable methods are only now beginning to appear and progress in this area has recently been reviewed in [1].

For nonpremixed combustion an economical description is possible through the conserved scalar formalism, [2, 3, 4]. In this approach the major species composition, temperature and density are related to a *strictly* conserved scalar quantity, the *mixture fraction.* Due to the nonlinearity of these state relations, account must be taken of the in¤uence of subgrid scale ¤uctuations and this is achieved by the introduction of a modelled form of the subgrid scale mixture fraction pdf (sgpdf). Some results from the simulation of a hydrogen-air turbulent diffusion ¤ame and for a model propane fuelled gas turbine combustor are presented. The overall level of agreement between the simulation results and measurements is quite good. The paper will provide an overview of current LES capabilities and future research needs for combusting ¤ows.

References

1. N. Branley and W.P Jones. Large eddy simulation of turbulent ¤ames. In *Proceedings ECCOMAS 2000*, Barcelona, Spain, September 2000.
2. N. Branley and W.P Jones. Large eddy simulation of turbulent non-premixed ¤ame. In *Eleventh Symposium on Turbulent Shear Flows*, pages 4.1–4.6, Grenoble, France, September 1997.
3. N. Branley and W.P. Jones. Large eddy simulation of a turbulent non-premixed swirling ¤ame. In W. Rodi, editor, *4th International Symposium on Engineering Turbulence Modelling and Measurements*, Corsica, France, May 1999.
4. N. Branley and W.P Jones. Large eddy simulation of a turbulent nonpremixed ¤ame. *Combustion and Flame*, 2001. to appear.

Large scale multi-agent transportation simulations

K. Nagel

Institut für Wissenschaftliches Rechnen, Department Informatik,
ETH Zürich, 8092 Zürich, Switzerland
nagel@inf.ethz.ch

It is now possible to micro-simulate the traf£c of whole metropolitan areas with 10 million travelers or more, “micro” meaning that each traveler is resolved individually as a particle. In contrast to physics or chemistry, these particles have internal intelligence; for example, they know where they are going. This means that a transportation simulation project will have, besides the traf£c microsimulation, modules which model this intelligent behavior. The most important modules are for route generation and for demand generation. Demand is generated by each individual in the simulation making a plan of activities such as sleeping, eating, working, shopping, etc. If activities are planned at different locations, they obviously generate demand for transportation. This however is not enough since those plans are in¤uenced by congestion which initially is not known. This is solved via a relaxation method, which means iterating back and forth between the activities/routes generation and the traf£c simulation.

From microscopic simulations to macroscopic material behavior

Stefan Luding

Iinstitut für Computeranwendungen 1 (ICA1), Universität Stuttgart,
Pfaffenwaldring 27, 70569 Stuttgart, Germany
email: lui@ica1.uni-stuttgart.de, http://www.ica1.uni-stuttgart.de/˜lui

One of the challenges in todays computer simulation is the question how to bridge the gap from the microscopic “atomistic” length to the macroscopic length scale of experimental observation.

A straightforward approach by just modeling and simulating all atoms in a macroscopic system is not possible due to the huge number of degrees of freedom. Therefore, one can reduce the size of the examined system so that a microscopic simulation of atoms is possible. However, the possible length of such a “probe” is in general too small in order to regard it as macroscopic. Therefore, the present study presents methods and tools in order to perform a so-called micro-macro transition. In a £rst step, microscopic simulations of a small sample lead to macroscopic laws describing the material in the framework of a macroscopic theory, as a second step. For granular materials, as an example, the grain properties are inserted into a discrete particle molecular dynamics and lead to the collective behavior of the dissipative many-particle system.

From a particle simulation, one can extract, e.g., the pressure of the system as a function of density. This equation of state allows a thermodynamical, macroscopic description of the material [1]. Here we focus on the hard sphere model which exhibits a disorder-order transition at a certain density. For low densities, the system resembles a dilute gas, for intermediate densities one has a disordered ¤uid, and for the highest densities, one obtains a solid with either disorder or order (evidenced by a crystal-structure). The elastic hard-spheres can be generalized by including inelasticity so that one ends up with a dissipative system for which, however, the micro-macro approach still can be applied.

From the algorithmic point of view, the model system is examined by an event-driven molecular dynamics simulation. One can compute the stress tensor and thus the pressure by summation over the momentum transfer per unit-time and volume. In the usual time-driven molecular dynamics, the procedure is similar, only that forces have to be measured. The stress tensor is derived for a dynamic system by means of kinetic-theory arguments, for a quasi-static system by means of an averaging over particle pairs [2], and also by means of a virtual displacement method.

Finally, several examples are presented where the above described methods were applied and where large-scale computation was used. Typical simulations involve 10^5 particles due to the ef£ciency of the event-driven algorithm.

References

1. S. Luding. Global equation of state of 2D hard sphere systems. *Phys. Rev. E*, 63:042201–1–4, 2001.
2. M. Lätzel, S. Luding, and H. J. Herrmann. *Macroscopic material properties from quasi-static, microscopic simulations of a two-dimensional shear-cell*. Granular Matter **2**/3, 123 (2000).

Instabilities in sheared loosed granular matter

J. Kertész[1], J. Török[1], M. Sasvári[1], D.E. Wolf[2], S. Krishnamurthy[3] and S. Roux[4]

[1] *Department of Theoretical Physics, Budapest University of Technology, Budafoki ut 6, H-1111 Budapest, Hungary*
[2] *Department of Theoretical Physics, Gerhard Mercator University Duisburg, D-45478 Duisburg, Germany*
[3] *Theoretical Physics, Oxford University, Oxford, OK1 3NP, UK*
[4] *UMR CNRS/Sain-Gobain, F-93303 Aubervillers Cedex, France*
e-mail: kertesz@phy.bme.hu

We have investigated the shear process in loose granular materials. If the process is carried out under the constrain of constant volume, a clustering instability occurs. This was studied in an inelastic hard disk gas sheared by two parallel bumpy walls (Couette-¤ow) [1]. In our molecular dynamics simulations we found a sensitivity to the asymmetries of the initial condition of the particle positions and velocities. The steady state is asymmetric where the deviation from (anti)symmetric hydrodynamic £elds gets stronger as the normal restitution coef£cient decreases. For the better understanding of this sensitivity we carried out a linear stability analysis of the former, kinetic theoretically obtained (anti)symmetric solution and found it to be unstable. The effect of the asymmetry on the self-diffusion coef£cient is also discussed.

For the case of shearing under constant pressure we have introduced a mesoscopic model for the formation and evolution of shear bands [2,3]. Numerical simulations and analytical calculations reveal that the system undergoes a non-trivial self-organization process which is governed by the motion of the shear band and the consequent restructuring of the material along it. High density regions are built up, progressively con£ning the shear bands in localized regions. This results in an inhomogeneous aging of the material with a very slow increase in the mean density, displaying an unusual glassy like

system-size dependence. The predicted density pattern formation and the slow dynamics should be accessible to experiments.

References

1. M. Sasvári, J. Kertész and D.E. Wolf: Instability of the symmetric Couette-¤ow in a granular gas: hydrodynamic £eld pro£les and transport, Phys. Rev. E. 62, 3817, (2000)
2. J. Török, S. Krishnamurthy, J. Kertész and S. Roux: Self-organization, Localization of Shear Bands and Aging in Loose Granular Materials, Phys. Rev. Lett. 84, 3851 (2000)
3. J. Török, S. Krishnamurthy, J. Kertész and S. Roux: Large strain shear of loose granular materials: Numerical and analytical study (preprint)

Wetting of a symmetrical binary ¤uid mixture on a wall

Nigel B. Wilding[1] **and Friederike Schmid**[2]

[1]*Department of Mathematical Sciences, The University of Liverpool, Peach Street, Liverpool L69 7ZL, UK.*
[2]*Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, D-33615 Bielefeld, Germany.*
wilding@liverpool.ac.uk

We study the wetting behaviour of a symmetrical binary ¤uid below the demixing temperature at a non-selective attractive wall. Although it demixes in the bulk, a suf£ciently thin liquid £lm remains mixed. On approaching liquid/vapour coexistence, however, the thickness of the liquid £lm increases and it may demix and then wet the substrate. We show that the wetting properties are determined by an interplay of the two length scales related to the density and the composition ¤uctuations. The problem is analysed within the framework of a generic two component Ginzburg-Landau functional (appropriate for systems with short-ranged interactions). This functional is minimized both numerically and analytically within a piecewise parabolic potential approximation. A number of novel surface transitions are found, including £rst order demixing and prewetting, continuous demixing, a tricritical point connecting the two regimes, or a critical end point beyond which the prewetting line separates a strongly and a weakly demixed £lm. Our results [1] are supported by detailed Monte Carlo simulations of a symmetrical binary Lennard-Jones ¤uid [2] at an attractive wall.

References

1. F. Schmid and N.B. Wilding. Phys Rev. E63, 031201 (2001)
2. N.B. Wilding, F. Schmid and P. Nielaba, Phys. Rev. E58, 2201 (1998).

Parallel tempering algorithm to equilibrate glassy systems

W. Kob[1], K. Binder[2], C. De Michele[3], F. Sciortino[3], T. Stühn[2], and R. Yamamoto[4]

[1] *Laboratoire des Verres, Université Montpellier II, 34095 Montpellier, France*
[2] *Institut für Physik, Johannes-Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany*
[3] *Dipartimento di Fisica, Universitá di Roma "La Sapienzá", P.le A. Moro 2, Roma, I-00185, Italy*
[4] *Department of Physics, Kyoto University, Kyoto 606-8502, Japan*
e-mail: kob@ldv.univ-montp2.fr

The relaxation time of most disordered systems (structural glasses, spin glasses, polymers in disordered media, etc.) increases dramatically if their temperature is lowered. The microscopic mechanism for this slowing down is presently still not well understood and hence the focus of many experimental as well as theoretical efforts. In recent years also computer simulations have increasingly been used to study these systems and have contributed signi£cantly to increase our understanding. However, most of these numerical investigations have use plain molecular dynamics or Monte Carlo algorithms with local moves to equilibrate the systems. Hence these types of approaches limits the range of temperatures at which the systems can be studied *in equilibrium* to values at which the relaxation dynamics is about 10^5 times longer than the typical microscopic time scale of the local motion of the particles (this corresponds to typical length of simulations of $O(10^8)$ time steps). In order to access the experimentally relevant temperature range one would need to equilibrate the systems at temperatures at which the relaxation time is on the order of seconds, i.e. around 10^{12} times the microscopic time scale (10^7 time longer than what is currently feasible). However, in principle it is possible to devise Monte Carlo schemes which, by using unphysical moves, are able to equilibrate the system also at a very low temperature. With the help of such algorithms it would therefore be possible to study the equilibrium properties of glassforming systems also at low temperatures and to improve considerably our understanding of these systems.

In this talk we discuss one possible algorithm to achieve this, the so-called parallel tempering method[1]. In this method one works with an extended ensemble in that several independent systems are simulated simultaneously at different temperatures. The algorithm allows that periodically two subsystems swap their temperature (ful£lling the condition of detailed balance) thus allowing each system to propagate faster in con£guration space. We have tested the ef£ciency of this algorithm for two types of glass forming system: A realistic model of silica (SiO_2) and a binary mixture of Lennard-Jones particles. We £nd that for the case of silica the algorithm works well in that it allows to equilibrate the system around 100 times faster than with conventional algorithms. A similar speedup is seemingly obtained for the case of the Lennard-Jones system. However, a careful analysis of the "equilibrated" data by means of the inherent structures shows that in fact the system has not yet been equilibrated, despite the fact that tests for equilibration, like histogram-reweighting etc, seem to work well [2, 3]. We speculate on the reason why the algorithm seems to work ef£ciently in on case but not in the other.

References

1. K. Hukushima and K. Nemoto, J. Phys. Soc. Jpn., **65**, 1604 (1996); R.H. Swendsen and J.S. Wang, Phys. Rev. Lett., **57**, 2607 (1996). K. Hukushima, H. Takayama, and H. Yoshino, J. Phys. Soc. Jpn., **67**, 12 (1998).
2. R. Yamamoto and W. Kob, Phys. Rev. E **61**, 5473 (2000).
3. W. Kob, C. Brangian, T. Stühn, and R. Yamamoto, p. 153 in *Computer Simulation Studies in Condensed Matter Physics* XIII, eds. D.P. Landau, S.P. Lewis and H.B. Schüttler, Springer, 2000.

Turbulence in dilute polymer solutions: A phase diagram

Bruno Eckhardt[1], **Jochen Kronjäger**[1]
and Jörg Schumacher[1,2]

[1] *Fachbereich Physik, Philipps Universität Marburg, 35032 Marburg, Germany*
[2] *Department of Mechanical Engineering, P.O. Box 208284, Yale University, New Haven, CT 06520-8284, USA*
(+49) 6421-2821316, (+49) 6421-2824511, bruno.eckhardt@physik.uni-marburg.de

The interaction between the small scale velocity gradients in a turbulent ¤ow and long ¤exible polymers and can trigger a coil-stretch transition in the polymers. We analyze this transition within a direct numerical simulation of shear turbulence in an Oldroyd-B model for the polymer. As in our simulations of Newtonian shear turbulence we use a volume force to maintain the gradient [1].

In the coiled state the trace of the con£guration tensor (a measure of the radius of gyration of the molecules) has an algebraic distribution with an exponent in agreement with the analytical predictions of Balkovsky et al [2]. The exponent decreases as the relaxation time of the polymer increases and eventually becomes non-normalizable: this marks the transition to the stretched state. Before this transition the effects on the ¤ow are minimal.

In the stretched state feedback with the ¤ow is essential and limits the stretching of the polymer. The distribution becomes very wide without clear scaling, except for the indications of an algebraic increase towards the maximum: this is a remnant of the algebraic law found below the transition.

Theoretical arguments of Balkovsky et al. [2] suggest that for stretched polymers there should be a sharp cut-off in the con£gurations, rather than the broad form we observe. We trace this difference back to the fact that the polymer concentration is small and most of the dissipation is carried by the solvent rather than the polymer.

We conclude that four cases have to be distinguished, characterized by the polymer being coiled or stretched and by the dissipation being carried predominantly by the solvent or the polymer. The characteristics of the polymer con£gurations and ¤ow £elds will be summarized and related to other simulations [3] and experiments [4].

References

1. Schumacher, J. and Eckhardt, B. (2000): On statistically stationary homogeneous shear turbulence, Europhys. Lett. **52**, 627–632.
2. E. Balkovsky, A. Fouxon and V. Lebedev, Turbulent dynamics of polymer solutions, Phys. Rev. Lett. **84**, 4765 (2000).
3. T. Becker and B. Eckhardt, Turbulence in a Maxwell Fluid, Z. Phys. B **101**, 461 (1996).
4. A. Groisman and V. Steinberg, Elastic turbulence, Nature **405**, 53 (2000).

Intermittency and multiscaling in turbulence

Mogens H. Jensen

The Niels Bohr Institute
Blegdamsvej 17, DK-2100 Copenhagen, Denmark
+45 35325371, mhjensen@nbi.dk

Over the last decades it has become clear that the ¤uctuations of the velocity £eld in turbulence, over small length scales, do not follow a Gaussian statistics. Instead the distribution function has a form like a stretched exponential where large events are important and must be counted into the statistics.

The existence of large events are often related to the presence of atypical scaling behavior, called multiscaling. This is a phenomenon which calls for an in£nity of independent scaling exponents[1]. We give a brief review of these properties in fully developed turbulence. In order to get a deeper understanding of the problem, we introduce approximative models for turbulent ¤ows, called shell models and discuss large events and multiscaling within this framework[1]. We propose a new approach where one can "invert" the formulation of multiscaling in order to monitor the complement of the large events, and we discuss under which circumstances the two formalisms are related[2].

References

1. T. Bohr, M.H. Jensen, G. Paladin and A. Vulpiani, "Dynamical Systems Approach to Turbulence", Cambridge University Press (1998).
2. M.H. Jensen, "Multiscaling and Structure Functions in Turbulence: An Alternative Approach", Phys.Rev.Lett. 83, 76 (1999).

The DataGrid as tool for global high energy physics computing

Ingo Augustin

CERN
1211 Geneva 23
Switzerland
Tel: +41 22 767 1470
Ingo.Augustin@cern.ch

The DataGridcite [1] project started 2001 as an joint European effort to tackle the computing needs of various user communities. The main users are High Energy Physics (HEP), bio-informatics and Earth observation. The biggest challenges in terms of data throughput and amount come from HEP[2]. The four Large Hardon Collider (LHC) experiments that will commence operations in spring 2006 will each record more than one PetaByte of data per year. The sustained data rates will amount up to 1.2 GB/sec.

The LHC computing model is based on a hierarchical multi-Tier model. In this model, for each experiment, raw data storage and reconstruction will be carried out at a Tier0 centre. Analysis, data storage, some reconstruction, Monte-Carlo data generation and data distribution will mainly be the task of several (national or supra-national) Regional Tier1 centres, followed by a number of (national or infra-national) Tier2 centres, by (institutional) Tier3 centres or workgroup servers, and by end-user workstations (Tier4). The CERN-based Tier0+Tier1 hardware for all LHC experiments should be installed as a single partitionable facility [2].

Hundreds of institutes from all over the world participate in the experiments. This alone already precludes the straightforward management and replication of the data. Nevertheless all physicists should have similar access to the data, irrespective of their location. Additional constraints arise from the limited funding for computing in the LHC projects. The price for CPU power (millions of SpecInt95 needed) led to the decision to use PC farms. This of course introduces new operational challenges. Additional hardware architectures might have to be taken into account, requiring suf£cient portability of any developed code.

The emerging GRID technologies [3] seem to provide the necessary elements to address the LHC computing requirements. The European Union funded DataGrid project will develop the means to operate such large farms (Tier0 & Tier1 centres) with the necessary middleware to schedule jobs and data transfers on a world-wide basis.

The presentation will cover the current architecture and developments in the DataGrid collaboration, as well as plans how to exploit its results.

References

1. http://www.datagrid.cnr.it/
2. Report of the Steering Group of the LHC Computing Review, S. Bethge et al., CERN/LHCC/2001-004
3. See e.g. The GRID, Blueprint for a New Computing Infrastructure, I. Foster and C. Kesselmann ed., ISBN 1-55860-475-8

Dedicated computing for lattice Gauge theories: The APE(s) projects

R. Tripiccione

INFN - Sez. di Pisa
Via Livornese
56010 S. Piero a Grado (PI)
Italy
raffaele.tripiccione@pi.infn.it

In this paper I review the physics goals of Lattice Gague Theory (LGT) and the corresponding computational requirements, in terms of both computing architecture and performance. I brie¤y review several projects that have developed massively parallel computer architectures optimized for LGT. Finally, I describe in details the hardware and software architecture, the status and future plans of one such project (APE), carried out jointly by DESY, INFN, and the University of Paris Sud.

Simulation of population growth and structure of the population

A.Z.Maksymowicz

Faculty of Physics and Nuclear Techniques, University of Mining and Metallurgy, al.Mickiewicza 30, 30-059 Cracow, Poland

amax@agh.edu.pl

Population growth and biological ageing is good example of the entry of physicists to more exotic £elds. Population evolution $n(t)$, in the simplest logistic model approach (and still useful as a test and/or as a reference case), is controlled by a balance between death toll due to limited environmental capacity N and birth rate B of those which survived, providing they reached reproduction age R. The most widespread axesual Penna model [1] applied here introduces genetic load as alternative cause of elimination of an individual at age a when number m of activated 'bad' mutations exceeds a threshold value T. (See also [2] for reviews.) The genome is represented by a string of bits with '1' as the bad mutation, coded on the computer word. The genome is inherited from the parent, and additional M bad mutations randomly distributed over the baby's genome are delivered at birth time. Then m is number of $active$ mutations '1', that is disclosed on bit positions from 0 to actual age a of an individual. The outcome of the simulation is the population $n(a, m)$ which may be compared with statistical data on populations. We may manipulate model parameters (N, B, R, M, T) to get results closer to the statistical data.

In this paper we also account on more detailed characteristics of genome to bring out structure $\Delta(m)$ of genome in terms of sequences of bits for given m, and its role on overall population structure $n(a, m, \Delta(m))$ at equilibrium. The main £ndings are: $1)$ (obvious) there are different time scales for different quantities extracted from simulation, which requires quite different numbers of iterations to reach the equilibrium; $2)$ (less obvious) even if $n(a)$ is not sensitive to characteristics of initial population, $n(a, m)$ still carries some replica of the past; $3)$ structure $\Delta(m)$ of gemomes shows very signi£cant marks of the history and, therefore, may be used to trace the depth of the past, perhaps even to the initial stages of the evolution. For example, unexpectedly the nearly ideal population at the Beginning establishes poorer £nal population in the sense of more frequent bad mutations.

Evolution and biological ageing is believed to be governed by three main factors, oxygen radicals, longevity genes and bad mutations. Only genetic deaths is included in the Penna model. However, this model is very ¤exible for introduction of anew ingredients in the life game, and so the next step should bring modeling which may cover more realistic facts. Most of the simulations were carried up on HP EXEMPLAR machine at the Academic Computer Centre CYFRONET in Kraków. Typical run takes couple of hours for population of about $n = 10^6$.

References

1. T.J.P. Penna, *J. Stat. Phys.* **78** (1995) 1629.
2. S.Moss de Oliveira, P.M.C. de Oliveira and D.Stauffer, *Evolution, Money, War and Computers*, Teubner, Stuttgart-Leipzig, 1999.

Multi-fractal nature of stock exchange prices

M. Ausloos[1] **and K. Ivanova**[2]

[1] *SUPRAS and GRASP, Institute of Physics, B5, University of Liège, B-4000 Liège, Belgium*

[2] *Pennsylvania State University, University Park, PA 16802, USA*

Tel: 32 4 366 3752; Fax: 32 4 366 2990; e-mail: marcel.ausloos@ulg.ac.be

The authors analyze the multifractal structure of the temporal dependence of several currency exchange rates (XR), by means of the calculation of its Hurst exponent H(q). The main qualitative result is that market evolution is driven by a hierarchy of multiple "information levels". The multifractal approach[1, 2, 3] is used to estimate the (q-th) order moments of the structure functions and the singular measures, as constructed from the data. The method seeks for various self-af£nity scales. The analysis is done on the absolute value of the price variations and not on the price variations themselves. This approach leads to characterizing the nonstationarity and intermittency pertinent to such £nancial signals as if produced by nonlinear dynamical processes. The value of the roughness parameter (H_1) is consistent with that obtained for the same data using different methods of analysis, like the DFA. The degree of intermittency C_1 has been also estimated.

In the (H_1, C_1) phase diagram, the currency exchange rates are dispersed in a wide region around the Brownian motion value ($H_1 = 0.5, C_1 = 0$) and have a signi£cantly intermittent component ($C_1 \neq 0$). Moreover, the multifractal behavior of the XR is consistent with the multi-af£ne properties of other turbulent phenomena[4].

The analysis shows the presence of correlated ¤uctuations. A concrete explanation of their appearance and of the differences for different cases seems related to the "strength" of the currencies. The discussion on their relevance in the understanding of the processes that underlie this "macroscopic" market index remains speculative in view of the lack of an appropriate experimental device. Nevertheless a non exhaustive list of results on turbulence and £nancial markets[5] is presented for asserting the analogy.

References

1. A. Davis, A. Marshak, W. Wiscombe, R. Cahalan, *J. Geophys. Research* **99**, 8055 (1994).
2. N. Vandewalle and M. Ausloos, *Int. J. Mod. Phys. C* **9**, 711 (1998).
3. K. Ivanova and M. Ausloos, *Eur. Phys. J. B* **8**, 665 (1999); Err. **12**, 613 (1999)
4. K. Ivanova and T. Ackerman, *Phys. Rev. E* **59**, 2778 (1999).
5. Th. Lux and M. Ausloos, "Market Fluctuations I: Scaling, Multi-scaling and their Possible Origins", in *Facets of universality in complex systems: - climate, biodynamics and stock markets*, A. Bunde and H.J. Schellnhuber, Eds. (Springer, Heidelberg, in press)

On the distribution function of the information speed in computer network

Lev N. Shchur

Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia

telephone +7-095-7029317, fax +7-095-9382077, e-mail shchur@landau.ac.ru

For Internet user the most important parameter of the network access is the speed with which he receiving documents. The daily example is the browsing of preprint and article archives (xxx.lanl.gov, publish.aps.org, elsevier.nl, iop.org, etc.), looking for the news and weather, booking tickets, making reservations, etc.

The speed rate of the document retrieving could be de£ned as the ratio of size of the requested document to the time elapsed from the request to the receiving of the full document. This speed rate are known to have log-normal distribution in the simplest case of measurement down between two £xed sites of network qnd under certain conditions. This is due to the relatively rare events of the extremely slow network response.

The speed rate measured at the £xed site of the all documents retrieved from the given domain, say for all documents requested by user of Aachen Technical University from British Universities ac.uk domain, would be de£nitely multipeaked. This is a re¤ection of several network features we would discuss. The simple example will be discussed in details which provide distribution composed with two log-normal distributions. Tuning some external parameter the absolute maximum of distribution could be positioned at the one or another center of the underlying distributions. Thus, the £rst-order phase transition could be easily realised in computer network.

In physics we understand experiment as a process of measurements which is repeatable under some given external conditions. The possibility of the experiments in that sense with the Internet traf£c is discussed and example of some realization will be given.

Emergence of scaling in complex networks: from the topology of the www to the structure of the cell

Albert-László Barabási

Department of Physics, University of Notre Dame, Notre Dame, IN 46556, USA.

alb@nd.edu, http://www.nd.edu/~alb

Systems as diverse as the world wide web [1] or the cell [2, 3] are described by networks with complex topology. Traditionally it has been assumed that these networks are random. However, recent studies indicate that such complex networks are the result of self-organizing processes governed by simple but generic laws [4], resulting in topologies strikingly different from those predicted by random networks. I will discuss the implications of these £ndings on the error and attack tolerance of the Internet [5], the robustness of the cells [2, 3], and other properties of complex evolving networks.

References

1. Albert, R., H. Jeong and A.-L. Barabási, 1999, Nature **401**, 130.
2. Jeong, H., B. Tombor, R. Albert, Z. N. Oltvai and A.-L. Barabási, 2000, Nature **407**, 651.
3. Jeong, H., S. Mason, A.-L. Barabási, and Z.N. Oltvai, Nature **411**, 41 (2001).
4. Barabási, A.-L. and R. Albert, 1999, Science **286**, 509.
5. Albert, R., H. Jeong and A.-L. Barabási, 2000, Nature **406**, 378.

Cosmological implications from observations of type Ia supernovae

Bruno Leibundgut

European Southern Observatory
Karl-Schwarzschild-Strasse 2
D–85748 Garching
Germany

+49 89 320 06 295, +49 89 320 06 480, bleibundgut@eso.org

The observations of distant Type Ia Supernovae (SNe Ia) have provided a major surprise for cosmology. The faintness of the distant supernovae compared to the expectation of even the most extreme model, i.e. an empty universe, has forged cosmology out of the simple matter-dominated picture and added a new, strange, component. Since next to nothing is know about this new constituent of the universe, it is generally referred to as "dark energy."

Although the measured effect is minimal, about 20% at a redshift of about 0.5, i.e. 5 billion years ago, it has been detected in data sets of two independent groups. Data by the High-z Supernova Search team is more than 2σ, while the Supernova Cosmology Project still £nds a 1.5σ signi£cance. An Einstein-de Sitter model ($\Omega_M = 1, \Omega_\Lambda = 0$), the 'standard model' of a few years ago, is excluded at high signi£cance. To explain the dimness of the supernovae a negative–pressure component must have accelerated the expansion of the universe over the last few Gyr. This result very nicely complements the measurements of the cosmic microwave background and determinations of the matter density. It further solves the long-standing problem of the dynamical age of the universe (for a review see [1])

This result comes at the end of a decade where SNe Ia have been discussed as possible standard candles and progress has yielded a way to normalize the peak luminosity of SNe Ia so that highly accurate distances can be derived. The physics of the explosion and the radiative transport in SNe Ia remains an area of active research. The observed correlations between peak luminosity, light curve shape, colors, line strengths, and line widths are so far unexplained (e.g. [2]).

Without some understanding of the physics, it will not be possible to provide clear guidelines as to whether evolution could have altered the peak luminosity of the SNe Ia ([3]). Recent indications that the color of distant supernovae is bluer than in the nearby sample could hint at evolutionary effects. Other possible explanations for the faintness of the distant are inter-galactic dust and gravitational lensing. Dust grain sizes would have to be signi£cantly different and selectively distributed to have an impact on the supernova result. The bluer colors of the distant supernovae are a further indication that dust may not be important. At the distances of the present supernova sample gravitational lensing is unlikely to be a signi£cant systematic effect.

There is a way to unambiguously determine whether the universe indeed contains a negative-pressure component. During the very early phases the universal expansion should have been decelerated due to its matter content. Only later did the dark energy take over. First indications for such an effect have been found and further observations are planned ([4]).

References

1. Leibundgut, B., 2001, Ann. Rev. Astr. Astrophys. 39, 67
2. Pinto, P. A., Eastman, R. G., 2000, Astroph. J., 530, 757
3. Hillebrandt, W., Niemeyer, J. C., 2000, Ann. Rev. Astr. Astrophys. 38, 191
4. Riess, A. G., et al., 2001, Astroph. J., in press (astro-ph/0104455)

Simulation of hadronic particle production in astrophysical environments

Ralph Engel

Bartol Research Institute, University of Delaware,
217 Sharp Lab, Newark, DE 19716, U.S.A.
(302) 831-0491, (302) 831-1843, eng@lepton.bartol.udel.edu

Hadronic particle production is a common process in astrophysical environments. High energy cosmic rays and gamma rays interact with matter at the production or acceleration site, during propagation and at Earth. The production of secondary particles is inherently linked to energy loss or complete absorption of the primary particle. In both cases the spectrum of cosmic rays is modi£ed. Hence the primary and secondary particle spectra carry important information on the astrophysical sources and the surrounding matter and radiation £elds as well as the intergalactic and interstellar medium.

We will discuss the requirements on the simulation of hadronic interactions and its realization in form of Monte Carlo calculations, using the example of ultra-high energy cosmic rays. Ultra-high energy cosmic rays are strongly interacting particles with an energy greater than 5×10^{10} GeV. Although observed in large air shower experiments, these cosmic rays are theoretically not understood. In particular their astrophysical sources and elemental composition are unknown [1].

The interpretation of data on ultra-high energy cosmic rays relies on the simulation of hadronic particle production over an extremely wide energy range. In addition, the important phase space of particle production is different from that measured at collider experiments.

In many of the proposed acceleration scenarios cosmic rays interact with dense radiation £elds at the source. At high energy, hadron production processes become important and give rise to secondary photon and neutrino ¤uxes. Depending on the model considered, the energies available for particle production cover the range from the particle production threshold up to $\sqrt{s} \sim 1000$ GeV.

The propagation of ultra-high energy cosmic rays is mainly governed by energy losses due to the interaction with photons of the cosmic microwave background. These interactions are typically of very low energy in the center of mass system, just above the particle production threshold and can be simulated with high precision [2].

The detection of the highest energy cosmic rays is based on the measurement of the secondary particles produced in extensive air showers. The simulation of these showers poses a challenge to currently applied simulation methods [3, 4]: the hadronic interaction models have to be extrapolated to c.m.s energies of about 400 TeV and the number of secondary particles produced in such high-energy showers is of the order of 10^{10}, photons not counted.

References

1. M. Nagano and A.A. Watson, Rev. Mod. Phys. **72**, 690 (2000).
2. T. Stanev, R. Engel, A. Mücke, R.J. Protheroe, and J. Rachen, Phys. Rev. **D62** (2000) 093005.
3. J. Jaime Alvarez-Muñiz, R. Engel, P. Lipari, J.A. Ortiz, and T. Stanev: *Ef£cient simulation of ultra-high energy air showers*, proceedings of 27th ICRC, Hamburg, Aug. 7-15, 2001.
4. R. Engel, T.K. Gaisser, and T. Stanev: *Extrapolation of hadron production models to ultra-high energy*, proceedings of 27th ICRC, Hamburg, Aug. 7-15, 2001.

Computational particle physics with the cluster computer ALiCE

N. Eicker, H. Neff, Th. Lippert, B. Orth, K. Schilling

Fakultät für Physik, Universität Wuppertal, 42097 Wuppertal, Germany
lippert@theorie.physik.uni-wuppertal.de

Quantum Chromodynamics (QCD) is the gauge theory of the strong forces, mediated by exchange of gluons between the constituent particles of matter, the quarks. In gauge theories, the coupling ”constant” depends on the typical momenta of the problem under consideration. At momenta comparable to light hadronic masses (i.e. mesons like the pion and the rho) the coupling of QCD becomes large. To solve QCD in this regime so-called ”non-perturbative” techniques like lattice QCD (LQCD) are required, because perturbation theory fails for coupling constants in the range of 1.

LQCD works by computer simulations of the gluonic and fermionic £elds on a 4-dimensional space-time lattice of Euclidean metrics. Typically, an ensemble of representative £eld con£gurations is generated by means of stochastic Monte Carlo methods as applied in statistical physics. Subsequently, observables which are functionals of the £elds are computed in form of statistical averages over the ensemble.

In recent years LQCD was established as the most promising technique to deal with non-perturbative aspects of £eld theories. This is demonstrated by the efforts of the elementary particle physics community to provide the huge compute power required by such ab-initio computer experiments. On one hand, systems dedicated for LQCD number crunching are constructed: in Europe, DESY/INFN together with other European institutes are jointly developing the Multi-Tera¤ops system apeNEXT. Columbia university (USA) and UKQCD (UK) together with IBM are building the 10 T¤ops QCDOS systems. In Japan, the group at Tsukuba university is heading for 100 T¤ops.

As an alternative, commodity-off-the-shelf (COTS) cluster computers promise to provide a cost-effective pathway towards Tera-computing for LQCD. The Hungarian group at Eïvös University has demonstrated the cost-effectiveness of COTS by their poor-mans-supercomputer. In the near future, Jefferson Lab, Fermilab and MIT are going for Multi-Tera¤ops cluster systems.

In my talk, I am going to present results from LQCD simulation projects carried out on a pre-Tera¤ops cluster system, the 128-node Compaq-DS10/Myrinet cluster ALiCE at Wuppertal University. After its £nal upgrade in October 2000, our general purpose multi-user platform provides a total compute power of 160 G¤ops. I will focus on two projects, (i) the truncated eigenmode algorithm (TEA), a new approach to compute ¤avor-singlet quantities in LQCD, which e.g. determine the mass of the eta’ meson, and (ii) simulations of QCD with dynamical fermions by use of the hybrid Monte Carlo algorithm, carried out in the framework of the GRAL project. For TEA, several hundred low-lying eigenvectors of the fermionic matrix with dimension $\mathcal{O}(10^6)$ have to be computed and stored for $\mathcal{O}(10^2)$ con£gurations. Besides the presentation of very encouraging physics results I will compare performances and I/O handling between ALiCE and the Cray T3E. The GRAL project (Going Realistic and Light) aims at a mass ratio between pion and rho meson below 0.5 that will allow the rho meson to decay into two pions, a £rst attempt with Wilson fermions to bring the realistic situation onto the lattice. In the GRAL context I am going to present performance comparisons between ALiCE and APEmille.

Hydromagnetic turbulence in computer simulations

Axel Brandenburg[1] **and Wolfgang Dobler**[2]

[1]*NORDITA, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark*
[2]*Department of Mathematics, University of Newcastle, NE1 7RU, UK*
Phone +45 353 25 228, FAX +45 353 89 157, brandenb@nordita.dk

Hydromagnetic processes play an important role in many astrophysical systems (e.g. stars, galaxies, accretion discs). This is because the medium is hot enough to be partially or fully ionized. Because of the huge scales involved the medium is usually turbulent, provided there is an instability (shear, convection) facilitating the cascading of energy down to small scales.

In ordinary turbulence research it has been a long standing tradition to solve the equations in spectral space giving the best possible accuracy. This is indeed a natural choice for incompressible problems with periodic boundaries, but it is no longer optimal in many astrophysical circumstances. It is argued that lower order spatial derivatives schemes are unacceptable in view of their low overall accuracy, even when mass, momentum, and energy are conserved to machine accuracy. High order £nite difference schemes are therefore found to be quite ef£cient and physically appropriate. They are also easily and ef£ciently implemented on massively parallel computers. High order schemes also yield suf£cient overall accuracy. Our code uses centered £nite differences which make the adaptation to other problems simple. Since the code is not written in conservative form, conservation of mass, energy and momentum can be used to monitor to quality of the solution. A third order Runge-Kutta scheme with $2N$ storage [1] is used for calculating the time advance.

A number of tests ranging from advection to shock problems are presented and their accuracy is considered in relation to other schemes. We then turn to applications of astrophysical turbulence where the driving is either through explicit forcing functions or through instabilities (convection, magnetic shear ¤ow instability). Numerically, the magnetic £eld is represented in terms of the magnetic vector potential, which provides an ef£cient way to ensure solenoidality of the £eld. Contrary to popular belief, such schemes do not suffer additional loss of accuracy: the second derivative required to calculate the current density from the vector potential is compensated by saving a derivative when evolving the magnetic vector potential itself.

A full description of the code is given in Ref. [2]. Applications to the problem of the inverse cascade phenomenon in hydromagnetic turbulence can be found in Ref. [3]. Here the turbulence is driven by explicit forcing functions. For references to naturally driven turbulence in stellar convection zones or accretion discs with strong shear see Ref. [4]. One of our most recent applications concerns the problem of resistively limited growth in models of stellar dynamos; see Ref. [5].

References

1. Williamson, J. H., J. Comp. Phys. 35, 48 (1980)
2. Brandenburg, A., in Advances in non-linear dynamos, ed. A. Ferriz-Mas & M. Núñez Jiménez (2001); also available under http://www.nordita.dk/~brandenb/papers/rev.ps.gz
3. Brandenburg, A., Astrophys. J. 550, 824 (2001)
4. Brandenburg, A., et al. Astrophys. J. 446, 741 (1995); J. Fluid Mech. 306, 325 (1996)
5. Brandenburg, A., & Dobler, W., Astron. Astrophys. 369, 329 (2001)

Oral Contributions

On new ef£cient algorithms for PIMC and PIMD

Martin H. Müser and Florian Krajewski

Institut für Physik, WA 331; Johannes Guntenberg-Universität
55099 Mainz; Germany

Tel: [++49] 6131 392-3646, Fax: [++49] 6131 392-5441, e-mail:
martin.mueser@uni-mainz.de

We report on new path-integral Monte Carlo methods for continuous degrees of freedom that incorporate information of the exact two-particle density matrix ρ. The calculation of the diagonal and non-diagonal components of ρ is outlined in [1] for the Coulomb potential, but it can be easily generalized to other central potentials. In the simulations, the potential energy between two interacting particles as well as the masses are effective properties that converge suf£ciently fast to their real values as the Trotter number becomes large.

Furthermore, new primitive estimators [2] for the calculation of elastic constants and the kinetic energy are proposed for PIMD simulations [3]. The variance of these estimators does not increase with Trotter number (unlike usual primitive estimators). The estimators are also applicable to the gas phase, where standard virial estimators turn out to fail. Applications of our methods include solid helium III [2], solid argon [2], and α-quartz [4], far below their respective Debye temperatures.

We will also comment on some important details of the implementation of our PIMD code. This concerns in particular the choice of the masses that are attributed to eigenmodes of the free classical chain representing the quantum mechanical point particle and thermostatisation [4].

References

1. E.L. Pollock, Comp. Phys. Comm. 52, 49-60 (1988).
2. P. Schöffel and M. H. Müser, Phys. Rev. B (submitted).
3. M.E. Tuckerman et al., J. Chem. Phys. 99, 2796-2808 (1993).
4. M. H. Müser, J. Chem. Phys. (in press)

Finite-temperature Lanczos algorithm study on pseudogap in high-T_c superconductors

Tôru Sakai[1] **and Yoshinori Takahashi**[2]

[1]*Tokyo Metropolitan Institute of Technology, Tokyo 191-0065*
[2]*Himeji Institute of Technology, Hyogo 678-1297*
TEL and FAX +81-791-58-0150, sakai@sci.himeji-tech.ac.jp

The pseudogap phenomena of the high temperture superconductors have attracted a lot of interest in the £eld of the condensed matter physics. They were observed as a broad peak in the temperature dependence of the NMR relaxation rate, the magnetic sucseptibility, the conductivity, the neutron scattering intensity and the angle-resolved photoemission etc. in the underdoped high-T_c cuprate superconductors. The pseudogap is supposed to be related to the mechanism of the superconductivity, but the origin is still an open question. In the previous work of the present authors[1, 2], the exact diagonalization of the t-J model on the $\sqrt{10} \times \sqrt{10}$ cluster with one hole suggested that the gap-like behavior is closely related to the growth of the antiferromagnetic short-range order. However, the study of the single-hole system is not enough to clarify some features of the superconducting systems where the hole pairing is an essential effect. In the present work, the t-J model on the 4×4 cluster with two holes is investigated by the £nite-temperature Lanczos algorithm using the random sampling of the initial vector.[3] The temperature dependence of the dynamical sucseptibility $\mathrm{Im}\chi(q,\omega)$ and the spin correlation functions is evaluated by the method. The calculated $\sum_q \mathrm{Im}\chi(q,\omega)$ for small ω and the static magnetic sucseptibility χ exhibit a gaplike behavior around the characteristic temperature where the Q ($=(\pi,\pi)$) component of the Fourier transformation of the spin correlation function grows signi£cantly. It con£rms that the pseudogap phenomena are caused by the enhancement of the antiferromagnetic spin correlation even for the two-hole system with the singlet ground state. Thus the conclusion is expected to be valid in the bulk systems. It is also found that the psedogap phenomena are almost indepnedent of the external magnetic £eld, which is consistent with the recent high magnetic £eld measurement.[4]

References

1. T. Sakai and Y. Takahashi, J. Phys. Soc. Jpn. **67** (1998) 2630.
2. T. Sakai and Y. Takahashi, J. Phys. Soc. Jpn. **70** (2001) 272.
3. J. Jaklic and P. Prelovsek: Phys. Rev. Lett. **74** (1995) 3411.
4. G.-q. Zheng et al.: Phys. Rev. B **60** (1999) R9947; Phys. Rev. Lett. **85** (2000) 405.

A computational study of some Josephson junction circuits

P. H. Borcherds

School of Physics and Astronomy, The University of Birmingham, B15 2TT

p.h.borcherds@bham.ac.uk

A Josephson junction is a nonlinear circuit element: the current through an ideal Josephson junction is proportional to the sine of the integral of the voltage across the junction. The work has been carried out both numerically and also using an electronic simulation of a Josephson junction interfaced to a computer. It will be demonstrated that there are real advantages in studying this system in these ways. For example, it is possible to make measurements on the models which cannot be made on a real junction; leading to a better understanding of some of the phenomena observed.

By interfacing an electronic simulation of a Josephson junction to a (digital) computer one obtains the advantages of an analogue computer: very high speed at very low cost, without the disadvantage of intrinsically low accuracy in the results.

When studying a nonlinear dynamical system one very often does not know in advance what sort of qualitative behaviour to expect: this means that one has to rely on the experimental expertise and intuition of the investigator. This in turn requires that there must be a good visual display, that the investigator can easily change the “experimental” conditions and that the system must respond reasonably rapidly to such changes. An electronic simulation is very satisfactory for pilot studies, as will be explained.

We have investigated the McCumber model of a junction (an ideal junction shunted by a capacitor and a resistor), sometimes in parallel with an LCR circuit, driven by a steady current, and sometimes a superimposed alternating current. In both the numerical and the electronic simulations the driving currents and the circuit parameters can be adjusted. Usually the driving current is varied (slowly), while keeping the component values £xed.

Our observations, obtained by varying the driving current, include:

1. A period doubling sequence leading to chaos, with windows of order in the chaos
2. “Fractional quantum effects” in the voltage-current characteristic.
   When there is a superimposed sinusoidal current (simulating an rf £eld) the voltage current characteristic exhibits steps whose height is proportional to the ¤ux quantum. Both for real junctions and in our simulations one £nds step heights which are a fraction (e.g. one third) of the expected height. This observation will be explained.
3. The Lyapunov exponents of the junction plus LCR circuit (in 4 dimensional phase space) have been studied: over much of the current range, two of the four exponents are degenerate, but there is a small region, outside the chaotic regime, where the degeneracy is lifted. This will be discussed.

Some of the advantages of a computational physics approach are shown in this work. In real Josephson junctions the voltage steps are measured in microvolts for a frequency measured in gigahertz: this is experimentally dif£cult. In a simulation the steps can be measured in volts, at a frequency of a few kilohertz. However there are also more fundamental advantages: it is possible to measure the currents through each of the three components of the McCumber model. In a real junction, such measurements are obviously impossible. It would also not be possible to measure Lyapunov exponents in a real system. It can therefore be seen that Computational Physics can, in some circumstances, provide information not obtainable in any other way.

Ab-initio prediction of complex magnetic structures in low dimensions

G. Bihlmayer, Ph. Kurz, F. Förster and S. Blügel

Institut für Festkörperforschung (IFF), Forschungszentrum Jülich, D-52425 Jülich, Germany

tel.: (+49) 02461 614677, fax: 02461 612620, e-mail: G.Bihlmayer@fz-juelich.de

In the last few years using modern, massively parallel supercomputers, the parameter-free calculation of complex, low-dimensional magnetic structures has become possible. The basic understanding of these structures is of signi£cant importance for the magnetic recording industry and for other nanotechnological applications. We present a detailed account of the implementation and application of a formalism that allows to calculate complex, non-collinear magnetic structures in the FLEUR code, a program based on the full-potential linearised augmented planewave (FLAPW) method. This method relies on the vector spin-density formulation of density functional theory with a (locally) collinear magnetic exchange-£eld in the vicinity of the atoms.

Strategies to apply this computationally demanding formalism (which requires the solution of large, generalised and complex eigenvalue problems) to realistic systems, e.g. a two-level parallelisation of the code and algorithmical modi£cations to extend the scalability of the program, will be discussed in detail. Special emphasis will be put on the investigation of surfaces, which are embedded in semi-in£nite vacuum to avoid the computational overhead of conventional repeated-slab calculations. Exploiting further symmetries, we can apply our method to even larger, more realistic, systems.

At present three approaches to deal with non-collinear magnetism are implemented: (i) arbitrary commensurate spin-structures by employing a (intra-atomic non-collinear) constraint-£eld, (ii) incommensurate spin-spirals and (iii) the relaxation of the spin directions. Technical aspects as well as several recent results of calculations, e.g. of fcc-Fe, Mn(100) and (111) monolayers are presented. Apart from commensurate spin structures we also discuss the calculation of materials with incommensurate spin spirals. We show how to explore the magnetic phase diagrams by relaxation of the spin directions and calculations with constrained spin directions. A systematic approach to the investigation of the magnetic ground-state of a system is the combination of these ab-initio calculations with model Hamiltonians. With this method, a new ground state for the Mn/Cu(111) system has been found [1].

References

1. Ph. Kurz, G. Bihlmayer, K. Hirai and S. Blügel, Phys. Rev. Lett. **86**, 1106 (2001).

Quasi-ab initio molecular dynamics simulations of atomic scale structures on metal surfaces

V.S. Stepanyuk[1,2], **D.I. Bazhanov** [1,3], **A.N. Baranov** [1,3]
and W. Hergert [2]

[1] *Max-Planck-Institut für Mikrostrukturphysik,*
Weinberg 2, D-06120 Halle, Germany
[2] *Martin-Luther-Universität Halle-Wittenberg,*
Friedemann-Bach-Platz 6, D-06108 Halle, Germany
[3] *Solid State Physics Department, Moscow State University, 119899 Moscow, Russia*
0345 5525 445, 0345 5525 446, hergert@physik.uni-halle.de

Using KKR Green's function method and density functional theory we present a novel approach for calculations of many body interatomic potentials for transition metal nanostructures on metal surfaces. [1]

Potentials are formulated in the second-moment tight binding approximation. The parameters of potentials are optimized simultaneusly by including in the £t the results of the £rst principle calculations of selected cluster-substrate properties, forces acting on adatoms on the surface, and ab initio and experimental bulk properties. Such approach allows one to reproduce well the bulk and surface properties of the system under investigation.

Magnetic effects on the interatomic interactions are investigated by means of £tting to the results of both spin-polarized and non-magnetic calculations for transition metal clusters on metal surfaces.

Several examples of the most recent applications of our method are presented. We concentrate on relaxations and atomistic processes in the early stages of Co and Fe thin £lm growth on the Cu(001). [2] to an unusual shape evolution in mesoscopic islands. [3]

We show that strain relief has a strong impact on the growth process leading

We demonstrate that magnetism effects the shape of clusters and promotes their sinking into the substrate. We reveal the in¤uence of magnetic interactions in mesoscopic islands on the 2D-3D structural transitions.

References

1. N.A. Levanov, V.S. Stepanyuk, W. Hergert, et al., Phys. Rev. B **61**, 2230 (2000).
2. V.S. Stepanyuk, D.I. Bazhanov, W. Hergert, Phys. Rev. B **62**, 4257 (2000).
3. V.S. Stepanyuk, D.I. Bazhanov, A.N. Baranov, W. Hergert, P.H. Dederichs, J. Kirschner , Phys. Rev. B **62**, 15398 (2000).

Dynamic critical behavior of the classical anisotropic BCC Heisenberg antiferromagnet*

Shan-Ho Tsai, Alex Bunker, and D.P. Landau

Center for Simulational Physics, University of Georgia, Athens, GA 30602

Telephone: 1 706 542 3460, Fax: 1 706 542 2492, Email: tsai@hal.physast.uga.edu

Realistic models for the dynamic behavior of magnetic materials can be constructed from simple spin models; however, the theoretical analysis of experimentally accessible quantities, such as the dynamic structure factor, is usually too demanding for analytical methods. Computer simulations can now provide information about dynamic critical behavior of model magnetic systems that is amenable to direct and quantitative comparison with experimental results. Simulations can also yield new insights into long-standing controversies between theory and experiment or between competing theories.

In this paper we study the effect of single-site uniaxial anisotropy on the critical dynamics of a classical Heisenberg antiferromagnet on a body-centered cubic lattice with nearest-neighbor interactions only. Examples of good physical realizations of this model are MnF_2 [1] and FeF_2 [2] with weak and strong anisotropy, respectively.

The dynamic behavior of this model is investigated through large-scale spin-dynamics simulations, using lattices with linear size $L \leq 60$, and both vector and massive-parallel programs. Time evolutions of spin con£gurations were determined numerically from coupled equations of motion for individual spins using an algorithm implemented by Krech *et al* [3], which is based on fourth-order Suzuki-Trotter decompositions of exponential operators. The dynamic structure factor $S(q, \omega)$ was calculated from the space- and time-displaced spin-spin correlation function. Dynamic £nite-size scaling theory was used to estimate the dynamic critical exponent of the system.

Results for the transverse and the longitudinal components of $S(q, \omega)$ show that while the former is propagative, with a relatively short time scale, the latter is diffusive and its computation requires very long time integrations. Preliminary dynamic £nite-size scaling analyses for the weakly anisotropic case show that the asymptotic region is very narrow, thereby an accurate estimate of the dynamic critical exponent requires the usage of very small values of the momentum transfer q, accessible only with very large lattice sizes. Although not yet conclusive, our results favor the predictions by the renormalization group theory [4] over theoretical results of a dynamic scaling argument [5].

Because of dif£culties for experiments to probe the critical region, experimental data have not yet been able to distinguish between competing theories. While limited by £nite lattice size and £nite integration time, simulations offer the hope of shedding light on the differences between theories and experiment.

*Supported by the National Science Foundation and San Diego Supercomputing Center.

References

1. M.P. Schulhof, R. Nathans, P. Heller, and A. Linz, Phys. Rev. B **4** 2254 (1971)
2. M.T. Hutchings, M.P. Schulhof, and H.J. Guggenheim, Phys. Rev. B **5** 154 (1972)
3. M. Krech, A. Bunker, and D.P. Landau, Comput. Phys. Commun. **111**, 1 (1998)
4. P.C. Hohenberg and B.I. Halperin, Rev. Mod. Phys. **49**, 435 (1977)
5. E. Riedel and F. Wegner, Phys. Rev. Lett. **24**, 730 (1970)

Strong electrostatic interactions in colloidal systems

René Messina, Christian Holm and Kurt Kremer

Max-Planck-Institut für Polymerforschung, Ackermannweg 10,
55128, Mainz, Germany

Tel +49 6131 379 148, Fax +49 6131 379 100, messina@mpip-mainz.mpg.de

We investigate spherical macroions in the strong Coulomb coupling regime within the primitive model in salt-free environment. We £rst show that the ground state of an isolated colloid is naturally overcharged by simple electrostatic arguments illustrated by the Gillespie rule [1, 2]. We furthermore demonstrate that in the strong Coulomb coupling this mechanism leads to ionized states and thus to long range attractions between like-charged spheres. Using molecular dynamics (MD) simulations we studied in detail the counterion distribution for one and two highly charged colloids for the ground state as well as for £nite temperatures. We compare our results in terms of a simple version of a Wigner crystal theory and £nd excellent qualitative and quantitative agreement.

We showed that for two *like-charged* macroions (symmetric case), an initially randomly placed counterion cloud of their neutralizing divalent counterions may not be equally distributed after relaxation, leading to two macroions of opposite net charges [1, 2]. The resulting con£guration is metastable, however separated by an energy barrier of several $k_B T_0$ when the bare charge is suf£ciently large, and can thus survive for long times. Such con£guration possess a natural strong long range attraction.

However, if the symmetry in the surface macroion charge density σ (*both* macroions are negatively charged) is suf£ciently broken, the ionized state is *stable*. The ground state of such a system is mainly governed by two important parameters,namely the asymmetry in the counterion concentration determined by $\sqrt{\sigma_A} - \sqrt{\sigma_B}$, and the colloid separation *R* [1, 3].

More recently, we carried out MD simulations to elucidate the effect of colloidal charge discretization [4]. Instead of considering a central bare charge, as it is traditionally done, we distribute *discrete* charges randomly on the sphere. One important result of this study is that, in the strong Coulomb coupling, the charge inversion is still effective when the macroion structural charge is carried by discrete charges distributed randomly over its surface area. We have shown that the intrinsic electrostatic potential solely due to the surface colloidal microions strongly vary from point to point on the macroion sphere. When counterions are present, it leads to a pinned structure where every counterion is associated with one colloidal charge site. Furthermore we observed a pure phonon-like behavior (counterion vibration with small lateral motion) at room temperature.

References

1. R. Messina, C. Holm, and K. Kremer, submitted to Phys. Rev. E. - cond-mat/0101263.
2. R. Messina, C. Holm, and K. Kremer, Phys. Rev. Lett. **85**, 872 (2000).
3. R. Messina, C. Holm, and K. Kremer, Europhys. Lett. **51**, 461 (2000).
4. R. Messina, C. Holm, and K. Kremer, Eur. Phys. J. E **4**, 363 (2001).

Optimal shapes of compact strings

C. Micheletti[1] **A. Maritan**[1]**, A. Trovato**[1]
and J. Banavar[2]

[1] *International School for Advanced Studies (S.I.S.S.A.), Via Beirut 2-4, 34014 Trieste, Italy*

[2] *The Pennsylvania State University, University Park, Pennsylvania 16802, USA*

Tel: +39 0402246463, Fax: +39 0403787528, michelet@sissa.it

Optimal geometrical arrangements, such as the stacking of atoms, are of relevance in diverse disciplines [1]. A classic problem is the determination of the optimal arrangement of spheres in three dimensions in order to achieve the highest packing fraction; only recently has it been proved [1] that the answer for in£nite systems is a face-centred-cubic lattice. This simply stated problem has had a profound impact in many areas ranging from the crystallization and melting of atomic systems, to optimal packing of objects and subdivision of space. Here we study an analogous problem–that of determining the optimal shapes of closely packed compact strings. This problem is a mathematical idealization of situations commonly encountered in biology, chemistry and physics, involving the optimal structure of folded polymeric chains. The problem is tackled by a stochastic optimization techniques which exploits ideas developed recently in the context of ideal knot shapes [2]. In particular, for a £xed con£ning boundary (a box, or upper limit to radius of gyration) we search for the (discretised) centerlines of the thickest tube that can be accomodated. The maximum thickness can be limited by local tight bends or by the close approach of distant parts of the tube. We £nd that, in cases where boundary effects are not dominant, helices with a particular pitch-radius ratio are selected. Strikingly, the same ratio (to within 1%) is observed in helices in naturally-occurring proteins [3]. It is also shown, that, to the same accuracy also the double helix of DNA satisfy an analogous optimal ctriterion [4].

References

1. Sloane, N. J. A., Kepler's conjecture con£rmed, *Nature* **395**, 435-436 (1998).
2. Gonzalez, O. and Maddocks, J. H., Global curvature, thickness and the ideal shapes of knots, *Proc. Natl. Acad. Sci. USA* **96**, 4769-4773 (1999).
3. A. Maritan, C. Micheletti, A. Trovato and J. Banavar, *Nature*, 406, 287-290 (2000).
4. Stasiak, A. and Maddocks, J., *Nature*, 406, 251-253 (2000).

Molecular dynamics study of polyelectrolyte brushes

Christian Seidel

Max-Planck-Institut für Kolloid- und Grenz¤ächenforschung,
Am Mühlenberg, D-14476 Golm, Germany

phone: (+49/0)-331-567 9608, fax: (+49/0)-331-567 9612,
e-mail: seidel@mpikg-golm.mpg.de

Polyelectrolytes, i.e., charged polymers, have received a lot of attention in recent years. Polyelectrolyte brushes consisting of charged polymers which are densely end-grafted to a surface form the subject of substantial interest by theory and experiment. They are also interesting from the point of view of applications. Molecular dynamics simulations provide an excellent means to study polymer systems. We have performed stochastic molecular dynamics simulations of polyelectrolyte brushes at various grafting densities with both completely charged and partially charged chains. A freely jointed bead-chain model was adopted, where the monomers are connected by nonlinear springs and end-grafted to a rigid surface. The counterions are explicitly modeled as charged particles. A special feature of brush simulations consists in the 2D+1 slab geometry of the problem. The simulation box is periodic in lateral directions and £nite in z-direction perpendicular to the grafting surface. To sum the full Coulomb interaction in a 2D+1 geometry we use an approach proposed by Lekner and modi£ed by Sperb [1].
A number of theoretical models have been suggested for effective attractions between likely charged rigid rods and for chain collapse in solutions of ¤exible polyelectrolytes. For the £rst time, we have observed a similar chain collapse in strongly charged polyelectrolyte brushes [2, 3]. The salient feature of the collapsed phase, not explained in previous theories for polyelectrolyte brushes, is that the monomer density stays constant as the grafting density and the polymer length is varied. For moderate strength of the Coulomb interaction, we £nd that the counterions are completely con£ned to the brush layer. In addition, although the Bjerrum length λ_B (which sets the interaction strength) is smaller than the average charge separation on the chain, strong counterion condensation is observed. Reducing the degree of charging f we £nd a crossover from the collapsed regime where the brush height scales linearly with the grafting density ρ_a to a neutral brush behavior with a height proportional to $\rho_a^{1/3}$ [4].
The nature of the collapsed phase can be understood on the basis of a simple scaling model. Including a Debye-Hückel correlation term in the total free energy, indeed generates a new collapsed regime where the attractive Debye-Hückel interaction is balanced by the second virial of monomers and counterions [4]. The theoretical model predicts that the brush properties are dependent on the ratio between second virial v_2 and Bjerrum length λ_B. Simulation results indicate a non-monotonic behavior of the brush thickness when λ_B is varied [2]. Reducing λ_B we obtain a stretching up to about $2/3$ of contour length before the coupling between polyelectrolyte charge and counterions becomes too weak and the brush relaxes back into a quasi-neutral con£guration. Systematic studies of the dependencies on interaction strength and second virial con£rm the predictions of theory. Decreasing v_2 by reducing the counterion size we £nd the chain collapse to be enhanced. On the other hand, on decreasing λ_B the collapse disappears and the brush is shifted towards so-called osmotic behavior.

References

1. J. Lekner, Physica A 176, 524 (1991), R. Sperb, Mol. Simulation 13, 189 (1994).
2. F.S. Csajka, C.C. van der Linden, C. Seidel, Macromol. Symp. 146, 243 (1999).
3. F.S. Csajka, C. Seidel, Macromolecules 33, 2728 (2000).
4. F.S. Csajka, R.R. Netz, C. Seidel, J.-F. Joanny, Eur. Phys. J. E to appear (2001).

Large-scale computer simulation of local segmental dynamics in amorphous atactic polystyrene

A.V. Lyulin and M.A.J. Michels

Department of Applied Physics, Eindhoven University of Technology
and Dutch Polymer Institute, P.O.Box 513 5600 MB Eindhoven, The Netherlands
phone +31(0)40 247 4253, fax +31(0)40 244 5253, e-mail a.v.lyulin@tue.nl

The underlying mechanisms of plastic deformation in amorphous polymers remain an open question. The dif£culties of understanding the basic mechanisms governing amorphous polymer behaviour stem from the complex microstructure and microstructural relaxation that dominate the material response. Very recent work[1] suggests that collective segmental dynamics plays a key role here. The goal of this work is to provide better understanding of the contribution of the inter- and intramolecular interactions in amorphous polymers to quasielastic properties and dynamic mechanical stress-strain behaviour. The most challenging question is whether the difference in the segmental mobility of different amorphous polymers (e.g., polystyrene and polycarbonate) can explain the obvious difference in their mechanical response.

In the present work molecular dynamics NPT simulations of bulk atactic polystyrene (PS) were performed in a temperature range from 100K to 600K and in a broad pressure range from 1 bar to 10 kbar. The force-£eld parameters employed are taken mostly from [2]. Simulations were performed up to 10-20 ns with the leap-frog algorithm at a time step of 2 fs.

The MD-determined speci£c volume vs temperature curves are in a good agreement with experimental data at different values of the applied pressure. The measured glass transition temperature, T_g, is displaced, as expected, to somewhat higher temperature than the longer-time experimental value. Calculated statistical properties (radius of gyration, end-to-end distance, distribution function of torsional angles) weakly depend on temperature and pressure in the whole P-T region studied here.

Local dynamical properties in the vicinity of T_g have been investigated. Translational mobility was studied in broad temperature and pressure range by measuring the mean square translational displacement of beads as a function of time. The long time asymptotic slope of these dependencies is close to 0.5 at $T > T_g$ at all applied pressures, showing diffusive behaviour. Local translational motion is essentially frozen in the glassy state, but the onset of diffusive behaviour can already be recognized in sub-T_g simulation data. Legendre polynomials of the £rst, $P_1(t)$, and second, $P_2(t)$, order have been calculated for the bonds in the main chain and along the phenyl side groups, through these the change in orientational and translational mobility with different positions along the PS chain and its temperature and pressure dependencies were examined. The calculated orientational relaxation time was almost constant in the middle part of the chain more than 3-5 monomer units away from the chain ends, decreasing drastically by a factor of 5 toward the chain ends.

The uniaxial deformation of amorphous PS has been studied for the £rst time using the loose coupling constant pressure algorithm of Brown and Clarke, [3]. The PS sample was subjected to a gradually increasing uniaxial tension by changing one of the components of the applied pressure tensor. Results on the yield and plastic behaviour at low temperatures will be discussed.

References

1. See e.g. B. Brule, J.L. Hallary, L. Monnerie, 11th Intern Conf Deformation, Yield and Fracture of Polymers, Cambridge (UK), April 2000, Book of Abstracts, IOM Communications Ltd.
2. M. Mondello et al, Macromolecules, 1994, 27, 3566.
3. D. Brown, J.H.R. Clarke, Macromolecules, 1991, 24, 2075.

Dynamics of droplet spreading

A. Milchev[1,2] **and K. Binder**[2]

[1] *Institute for Physical Chemistry, Bulgarian Academy of Sciences, 1113 So£a, Bulgaria*

[2] *Institut für Physik, Johannes-Gutenberg-Universität, Staudinger Weg 7, 55099 Mainz, Germany*

[1] *phone:+3592727550, fax: +35929712688, e-mail: milchev@ipchp.ipc.bas.bg*

The spreading dynamics of polymer droplets in condition of complete wetting on an ideally ¤at and structureless solid substrate has been studied by a Monte Carlo simulation, using a coarse-grained bead-spring model of ¤exible macromolecules. For the £rst time we £nd evidence in a computer experiment that Tanner's law[1] for the growth of the droplet radius $\left\{r(t) \propto t^{1/10}\right\}$ and contact angle $\left\{\theta \propto t^{-0.3}\right\}$ holds on nanoscopic scales. The density pro£les, Fig.1, con£rm earlier predictions[2] that the central cap-shaped region of the droplet shrinks at the expense of a transition region ("foot") surrounded by a *precursor £lm* which is roughly one monolayer thick. At later times the precursor £lm breaks into individual polymer chains and advances in a typically diffusive manner as observed in experiment[3]. The con£rmed validity of Tanner's law down to nanoscopic scales appears rather remarkable given that

Fig. 1. Contour diagrams of the radial density of a droplet, consisting of 128 polymer chains each of $N = 32$ monomers, before and after (time $t = 4.10^6$ MCS) the adsorption strength of the substrate potential has been switched from partial to complete wetting. Adjacent isolines are shifted by $1/18$ of the bulk density of the melt. An attractive potential $V_{wall} \propto 1/z^3$ acts on the drop in z-direction.

the law was derived from macroscopic hydrodynamics[1]. It supports our recent £nding[4] that typical macroscopic quantities which characterize wetting, such as Young's angle or surface tension, retain meaning even at scales where one goes over from continuous to discrete description of matter.

High ef£ciency of our off-lattice Monte Carlo algorithm is achieved by means of integer-based binary arithmetics in combination with link-cell lists while the necessary statistical accuracy required averaging on a parallel computer with 128 PES.

References

1. L. H. Tanner, J. Phys. D **12**, 1473(1979).
2. P. G. de Gennes, Rev. Mod. Phys. **57**, 825(1985).
3. F. Heslot, A. M. Cazabat, and P. Levinson, Phys. Rev. Lett. **62**, 1286(1989)
4. A. Milchev and K. Binder, J. Chem. Phys. (2001, in press).

Large shear deformation of particle gels studied by Brownian dynamics simulations

A.A. Rzepiela

Mathematical and Statistical Methods Group, Wageningen University, Dreijenlaan 4, 6703 HA Wageningen, The Netherlands

e-mail: Anna.Rzepiela@mat.dpw.wag-ur.nl, fax:+31317483554

Colloidal particle gels form an extensively bonded network consisting of weakly bonded colloidal particles interpenetrated by a suspending ¤uid. Structure of such a gel can be described with fractal analysis [1], and it is strongly determined by the aggregation kinetics and reorganisation of the system [2]. The concentration of particles in those systems can be quite low, but the mechanical properties are still dominated by the network rather than by the interpenetrating ¤uid.

When a colloidal gel is put under stress its equilibrium structure is £rst deformed and £nally destroyed. The deformation behaviour is related to the structure of the gel and its reversibility depends both on the duration and the size of the acting force. Often gels do not exhibit clear fracture but show a yielding transition from elastic to a viscous regime. Many models were previously developed to describe shear deformation and ¤ow of aggregating colloidal suspensions [3, 4]. They describe a wide range of colloid volume fractions, up to $\phi = 0.64$, and a wide range of shear rates but generally, small strains. Also models were developed to describe brittle versus ductile fracture behaviour under strain for crystal solids [5].

Here we report on a large non-af£ne shear deformation of particle gels. In contrast to af£ne, non-af£ne deformation omits ¤ow £elds in the bulk of the system and the shear forces act on the perpendicular surfaces of the material. This technique, to our knowledge not used before for studying shear gel deformation, is a better model of a real rheological experiment as the network, not the suspending ¤uid, determines the mechanical response of a gel. In the non-af£ne deformation model the system evolves to greater relative strains before it ruptures or yields as the system reorganisation plays more important role.

Brownian Dynamics simulations have been performed within a ball and string model. We consider a system of 10 000 elastic spheres placed in a periodic 3D cubic box with volume fraction $\phi = 0.1$. The particles interact through potentials modelled by a harmonic central repulsion and non-central bonding attraction, upon stretching bonds may break.

We report on the large non-af£ne deformation behaviour of particle gels in a range of shear rates. In the used range of model parameters we observe a wide range of rheological behaviour, and it was possible to distinguish a ductile fracture and a yielding transition. We support the £ndings with available data and discuss the microstructure mechanism of the processes identi£ed. Presently we are implying modi£cations to our model to also include brittle fracture.

References

1. M. Mellema, J.H.J. van Opheusden and T. van Vliet, *J.Chem.Phys* **111**, 6129 (1999).
2. A.A. Rzepiela, J.H.J. van Opheusden and T. van Vliet, *J. Coll. Int. Sci.*, submitted.
3. L.E. Silbert and J.R. Melrose, *J. Rheol* **43**, 673 (1999).
4. A.A. Potanin and W.B. Russel, *Phys. Rev. E* **53**, 3702 (1995).
5. S.J. Zhou, P.S. Lomdahl, A.F. Voter, B.L. Holian, *Eng. Frac. Mech.* **61**, 173 (1998).

Chaotic ionization of non-classical alkali Rydberg states – computational physics beats experiment

Andreas Krug[1,2] **and Andreas Buchleitner**[1]

[1] *Max-Planck-Institute for Physics of Complex Systems, Nöthnitzer Str. 38, D-01187 Dresden*
[2] *Max-Planck-Institute for Quantum Optics, Hans-Kopfermann-Str. 1, D-85748 Garching*

phone (++49+351) 8712211, fax (++49+351) 8712299, e-mail abu@mpipks-dresden.mpg.de

Highly excited atoms (’Rydberg atoms’) exposed to strong electromagnetic £elds are experimentally accessible, perfect low-dimensional micro-laboratories which display fundamental phenomena of coherent quantum transport in disordered media (Anderson localization, conductance ¤uctuations), together with the characteristic “£ngerprints of chaos” of dynamical systems with a mixed regular-chaotic classical phase space structure (nondispersive wave-packets, scarred wave functions, chaos-assisted tunneling). However, due to the complexity of their spectral structure involving multiply degenerate continua and, possibly, quantum scattering off a multielectron core, these objects remained so far unaccessible to a rigourous theoretical/numerical treatment. As a matter of fact, the atomic ionization problem is characterized by a density of states which scales as n_0^5, $n_0 \simeq 30 \ldots 100$ the principal quantum number of the atomic initial state, and multiphoton processes of order $15 \ldots 120$. Consequently, an accurate numerical treatment without any essential approximation amounts to the diagonalization of a complex symmetric, banded generalized eigenvalue problem with a typical dimension of approx. 1000000, and a bandwidth around 6000. To determine the atomic ionization probability under external driving at given frequency and amplitude, approx. 5000 eigenvalues in the vicinity of the unperturbed energy of the initial atomic state have to be extracted.

Such requirements represent a formidable challenge for the most advanced computational techniques and facilities. Combinig group theoretical methods, R-matrix and Floquet theory, complex dilation of the Hamiltonian [1], and an intelligent, parallel implementation of the Lanczos algorithm with excellent scalability (with a Cholesky decomposition, the actual Lanczos iteration, and a matrix inversion as the fundamental building blocks), we recently succeeded to tackle this problem. Access to the currently largest, massively parallel supercomputer available in the academic realm, the Hitachi SR8000-F1 of the Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften, has been absolutely crucial for the realization of this project.

With our latest results, we now understand [2] the apparently enhanced ionization of non-hydrogenic alkali Rydberg states under periodic driving, as compared to Rydberg states of atomic hydrogen [3], an experimental observation which remained unexplained and questionable for more than one decade. This highlights the important role of computational physics for the understanding of complex quantum transport phenomena.

The talk will discuss basic aspects of the numerical treatment, and touch upon the abovementioned, longstanding puzzle of atomic ionization dynamics, in the light of a direct comparison between laboratory and numerical experiments.

References

1. A. Krug and A. Buchleitner, Europhys. Lett. **49**, 176 (2000)
2. A. Krug and A. Buchleitner, Phys. Rev. Lett. (2001), in print
3. Panming Fu et al., Phys. Rev. Lett. **64**, 511 (1990); M. Arndt et al., Phys. Rev. Lett. **67**, 2435 (1991); P. M. Koch and K. A. H. v. Leeuwen, Phys. Rep. **255**, 289 (1995)

Improving the Dirac operator in lattice QCD

Christof Gattringer[1] **and C. B. Lang**[2]

[1] *Inst. f. Theoret. Physik, Univ. Regensburg, Universitätsstr. 31, D-93053 Regensburg, Germany*

[2] *Inst. f. Theoret. Physik, Universität Graz, A-8010 Graz, AUSTRIA*

+43 (316) 380 5246, fax: +43 (316) 380 9820, christian.lang@uni-graz.at

Recently various new concepts for the construction of Dirac operators in lattice QCD have been introduced. A common property of these operators is that they – at least approximately – satisfy the so-called Ginsparg-Wilson condition (GWC)[1]. Such operators obey the Atiyah-Singer index theorem and violate chiral symmetry only in a modest and local form. In earlier work [2] we suggested a method to systematically expand the lattice Dirac operator in terms of simple lattice operators and to turn the GWC into a large algebraic system of coupled equations for the expansion coef£cients. The solution for a £nite parameterization leads to an approximate Ginsparg-Wilson operator.

Such an improved Dirac operator has been constructed in 2-d for the Schwinger model [3] and also for Quantum Chromodynamics in 4-d [4], where an analysis of its spectrum revealed intriguing properties.

One of the expected advantages is a better performance when used as a starting point for the determination of the overlap Dirac operator, which satis£es the GWC exactly, but is usually computationally extremely expensive. Here we present studies in 4-d for more realistic SU(3) gauge con£gurations with non-trivial topological content, including model con£gurations with instantons. We study the ¤ow of eigenvalues and we compare the numerical stability and ef£ciency of the improved operator with that of others in this respect.

References

1. P.H. Ginsparg and K.G. Wilson, Phys. Rev. D 25 (1982) 2649.
2. C. Gattringer, hep-lat/0003005.
3. C. Gattringer and I. Hip, Phys. Lett. B 480 (2000) 112.
4. C. Gattringer, I. Hip and C. B. Lang, hep-lat/0007042, Nucl. Phys. B in press.

Universal ¤uctuations of Dirac spectra in QCD

Steffen H. Meyer

Theoretische Physik, Fachbereich Physik, D-67663 Kaiserslautern, Germany

phone: 0049 631205 2272, fax: 0049 631205 3907, e-mail: smeyer@physik.uni-kl.de

Hadronic properties, such as the lightness of the pion masses and the absence of parity doublets in the meson sector, strongly indicate that chiral symmetry is broken spontaneously in QCD. A great deal of insight in such nonperturbative phenomena has been obtained from extensive lattice QCD simulations over the last two decades. But what is the particular physical mechanism in QCD which is responsible for chiral symmetry breaking is still a matter of strong debate.

Recently the view of the QCD vacuum as a strongly disordered system due to the non abelian gauge £elds has led to the conjecture [1], that chiral symmetry breaking is manifest in the universal distribution of the low lying eigenvalues of the lattice Dirac operator and therefore can be described by Random Matrix Models. This conjecture has £rst been con£rmed by lattice gauge theory simulations for quenched $SU(2)$ [2] and dynamical staggered fermions [2] and later for all different values of the Dyson symmetry index [3].

A very interesting question is whether the eigenfunctions of the corresponding eigenvalues of the lattice Dirac operator can be exponentially localized . This phenomenon is called Anderson localization for a metal-insulator transition when the disorder becomes suf£ciently strong. Therefore, if chiral symmerty is spontaneously broken, the eigenfunctions of the Dirac operator must be spatially extended. Indeed, our £rst results for quenched $SU(2)$ gauge theory with staggered fermions are in agreement with these expectations [4].

The calculation of the spectrum of the Dirac operator is performed on a CRAY T3E dividing the physical four dimensional lattice into non-overlapping sublattice of equal size. We use a k-step Arnoldi method for approximating the low lying eigenvalues and corresponding eigenvectors. For details of the performance and scalability measurements of the implementation see [5].

In conclusion, the high-statistics study of the eigenvalue spectrum of the lattice QCD Dirac operator with particular emphasis on the low- lying eigenvalues and eigenvectors provides strong evidence for Random Matrix universality. In addition, these results indicate a novel link to disordered systems in condensed matter physics.

References

1. E.V.Shuryak and J.J.M.Verbaarschot, Nucl.Phys. **A560**, 306 (1993)
2. M.E.Berbenni-Bitsch, S.Meyer, A.Schäfer, J.J.M. Verbaarschot, and T.Wettig, Phys.Rev.Lett.**80**,1146 (1998)
   M.E.Berbenni-Bitsch, S.Meyer, and T.Wettig, Phys.Rev. D **58**, 071502 (1999)
3. for a recent review, see J.J.M. Verbaarschot and T.Wettig, hep-ph/0003017, June 2000, to be published
4. M.E.Berbenni-Bitsch and S.Meyer, to be published
5. M.E.Berbenni-Bitsch and S.Meyer ,in High Performance Computing in Science and Engineering '99, E.Krause and W.Jäger (Eds.),Springer-Verlag.

Anisotropic scaling and generalized conformal invariance at Lifshitz points

Malte Henkel[1] **and Michel Pleimling**[1,2]

[1] *Laboratoire de Physique des Matériaux, Université Henri Poincaré Nancy I, B.P. 239, F – 54506 Vandœuvre lÆs Nancy Cedex, France*
[2] *Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, D – 91058 Erlangen, Germany*

phone +33 3 83 91 2725, fax +33 3 83 91 2083, henkel@lpm.u-nancy.fr

The modern understanding of critical phenomena is governed by the notion of scale invariance. We are interested in systems with strongly anisotropic critical points, where the value of the anisotropy exponent θ differs from unity. In these cases, the two-point function satis£es the scaling form

$$C(\vec{r}_\perp, r_\parallel) = r_\perp^{-2x}\, \Omega(r_\parallel r_\perp^{-\theta}) \tag{1}$$

where $r_\parallel$ and $\vec{r}_\perp$ are the distances parallel and perpendicular to a chosen axis, x is a scaling dimension, θ is the anisotropy exponent and $\Omega(v)$ is a scaling function. Scale invariance alone is not enough to determine the form of the function $\Omega(v)$. While dynamical scaling (1) occurs in critical dynamics or in true non-equilibrium phase transitions, it is also observed at strongly anisotropic equilibrium criticality as for example Lifshitz points encountered in systems with competing interactions. The simplest model for these is the ANNNI model [1].

A recently proposed generalization of conformal invariance involving local space-time-dependent scale transformations for anisotropy exponents $\theta = 2/N \neq 1$ [2] leads to a differential equation for $\Omega(v)$ which can be solved explicitly. In this contribution, the idea of local scale invariance is tested in the ANNNI model by checking the resulting expressions for $\Omega(v)$.

We present the numerical computation and thorough analysis of the critical spin-spin correlation function at the uniaxial Lifshitz point of the ANNNI model [3]. The data are obtained by simulating systems of anisotropic shape (taking into account the special £nite-size effects coming from the anisotropic scaling) with a newly developed variant of the Wolff cluster algorithm involving the ¤ipping of clusters containing spins of both signs and specially suited for the study of systems with competing interaction [3]. This enables us to simulate in the vicinity of the anisotropic critical point systems far larger than in previous studies. The location of the Lifshitz point is determined with a high precision. Much more reliable values for the Lifshitz point critical exponents are obtained than previously. Our estimations for the critical exponents are: $\alpha = 0.18(2)$, $\beta = 0.238(5)$ and $\gamma = 1.36(3)$. For the computation of the spin-spin correlation function we adapt a recently presented very ef£cient method [4] to systems with competing interactions. In the present study the scaling (1) is veri£ed for the £rst time.

A comparison of the numerically computed scaling function with the analytical expression for $\Omega(v)$ derived under the assumption of local scale invariance yields excellent agreement. The con£rmation of the applicability of local scale invariance to this situation suggests a new dynamical principle for the description of equilibrium systems with anisotropic scaling.

References

1. W. Selke, in *Phase Transitions and Critical Phenomena*, Vol.15, edited by C. Domb and J.L. Lebowitz (Academic Press, New York, 1992).
2. M. Henkel, Phys. Rev. Lett. **78**, 1940 (1997).
3. M. Pleimling and M. Henkel, submitted.
4. H. G. Evertz and W. von der Linden, cond-mat/0008072.

Distribution of instanton sizes in a simpli£ed instanton gas model

Gernot Münster and Christel Kamp

Institut für Theoretische Physik, Universität Münster, Wilhelm-Klemm-Str. 9, D-48149 Münster, Germany

Tel. 0251-8334911, Fax: 0251-8336328, munsteg@uni-muenster.de

In non-abelian gauge theories different topologically nontrivial con£gurations have been made responsible for non-perturbative features. An important class are instantons, which are solutions of the Euclidean £eld equations with non-vanishing topological charge. They give contributions to the saddle-point approximation of Euclidean functional integrals, which lead to non-perturbative effects. For a review see [1].

In recent years much effort has been devoted to lattice Monte Carlo calculations of properties of the instanton ensemble [2]. Of central importance is the distribution of instanton sizes, which is related to the infrared problem of nonperturbative instanton contributions.

In this work we investigate the distribution of instanton sizes in the framework of a simpli£ed model for ensembles of instantons. This model takes into account the non-diluteness of instantons. The infrared problem for the integration over instanton sizes is dealt with in a self-consistent manner by approximating instanton interactions by a repulsive hard core potential. This leads to a dynamical suppression of large instantons. The characteristic features of the instanton size distribution are studied by means of analytic and Monte Carlo methods. In one dimension exact results can be derived. In higher space-time dimensions we employed analytical approximations as well as Monte Carlo simulations. The numerical Monte Carlo calculations are done in the grand canonical ensemble. We have developped and implemented the appropriate algorithm and performed simulations for different sets of parameters.

In any dimension we £nd a power law behaviour for small sizes, consistent with the semi-classical results. At large instanton sizes the distribution decays exponentially. The results are compared with those from lattice simulations, e.g. [3]. The results indicate that our simpli£ed model reproduces the main features of instanton ensembles with a dynamical infrared cut-off.

References

1. T. Schäfer and E. Shuryak, Rev. Mod. Phys. 70 (1998) 323, hep-ph/9610451.
2. J.W. Negele, Nucl. Phys. Proc. Suppl. 73 (1999) 92, hep-lat/9810053.
3. Ph. de Forcrand, M. García Pérez and I.-O. Stamatescu, Nucl. Phys. B 499 (1997) 409, hep-lat/9701012.

The fractal dimension of the critical ¤uctuations in Abelian gauge theories

Joakim Hove, Sjur Mo, Asle Sudbø

Department of physics
Norwegian University of Science and Technology, N-7491 Trondheim, Norway
+47 73 59 36 37, +47 73 59 77 10, hove@phys.ntnu.no

The geometric properties of the critical ¤uctuations in abelian gauge theories such as the Ginzburg-Landau model are analyzed in zero background £eld. Using a dual description, we obtain scaling relations between exponents of geometric and thermodynamic nature. In particular we connect the anomalous scaling dimension η of the dual matter £eld to the Hausdorff dimension D_H of the critical ¤uctuations.

Anderson has proposed the breakdown of a generalized rigidity associated with proliferation of defect structures in an order parameter as a general feature of 2nd order phase transitions . In the context of three-dimensional super¤uids and extreme type-II superconductors, this has been demonstrated explicitly[1]. In this case the topological defects are closed loops of quantized vorticity, and this paper concerns their geometrical properties.

We will mainly concentrate on the £eld theory

$$H_\psi = m_\psi^2 \left|\psi\right|^2 + \frac{u_\psi}{2}\left|\psi\right|^4 + \left|\nabla\psi\right|^2, \tag{1}$$

i.e. a neutral $|\psi|^4$ theory. The critical ¤uctuations of this theory are closed vortex loops. These loops have long range interactions, and can be described by a *dual* £eld theory where the matter £eld ϕ is coupled to a gauge £eld $\mathbf{h}$ mediating long range interactions.

Hence by studying the vortex tangle from Eq. 1 we can also learn about the critical properties of the dual theory. In particular we have found a relation relating the *anomalous dimension* η_ϕ of the ϕ £eld to the *geometrical properties* of the vortex tangle. These can be summarized by the exponents Δ, α and η_ϕ. $\langle|\mathbf{x}-\mathbf{y}|^2\rangle \propto N^{2\Delta}$, $D(N) \propto N^{-\alpha}$ and $G(\mathbf{x},\mathbf{y}) = \sum_N P(\mathbf{x},\mathbf{y};N) \propto |\mathbf{x}-\mathbf{y}|^{2-d-\eta}$. For a non-interacting walker these exponents can be found analytially, $(\Delta,\alpha,\eta) = (1/2, 5/2, 0)$. For the interacting walker we can not £nd the exponents excatly, but by invoking a scaling form for the probability $P(\mathbf{x},\mathbf{y};N)$ we £nd the scaling relations

$$\eta_\phi + \frac{1}{\Delta} = 2, \qquad \frac{1}{\Delta} = \frac{d}{\alpha - 1}. \tag{2}$$

We have done MC simulations on the 3DXY model[2], which corresponds to the lattice version of Eq. 1 in the $|\psi| = C$ approximation. From the phase distribution of the matter £eld we can extract vortex loops, and determine the exponent α. We have found the numerical value $\alpha = 2.31$, corresponding to $\eta_\phi = -0.29$ and $\Delta^{-1} = D_H = 2.29$. The deviations from the Gaussian values indicate that the vortex tangle is self-seeking, i.e. it packs space more ef£ciently than a random walker. This has implications for the possibility of a £nite £eld transition.

References

1. A. K. Nguyen and A. Sudbø, Euro. Phys. Lett. **46**, 780 (1999); A. K. Nguyen and A. Sudbø, Phys. Rev. B **60**, 15307 (1999).
2. J. Hove and A. Sudbø, Phys. Rev. Lett. **84**, 3426 (2000), J. Hove, S. Mo and A. Sudbø, Phys. Rev. Lett. **85**, 2368 (2000).

Coupling molecular dynamics and continuum dynamics

G. Wagner[1,2], E.G. Flekkøy[2,3], J. Feder[2,3] and T. Jøssang[2,3]

[1] *Dept. of Physics, Technion Institute of Technology, 320000 Haifa, Israel*
[2] *Fracton as, Tåsenveien 74C, 0873 Oslo, Norway*
[3] *Dept. of Physics, University of Oslo, PB 1048 Blindern, 0316 Oslo, Norway*
Tel: +972 4 829 3546 *e-mail:* wagner@fractal.tau.ac.il

Molecular Dynamics (MD) is one of the most powerful methods to study the behavior of many-body systems on a microscopic scale. The limiting factor in such simulations is the immense computational effort that is required. MD simulations usually can cover only a short range in time and space. For this reason, MD can in general not be used to study dynamical processes that take place on macroscopic length scales.

Macroscopic processes must be described more ef£ciently by continuum equations – the underlying assumption being that the atomic character of matter is largely irrelevant on super-atomic length scales. There are, however, processes in which this assumption is known to be incorrect. For instance, in sliding friction the atomic interactions in a region of microscopic size (the surfaces in contact) conspire to forces that affect a sliding body on a macroscopic scale.

The obvious solution is to bring the two descriptions together in a seamless fashion. In such a hybrid simulation, most of the represented volume is represented by a continuum while a small region is represented using MD. The two domains are separated by an interface providing a coupling mechanism. Simulations of this sort have been successful in the context of solid crystals [1]. Simulations of a liquid state have so far been limited to highly symmetric setups [2] or steady-state scenarios [3].

We report on a new and general scheme to build such a coupling mechanism, based on a mutual and symmetric exchange of ¤ux densities – mass ¤ux, momentum ¤ux, and energy ¤ux – across the interface. The quantities associated with the ¤uxes are conserved by construction. The present work is a signi£cant extension of a coupling scheme presented earlier by some of us [4].

We consider two domains that are controlled by continuum dynamics (the compressible Navier-Stokes equations) and by particle dynamics (MD employing a Lennard-Jones potential), respectively. We measure the continuum mass ¤ux, momentum ¤ux, and energy ¤ux at the boundary of the continuum domain, and simultaneously average the complementary particle ¤ux quantities at the boundary of the particle domain. We then £nd the arithmetic mean of the pairs of ¤ux and impose the mean ¤ux as boundary conditions onto both the continuum domain and the particle domain.

In our contribution, the approach and some aspects of its implementation will be described, and we present some simple test applications.

References

1. F. Abraham, J. Broughton, N. Bernstein, and E. Kaxiras, Europhys. Lett. **44**, 783 (1998).
2. S. T. O'Connel and P. A. Thompson, Phys. Rev E **52**, 5792 (1995).
3. N. G. Hadjicostantinou and A. T. Patera, Int. J. Mod. Phys. C **8**, 967 (1997).
4. E. G. Flekkøy, G. Wagner, and J. Feder, Europhys. Lett. **52**, 271 (2000).

Determining the density of states for classical statistical models: A random walk algorithm to produce a ¤at histogram

David P. Landau and Fugao Wang

Center for Simulational Physics,
The University of Georgia, Athens, Georgia 30602, USA
1-706-542-2908(phone),1-706-542-2492(fax),
dlandau@hal.physast.uga.edu

We describe an ef£cient and general Monte Carlo algorithm using a random walk in energy space to obtain a very accurate estimate of the density of states for classical statistical models [1, 2]. The density of states is modi£ed at each step when the energy level is visited to produce a ¤at histogram. By carefully controlling the modi£cation factor, we allow the density of states to converge to the true value very quickly, even for large systems. From the density of states at the end of the random walk, we can estimate thermodynamic quantities such as internal energy and speci£c heat capacity by calculating canonical averages at essentially any temperature.

Using this method, we not only can avoid repeating simulations at multiple temperatures, but can also estimate the Gibbs free energy and entropy, quantities which are not directly accessible by conventional Monte Carlo simulations. This algorithm is especially useful for complex systems with a rough landscape since all possible energy levels are visited with the same probability. As with the multicanonical Monte Carlo technique [3], our method overcomes the tunneling barrier between coexisting phases at £rst-order phase transitions.

We apply our algorithm to both 1st and 2nd order phase transitions to demonstrate its ef£ciency and accuracy. We obtained direct simulational estimates for the density of states for two-dimensional ten-state Potts models on lattices up to 200×200 and Ising models on lattices up to 256×256. Our simulational results are compared to both exact solutions and existing numerical data obtained using other methods [3, 4]. Applying this approach to a 3D $\pm J$ spin glass model we estimate the internal energy and entropy at zero temperature; and, using a two-dimensional random walk in energy and order-parameter space, we obtain the (rough) canonical distribution and energy landscape in order-parameter space. Preliminary data suggest that the glass transition temperature is about 1.2 and that better estimates can be obtained with more extensive application of the method. This simulational method is not restricted to energy space and can be used to calculate the density of states for any parameter by a random walk in the corresponding space.

References

1. F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).
2. D. P. Landau and K. Binder, *A Guide to Monte Carlo Methods in Statistical Physics*, (Cambridge U. Press, Cambridge, 2000).
3. B. A. Berg and T. Neuhaus, Phys. Rev. Lett. **68**, 9 (1992).
4. J. S. Wang, T. K. Tay and R. H. Swendsen, Phys. Rev. Lett. **82**, 476 (1999).

A cluster Monte Carlo algorithm for 2-dimensional spin glasses

Jérôme Houdayer

Institut für Physik, Johannes Gutenberg Universität, D-55099 Mainz, Germany
phone: 00 49 6131 3923645, fax: 00 49 6131 3925441,
e-mail: jerome.houdayer@polytechnique.org

The understanding of Ising ferromagnets has been greatly enhanced by fast Monte Carlo (MC) simulations using cluster algorithms [1]. Unfortunately this technique cannot be directly applied to disordered models such as spin glasses (SG) because of frustration. Attempts have been made to generalise this method but the resulting algorithms are complicated and the speed increase not impressive. Other techniques such as exchange MC (EMC) (also called parallel tempering) allow big improvements over standard one-spin ¤ip MC and are widely used for SG. Nevertheless the sizes and temperatures accessible to simulations are still not enough to clearly solve many important issues (see [2] for a review on SG simulations).

We present a new cluster MC algorithm for 2-dimensional SG which is several orders of magnitude faster than previous MC techniques (namely EMC). It thus gives access to sizes and temperatures which were unreachable before. This new algorithm can treat any Ising spin system whatever the interactions and the magnetic £eld so long it is 2-dimensional with nearest neighbor interactions. Note that transfer matrix methods which are widely used for 2-dimensional systems are restrained to "small" sizes, usually no more than $16 \times \infty$ which appears not to be enough to answer certain questions. With our new tool we have studied the problem of the SG transition in the 2-dimensional $\pm J$ Edwards-Anderson (EA) model for which several questions are still unsettled. In particular the value of the critical temperature (zero or not) and the nature of the divergences (power laws or exponentials) are still debated.

Using this new algorithm we have simulated systems of size up to 100^2 down to temperature $T = 0.1$ (!). We present strong evidence that $T_c = 0$ and that the correlation length follows an exponential law: $\xi \sim e^{2\beta J}$, which is different from the standard lore (namely $\xi \sim T^{-\nu}$).

This work has already been submitted [3]. New results are expected to be obtained before the conference takes place (in particular concerning the 2-Dimensional SG with Gaussian couplings).

References

1. R. Swendsen and J.-S. Wang, *Phys. Rev. Lett.*, **58** (1987) p. 86.
2. E. Marinari, G. Parisi and J.J. Ruiz-Lorenzo,
   In A. P. Young ed. *Spin Glasses and Random Fields*, World Scienti£c, Singapore (1998).
3. J. Houdayer, *Submitted to Eur. Phys. Jour. B*, cond-mat/0101116.

Pattern formation and coherent structures in collective models from accelerator physics

Antonina N. Fedorova and Michael G. Zeitlin

Russian Academy of Sciences, Institute of Problems of Mechanical Engineering,
Mathematical Methods in Mechanics Group
V.O., Bolshoj pr., 61, 199178, St. Petersburg, Russia

tel: +7-812-3214776, fax: +7-812-3214771, E-mail: zeitlin@math.ipme.ru
http://www.ipme.ru/zeitlin.html, http://www.ipme.nw.ru/zeitlin.html

We consider the applications of a new numerical-analytical technique which is based on the methods of local nonlinear harmonic analysis or wavelet analysis to three nonlinear beam/accelerator physics problems which can be characterized by collective type behaviour: some forms of Vlasov-Maxwell-Poisson equations, RMS envelope dynamics, the model of beam-beam interactions. Such approach may be useful in all models in which it is possible and reasonable to reduce all complicated problems related with statistical distributions to the problems described by systems of nonlinear ordinary/partial differential equations with or without some (functional)constraints.

Wavelet analysis is a relatively novel set of mathematical methods, which gives us the possibility to work with well-localized bases in functional spaces and gives the maximum sparse forms for the general type of operators (differential, integral, pseudodifferential) in such bases. Our approach is based on the variational-wavelet approach from [1]-[3], which allows us to consider polynomial and rational type of nonlinearities.

The solutions are represented via the multiscale/multiresolution decomposition in nonlinear high-localized eigenmodes which correspond to the full multiresolution expansion in all underlying time/space scales (in the generalized space coordinates or phase space coordinates and time coordinate). We construct expansions into the slow part and fast oscillating parts. So, we may move from coarse scales of resolution to the £nest one for obtaining more detailed information about our dynamical process. The £rst terms correspond on the global level of function space decomposition to resolution space and the second ones to detail space. In this way we give contribution to our full solution from each scale of resolution or each time/space scale or from each nonlinear eigenmode. The same is correct for the contribution to power spectral density (energy spectrum): we can take into account contributions from each level/scale of resolution.

In contrast with different approaches we do not use perturbation technique or linearization procedures and represent dynamics via generalized nonlinear localized eigenmodes expansion. So, by using wavelet bases with their good (phase)space/time localization properties we can construct high-localized coherent structures in spatially-extended stochastic systems with collective behaviour.

In all these models numerical modelling demonstrates the appearence of coherent structures and stable pattern formations.

References

1. Variational Approach in Wavelet Framework to Polynomial Approximations of Nonlinear Accelerator Problems, American Institute of Physics , Conf. Proc., vol. 468, Nonlinear and Collective Phenomena in Beam Physics, pp. 48-68, 1999.
2. Variational-Wavelet Approach to RMS Envelope Equations, Proc. 2nd Advanced Accelerator Workshop on The Physics of High Brightness Beams pp.235–254, World Scienti£c, 2000
3. Localized Coherent Structures and Patterns Formation in Collective Models of Beam Motion, Quantum Aspects of Beam Physics, World Scienti£c,2001; Los Alamos preprint,physics/0101007.

Vlasov Poisson solver for density enhancement near ions at rest in magnetized electron plasmas

C. Heerlein and C. Toepffer

Institut für Theorietische Physik II, Universität Erlangen, Staudtstr. 7, 91058 Erlagen, Germany

Fon: +49(0)9131-8528459, Fax: +49(0)9131-8528907, e-mail: heerlein@theorie2.physik.uni-erlangen.de

Numerous experiments have recently investigated on ion-electron recombination in electron coolers, e.g. [1]. A common feature is an enhancement of the recombination rate with respect to the standard theory of recombination. So far this effect lacks a satisfactory theoretical explanation. Recent theoretical studies in the £eld concentrate on an examination of the density enhancement near the ion. This is a strongly nonlinear process, such that the standard Debye shielding is not applicable. Various simulations have been performed using molecular dynamics [2]. Due to statistical noise this faces serious problems in predicting densities close to the ion.

As under experimental conditions the plasma parameter is extremely small, collisions between electron are extremely rare. So the description of the Vlasov Poisson equation suits well reality. However the Vlasov Poisson problem is formulated in a six-dimensional phase space, and its vast volume inhibits a numerical solution on a complete phase space grid with an affordable amount of CPU power. But in comparison with test particles methods, e.g. particle-in-cell, a solution on the grid shows better scaling and less numerical noise for local observables such as the density. Further the noise of particle-in-cell simulations introduces arti£cial thermalization [3]. This problem is also circumvented by usage of a grid method. Hence our approach is to reduce the complexity of the Vlasov Poisson system by utilizing the cylindrical symmetry of the problem with respect to the direction of the magnetic £eld. This formally introduces coordinate singularities into the Vlasov Poisson equation, which however can be overcome by a characteristics method.

We have been able to construct a stable numerical method on the grid, which is applicable to arbitrarily large disturbances from equilibrium. The algorithm relies on a second order splitting scheme [4] jointly with third order interpolation. The Vlasov operator is split in two partial propagators. The £rst of which already contains the single particle orbits with the ionic and magnetic £eld, and the second adds the self consistent electric £eld obtained by Gauß's law. The method can be massively parallelized in angular momentum slices with high ef£ciency.

In a uniform electron plasma our calculation inserts an resting ion at time $t = 0$. For large radii, where the density enhancement is small, the results agree with the Debye screening of linear theory. Of primary interest is the region close to the ion, there our £rst calculations yield a strongly nonlinear density enhancement. A large fraction of this density enhancement stems from bound electrons, captured at $t = 0$. These electrons are not accounted for in standard recombination theory. This might provide a qualitative explanation for the observed recombination enhancements. A quantitative description, of course, requires a more realistic modeling of the initial conditions describing the merging of electron and ion beams.

References

1. O. Uwira, A. Müller, et al., Hyper£ne Interactions 108 (1997) 149
2. Q. Spreiter, C. Toepffer, Hyperf. Interac. 114 (1998) 245
3. P.-G. Reinhard, E. Suraud, Ann.Phys. 239 (1995) 193 and 216
4. C.Z. Cheng, G: Knorr, J.Comp.Phys. 22, 330 (1976)

Abstract withdrawn by the author

Modelling (001) surfaces of II-VI semiconductors

M. Ahr and M. Biehl

Institut für Theoretische Physik und Astrophysik,
Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Phone: +49 (0)931 888 4908 Fax: +49 (0)931 888 5141
E-mail: ahr@physik.uni-wuerzburg.de

We present a novel lattice-gas type model which reproduces the surface reconstructions and many other features of II-VI semiconductors in an MBE environment. We focus especially on (001) surfaces of CdTe [1]. Under vacuum conditions these surfaces are always metal terminated. At low temperatures, a $c(2\times2)$ reconstruction with coverages $\leq 1/2$ is observed, in which the Cd atoms arrange in a checkerboard like con£guration. A reordering occurs at a temperature of $\approx 300K$, above which a (2×1) ordering in rows dominates on a *sublimating* surface. Under a Te ¤ux, the surface is Te-terminated. For small ¤uxes, the Te coverage is ≈ 1 and the Te atoms dimerize.

We model the surface in *thermal equilibrium* by a two-dimensional array of Cd sites $\{n_{xy}\}$ which can be either occupied ($n_{xy}=1$) or empty ($n_{xy}=0$) [2]. The energy of the surface is represented by effective pairwise interactions of atoms. Electron counting rules forbid the simultaneous occupation of nearest neigbour (NN) sites in the $[1\overline{1}0]$ direction. There are couplings ϵ_x and ϵ_d between NN in $[110]$ direction and next nearest neighbours, respectively. These parameters are chosen in aggreement with recent DFT calculations [3], which have shown that the surface energy per site of a $c(2\times2)$ reconstrution is $\leq 0.03eV$ smaller than that of a (2×1) reconstruction. Investigation of this model by means of Monte-Carlo and Transfer Matrix techniques shows an order-disorder phase transition. At low temperature T, the system is in a $c(2\times2)$ phase with long range order, while at high T, it is in a *globally* disordered phase. However, the *local* environment of an atom is dominated by the (2×1) rows. This is consistent with the experimental observation of "small domains" in the (2×1) reconstruction. This model may be extended to include Te dimerization, which leads to a more complicated phase diagram.

The planar lattice gas can be extended to a model of a three-dimensional crystal [4]. Inside the bulk, there is an isotropic attraction between the particles and their NN. While there is no difference in the interactions of Te atoms between bulk and suface, Cd atoms on the surface interact via the anisotropic interactions ϵ_x, ϵ_d and a NN exclusion in $[1\overline{1}0]$ direction. A reasonable choice of parameters yields Cd terminated surfaces under vacuum. Monte Carlo simulation shows, that this model qualitatively reproduces many of the characteristic features of CdTe(001) which have been observed during sublimation and ALE: (a) On a sublimating surface the reordering of Cd atoms on the surface is qualitatively preserved. The *nonequilibrium* nature of sublimation even enhances the dominance of (2×1) ordering in the high temperature regime. (b) Exposure to a ¤ux of pure Cd leads to a re-appearance of the $c(2\times2)$ reconstruction at temeratures above the transition. Under a small Te ¤ux, the Cd coverage decreases and the remaining Cd atoms prefere the (2×1) ordering even at low temperatures. (c) Our model reproduces the experimental observation of ALE growth at a rate of ≈ 0.5 monolayers per cycle. An inclusion of Te dimerization in this model is currently under developement.

References

1. J. Cibert, S. Tatarenko. Defect and Diffusion Forum, **150-151** 1 (1997)
2. M. Biehl, M. Ahr, W. Kinzel, M. Sokolowski, T. Volkmann. Europhys. Lett. **53**(3), 169 (2000)
3. S. Gundel, A. Fleszar, W. Faschinger, W. Hanke. Phys. Rev. B **59**, 15261 (1999)
4. M. Ahr, M. Biehl, unpublished (cond-mat/0010133)

Monte Carlo simulations of Ge quantum dots on Si(100): stress £elds and intermixing

Ph. Sonnet[1] **and P. C. Kelires**[1,2]

[1] *Foundation for Research and Technology-Hellas (FORTH), P.O. Box 1527, 711 10 Heraclion, Crete, Greece*

[2] *Physics Department, University of Crete, P.O. Box 2208, 710 03 Heraclion, Crete, Greece*

(30)-81-394223, (30)-81-394201, kelires@physics.uoc.gr

Germanium quantum dots (QDs) on Si(100) surfaces are nanostructures of great fundamental and technological interest. They are promising candidates for optically active devices with strong photoemission signal [1]. Although intensively studied, both experimentally and theoretically, several issues about them remain unclear. For example, there is a signi£cant gap in our knowledge about the atomistic description of these nanostructures, especially regarding the stress £elds and the chemical composition pro£les within the islands. From the point of view of theory, this shows the dif£culty in simulational approaches to equilibrate compositionally inhomogeneous environments in semiconductors.

We present here a detailed theoretical atomistic description of Ge QDs on Si(100). We extract, for the £rst time, the stress £elds and the composition pro£les within the islands and at the interfacial regions. This is made possible by implementing a state-of-the-art Monte Carlo (MC) algorithm [2, 3] in the semigrand canonical ensemble. This MC algorithm allows for complete equilibration of the system, topological and compositional, at typical growth temperatures ($\sim$ 800 K). It is based on Ising-type identity ¤ips that are driven by the appropriate chemical potential difference. The success rate of these switches is enhanced by a ¤ip-relaxation technique [3]. The interatomic interactions are modeled using the well established empirical potentials of Tersoff for multicomponent systems [4]. We map the strain £elds by calculating the atomic level stresses [2], pertained to local incompatibilities and rigidity. Compositional equilibration is achieved also at the local level by calculating the average site occupancies over the statistical ensemble.

The local analysis of the stress £eld within the pure Ge islands, before any intermixing, shows that sites in the periphery and as approaching the top of the dot are under tensile stress, while sites in the interior and as approaching the wetting layer (the base) are under compressive stress. The wetting layer is under compressive stress, while the Si substrate layers below the dot are under tensile stress. These stress conditions drive interdiffusion (note that due to size Ge atoms prefer occupying sites under tension and vice versa for Si). We £nd that Ge atoms enrich the surface at the top and the periphery, while Si atoms intrude into the interior regions and the wetting layer. Outdiffusing Ge atoms enrich the area of the substrate below the dot. We £nd a limiting diffusion depth in the substrate of 8-10 monolayers. For this limit, we estimate a maximum Si fraction in the QD of $\sim$ 50%.

References

1. O.G. Schmidt, C. Lange, and K. Eberl, Appl. Phys. Lett. **75**, 1905 (1999).
2. P.C. Kelires and J. Tersoff, Phys. Rev. Lett. **63**, 1164 (1989).
3. P.C. Kelires, Phys. Rev. Lett. **75**, 1114 (1995).
4. J. Tersoff, Phys. Rev. B **39**, 5566 (1989).

Different types of scaling in epitaxial growth

L. Brendel[1], B. Hinnemann[1,2], H. Hinrichsen[1,3], A. Schindler[1], M. von den Driesch[1], F. Westerhoff[1], and D. E. Wolf[1]

[1] *Department of Physics, Gerhard-Mercator-University Duisburg, D-47048 Duisburg, Germany*
[2] *Department of Physics, Technical University of Denmark, DK - 2800 Lyngby, Denmark*
[3] *Fachbereich 8, Universität GH Wuppertal, D-42097 Wuppertal, Germany*
phone: +49 203 379 2816, e-mail: d.wolf@uni-duisburg.de

In epitaxial thin £lm or multilayer growth one is interested in growing some material on a substrate of a different material with a sharp interface. However, often the interfaces are not as sharp as one wants them in order to extract and investigate the new physical phenomena of heterostructures which may be the basis e.g. for future electronic devices. Reasons may be the roughness of the surface, which becomes the interface upon further growth, or interdiffusion. Numerous microscopic mechanisms have been proposed and investigated in this context, and in most of these models scaling laws were found. These results provide insight, which helps analyzing and improving the quality of thin £lm and multilayer growth.

The computational method we use are kinetic Monte Carlo simulations. For molecular beam epitaxy, the simulation parameters are the rates of thermally activated atomic processes at the growing surface and the deposition rate. Recently an alternative growth technique, pulsed laser deposition, has also attracted much interest. In this case the deposition rate is replaced by two parameters, the pulse intensity and frequency.

Recently we have investigated three new scaling phenomena in this context:

- Vertical exchange of adatoms and substrate atoms leads to a concentration pro£le, which decays like a power law with exponent -2 into the growing £lm. This implies a diverging width of the interdiffusion zone. For an exchange rate that is not in£nitely fast compared to the hopping rate of adatoms, as well as for £nite system size, the power law is exponentially cut off at a critical thickness of the growing £lm [1].
- In the widespread case, where layer-by-layer growth is spoiled by Ehrlich-Schwoebel barriers inhibiting interlayer transport of adatoms, strained layer growth may help. This prediction is based on the numerical results for the power law dependence of the critical £lm thickness on the growth parameters [2].
- We have shown that the island density on surfaces growing by pulsed laser deposition exhibits an unusual type of scaling as function of pulse intensity and deposition time. A data collapse is found for the ratios of the logarithms of these quantities, whereas conventional scaling as observed in molecular beam epitaxy involves ratios of powers [3].

References

1. M. von den Driesch, D. E. Wolf, *Interfacial mixing in heteroepitaxial growth*, preprint.
2. L. Brendel, A. Schindler, D. E. Wolf *Strain effects in layer-by-layer growth*, preprint.
3. B. Hinnemann, H. Hinrichsen, D. E. Wolf, *Unusual scaling for pulsed laser deposition*, preprint.

Molecular dynamics study of martensitic transformations in sintered Fe-Ni nano-particles

K. Kadau and P. Entel

Theoretische Tieftemperaturphysik Gerhard-Mercator-Universität Duisburg
Lotharstraße 1, 47048 Duisburg, Germany
+49-203-379-3331, +49-203-379-2965, kai@thp.uni-duisburg.de

Here we report on the £rst molecular dynamics simulations of martensitic transformations -i.e. structural transformations from fcc to bcc- in sintered Fe-Ni nano-particles. The atomic interactions were described by an embedded-atom method (EAM) potential specially designed to model the Fe-Ni system [1]. Simulations were carried out by applying a constant pressure and temperature ensemble (NPT-ensemble) [2] to 32 nano-particles each containing approx 1000 atoms. The nano-particles initially were placed with random crystallographic orientation on an fcc lattice such that the nano-particles attract each other. After relaxation for 150 ps at a temperature of 800 K and pressure of 0 GPa the pressure was increased in order to consolidate the sample. Subsequent cooling to lowest temperatures allow the study of the temperature induced martensitic transformation at pre-existing defects [3].

Fig. 1. Time evolution of thermal sintering of $Fe_{80}Ni_{20}$ nano-particles after 54 ps (left) and 90 ps (right). For clari£cation only a slice of about 0.5 nm of the system is shown, whereby Fe- and Ni-atoms are marked dark and bright, respectively.

References

1. R. Meyer and P. Entel, *Martensite-austenite transition and phonon dispersion curves of* $\mathrm{Fe}_{1-x}\mathrm{Ni}_x$ *studied by molecular-dynamics simulations*, Phys. Rev. B **57**, 5140 (1998).
2. D. C. Rapaport, *The Art of Molecular Dynamics Simulation*, Cambridge University Press., Cambridge 1995.
3. K. Kadau, P. Entel, T. C. Germann, P. S. Lomdahl, and B. L. Holian, *Large-scale molecular-dynamics study of the nucleation process of martensite in Fe-Ni alloys*, J. Phys. IV (Paris) (2001).

Abstract withdrawn by the author

First-principles molecular-dynamics simulations of the sticking of Ga and N gas-phase atoms on wurtzite GaN surfaces

Min-Hsiung Tsai

Department of Physics, National Sun Yat-sen University, Kaohsiung 804, Taiwan

886-7-525-3729,886-7-525-3709,tsai@mail.phys.nsysu.edu.tw

GaN is an important material of technological and fundamental interest. The £rst step to understand the growth mechanism of GaN thin £lms is to study the sticking of gas-phase Ga and N atoms on the GaN surfaces. We employ the £rst-principles molecular-dynamics (MD) simulation method to simulate the approach, migration and settlement of gas-phase Ga and N atoms on the GaN surfaces. The trajectories of the incoming Ga and N atoms will show how they move and where they settle on the surface. Their velocities as a function of time will provide information about energy transfer and kinetic energy evolution. The £rst-principles MD method used in this study originates from Sankey and Niklewski's multicenter MD method[1]. The current version calculates charge densities and corresponding potentials self-consistently[2]. Since the chemisorption energy has an order of 1eV, the incoming atom has a very high temperature when it reaches the surface. Without heat dissipation, the surface will be unrealistically heated up. To simulate heat dissipation within the repeated slab surface model, we take away part of the kinetic energies of substrate atoms transferred from the incoming atom according to the experimental thermal conductivity. We have considered two systems. The £rst system has Ga gas-phase atoms and a N-terminated $GaN(000\bar{1})$ surface. The second system has N gas-phase atoms and a monolayer Ga adlayer covered N-terminated $GaN(000\bar{1})$ surface. For the £rst system, we £nd that when the Ga gas-phase atom impinges the N-terminated $GaN(000\bar{1})$ surface from above the atop site, it recoils back into vacuum, despite the large Ga/N mass ratio. This property re¤ects that the N surface atom is strongly bonded [3]. When the incoming Ga atom impinges from above the bridge site, it moves towards and settles at the H_3 site. When it impinges from above the H_3 site, it moves down and settles at the H_3 site. The bridge- and H_3-site results suggest that the H_3 site is the chemisorption site for a low coverage Ga adlayer. For the second system, the incoming N atom recoils back into the vacuum, when it approaches the surface from above the atop site. When it impinges the surface from above the bridge site of two Ga adatoms, it migrates on the surface initially. When it arrives at a position above a surface N atom, it drops down through the Ga adlayer and combines with that N surface atom and a nearby Ga adatom. This property re¤ects a stronger N-N bond than the N-Ga bond and the multiple bonding nature of the N atom. This study is a £rst attempt to use £rst-principles MD simulations to understand the sticking of gas-phase Ga and N atoms on the GaN surfaces. We are able to elucidate some interesting properties of the movement incoming of Ga and N atoms as they approach and settle on the surface.

References

1. O. F. Sankey and D. J. Niklewski, Phys. Rev. B40, 3979 (1989).
2. M.-H. Tsai and K. C. Hass, Phys. Rev. B52, 16420 (1995).
3. M.-H. Tsai, O. F. Sankey, K. E. Schmidt, and I. S. T. Tsong, Phys. Rev. B, submitted.

How pearl-necklaces unwind

Christian Holm and Hans-Jörg Limbach

Max-Planck-Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany

Tel: 06131-238224, Fax: 06131-379100, Email: holm@mpip-mainz.mpg.de

We will present a detailed MD simulation study of polyelectrolytes in poor solvent where we take explicitly care of the counterions [1]. All charges interact via the full Coulomb interaction, and we employ a FFT accelerated version of the Ewald sum (P3M) for calculation of the electrostatics[2]. The number of chains varies between 5 and 15, with chain lengths between 100 and 400 monomers. For the longer chains we can observe up to £ve pearls. For our strongly charged polyelectrolytes we £nd a signi£cant portion of counterions close to the chains, already even below the Manning threshold, and much stronger than for the case of polyelectrolytes in good solvent. Around the Manning threshold we observe pearl-necklace structures[3], which have not a well de£ned pearl number. We £nd that these ¤uctuations are strongly coupled to the distribution of the counterions. These structures are, however, still stable even when condensed counterions are present. Upon increasing the electrostatic interactions further, we can reach the transition point, where theses necklaces become unstable and collapse into a single globule. Measurements of the osmotic coef£cient and of the structure factors are provided. The calculated form factors of the single chains show structural features hinting towards the necklace structure, which could be observable in experiments.

In a second stage of our investigations we start to apply an external force to a single chain. This in principle will lead to an unwinding of the pearl structures. However, we observe that the pearl number will £rst increase[4]. It is only at a later stage, that they start to unwind. This behavior is consistent with the discussion in the paper of Tamashiro and Schiessel (Macromolecules **33**, 5263, (2000)). We provide force-extension curves for several simulated systems, and discuss the strong in¤uence of the counterions on the sharpness of the unwinding transition. We also comment under which circumstances the recently predicted zick-zack curves of Tamashiro and Schiessel and Vilgis *et. al* (Eur. Phys. J E **2**, 289, 2000) should be observable.

In addition we will present some simulational video sequences to visually support our arguments.

References

1. U. Micka, C. Holm, and K. Kremer, Langmuir **15**, 4033 (1999).
2. M. Deserno, C. Holm, J. Chem. Phys.**109**, 7678 (1998); 7694 (1998).
3. H.J. Limbach, C. Holm, K. Kremer, in preparation.
4. H.J. Limbach, Ph.D. thesis, University of Mainz, May 2001.

Sequence design of AB-copolymers: Conformation-dependent scheme

V.A.Ivanov[1], **P.G.Khalatur**[2], **and A.R.Khokhlov**[1]

[1]*Physics Department, Moscow State University, Moscow 117234, Russia*
[2]*Department of Physical Chemistry, Tver State University, 170002 Tver, Russia*
+7 (095) 939-4756, +7 (095) 939-2988, ivanov@polly.phys.msu.su

We present our most recent results on the so-called conformation-dependent sequence design scheme for AB-copolymers proposed for a £rst time in [1]. The original idea was to prepare the primary structure of synthetic AB-copolymer chain (i.e. the sequence of monomer units of A- and B-types along the chain) using some particular spatial conformation of a homopolymer chain. It was most natural to take a globular conformation as such ”parent” conformation and use the criteria of being inside the dense core or at the globular surface to divide monomer units in two types. However, other dividing criteria [2] and other ”parent” conformation (i.e. a chain adsorbed on a plane surface [3]) were also considered. It was shown in [1, 2, 3] that such sequence design scheme leads to the effect of ”memorizing” of some important features of the ”parent” conformation.

Here we will present our recent £ndings on the statistics of sequences obtained by means of such design scheme. We have shown, both by exact analytical calculations and by computer simulation, that protein-like AB-copolymers obey the Levy-¤ight statistics [4].

We have performed the detailed study of stability against aggregation for AB-copolymers with designed ”protein-like” primary sequences. First, we report the computer simulation results for two copolymer chains brought in close contact with each other, and discuss the conditions at which they do not aggregate. Second, we consider a block-copolymer chain composed of two different AB-copolymers with designed sequences. Computer simulation was performed at such values of parameters when it is most favorable for both sequences to form a dense core covered by a loose shell. We discuss the conditions at which the globular conformation of block-copolymer chain will consist of only one common core or of two separate cores.

We report also our new results on computer simulation of several important modi£cations of originally proposed scheme, namely, we have introduced strongly associating monomer units (C-units) in the primary AB-sequence and studied their effect on conformational properties of copolymer globules. Another modi£cation is the ”double selection” scheme when we select only those sequences from all designed ”protein-like” ones that have the most fast collapse kinetics.

We acknowledge the £nancial support from INTAS, NATO and Russian Foundation for Basic Research.

References

1. A.R.Khokhlov, P.G.Khalatur, *Physica A* **249** (1998) 253; *Phys.Rev.Lett.* **82** (1999) 3456.
2. A.V.Chertovich, V.A.Ivanov, A.A.Lazutin, A.R.Khokhlov, *Macromol.Symp.* **160** (2000) 41.
3. E.A.Zheligovskaya, P.G.Khalatur, A.R.Khokhlov, *Phys.Rev.E* **59** (1999) 3071.
4. E.N.Govorun, V.A.Ivanov, A.R.Khokhlov, P.G.Khalatur, A.L.Borovinsky, A.Yu.Grosberg, submitted to *Phys.Rev.Lett.* (2001).

see I24

Excitons in conjugated polymers from £rst principles

J.-W. van der Horst[1], P.A. Bobbert[1], W.F. Pasveer[1], M.A.J. Michels[1], G. Brocks[2], and P.J. Kelly[2]

[1]*Dept. of Applied Physics, COBRA Research School, and Dutch Polymer Institute, P.O. Box 513, NL-5600 MB Eindhoven, The Netherlands*
[2]*Dept. of Applied Physics, Twente University, P.O. Box 217, NL-7500 AE Enschede, The Netherlands*
tel.: +31.40.2474352, fax: +31.40.2445253, P.A.Bobbert@tue.nl

Conjugated polymers are attracting a fast growing attention because of their fascinating opto-electronic behaviour. Despite intense research, many fundamental issues are not yet resolved, among which the magnitude of the exciton binding energy, very important for applications. Contradictory studies support a large ($\sim$ 1 eV or larger), medium ($\sim$ 0.5 eV), and small ($\sim$ 0.1 eV or smaller) binding energy. In this work we investigate the opto-electronic properties of these materials using three complementary *ab-initio* techniques: (a) density-functional theory to calculate ground state properties, (b) GW theory to calculate one-particle excitations, and (c) an *ab-initio* solution of the Bethe-Salpeter equation to calculate two-particle optical excitations, excitons. We consider three situations: (I) an isolated polymer chain, (II) a chain embedded in a dielectric medium, and (III) a polymer crystal.

Situation I leads to an optical gap in good agreement with experiment for the polymers poly-phenylene-vinylene (PPV)[1] and polythiophene (PT)[2], with rather large values for the exciton binding energies (0.9 eV and 1.85 eV, respectively). However, calculations for PT in situation II show that the optical gap of a polymer chain embedded in a dielectric medium, with dielectric properties derived from those of a single chain, is virtually the same as that of an isolated chain, whereas the exciton binding energy (0.76 eV for PT) is much reduced[2]. Bulk screening effects reduce both the quasiparticle band gap and the exciton binding energy, leaving the optical gap unchanged. The excitonic properties (spectra, radiative lifetimes, polarizabilities) obtained for situation II agree very well with experiment, either for bulk polymers[3], or dissolved polymers[4].

Situation III leads to small binding energies $\sim$ 0.1 eV, and to results that disagree with several experiments. The reduction of the binding energy compared to situation II is mainly caused by hybridization effects among the chains. We attribute the disagreement to the fact that in real samples polymer chains are more or less randomly packed, suppressing hybridization. Therefore, in most cases situation II describes reality better than situation III. An interesting exception occurs in ladder-type poly-para-phenylene (LPPP), which has very stiff chains and is expected to be more prone to crystal formation than other polymers. Recent STM experiments, in which the local quasiparticle band gap is measured, reveal regions with a relatively low ($\sim$ 0.1 eV) exciton binding energy and regions where it is much higher. One interpretation is that the former regions consist of crystalline aggregates, whereas in the latter regions random packing occurs. This sheds interesting light on the debate about the magnitude of exciton binding energies in conjugated polymers: this quantity may critically depend on sample preparation, and different binding energies may even coexist in one sample.

References

1. M. Rohl£ng and S.G. Louie, Phys. Rev. Lett. **82**, 1959 (1999).
2. J.-W. van der Horst, P.A. Bobbert, M.A.J. Michels, G. Brocks, and P.J. Kelly, Phys. Rev. Lett. **83**, 4413 (1999).
3. J.-W. van der Horst, P.A. Bobbert, M.A.J. Michels, H. Bässler, to be published in J. Chem. Phys. **114**, 2001.
4. J.-W. van der Horst, P.A. Bobbert, P.H.L. de Jong, M.A.J. Michels, L.D.A. Siebbeles, J.M. Warman, G. Gelinck, and G. Brocks, Chem. Phys. Lett. **334**, 303 (2001).

Electronic structure at a new level of complexity with parallel FLAPW

W.Mannstadt[1] A.Canning[2] and A.J.Freeman[3]

[1]*Fachbereich Physik und Zentrum fur Materialwissenschaften, Philipps University Marburg*
[2]*NERSC LBL, Berkeley*
[3]*Department of Physics, Northwestern University, Evanston*
wolfgang.mannstadt@physik.uni-marburg.de, phone:+49-6421-28-24138

Simulating real materials has become increasingly more important in understanding a variety of modern topics in solid state and surface physics as well as quantum chemistry. The increasing number of new experimental techniques, many of which can now probe the electronic structure, coupled with the development of an increasing variety of new materials with new properties has driven the need for a more accurate theoretical understanding at the atomic scale. This has led to the increased use of £rst principles methods where the quantum mechanical behavior of the electrons is explicitly treated. In materials science, density functional theory provides the modern theoretical framework for a tractable quantum mechanical treatment of the electrons and hence of those properties which allow the accurate simulation of new materials and their behavior, on the computer. Many of these technologically important new materials, such as nanostructures, and their associated properties require the study of systems of the order of hundreds of atoms or more, that is beyond the reach of £rst principles codes on a serial computer. The FLAPW method is widely accepted as one of the most accurate £rst principles electronic structure methods available today. With an increasing interest in more complex structures however, the large computational demands required by this highly precise method have limited its usage. Our newly developed massive parallel FLAPW code (P-FLAPW)[1] for £lm and bulk geometry allows to overcome these limitations. Complex surface structures, involving catalysis and growth processes and dilute impurities in semiconductors, to name a few, can now be treated at the highest level of accuracy using several hundred atoms in the unit cell. With this new methodology nanoscale physics is accessible from £rst principles treating all electrons with no shape approximation for the potential and charge density. We discuss the physics of dilute impurities in semiconductors such as Er doped Si with up to 256 atoms, todate. The location of the impurity states as well as the relaxation around the impurity is discussed as a function of the doping concentration. Furthermore we present recent results of hydrogen defects on hydrogen terminated Si surfaces and their in¤uence on the electronic properties of the surface. In particular we discuss the local electronic density of states (LDOS) relevant for NMR studies on such surfaces.

References

1. A. Canning,W. Mannstadt and A.J. Freeman, Comp. Phys. Comm. 130,(2000) 233

P-FLAPW: A large scale parallel all electron £rst principles code

A. Canning[1], **W. Mannstadt**[2] **and A.J. Freeman**[3]

[1]*NERSC, Lawrence Berkeley National Laboratory, Berkeley, CA94720.*
[2]*Fachbereich Physik, Philipps Universität Marburg, 35032 Marburg.*
[3]*Department of Physics and Astronomy, Northwestern University, Evanston, IL60208.*
tel: (510) 495 2962, FAX: (510) 486 5812, email: canning@nersc.gov

In the last ten years electronic structure calculations based on £rst-principles methods that treat the electrons quantum mechanically with no free parameters, have become an integral part of material science research. In the majority of computer centers around the world, £rst-principles codes have become the largest consumer of computer cycles. These £rst-principles methods are accurate enough to give good predictions for the properties of new materials while still being able to treat large enough systems to be of technological importance. This major advance in computational materials science has been due to both the development of new computationally ef£cient methods as well as more and more powerful computers. The FLAPW (full-potential linearized-augmented plane-wave) method [1, 2] is one of the most accurate and heavily used density functional theory based £rst-principles methods for determining electronic and magnetic properties of crystals and surfaces. In the past the FLAPW method has been limited to system sizes below about a hundred atoms due to the lack of an ef£cient parallel implementation to exploit the power and memory of parallel computers. This has greatly limited the materials/properties that can be studied with this method as many new materials such as nanostructures require the study of systems on larger length scales than is possible with serial codes. In this work we present a novel ef£cient parallelization of the FLAPW method based on division among the processors of the plane-wave components for each state. With our parallel code P-FLAPW, we can study systems an order of magnitude larger than was previously possible using parallel supercomputers such as the Cray T3E and IBM SP. To test the performance of the code we ran different sized systems of bulk silicon, with and without inversion symmetry and bulk palladium, with inversion symmetry. The FLAPW method is particularly well suited to studying transition metals. We have run bulk silicon systems on a Cray T3E and IBM SP on up to 512 processors for systems of 125 to 686 silicon atoms and bulk palladium of 128 to 343 atoms. The performance is extremely good with close to linear speed-up curves with increasing processor counts providing we do not try and run a small system on a large number of processors.

In conclusion with our new ef£cient parallel implementation of the FLAPW method, we can now study new materials and phenomena that were previously not accessible. Complicated surface structures, related to catalysis and growth processes as well as impurities in semiconductors, can now be accurately treated with large unit cells. This research used resources of the National Energy Research Scienti£c Computing Center, which is supported by the DOE Of£ce of Energy Research. Work at Northwestern supported by the NSF through its materials research center. We would like to thank the John von Neuman Institute für Computing at the Forschungszentrum, Jülich for giving us access to run on 512 processors. Some results present in this paper were previously published in [3]

References

1. E.Wimmer, H.Krakauer, M.Weinert, and A.J.Freeman, Phys. Rev. B **24,** 864 (1981), and references therein
2. M.Weinert, E.Wimmer, and A.J.Freeman, Phys. Rev. B **26,** 4571 **140,** A1133 (1965).
3. A.Canning, W.Mannstadt and A.J.Freeman, Comp. Phys. Comms. **130**, 233 (2000).

Monte Carlo calculations of the microstructure of solids and liquids

Klaus A. Gernoth
Department of Physics, UMIST, PO Box 88, Manchester M60 1QD, UK
+44 (0)161 200 3679, +44 (0)161 200 4303, K.A.Gernoth@umist.ac.uk

Path integral Monte Carlo (PIMC) techniques are amongst the most powerful computational methods for exact numerical calculations of macroscopic and microscopic statistical properties at £nite temperatures of a large variety of condensed matter systems of current theoretical and experimental interest. These include the liquid and solid phases of rare gas elements, adsorbed £lms, super¤uid helium, or polyethylene, to name just a few examples. Physical quantities that may be computed exactly by means of the PIMC approach and compared directly to experimental results, where available, include the kinetic, potential, and total energy, the (angle-averaged) radial distribution function, or neutron scattering cross sections.

In particular, inert gas solids and liquids have been and are being extensively investigated with Monte Carlo methods [1–3] and many of their properties have been researched also experimentally [2] and are well documented. However, in these Monte Carlo studies hardly any attention has ever been paid until recently to the many fascinating and perplexing details of point and space group symmetries in crystals and to breaking of these symmetries in the liquid-solid phase transition. Here we focus on exact Fourier path integral Monte Carlo (FPIMC) calculations of the local one-body density and of the *full* two-body density of noble gas crystals [3] and on symmetry-breaking in these microscopic quantities in FPIMC simulations of spontaneous crystallization.

The numerical FPIMC calculations [3] are carried out by employing the formal results of a thorough mathematical analysis of point and space group symmetries in the one- and two-body densities. The quantities that are computed by means of the exact group-theoretical FPIMC method [3] are related to the scattering cross sections that can be measured in neutron scattering and X-ray diffraction experiments. Numerical results are presented for solid natural argon in the hexagonal close-packed (hcp) structure at the experimental triple point temperature of argon. The experimental signi£cance of this particular system is pointed out. The exact group-theoretical FPIMC approach is further employed in studies of point and space group symmetry-breaking in the liquid-solid phase transition. Numerical results on symmetry-breaking in the one-body density and in the *full* two-body density obtained in an FPIMC simulation of solidi£cation of liquid natural argon are presented.

The group-theoretical FPIMC method has the potential of opening novel avenues of analyzing the structure of materials and of casting a new light on symmetry-breaking in phase transitions. The computational and formal techniques of the group-theoretical FPIMC approach presented here might turn out to become valuable also for other theories and computational methods, such as, for example, the theoretical treatment of phase transitions in liquid crystals, electronic structure calculations, molecular dynamics computations [4] of the spatial microstructure of crystals, or computer simulations of adsorbed solid and liquid £lms and of their phase transitions.

References

1. A. Cuccoli et al., *Phys. Rev. B* **47** (1993), 14923.
2. D. N. Timms at al., *J. Phys.: Condens. Matter* **8** (1996), 6665.
3. K. A. Gernoth, *Ann. Phys. (N.Y.)* **285** (2000), 61–137.
4. M. P. Allen and D. J. Tildesley, “Computer Simulation of Liquids,” Clarendon Press, Oxford, 1987.

A domain partition approach to parallel adaptive simulation of dynamic threshold voltage MOSFET

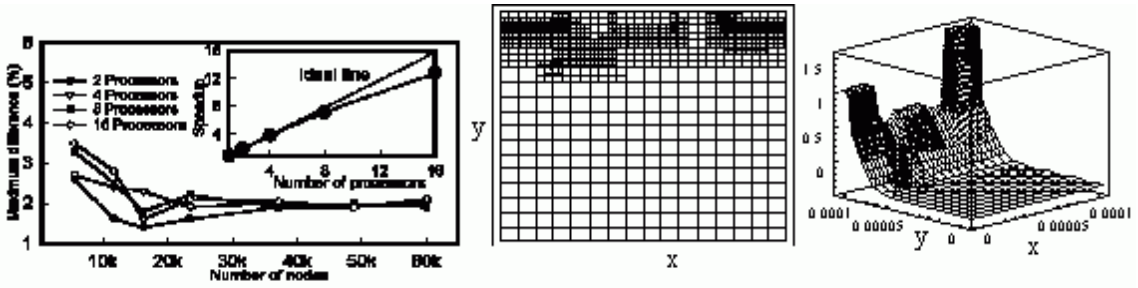
Yiming Li[1], **Tien-Sheng Chao**[2], **and S. M. Sze**[1]

[1] *Institute of Electronics, National Chiao Tung University, Hsinchu, Taiwan*
[2] *National Nano Device Laboratories, Hsinchu, Taiwan*
Corresponding address: P.O. Box 25-178, Hsincu 300, Taiwan
Email: ymli.ee87g@nctu.edu.tw and Tel. 886-930-330766

Computer-aided simulation of semiconductor device and physics provides the capability for a software-driven approach to explore new physics and devices. In recent years, a novel device structure so called dynamic threshold voltage MOSFET (DTMOS) has been studied for an alternative way to improve the conventional submicron MOSFETs I-V characteristics at ultra low supply voltage applications [1]. Experimental fabrication and measurement has illustrated primarily that the DTMOS scheme appears to be very promising for future low-power and high-speed circuit applications [1]. Some theoretical studies for this new device have been of great interests [2] with simpli£ed compact or conventional MOSFET numerical modeling approaches.

In this paper, a new parallel adaptive semiconductor device simulation using the dynamic load balancing approach is presented and successfully applied to fast simulate and study the physical characteristics of DTMOS. The developed simulator based on adaptive £nite volume (FV), dynamic domain decomposition, posteriori error estimation, and monotone iterative (MI) methods has been developed and implemented on a 16-processors Linux-cluster with message passing interface (MPI) library. Hydrodynamic DTMOS partial differential equations are discretized £rstly with FV method and hence a large-scale system of nonlinear algebraic equations is obtained. The nonlinear algebraic system is then solved with the MI method [3, 4]. A physical based unstructured mesh re£nement rule with posteriori error estimation has also been developed for the quality control of computed results. Due to the robust features of the method, such as global convergence and parallel algorithm, the proposed parallel domain decomposition algorithm reduces signi£cantly the execution time up to an order of magnitude.

The right two Figs. show an adaptive re£nement mesh and computed electrostatic potential for a DTMOS at $V_D = 1.5V$ and $V_G = 1V$. Furthermore, the left Fig. demonstrates the parallel speedup and loand balancing on a 16-processors Linux-cluster with MPI. In a short conclusion, a domain partition approach to parallel adaptive simulation of DTMOS device has been presented. Achieved adaptive re£nement, parallel performance and comparison with the measured data are tested to show the computational ef£ciency and accuracy of the method.



References

1. S. J. Chang, C. Y. Chang, et al., IEEE Trans. Elec. Dev. **47** 2379 (2000).
2. F. Assaderaghi, D. Sinitsky, et al., IEEE Trans. Elec. Dev. **44** 414 (2000).
3. Y. Li, et al., Prof. IEEE VLSI-TSA, 27, (1999).
4. N. Mastorakis, Recent Advances in Applied and Theoretical Mathematics, World Scienti£c, (2000).

Computer simulation of radiation effect on the electronic properties of carbon nanotubes

Yu.I. Prylutskyy[1] **and M.V. Makarets**[2]

Department of [1] *Biophysics and* [2] *Physics,*
Kyiv National Shevchenko University,
Volodymyrska Str., 64, 01033 Kyiv, Ukraine
+380 44 266 22 76, 252 08 27, prylut@biocc.univ.kiev.ua

The advance of high technologies involves creation of materials and devices with new properties. The effective method for this creation is radiation of matter by particles. As known, the most effect of the particle beam technology has been achieved in the microelectronics. Now this technology is intensively investigated with the purpose of creating and modi£cation the different nanostuctures [1].

Single-walled carbon nanotubes (SWCNT) demonstrate unique physical properties [2]: a diameter-dependent character of conductivity (semiconducting or metallic); a high mechanical strength; an ultimate ¤exibility; a unique capacity for hydrogen storage; a high ef£ciency of a low-£eld electron emission. Due to these properties the SWCNT are very promising for applications in nanoelectronics, nanomechanics and in vacuum electronics (as a cathode material for ¤at panel displays). At present time, in the literature the in¤uence of the particle radiation on the structure and electronic properties of SWCNT are not currently known, and this problem is very important for nanotechnology.

In present work we have carried out the following researches using the molecular dynamics and quantum chemistry tight-binding and semi-empirical PM3 methods [3]:
1. Theoretical modelling of structure of SWCNT under radiation (electron, heavy-ions and γ-beams).
2. Theoretical and computer modelling of spatial distributions of: a) projectiles and energy losses; b) electronic excitations and ionization of carbon atoms; c) radiation defects and kind of theirs.
3. Theoretical study of the electronic spectra and the density of states calculations for the SWCNT under radiation.

As a result the threshold energy for knock-on damage to the SWCNT has been estimated. It was found that the presence of pentagon-heptagon pairs as the local radiation defects in the geometrical structure of SWCNT leads to the formation of the heterojunction. The possible mechanisms of interaction of low- and high-energy particle beams with SWCNT were analyzed in detail.

References

1. D. Fink, and R. Klett. Braz. J.Phys. 25, 54 (1995).
2. R. Saito, G. Dresselhaus, and M.S. Dresselhaus. Physical Properties of Carbon Nanotubes (Imperial College Press, Singapore, 1998).
3. Yu.I. Prylutskyy, S.S. Durov, O.V. Ogloblya, E.V. Buzaneva, and P. Scharff. Comput.Mat.Sci. 17, 352 (2000).

A new ab-initio approach for the calculation of NMR chemical shifts in periodic systems

Daniel Sebastiani[1] **and Michele Parrinello**[2]

[1]*Max-Planck-Institute for polymer research, Ackermannweg 10, D-55128 Mainz, Germany, email: sebastia@mpip-mainz.mpg.de*
[2]*Max-Planck-Institute for solid state research, Heisenbergstraße 1, D-70569 Stuttgart, Germany, email: prr@prr.mpi-stuttgart.mpg.de*

Nuclear magnetic resonance (NMR) properties, in particular NMR chemical shifts, can provide important insight into the physics and chemistry of microscopic systems. Coordination numbers, bonding distances and other structural information can be extracted from measured resonance lines and attributed to individual atoms. Due to this ability, NMR spectroscopy has become one of the most widespread analysis tools in structural chemistry.

Many empirical rules exist to relate chemical shifts to conformational properties, but they are unable to take into account any but the simplest quantum effects involved in the problem. Since several decades, many methods for computing NMR lines have been developed in quantum chemistry, but they are all restricted to isolated systems in the gas phase. A £rst generalization to extended systems has been developed only a few years ago by F. Mauri et. al. [1]. They showed that nuclear magnetic resonance lines can also be calculated under periodic boundary conditions. However, the approach is computationally relatively expensive and involves the numerical evaluation of a differentiation.

In this paper, an alternative approach [2] is presented which avoids some of the drawbacks of the Mauri method. The new approach is computationally more ef£cient, in particular for large disordered systems. The formalism is based on Kohn-Sham density-functional theory [3] and exploits the exponentially decaying nature of localized Wannier orbitals. It is implemented in a plane-wave pseudopotential scheme and can be applied to crystalline and amorphous insulators under periodic boundary conditions, as well as to isolated molecules.

The performance of the new method is demonstrated on a series of test systems, as well as by several applications on larger organic systems, such as polymers. In combination with Car-Parrinello molecular dynamics [4], it allows an ef£cient sampling of the phase space of complex systems at £nite temperature. This statistical average is crucial for a realistic calculation of the NMR spectrum as soon as the considered system evolves dynamically.

The results are in good agreement with experiment and with calculations that use other theoretical methods.

References

1. F. Mauri, B. Pfrommer and S. Louie, *Phys.Rev.Lett.* **77**, 5300 (1996)
2. D. Sebastiani and M. Parrinello, *J.Phys.Chem.A*, accepted for publication (2001)
3. P. Hohenberg and W. Kohn, *Phys.Rev.* **136**, B 864, (1964); W. Kohn and L.J. Sham, *Phys.Rev.* **140**, A1133, (1965)
4. R. Car and M. Parrinello, *Phys.Rev.Lett.* **55**, 2471 (1985)

On the parallelization of molecular dynamics codes

G.P. Trabado, O. Plata and E.L. Zapata

Dept. Computer Architecture, University of Málaga, Spain

{*guille,oscar,ezapata*}*@ac.uma.es*

Codes simulating large particle systems present a high degree of spatial data locality and a signi£cant amount of independent computations. However, current parallelization strategies are based on manual restructuring of sequential programs and the introduction of communications speci£c for the problem structure [1]. Other solutions reside on the design of libraries intended for solving data distribution and communication in the parallelization of short-range molecular dynamics (MD) codes, although they are mostly oriented to the design of new code [2]. In this paper we propose a new methodology which reduces manual intervention in the parallelization of existing short-range MD sequential codes. Our method extends the programming language to allow programmers to express the data parallelism of the problem, so that the compiler is in charge of code restructuring and insertion of communication support. We also provide an ef£cient design of the runtime support for parallelization.

Short-range MD codes usually apply optimizations like the link-cell and the neighbor lists (Verlet lists) methods to reduce computational cost. These methods increase the algorithmic complexity of the program (indirection arrays updated periodically), dif£culting greatly its parallelization. Code restructuring usually requires full rewriting of the program as those computational structures (link-cell, Verlet lists) do not allow clean partitioning in well-de£ned computational domains. However, this fact contradicts the high spatial locality that the problem exhibits. An automatic alternative to code restructuring is the inspector-executor approach, but with a high penalty in the analysis time and in the size of the control data structures [3].

Our approach takes advantage of the knowledge about the problem nature to minimize the parallelization costs but with minimal changes to the original sequential program [4]. First, problem data is distributed across processors using a value-based irregular decomposition. Each processor analyzes locally assigned data and a communication schedule is generated. This schedule only contains that data which is likely to be used in the neighboring domains. As each processor is able to generate its schedule based only on local data, only a one-way communication stage is required (minimizing synchronization between processors). The distribution of computations involves replication of a small percentage of operations, avoiding a subsequent communication stage to propagate results to other processors.

As a result of our research, we have designed a runtime support with optimal methods to help in the parallelization of MD sequential codes. We have also proposed extensions to HPF to express data parallelism in MD applications, as well as compilation techniques to automatically generate ef£cient parallel code. Finally, we have applied our semi-automatic method to real MD applications (based on the Lennard-Jones potential) obtaining similar performance than using manual restructuring.

We conclude that it is possible to guide the compiler to parallelize complex scienti£c applications (MD simulations), with a performance similar to the best manually parallelized codes.

References

1. S. Plimpton, J. Comp. Phys., 117, 1-19, March 1995.
2. S.G.Srinivasam, et.al., Comp. Phys. Comm., 102, 28-43, 1997.
3. R. Ponnusamy, et.al., IEEE Trans. Par. Distr. Proc., 6 (8), 815-831, Aug. 1995.
4. G.P. Trabado, et.al., 10th Work. Lang. Comp. Par. Comp. (LCPC'97), 218-234, Aug. 1997.

Expanded ensemble Monte Carlo method for free energy calculations

P.N.Vorontsov-Velyaminov[1] **and A. P. Lyubartsev**[2]

[1] *Faculty of physics, St.Petersburg State University, 198504, St.Petersburg, Russia*
[2] *Division of Physical Chemistry, ArrheniusLaboratory, University of Stockholm, S-10691, Stockholm, Sweden*
voron.wgroup@pobox.spbu.ru

Calculation of the free energy in computer simulations is generally a substantially more dif£cult computational problem than calculation of structural properties. On the other hand, knowledge of the free energy and related thermodynamical properties is extremely important for understanding of many processes and phenomena in physics, chemistry and biology. Almost ten years ago the authors of this report suggested an approach called the expanded ensemble MC method [1] which soon has proven to be very ef£cient and precise in computing free energies. In this report we shall review the basis of the method, its most important applications and facilities. We shall try also to trace the relationship of this method to relevant approaches developed by other simulation groups.

The partition function of the expanded ensemble is composed as a sum of partition functions of canonical ensembles with an additional (expansion) parameter. This parameter can be either temperature or volume or a degree of insertion of a new molecule, or any other parameter of the Hamiltonian. The Monte Carlo simulation scheme in the expanded ensemble consists of two kinds of steps – usual particle shifts and changes of the expansion parameter. The distribution over the expansion parameter provides us free energy differences between the subsystems. In order to make this distribution as close to homogeneous as possible additional (balancing) factors are determined in a certain preliminary procedure. The method can be easily generalized for the case of constant-pressure (NPT) ensemble for calculations of the Gibbs free energy. It has been also implemented within the molecular dynamics simulations.

The expanded ensemble method has been applied for calculation of free energies in a model electrolyte system, a system of Lennard-Jones particles, water, ionic solutions with explicit water molecules. During last years several applications to compute solvation free energies of relatively large organic molecules in water have been reported. Also, the method has been applied to computations of chemical potential in model polymer systems.

Besides the free energy computation, the expanded ensemble method turned out to be a very ef£cient way to treat the 'multiple minima', or 'metastable states' problem. In this connection, attempts to use the expanded ensemble method in 'protein folding' problem have been made.

The method is promising in treatment of systems at high density, low temperature, with rough multiminima potential landscape, in presence of complicated molecular components.

References

1. A. P. Lyubartsev, A. A. Martsinovski, S. V. Shevkunov, and P. N. Vorontsov-Velyaminov, J.Chem.Phys., **96**, 1776 (1992)

CFD simulations of turbulent reactive ¤ows with supercomputing for hydrogen safety

W. Rehm[1] **W. Jahn**[1] **R. Vogelsang**[2] **B. L. Wang**[1]

[1] *Forschungszentrum Jülich, ISR1, D-52425 Jülich, Germany*
[2] *Silicon Graphics (SGI), c/o Forschungszentrum Jülich, ZAM, D-52425 Jülich, Germany*

+49 2461-61-6032, +49 2461-61-8250, w.rehm@fz-juelich.de

Generally, £re- and explosion protection is an important safety issue in most of the engineering areas. For instance, the prediction of hydrogen explosion loads in safety enclosures under severe accident conditions is relevant for nuclear reactor containments and hydrogen demonstration plants with fuel cells or hydrogen driven vehicles. Contextually, special veri£cation tests of reactive £eld codes and validation tests of calculations have been performed for speci£c reacting ¤ows in complex geometries. The turbulent combustion modes considered are related to de¤agration, transition (DDT), and detonation in explosive hydrogen-air mixtures. Hereby, experimental and numerical results were compared on integral- and laboratory scales, obtaining a high temporal and spatial resolution of complex ¤ows in the numerical simulations. Therefore, a modern £eld code cluster (MFCC) was established with new versions of the reactive Navier-Stokes/Euler ¤ow solver codes: AIXCO, CFX, COM for fast ¤ames (de¤agrations) and DET, IFSAS, SHOCKIN for rapid ¤ames (detonations), including vector- and parallel processing capabilities. For benchmark calculations, most of these codes have been ported successfully to the heterogeneous CRAY-J90/T90/T3E supercomputer complex at FZ-Jülich, running in the sequential, moderate parallel or massively parallel mode with promising performances and good speedup factors[1].

As a result, the reduction of the computing time per allocated processor allows appropriate mesh re£nement with unstructured or adaptive grids and robust algebraic multi-grid solvers together with higher order turbulence- and combustion models of multi-¤uids and multi-reactions. Consequently, we have provided RANS/VLES/LES/DNS ¤ow solver algorithms in combination with the ¤amelet concept (FC), the eddy dissipation model (EDM) or probability density functions (PDF). In the scope of joint research project activities funded by HGF-Bonn and EC-Brussels, massively parallel processing (MPP) software systems (e.g. AIXCO and CFX-5) have been developed on the CRAY-T3E with maximum number of 512 processor nodes (600 MHz) for high-performance supercomputing (HPSC), based on domain decomposition with message passing tools, using MPI and PVM or HPF routines. Hence, we use multi-block un/structured pre-processing (PATRAN/BUILD) as well as online post-processing (AVS/FIELDVIEW) with meta-supercomputing clusters for huge computer resources, solving the input/output bottleneck of large computing domains within practicable computing times. In summary, the applied computational ¤uid dynamics (ACFD) with supercomputing makes it possible to explore the scienti£c/technical aspects of £re- and explosion protection in more detail for realistic safety enclosures of nuclear and conventional energy systems, especially for the hydrogen safety behaviour.

References

1. R. Klein, W. Rehm: Models and Criteria for Prediction of De¤agration-to-Detonation Transition (DDT) in Hydrogen-Air-Steam Systems under Severe Accident Conditions, in Energy Technology, Volume 9, Forschungszentrum Jülich.

A nonlinear wave dynamical model for two-phase ¤ows and its numerical solutions

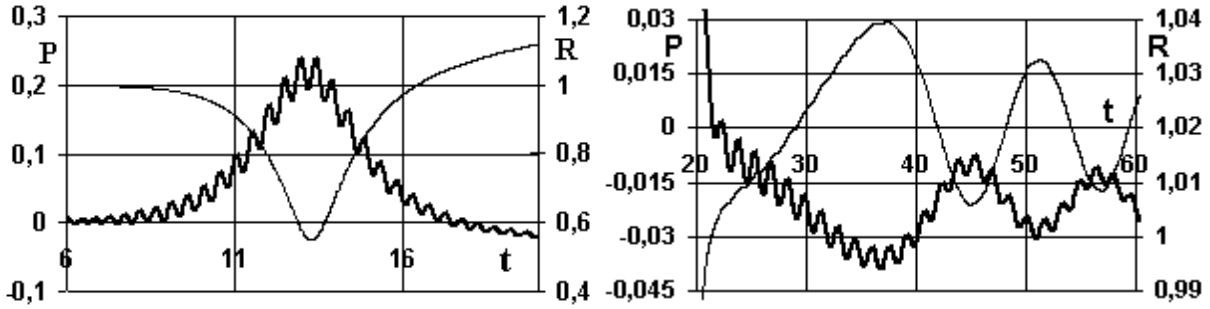
Din Cher Kim

High Informatics College of Novosibirsk State University,
35 Russkaya St., Novosibirsk 630058, Russia
Tel. (3832)344467, fax (3832)343783, dckim@dat.ict.nsc.ru

The clari£cation of the models for bubbly liquids remains one of the elusive goals of mechanics heterogeneous media. Consistent experimental veri£cation of theoretical models has not been forthcoming, owing, on the one hand, to the mathematical dif£culties of dealing with highly nonlinear equations of bubbly ¤ow, posing challenges to the numerical algorithms, and, on the other hand, experiments are also dif£cult to perform. In this connection a new approach has been put forward, called ”a nonlinear wave dynamical model for liquid containing gas bubbles,” and new accurate numerical technique has been developed to retrieve the main real features of the two-phase ¤ow from direct numerical modeling [1]. The large variety of existing models which might be relevant to bubbly ¤ows naturally raises the need for some criterion to distinguish the most adequate among them. We demonstrate that, in contrast with what was previously believed, these well-known models are not in Lagrangian frame. At closer look at these models reveals that they are the particular case of our model.

Two main equations in the computer program are the generalized Lighthill inhomogeneous wave equation and complete bubble dynamics equation. Based on the numerical technique, that is a combination of a £nite difference method for the PDE and a fourth-order Runge-Kutta scheme for the high nonlinear ODE, various numerical experiments have been carried out. We discover a fundamentally new kind of solitary wave called ”an oscillatory soliton” and asymmetry pulse body transforming into a train of spatial solitary waves. The nature of solitary wave oscillations, solitary wave with oscillatory structure, solitary-wave tail, positive wave packet, and other wave dynamical phenomena in bubbly liquid are clari£ed. This model has been successfully applied to describe pressure transients in a tube conveying two-phase ¤ows. We reveal novel oscillatory water-hammer with £ne structure, the effect of closing time for water-hammer, radiation of high-harmonic precursor, and other effects for the £rst time.

There is very reason to expect that the oscillatory soliton found here will also occur in two and three dimensions. Similar the oscillatory solitons are to be expected in general for other physical and mechanical problems. The proposed model is easily amenable to parallel programming.



The oscillatory soliton (left) and subharmonic generation at the solitary-wave tail (right).

References

1. Kim, D., Nonlinear Exactly Solvable Wave Dynamical Model for Liquid Containing Gas Bubbles, in *15th International Symposium on Nonlinear Acoustics*, Gottingen, Germany, 1-4 September 1999, pp. 493-496.

Small scale statistics of turbulence at high Reynolds numbers by massive computation

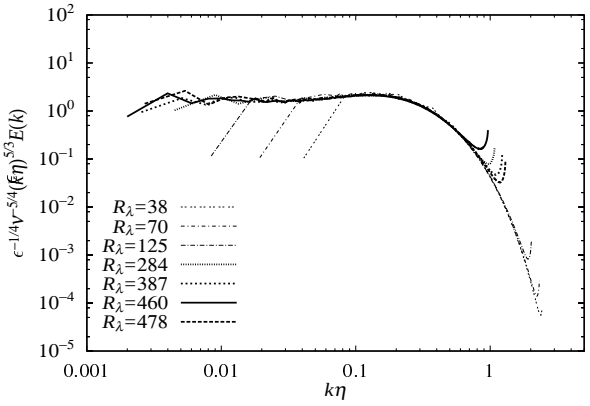
Toshiyuki Gotoh

Nagoya Institute of Technology, Gokiso, Showa-ku, Nagoya 466-8555, Japan
Tel: +81-52-735-5377, Fax: +81-52-735-5401, e-mail: gotoh@system.nitech.ac.jp

Direct numerical simulation (DNS) of turbulence, a simulation without any models of motions with scales below grid size, provides us a powerful tool to study the turbulence. It can compute any quantities without deformation of the £eld and provides us a lot of image of the £eld, from which we can understand how the turbulent £eld behaves. However, range of scales resolved in DNS of the turbulent ¤ow has been limited, and the Reynolds number of the turbulence has not been large enough to study the inertial range where the universal statistical laws for the turbulence is expected.

We have performed a series of DNS of steady homogeneous turbulences of three dimensional incompressible ¤uid with very high resolution up to $N = 1024^3$.[3] Range of the Taylor microscale Reynolds number is between 38 and 460. Navier-Stokes equation was integrated in the wavevector space in terms of 4th order Runge-Kutta-Gill method. Convolution sum for the nonlinear term was done by using pseudo spectral method. Computations were performed using a Fujitsu VPP700E vector parallel machine with 16 processors at RIKEN, and a Fujitsu VPP5000/56 with 32 processors at the Nagoya University Computation Center. FFT has been developed for the machines and core memoy requires more than 128GB. It took more than 500 hours for computations for the highest Reynolds numbers.

For the £rst time, the inertial rnage energy spectrum $E(k) = K\epsilon^{2/3}k^{-5/3}$ has been clearly observed and compared with the experimental data. It is found that the universal constant K is 1.65 ± 0.05, very close to the experimental value, $K = 1.62 \pm 0.17$.[2] Also Kolmogorov's $4/5$ law, $\left\langle \delta u_r^3 \right\rangle = -4/5\epsilon r$, the only exact result in the turbulence theory, where $\delta u_r = u(x+r) - u(x)$ is the longitudinal velocity difference, has been examined. The scaling exponents ζ_p of $\langle \delta u_r^p \rangle \propto r^{\zeta_p}$ were computed directly between about $60\eta \sim 5\lambda$ and 500η, where η is the dissipation length and λ is Taylor's microscale. They are anomalous re¤ecting the intermittency of the turbulence, and consistent with the experimental data. More is obtained for the probability density functions for velocity differences. To author's knowledge, these are the £rst DNS data in the inertial range and provide us new feature of the inertial and dissipation ranges.



Scaled energy spectra, $\epsilon^{-1/4}\nu^{-5/4}(k\eta)^{5/3}E(k)$. The inertial range is $0.007 \leq k\eta \leq 0.04$ and $K = 1.65 \pm 0.05$.

References

1. A. S. Monin and A. M. Yaglom, *Statistical Fluid Mechanics* (MIT, Cambridge, MA 1975) Vol. 2.
2. K. R. Sreenivasan, Phys. Fluids. **7**, 2778 (1995).
3. T. Gotoh and D. Fukayama, Submitted to Phys. Rev. Lett. (2000).

Study of the distribution functions in minimal model market

A. Chakraborti, S. Pradhan and B. K. Chakrabarti

Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Calcutta-700064.

Tel:091-33-3375345,fax:091-33-3374637,e-mail:anirban@cmp.saha.ernet.in

An economic market is a commonly encountered self-organising system or network, whose dynamics profoundly affects us all. Its dynamics is no doubt very intriguing. In statistical physics models of interacting systems, self-organisation [1] has been seen to emerge in the global aspects of the system which consists of a large number of simple dynamical elements having local interactions and dynamics, as also observed by Adam Smith (1776) in the market consisting of sel£sh agents. Economists noted that dynamics, which takes the system to equilibrium, is greatly facilitated by 'paper money' (rather than the direct commodity exchanges as in barter economy) which does not have any value of its own, but can be considered as a good 'lubricant' [2, 3]. Also, when the (paper) money supply gets changed, it does not just scale up (for increased money supply) or down (for decreased money supply) the commodity prices, the (self-organising) dynamics towards equilibrium gets seriously affected.

We have studied here numerically the steady state distributions $P(m)$ and $P(q)$ of money and commodity in a model consisting of £xed number of agents N, total commodity Q and total money M in the market. Only one commodity is considered for trade and its price is taken to be £xed (at unity) and it does not change with the money supply in the market. The subsistence commodity level q_0 of all the agents is the same and each of them would like to purchase the de£cit amount $(q_0 - q_i)$ from the agents having $q_i > q_0$, in exchange of its own money. Apart from the basic urge to reach the subsistence level, all the agents would like to maximize their money. The second instinct allows the agents with excess commodity (over q_0) to £nd hungry partners and to sell-off the excess. The dynamics considered here is the short time (or daily) dynamics. Additionally, we consider a long time (or yearly) dynamics, which reshuf¤es mildly but randomly the amounts of money and commodity of each agent. We de£ne $g = q_0/ < q >$ and $< q > = Q/N$. The resulting distributions follow from the successive applications of the local directed dynamics, followed by a randomization in the quantities. We consider two cases: unfrustrated case ($g < 1$) where in principle every agent can be satis£ed, and frustrated case ($g > 1$) where not all can be satis£ed. We concentrate on the quantity $P(q_0)$ which gives the steady density of agents in the market who can satisfy the basic requirement of commodity (q_0). It is most signi£cant in the frustrated cases where there is not enough commodity in the market to satisfy the basic requirements for everyone. It grows and the distribution of commodity among the agents is facilitated, with the supply of money M in the market. We see that $P(q_0) = g$ for $g < 1$ and $P(q_0) \simeq g\exp(-g)/(g - 1 + \exp(-g))$ for $g > 1$, where the money supply M is much greater than M_0, the optimal money required in the market. The analytic expressions for the distributions ($P(q_0)$ in particular) were obtained using simple formalisms of statistical physics and agree well with the numerical results obtained. The above observations are quite interesting when compared in the context of kinetic theory of gases [4]. Also, we do not observe any critical (singular) behaviour in the distribution functions, although self-organisation obviously occurs.

References

1. P. Bak, *How Nature Works: The Science of Self-Organised Criticality*, Springer, New York (1996)
2. A. Chakraborti and B. K. Chakrabarti, *Eur. Phys. J. B*, **17**, 167-170 (2000); A. Chakraborti, S. Pradhan and B. K. Chakrabarti, *cond-mat/0012405.*
3. P. A. Samuelson, *Economics*, 16th Edition, McGraw-Hill Inc., Auckland, 29-32 (1998).
4. L. D. Landau and E. M. Lifshitz, *Statistical Physics*, Butterworth-Heinemann, Oxford, 79-82 (1998).

Are hierarchical Weierstrass walks present on a stock market?

R. Kutner

Institute of Exper. Physics, Warsaw University, Hoża 69, Pl-00681 Warsaw, Poland
phone/fax:+004822 8536980, e-mail address: erka@fuw.edu.pl

In this work we give arguments that the hierarchical Weierstrass walks model (HWWM) is able to describe stochastic aspects of high-frequency empirical stock market data regarding, e.g., price changes of £nancial indexes such as S&P 500 index or Xerox stock one traded in the New York Stock Exchange [1]. The formalism of the model was introduced in our initial paper [2] together with the Monte Carlo algorithm based on toss, analogously as in "Petersburgh paradox" which is able to numerically study individual time evolution of a given index measured at different time horizons as well as different moments, correlation functions and different types of statistics. The HWWM is in principle a version of a continuous-time random walk (CTRW) with waiting-time distribution (WTD) de£ned by the hierarchical superposition of local conditional propability densities for a single increment in £nancial space and trading time. Such a form of WTD leads to results which, with good approximation, agree with Mandelbrot hipotesis [3] of stochastic self-similarity in the time evolution of the stock indexes. For example, it is possible to reproduce, with controlled accuracy, the non-Gaussian scaling and leptokurtic property of £nancial empirical data. Of course, the HWWM reproduces, among others, Lévy walks which seems to be more proper than Lévy ¤ights, since an increment of any stock price has £nite velocity and it is not instantaneous. Moreover, it exhibits a coupling between £nancial space variables and the trading time, which seems to be an important feature of £nancial empirical data; the simpli£ed, separable hierarchical models were reviewed in ref. [4]. Thanks to HWWM we were able to prepare a two-dimensional "phase diagram", based on the analysis of the second moments (of the individual and summarized increments), which classi£es all types of the diffusion of stock market index from sub-, through normal, super-, ballistic, hyper-, to Richardson diffusion and £nally the Lévy walks. Concluding, we suppose that the possibility of construction the hierarchical Weierstrass walks model is essentially based on a spontaneous hierarchical grouping of investors on a stock market according to the magnitude of invested capital. It is relatively easy to extend our model to include a persistent, constant trend (drift) were £nancial empirical data really to exhibit such phenomena.

References

1. R. N. Mantegna and H. E. Stanley, *An Introduction to Econophysics. Correlations and Complexity in Finance* (Cambridge Univ. Press, New York 2000).
2. R. Kutner and M. Regulski, Physica A **264** (1999) 107.
3. B. B. Mandelbrot, *Fractals and Scaling in Finance* (Springer-Verlag, New York 1997).
4. W. Paul and J. Baschnagel, *Stochastic Processes. From Physics to Finance* (Springer-Verlag, Berlin 1999).

Modelling traf£c ¤ow for a single-lane urban roundabout

Ruili Wang and Heather J. Ruskin

School of Computer Applications, Dublin City University, Dublin 9, Ireland.

Tel: 353-1-700-5513, Fax: 353-1-700-5442, e-mail: hruskin@compapp.dcu.ie

Traf£c ¤ow at a single-lane roundabout in an urban network is modelled using cellular automata. Roundabouts without traf£c lights are controlled through driver self-organisation and by the offside priority rule, (by which a vehicle entering gives way to one already on the roundabout). Three aspects of roundabout performance in particular have been studied. The £rst, looks at overall throughput, (the number of vehicles, which navigate the roundabout in a given time), for different geometries, arrival and turning rates. The second investigates changes in queue-length, delay-time and vehicle density for an individual road. The third considers the impact of driver choices on throughput and operation of the roundabout.

The roundabout is modelled as a ring of n cells, where each cell may be either occupied or vacant, with deterministic update rule. Before driving onto the roundabout, vehicles are randomly assigned turning directions, with speci£ed probabilities. Car arrivals are random with arrival rates, (the probability that a car arrives at an entrance in a given time step), in the range 0.05 to 0.95. The geometry of the roundabout is also varied to include from three to £ve entry/exit roads and two different sizes, *n = 16* and *32* cells respectively.

Throughput does not appear to depend on roundabout size or road-spacing, given similar topology, (number of entry/exit roads), and other parameters held constant. However, different throughput levels are observed when the topology is changed. Clearly, the entrances are bottlenecks in terms of smooth operation.

In general, throughput increases with arrival rate and reaches a maximum when the arrival rate reaches a critical value on one or more roads. Critical arrival rates for all roads depend on roundabout topology and direction of travel when leaving the roundabout. The throughput decreases as right-turning rate increases, (for cars driving on the left). The queue-length of an individual road rapidly achieves maximum as its arrival rate is increased, with critical arrival rate again dependent on topology and the arrival rates at other entry points. Over 10,000 time steps, the maximum queue-length or saturation of a given entry road was observed to occur within a few hundred time steps for arrival rates > 0.45 on the given road. The delay for any car seeking entry onto the roundabout was found to depend not only on the queue-length but also on factors, such as driver opportunity. Queue formation also occurred at car densities lower than the maximum density for free ¤ow, quoted in earlier work.

Driver behaviour at roundabout entrances was randomly categorised as *rational*, (when optimum conditions of entry are realised), *tardy* and *radical*, with speci£ed probabilities. Rational behaviour leads to free-¤ow on the roundabout for all arrival/turning rates considered, whereas radical decisions lead rapidly to roundabout congestion and tardy decisions to decrease in throughput and increase in queue-lengths. Assigned probabilities are clearly subjective and would bene£t from calibration on real data, but equally are unlikely to be standard for real traf£c systems.

References

1. Chopard, B., Dupuis, A., and Luthi, P., (1998) Traf£c and Granular Flow'97, World Scienti£c, pp. 153-168.
2. Hyden, C. and Varhelyi, A., (2000) Accident Analysis Prevention 32, pp. 11-23.
3. Yakawa, S., Kikuchi M and Tadaki, S., (1994) J. Phys. Soc. Jpn., 63, No. 10, pp. 3609-3618.

Molecular dynamics simulation of the nanoparticles transfer in gases and liquids

Rudyak V.Ya. and Belkin A.A. and Kharlamov G.V.

Novosibirsk State University of Civil Engineering, Leningradskaya, 113, 630008, Novosibirsk, Russia

(3832)668014, fax: (3832)161107, rudyak@ngasu.nsk.su

The numerical simulation of transfer processes of the nanoparticles (the particles with the sizes are of the order of $10 \div 10^2$ nm) in dense gases and liquids is the aim of present paper. The evolution of hard spheres heterogeneous system consisting of the homogeneous molecular system of hard spheres with radius r and mass m in which the dispersed particle with radius R and mass M dip into is investigated. We will use the molecular dynamics method. The mass ratio is equal to $M/m = 10^{-2} \div 300$. In our calculations the ratio of molecule and particle radii is equal to $R/r = 2 \div 4$. We used from 2 until 10 thousand molecules. The velocity autocorrelation functions, the pair equilibrium correlation function, the pressure dependance on concentration of the dispersed particles were analyzed. The diffusion coef£cient and viscosity of considered media were calculated.

In particular we will discuss two obtained results. The £rst one is the investigation of small dispersed particle in¤uence on liquid-solid phase transition. It was shown that the character of the phase transition change essentially if a large dispersed particle is immersed into homogeneous liquid. In this case the phase transition takes place at higher densities and pressures. Moreover, the pressure of the mixture is less then one-phases one with the same density α in liquid state and more then one-phase system pressure in solid state. The phase transition in heterogeneous system has geometrical nature as in homogeneous one and therefore the variation of the characteristic value of the phase transition density is easily explained by the screening effect.

The second result is connected with the calculation of the nanoparticle autocorrelation velocity function. The calculations showed, that in liquids and very dense gas the dependence of the autocorrelation velocity function of heavy ($M > 5m$) smooth particles is well approximated by the sum of two exponents with different relaxation times

$$\psi_{vv} = a_1 \exp(-t/\tau_1) + a_2 \exp(-t/\tau_2). \quad (1)$$

Equation (1) show, that nanoparticle velocity relaxation is characterized by two mechanisms (as a minimum). From our viewpoint, the £rst is connected with interactions of a particle with separate molecules and small group of molecules. Another mechanism is connected with the particle interaction with carrier medium micro¤uctuations. It is important, that the second branch of the autocorrelation velocity function for nanoparticle is exponential and is greatly different from power dependence, which is characteristic of one component system of hard spheres. If the carrier density is reduced, the difference between relaxation times τ_1 and τ_2 is also reduced, and the autocorrelation function was described by the exponential curve for suf£ciently small densities.

The same results were obtained, when benzol and freon-12 diffusion in hydrogen environment with pressure $8 \div 29 \;\; MPa$ was calculated. The last part of the paper was devoted with calculation of the nanoparticles diffusion coef£cients. Then calculated values is compared with the experimental data.

This work was supported by the Russian Foundation for Basic Researches (grants No. 00-15-96164).

The wonderful world of granular ratchets

D. C. Rapaport

Physics Department, Bar-Ilan University, Ramat-Gan 52900, Israel

tel: +972-3-5318048, fax: +972-3-5353298, e-mail: rapaport@mail.biu.ac.il

Granular media embody properties of solids, liquids and gases, but studies of the granular state continue to produce surprising results that are unique to this class of matter. Computer modeling is important, due to the fact that once the ability to reproduce experiment has been demonstrated it can be used to explore the mechanisms involved. A recently reported example of unusual behavior in granular matter involves a granular layer that is vibrated vertically by a base whose surface pro£le consists of sawtooth-like grooves. Experiment [1] reveals the occurrence of horizontal ¤ow whose direction and magnitude depend on the parameters of the system in an apparently complex manner. Detailed simulations of this phenomenon [2] demonstrate that the induced ¤ow rate actually varies with height within the granular layer and, even more surprisingly, that oppositely directed ¤ows can exist simultaneously at different levels.

A combination of this phenomenon and the familiar effect of vertical size segregation under vibration [3] suggests an entirely new mechanism for separating the components of a granular mixture according to particle size. If the upper and lower layers of the material move horizontally in opposite directions, and the larger particles climb towards the top of the layer, then some degree of horizontal separation of large and small particles will result. Simulations [4] reveal that this behavior actually occurs, and that a high degree of segregation can be achieved.

The computations employ the same models used in previous work [5], with interparticle interactions that account for grain shape, inelastic collisions and friction. The simulations allow a detailed examination of the dependence of horizontal ¤ow velocity on the height within the granular layer. Near the base the behavior is dominated by ratcheting, in which the grains tend to climb up the shallow tooth edge; on the other hand, tooth asymmetry affects the upper levels in the opposite fashion, with the grains being tossed in the reverse direction. Simulations involving a bimodal distribution of particle sizes clearly demonstrate the novel horizontal segregation effect in both two and three dimensions; separation occurs even when the particle sizes do not differ greatly, suggesting a fairly sensitive mechanism.

On a more general level, while the familiar role of computer simulation as applied to granular media is in attempting to reproduce experimental behavior, here the process has been reversed and simulation has identi£ed a previously unknown granular ¤ow phenomenon. It remains to be seen whether real granular matter obeys these predictions; if this is the case, then since separation is an important component in the processing of bulk granular materials such an approach could be of industrial value.

References

1. Z. Farkas, *et al*, Phys. Rev. E **60** (1999) 7022.
2. M. Levanon, D. C. Rapaport, (2000, submitted).
3. A. D. Rosato, *et al*, Phys. Rev. Lett. **249** (1987) 1038.
4. D. C. Rapaport, (2001, submitted).
5. D. Hirshfeld, D. C. Rapaport, Phys. Rev. E **56** (1997) 2012.

Friction between Si tip and (001)-2×1 surface: a molecular dynamics simulation

C. Jun[1,2] **and J.-S. Wang**[2]

[1] *Singapore-MIT Alliance and Department of Computational Science, National University of Singapore, Singapore 119260, Republic of Singapore*
[2] *Department of Physics, Beijing Normal University, Beijing 100875, China*
Tel:65-8746880, Fax:65-7746756, Email:wangjs@cz3.nus.edu.sg

A dynamical interaction between a tip and a substrate involves cohesion, wear, adhesion, friction, diffusion, and etc. It is closely related to an indentation process and an interfacial phenomenon in nano-material science. It has been widely explored both theoretically and experimentally[1, 2]. However, in the recently theoretical works there exists an obvious weakness, i.e., due to the limitation of computer resources the speed the tip advances over substrate is required to be greater than 1.0 m/s.[2]. In the experiments, the velocity is only at the range from $\mu m/s$ to mm/s[1, 2]. The experimental and the simulation velocities are quite different from each other. For this reason, we may question the conclusions from those simulations. In order to investigate this problem, as an example, we simulate the interaction of a Si tip and its (001)-2 $\times$ 1 surface by molecular dynamics method. Our aim is to present a new and reasonable method to describe the friction phenomenon of nano-materials theoretically.

In the simulations, the computational cell consists of a Si tip and a Si substrate. The Si tip is placed over the Si substrate. Periodic boundary conditions are used in the two dimensions parallel to the surface plane. In the third dimension, £xed boundary conditions are established by static atoms in the bottommost layers of substrate and the topmost layers of the tip. The positions of the static atoms are £xed at their bulk lattice sites. In this work two methods are used. In the £rst method, the static atoms of the tip are displaced in the direction of sliding each MD time step and the dynamic atoms are relaxed simultaneously. This is a traditional method and has been widely used in the study of a tip-substrate system.[2]. In the second method, the tip is £xed over the substrate while its dynamic atoms are relaxed for 1000 time steps. Then the static atoms of the tip advance 0.05 Å) along the direction of sliding. The process is repeated. For all of the simulations, the temperature of dynamic atoms is controlled by Hoover dymamics equation[3]. Before the simulations are performed for the system by the MD, a conjugate gradient method has been used to relax the tip and the substrate of the system, respectively. In all of the cases we simulate a constant height scan of a tip over a substrate.

It is found that if the tip and the substrate approach each other closely enough, for the two schemes a wear occurs under slip-stick way, but their details are quite different from each other. We present a detailed explanation for this phenomenon and conclude that different from the £rst method, at large mean velocity (several m/s) the tip moves, the second method may be used to simulate a quasi-equalibrium process. In experiments, the tip and the substrate interact on each other in a quasi-equalibrium process. Thus the second scheme is more appropriate for the description of experimental situations. In additions, we £nd that the friction properties of nano-materials are related to a sliding direction.

References

1. see, for example, S. Nasuno, A. Kudrolli, and J. P. Gollub, Phys. Rev. Lett. **57**, 949(1997)
2. see, for example, T. Cagin, J. Che, M. N. Gardos, A. Fijany, and W. Goddard, Nonotechnology, **10**, 278(1999)
3. W. G. Hoover, in "Simulation of Molecular Dynamics", (Verlet-Spring, 1986)

A numerical study of the 10 states Potts glass

Claudio Brangian[1] **Walter Kob**[2] **and Kurt Binder**[1]

[1] *Institut für Physik, Johannes Gutenberg Universität, Staudinger Weg 7, D-55099 Mainz, Germany*

[2] *Laboratoire des Verres, cc69, Université Montpellier II, 34095 Montpellier Cedex 05, France*

e-mail: Claudio.Brangian@Uni-Mainz.DE

A complete understanding of the glass transition of a ¤uid and what structural features really distinguish the solid glass from the liquid from which it was formed, are still challenging problems. While some researchers attribute glassy freezing to the (hypothetical) vanishing of the con£gurational entropy at the "Kauzmann temperature", which is lower than the experimental glass transition temperature, others emphasize the dynamical transition at the critical temperature of mode coupling-theory from the ergodic ¤uid to a non ergodic state.

A class of disordered spin models has been found which exhibit a uni£ed scenario and has a lot in common with the structural glass phenomenology [1]. One of these models is the p-state in£nite range Potts glass with $p > 4$, which presents both, a dynamical phase transition, and a static one at a lower temperature. In this model every spins interacts with all the others, irrespective of distance. Interactions are taken from a Gaussian distribution. It is well established that one has both a dynamical transition where the relaxation time of the spin-spin autocorrelation function diverges at a temperature T_D and a static transition at a lower temperature T_0 where a glass order parameter appears discontinuously, and both the internal energy and the entropy as functions of temperature present a kink.

In order to understand better the behavior of the model for £nite number of spins and the approach to the thermodynamic limit, we have performed extensive Monte Carlo simulations of the $p = 10$ Potts glass. Comparing results for system sizes $N = 160, 320, 640, 1280$ and 2560 at temperatures above the dynamical transition temperature T_D, the extrapolation of dynamic properties to the thermodynamic limit is studied for this model, and a dynamical £nite size scaling behavior near T_D is proposed [2]. For the two smallest system sizes, also the behavior in the spin glass phase down to a temperature $T = 0.7$ ($\approx 60\%$ of the transition temperature) is obtained. Well-equilibrated con£gurations are obtained with the parallel tempering method [3, 4], which is also useful for properly establishing static properties, such as the order parameter distribution function $P(q)$. The autocorrelation function at low T exhibits a two-step decay, and a scaling behavior typical of supercooled liquids, the time-temperature superposition principle, is observed. The parallel tempering method helped us giving access to a low-temperature region otherwise not accessible with standard single-spin ¤ip Monte Carlo moves.

References

1. A review can be found in: T.R. Kirkpatrick and D. Thirumalai, Transp. Theory Stat. Phys. **24**, 927 (1995).
2. C. Brangian, W. Kob, and K. Binder, Europhys. Lett., in press (2001); preprint cond-mat/0009475.
3. K. Hukushima and K. Nemoto, J. Phys. Soc. Jpn. **65**, 1604 (1996).
4. W. Kob, C. Brangian, T. Stühn, and R. Yamamoto, in *Computer Simulation Studies in Condensed Matter Physics* XIII, eds. D.P. Landau, S.P. Lewis and H.B. Schüttler, Springer, 2000.

Simulation of electron-electron scattering in semiconductor devices by the local iterative Monte Carlo technique

Jürgen Jakumeit

Institute for Algorithm and Scienti£c Computing (SCAI),
GMD-German National Research Center for Information Technology,
Schloß Birlinghoven, 53754 Sankt Augustin, Germany
02241/14-2746, -2181, jakumeit@gmd.de

The simulation of electron-electron scattering in semiconductor devices by means of MC simulations is complicate, since the scattering rates depend on the electron distribution itself and a two particle scattering has to be simulated for the short range direct interaction of electrons. We introduced the local iterative Monte Carlo (LIMO) algorithm in order to reduce the computation time of Monte Carlo (MC) simulations of electron transport in semiconductor devices by a more ef£cient use of the computational resources. [1, 2] In this contribution we focus on the possibilities for an effective treatment of electron-electron scattering within the LIMO approach.

Two properties of the LIMO algorithm simplify the simulation of electron-electron interaction effects compared to standard MC algorithms. First, the energy distribution of electrons is known at each iteration of the LIMO algorithm. LIMO does not simulate the ¤ight of an ensemble of electrons through the device like standard MC algorithms but changes the distribution iteratively by applying many MC simulations of short ($\sim 10^{-14}$ sec.) electron trajectories. Therefore, the electron distribution is always accessible and the self-consistent electron-electron scattering rates can be calculated directly using Fermi's Golden Rule. Secondly, the partner electron for a short range electron-electron scattering can be created out of the distribution and returned to the distribution for each scattering process. In standard MC algorithms a computational expensive search for a partner electron from the ensemble of model electron is necessary and the correct treatment of energy and momentum of both electrons is more complicate. Both properties together lead to a less computational expensive treatment of electron-electron scattering.

The LIMO approach to electron-electron scattering was used for the investigation of hot electron effects in short channel MOSFETs. The exemplary MOSFETs from the well-tempered MOSFET project [3] with channel length 90 nm, 50 nm and 25 nm were taken for this investigation. The results reveal that the long range electron-plasmon scattering leads as additional relaxation mechanism to a reduction of the distribution while the short range direct interaction increases the high energy tail of the distribution. Substrate I_s and gate current I_g were calculated from the simulated electron distributions for the analysis of hot electron effects. With electron-electron interaction an excellent agreement with measurements could be achieved.

In conclusion, the results for short channel Si-MOSFETs proof, that the LIMO technique is an effective MC approach for complicate problems like the simulation of electron-electron scattering in semiconductor devices. It may be promising to transfer the basic idea of the LIMO approach, the iterative application of small MC steps to a distribution, to other applications.

References

1. J. Jakumeit, U. Ravaioli, *Semiconductor transport simulation with the Local Iterative Monte Carlo Technique*, accepted for the April 2001 issue of IEEE Trans. Electron Devices
2. J. Jakumeit *Computational Aspects of the Local Iterative Monte Carlo Technique*, Int. J. Mod. Phys. C, **11**, 2000, S. 665
3. http://www-mtl.mit.edu:80/Well

Abstract withdrawn by the author

Dynamic subgrid-modeling in large-eddy simulations of magnetohydrodynamic turbulence

Wolf-Christian Müller, Bernard Knaepen, Olivier Debliquy and Daniele Carati

Euratom-Belgian State Association, Physique statistique et des plasmas, CP 231, Campus Plaine, Université Libre de Bruxelles, 1050 Bruxelles, Belgium.

Email: Wolf.Mueller@ipp.mpg.de

The large-eddy simulation (LES) approach is adapted for fully developed incompressible magnetohydrodynamic (MHD) turbulence and tested by comparison to high-resolution direct numerical simulations. Due to the large number of degrees of freedom, inherent to turbulent MHD ¤ows, the Reynolds numbers reached in direct numerical simulations of such systems are still many orders of magnitude lower than the values observed in nature, e.g., in astrophysical systems like the solar wind. The LES technique aims at overcoming this dif£culty by directly computing only the largest turbulent scales of motion while incorporating the in¤uence of the small-scall ¤uctuations through a subgrid-model. This scale-separation is achieved by application of a spatial £lter to the turbulent £elds [1]. The MHD equations for the £ltered velocity ($\overline{\mathbf{v}}$) and magnetic ($\overline{\mathbf{b}}$) £eld then read

$$\begin{aligned} \partial_t \overline{\mathbf{v}} &= -\nabla\cdot(\overline{\mathbf{v}}\,\overline{\mathbf{v}} - \overline{\mathbf{b}}\,\overline{\mathbf{b}} + \boldsymbol{\tau}^v) + \nu\Delta\overline{\mathbf{v}} - \nabla\overline{p}\,, \\ \partial_t \overline{\mathbf{b}} &= -\nabla\cdot(\overline{\mathbf{v}}\,\overline{\mathbf{b}} - \overline{\mathbf{b}}\,\overline{\mathbf{v}} + \boldsymbol{\tau}^b) + \eta\Delta\overline{\mathbf{b}}\,, \\ \nabla\cdot\overline{\mathbf{v}} &= \nabla\cdot\overline{\mathbf{b}} = 0\,, \end{aligned}$$

with the effective £ltered pressure $\overline{p}$, the kinematic viscosity ν and the magnetic diffusivity η. The £ltered-scale stress tensors $\boldsymbol{\tau}^v$ and $\boldsymbol{\tau}^b$ depend on the turbulent scales that have been £ltered out, consequently they have to be modeled using the resolved scales of motion. Here, the turbulent system is represented by a cube of edge length 2π wherein the £ltered MHD equations are solved by a pseudospectral algorithm with explicit time-stepping and periodic boundary conditions. The free parameters of all applied subgrid-models are calculated self-consistently during run-time with the dynamic procedure £rst proposed by Germano *et al.* [2].

The performance of different gradient-diffusion type subgrid-models (see e.g. [3]) is evaluated in LES with a maximum of 64^3 spectral modes by using data stemming from high-resolution direct numerical simulations of decaying and forced MHD turbulence with up to 512^3 spectral modes [4]. *A priori* tests on the correlation between exact and modeled subgrid-stresses together with *a posteriori* tests on the probability density functions of the £eld increments, the energy and energy transfer spectra and the temporal development of important macroscopic quantities like kinetic and magnetic energy, the ideal invariants cross helicity $\int_V dV\,\mathbf{v}\cdot\mathbf{b}$ and magnetic helicity $\int_V dV\,\mathbf{A}\cdot\mathbf{b}$, $\mathbf{A}$ being the components of the magnetic vector potential, show that the turbulent dynamics is well captured by the different subgrid-models at a substantially reduced spatial resolution of 64^3 modes. All observations con£rm convincingly the general applicability of the dynamic procedure LES technique to homogeneous MHD turbulence and allow a clear ranking of the used subgrid-modeling techniques.

References

1. A. Leonard, Ad. Geophys. **18 A**, 237 (1974).
2. M. Germano, J. Fluid Mech. **238**, 325 (1992).
3. J. Smagorinsky, Month. Weather Rev. **91**, 99 (1963).
4. D. Biskamp and W.-C. Müller, Phys. Plasmas **7**, 4889 (2000).

Fluid ¤ows in narrow channels

Zbigniew A. Walenta[1], **Anna Kucaba-Pietal**[2] **and Zbigniew Peradzynski**[3]

[1]*Institute of Fundamental Technological Research, Polish Academy of Sciences, Swietokrzyska 21, 00-049 Warszawa, Poland*
[2]*Rzeszow University of Technology, Dept of Fluid Mechanics and Aerodynamics, Powstancow Warszawy 8, 35-959 Rzeszow, Poland*
[3]*University of Warsaw, Institute of Applied Mathematics and Mechanics, Banacha 2, 02-097 Warszawa, Poland.*
tel. +48 22 8269803, fax +48 22 8269815, e-mail zwalenta@ippt.gov.pl

Recent experimental results [4] indicate, that the microscale ¤ows are essentially different from ¤ows in large scale and the continuum, Navier-Stokes approach is not suitable for explaining the observed microscale phenomena. However, there exist some experimental data, which agree with the theory of micropolar ¤uids [2], also based on the assumption of a continuous medium.

The micropolar ¤uid theory is widely used for description of real ¤uids with internal structure ([4] and the papers cited there). This theory is being developed rapidly because of its possible applications (in tribology, biotribology, for microchannel ¤ows, in magnetorheology, etc.).

The experiments and esimations indicate, that for real ¤ows the micropolar effects are important only if the width of the channel is comparable to the dimensions of the ¤uid particles. Otherwise the classical Navier-Stokes desription is adequate. For such narrow channels, however, the assumption of continuous medium seems not to be justi£ed.

The problem of validity of the micropolar ¤uid model for the ¤ows through narrow channels is open. Solution is becoming urgent [3], since the area of possible applications is still increasing.

This paper presents the results showing to what an extent the theory of micropolar ¤uids may be applied to ¤ow through a channel, whose width is comparable to the dimension characteristic for the molecular structure of the medium (mean free path, average distance between the molecules or diameter of the molecule – whichever is the largest).

We present the results of the numerical simulation of the ¤ow considered as a motion of separate particles. The methods of Molecular Dynamics and Direct Monte-Carlo Simulation are employed. The model of collisions takes into account rotation of the molecules. Large number of the performed numerical simulations makes it possible to obtain the average distributions of velocity. These are compared with solution of the Eringen Equations [1] for the Poiseuille ¤ow.

The comparisons are presented for various values of the geometric and ¤ow parameters: various values of the ratio of the characteristic molecular dimension to the channel width, various numbers of the particles, various models of the interactions of the particles with walls, various initial positions of the particles.

References

1. Eringen A.C., J. Math. Mech.16, 1, 1–16, 1966,
2. Papautsky J. Brazzle J. Amel T. Frazier B., Microelectromech. Sys., Proc. EMBS 97, Chicago, II Oct. 30 – Nov. 2, 2281–2292, 1997.
3. Pfahler J. Harley J. Bau H., Sensors and Actuators, Vol. A21-23, 431–434, 1990.
4. Yager P.P. Brody P., Proc. Solid-State Sensor and Actuator Workshop, Hilton Head, S.C., June 2-6, 105–108, 1996.

Simulation of ¤uid ¤ow in the presence of particles

Witold Alda[1], **Witold Dzwinel**[1] **and Jacek Kitowski**[1,2]

[1]*Institute of Computer Science, AGH, al. Mickiewicza 30*
30-059 Cracow, Poland
[2]*ACK CYFRONET-AGH, Nawojki 11, 30-950 Cracow, Poland*
phone: +48 12 617 35 20, e-mail: alda@uci.agh.edu.pl

In the paper we present and compare two different approaches of ¤uid ¤ow simulation in the presence of interacting particles. The £rst model is based on works of Schwarzer et al. [1, 3]. The continuous model of ¤uid is described by Navier-Stokes equations and numerically solved by Finite Elements in order to increase the ¤exibility of boundary conditions. Particle-particle visco-elastic interaction calculations are accelerated by applying fast MD algorithms. Particles interact with the ¤uid locally, i.e. in the element in which they are placed. The ¤uid acts on the particle with the reaction and lubrication forces. We assume stationary, laminar ¤ow of Newtonian incompressible viscous ¤uid for small values of Reynolds number, with particles either immobile or moving along the ¤ow or due to gravity. The computer experiment assumes two phase ¤ow through porous medium with particle convection/sedimentation. The original simulation code has been elaborated for both 3D and 2D systems. In the example, a ¤ow trough curved pipe with immobile particles distributed on random is shown in Fig.1a,b. Certain irregularities of the velocity distribution due to the presence of particles can be seen in Fig.1a.

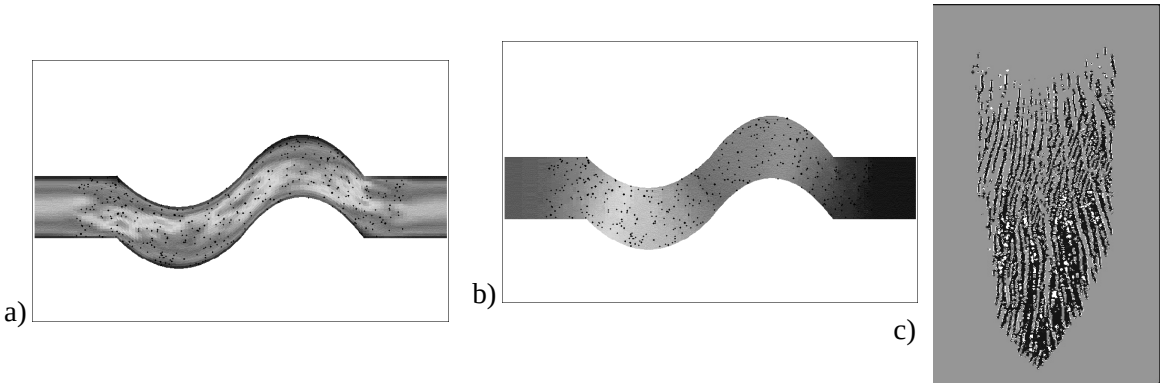


Fig. 1. Distribution of total velocity (a) and pressure (b) in the ¤ow through S shaped pipe £lled with particles. (c) The multiresolution structures emerging in mesoscopic simulation of colloidal agglomerate accelerated in complex ¤uid

Different approach has been employed for simulating a granular medium dispersing (fragmenting) in the complex ¤uid. For example, in tiny blood vessels the large blood cells are of comparable size to the granular microstructures such as thrombus or medicines. In this case, the complex ¤uid - blood - cannot be simulated by using continuum models. In Fig.1c, we present the result of 2-D simulation of colloidal agglomerate in a periodic box fragmenting in the complex ¤uid. The colloidal beds are modeled employing singular DLVO forces while the bulk of ¤uid is simulated with ¤uid particles. The ¤uid particles interact with dissipative forces such as in [4]. In result, the complex multiresolution structures emerge.

References

1. Schwarzer S., 1995, Phys. Rev. E 52, 6461
2. Kalthoff W., Schwarzer S, Ristow G. and Herrmann H., 1996, Int. J. Mod. Phys. C 7, 883
3. Hoef¤er K, Mueller M., Schwarzer S, and Wachmann B., in High Performance Computing in Science and Engineering, E. Krause, W. Jeager eds., Springer, Berlin, 1998.
4. Espanol, P., 1998, Phys. Rev. E 57, 2930.

APE – T¤ops computers for theoretical particle physics

Karl Jansen, Norbert Paschedag, Dirk Pleiter, Hubert Simma and Peter Wegner

John von Neumann Institute for Computing (NIC) & Deutsches Elektronen-Synchrotron (DESY), Platanenallee 6, D-15738 Zeuthen, Germany

(49)33762-77-381, (49)33762-77-330, Dirk.Pleiter@desy.de

At several European sites the commissioning of large installations of APEmille computers will be £nished in spring 2001. These machines make another 2 T¤ops of computing power available for numerical simulations in theoretical particle physics. APEmille is the most recent generation of APE computers. The previous generation APE100 has been intensively used for many years by several international research collaborations.

In this talk we describe the APEmille computers and report on our experiences running these machines. APEmille is a massively parallel computer which was designed by the APE project (”Array Processor Experiment”) at INFN (Istituto Nazionale di Fisica Nucleare) in collaboration with DESY (Deutsches Elektronen-Synchrotron). The building blocks of APEmille are crates which consist of 16 processing boards each. Each crate has a peak performance of 67 G¤ops. There are 8 processors per board which are specially designed for complex arithmetics. The nodes are connected in a three-dimensional topology by a fast synchronous low-latency communication network.

The John von Neumann Institute for Computing (NIC) runs seven APEmille crates at DESY Zeuthen. This installation is mainly used to simulate QCD with dynamical fermions. Before that usually virtual quark loops have been neglected. This approximation is conventionally referred to as ”quenching”. During this talk we will give a survey on the different collaborations and their research topics. These collaborations cover most of the key issues of this £eld, like hadronic spectroscopy or calculation of fundamental parameters of the theory (e.g. quark masses).

In the remaining part of the talk we will focus on the algorithms used in simulations of QCD on the lattice and discuss the hardware requirements. The main challenge in lattice QCD simulations arises from the fermionic degrees of freedom. From a numerical point of view the fast computation of the discretized Dirac operator and the availability of ef£cient algorithms e.g. for the inversion of very large sparse matrices are crucial.

Large scale & grid computing with Cactus

G. Allen[1], W. Benger[1,2], T. Dramlitsch[1], T. Goodale[1], H. Hege[2], G. Lanfermann[1], A. Merzky[2], T. Radke[1], E. Seidel[1,3] and J. Shalf[4]

[1]*Max-Planck-Institut für Gravitationsphysik, Albert-Einstein-Institut, Golm*
[2]*Konrad-Zuse-Zentrum für Informationstechnik, Berlin (ZIB)*
[3]*National Center for Supercomputing Applications, Champaign, IL*
[4]*Lawrence Berkeley National Laboratory, Berkeley, CA, (LBNL)*

Cactus[1] is an open source problem solving environment designed for scientists and engineers. Its modular structure facilitates parallel computation across different architectures and collaborative code development between different groups. The Cactus Code originated in the academic research community, where it has been developed and used over many years by a large international collaboration of physicists and computational scientists. We discuss here how the intensive computing requirements of physics applications now using the Cactus Code encourage the development and use of Grid computing techniques. We detail capabilities for large scale computing now available and under development within the framework[2], including

Cactus Computational Toolkit: A set of modules usable by any application providing functionality such as checkpointing, parallel I/O, parallel interpolators and reduction operators, as well as coordinates systems, boundary conditions, and elliptic solvers.
Accessibility to Resources: A *Cactus User Portal* to provides a easy-to-use interface for using remote machines, in both a local and Grid environment, providing code assembly, resource £nding and authentication, executable staging, and simulation monitoring and steering.
Remote File Access: Large-scale computer simulations generate large-scale data sets. Conventional analysis and visualization then becomes prohibitively resource-intensive when remote simulation data must be moved to a local machine for processing. Enhancements to the *Hierarchical Data Format* HDF5 I/O library, allow existing I/O layers to operate directly on remote £les which are uniquely addressed by their URL.
Remote Visualization, Monitoring and Steering: Remote visualization is the capability to visualize data (possibly in a virtual £le streamed live from a running simulation) from a remote resource with a client on a local machine, eliminating the need to move enormous amounts of data between machines. Cactus provides several different implementations of data streaming. which can be viewed using various visualization tools (e.g. [3]). Scientists using large scale remote resources have to cope with different accounts, networks, operating systems, and queuing systems. Cactus alleviates many of these problems with a module which provides a simulation with its own webserver providing detailed simulation information viewable from any remote web browser. The web interface can also be used for steering: e.g. pausing or terminating a simulation, as well as changing the values of parameters, for example changing data output properties.
Dynamic and Distributed Grid Computing: Distributing a single simulation across multiple resources provides the means to run large simulations or to run simulations immediately. Cactus applications are easily distributed using the Globus Toolkit. We are developing a *Grid Application Toolkit* to exploit the Grid for new dynamic application scenarios.

References

1. Cactus Code homepage: http://www.cactuscode.org
2. G. Allen, W. Benger, T. Goodale, H. Hege, G. Lanfermann, A. Merzky, T. Radke, E. Seidel, J. Shalf, "Cactus Tools for Grid Applications", submitted to *Cluster Computing*, (2001), [http://www.cactuscode.org/CacPapers/CactusTools.ps.gz]
3. Amira: http://amira.zib.de, IBM Data Explorer: http://www.research.ibm.com/dx, LCA Vision: http://zeus.ncsa.uiuc.edu/ miksa/LCAVision.html.

Abstract withdrawn by the author

Growth & structure of the world-wide web: Towards realistic modeling

Bosiljka Tadić

J. Stefan Institute, 1001 Ljubljana, Slovenia

phone: +386-1-4773767; fax: +386-1-4773716; e-mail: Bosiljka.Tadic@ijs.si

The world-wide Web is a directed graph with nodes representing Web pages and arcs representing the hyperlinks between pages [1, 2, 3]. Recent large-scale measurements [2] show that both outgoing and incoming links in the Web exhibit hierarchical organization with different scaling exponents. In addition, the size of connected component has scaling behavior and a giant component in the center. This complex structure of the real Web remains elusive for simpli£ed modeling of generic social networks with only dynamics of incoming links that is governed by preferential attachment rules [4]. Applying a generalized random-graph theory to study structure of the Web the authors in Ref. [3] have demonstrated how a giant component can occur in directed graphs. In their approach, however, it is necessary to assume the "right" distributions of incoming and outgoing links in order to get a quantitative agreement.

Here we present a *growth* model [1] of directed graphs in which we show, £rst, how the correct distributions of outgoing and incoming links emerge from the growth rules and, second, we explore the structure of the grown network by numerical simulations. We suggest the dynamic rules that are motivated by the policies of agents in the real world-wide Web. The key features of the model are: (i) *link correlations*—the incoming links are driven by the dynamics of outgoing links, (ii) *link updates*—the links of the network are rearranged at the pace at which the network grows, and (iii) *bias activity* of agents and *bias attachment* of links. These rules lead to the structure of links that is speci£c to the Web. We use numerical simulations with the above described dynamic rules to grow a large network. We then measure the probability distributions of node ranks. The emergent hierarchical organization both of outgoing links and incoming links compares well with the real Web. A single control parameter—ratio of the updated versus added links per time step is estimated from the comparison with the available empirical data [2].

We then explore the structure of the network using two different approaches. First, we mimic the Web crawls starting from a random node in the network to determine size and depth of connected components. We show that for the above estimated value of the control parameter the size distribution with the giant component occurs which is in agreement with the empirical data [2]. Second, we simulate a random walker on the network to determine the local properties of the structure. We also discuss possible scenario when the control parameter is freely varied.

References

1. B. Tadić, cond-mat/0011442; Physica A: Statistical Mechanics and its Applications **293**, 273 (2001).
2. A. Broder *et al.*, Computer Networks 33, 309 (2000).
3. M.E.J. Newman *et al.*, cond-mat/0007235; M.E.J. Newman, private communication.
4. S. Dorogovtsev *et al.*, Phys. Rev. Lett. **85**, 4633 (2000).

A model for proportional voting process

A. T. Bernardes
Departamento de Física, Universidade Federal de Ouro Preto, Campus do Morro do Cruzeiro, 35400-000, Ouro Preto-MG, Brazil
atb@iceb.ufop.br

Recently, Costa-Filho *et al.* [1] have shown that distributions of votes per candidate for the 1998 elections in Brazil follow a power law distribution, with exponent $\simeq -1.0$. They obtained the same result for the whole country (candidates for a seat as federal deputy) as well as for the state of São Paulo (candidates for a seat as state deputy). The same behaviour was observed in the 2000 elections for city representatives. Elections are processes where a vote is supposed to be obtained as a result of convincing arguments. This can be done by the candidate/party or other voters. Thus, it can be compared with a physical process of clustering. However, usual models of formation of clusters (as percolation, for instance) may give exponents $\simeq -2.0$ (square lattice).

In this work, a modi£ed version of the Sznajd model [2] is used to simulate proportional elections. A square lattice of size $L \times L$ represents the set of voters. A number of N candidates is de£ned in the beginning of the simulation. The value n of a site S on the lattice represents that this voter has given the vote to that candidate n. The model has two different stages: First, the initial condition is de£ned and, after that, the electoral campaign is simulated.

The £rst stage starts with an empty lattice, meaning that there are no votes. Then, all the sites are visited at random. For each visit, a candidate randomly chosen tries to convince the voter. This candidate has a probability $P_c = (n/N)^2$ (the probability of convincing) of being accepted. If the candidate is accepted by that voter, now the voter tries to convince its neighbourhood, once again with probability P_c: for each neighbouring site that has the same value of the candidate chosen before, all the six neighbouring sites of this bond of two sites will assume the same value (as in the usual Sznajd prescription). If nobody had chosen the same candidate, only the originally selected voter was changed.

In the second stage, a usual Sznajd process is performed. A site and one of its four neighbours are chosen at random. If the two sites have the same value (they vote in the same candidate) all the six neighbours change to vote in that candidate.

As in real elections, one does not wait for a kind of equilibrium state, but count the votes for different times, i.e., it is done the analysis during the transient time, $1 \ll t \ll L^2$. For simulations with $\simeq 10^8$ voters and 2000 candidates, a power law behaviour with exponent -1.09 was obtained, similar to that observed experimentally [3].

References

1. R.N. Costa-Filho, M.P. Almeida, J.S. Andrade Jr., and J.E. Moreira, Phys Rev E **60**, 1067 (1999).
2. K. Sznajd-Weron and J. Sznajd, Int. J. Mod. Phys. C **11**, 1157 (2000); D. Stauffer, A.O. Sousa and S. Moss de Oliveira, Int. J. Mod. Phys. C **11**, 1239 (2000).
3. U.M.S. Costa, A.D. Araujo, A. T. Bernardes and D. Stauffer, Int. J. Mod. Phys. C, in press (2001)

Computational physics programme in research and teaching - An african experience

C. V. Sheth
Physics Department, University of Zambia,
P. O. Box 32379, Lusaka, Zambia.
E-Mail: csheth@natsci.unza.zm

Physics as a discipline has played an important role in the development of science and technology world over. Countries with strong physics programme are ones who come up with new technologies and new discoveries. The third world countries and the majority of these being in Africa, suffer from many problems in having a good physics programmes in research and teaching. The contributing factors are: (i) shortage of £nancial resources, (ii) shortage of trained manpower, (iii) lack of basic technical infrastructure.

The availability of powerful PC's at an affordable price, the internet and networking facilities, have opened up new opportunities in teaching, research and information exchange in third world countries. It is now possible to have research and teaching opportunities in computationally intensive calculations, modeling of realistic current problems and a possibility of global collaborations in experimental work through remote terminals. Computational physics programmes at undergraduate and graduate level is seen to prepare a physicist for global collaboration . The author £nds, in the context of third world countries , in particular at the University of Zambia, Lusaka, Zambia, the students and staff greatly bene£ting in research and teaching through computational physics. The programme currently offered is explained which can be a model programme for many countries.

The recent advances in computer software, especially in programming languages has brought in a certain amount of confusion. There is in existence a diverse adoption of operating systems, programming languages and the use of general purpose utility software packages. This results in limited communications between various groups, duplication in the development of software. There are a number of web sites of various institutions which have freely accessible software and other related resources. However, this is ineff£cient from the point of user since much of the time is spent in browsing before one could decide to use such a software. This re¤ects eventually into wastage of limited £nances. In conclusion, it is recommended to establish: (1)world body, supervising and recommending resources, standards and structure in computational physics(science), (2) an international resource centre wherein free software and utility packages can be accessed, (3) international contributions in £nances to establish a program to support and develop computational physics programmes in the third world countries.

References

1. ' The Conference on Computers in Physics Instruction '-Proceedings Aug 1-5, 1988, Raleigh, North Carolina, U.S.A. -Editors: E. F. Redish and J.S. Risley (Addison-Wesley, 1990).
2. ' Is Java for Scienti£c Programming '-Paul F. Dubois, Comput. Phys.11, 611 (1997).

Steady state two-phase bulk ¤ow in 2D porous media by network models

Henning Arendt Knudsen and Alex Hansen

Department of Physics, Norwegian University of Science and Technology, NTNU,NO-7491 Trondheim, Norway

+47 73593655, +47 73593372, Henning.Knudsen@phys.ntnu.no

Multi-phase ¤ow in porous media is a problem encountered in oil recovery and hydrology. The problem has a very complex nature since it involves the topology of the porous media, the number of phases present, the properties of these phases, *e.g.*, viscosity and wettability, and the ¤ow conditions, *e.g.*, global pressure gradients and distances from inlets and outlets.

In particular, for two phase ¤ow, a lot of experimental work has been done in order to £nd average ¤ow properties of the two phases in speci£c porous media, properties which are applicable to oil production, see *e.g.*[1] . The theoretical understanding of two-phase ¤ow is growing, but still there is much to be done in order to bridge the gap between ¤ow properties on porelevel and macroscopic ¤ow properties. Experimentally there has been done work on two-dimensional steady state ¤ow, which reveals the complex nature of bubble dynamics and the need of a deeper understanding[2].

We present work done on a pore level network model. In two dimensions we simulate two-phase ¤ow within a network of tubes. For each time step a discrete Poisson problem with time-dependent coeff-isients is solved for the pressure within the model. The time evolution is found by Euler integration. The boundary conditions are biperiodic, which allows the system to run for a long time, and thus reach a steady state. Previous simulations on this scale and level of details have concerned invasion processes[3]. The present work goes beyond the front phenomena of one ¤uid displacing another and look at bulk behaviour far from inlets and outlets where complex bubble dynamics occur.

Simulations on this model provides average ¤ow properties, namely the fractional ¤ow of each phase, and the corresponding global pressure gradient. These properties can be translated into the language of relative permeabilities and mobilities. The properties are known to be functions of many parameters such as the capillary number, which physically is the ratio between viscous forces and capillary (interfacial) forces, the viscosity ratio between the two phases, and the width of the size distribution of the pores of the porous media.

The many free variables of the problem make a numerical approach particularly interesting since the behaviour of the macroscopic properties can be studied as a function of the microscopic properties in a systematic way. To the £rst end, these simulations contribute to reveal the structure of these dependencies. Second the method can hopefully be developed further and thus provide results for speci£c rock and ¤uid systems.

References

1. F. A. L. Dullien, *Porous Media: Fluid Transport and Pore Structure* (Academic Press, San Diego, 1992).
2. D. G. Avraam and A. C. Payatakes, Trans. In Porous Media **20**, 135 (1995).
3. E. Aker, K. J. Mâløy, and A. Hansen, Phys. Rev. E **58** (1998).

Multicanonical simulations of some peptides

H. Arkın[1], **F. Yaşar**[1], **T. Çelik**[1]
B. A. Berg[2,3] **and H. Meirovitch**[3]

[1] *Dept. of Physics, Hacettepe University, Beytepe 06532, Ankara.*
[2] *Dept. of Physics, Florida State University, Tallahassee, USA*
[3] *CSIT, Florida State University, Tallahassee, USA*

(+ 90 312 297 7229, Fax: + 90 312 299 2037, tcelik@hacettepe.edu.tr)

A brief discussion of the multicanonical simulation method [1] will be given and the results of our simulations of some short peptides will be presented. The determination of the a priori unknown multicanonical weight factors by recursion will be shown. The intermediate steps of the simulation method starting from a given sequence as the input leading to the folded three dimensional structure and the minimization procedure will be presented [2]. The comparison to the canonical simulations at £xed temperature and the effectiveness of the multicanonical simulation method will be discussed [3].

References

1. B. A. Berg and T. Çelik, Pys. Rev. Lett. 69 (1992) 2292.
2. F. Yaşar, T. Çelik, B. A. Berg and H. Meirovitch, J. Comput. Chem. 21 (2000) 1251.
3. H. Meirovitch and E. Meirovich, J. Comput. Chem. 18 (1997) 240.

New algorithms and the statistical physics of protein folding

Ulrich H.E. Hansmann
Department of Physics, Michigan Technological University, Houghton, MI 49931-1295, USA
hansmann@mtu.edu

The protein-folding problem is to understand for a given protein the relation between its sequence of amino acids and the set of thermally accessible conformations; and to comprehend the mechanism by which the protein folds into its biologically active structure.

In principle, such questions can be studied by computer simulations. However, the energy landscape of proteins is characterized by a multitude of local minima separated by high energy barriers. Hence, low temperature simulations by canonical molecular dynamics or Monte Carlo will get trapped in con£gurations corresponding to one of these local minima. We show how this so-called multiple-minima problem can be overcome by new simulation techniques such as *parallel tempering* and *generalized-ensemble* algorithms.

We demonstrate the effectiveness of this approach for protein simulations, and study these molecules from a statistical physics point of view. The free energy landscape and structural transitions in small proteins are evaluated. For some homopolymers, a set of critical exponents is calculated which characterizes transitions in these systems.

References

1. U.H.E. Hansmann and Y. Okamoto, in *Annual Reviews in Computational Physics VI*. Edited by Stauffer D. Singapore: World Scienti£c; (1999) 129.
2. U.H.E. Hansmann, Y. Okamoto and J.N. Onuchic, *Proteins* **34** (1999) 472.
3. U.H.E. Hansmann *Eur. Phy. J. B*, **12** (1999) 607;
   N.A. Alves and U.H.E. Hansmann, *Int. J. Mod. Phys. C*, **11** (2000) 301.
4. N.A. Alves and U.H.E. Hansmann, *Phys. Rev. Let.*, **84** (2000) 1836.

Magnetorotational supernova explosion. Simulation Lagrangian implicit numerical method on triangular grid with grid reconstruction

S.G.Moiseenko[1], **N.V.Ardeljan**[2] **and G.S.Bisnovatyi-Kogan**[1]

[1]*Space Research Institute Profsoyuznaya str. 84/32 Moscow 117810, Russia*
[2]*Department of Computational Mathematics and Cybernetics, Moscow State University Vorbjevy Gory, Moscow B-234 119899, Russia*
phone: 7 095 333 45 88, fax: 7 095 310 70 23 e-mail: moiseenko@mx.iki.rssi.ru

We investigated a problem of the magnetorotational supernova star explosion using specially developed original implicit Lagrangian numerical scheme on triangular grid with grid reconstruction.

Magnetorotational mechanism is based on the idea that initial poloidal magnetic £eld due to the differential rotation of the star produces toroidal magnetic £eld which grows with time and transforms part of the gravitational energy of the star to the energy of explosion [1]. Usual values of the magnetic £elds in stars are rather weak $\alpha = E_{mag}/E_{grav} = 10^{-6} - 10^{-8}$ (E_{mag} - initial magnetic energy, E_{grav} - initial gravitational energy). The smallness of α that value is the main problem for the numerical solution, because the problem has 2 very different timescales: £rst is very small one corresponding to the large sound speed in the central parts of the star, second timescale is huge and corresponds to the slow evolution of the toroidal component of the magnetic £eld. Set of MHD equations becomes stiff and its stiffness is characterized by the parameter α.

Application of the completely conservative implicit Lagrangian scheme on triangular grid with grid reconstruction [2] allows us to make large time steps (usually about 100-300 Courant time steps). It is known that one of the main dif£culties for the application of the Lagrangian schemes is grid distortion. We use specially developed procedure of grid reconstruction procedure, which allows us to restore the triangular grid and recalculate its parameters in conservative way. Grid reconstruction procedure showed its ef£ciency for the problem of the collapse of the rapidly rotating cold protostellar problem [3].

As result of our simulations we get ampli£cation of the toroidal magnetic £eld and transformation of the part of the energy of the star to the energy of the explosion. Part of the matter - $\sim 7\%$ of the mass of the cloud ($\sim 3.3\%$ of the £nal gravitational energy of the cloud) - gets radial kinetic energy which is larger than its potential energy and can be thrown away to the in£nity. It carries about 30% of the initial angular momentum of the cloud. This effect is important for angular momentum loss in the processes of stellar formation, and for the magnetorotational mechanism of explosion suggested for supernovae [4].

References

1. Bisnovatyi-Kogan G.S.: 1970 Astronomicheskij Zhurnal. **47**, 813 (Soviet Astronomy 1971, **14**, 652).
2. Ardeljan N.V., Kosmachevskii K.V.:1995 Computational and Mathematical Modelling 1995 **6**, 209
3. Ardeljan N.V., Bisnovatyi-Kogan G.S., Kosmachevskii K.V., Moiseenko S.G.: 1996 Astron.& Astrophys. Supl. Ser. **115**, 573.
4. Ardeljan N.V., Bisnovatyi-Kogan G.S., Moiseenko S.G.: 2000 Astron.& Astrophys. **355**, 1181.

The effects of cosmic rays on the large scale structure formation in the universe

Dongsu Ryu[1], **Hyesung Kang**[2], **and Peter L. Biermann**[3]

[1] *Chungnam National University, Daejeon 305-764, Korea*
[2] *Pusan National University, Pusan, 609-735, Korea*
[3] *Max-Planck Institute for Radioastronomy, Bonn, Germany*
82-42-821-5466 (phone), 82-42-822-8380 (fax), ryu@canopus.chungnam.ac.kr

Clusters of galaxies and large scale structures may contain a signi£cant amount of cosmic rays and magnetic £elds embedded in the hot gas detectable in X-rays; the energy output from growing black holes at the centers of galaxies in addition to supernovae and GRBs leads naturally to a scenario, where the intergalactic medium in analogy to the interstellar medium is £lled with energetic particles, and permeated by magnetic £elds. Recent hard X-ray and extreme ultra-violet observations indicate that cosmic rays may be energetically as important as the hot gas in clusters; the two components are in pressure equipartition[1]. Observations of rotational measure shows that the energy in magnetic £eld can also be a signi£cant fraction of gas energy[2] in intracluster medium. Here we present the exploration of large scale structure formation through numerical simulations which include the injection of cosmic rays from cosmic black holes and their subsequent evolution, in order to see a) to what degree structure formation is in¤uenced by cosmic rays ejected from black holes and b) which observables will make good tests for the effects of energetic particles as well as magnetic £elds. A cosmological hydrodynamic code which can follow the evolution of dark matter, gas, magnetic £eld, and cosmic rays has been used[3]. This represents the £rst work where the dynamical role of cosmic rays is studied in the context of the simulations for the large scale structure formation. Magnetic £elds are included in the simulations too, but they are expected to play only a minor role dynamically. The cosmic structures, when the effects of cosmic ray pressure are accounted, are spreaded more widely. The density and temperature peaks are reduced. The density power spectrum is suppressed in the scale of $\sim 10h^{-1}$ Mpc and smaller.

References

1. Blasi, P. 1999, The Astrophysical Journal, 525, 603
2. Clarke, T. E., Kronberg, P. P. & Böhringer, H. 2001, The Astrophysical Journal Letters, 547, L111
3. Ryu, D., Ostriker, J. P., Kang, H. & Cen, R. 1993, The Astrophysical Journal, 414, 1

Performing and analysing cosmological simulations with FLY and AstroMD

V. Antonuccio-Delogu[1], U. Becciani[1], D. Ferro[1], A. Germaná[1], A. Pagliaro[1], F. Buonomo[2], C. Gheller[2]

[1] *Osservatorio Astro£sico di Catania - Catania*
[2] *CINECA - Casalecchio di Reno*
Tlf: +39 095 7332317, Fax: +39 095 330592, e-mail: ube@sunct.ct.astro.it

This contribution is primarily concerned with FLY, an optimized muti-platform tree N-body code allowing to evolve three-dimensional self-gravitating collisionless systems with a large number of particles ($N \geq 10^7$). FLY (**F**ast **L**evel-based N-bod**Y** code) is a fully parallel code based on the octal-tree algorithm introduced by Barnes and Hut in 1986 [1]. It adopts periodic boundary conditions implemented by means of the Ewald summation technique. FLY is based on the one-side communication paradigm to share data among the processors that access remote private data avoiding any kind of synchronism. The code was originally developed on a CRAY T3E system using the *Shmem* library and it was ported on SGI ORIGIN systems and on IBM SP (on the latter making use of the *Lapi* library). FLY can advance more than 53,000 particles/second in runs using 16,777,216 particles in clustered conditions, on a Cray T3E with 64 processors. In the latest version of the code, which is included in the £rst publicly available release, we have also implemented a new "grouping" scheme ([3]), and we will describe in detail the tradeoff between numerical accuracy and performance gain which can result from the adoption of this algorithmic advance. FLY is an open source free code available at http://www.ct.astro.it/¤y/.

FLY has been integrated within AstroMD (http://www.cineca.it/astromd), a freely available analysis and visualization tool speci£cally designed to deal with the visualization and analysis of astrophysical data. AstroMD started as a joint project of our Institutions, and has been now funded under the EC V Framework Programme, involving in its development other european research institutions. It allows the user to compute interactively relevant point statistics like correlation functions, power spectra, Minkowski functionals, on user-speci£ed subsets of data, and to compute model-dependent quantities for user-selected groups of points, like magnitudes and colours. In this talk we will show the capabilities od AstroMD on a series of high-resolution cosmological simulations of the Large Scale Structure of the Universe we have recently performed. Even on medium-size computational systems like portable computers with 128 MB RAM AstroMD allows a quick interactive analysis of large simulations, and conversions among different popular data formats (HDF, TIPSY, binary) and image formats. Finally, we will discuss the possible future extensions and optmizations of these software packages.

References

1. Barnes, J.E. and Hut, P., 1986, Nature, 324, 446
2. Becciani, U., Ansaloni R., Antonuccio-Delogu, V., Erbacci, G., Gambera, M., Pagliaro, A., 1997, Comp. Phys. Comm., 106, 1
3. Becciani, U., Antonuccio-Delogu, V., 2000, J. Comput. Phys., 163, 118
4. Hockney, R.W., Eastwood, J.W., 1981, Computer simulation using particles ed. Mcgraw-Hill International, New York

Computation of relativistic electron acceleration, transport and emissions in complex astrophysical ¤ows

T. W. Jones[1], **I. L. Tregillis**[1] **and D. Ryu**[2]

[1]*School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, USA*
[2]*Department of Astronomy and Space Science, Chungnam National University, Daejun 305-764, Korea*
voice: 612-624-8546, fax: 612-626-2029, twj@astro.umn.edu

Relativistic hadrons and leptons are ubiquitous constituents in astrophysical environments. These so-called “cosmic-rays” (CRs), which re¤ect the breakdown of thermodynamic behaviors in collisionless plasmas, particularly at shocks, can carry substantial portions of the energies in violent plasma ¤ows. Their radiations, especially as seen from the electronic components, often are critical diagnostic tools for the associated phenomena. Detailed computation of the microphysics responsible for CR acceleration at shocks and subsequent transport is very dif£cult, since it is based on processes that are not fully understood. The processes also span length and time scales ranging upwards several orders of magnitude from close to the smallest dissipative scales. We have developed a variety of numerical approaches to this problem. Here we report on a new method and its application for simulating acceleration and transport of relativistic electrons in the context of highly driven astrophysical MHD ¤ows [1], [2], [3].

Our computational method involves a simple £nite volume scheme for solving the relevant Fokker-Planck equation (the so-called “diffusion-convection equation”). It is designed to take advantage of the severe mismatch between electron transport scales and scales generally treated in the global dynamics. This treatment is followed simultaneously with a TVD MHD scheme for the underlying bulk plasma ¤ow [4].

In this presentation we will describe our results from the £rst fully 3D simulations of radio galaxy jets and their environmental interactions that include explicit energy-dependent transport of the nonthermal relativistic electrons, as well as direct calculations of nonthermal radio and X-ray emissions from the simulated objects. This enables us to produce “synthetic observations” of the objects using the same tools as observational astronomers, so that we can explore meaningful relationships between internal dynamics and such observed properties as surface brightness, spectra and polarization. All previous attempts to do this have been based on *assumed* connections between dynamics and emissions.

The simulations show clearly that shock structures in radio galaxy ¤ows are very complex, and that this impacts in a fundamental way on the character of particle acceleration in the ¤ows. That, in turn casts strong doubts on many of the conventional interpretations of emission spectral and brightness patterns. At the same time these more complete simulations are allowing us to de£ne more clearly how we can determine actual physical conditions from observations.

This work is supported by the National Science Foundation, NASA, KOSEF and the University of Minnesota Supercomputing Institute.

References

1. B. I. Jun & T. W. Jones 1999, ApJ, 511:774-791
2. T. W. Jones, D. Ryu & A. Engel 1999, ApJ, 512:105-124
3. I. L. Tregillis, T. W. Jones & D. Ryu 2001, ApJ, submitted
4. D. Ryu, F. Miniati, T. W. Jones & A. Frank 1998, ApJ, 509:244-255

Estimates of arrival directions of giant air showers

E.E.Antonov[1], **I.L.Buylova**[1], **L.G.Dedenko**[1], **G.F.Fedorova**[2], **A.V.Glushkov**[3], **V.A.Kolosov**[3], **T.M.Komissarova**[1], **M.I.Pravdin**[3], **Yu.P.Pyt'ev**[1], **T.M.Roganova**[2], **I.E.Sleptsov**[3]

[1] *Department of Physics, M.V.Lomonosov Moscow State University, 119899 Moscow, Russia*

[2] *Scienti£c and Research Institute of Nuclear Physics, M.V.Lomonosov Moscow State University, 119899 Moscow, Russia*

[3] *Institute of Space Physics and Aeronomy, Siberian Branch of the Russian Academy of Sciences, 677891 Yakutsk, Russia*

telephone: (095)939-14-89, fax: (095)939-14-89, e-mail:ddn@dec1.npi.msu.su

The arrival directions of giant air showers generated in the atmosphere by primary cosmic ray particles with energies above $\sim 5 \cdot 10^{19}$ eV may be connected with possible extragalactic sources, because the Larmor radius of such particles is too large. Besides it was suggested that primary particles with enormous energies may be neutrons [1]. In this case it is possible to avoid the energy loss in interactions with the microwave background radiation and arrival directions will strongly point to sources. Thus it is of primary importance to decrease possible errors in the estimates of arrival directions of giant air showers. To estimate the arrival direction of a giant air shower one has to have any model of its space-time structure. The simplest model of the shower time front is a model of the ¤at front when all particles are located in this front plane. It was shown [2] that possible errors in estimates of the zenith and azimuthal angles which characterize the arrival directions may be as large as 5^o or even more. The χ^2 method gives very large values of χ^2. That means that this model is inconsistent with the data. Much more realistic model of a shower time front was suggested by Linsley. Calculations [3] displayed that both the shower disk thickness and the average time delay depend on energy of primary particles. So the calculated shower time front for both electrons and muons may £t the data and thus provide better accuracy. The standard mathematical procedure to interpret data is the χ^2 method. This method leads to reasonable estimates of the zenith and azimuthal angles. In some cases the minimax procedure may be utilized to interpret data. It was shown,that the possible error in estimates of the zenith and azimuthal angles may be decreased up to 0.5^o. At last the fuzzy uncertain variables and the possibility theory are suggested here to use for interpreting the data. Calculations were carried out in terms of the quark-gluon string model for primary protons and observation level of 1020 g/cm^2. The Landau- Pomeranchuk-Migdal effect and interactions of neutral pions the with nuclei in the atmosphere at high energies are taken into account. The Monte-Carlo method was used for primary protons while cascades from numerous charged pions were considered with the help of cascade equations. Though experimental statistics is very low no evidence is found to prefer any directions. Thus the isotropic distribution of the arrival directions of giant air showers with energies above 10^{19} eV seems to £t data.

References

1. S.Coleman and S.L.Glashow, Phys. Rev. D **59** 116008 (1999).
2. E.E.Antonov, L.G.Dedenko, G.F.Fedorova, Glushkov A.V. et al., Proc. 26th ICRC, Salt Lake City, USA, **1**, 449 (1999).
3. A.M.Anokhina, L.G.Dedenko, G.F.Fedorova, V.I.Galkin et al., Phys. Rev. D **60** 033004 (1999).

Estimation of the attenuation length of the charged particle density at 600 metres from the shower axis

E.E.Antonov[1], **L.G.Dedenko**[1], **G.F.Fedorova**[2], **E.Yu. Fedunin**[1], **A.V.Glushkov**[3], **V.A.Kolosov**[3], **M.I.Pravdin**[3], **T.M.Roganova**[2], **I.E.Sleptsov**[3]

[1] *Department of Physics, M.V.Lomonosov Moscow State University, 119899 Moscow, Russia*

[2] *Scienti£c and Research Institute of Nuclear Physics, M.V.Lomonosov Moscow State University, 119899 Moscow, Russia*

[3] *Institute of Space Physics and Aeronomy, Siberian Branch of the Russian Academy of Sciences, 677891 Yakutsk, Russia*

telephone: (095)939-14-89, fax: (095)939-14-89, e-mail:ddn@dec1.npi.msu.su

The observations of the giant air showers with energies well in excess of 10^{20} eV put forward a very dramatic puzzle to the cosmic ray astrophysics. Billions secondary particles produced in interactions with the atomic nuclei and decay processes in the atmosphere are spread to distances of about a few kilometres from the shower axis at ground level. The density of charged particles at 600 m from the shower axis is used as a reliable indicator of energy of individual vertical showers. As giant showers are assumed to be isotropic one needs the attenuation length of the signal in a standard scintillator at 600 m from the shower axis to recalculate observed signal to a vertical shower. This attenuation length usually was estimated indirectly by taking cuts of constant intensity in signal spectra for showers of different zenith angle bins. The reliability of such procedure for the total number of secondary particles was analysed [1, 2]. As for the signal at 600 m this reliability is investigated in this paper. Besides some more methods are also discussed. The £rst one is related to the longitudinal development of signal and the last one to calculations of signal for a vertical shower with the same energy.

Calculations were carried out in terms of the quark-gluon string model for primary protons and observation level of 1020 g/cm^2 for showers with various zenith angles. The Landau-Pomeranchuk-Migdal effect and neutral pions interactions are taken into accunt at high energies. The Monte Carlo method was used for primary protons while cascades from numerous charged pions were considered with the help of transport equations [3]. Nearly 10^5 showers were simulated with various energies and zenith angles using a cluster of computers. Then signal spectra were calculated assuming the standard energy spectrum of the primary particles. At last taking cuts of the signal spectra one can obtain the development curve for a signal and estimate the attenuation length. The longitudinal development of a signal was calculated to estimate the attenuation length in the individual showers. The applicability of the last method is straightforward.

As a result the value of $530 \pm 60\ g/cm^2$ was estimated for the attenuation length by the constant intensity cuts method which should be compared with $520 \pm 70\ g/cm^2$ found experimentally. The longitudinal development gives $350 \pm 12\ g/cm^2$ while calculations for vertical and inclined showers lead to various attenuation lengths of $300 - 400\ g/cm^2$. The standard method of the constant intensity cuts usually used may decrease energy estimates by factor $\sim 1.1 - 2$.

References

1. L.G.Dedenko, Proc. 14th ICRC, Munich, Germany, **8**, 2857 (1975).
2. T.K.Gaisser, A.M.Hillas, Proc. 15th ICRC, Plovdiv, Bulgaria, **8**, 353 (1977).
3. A.M.Anokhina, L.G.Dedenko, G.F.Fedorova, V.I.Galkin et al., Phys. Rev. D **60** 033004 (1999).

Poster Session A

Magnetic quantum tunneling in systems of dipolar Ising spins

Juan J. Alonso[1] **and Julio F. Fernández**[2]

[1]*Departamento de Física Aplicada 1, Universidad de Málaga, E-29071 Málaga (Spain)*

[2]*Departamento de Física de la Materia Condensada, Facultad de Ciencias, E-50009 Zaragoza (Spain)*

phone 34.952132039, fax 34.952132000, e-mail jjalonso@darnitsa.cie.uma.es

Crystals of interacting molecular magnets such as Fe8 and Mn12 acetate have been actively investigated during the last years because strong evidence of Magnetic Quantum Tunneling (MQT) has been observed in such systems at very low temperatures [1]. Crystals of these materials can be considered as ensembles of identical dipoles of spin $S = 10$ with a strong Ising anisotropy. At temperatures well below $360mK$ these systems exhibit a crossover from thermally activated MQT to a temperature independent behaviour where the relaxation of the magnetization was found to be nonexponential [2]. According to the present theory dynamic nuclear spin and the evolving distribution of the magnetic dipole £elds play an important role [3]. This is because the resonance condition condition that must be met to MQT to take place is only satis£ed if the local magnetic £eld is within some window W. Prokof'ev and Stamp have proposed that the value of W is enhanced by the ¤uctuating hyper£ne £elds generated by magnetic nuclei. Experimental determination of W is therefore important.

Wernsdorfer *et al.* [4] have performed experiments that yield the distribution of dipolar £elds by assuming the Prokof'ev and Stamp theory. An unexpected "hole" has been observed to develop in the distribution in the very short time regime, and from its width δh, the value of W has been inferred. However, the relation between W and the observed value δh is not well established.

This relation can be investigated by means of Monte Carlo simulations, since, in contrast with experiments, the value of W can be varied. In our contribution we will present numerical simulations for systems of Ising spins with dipolar interactions. As in tunneling experiments at very low temperature, in our simulations spin transitions are allowed between two states only if the energy changes by a suf£ciently small amount, less than W. We have computed the time evolution of the dipolar £eld distribution $P(H)$ after the system temperature is suddenly lowered from the paramagnetic phase to a temperature well below the ordering temperature. As in tunneling experiments performed in Fe_8 clusters near $40mK$, a "hole" develops very rapidly in $P(H)$ as time goes on. We have studied the relation between this hole width and W. We have found that $W \sim \delta h$ only if $kT < \delta h$, wich enables one to infer the value of W from experiments.

References

1. B. Schwarzschild, *Physics Today*, **50**, (1), 17 (1997).
2. C. Sangregorio, T. Ohm, C. Paulsen, R. Sessoli, D. Gateschi, *Phys. Rev. Lett.* **78**, 4645 (1997).
3. W. Wernsdorfer, T. Ohm, C. Sangregorio, R. Sessoli, D. Mailly and CPaulsen, *Phys. Rev. Lett.* **82**, 3903 (1999).
4. N.V.Prokof'ev and P.C.E. Stamp, *Phys. Rev. Lett.* **80**, 5794 (1999)

Target heating during ion-solid interactions

Christo Angelov, Nikolai Kirov

Institute for Nuclear Research and Nuclear Energy, BAS, So£a 1784, Bulgaria
Technical University, So£a, Bulgaria

Ion implantation apparatus can produce beams of suf£cient power density to raise the temperature of the implanted material by hundreds of degrees. The £nal temperature, which can be exceed the melting point in some cases, depends on such factors as the beam power density, the total accumulated dose and the number of wafers over which the beam passes during one implant cycle. The resulting heating and cooling curves have been calculated using a model of Parry and Komarov which includes the effects of ion beam heating, radiative cooling, conductive cooling and reirradiation from the surroundings. Ion beam power density was varied from 0.05 to 100 W.cm^{-2}. The values of target temperature were computed for different stages of target heating up to the point where thermal equilibrium is attained. For the system studied, conductive cooling in vacuum is less reliable and generally less effective than radiating cooling, unless conductive grease can be used. In the case of pre-existing surface amorphous layer with a well-de£ned amorphous-crystal (a-c) interface, for a given ion ¤ux (assuming pure beam heating only) either amorphization or crystallization may occur depending on the substrate temperature. Accordingly, the a-c interface will move either to greater or towards the surface. Preliminary calculation of this so-called reverse temperature (target temperature at which the processes of ion-beam induced amorphization and crystallization are balanced) is very important for choosing of basic implantation parameters. Computer simulation of target heating during ion-solid interactions is intended to the use of existing ion implantation systems. Although silicon is used in the examples, the procedure can easily be generalised to other target materials.

Diffusion in Cayley tree structures

Panos Argyrakis

Panos Argyrakis Department of Physics University of Thessaloniki P.code: 54006, Thessaloniki, Greece

e-mail: panos@physics.auth.gr , tel: +30-31-998043, fax: +30-31-998042

Diffusion properties for particles in disordered systems have been notoriously peculiar and dif£cult to predict. For example, in fractal structures it is well-known that diffusion is slowed down from the normally expected. Similar ideas pertain at the so called low-dimensional systems (d¡3, such as d=1 or d=2), or quasi 1-dimensional systems. In the current study we employ the so called Cayley tree structures. These are well known for a long time, at least as theoretical models of structures for which we can not de£ne their dimensionality as usual. Or we can say that their dimensionality is in£nity.[1] The interest in these systems stems from the fact that recently the new dendrimer molecules were synthesized, and these can be directly modeled as Cayley trees. These are large molecular systems, which for a long time eluded direct synthesis. However, since their synthesis about a decade ago they have been proven quite promising candidates for systems for which one could control the energy transfer process by varying the size, generation order, and branching ratio of the system at hand [2].

In the present study we perform computer simulations of the diffusion of particles on Cayley tree structures. We model the process with a usual random walk, and monitor such properties as at the mean-square displacement, the number of sites visited at least once, the survival probability in the presence of randomly distributed traps, etc. We compare these to the case of normal dimensionalities. We vary as a parameter the generation order, g, of the structure, and the coordination number, z, as these are the two parameters that limit the size of the system. The random walk procedure has no dif£culties at all. However, there are some inherent dif£culties encountered at the system boundaries. Due to the nature of the structure all system nodes are very close to the boundary, say at a distance of the order of g sites. Thus one encounters £nite size effects almost immediately. This makes it impossible to store the entire structure in the computer memory. For example, at g=20 and z=3 we have of the order of 10 million nodes, and the number grows extremely fast. It is thus impossible to simulate large size Cayley trees directly, due to memory limits. We, therefore, resorted to new algorithms that do not store the entire structure in memory, but only the parts used, or the index of the path traced by the diffusing particles. These algorithms will be described in detail.

Our results show that for the distance traversed, diffusion is ballistic, i.e. the distance is proportional to time, rather than the square root of time as in normal diffusion. The number of sites visited is also linearly proportional to time, making this case equivalent to the 3-dimensional normal lattice diffusion. The reason that we observe such behavior is that because of the branching, the number of pathways away from the point of origin is always larger towards the direction of the periphery, rather than towards the direction of the central core. This makes the random walk effectively a ”biased” walk, which, has, of course, very different behavior from the normal random walk. Models of how this can be corrected also also discussed. Our conclusions are that for diffusion on Cayley tree structures (dendrimer molecules) there is no universal behavior which collectively resembles diffusion in structures of any given dimensionality. Implications to recent experimental data are discussed.

References

1. B.D.Hughes and M.Sahimi, J. Stat. Phys., 29(1982)781
2. P.Argyrakis and R.Kopelman, Chem. Phys., 261(2000)391

Molecular dynamics analysis of coalescence behavior in the nanorods formation

J. A. Ascencio, and H. B. Liu.

Instituto Nacional de Investigaciones Nucleares. Km. 36.5 Carr. Mex-Tol, Ocoyoacac, Mxico. 52045, Mxico.

ascencio@nuclear.inin.mx

Gold nanorods present very interesting properties such as the enhancement of the ¤uorescence by a factor 10^6 compared with the gold metal (Mohamed, 2000) and because of large aspect ratio appear as promising for being used in nanomachines. Most of the studies on gold nanorods have used nanorods synthesized by electrochemical methods.

In the present work, we report the growth of gold nanorods using the bio-reduction method described by Gardea-Torresday with some modi£cations. We study the structure of the gold nanorods obtained by colloidal methods using high resolution TEM, dark-£eld images in the TEM, HREM image simulation and electron diffraction. In contrast to the report of Wang, who found no defects on the short nanorods and a single twin line in long ones, in our method we found that the gold nanorods show several parallel twins and in some cases follow the symmetry of the pentagonal twinned structure. The differences between electrochemical and bio-reduction methods give new insight on the nature of the gold nanorods.

Based on the experimental results, we apply molecular dynamics methods in order to analyze the dynamical behavior that are present in the colloidal process of coalescence. Multiple twins nanoparticles are studies at different dynamics conditions to get enough information about how nanoparticles coalescence produce nanorods. Gold con£gurations are studied with different models, and the conditions to produce nanorods are considered.

The results have shown that multiple twinned nanoparticles coalescence induce the formation of multiple twinned nanorods, the sequence of obtained models are analyzed as a continuous movie, and also by calculating the corresponding HREM images for each model, which help to compare directly the experimental and theoretical results.

In this work, we present the molecular dynamics results and their corresponding comparison to corroborate the analysis of the coalescence process.

Molecular dynamics study of cluster formation via vaporized media condensation

I. M. Assatourova

St. Petersburg State Technical University, Politechnicheskaya Street 29, 195251
St.-Petersburg, Russia

Phone: +7-812-5347436, Email: assatourova@AK5744.spb.edu

Simulation of granular materials using particles can be based on the two different approaches. According to the £rst one each grain is associated with the single computer particle [1]. Unfortunately the understanding of the general form of the force and moment interactions between the material grains is very incomplete, and this fact limits harshly the possibilities of such modeling. Another approach is based on representation of each grain as a cluster of computer particles, possessing monocrystal or random packing [2]. The computer particles can be associated with the atoms or molecules of the substance (conventional molecular dynamics), or they can be used as a kind of £nite elements for the grain modeling. Then interaction between grains is calculated automatically in the process of the simulation using interatomic potentials, which are much better developed [3].

The particle cluster can be formed by pure geometrical methods [4], but the preferable way is forming of the grains by the process of condensation of the vaporized mixture of the particles. The condensation process is performed as following. Firstly a random initial distribution of the particle coordinates and velocities is being set, forming initial conditions for the simulation. Then the system motion is simulated under the action of the interparticle potentials and small dissipative forces. The dissipation is intended for the kinetic energy removal from the system. Due to the total energy decreasing the particles coalesce forming grains.

In the presented work in¤uence of the several factors on the coalescence process is investigated. Firstly it is shown that the initial density in the vaporized state has strong in¤uence on the size and shape distribution of the obtained grains. Comparison of the results of 2D and 3D simulations shows that in the 2D case the coalescing is much more inclined to forming monocrystal structure then in the 3D case, where amorphous packings are likely to appear for a wide range of the simulation conditions. One of the main subjects of interests in the current investigation is in¤uence of the type of interparticle potentials on the grain formations, and vice versa, constructing of the interparticle potentials allowing to obtain the desired grain distributions. Mainly the pair potentials are considered. It is shown that the short-range potentials (e. g. high order Mie potentials) are producing irregular grain shapes, when a long range potentials (e. g. low order Mie potentials) result in spherically symmetrical grains. For some long-range potentials it is proved that the related substance can not reach the solid state even for the lowest temperatures, being always in the liquid or gas state.

Applications of the presented technique to constructing nanocrystal materials and modeling mechanical properties of the £ne powders are considered.

References

1. M. L. Falk, J. S. Langer. *Physical Review E*, 1998, 57(6), 7192–7205.
2. A. M. Krivtsov, M. Wiercigroch. *Proc. of XXVIII Summer School "Actual Problems in Mechanics"*, 2000, St. Petersburg, Russia.
3. R. Car, M. Parrinello. *Physical Review Letters*, 1985, 55(22), 2471–2474.
4. J. Schiotz, T. Vegge, F. D. Di Tolla, K. W. Jacobsen. *Physical Review B*, 1999, 60(17), 11971–11983.

Fully solvated molecular dynamics simulations of duplexes formed by modi£ed oligonucletides with nonisosteric phosphonate and xylo internucleoside linkages and their natural counterpart

Ivan Barvík, Jr., Josef Štěpánek and Jiří Bok

Institute of Physics, Charles University, Ke Karlovu 5, 12116 Prague 2, Czech Republic

tel. (00-420-2) 21911342, fax (00-420-2) 24922797, ibarvik@karlov.mff.cuni.cz

The concept of antisense nucleic acids represents a perspective approach in chemotherapy, promising to inhibit selectively unwanted gene expression by creation of a helical complex with target mRNA or DNA (carrying sense genetic information) [1]. The oligonucleotides with natural chemical composition have been, however, found unsuitable for in vivo applications because of their insuf£cient resistance against nucleases. A number of phosphonate-based mononucleotide analogs containing an O-(phosphono)methyl group instead of the natural phosphonomonoester one were found to be potent antivirals: this indicates enzyme stability of the phosphonate -O-P-CH2-O- bond. The present work deals with the nonisosteric phosphonate analog (3-O-PO2-CH2-O-5) of the natural phosphodiester internucleoside linkage (3-O-PO2-O-5). Three Watson-Crick double helical structures consisting of a natural deoxyadenosine and a complementary - natural, xylo/phosphodiesteric, and xylo/phosphonate - thymidine 15-mer were used as model systems. Impact of the internucleoside linkage modi£cation on the ability of the modi£ed oligonucleotides to hybridize with a natural DNA strand, was studied by molecular dynamics simulations. The nucleic acids were surrounded by a periodic box of 10000 TIP3P water molecules. Fully solvated trajectories were computed using the AMBER 5.0 software package. The implemented force £eld doesnt contain force constants needed to describe the modi£ed parts of the phosphonate analogs [2]. The completion was made on the base of ab initio calculations on the CH3-O-CH2-PO2-O-CH3 model system. By the molecular dynamics simulations the optimal conformation of modi£ed internucleotides linkages was determined and the deformation of relevant duplexes was described using the classical helical parameters.

In acknowledgments, this work was supported by grants of the Ministry of Education, Youth, and Sports of the Czech Republic (project No. VS 97113), of the Grant Agency of the Czech Academy of Sciences (project No. A 4055902), and of the Grant Agency of the Czech Republic (project No. 203/01/1166). The results were partially obtained by usage of computational facilities of Supercomputing centres of Charles University in Prague and Masaryk University in Brno.

References

1. E. Uhlmann and A. Peyman, 1990; Chem. Rev. 90: 544-584.
2. W. D. Cornell et al., 1995; J. Am. Chem. Soc. 117: 5179-5197.

Toughness dependence on failure regimes

I. L. Menezes-Sobrinho[1], **A. T. Bernardes**[2], **and J. G. Moreira**[3]

[1]*Departamento de Física, Universidade Federal de Viçosa, 36570-000 Viçosa, MG, Brazil*

[2]*Departamento de Física, Universidade Federal de Ouro Preto, 35400-000 Ouro Preto, MG, Brazil*

[3]*Departamento de Física, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, C.P 702, 30123-970 Belo Horizonte, MG, Brazil*

atb@iceb.ufop.br

A sort of computational models describing the fracture of distinct materials have been developed in recent years. For many of them, the high degree of correlations between its constituents leads to a high computational cost. On the other hand, models for fracture in £brous materials are very simple. A bundle of unidirectional £bers form a system with low degree of correlations allowing the simulation of large scale fracture processes.

Two basic regimes can de found: a catastrophic and a shredding [1]. In the catastrophic regime the fracture pro£le is reasonably smooth, while in the shredding regime it is very rough. A parameter of easy physical interpretation used to characterize fracture surfaces is the roughness. The roughness has a direct relation with the fractal dimension, which characterizes the fractal character of the fracture surface. Therefore, a high fractal dimension indicates a very rough fracture pro£le. Another important parameter in the study of fracture, is the fracture toughness. This quantity measures the amount of energy that a material can absorb before it breaks. The fracture toughness is intimately related to the amount of cracks that appear in the material. Therefore, the larger the number of cracks in the sample, the more energy will be absorbed before fracture occurs.

In the present paper, we simulated a model for fracture in £brous materials which allows us to obtain the fracture pro£le. We calculate the pro£le roughness and used it to de£ne the transition between the fracture regimes. We also investigate the relationship between the fracture roughness and toughness for £brous materials.

Our model consists of a bundle of N_0 parallel £bers all with the same elastic constant k. In order to simulate the height of the sample, the £bers are divided in η segments with the same length. The £ber bundle is £xed at both ends to two parallel plates, which are pulled apart. Each £ber has a rupture probability which depends on its deformation and the number of unbroken neighbouring £bers. When a £ber breaks, during the pulling process, a crack may growth through the material [2].

We obtained the fracture pro£le and evaluate its roughness and toughness. We show that in the catastrophic regime the roughness of the fracture pro£le is reasonably smooth. In the shredding regime, in which slow cracks are formed in the material, the fracture pro£le is very rough. In this regime the energy necessary to break the material is higher than in the catastrophic regime. Our results indicate that the roughness is related to the fracture toughness.

References

1. I. L. Menezes-Sobrinho, J. G. Moreira, and A. T. Bernardes, Eur. Phys. J. B. **13**, 313 (2000).
2. Menezes-Sobrinho, I.L., Bernardes, A.T. and Moreira, J.G., Phys. Rev. E, **63**, 25104 (2001);

Terrace sizes, slope selection and the role of desorption in unstable epitaxial growth

Michael Biehl[1], **Martin Ahr** [1], **Martin Kinne**[2], **Wolfgang Kinzel**[1], **and Stefan Schinzer**[1]

[1] *Julius–Maximilians–Universität Würzburg, Institut für Theoretische Physik und Astrophysik, Am Hubland, 97074 Würzburg, Germany*

[2] *Friedrich–Alexander–Universität Erlangen–Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany*

+49 931 888 5865, +49 931 888 5141, biehl@physik.uni-wuerzburg.de

Epitaxial growth has become a standard method for the production of high–quality crystals and £lms. Signi£cant effort has been devoted to a theoretical understanding of the many morphologies and scaling behaviors that can be observed, see e.g. [1]. Here, we address the frequently observed phenomenon of mounds in unstable growth which has attracted considerable interest in this context.

A solid–on–solid model of epitaxial growth is re–visited [2, 3]. In the model, single particles are deposited on a growing surface. Arriving adatoms are locally incorporated or perform a random diffusion until they stick irreversibly to lateral binding partners. A restriction of the diffusion process is due to the presence of an Ehrlich–Schwoebel (ES) barrier which hinders downward moves at step edges. Incorporation and the ES–effect result in slope dependent upward and downward particle currents, which compete on the surface.

In continuous models of unstable growth, slope dependent particle currents are frequently introduced in an *ad hoc* fashion [1]. Here, we discuss the microscopic mechanisms yielding these currents in the framework of solid–on–solid systems. To our knowledge, we present the £rst discrete model which allows for calculating the distribution of terrace sizes and the resulting currents on a stepped surface. The cancellation of competing up– and downward currents gives rise to the selection of a stable *magic slope* which is evaluated as well.

The results are exact for an in£nite ES–barrier and we £nd a Poisson distribution of terrace sizes in this limit. In general, an approximation allows for a self–consistent numerical treatment. Kinetic Monte Carlo simulations of the growth process show very good agreement with the theoretical £ndings.

Our results complement those of a BCF–like treatment [1] which neglects ¤uctuating terrace sizes. Further, the frequency of terrace sizes differs signi£cantly from the frequently assumed geometric distribution on vicinal surfaces.

Extending the results of [4], we include desorption in the model and study its in¤uence on the statistical properties of the growing surface. We observe in Kinetic Monte Carlo simulations, that an increasing desorption rate triggers a transition from mound structures with slope selection to self–af£ne, rough growth.

References

1. A. Pimpinelli and J. Villain, *Physics of Crystal Growth*, Cambridge University Press, 1998.
2. M. Biehl, W. Kinzel, and S. Schinzer, Europhys. Lett. **41**, 443, 1998.
3. S. Schinzer, M. Kinne, and W. Kinzel, Surface Science **439**, 191, 1999.
4. M. Biehl, M. Ahr, M. Kinne, W. Kinzel, and S. Schinzer, preprint (2001), cond-mat/0102166.

Propagation of nonlinear surface polaritons in 2D electron system

N.N. Beletskii and Y.V. Bludov

Usikov Institute for radiophysics and electronics, NAS of Ukraine. 12, Acad. Proscura st., Kharkov, 61085, Ukraine.

tel.: +38-0572-448-331, , fax: +38-0572-441-105, e-mail: bludov@ire.kharkov.ua

Surface polaritons (SP) in nonlinear media possess some new unusual features in comparison with SP in linear media. For example, an excitation of SP becomes possible without using prisms and periodical structures. It can occur when wave train falls directly upon the interface [1].

The paper deals with the theoretical investigation of surface polaritons (SP) in in£nitely extended two-dimensional electron system (2DES), placed at the boundary ($z = 0$) between linear and nonlinear media. We considered that the region $z < 0$ is occupied by linear uniform medium with dielectric constant ε_1 and the region $z > 0$ is occupied by the nonlinear medium which dielectric tensor possesses only diagonal components. We supposed that tensor depends upon the electric £eld E_x only and it's components take the form: $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon + \rho|E_x|^2$, $\varepsilon_{zz} = \varepsilon_0$. We consider only the case $\rho < 0$. A constant quantizing magnetic £eld is directed perpendicularly to 2DES along axis z.

For obtaining the dispersion relation we used Maxwell equations with standard boundary conditions at interface. We consider that tangential components of electric £eld are continuous across the interface $z = 0$, and tangential components of magnetic £eld are discontinuous across the interface due to presence of currents in 2DES. Due to the fact that dielectric tensor of nonlinear medium depends upon component E_x only, the nonlinear differential equation for E_x component can be solved analytically. But the differential equation for E_y component should be solved numerically by £nite element method. In our paper we used the formulas for high-frequency 2DES conductivity tensor under the quantum Hall effect conditions obtained in papers [2].

It is shown, that in the case of such type nonlinearity SP's exist only in the case when $E_x(0) \leq E_{max} = \sqrt{2\varepsilon/|\rho|}$. A new additional mode of SP – nonlinear surface polariton (NSP) appears in the SP spectrum, which has no analog in linear case. The dispersion curve of NSP exists at frequencies of the order of cyclotron resonance (CR) and has a spectrum end-point lying on the light line $\omega = k\, v_d$ (where $v_d = c/\sqrt{\varepsilon}$ is the velocity of light in the dielectric medium). Notice that at the long-wave region (for small values of k) the NSP possesses normal dispersion but at short-wave region NSP possesses anomalous dispersion. At the same time a resonant interaction between the NSP and the usual SP mode occurs in the vicinity of CR subharmonic. With the increasing of Landau-level £lling factor of 2DES the resonant interaction point shifts to the longer-wave region. It's found that the E_x component of NSP electric £eld in the region $0 < z < z_0$ increases with the increasing of z and $E_x(z_0) = E_{max}$ (here z_0 is the depth of localization). At the same time the value of E_x decreases with the increasing of z in the region $z_0 < z < \infty$. Notice that the electric £eld $E_y(z)$ decreases monotonely with the increasing of z.

Notice, that with the increasing of $E_x(0)$ a low frequency mode of usual SP shifts to the higher-frequency region and NSP shifts to the lower-frequency region. When $E_x(0) = E_{max}$, the dispersion curves of usual SP and NSP coincide.

References

1. Marcuse D. // Appl. Opt. **19**, 3130(1980)
2. Aronov I.E., Beletskii N.N. // J.Phys.: Condens. Matter **8**, 4919(1996)

Melting of metallic clusters studied by *ab initio* electronic structure methods

S. A. Blundell and Rajendra R. Zope

Département de Recherche Fondamentale sur la MatiÁre Condensée
CEA-Grenoble, 17 rue des Martyrs, F-38054 Grenoble CEDEX 9, France
tel: (+33) 476885939, fax: (+33) 476885160, sblundell@cea.fr

Most statistical simulations of atomic and molecular clusters have been based on semiempirical interatomic potentials such as the Lennard-Jones or embedded-atom model potentials, which have a simple analytic parametrization and are computationally cheap. However, recent experiments measuring the caloric curves of small sodium clusters [1] show an irregular variation of cluster melting point with respect to cluster size, with pronounced maxima at the puzzling sizes of $N = 57$ and $N = 142$. This points to a subtle interplay between geometric effects and electronic shell effects, which is dif£cult to incorporate in a semiempirical potential, and a precise theoretical explanation is so far lacking.

In this paper we address the possibility of making an accurate extraction of statistical quantities such as the ionic entropy and the ionic speci£c heat using an *ab initio* interatomic potential derived from density functional theory. Several novel approaches will be discussed. First, extending earlier work on the temperature dependence of the polarizability [2], we use an $O(N)$ density-based parametrization of the electron kinetic energy, and sample the ionic phase space by means of microcanonical molecular dynamics, with a Car-Parrinello-type propagation of the electron density. The ionic entropy is extracted by multiple histogram methods. We present statistically well-converged caloric curves for clusters of size up to $N = 147$. Second, we consider a Kohn-Sham approach, with both *ab initio* and soft, phenomenological pseudopotentials. Here the phase space is sampled both by molecular dynamical and also by Monte Carlo methods, including parallel tempering Monte Carlo to help improve the ergodicity of the sampling.

We £nd that the smaller clusters prefer a multi-step melting process, proceeding via isomerization and rearrangement processes. The larger clusters $90 < N < 147$ considered show a one-step melting process, with simultaneous melting of all ionic shells, and a corresponding pronounced single peak in the ionic speci£c-heat curves. Using the density-based approach, we £nd a pronounced maximum in the melting point at a size of $N = 55$, in disagreement with the experimental maximum at $N = 57$. Prospects for improving the accuracy of the density functional, and of extending the calculations to larger sizes, will be discussed.

References

1. M. Schmidt *et al.*, Phys. Rev. Lett. **79**, 99 (1997); M. Schmidt *et al.*, Nature **393**, 238 (1998).
2. S. A. Blundell, C. Guet, and R. R. Zope, Phys. Rev. Lett. **84**, 4826 (2000).

Optical spectra of indium bromide: Theory and experiment

M.I. Kolinko and O.V. Bovgyra

Ivan Franko National University of Lviv,
1 Universytetska Str., Lviv 79602, Ukraine
tel: +380 322744127, fax: +380 322 727981, kolinko@franko.lviv.ua

The layered indium bromide single crystals that have been synthesized comparatively lately, as well as other representatives of A^3B^7 family are being intensively investigated from the point of view of the unique combination of their optical properties.

The most complete and easy-to-interpret information about the peculiarities and parameters of the electronic spectra are contained in the complex of fundamental optical functions. The determination of the optical function spectra in the broad energy region for different light polarizations has been accomplished on the basis of low-temperature experimental re¤ection spectra using the Kramers-Kronig technique.

In order to get precise information on band-structure parameters for the £rst time we carried out £rst-principle self-consistence calculations using the method of a nonlocal norm-conserving pseudopotentials [1]. To obtain the $\mathbf{k}$-space band dispersion diagram the energies have been tabulated at 535 points on edges and high symmetry lines in the irreducible part of the Brillouin zone. The charge density distribution $\rho(\mathbf{r})$ was calculated by the method of special points [2]. In the calculations of density of states $N(E)$ and imaginary part of the dielectric function ε_2 the tetrahedron integration method was used. The detail explanation of the theoretical framework and main approximations used are presented in [3].

The comparison of experimental results with the data of theoretical calculations of energy band structure of InBr enabled us to make the identi£cation of the main peaks in the spectra of re¤ectivity and dielectric function. The $\mathbf{k}$-space identi£cation of the substantial structures has been accomplished on the basis of study of the electron density distribution $\rho(\mathbf{r})$ for the occupied and virtual states, band diagram and using group theory analysis as well. The re¤ection spectra show a complex structure of up to 10 peaks for each polarization direction in the range 2-15 eV. On the whole, this structure is assigned to the transitions from valence bands of Br $4p$ and In $5s, 5p$. The top valence band is formed predominantly by cation $5s$ orbitals, and the bottom conduction band by $5p_z$ In orbitals. Thus, the £rst direct exciton transition observed at 2.33 eV for $\mathbf{E}\|\mathbf{c}$ takes place in the cationic sublattice. The structure that appears in the spectra in the region up to 15 eV is due to transitions from the halogen $4s$ states. At about 19 eV the sharp doublet structure was observed due to the metal core d-states. The analysis of the calculated dielectric functions shows that there is an in¤uence of both van Hove singularities and volume effects on the formation of the electron spectra in InBr. In general, qualitatively good agreement with experiment is found, but all peak positions are somewhat shifted to lower energies since the local density approximation underestimates the optical band gaps. The inclusion of empirical lifetime and self-energy corrections improves the theoretical-experimental agreement.

The results obtained allow for the £rst time the optical spectra of InBr to be identi£ed, and can serve as a basis for understanding the physical mechanisms in strongly anisotropic compounds.

References

1. G.B. Bachelet, D.R. Hamann, M. Schlüter, Phys. Rev. B. **26**, 4199 (1982).
2. D.J. Chadi and M.L. Cohen, Phys. Rev B. **8**, 5747 (1973).
3. M.I. Kolinko, I.V. Kityk and A.S. Krochuk, J. Phys. Chem. Solids **53**, 1315 (1992).

Estimation of electrical durability of dielectrics

I.A. Brigadnov

North-Western State Technical University
Millionnaya 5, St. Petersburg, 191186, Russia
phone:+7-812–514-9109, fax:+7-812–311-6016, e-mail:brigadnov@nwpi.ru

The electrical state of a medium in a given domain $\Omega \subset R^3$ is characterized by the bulk and surface density of charges ($\rho : \Omega \to R$ and $g : \Gamma^2 \subset \partial\Omega \to R$, respectively) and by vectors of electrical tensity, electrical induction and electrical current density $E, D, J : \Omega \to R^3$, respectively [1]. Vector D is introduced by the rule $D = \varepsilon_0 E + P$, where $\varepsilon_0 \approx 8.85 \cdot 10^{-12}$ is the electrical constant and $P \in R^3$ is the vector of polarization. For the electrical tensity the scalar potential u is introduced such that $E = -\nabla u$. The polarization and ionization properties of dielectrical medium are discribed by two constitutive ralations $D = \hat{D}(x, E) : \Omega \times R^3 \to R^3$ and $J = \hat{J}(x, E) : \Omega \times R^3 \to R^3$.

In electrostatics it is assumed that an external source of the electrical £eld compensates the work of the electrical current in the dielectric. In accordance with the classical Thomson's principle [1] the variational formulation of the electrostatical boundary-value problem (BVP) is used taking into account the current of conductivity.

In powerful electrical £elds the nonlinear phenomena of polarization saturation ($|P| \le P_* < +\infty$) and essential ionization ($|J|/|E| \gg \varepsilon_0$) must be taken into account [1]. The complementary physical parameter of dielectrical medium $\lambda > 0$ always exists such that $\left|\hat{D}(x, E) - \hat{J}(x, E)\right| \le \lambda(x)$ for every $E \in R^3$ and almost every $x \in \Omega$. As a result, *the limiting analysis problem* (LAP) is formulated as the following original variational problem

$$t_* = \inf \left\{ \int\limits_\Omega |\nabla u(x)| \lambda(x)\, dx : \; u \in W^{1,1}(\Omega);\; u(x) = u^0(x),\; x \in \Gamma^1;\; \int\limits_\Omega \rho u\, dx + \int\limits_{\Gamma^2} g u\, d\gamma = 1 \right\},$$

where u^0 is a given potential on $\Gamma^1 = \partial\Omega \setminus \Gamma^2$ with $\mathrm{area}(\Gamma^1) > 0$. If $t_* > 1$ then the electrostatical BVP has no solution. From the physical point of view this effect is treated as a loss of the electrostatical balance, i.e. as beginning of the electrical puncture of dielectric.

From the mathematical point of view LAP is non-correct because its solution belongs to the space $BV(\Omega) \supset W^{1,1}(\Omega)$ of scalar functions with bounded variations having the generalized gradient as the bounded Radon's measure. As a result, LAP needs a relaxation. We propose *the partial relaxation* of LAP which is based on the special discontinuous £nite-element approximation [2].

After this approximation LAP is transformed into the system of non-linear algebraic equations which can be *ill conditioned.* Therefore, for the numerical solution the decomposition method of adaptive block relaxation is used because it practically disregards the condition number of the global stiffness matrix [3]. The appropriate numerical results show that for £nding the main parameter t_*, the proposed technique has the qualitative advantage over the standard continuous £nite-element approximations.

References

1. Tamm, I.E. *Bases of the Electricity Theory*, Nauka: Moscow, 1989 (in Russian).
2. Brigadnov, I.A. Discontinuous solutions and their £nite element approximation in non-linear elasticity. *Advanced Computational Methods in Engineering*, eds. R. Van Keer, B. Verhegghe, M. Hogge & E. Noldus, Shaker Publishing B.V.: Maastricht, 1998. pp. 141–148.
3. Brigadnov, I.A. Numerical methods in non-linear elasticity. *Numerical Methods in Engineering*, eds. J.-A. Desideri, P. Le Tallec, E. Onate, J. Periaux & E. Stein, Wiley: Chichester, 1996. pp. 158–163.

Phase constitution of Ni-based quaternary alloys studied by Monte Carlo simulation

Jiří Buršík

Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Žižkova 22, 616 62 Brno, Czech Republic

Tel.: +420 5 41636473; fax: +420 5 41218657; bursik@ipm.cz

Further improvement of advanced Ni-based superalloys calls for deeper understanding of the phase transitions and better description of phase equilibria at service temperatures [1]. Owing to rather complex alloying of these alloys it is extremely difficult to apply the standard methods of thermodynamic modelling. Advanced superalloys contain typically over six alloying elements; on the other hand the present assessments of thermodynamic parameters for phase diagram calculations are usually dealing with ternary or even binary subsystems. Another class of promising methods of prediction of phase constitution of alloys is based on the computer modelling at the atomic level. These methods are very suitable especially for modelling of the order–disorder phase transitions. This is exactly the case of Ni-based superalloys where the superior mechanical properties at high temperature can be attributed to the dispersion of coherent precipitates of an ordered phase (γ') distributed in a disordered ductile matrix (γ).

The aim of this paper is to study ordering processes in Ni-based quaternary systems using a Monte Carlo simulation technique. This method is well established and used in many branches of solid state physics including this particular problem [2]. To simulate the ordering processes in our systems the Ising Hamiltonian was used to express the configurational energy of the system. Pair interactions were introduced by means of phenomenological Lennard-Jones potentials [3]. The impact of the interaction range on the results was studied by taking into account either only the nearest and next nearest neighbours or also more distant pair interactions up to third coordination sphere. The ordering process itself was realised by direct atomic pair exchanges (Kawasaki dynamics). The value of an average lattice parameter was readjusted periodically during the calculation.

The primary output of Monte Carlo simulation are time series of real-space snapshots of the atomic arrangement at given annealing temperature and chemical composition. From these data follows the correlation between short range order parameters and metric parameters of ordered domains. The most important result for practical purposes is the evaluation of the site preferences of alloying elements in the γ and γ' phases. Although qualitative agreement between the simulation output and experimental literature data can be stated, the results indicate that for satisfactory quantitative agreement resulting in realistic phase diagrams the Lennard-Jones potentials are to be improved or replaced by a different type of potential. The empirical many-body potential of a Finnis-Sinclair type [4] seems to be a suitable candidate.

The work has been supported by the Grant Agency of Czech Republic as the project No. 202/01/0383.

References

1. High-Temperature Ordered Intermetallic Alloys, I. Baker et al, eds, MRS, Pittsburgh, Pennsylvania, 1993.
2. Y. Saito and H. Harada: Mater. Sci. Eng. A 223 (1997) 1.
3. M. Enomoto and H. Harada: Metall. Trans. A 20 (1989) 649.
4. M. W. Finnis and J. E. Sinclair: Phil. Mag. A 50 (1984) 45.

First principle investigation of the intermediate range order in disordered materials: the case of $SiSe_2$

Massimo Celino[1] **and Carlo Massobrio**[2]

[1]*ENEA, HPCN Project, CR Casaccia, CP2400, 00100 Roma AD, Italy*
[2]*IPCMS, CNRS, 23 rue du Loess, F-67037 Strasbourg, France*

Tel.: +39-06-30483871, Fax: +39-06-30484230
Email: massimo.celino@casaccia.enea.it

The atomic structure of disordered materials is not yet well understood, mostly because of dif£culties to link observations in reciprocal space to unambiguous feature in real space. This situation is even more striking in the case of covalent AX_2 disordered materials, which are characterized by intermediate range order (IRO), as revealed by several diffraction experiments [1]. The establishement of IRO (the level of structural organization beyond nearest-neighbors) is accompanied by the appearance of the £rst sharp diffraction peak (FSDP) in the total structure factor at values of the momentum transfer typically half that of the main peak. Recently the $GeSe_2$ material, both in the amorphous and in the liquid phase, has been widely studied and characterized by classical and £rst principle molecular dynamics (FPMD) simulations. In particular, it appears clear that the better performances of FPMD are crucial to describe correctly the atomic bonding. Moreover, it has been recently shown, in the case of liquid $GeSe_2$, that the role of the ionicity and the presence of homopolar bonds, not well described by classical potentials, are essential to reproduce the main features in the partial structure factors [2].

In this framework, FPMD simulations of $SiSe_2$ can play a key role in the understanding of this class of materials. $SiSe_2$ has a very peculiar crystalline structure, in which all $SiSe_4$ tetrahedra share two Se atoms, i.e. are edge-shared connected, leading to a molecular network with macroscopic extension in one dimension. The question arises as to which extent this peculiar structure will persist in the disordered phase and which information can be gained on the correlation between the connectivity of the tetrahedra and the appearance of the FSDP. In this respect it should be stressed that classical molecular dynamics models are not compatible with the existence of homopolar bonds, which might alter the chemical order within the network.

FPMD simulations of the glassy $SiSe_2$ system are performed in the framework of Car-Parrinello technique in which electronic structure is described within density functional theory and evolves self-consistently during the ionic motion [4]. A GGA for the exchange and correlation energy is adopted. Simulations are carried out at constant volume and constant temperature.

Two disordered structures are produced: the £rst one from a completely random initial con£guration and the second one from an initially ordered arrangement with edge-shared tetrahedra only. We provide a full picture of the atomic con£guration for the liquid and for the amorphous structure in terms of partial structure factors, pair correlation functions, bond angle distributions and a ring statistics. This reveals that the regular tetrahedral network is disrupted by homopolar bonds. Moreover, both corner sharing and edge sharing connections are present, in marked contrast with the crystalline arrangement consisting of edge-sharing connections only. Analogies and differences with other disordered network-forming materials (SiO_2, $GeSe_2$) will also be discussed.

References

1. S. R. Elliott, Nature (London) **354**, 445 (1991).
2. C. Massobrio, A. Pasquarello, R. Car, Phys. Rev. Lett. **80**, 2342 (1998); J. Am. Chem. Soc. **121**, 2943 (1999).
3. G. Antonio, R. K. Kalia, A. Nakano, P. Vashishta, Phys. Rev. B **45**, 7455 (1992).
4. R. Car, M. Parrinello, Phys. Rev. Lett. **55**, 2471 (1985).

Calculation of linear and nonlinear optical properties of granulated multilayers

D.R. Barskii, I.N. Cherichihin and E.D. Mishina

Moscow Institute of Radioengineering, Electronics and Automation, prosp. Vernadskogo 78, 117454 Moscow, Russia

igor_vnd@mtu-net.ru

Nanoscale materials play more and more important role in the modern electronics and optoelectronics. New properties of multilayers and quantum dots, including effects of quantum con£nement and local electromagnetic £eld enhancement have been observed and already utilized; the recent fascinating example is presented in [1]. The properties of multilayers and quantum dots can be varied in a speci£ed way by variation of geometrical parameters and adjacent materials. Recently the fabrication and optical properties of even more complicated multilayered structure has been reported [2], in which one of two altering layers represents a nanoparticle array. Although linear optical properties of both multilayers and quantum dots can be obtained separately in the frames of already classical problems, there is no adequate description for the whole system. The problem of nonlinear optical properties of multilayers and nanoparticles is more recent [3] and not generalized yet even for separate systems.

In this paper, we present the results of self-consistent calculation of linear optical properties (re¤ectivity, transmittance and absorbance) and nonlinear optical properties (second harmonic generation intensity) of multilayers, in which one of two periodic layers is a semiconductor, and the second one consists of metal nanoparticles embedded in a semiconductor matrix.

Optical properties of nanoparticles are described by Mie theory. The dielectric function of individual particle is described by Drude model. Logarithmic distribution of particle size is taken into account. Matrix approximation is used for treating both linear and nonlinear optical properties of multilayers. Comparison of our exact solution approach with the effective media approximation applied either for nanoparticles layer or to the whole structure is presented.

The program is written in C++. The program allows, using selected panels to display the dependences of optical properties as functions of the wavelength, the number and the thickness of the layers. With the use of the program on-line alteration of the angle of incidence, and the size of the particle is possible. The program allows us also to £t experimental data. The program is user-friendly and compatible with LabView environment.

The results of calculation of linear optical properties are checked for the Cu/CuO_2 multilayered structure [3] with the thickness of the layers varied in the range of 0.8 - 2 nm and 11-20 nm for CuO_2 and copper composite respectively and the size of particles in copper composite layer varied in the range of 10-30 nm. It is shown, that our exact solution approach gives much closer approximation to experimental results than effective media calculations. New spectral features and enhancement of the SHG intensity in such structures are predicted. Optimal layer/particle con£guration for the best display of these features is suggested. We show that the model and the program could be very powerful, particularly while applying simultaneously with experimental studies of linear and nonlinear optical properties of granulated multilayered nanostructures.

References

1. L.A. Peyser, A.E. Vinson, A.P. Bartko, R.M. Dickson, Science. **291**, 103 (2001).
2. J.A. Switzer, C-J. Hung, E.W. Bohanman, M.G. Shumsky, T.D. Golden, and D.C. Van Aken, Adv. Materials **9**, 334 (1977).
3. B. Koopmans, M.G. Koerkamp, Th. Rasing, H.van der Berg, Phys. Rev. Lett. **74**, 3692 (1995).

On short life energy ¤uctuations in low dimensional systems

Dan Chicea and Dorin Gh. Stoicescu

Physics Dept., University Lucian Blaga, Str. Dr. Ion Ratiu nr. 7-9, Sibiu, 2400, Romania

telephone: 40-95-789781, fax: 40-69-216617, e-mail: dchicea@univ.sibiu.ro

A computer experiment to analyze the behavior of a light ion inside the lattice of a heavier element has been designed and performed. We de£ne the short life energy ¤uctuation of an ion or atom , here after SLEF, to be the time interval during which the energy of the ion has a value higher than a speci£c threshold for a certain number of consecutive interactions [1].

First a one dimensional system was considered. A statistical collection was generated by computer and the host lattice ions had a Maxwell velocity distribution. The light ion started it's hypothetical evolution through the lattice having an initial energy equal with the thermal energy. A random number generator was used to select from the collection the host lattice ion for the next collision. An elastic collision in one dimension was considered and the host lattice ion energy and velocity after collision was recorded back and kept as initial values for the next collision. Both the energy and the velocity of the light ion were recorded after each interaction. Each target ion has been collided twenty times as an average. This number was selected because for a lower number of collisions the host lattice ions distribution was found to be distorted from the Maxwell shape.

After the hypothetical experiment was completed, the recorded values of the energy of the light ion were analyzed and the SLEFs were identi£ed. We found from this experiment that the energy distribution of the light ion is shifted towards higher energies that the thermal energy, the higher the mass number is the bigger is the shift. Another interesting result is that SLEFs were found in a surprisingly large amount, meaning that during a considerable part of the experiment time the energy is a few times higher that the thermal energy [2], [3].

The model was extended to a two - dimensional system, using the same algorithm. Elastic collisions in two dimensions were considered this time. SLEFs were identi£ed after the experiment analyzing the recorded values of the light ion energy after each interaction. Different ways of modeling the motion of each host ion lattice were investigated and work is still in progress.

Certain differences were found between the one and the two - dimensional models. The differences between the predicted energy distribution shift are analyzed. Results are discussed in connection with the experimental data on certain lattices like Palladium and Titanium that can absorb Hydrogen isotope ions in an unusually large amount.

References

1. K.R. Rao, S. L. Chaplot, ”Computer Experiments Concerning Palladium - Deuterium Lattices - Implications to Phenomenon of Low Energy Nuclear Reactions”, Fusion Technology vol. 30, pg. 355, Dec. 1996.
2. K.R. Rao, S. L. Chaplot, ”Phonons in Condensed Matter Physics”, p. 3, R.K. Singh and S.P. Sanyal Eds. Wiley Eastern Delhi, 1990.
3. L. Chaplot, ”Phonons in Condensed Matter Physics”, p. 149, R.K. Singh and S.P. Sanyal Eds. Wiley Eastern Delhi, 1990.

The ampere force computation

Dan Chicea
Physics Dept., University Lucian Blaga, Str. Dr. Ion Ratiu nr. 7-9, Sibiu, 2400, Romania
telephone: 40-95-789781, fax: 40-69-216617, e-mail: dchicea@univ.sibiu.ro

A law for the mechanical force between two current elements, experimentally deduced in 1820 by Ampere and recently demonstrated by Rambaud using the Maxwell-Lorentz- Einstein electromagnetic laws [1], states that an electric current ¤owing through a straight conductor should place it in tension. For two randomly oriented current elements the result is the same as the force computed by the Biot-Savart law, while for two currents which are placed on the same axis as the current ¤ows, the Ampere forces predict repulsive force while Biot-Savart formula predicts a null force [2].

A nondimensional quantity, named reduced force was derived and used for computations; the real force was then calculated by multiplying it with the total current. The total current was divided in £nite elements and the interaction force between two parts of the conductor was calculated. A direct analysis of the method was done to validate the results.

The distribution of the Ampere forces in the conductor section, for different sections was calculated and data is plotted in 3D. Then the interaction force between two parts of the conductor was computed and the calculated values were compared with the experimental data on wire fracturing as a result of the Ampere forces produced by electric currents in the range of hundreds of KiloAmpers [3].

A speculation on the possibility of Ampere forces acting as an ion acceleration mechanism to explain anisotropy of the neutron emission from a frozen Deuterium £ber explosion is presented as a conclusion [4].

References

1. Graneau, P. - First indication of Ampere tension in solid electric conductors, Phys. Lett. A 97 (1983), no. 6, p. 253.
2. Rambaut, M. - Macroscopic non-relativistic Ampere EM interactions between current elements re¤ect the conducting electron accelerations by the ion’s electric £elds, Phys. Lett. A 154 (1991), no. 5,6, p. 210.
3. Nasilowski, J. - Exploding wires, Plenum, New York, 1964.
4. Graneau, P. and Graneau, N. - The role of Ampere forces in nuclear fusion, Phys. Lett. A 165 (1992), p. 1.

Simulation of peculiarities of lowtemperature luminescence of cadmium tungstate crystals doped with Dy^{3+} ions

Chukova O.V., Nedilko S.G., Scherbatskiy V.P., Sheludko V.I.

Physics Faculty, Taras Shevcheenko National Kyiv University 6, acad. Hlushkov Ave., 03680 Kyiv, Ukraine

+380 44 2664036, +380 44 2664036, chukova@ups.kiev.ua

Properties of electron-vibration interaction in luminescence centers in solid state are displaying in the $I(\nu)$ spectral distribution and I(t) intensity ($\eta(T)$ yield) of luminescence and their temperature dependencies. Tungstate crystals have attracted a much attention in the last years correspondingly to their wide application as scintillators. Rare-earth (RE) ions are widely used for doping various tungstate crystals because they can cause some desirable changes of the physical properties of these crystals. At the same time, RE ions can be a luminescent probe for investigation of a crystal matrix. [1].

Absorption, excitation and luminescence spectra of $CdWO_4$ crystals doped with Dy^{3+} ions (CWO-Dy) contain on the background of nonstructural matrix emission the narrow spectral lines caused by the inner transitions in $4f^n$ shall of $Dy3^+$ ions. In order to identify spectral lines we have carried out computer simulation of average values of energy matrix for Dy^{3+} ions in CWO crystal using parameterisation procedure for impurity ions in crystals. Obtained $F^k(nl, nl)$ parameters were used for solution of a direct spectroscopy task - calculation of the energies of all actual in the absorption and luminescence levels of impurity ion and study of probabilities of radiation transitions using Judd-Ofelt's theory. [2].

In order to describe observed anomalous behavior of I(T) dependence of Dy^{3+} luminescence intensity on temperature at 477 nm excitation, we have £rstly described luminescence intensity by solution of two kinetic rates describing populations of the F_1 lowest excited sublevel and F_2 effective level the center of Stark multiplet. Then we have expanded this solution by interaction of electron absorption transition with a photon and a phonon taking into account respective temperature distribution as well as background emission of defect matrix. Therefore we have obtain the follow expression for the anomalous luminescence intensity:

$$I_L(T) = I_L(0)\left[1 + \frac{C}{\left(1 + A\exp\left(\frac{-\Delta E_{12}}{kT}\right) + B\exp\left(\frac{-E_a}{kT}\right)\right)\left(\exp\left(\frac{\hbar\nu_{ph}}{kT}\right) - 1\right)}\right]$$

where $\Delta E_{12} = 160cm^{-1} = E_2 - E_1$; A, B, C are parameters. Then using variation method we have obtained the value of parameters giving the best approximation of experimental results. There are 90, $2 * 10^9$ and 480 for A, B, and C respectively. The activation energy $E_a = 3700cm^{-1}$ and energy of additional photon taking part in this case in two-photon excitation of luminescence $\nu_{ph} = 120cm^{-1}$. The calculated value of ν_{ph} is closed to frequency of CWO lattice's phonon. Therefore, computer modeling of anomalous I(T) behavior allow us to establish two photon excitation of this luminescence and interaction of inner electron transition in impurity ions with host lattice's phonon in Dy^{3+} doped CWO crystals.

References

1. M.Nikl, Phys. Stat. Sol. (a) 178, 595 (2000).
2. W.T.Carnall Handbook on the Physics and Chemistry of Rare-Earth. New-York (1979)

Visualization of Coulomb correlations in £nite metallic systems

Florin Despa R. Stephen Berry

Department of Chemistry, The University of Chicago, Chicago, Illinois 60637

The way electrons are correlated in a three-body system such as He^{**} or the valence electrons of Mg can be inferred from the probability distribution implied by their wavefunction.[1] This method provided a vivid and precise way to depict the correlation of two electrons. For the system of more particles, we have yet to £nd a comparably powerful approach because too much information is contained in the wave function and we do not know how to extract what is relevant in a manner adaptable to pictures. An exception emerges, obviously, for the high-density limit of the Fermi ¤uid where a collective description of electrons is likely to be optimal.

Working toward extracting insights from the probability density $|\Psi|^2$ and making use of the quasi-classical description for the (valence) electron gas,[2, 3] we develop here an analytical ansatz which allows us to £nd and visualize the effective electrostatic potential and Coulomb correlations in multi-center problems. We focus on their interpretive aspects and speci£cally on extracting insights regarding the geometric effects of Coulomb correlations for any given spatial disposition of ionic cores. Also, we explore the case of a foreign metal atom doping a otherwise-homogeneous cluster of metallic atoms. This approach provides us with a direct visualization of the way both the screening effect and the Coulomb correlations change with changes of the location of the impurity. This analysis is important in the context of recent observations of the role played by composition and geometry in changing the physical properties of metallic clusters.[4]

References

1. see, for review, R.S. Berry, in *The Lesson of Quantum Theory*, edited by J. deBoer and O. Ulfbeck (North-Holland, Amsterdam, 1986)
2. N.H. March, W.H. Young, and S. Sampanthar, in *The Many-Body Problem in Quantum Mechanics* (New York, Dover, 1995)
3. F. Despa, Phys. Rev. **B57** 7335 (1998)
4. M. Heinebrodt, N. Malinowski, F. Tast, W. Branz, I.M.L. Billas, and T.P. Martin, J. Chem. Phys. **110** 9915 (1999); W. Bouwen, F. Vanhoutte, F. Despa, S. Bouckaert, S. Neukermans, L. Theil Kuhn, H. Weidele, P. Lievens, and R.E. Silverans, Chem. Phys. Lett. **314** 227 (1999)

SiC(0001) surfaces: Stacking defects and the implications for the epitaxial growth of silicon carbide

G. Borghi[1], **R. Di Felice**[1], **C. M. Bertoni**[1] **and A. Catellani**[2]

[1]*INFM UnitÁa di Modena and Dipartimento di Fisica, UniversitÁa di Modena e Reggio Emilia, via Campi 213 A 41100 Modena Italy*

[2]*CNR-MASPEC, Parco Area delle Scienze 37a, 43010 Parma, Italy*

0039-059-2055301, 0039-059-367488, rosa@unimo.it

Wide-bandgap semiconductors have suitable properties for applications in high temperature and high power electronics. Among them, Silicon Carbide has received particular attention [1].

A very peculiar feature of SiC is the existence of many polytypes [2], with small energy differences between them. The relative stability of SiC polytypes in the bulk form has been extensively studied theoretically and experimentally. On the contrary, the effect of the presence of a surface on the stacking properties of the material has been scarcely investigated.

We present the results of ab-initio calculations for different SiC(0001)-$\sqrt{3} \times \sqrt{3}$ surfaces: this type of reconstruction is well known for SiC(0001) [3], despite its microscopic nature is still controversial [4]. Several geometries are selected, in order to get insight into the stacking properties of SiC at the surface termination. Moreover, we study the modi£cations of the polytype energetics in the proximity of a surface may affect the growth of Silicon Carbide.

Recently, Starke and coworkers have observed by Scanning Tunneling Microscopy (STM) that a cubic stacking sequence is favorable to occur at the surface of 4H-SiC(0001) [3]. We investigate the microscopic details of this effect by performing total energy and electronic structure calculations for both 3C-SiC(0001) and 4H-SiC(0001), varying the stacking of the outermost layer from cubic (3C) to hexagonal (2H). We have studied also other structure to take into account different possible subsurface terminations of the 4H substrate.

We £nd that the energy differences between different stacking sequences are enahnced at the surface with respect to the bulk: the zincblende-type termination is favorable by about 100 meV/pair, independently of the polytype of the underlying substrate. Note that the energy differences between bulk polytypes are of the order of few tens of meV/pair. In thermodynamic equilibrium, the most favorable deposition condition is a 3C overlayer on top of 3C-SiC. Instead, if a 4H-SiC substrate is employed, which in the bulk phase is more stable than 3C-SiC, the formation of a surface favors a stacking transformation and possible stacking mismatch boundaries, in agreement with the recent experimental £ndings.

In summary, our results suggest that it is possible to stabilize the cubic polytype via a controlled layer-by-layer deposition.

References

1. H. Morkoç, S. Strite, G.B. Gao, M.E. Lin, B. Sverdlov, and M. Burns, J. Appl. Phys. **76**, 1363 (1994).
2. N.W. Jepps and T.F. Page, Prog. Cryst. Growth Charact. **7**, 259 (1983); F. Bechstedt, P. Käckell, A. Zywietz, K. Karch, B. Adolph, K. Tenelsen, and J. Furthmüller, phys. stat. sol. (b) **202**, 35 (1997).
3. U. Starke, J. Schardt, J. Bernhardt, M. Franke, and K. Heinz, Phys. Rev. Lett. **82**, 2107 (1999).
4. M. Rohl£ng and J. Pollmann, Phys. Rev. Lett. **84**, 135 (2000).

Examination of the Li^+-water potential derived from $ab\ initio$ MD in a wide temperature range

A. V. Egorov[1], A. V. Komolkin[1], V. I. Chizhik[1], P. V. Yushmanov[1], A. P. Lyubartsev[2], and A. Laaksonen[2]

[1]*Institute of Physics, St. Petersburg University, Ulianovskaya 1, 198904, St. Petersburg, Russia*

[2]*Division of Physical Chemistry, Arrhenius Laboratory, Stockholm University, SE-106 91, Stockholm, Sweden*

+7 812 4284362, +7 812 4287240, egorov@esr.phys.spbu.ru

Understanding the microstructure of aqueous electrolyte solutions is a fundamental problem of physical chemistry. However, the direct experimental determination of solution microscopic characteristics is dif£cult in general. On the other hand, the computer simulations, which are widely used to obtain various type of information about ionic solution, are as good as the interaction potentials describing the interactions between water molecules and ions. Different ion–water interaction models show a wide spread of potential parameters. For instance, for Li^+ cation, described by Lennard-Jones (LJ) type of potential, the differencies in existing parameter values lead to a change of the ion coordination number from 4 to 6 (see [1]). $Ab\ initio$ molecular dynamics (MD) simulations, in which the forces are determined from quantum chemical calculations, are computationally very expensive and have the limited statistics (the typical simulation times does not exceed the tens of picoseconds). This does not allow to evaluate with high accuracy many properties of the solutions, for instance, the self-diffusion coef£cients of the ions. A possible alternative, studied in the prersent work, is to use the $ab\ initio$ MD for derivation of more reliable effective potentials for classical computer simulations.

In this study we employ the Li^+-water potential calculated previously in [2] on the basis of $ab\ initio$ MD simulation data. The non-electrostatic part of the Li^+ potential has a simple exponential form: $V_{eff}(r) = A \cdot exp(-Br)$. In the present work this potential is tested in classical MD simulations of LiCl aqueous solution in a wide temperature range (from -30 to 120^0C). The simulations are carried out in a canonical NVT ensemble in a cubic periodic cell, £lled with 323 water molecules, 10 lithium cations, and 10 chlorine anions, corresponding to 1.7 molal LiCl aqueous solution. The temperature was kept constant by using the standard Berendsen method. The equations of motion were solved using the standard Verlet leap-frog algorithm with a time step of 0.5 fs. Each simulation consisted of 100 ps of the equilibration and 500 ps of the data collection. Two water models were used for simulations: three-site SPCE and £ve-site ST2. The Cl^--water exponential potential parameters were taken from [3], and the ion-ion interactions were determined by applying the usual sum rules.

The structural properties of LiCl ion solution, calculated in the present simulations, are compared with the previous results obtained for potential of LJ type and with the experimental data on NMR-relaxation [4]. Also, the temperature dependence of the lithium ion self-diffusion coef£cients is compared with the experimental results measured by means of NMR spin-echo experiments.

References

1. A. V. Egorov, A. V. Komolkin, V. I. Chizhik, J. Mol. Liq. **89**, 47 (2001).
2. A. P. Lyubartsev, K. Laasonen, A. Laaksonen, J. Chem. Phys. **114**, 3120 (2001).
3. D. G. Bounds, Mol. Phys. **54**, 1335 (1985).
4. V. I. Chizhik, Mol. Phys. **90**, 653 (1997).

Three body bound state calculations with three body forces without angular momentum decomposition

Ch. Elster[1,2]**, H. Liu**[2]**, and W. Glöckle**[3]

[1]*Inst. für Kernphysik, Forschungszentrum Jülich, Jülich, Germany*
[2]*Inst. for Nuclear and Particle Physics, Ohio University, Athens, USA*
[3]*Inst. für Theoret. Physik II, Ruhr-Universität Bochum, Bochum, Germany*
+(740) 593-1697 , +(740) 593-0433, elster@ohiou.edu

The objective of the presented work is to carry out few nucleon calculations without the traditionally employed angular momentum decomposition. It is well known that nuclear scattering at intermediate energies of a few hundred MeV requires quite a few angular momentum states in order to achieve convergence of e.g. scattering observables. Presently employed computational methods for three nucleon (3N) scattering at higher energies using conventional partial wave expansions have intrinsic limitations, since with increasing energy the number of channel quantum numbers strongly proliferates, leading to increasing numerical dif£culties with respect to accuracy as well as storage requirements.
This is especially the case, when one wants to consider genuine three-nucleon force (3NF) effects. The computational dif£culty, which limits at present calculations based on partial wave decomposition, stems from the fact, that a 3N calculation is carried out in Jacobi variables, whereas a typical form of a 3NF has the form of two consecutive meson-exchange propagators between e.g. particles 1 and 2, then particles 2 and 3. The 3NF has to be expressed as function of the Jacobi momenta and then be decomposed into partial wave form. Although this is possible [1], one obtains such an enormous amount of coupling coef£cients that their number is at the limit of storage and memory capabilities of the largest computer architectures.
This is the very point why it is absolutely crucial to abandon the method of angular momentum decomposition and develop a new approach based on vector momenta only. In a formulation without partial waves the coordinate transformation inherent in including a 3NF as well as the application of permutation operators is 'only' an evaluation of the functions at shifted arguments. Of course, the 3NF depends on vector variables, that is magnitudes and angles, which are in part integration variables, and the incorporation in the 3N equations requires multidimensional interpolations. The Faddeev equation for 3 identical particles including a 3NF, V_4, is given by $|\Psi\rangle = G_0\,[tP + (1 + tG_0)V_4(1 + P)]\,|\Psi\rangle$. Here $G_0^{-1} = E - \frac{p^2}{m} - \frac{3}{4m}q^2$ is the 3N propagator, **p** and **q** the Jacobi momenta, and E the ground state energy to be determined. The operator t represents the off-shell two-body t-matrix, whereas P describes cyclic permutations for t acting between particles 2 and 3. As two-body force we concentrate on a superposition of an attractive and repulsive Yukawa interaction, representing typical features of the NN force.
The discretized Faddeev equation (neglecting spin and isospin degrees of freedom) is an integral equation in 3 variables on typical grids of 90*100*42 (momentum magnitudes p,q, and angle between the two vectors). The eigenvalue equation is solved iteratively by Lanczo's type techniques, here the method of iterated orthogonal eigenvectors. The bound state equation was successfully solved using 2N forces alone [2], and its numerical feasibility and accuracy established. Here we present results including the scalar 3NF and study its effects on the energy eigenvalue and the 3N wave function, as well as accuracy of our numerical implementation.

References

1. D. Hüber, H. Witala, A. Nogga, W. Gl"ockle, H. Kamada, Few Body Systems **22**, 107 (1997).
2. Ch. Elster, W. Schadow, A. Nogga, W. Glöckle, Few-Body Systems **27**, 83 (1999).

Six-state model of glassy crystal cyanoadamantane. Monte Carlo simulations

Robert Fabanski[1,2], Bogdan Kuchta[1], Lucyna Firlej[2], and Marc Descamps[3]

[1] *Instytut Chemii Fizycznej i Teoretycznej, Politechnika Wroclawska, Wybrzeze Wyspianskiego 27,50-370 Wroclaw, Poland*

[2] *Groupe de Dynamique des Phases Condensées; Université Montpellier II, Pl. E. Bataillon, 34095 Montpellier Cedex 05, France*

[3] *Laboratoire de Dynamique et Structure des Matériaux Moléculaires, UA CNRS 81, Université Lille 1, Villeneuve d'Ascq, France*

tel. (004871)3203854, fax (004871)3203364, fabianski@kchf.ch.pwr.wroc.pl

Glassy crystals have been objects of extensive studies for many years. Among them, ethanol, cyanoadamantane (CNadm) and its mixed crystals (so called cyanoadamantane family) have been model systems. In case of CNadm, glassy phase is obtained when the rotationally disordered (plastic) cubic phase is supercooled after deep quenching. At high temperature, the orientational disorder of molecules, which occupy lattice sites of fcc structure (Fm3m space group symmetry), is formed by dynamical, random distribution of molecular long axes among six orientations corresponding to six crystallographic directions (along [$\pm$100], [$\pm$010], [$\pm$001]. Below 180 K CNadm transforms into an orientational glass phase[1]. This transformation and a process of ordering of the supercooled, metastable phase have already been described both by experimental study[2] and phenomenological theory[3] as well. A decrease of con£gurational entropy on approaching the glass transition as seen in experiment corresponds to the development of an antiferroelectric short range order[2] and frustrated tetragonal local orderings (domains) as explained by Luty *et al.*[3]

Different time scales of dynamics and high activation barriers for molecular ¤ips in plastic phase lead to problems of insuf£cient sampling of the con£gurational space in computer simulations of such systems. Probability of ¤ips is very low and that causes simulations to be quasi-ergodic. Quasi-ergodicity (also called broken ergodicity) may yield results which are completely wrong. To decrease non-ergodicity of computer simulations, a preferential sampling instead of conventional Metropolis algorithm can be used[4] or an appropriate model of a system can be created. In case of more sophisticated algorithms (preferential and/or non-Boltzmann sampling) we need to take into account a usually considerable prolongation of awaiting results. If we want to use "fast" standard Metropolis method for such systems, we should construct a simple, but accurate model, in which all relevant features of a system are preserved.

In this paper we want to present results of implementation of a six-state spin model of cyanoadamantane crystal in Monte Carlo calculations. Our work offers a new approach to deal with problems of broken ergodicity in simulations of CNadm and similar systems. This approach has allowed not only to observe phase transition and metastable states but also to signi£cantly improve ergodicity of computer simulations of this system.

References

1. M. Bee, J. P. Amoureux, and A. J. Dianoux, *Mol. Phys.* **41**, 325(1980); B. Kuchta, M. Descamps, and F. Affouard, *J. Chem. Phys.* **109**, 6753(1998).
2. J. F. Willart, M. Descamps, and J. C. van Miltenburg, *J. Chem. Phys.* **112**, 10992(2000).
3. T. Luty, K. Rohleder, J. Lefebvre, and M. Descamps, *Phys. Rev. B* **62**, 8835(2000).
4. B. Kuchta, M. Descamps, and J. F. Willart, *Chem. Phys.* **243**, 169(1999).

Monte Carlo simulations of carbon-based structures based on an extended Brenner potential.

A. Fasolino and J.Los

Institute of Theoretical Physics, University of Nijmegen, Toernooiveld 1, 6525ED Nijmegen, The Netherlands

0031-24-3652222, 0031-24-3652120, fasolino@sci.kun.nl

The discovery of fullerene has awakened an increasing interest in carbon based nanostructures. Since then an incredible amount of new forms of solid carbon have been synthesized either with graphitic-like or mixed diamond-graphitic bonding. Lately much attention is also been given again to the process of diamond graphitization which is known since 1920 but which is still not understood [1]. Beside the fundamental interest, understanding the structure and transformation of carbon under different conditions is technologically relevant for coatings, growth and machining of diamond and new superhard materials. It is noteworthy how many open questions exist and how many unexpected results have recently come out for this elemental material. It is therefore important to develop predictive schemes to treat diamond, graphite and mixed bonding with approaches able to deal with large structures which are beyond the possibility of ab initio calculations.

Our approach is based on the use of a state of the art phenomenological potential due to Brenner [2]. which is accurate enough to describe both types of bonding and simple enough to deal with very large samples. This classical potential makes the bond energy dependent on the local environment via a many body term which depends on bond length, angle and coordination.

We have demonstrated, by extended grand-canonical Monte Carlo simulations[3], the very high accuracy of the empirical many-body Brenner potential for carbon structures by a detailed comparison of its structural predictions with those of *ab-initio* studies for known reconstruction of the diamond (100) and (111) surfaces. In addition to the minimal energy unbuckled undimerized Pandey (2×1) (π-bonded) chain reconstruction we £nd three new meta-stable states, very near in energy, with surface atoms in three-fold graphite-like bonding. The absence of consensus on the structural details and electronic structure of the clean (111) surface might be related to these surface structures, which are peculiar of carbon and have never been considered so far.

Furthermore, we suggest a new parametrisation to extend the Brenner potential beyond its cut-off radius of 2 Å. This extension allows us to reproduce the long-range interplanar interactions in graphite. Preliminary results on the diamond surface graphitisation obtained by use of the extended Brenner potential are presented.

References

1. see e.g. Y.G. Gogotsi, A. Kailer, K.G. Nickel, Nature, **401**, 663 (1999).
2. D.W. Brenner, Phys. Rev. B **42**,9458 (1990)
3. A. V. Petukhov, D. Passerone, F. Ercolessi, E. Tosatti, A. Fasolino, Phys. Rev. B **61**, R10590 (2000); A. V. Petukhov, A. Fasolino, Phys. Stat. Sol. a **181**, 109 (2000).

Computer simulation of femsosecond pulse propagation in bulk dielectric samples

T.V.Smirnova, O.M.Fedotova, and O.K.Khasanov

Institute of Physics of Solids and Semiconductors, NAS, 17 P.Brovki Str.; 220072 Minsk, Belarus

khasanov@ifttp.bas-net.by; tel.: +375 172 841117; fax: +375 172 840888

Processes occurring when intense femtosecond laser pulses are focused into the bulk of dielectric materials are investigated. Experimentally it was found [1] that for femtosecond laser irradiation no indication of plasma formation or catastrophic self-focusing could be seen in the bulk. We compare the results of numerical modeling with experiments. Possible reasons for the absence of laser-induced breakdown in bulk media observed in [1] are discussed. The necessity of solving the self-consistent problem for the evolution of both the pulse £eld and the material parameters is noted. The only change of the refraction index due to normal (Kerr) dispersion leads to beam self-focusing in the medium. However, as the beam intensity increases, some processes , such as an avalanche , multiphoton absorption, or tunneling, may lead to ionization [2] , and as result, plasma induced defocusing needs to be included.

As known, femtosecond pulse propagation is described by (2+1)-D nonlinear Schrodinger equation. We analyze it numerically taking into account a group velocity dispersion, diffraction, and the polarization change due to non-linear refractive index change, multiphoton absorption and electron plasma formation. As is shown in [2], for femtosecond pulses namely the multiphoton absorption is dominant mechanism of ionization. To realize the numerical experiment, the following steps were performed. For the equation solving we use split-step method on $3-D$ grid (r,z,t) [3]. Linear diffraction is calculated according to a Crank-Nickolson scheme. The computer code was worked out in Fortran. The reliability of the code was tested when the number of steps in each direction was doubled and the phase difference between two adjacent points on the $3-D$ grid was controlled.

Under non-stationary conditions the pulse exhibits asymmetrical splitting. Its character is analyzed in dependence on the sample thickness, on the group velocity dispersion, on the relation between the input beam power and the self-focusing threshold. If the input beam power is slightly more than the threshold, the space-time focusing acts to push the peak intensity towards the rear of the pulse. At higher power the pulses become well separated in time and are considerably shorter than the initial pulse. At the same time, the front pulse becomes higher in amplitude than the rear pulse. As the power is increased further, the split pulses become shorter in time. With increasing the pulse duration, the beam self-focusing becomes stationary. Results are in agreement with [4]. It is substantiated to add the equation for carrier generation [2] for solving self-consisted task to estimate the contribution of the plasma formation in the refraction index.

References

1. D. von der Linde and H. Schuler, J. Opt. Soc. Am. B, **13**, 216 (1996).
2. B.Rethfeld, A.Kaiser, M.Vicanek, and G.Simon. High-power laser ablation , SPIE V. **4065**, 356 (2000)
3. O. G. Kosareva, V. P. Kandidov, A. Brodeur, et al. Opt. Lett. **22**, N.17, 1322 (1977).
4. J. K. Ranka, R. W. Schrimmer and A. Gaeta.. Phys.Rev.Lett. **77**, N.18, 3783 (1996).

ab initio Density functional study of GaAs clusters

T. B. Boo and Y. P. Feng

Department of Physics, National University of Singapore, Singapore 119260

Tel: (65) 874 2960, Fax: (65) 777 6126, phyfyp@nus.edu.sg

Clusters formed by multi-elements are interesting because of their composition dependent properties. Such composition dependence allows control of material properties by varying the cluster composition, in addition to the cluster size. It is therefore important to study the composition dependence of properties of composite clusters.

We have used £rst principle electronic structure calculation to study composition dependence of properties of GaAs clusters[1]. Ground-state structures of these clusters are explored using the *ab initio* density functional theory with the generalized gradient approximation. Structural, chemical and electronic properties of the clusters and their dependence on the composition of the clusters are investigated.

We have determined the structures and calculated properties of the Ga_mAs_n clusters for $n + m = 6, 8, 10, 12$ and 14. It is found that on substitutional Ga doping, the GaAs clusters become less cohesive, less stable in electronic structure, and highly susceptible to external electric £eld. Due to the elemental electronegativity, As-rich clusters favor strong and short As-As bonds; Ga-rich clusters favor weak and long Ga-Ga bonds; and stoichiometric clusters favor even stronger and shorter Ga-As bonds. All clusters are electronegative in nature. It is energetically feasible to form anionic clusters. Bonding of stoichiometric clusters are found highly ionic. Red-shift is observed in the *ab initio* photoabsorption spectrum on substitutional Ga doping and is more prominent for the stoichiometric or As-rich clusters.

Charge is transferred from Ga atoms to As atoms and the amount of charge transferred is distinctly peaked at the stoichiometric ratio. The bonding ionicity can be characterized by the atomic charge promoted from the Ga $4s$-orbitals to the As $4p$-orbitals. This charge promotion becomes more signi£cant as the cluster becomes larger. These general trends are followed by all clusters being studied with small variations.

References

1. Y. P. Feng, H. H. Kwong, T. B. Boo and H. K. Quek, paper presented at CCP2000, Gold Coast, Australia (to appear in Computer Physics Communication).

Computer aided estimation of the lifetime of a material by the thermo-gravimetric analysis

Mariana Georgescu[1] **Mihaela (Dumitru) Ghelmez, B.Dumitru, M.Georgescu and S.Serban**[2]

[1] *Macromolecular Materials and Membranes Research Centre, Bucharest, Romania*
[2] *Politehnica University of Bucharest, 77 206 Bucharest, Romania*
Tel:(+40 1)410 45 42, Fax:(+40 1)410 44 88, e-mail:dem@physics.pub.ro

The paper presents an experimental and computers study of a large used material in industrial applications, namely the terpolymer acrylonitrile-butadiene-styrene (ABS). The purpose of this study was to estimate the lifetime of this material, by means of the thermo-gravimetrical analysis (TGA). This method establishes the kinetic parameters of the material decay, giving information on the thermal stability of the material. [1].

This information is very useful especially for the long term and large scale used products in the technical £eld (nuclear plants, underground pipelines, ¤oors etc). The computer program TGA Kin.V-4.0 Du Pont Instruments processed the experimental data obtained with the THERMAL ANALYSIS 2100 Du Pont. The paper presents £rst the experimental method and conditions for getting the lifetime of the ABS [2].

The experimental setup takes advantage of an interface for computer data processing and computer control. A series of graphs for the thermal stability were obtained. Decay levels of 2.5

Since most of polymers decay by a £rst kind kinetics reaction, we used it for our calculations. Taking into account the sample weight, the heating speed, the initial and £nal temperature and the chosen level in the decay process, the activation energy can be determined and then the lifetime of the material. [4].

For a lifetime value, the maximum temperature for practical use can be estimated. Comparative and detailed computer results are presented. This method can be also applied for characterizing - by means of thermal methods - the thermo-stable polymers, elastomers, thermoplastics, and synthetically £bers. Alternative thermo-analitical methods (as the differential calorimetric method-DSC, and DSC under pressure) are discussed.

References

1. R.F.Schwenker, P.D.Garn, ”Thermal Analysis”, Academic Press, New York, Vol.1, 2, 1969
2. M. Georgescu and C. Hagiopol, ”Emulsion copolymerization of styrene”, Synthetic Polymer Journal, 1, 59-61, 1994
3. M.Ghelmez (Dumitru), ”Nonlinear Optical Effects in Biological Membrane Simple Models” -Monograph, Ed. Printech Bucharest, 2000
4. J.H.Flynn et al., Polym. Lett., B4, 323, 1966; D.J.Toop, IEEE Trans.Electr.Ins. El-6, 2, 1971

Explicit kinetic functionals for diatomic molecules

David García-Aldea[1,2] and J. E. Alvarellos[2]

[1]*Dpto. Teoría de la Materia Condensada. ICMM. CSIC*
[2]*Dpto. Física Fundamental. Facultad de Ciencias. UNED*
Tel:+034913987636, fax:+034913986697, email:dgaldea@£sfun.uned.es

Density Functional Theory (DFT)[1] is one of the most widely used methods for *ab initio* calculations of the structure of atoms, molecules, crystal, surfaces, and their interactions. Unlike the Hartree-Fock method, DFT allows molecular dynamics calculations (e.g. using the *Car-Parrinello* method) for large systems, due to a smaller computational cost. Even more, it allows the use of *orbital-free functionals* for the description of the kinetic energy, avoiding the self-consistent soluction of Schrödinger-like equations. In this case, some numerical problems are still unsolved. We present a new algorithm for a such a *complete* DFT calculation, implemented in a diatomic molecule using different explicit kinetic functionals. For any system of electrons, the DFT, proves the existence of a density functional $E[n]$ for the total energy such that it reaches its minimum value at the density distribution of the ground state. The functional $E[n]$ may be separated into an intrinsic nonelectrostatic term $G[n]$, the interactions between the electrons and the external potential $V[n]$ plus the repulsive Hartree energy, $J[n]$, due to the electronic density distribution. $G[n]$ itself is usually divided into a 'kinetic energy' term $T[n]$, which would be the full energy of a noninteracting electron system, plus an exchange and correlation term $Exc[n]$: [2]

$$E[n] = G[n] + V[n] + J[n] = T[n] + V[n] + J[n] + Exc[n].$$

In our approach, both the kinetic energy $T[n]$ and the exchange and correlation term $Exc[n]$ must be approximated by explicit functionals that only depends on the electron density. Some of former terms present numerical dif£culties when evaluated without the use of a basis set. Speci£cally, the Hartree energy term has a very great numerical cost in a real space calculation, due to those in£nite singularities in every point of space. We try to solve this problem by using a Fourier Transform. In Fourier space, the expression of the Hartree energy has only a singularity at the origin and so the integral is much easier to handle.

Due to the symmetry of our problem, we can use cylindrical coordinates, and we get a two dimensional integral instead the general three dimensional integral. We then manage to write a 1D-Fourier Transform plus 1D-Hankel Transform, instead of the original 3D-Fourier Transform of the electron density. This calculation is now computationally feasible. In this way, we can evaluate kinetic and total energies in a numerical scheme without the use of any basis set.

We have calculated the total energy of diatomics [3] using several kinetic energy functionals, including local, semilocal and non-local [4] approximations. The results can be reasonably compared with those obtained when using Hartree-Fock densities described by a basis set. Minimization of the total energy will give information about the quality of the kinetic density functional we use. The algorithm must be improved in order to speed up the calculation and to evaluate more properly the non-local part of the kinetic functionals.

References

1. P. Hohenberg and W. Kohn Phys. Rev. **136**, B864 (1964), W. Kohn and L.J. Sham Phys. Rev A **140**, 1133 (1965).
2. A. Nagy, Physics Reports 298 1-79 (1998).
3. K. Yonei, J. Phys. Soc.Japan **31**, 882 (1971); A.J. Thakkar Phys. Rev. A **46**, 6920 (1992); Chan, Cohen and Handy, J. Chem. Phys. **114-2**, 631 (2001).
4. E. Chacón, J. E. Alvarellos and P. Tarazona, Phys. Rev. B **32**, 7868 (1985); P. García-González, J. E. Alvarellos and E. Chacón, Phys. Rev. A **54**, 1897 (1996).

Chaos of two particles in the ding-a-ling model

P.Gawronski and K.Kulakowski

Faculty of Physics and Nuclear Techniques, University of Mining and Metallurgy,
al.Mickiewicza 30, 30-059 Cracow, Poland
+(4812)6173539, fax(4812)6340010,kulakowski@novell.ftj.agh.edu.pl

The ding-a-ling model is a member of the family of nonlinear many-body problems, among which the Fermi-Pasta-Ulam system is the most famous one. The smallest ding-a-ling system consists of two particles of equal masses. They move along a ring, and interact via elastic collisions. One of them is bound by a harmonic potential. In his seminal paper [1], Casati et al. suggested that this system shows a phase transition from chaotic to quasiperiodic behaviour, as the system energy increases. In our approach, the system is described by a set of coupled maps, which drive it from one to another collision of the particles. This kind of Poincare section is equivalent to a non-canonical transformation, and the phase-space volume is not preserved. We investigate a series of times $t(n)$ between subsequent collisions. The method applied is the numerical calculation of the box fractal dimension D of the phase portrait $t(n+1)$ vs $t(n)$ [2]. This method has been proved to be ef£cient in a similar application [3]. We show that the character of motion depends on the value of the ratio r of velocities of the particles. For values of energy larger than those from [1], we £nd chaotic behaviour for r close to unity. There, the phase portrait is a fractal. On the contrary, the system is quasiperiodic above some value of r, and the phase portrait is a closed curve. We conclude that for the latter case, the kinetic energy of the quicker particle can be treated as an adiabatic invariant of motion [4].

References

1. G.Casati, J.Ford and W.M.Visscher, Phys.Rev.Lett. 52 (1984) 1861.
2. H.Kantz and Th.Schreiber, Nonlinear Time Series Analysis, Cambridge University Press, Cambridge 1997.
3. P.Gawronski and K.Kulakowski, Int.J.Mod.Phys.C 11 (2000) 247.
4. A.J.Lichtenberg and M.A.Lieberman, Regular and Chaotic Dynamics, Springer-Verlag, New York 1992.

Numerical simulation of the modi£ed Ginzburg-Landau type equations for a Josephson junction

Z.D. Genchev[1] **and T.L. Boyadjiev**[2]

[1]*Inst. Electron. Bulg. Acad. Sci., 1784 So£a, Bulgaria.*
[2]*University of So£a "St. Kliment Ohridski",1163 So£a, Bulgaria.*
zgenchev@ie.bas.bg, todorlb@fmi.uni-so£a.bg

The formalism of Ginzburg-Landau (GL) provides a simple method to study the global properties of non-homogeneous superconducting structures. We investigate the well-known class of supercondicting/normal/superconducting (SNS) sandwiches with plane boundaries on the basis of modi£ed GL type equations [1] for the order parameter (wave function) $\psi(x)$, de£ned in the whole space as follows:

$$\psi'' + \left(1 - |\psi|^2\right)\psi = 0, \tag{1}$$

$$J = -\frac{i}{2}\left[\psi^*\psi' - \psi\psi^{*\prime}\right], \quad (-\infty < z < -d/2) \cup (d/2 < z < \infty), \tag{2}$$

$$\frac{m_s}{m_n}\psi'' - \frac{a_n}{|a_s|}\psi - \frac{b_n}{b_s}|\psi|^2\psi = 0, \tag{3}$$

$$J = -\frac{i}{2}\frac{m_s}{m_n}\left[\psi^*\psi' - \psi\psi^{*\prime}\right], \quad |z| < d/2. \tag{4}$$

The dimensionless constant J de£nes the supercurrent density as a function of phase offset $\Delta\phi$, the thickness of the normal layer d, and the parameters of the model which appear as constants in equations (3) and (4). When this dependence is a single-valued and analytical odd function of the phase offset $\Delta\phi$, the structure shows a Josephson behavior. We investigate numerically and analytically the supercurrent-phase relation and the crossover from the Josephson effect to bulk superconducting ¤ow by using the continuous analogue of the Newton's method [2].

We show that, due to different nonlinear terms in the normal and superconducting regions, the dependence $J(\Delta\phi)$ is not sinusoidal. The usually accepted dependence $J = j_c \sin(\Delta\phi)$ is justi£ed only for a restricted domain of values of the parameters $d, m_n/m_s, a_n/|a_s|$, and b_n/b_s. The in¤uence of the second term in the Fourier-decomposition $(\sim \sin(2\Delta\phi))$ is also investigated. We prove numerically that the essential deviation from sinusoidal relation is caused by the possible anisotropy of masses $(m_n/m_s \neq 1)$.

It is shown that the maximum (critical) current density j_c corresponds to a bifurcation point for the amplitude $|\psi|^2$ of the order parameter as we change the current density J.

When the anisotropy of masses is absent ($m_n/m_s = 1$) and the thickness d is very small, we recover the results given in [3].

References

1. Chapman S. J., Du Q., and Gunzburger M.D. (1993), A Ginzburg-Landau type Model of Supercoducting Normal Junction including Josephson Junctions, Preprint Oxford Univ.
2. Puzynin I. V.et al. (1999), The Generalized Continuous Analogue of Newton's Method for the Numerical Investigation of some Nonlinear Quantum-Field Models, in *Physics of Elementary Particles and Atomic Nuclei*, vol. **30**, No 1, AIP, p. 97.
3. Sols F. and Ferrer J. (1994), Crossover from the Josephson effect to bulk superconducting ¤ow, Phys. Rev. B **49** (22), p. 15913.

Electronic and magnetic structure of NiO(001) and NiO/Ag(001)

D. Ködderitzsch[1], W. Hergert[1], W. Temmerman[2] and Z. Szotek[2]

[1]*FB Physik, Martin-Luther-Universität Halle-Wittenberg, Friedemann-Bach-Platz 6, D-06108 Halle*

[2]*Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK*

0345 5525 445, 0345 5525 446, hergert@physik.uni-halle.de

An adequate description of strongly correlated systems, such as the antiferromagnetic insulating transition-metal monoxides (FeO, CoO, NiO), is not possible within the local spin density approximation to the density functional theory (LSDA-DFT) due to its mean-£eld treatment of the strong on-site Coulomb correlations. A better representation of the latter can be obtained within the self-interaction corrected (SIC) LSDA, which has been successfully applied to systems having strongly localised states, as, e.g., rare earth systems and transition-metal oxides. [1]

In this work we apply the self-interaction corrected LSDA formalism, as implemented in the TB-LMTO-ASA method, [2] to study the electronic and magnetic structure of transition-metal oxide (TMO) surfaces and thin oxide layers on metallic substrate. Here the NiO surface and the properties of up to 3 layers of NiO on the Ag(001) surface are investigated. We model the surface in a supercell approach by a series of repeated slabs consisting of up to seven layers of oxide separated by £ve layers of empty spheres, representing the vacuum. Relaxations at the surfaces are not taken into account. Having investigated different magnetic orderings in the bulk and in the slabs, we argue that the AFII phase is most energetically favoured. The layer resolved densities of states at the NiO(001) surface are also considered for different arrangements of spin orientations in the surface layers whilst keeping the inner layers in the antiferromagnetic ordering of type II (AF II). It is shown that the self-interaction corrected LSDA calculations can describe surface properties of TMO and thin TMO layers on metal substrates and their results used to interpret experiments on thin transition metal oxide £lms on metallic substrates in the scanning tunneling microscope.

Furthermore, to gain more insight into the nature of exchange interactions, a Heisenberg model has been £tted to both bulk NiO and NiO surface, respectively. Conventional LDA calculations (see [3]) for NiO bulk overestimate the exchange parameters for nearest and next-nearest Ni interactions by a factor of 3, with respect to experiments. [4] In contrast, the values of the exchange parameters obtained by the self-interaction corrected LSDA deviate from the experimental ones by less than 20 %. The corresponding Neél temperatures are estimated from this Heisenberg model.

References

1. Z. Szotek, W.M. Temmerman, H. Winter, Phys. Rev.B **47**,4029 (1993); A. Svane, O. Gunnarsson, Phys. Rev. Lett. **65**, 1148 (1990).
2. W.M. Temmerman, A. Svane, Z. Szotek, H. Winter, S.V. Beiden, 'Electronic Structure and Physical Properties of Solids', Lecture Notes in Physics, ed. H. Dreyssé, Springer-Verlag, 2000.
3. T. Oguchi *et al.*, Phys. Rev. B **28**, 6443 (1983).
4. M.T. Hutchings, E.J. Samuelsen, Phys. Rev. B **6**, 3447 (1972).

Energy relaxation and transfer in trimer

Pavel Heřman[1], Ivan Barvík[2] and Martin Urbanec[1]

[1] *Department of Physics, University of Hradec Králové, V. Nejedlého 573, 500 03 Hradec Králové, Czech Republic*
[2] *Institute of Physics of Charles University, Faculty of Mathematics and Physics, Ke Karlovu 5, CZ-121 16 Prague 2, Czech Republic*
tel.: (+42)049 5061186, fax: (+42)049 5513890,
e-mail: pavel.herman@uhk.cz

We considered the relaxation and equilibration in symmetric trimer coupled to a phonon bath. Energy transfer within the trimer occurs via resonance interactions and coupling between the trimer and the phonon bath occurs via modulation of the monomer energies by the phonons. We suppose totally uncorrelated baths for each site of trimer.

Using software package Mathematica [1] we compare model introduced by Čápek [2] with commonly used Redfield model (with the secular approximation) [3] and also with the Stochastic Liouville Equation model with Haken-Ströbl-Reineker parametrization [4]. We focus on the differences of these models.

We discuss two initial conditions:
a) The highest energy level in the trimer is initially occupied,
b) one local site (site 1) of the trimer is initially occupied.

We find that the diagonal elements of density matrix - probabilities of occupation in the representation of eigenstates are the same in all three models. But it is not the case of the off-diagonal elements of density matrix. If the off-diagonal density matrix elements vanish initially, they vanish in every following time in all three models (they are the same for the initial condition a). If the initial condition is local (initial condition b), the off-diagonal matrix elements have essential differences even in the long time limit.

References

1. S. Wolfram, The Mathematica Book, 4th ed. ,Wolfram Media/Cambridge University Press, 1999.
2. V. Čápek, Z. Phys. B99 (1996) 261.
3. A. G. Redfield, in Advances in Magnetic Resonance, Vol 1, ed. J. S. Waugh. Academic Press, New York - London, 1965, p. 1.
4. P. Reineker, in Exciton Dynamics in Moleculer Crystals and Aggregates, Springer Tracts in Modern Physics, Vol. 94, ed. G. Höhler, Springer, Berlin-Heidelberg, 1982, p.111.

Boundaries in collaborative virtual environments: How to classify them to introduce in a new awareness model

Pilar Herrero[1] **and Angélica de Antonio**[2]

[1] *Computer Science School. Universidad Politecnica de Madrid*
Campus de Montegancedo s/n. 28.660 Boadilla del Monte. Madrid (Spain) Tel.: +34 91 336 74 56 Email: pherrero@£.upm.es
[2] *Computer Science School. Universidad Politecnica de Madrid*
Campus de Montegancedo s/n. 28.660 Boadilla del Monte. Madrid (Spain)
Tel.: +34 91 336 69 25 Email: angelica@£.upm.es

The importance of awareness model has been underwritten by many studies and much interesting research has been undertaken in this research area.

Perhaps the most well known awareness model for Virtual Environments is *"The spatial Model of Interaction"*. This model was developed between 1991 and 1993 mixing the researches led by Professor Steve Benford at the *School of Computer Science and Information Technology*, in the Nottingham University, the researches led by Lennart E. Fahlén at *The Swedish Institute of Computer Science (SICS*) and the researches led by John Bowers at Royal Institute of Technology (KTH) in Stockholm (Sweden).

The spatial model, as its name suggests, uses the properties of space as the basis for mediating interaction. It was proposed like a way to control the ¤ow of information of our environment in CVEs (Collaborative Virtual Environments), allows objects in a virtual world to govern their interaction through the some key concepts: aura, awareness, focus, nimbus, adapters [1] and boundaries [3].

A lot of researches have been carried out starting from this model, some of them to rede£ne the model and another to rede£ne some of it key concepts. For example, Benford introduced boundaries as "Boundaries divide space into different areas and regions and provide mechanisms for marking territory, controlling movement, and in¤uencing the interactional properties of space" [2].

In this way, the goals of this work are three-fold:

1. To rede£ne and classify the different kind of boundaries in CVE, using some properties of space, as for example permeability, situation and dynamics [4].
2. To study how these boundaries can have an in¤uence in the perception process
3. To introduce how the above boundaries theory could be connected with some physical phenomenon (as for example the wave motion)

References

1. Benford, S.D., and Fahlén, L.E. ***A spatial model of interaction in large virtual environments***, in Proc. Third European Conference on Computer Supported Cooperative Work (ECSCW'93), Milano, Italy. Kluwer Academic Publishers, pp. 109-124.
2. Benford, S. D., Fahlén, L. E. and Bowers, J. M., ***Managing Mutual Awareness in Collaborative Virtual Environments***, in Singh, G.,Feiner, S. K., Thalmann, D. (eds.) Proc. ACM SIGCHI Symposium on Virtual Reality Software and Technology (VRST'94), Singapore, pp.223-236, August 1994, World Scienti£c: Singapore
3. Bowers, J., ***Modelling Awareness and Interaction in Virtual Spaces, Supplement*** to Proceedings of the 5th MultiG Workshop, Stockholm-Kista, May 17, 1993, pp. S9-S24.
4. Koleva, B. N., Benford, S. D. and Greenhalgh, C. M., ***The Properties of Mixed Reality Boundaries***, in Proceedings of the 6th European Conference on Computer Supported Co-operative Work (ECSCW'99), Copenhagen, September, 1999.

Computation of optical properties of Si-based photonic crystals

R. Hillebrand[1] **W. Hergert**[2]

[1]*MPI für Mikrostrukturphysik Halle, Weinberg 2, D-06120 Halle*
[2]*FB Physik, Martin-Luther-Universität Halle Wittenberg, Friedemann-Bach-Platz 6, D-06108 Halle*
+49 345 5582 911, +49 345 5511 223, hi@mpi-halle.de

Si-based 2D macroporous photonic crystals (PCs) have become of increasing interest, because of their extraordinary optical properties in the near IR. They are fabricated by electro-chemical pore etching of lithographically prestructured Si wafers, with pore diameters in the range of 1.5 μm - 0.5 μm having a pore depth of about 100 μm. [1] Experimental measurements can be interpreted, e.g., in terms of calculated photonic band structures (PBS), density of states and transmittance. Solving Maxwell's equations for the magnetic £eld yields an eigenvalue problem for the eigen frequencies of the system and the electromagnetic £eld modes.

For the given dielectric contrast between the silicon ($\epsilon_{Si} = 11.6$) and the pores (e.g. air $\epsilon_p = 1$), the dispersion of the bands can be controlled by the lattice type, the pore size and the cross section of the pores. The in¤uence of pore roundness de£ciencies on the PBS of 2D photonic crystal has been extensively studied. [2]

Dedicated regimes of electro-chemical PC fabrication [3] allow to modify the pore radius in the growth direction of the pore, providing 3D-like photonic structures in an ef£cient way.

It is the aim of the contribution to theoretically study whether this type of modulated pores can cause a vertical con£nement of the electro-magnetic modes. In particular, the optimum pore pro£le, i.e., strength and shape of diameter variations, has to be identi£ed. It has to be noted that most of the previous theoretical studies of photonic crystal waveguides have been restricted to purely 2D systems.

A frequency-domain method is used to solve Maxwell's equations for periodic dielectric structures with the model of the PC coded on a 3D supercell grid. Preconditioned block-iterative eigensolvers in a plane wave bases are used for a full-vectorial, three-dimensional solution. The method allows to calculate the frequency eigenstates and the electromagnetic £eld modes. [4].

The results are presented by band structure plots as well as 3D £eld distributions for varying parameter combinations.

We present a detailed investigation of the in¤uence of pore pro£le variations on the photonic band gaps, which control the in-plane guiding of the modes. In conclusion, the vertical con£nement of guided modes in photonic crystals, either radius-variation-based in modulated pores or index-variation-based in slabs, are compared.

References

1. A. Birner et al., Phys. Stat. Sol. (a) **165**, 111-117 (1998).
2. R. Hillebrand and W. Hergert, Solid State Communications **115**, 227 (2000).
3. J. Schilling et al., Appl. Phys. Lett. **78**, 1180-1182 (2001).
4. St. G. Johnson and J. D. Joannopoulos, Optics Express **8**, 173-190 (2001).

Cluster approach in calculations of electronic structure of defects in $PbWO_4$

Yu. A. Hizhnyi, S. G. Nedilko, and M. U. Bilyi

Physics Fclt., T. Shevchenko Kyiv Univ., 6 Glushkova av., Kyiv Ukraine

380 44 2662295, 380 44 2664036, hizhniy@phys.univ.kiev.ua

The increase in computational power of computers enables the researchers both to improve the methods of electronic structure calculations and to apply them to a wider range of the investigated objects. But in solid-state physics the majority of objects of calculation still require huge amounts of computational time, and all existing methods always have some classes of compounds, where they work less effectively than others. Therefore, the question of applicability of some method to some or other kind of compounds is no doubt the overriding problem for researchers. We think our work is interesting in this sense £rst of all for its somewhat unexpected consequence: the in¤uence of structure defects on the electronic structure of complex ion-covalent oxide crystals of lead tungstate $PbWO_4$ could be described with considerable degree of accuracy and credibility without use of supercomputers. We obtained quite informative results by ab-initio all-electron Restricted Hartree-Fock (RHF) calculation of the electronic structure of small-sized molecular clusters of $PbWO_4$ with single-atom defects.

Well known scintillator, lead tungstate $PbWO_4$ is assumed to be the working scintillation material for Large Hadron Collider project at CERN. Electronic structure calculations are necessary for successful clari£cation of the origin of it's luminescence centers. Electronic band-structure of lead tungstate was ab-initio calculated recently [1], but the properties of two important types of defects in lead tungstate have not ever been described in terms of electronic structure. It is well known, that oxygen vacancies V_o and molybdenum impurities signi£cantly affect luminescence properties of $PbWO_4$.

With the view of £nding the in¤uence of these defects on lead tungstate optical properties we issued another challenge: are we able to solve this problem effectively by force of a desktop computer? We applied all-electron RHF-calculation to small clusters contained two formula units of $PbWO_4$ (a half of the unit cell) in which V_o and W substitution by Mo were modelled. Comparing density of states (DOS), partial DOS and combined (interband) DOS calculated for defect and perfect structure representations by the clusters we determined the in¤uence of these defects on the character of interband optical transitions. Calculating molecular and atomic populations we estimated total electronic charges on constituent atoms and WO_4 molecular aninons and the degree of covalence of interatomic bonds for perfect crystal. Changes in these parameters that accompanied defects formation were also considered. We used calculated spatial distribution of electronic charge for investigation of the conditions of (Pb-WO_4)-type exciton autolocalization on WO_4, WO_3 and MoO_4 molecular complexes, that were recognized as luminescence emission centers in perfect and defective crystals. Furthermore, in this work we made an attempt to de£ne choice criteria for a minimal crystal fragment, need to be considered in order to determine the in¤uence of single-atom defects on the optical properties of $PbWO_4$-like crystals, if the calculation method uses LCAO formalism.

Taking our work as an instance we show, that whatever complex the investigated systems may be, such kind of approach in calculations will always be relevant as the £rst approximation, that should enhance the effectiveness of entire solution of the problem.

References

1. Zhang Y., Holzwarth N.A.W., Williams R.T.//Phys. Rev. B, 57 (1998) 12738

A Lattice–Boltzmann method for the simulation of transport phenomena in charged colloids

Jürgen Horbach[1] **and Daan Frenkel**[2]

[1]*Institute of Physics, University of Mainz, Staudinger Weg 7, 55099 Mainz, Germany*
[2]*FOM Institute of Atomic and Molecular Physics, Kruislaan 407, 1098 SJ Amsterdam, Netherlands*

Tel.: (06131) 3923641, Fax: (06131) 3925441, horbach@plato.physik.uni-mainz.de

The simulation of charged colloidal suspensions is a very challenging task because the typical relaxation time of the colloidal particles can be of the order of seconds or more whereas that of the solvent particles is normally of the order of picoseconds (e.g. water at room temperature). Furthermore the computation of the long–ranged Coulomb interactions require a lot of CPU time. Therefore conventional simulation methods like molecular dynamics or Monte Carlo are not well suited to study the dynamics in charged colloids.

A computational method which was successfully applied to colloidal systems is the so–called Lattice–Boltzmann method (for an introduction see [1]) which was developed to simulate hydrodynamics on a grid. We have developed a simulation scheme for charged colloids, based on this method, in which the dynamics of the solvent ions is solved on a coarse grained hydrodynamic level. In our method a set of non–linearly coupled electrokinetic equations is solved which consists of convective diffusion equations for the ion densities, the linearized Navier–Stokes equations for the mass densities, and the Poisson equation for the electrostatic potential.

We apply our method to the calculation of the reduced sedimentation velocity U/U_0 (U, U_0: sedimentation velocity for the charged and uncharged system, respectively) for a cubic array of charged spheres in an electrolyte. U/U_0 is determined as function of the dimensionless quantity κa (κ: inverse Debye length, a: radius of a sphere) for different volume fractions of spheres. For the limit of a weakly charged, isolated sphere in an unbounded electrolyte there exists an analytical solution which was £rst derived by Booth [2]. We show that we recover the result of Booth's theory with our method, and we compute the correction terms to this theory for higher charged spheres. Furthermore, we investigate the complex behavior of U/U_0 at larger volume fractions of macroions.

In conclusion we have developed a new simulation method for suspensions of charged colloidal particles which is based on the Lattice–Boltzmann method. We apply our method to the investigation of sedimentation phenomena. We show that we recover an analytical result for the limit of a weakly charged sphere in an unbounded electrolyte, and moreover we give physical insight into the behavior of the sedimentation velocity as a function of the volume fraction and the charge of the macroions.

References

1. A. J. C. Ladd, J. Fluid. Mech. **271**, 285 (1994).
2. F. Booth, J. Chem. Phys. **22**, 1956 (1954).

Study of thin £lm growth by means of computer simulation and image analysis

R. Hrach, J. Šimek and M. Kostern

Faculty of Mathematics and Physics, Charles University,
V Holešovičkách 2, 180 00 Prague 8, Czech Republic
+420 2 21912328, +420 2 6885095, rudolf.hrach@mff.cuni.cz

When preparing thin metal £lms deposited on dielectric substrates, a Volmer-Weber mechanism of three-dimensional nucleation and £lm growth takes place. The basic information about £lm properties in the initial stages of their growth can be derived from the analysis of £lm photographs from a transmission electron microscope as well as from atomic-force and scanning-tunnelling microscopes. For better understanding of processes, which take part during early stages of £lm growth, the technique of computer experiment combined with image analysis of simulated structures seems to be very useful. For the discussion of physical mechanisms taking part during thin £lm growth two sorts of models can be used - analytical models based on a numerical solution of rate equations and atomistic models performing operations with individual atoms of growing £lm. The atomistic models are time-consuming but better physical assumptions can be used in their construction.

Realistic atomistic models of £lm growth able to handle growth process in extremely large time scale of nearly 15 orders of magnitude (from the description of interaction of impinging atoms with substrates to the formation of semicontinuous layers) must consist of several sub-models with various time and space scales and with their outputs connected:

- The nucleation process is simulated by the detailed calculations of movements of individual atoms of deposited material and their interaction with atoms of the substrate. The algorithm used is the standard molecular dynamics method with forces obtained from inter-atomic potentials (see e.g. [1]). The £nite temperature of substrate and the cooling of impinging atoms is handled by the Nose's method [2].

- The formation of small clusters and their further growth is studied stochastically by the Energy minimization technique, where the probabilities of transitions between various states are compared with Boltzmann factors.

- Data from the £rst two models serve as input values for the kinetic Monte Carlo model. Atomistic Monte Carlo models are used for the simulation of thin £lm growth for a rather long time (e.g. [3]), however only present computational technique enable us to include realistic assumptions into models [4].

The results of simulation are compared with both the predictions of nucleation theory and with experimental data - TEM photographs of discontinuous metal £lms. For the analysis of these photographs as well as for the analysis of simulated micrographs, the basic algorithms of mathematical morphology together with some more advanced algorithms based on percolation theory and Fourier optics are used.

References

1. Ra£i-Tabar H., Physics Report 325 (2000) 239.
2. Nose S., J. Chem. Phys. 81 (1984) 511.
3. Hrach R., Starý V., Thin Solid Films 85 (1981) 285.
4. Adams J. B. et all., Thin Solid Films 365 (2000) 201.

Sheath evolution in electronegative plasmas

R. Hrach, V. Hrachová and M. Vicher

Faculty of Mathematics and Physics, Charles University,
V Holešovičkách 2, 180 00 Prague 8, Czech Republic
+420 2 21912306, +420 2 6885095, vera.hrachova@mff.cuni.cz

The understanding of processes in the boundary layer between plasma and immersed solids is very important in modern plasma-chemical technologies as well as in probe diagnostics of low-temperature plasma. Further, in contemporary plasma physics there is a considerable scienti£c and technological interest in the plasmas of electronegative gases as the presence of negative ions in¤uence the formation of the transient region, so-called sheath, between undisturbed plasma and substrate [1]. Third, dynamical processes in the sheath resulting either from applying step voltages to substrates or caused by internal instabilities in the plasma became an popular topic theme in the literature - e.g. [2], [3]. These processes are important for the implantation of ions and for technologies taking place at higher frequencies. All physical and chemical processes during plasma-solid interaction depend on plasma composition and further experimental parameters. As our understanding of these mechanisms is still incomplete, various mathematical and computational models have been suggested.

The transport of charged particles originating from undisturbed plasma to metal substrates immersed into plasma can be studied by various simulation techniques - by ¤uid modelling, by particle modelling or by solving Boltzmann kinetic equation. Most of authors use the ¤uid simulation. In our laboratory, the self-consistent particle simulation technique is preferred as it gives more information, although it is very time-consuming.

Our main task was to study dynamics of sheath formation in three-component plasma containing electrons, positive ions and negative ions under the in¤uence of voltage steps. The technique used was the standard self-consistent PIC-MC method: the distribution of electric £eld in the sheath was derived from the charge distribution by solving the Poisson equation, the equations of motion were solved by the Verlet algorithm, electrons, positive argon ions and negative oxygen ions were taken as charged species, scattering events were treated stochastically with mean free paths given by [4]. To be able to study the sheath dynamics, the identical time steps for both electrons and ions ought to be used.

In our contribution the steady-state distributions of electric potential in the sheath for various concentrations of negative ions, the transient electric £elds in the sheath caused by step substrate biases and the ¤uxes of all charged species were derived. The obtained results con£rmed the importance of negative ions in the sheath formation. It was found that at higher concentrations of negative ions, the sheaths of complex structure are created and the ¤uxes of both positive and negative particles are highly in¤uenced - resulting even in transient currents of reversed polarity. The calculations were extremely time-consuming, as a large number of particles were treated simultaneously and the standard techniques for increasing the performance of computation can be used for steady-state situations only. Therefore, the attention was devoted to the additional simulation techniques for the increase of effectiveness of simulation.

References

1. Chung T. H. et al., Jpn. J. Appl. Phys. 36 (1997) 2874.
2. El-Zein Y. et al., J. Appl. Phys. 70 (1996) 3853.
3. Vitello P., Jpn. J. Appl. Phys. 38 (1999) 4283.
4. Brown S. C.: The Fundamental Data on Electrical Discharges in Gases. In: Basic Data of Plasma Physics. AIP Press, New York (1994).

Variation effect on the insecticide activity of DDT analogs - A chemometoric approach

S.Itoh[1], M.Arai[2], K.Kobayashi[2], and U.Nagashima[3]

[1] *TOSHIBA R&D Center, Kawasaki, 212-8582, JAPAN*
[2] *Nnational Institute for Research in Inorganig Materials, Tsukuba, 305-0044, JAPAN*
[3] *National Institute for Advanced Interdisciplinary Research, Tsukuba, 305-8562, JAPAN*
+81-44-549-2113, +81-44-520-1801, satoshi.itoh@toshiba.co.jp

The £rst molecular of DDT, 2,2-bis (p-chlorophenyl) - 1,1,1-trichloroethane, have been synthesized over a hundred years ago, and it is more than a half century since the discovery of its insecticide effect against a wide variety of arthropos. Nevertheless, little speci£c knowledge about its toxicity is known. Since a microscopic mechanism for the toxicity to a living animal would be very complex, it is hard to investigate the mechanism detailed experimentally. On the other hand, QSAR (quantitative structure-activity relationship) or chemometric approach is a promising way to investigate bio-chemical activity of molecules. We have found previously that, based on the £rst principles electronic structure calculations and neural-net analysis, charge distributions in dioxin isomers are related to its toxicity, and the dioxin isomers containing a few Cl atoms, e.g. 1-MCDD, 2,3-DCDD and 1,2,3-TriCDD, are conjectured to show highly harmful as the same as 2,3,7,8-TCDD[1]. Quite recently, the harmfulness of such dioxin isomers are con£rmed experimentally by using spleen and thymus cells. Although we have no information concerning the toxicity mechanism of dioxin isomers against living cells, a combined method of the electronic structure calculations and neural-net approach shows a good predictability.

The molecular structure of the DDT analogs is written as $C(C_6H_4X)(C_6H_4Y)LZ$, where the molecule with X=Y=Cl, Z=H, and L=CCl_3 is p-p' DDT, and the molecule with X=Y=Cl, Z=H, and L=CCl_2H is p-p' DDD. For the DDT analogs, effects on the variation in the X,Y,Z, and L positions on the insecticidal activity are experimentally investigated by using house¤ies[2]. However, there is no report on the electronic structures of these DDT analogs as the authors as known. We have carried out the electronic structure calculation based on the density functional theory with a local approximation, and determined the most stable geometry of over 25 DDT analogs. The DDT analogs with large functional groups such as SCH_3 and OC_2H_5 shows small LUMO-HOMO gap energy in comparison with one of other DDT analogs. However there is little evidental chemical trend concerning the substitution of functional groups in the X and Y positions. In order to investigate the relationship between the electronic structures of the DDT analogs and the insecticidal activity, neural-net analysis has been carried out, where experimental insecticitad activities of the DDT analogs were user as teaching signals and Mulliken gross populations in the molecules were used as input signals. From this analysis, we have found that charge distribution at the carbon atoms of aryl groups is relevant to its insecticidal activities, and it is hard to £nd the relationship between the local electronic structures of substitutional groups X and/or Y and the insecticidal activities reported experimentally. We will discuss on possibility of neutralization of the toxicity of the DDT analogs based on the electronic structure calculation and the neural-net analysis.

References

1. S.Itoh, H.Ueki, M.Arai, K.Kobayashi, and U.Nagashima, in Proceedings of FOMMS2000 (Foundation of Molecular Modeling and Simulation), Keystone, USA, 2000.
2. R.L.Metcalf and T.R.Fukuto, Bull. W.H.O. 38 633 (1968), R.L.Metcalf, I.P.Kapoor and A.S.Hirwe, Bull. W.H.O. 44 363 (1971).

Quanti£cation of channels of plasma polymerisation using a chemical model based on mass spectrometry

D. F. Ihrig, J. Stockhaus, F. Scheide,
O. Winkelhake, O. Streuber

Maerkische Fachhochschule
University of Applied Sciences
Labor fuer Umwelttechnik
Frauenstuhlweg 31
D-58644 Iserlohn
Tel.: 02371/566-272, Fax: 02371/566-274

Goal of the project is a solvent free painting shop. The environmental technologies laboratory is developing processes of plasma etching and polymerisation. Polymerised thin £lms are £rst order corrosion protection and primer for painting.

Using pure acetylene we get very nice thin £lms which were not bonded very well. With air as bulk gases in acetylene it is possible to polymerise well bonded thin £lms which are stable £rst order corrosion protections and well primers.

Nitrogen is necessary to generate well bonded thin £lms. UV/Vis spectroscopy shows nitrogen oxide radicals in emission spectra of pure nitrogen and air. But nitrogen oxide is fully suppressed in presence of acetylene. IR spectroscopy shows only C=O, CH_2 and CH_3 groups but no nitrogen species.

Using a numerical model it is possible to calculate theoretical mass spectra. The adjustment of theoretical mass spectra to real measurement leads to speci£c channels of polymerisation which is driven by a couple of radicals. The chemistry of polymerisation is similar to photochemical production of ozone in the troposphere. With respect to this chemical processes it is possible to have an idea of pollutant production processes.

Modelling of the phase separation in a supersaturated solid solution

T. Ischenko[1], S.V. Demishev[1] and W. Gust[2]

[1] *General Physics Institute, Vavilov str. 38, 117942 Russia*
[2] *MPI Metallforschung, Seestr. 92, 70174 Stuttgart, Germany*

Decomposition of a solid solution is one of the phenomena often observed in materials science. A prominent and interesting object for investigation is a novel class of non-equilibrium superconducting metals – Al-based solid solutions produced by high pressure treatment that are characterised by a quite simple crystalline structure and rather strong electron-phonon interactions with vibrations of atomic clusters. The study of the temperature and time stability of such alloys, as well as the relationship between their microscopic properties and the mechanism of structure formation and evolution remains a challenge for the theory due to the great complicity of the problem.

A model describing the phase separation process in a supersaturated binary solid solution for a broad interval of supersaturation has been developed. The kinetic of the process and equilibrium structure obtained has been investigated by the Monte Carlo method. The probability of direct atom exchange in a solid solution has been calculated according to the new proposal that incorporates the effect of the energy difference between £nal and initial states of an exchange and the in¤uence of all the neighbouring atoms on the exchange considered. A new approach has been suggested to accelerate the simulation procedure for the time evolution of the system. The interatomic interaction up to the next-nearest neighbours has been taken into account. The lattice distortion produced by precipitation is included into consideration.

The dependence of the stable structure of the system on the temperature, solute atom concentration and the type of interatomic interaction is obtained as result of the computer simulation. The exponent of time dependence of the precipitate size is analysed as a function of different microscopic parameter of the model. It is found, that there is a correspondence between its value and the different separation regimes those can occur in a solid solution.

Contact dynamics simulations of compacting cohesive granular systems

D. Kadau, G. Bartels, L. Brendel, and D. E. Wolf

Theoretical Physics, University of Duisburg, 47048 Duisburg, Germany

+49-203-379-4227 (phone), +49-203-379-1681 (fax),

kadau@comphys.uni-duisburg.de

Contact dynamics is a simulation scheme which implements the excluded volume interaction of perfectly rigid particles and the solid friction law exactly. Hence, it is an important counterpart to molecular dynamics simulations where these singular interactions have to be regularized, especially for granular systems with lasting contacts [1].

Cohesive attraction in granular systems becomes more and more important as the grain size decreases. In the extreme case of nano-particles the cohesion is even one of the most important factors. For example it has to be taken into account when processing “nano-ceramics” by *sinter-forging*, i.e. pressure sintering at low temperatures [2]. There, the compaction by rearrangement of the grains for a large number of particles can be simulated by means of contact dynamics.

To that purpose, we developed and implemented a model of cohesion in the context of contact dynamics [3]. This model allows for a £nite range of the attractive interaction and will be compared to an alternative approach with the restriction to pure contact forces and a different treatment of persisting contacts and shocks. Since we model round particles, we introduced rolling friction, so that force chains are not destabilized by rolling. In practice this means we allow for the transfer of a torque through a contact, extending the concept of a point contact. The admissible torque is treated similar to Coulomb’s friction law, i.e. we use a torque threshold depending on the normal force.

The initial state of the simulated system shown in £gure 1 was prepared by means of ballistic deposition. Its behavior under compression for different cohesion and friction parameters is investigated. It turns out that rolling friction is crucial for a highly porous £nal state.

This work was performed within DFG-Sonderforschungsbereich 445 *Nano-Particles from the Gas-Phase : Formation, Structure, Properties.*

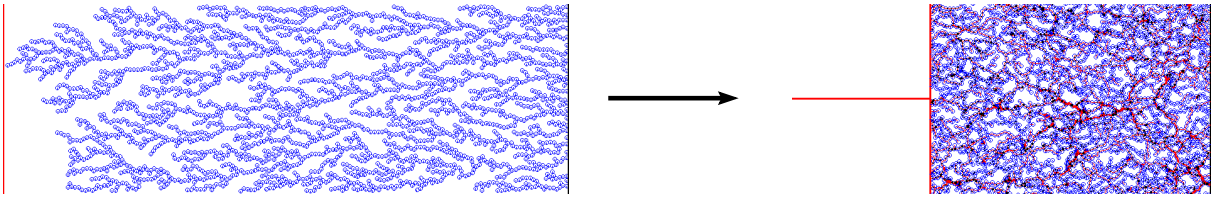


Fig. 1. Compaction of ballistic deposited cohesive grains

References

1. F. Radjai, J. Schäfer, S. Dippel and D. Wolf, J. Phys. I France **7**, 1053 (1997).
2. G. Skandan, H. Hahn, B. H. Kear, M. Roddy, and W. H. Roddy, Mat. Lett. **20**, 305 (1994).
3. G. Bartels, L. Brendel, D. Kadau, and D. Wolf *The modelling of cohesive granular matter within contact dynamics*, preprint.

Large-scale simulations of the £nite-temperature properties of the molecular assemblies Mn_6 and Ni_{12}

G. Kamieniarz[1], R. Matysiak[2], A. Caramico D'Auria[3], F. Esposito[3], and C. Benelli[4]

[1] *Computational Physics Division, Institute of Physics, A. Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland*
[2] *Institute of Technology, Pedagogical University in Zielona Góra, Poland*
[3] *Dipartimento di Scienze Fisiche, UniversitÁa di Napoli, Piazzale Tecchio, 80125 Napoli and INFM UnitÁa di Napoli, Italy*
[4] *Dipartimento di Chimica, UniversitÁa di Firenze, 50144 Firenze, Italy*
tel. +48 61 8273 071, fax +48 61 8257758, e-mail: gjk@amu.edu.pl

Assemblies of spins are interesting as objects providing the lower-size limit for magnetic nanoparticles. Among the fundamental questions they raise are the magnetic quantum tunneling and the quantum-size effects on the thermodynamical properties. The spin aggregates are embedded as the cores in the macromolecules with well-de£ned size, shape and stoichiometry. They are separated from one another by shells of ligand molecules and can be synthesized in macroscopically large samples in regular structures.

In our report a numerical transfer-matrix approach, based on the Suzuki-Trotter formula and the checkerbord decomposition, as well as an exact diagonalization technique exploiting the point-group symmetry and the properties of the shift operator are worked out in the framework of quantum statistical mechanics. The advantages of the quantum transfer-matrix (QTM) simulation method have been demonstrated for the macroscopic Haldane-gap and molecular-based magnetic chains [1]. The results are not subject to any statistical nor systematic errors and the macroscopic limit can be directly evaluated from the largest eigenvalue of the transfer matrix. For the £nite rings, however, all terms in the de£nition of the partition function bring some contribution, so that the computational complexity of the QTM method increases enormously.

To accomplish the exact numerical diagonalization in the case of the uniform spin variable $S = 1$ and $N = 12$ (appropriate for Ni_{12}), we selected the commuting operators: the z-component of the total spin $\mathcal{S}_z$, the mirror re¤ection operator $\mathcal{R}$ and an operator $\mathcal{K}$. The real operator $\mathcal{K}$ stands for $\mathcal{K} = \frac{1}{2}\left(\mathcal{P} + \mathcal{P}^{\dagger}\right)$, whose eigenvalues are $\lambda_k = \cos\frac{2\pi k}{N}$ with $k = 0, \ldots, \left[\frac{N-1}{2}\right]$, where $\mathcal{P}$ is a shift operator [2].

Both methods are applied, using the isotropic Heisenberg spin Hamiltonian and the large-scale simulations, to the title high nuclearity cyclic clusters Mn_6 (i.e. $[Mn(hfac)_2NITPh]_6$) [3] and Ni_{12} (i.e. $Ni_{12}(O_2CMe)_{12}(chp)_{12}(H_2O)_6(THF)_6$) [4] in order to model quantitatively their magnetic properties. The mesoscopic parameters for both molecules ($J/k_B = 350 \pm 10K$ and $J/k_B = 8.5 \pm 0.5K, g = 2.23 \pm 0.01$) are obtained from a £t of the theoretical susceptibility curves to the experimental results. For the Ni_{12} complex new experimental susceptibility data are also reported. We applied parallelized program written in Fortran Languange using Parallel Virtual Machine (PVM) utility on Cray T3E.

References

1. Caramico D'Auria A., Esposito F., Esposito U., Gatteschi D., Kamieniarz G. and Wałcerz S., J. Chem. Phys. **109**, 1613 (1998).
2. Caramico D'Auria A., Esposito F., Kamieniarz G., Matysiak R., J. Phys. C Cond. Matt. - accepted
3. Caneschi A., Gatteschi D., Laugier J., Rey P., Sessoli R., Zanchini C., J. Am. Chem. Soc.110, 1988 2795
4. Blake A.J., Grant C.M., Parsons S., Rawson J.M. and Winpenny R.E.P., J. Chem. Soc., Chem. Commun. 1994 2363

Finite-temperature quantum transfer-matrix simulations of the frustrated spin 1/2 chains

G. Kamieniarz[1], **M. Bieliński**[1], **H. Szymczak**[2] **and J.-P. Renard**[3]

[1] *Institute of Physics, Adam Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland*

[2] *Institute of Phisics, Polish Academy of Sciences*

[3] *Institut d'Electronique Fondamentale, Université Paris-Sud, Bâtiment 220, 91405 Orsay Cedex, France*

tel. +48 61 8273 071, fax +48 61 8257758, gjk@zawrat.amu.edu.pl

Both experimental and theoretical interest in quasi one-dimensional frustrated quantum spin systems has been strongly forced since 1993, when it was shown that the magnetic susceptibility of $CuGeO_3$ measured in all crystal directions drastically drops below $T_{SP} = 14.3K$. It was atributed to the spin-Peierls (SP) phase transition, which manifests itself when a system of quasi one-dimensional quantum spin chains undergoes dimerization due to lattice distortion.

To describe these properties, a $S = 1/2$ one-dimensional antiferromagnetic Heisenberg model of $CuGeO_3$ with nearest neigbour (nn) and next-nearest neigbour (nnn) interactions was proposed [1, 2], with the Hamiltonian in the form $H = -J\sum_{i=1}^{N}(S_iS_{i+1} + \alpha S_iS_{i+2}) + \sum_{i=1}^{N}(-1)^i\delta S_iS_{i+1}$, where N denotes the size of the chain, $J(< 0)$ and $\alpha(> 0)$ are the nn exchange integral and the ratio of the nnn exchange integral to the nn one, respectively. The parameter δ describes dimerization. Below T_{SP}, the value of δ is non-zero and the alternation of J has to be taken into account. So far, in order to estimate theoretically the J and α values, full diagonalization has been applied [1, 2, 3] to rings with $N \leq 18$ (e.g. 9 spin pairs at most). The £nite-size data have been extrapolated to the thermodynamic limit and compared to the susceptibility measurement results above the SP transition point. Also, newly developed density matrix renormalization group (DMRG) technique has been used to estimate the temperature dependence of dimerization parameter δ in the region below T_{SP} [4].

Here thermodynamical properties of the one-dimensional $S = 1/2$ Heisenberg model with dimerized nearest and uniform next-nearest neighbour interactions are studied by the numerically exact quantum transfer-matrix method and the results are applied to the quasi-one-dimensional magnetic systems $CuGeO_3$ and $Pb[Cu(SO_4)(OH)_2]$.

The Suzuki-Trotter formula is used to obtain a classical system with spin $\sigma = 3/2$ and effective interactions between nearest neigbours only [5]. The magnetic susceptibility curve is calculated and compared with experimental results performed in a wide temperature range, revealing the presence of frustration in the model proposed for CuGeO3 and $Pb[Cu(SO_4)(OH)_2]$. For the pure $CuGeO_3$, temperature dependence of the dimerization parameter below the spin-Peierls transition point is also estimated. The technique is extended for the £nite-chain segments and applied to the diluted $CuGeO_3$ obtained by the neutron beam with three different intensities. The corresponding sizes of segments are also estimated for all the samples.

References

1. J. Riera and A. Dobry, *Phys. Rev. B* **51**, 16098 (1995)
2. G. Castilla, S. Chakravarty and V. J. Emery, *Phys. Rev. Lett.* **75**, 1823 (1995)
3. K. Fabricius, A. Klümper, U. Löw, B. Büchner, T. Lorenz, G. Dahlenne, A. Revcolevschi, *Phys. Rev. B* **57**, 1102 (1998)
4. A. Klümper, R. Raupach and F. Schönfeld, *Phys. Rev. B* **59**, 3612 (1999)
5. G. Kamieniarz, M. Bieliński and J.P. Renard, *Phys. Rev. B* **60**, 14521 (1999)

Temperature dependence of vibrational properties of a Σ 5(310)[001] NiO grain boundary: A molecular dynamics study

T. E. Karakasidis [1,2]

[1]*Department of Civil Engineering*
University of Thessaly, Pedion Areos, 38334 Volos, Greece
[2]*Department of Computer Engineering, Telecommunications, and Networks*
University of Thessaly, Pedion Areos, 38334 Volos, Greece
tel: ++30.421.74054, fax: ++30.421.74169, email: thkarak@uth.gr

Grain boundaries (GBs) present a great interest in ceramics since these materials are often used in polycrystalline form. The reason for this is that many technologically interesting ceramic materials are prepared by powder sintering. GBs may seriously affect several properties such as conductivity, brittle fracture, creep etc [1]. The knowledge of the atomic structure in the boundary region as well as the dynamic properties of the atoms in this region helps understanding such effects. Atomistic simulations are well suited for such studies since they provide a microscopic description of the phenomena. Molecular Dynamics (MD) is one of the most appropriate ones as it can take into account explicitly temperature effects.

In the present work we focus on the study of vibrational properties of the ions in the GB region of a Σ 5(310)[001] NiO GB by means of MD simulations. The choice of the material and of the speci£c boundary lies on the fact that NiO has a relatively simple crystal structure (fcc) while there are simulation studies of the structural [2, 3], and diffusional [4] behavior of the speci£c GB showing its stability as a function of temperature.

The ionic interactions are described by a rigid ion potential developed for NiO. The simulations were performed in the canonical ensemble using the Nose Scheme, while the equations of motion were integrated using the Verlet algorithm with a timestep of 10^{-15}s. The phonon density of states (DOS) of the boundary region was calculated at room temperature in the directions parallel and perpendicular to the boundary plane. The obtained results are compared with those for the bulk region and conclusions are derived about the binding of the ions. We have also calculated the phonon DOS for various temperatures up to $0.80\mathrm{T}_m$, T_m being the melting point of the model system.

Mean square displacements (msd) of the ions in the GB region as a function of temperature in the direction perpendicular and parallel to the boundary plane have also been calculated and the results are compared with that of the bulk. There is evidence of an anisotropy in the two directions studied: the vibration amplitudes normal to the boundary plane are larger than in the direction parallel to it indicating that the ions are less tightly bound normal to the GB plane than parallel to it in accordance with the indications obtained from the DOS results.

References

1. Sutton A.P. and Balluf£ R.W. "Interfaces in Crystalline Materials", Oxford Univeristy Press (1996)
2. Meyer M. and Waldburger C., Mater. Sci. Forum v.126-128, pp. 229 (1993)
3. Karakasidis T. and Meyer M., Model. and Simul. in Materials Science and Engineering v.8 pp.117 (2000)
4. Karakasidis T. and Meyer M., Physical Review B v.55, pp. 13853 (1997)

Performance analysis of parallel molecular dynamics simulation of Lennard-Jones liquids on a small Beowulf cluster

T. E. Karakasidis [1] **N. Cholevas** [2] **A. Liakopoulos** [1]

[1] *Department of Civil Engineering, Hydromechanics Laboratory, University of Thessaly, Pedion Areos, 38334 Volos Greece.*
[2] *Department of Mechanical and Industrial Engineering, University of Thessaly, Pedion Areos, 38334 Volos, Greece.*
tel: ++30.421.74054, fax: ++30.421.74169, email: thkarak@uth.gr

Molecular Dynamics (MD) is a well established simulation method based on an atomic description of matter. MD is well-suited for the study of transport and structure properties as it can probe microscopic mechanisms not easily accessible by experiment and thus it is widely used in several areas of physics and materials science. MD provides us with a set of atomic trajectories, as they are determined by the interactions between the atoms and Newton's law of motion. Useful information is obtained about the system's properties through statistical mechanics since one can relate nearly any experimental property to the motion of atoms through the formalism of statistical mechanics [1]. However, even with present day computing power, MD is quite demanding in computer time if one attempts to simulate either very large systems or/and very long times [2].

The introduction of parallel computers initiated a great deal of research towards the development of parallel codes for computationally intensive problems. However the high cost of parallel computers had limited the availability of such machines to major and well-funded research centers. The emergence of Linux and the Beowulf project allowed the introduction of low-cost high-performance parallel computation to small research groups while many major labs created and operate vast such clusters.

In the present work we deal with the building of a small Beowulf cluster and the necessary transformation of a sequential MD code in order to run in parallel mode and to be used for the simulation of liquids. The cluster consisted of four PC's with Pentium III processors running under Linux and using MPI [3] which is a TCP/IP based protocol. The con£guration used was that of MPICH [3] although the same code can run also under LAM [3]. We discuss the changes made to the sequential code with an effort to maintain its readability. A Lennard-Jones potential was used to describe interactions between atoms. Such potential is widely used in simulations of model liquid systems. The simulation runs were performed in the microcanonical ensemble and several properties of the Leenard-Jones liquid were successfully reproduced. The methodology used was the atom decomposition method [2] in which each processor is assigned to deal with a given group of atoms. We examined the program performance for system sizes from 10^2 up to 10^5 atoms and also the scaling with the number of processors varying from 1 to 4. The in¤uence of the communication methods between processors was also examined. It was found that even such a small cluster could be a very useful and cost-effective solution for the realization of MD simulations of small Leenard-Jones liquid systems for real times up to 1μs within a reasonable execution time.

References

1. M. P. Allen and D.J. Tildesly "Computer Simulation of Liquids", Clarendon Press, Oxford (1987)
2. S. J. Plimpton, J Comp. Phys., v.117, p.1-19 (1995)
3. MPI Forum. Internatioanl Journal of Supercomputing Application v8, p.165-416 (1994)
   see also http://www-unix.mcs.anl.gov/mpi/

Perturbation theory and numerical calculations for the effective conductivity of two-dimensional structures

Isaak M. Khalatnikov

L.D. Landau Institute for Theoretical Physics,Russian Academy of Sciences,
Kosygina str. 2, 117334, Moscow, Russia
Landau Network - Centro Volta, Villa Olmo, via Cantoni 1, 22100 Como, Italy
Raymond and Sackler Faculty of Exact Sciences, School of Physics and Astronomy,
Ramat Aviv, 69978, Israel
Tel: 39-031-579827, Fax: 39-031-570174, landau@icil64.cilea.it

While the problem of the calculation of the effective conductivity of composite materials is well-known only few exact results was obtained until now. The most developed is the theory of the effective conductivity of the plane, because here one can use the property of duality between conductivity and resistence, which holds only for the two-dimensional Ohm's law. The most interesting result in this £eld is that by Dykhne [1], who has considered the plane covered by regions with two different conductivities σ_1 and σ_2. If the distribution of condictivities is stochastic and equal-weighted when $\sigma_{eff} = \sqrt{\sigma_1 \sigma_2}$. The same result holds also for some regular two-color structures on the plane (in particular, for chessboard) as was shown by Keller in his earlier paper [2].

In our recent paper [3], the perturbation theory together with convenient diagram technique for the solution of Laplace-type equation was developed. This technique allows to calculate perturbatively the tensor of effective conductivity for any periodic structures on the plane. We have reproduced the result of Keller -Dykhne by our perturbative method. Besides the components of the tensor of effective conductivity for the anisotropic three- color chessboard are calculated. It is shown that the isotropic (symmetric) part of effective conductivity calculated up to the sixth order of perturbation theory satis£es the Bruggeman effective medium equation for symmetric three-color structures with equally partitioned components. In another our paper [4]the asymptotic formula for the effective conductivity of the isotropic three-color (three-conductivity) rhombic tesselation in the plane is obtained for the case when one conductivity is much smaller that the two others. The tentative formula for this rhombic tesselation $\sigma_{eff} = \frac{(\sqrt{\sigma_1}+\sqrt{\sigma_2}+\sqrt{\sigma_3})\sqrt{\sigma_1\sigma_2\sigma_3}}{\sqrt{\sigma_1\sigma_2}+\sqrt{\sigma_1\sigma_3}+\sqrt{\sigma_2\sigma_3}}$ is suggested and discussed.

The application of our perturbative technique for more complicated tesselations of the plane such as three-color hexagonal (honeycomb) or rhombic tesselations encounter some claculational dif£culties connected with the fact the the structure of Fourier coef£cients corresponding to these tesselations is very complicated. Using the numerical calculations one can get the neccessary estimations for the corresponding diagrams which can allow to check different tentative formulas for the compicated (and interesting from the physical point of view) tesselations of the plane [5].

References

1. A.M. Dykhne, Sov. Phys. JETP 32, 63 (1970).
2. J.B. Keller, J. Math. Phys. 5, 548 (1964).
3. I.M. Khalatnikov and A.Yu. Kamenshchik, JETP 91, 1261 (2000).
4. I.M. Khalatnikov and A.Yu. Kamenshchik, JETP Lett. 72, 341 (2000).
5. I.M. Khalatnikov, A.Yu. Kamenshchik and A.V. Toporensky, work in progress.

Computer modeling of interface structure in Al-Be system

E. Abramov, A. Kiv, G. Zamir

Department of Materials Engineering, Ben-Gurion University of the Negev
84105 Beer-Sheva, P.O. Box 653
Tel +972-8-6460461, E-mail: kiv@bgumail.bgu.ac.il

The Molecular Dynamics method was applied to obtain a realistic picture of interface structure in the Al-Be system. The calculations were performed for three cases corresponding to real conditions of Al-Be interface formation

The liquid Al-Be mixture is slowly becoming cool from high temperatures (T¿1560K). In this case it is worth while to consider a process when Al phase is forming on the Be substrate.

The liquid Al-Be mixture is quickly becoming cool from high temperatures (T¿1560K) to low temperatures (T¡ 400K). Because of thermal conductivity of liquid Al is somewhat larger than the corresponding one of Be one may to suppose that Al in favorable cases £rst will form the solid phase.

Then in the simulation procedure Be layers have to be deposited on the Al substrate.

Low temperature decay of Al-Be solid solution may proceed in conditions of irradiation by fast particles (for example, in nuclear reactor). These processes are similar to low temperature aging of metal alloys and solid solutions. The stochastic rise of nucleation centers of new eliminated phases takes place. This case is differed from two previous ones and corresponds to relaxation of two structures which came into contact without growth of layers step by step.

We used potential functions which were obtained by ab-initio method, but applied them to calculations of real Al-Be interface structure by using classical MD scheme. The calculation scheme allows to investigate both interface features and bulk properties.

It was established that at the £rst stages of Al (Be) layers growth on the Be(Al) substrate the boundary disordered phase (BDP) arises. The mixing of Al and Be atoms in the BDP is observed. The degree of boundary disorder depends on the temperature conditions of Al-Be interface formation and on the nature of substrate. We obtained essentially different characteristics of microstructure of Al-Be interface for the deposition of Al layers on Be substrate and for the contrary case.

In the case of the low temperature decay of Al-Be solid solution under the irradiation by fast particles the interface layers, as a rule, are more homogeneous. We observed the clearly expressed island structure of Be layers in the Al – Be interface region. In other cases the interface layers also were inhomogeneous.

Some Be atoms from the boundary layers penetrate through the restored Al planes and appear at the large distances from the boundary in the Al lattice. In consequence the density of Be atoms in the interface region decreases.

Some Al atoms penetrate to the £rst layers of the substrate. Approximately 5% of Be atoms are found in the nearest layers of Al. So the formation of thin eutectic layers in a boundary region takes place.

The asymmetry of BDP relatively the boundary may give information regarding the nature of substrate in the Al-Be system and about the mechanism of Al-Be interface formation.

Wave packet molecular dynamics simulations of hydrogen at Mbar pressures

M. Knaup, P.-G. Reinhard, C. Toepffer, and G. Zwicknagel

Institut für Theoretische Physik II, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Tel.: ++49-9131/85-28457, Fax: ++49-9131/85-28907, email: knaup@theorie2.physik.uni-erlangen.de http://www.theorie2.physik.uni-erlangen.de/~knaup

We study hydrogen at Mbar pressures using semi-quantal "Wave-Packet-Molecular-Dynamics" simulations, in which the electrons are represented by anti-symmetrized Gaussian wave packets described by parameters which follow a pseudo-Hamiltonian dynamics. With this method we can simulate up to $N \approx 250$ electrons and the same number of protons on an ordinary PC, and about $N \approx 1000$ electrons on a parallel computer.

In our model we describe the protons classically, i.e. by the positions $\vec{R}_I$ and momenta $\vec{P}_I$ in a periodically continued box with boxlength L, whereas the electrons are represented by a N-particle Slater-sum

$$\Psi(\vec{x}_1, \ldots, \vec{x}_N) = \frac{1}{\sqrt{N! \det(\mathbf{O})}} \sum_{\sigma \in \mathcal{P}} \mathrm{sgn}(\sigma) \prod_{s=1}^{N} \varphi_{\sigma_s}(\vec{x}_s) \, .$$

Here, $\mathcal{P}$ is the set of permutations of order N, and $\mathbf{O}$ is the overlap-matrix $O_{kl} = \langle \varphi_k \,|\, \varphi_l \rangle$.

For the one-particle wavefunctions we make an ansatz of periodic Gaussian wave packets [1]:

$$\varphi_s(\vec{x}_s) \;\propto \sum_{\vec{n} \in \mathbb{Z}^3} \exp\left[-\left(\frac{3}{4\gamma_s^2} + \frac{i p_{\gamma_s}}{2\hbar\gamma_s} \right) (\vec{x}_s - \vec{r}_s - \vec{n}L)^2 + \frac{i}{\hbar} \vec{p}_s \, (\vec{x}_s - \vec{r}_s - \vec{n}L) \right] .$$

with the 8 variational parameters $\{\vec{r}_s, \, \vec{p}_s, \, \gamma_s, \, p_{\gamma_s}\}$.

For a given Hamilton operator $\hat{H}$, one can derive the time evolution of the system from the time-dependent variational principle [2]

$$\delta \int \langle \, \Psi \, | \; i\frac{\partial}{\partial t} - \hat{H} \; | \, \Psi \, \rangle \, \mathrm{d}t \; = \; 0 \, .$$

This results in equations of motion for the variational parameters with a pseudo-classical Hamilton function $\mathcal{H} = \langle \, \Psi \, | \, \hat{H} \, | \, \Psi \, \rangle$.

This method allows to simulate hydrogen at densities of the order of the solid-state density and various temperatures, covering the wide range from a molecular solid state, over a liquid up to a fully ionized plasma. From these simulations we extract pressure, pair correlation functions, autocorrelation functions of current and velocity as well as the resulting transport coef£cients. Our results are in quite good agreement with both experiments and other theoretical approaches.

References

1. M. Knaup, P.-G. Reinhard, and C. Toepffer, *"Wave Packet Molecular Dynamics Simulations of Deuterium in the Region of Laser Shock-Wave Experiments"*, preprint 2000, to be published in Contrib. Plasma Phys. (proceedings of PNP-10, September 2000)
2. P. Kramer, M. Saraceno, *"Geometry of the Time-Dependent Variational Principle in Quantum Mechanics"*, Lecture Notes in Physics 140, Springer Verlag 1981

Justi£cation of the ”net” model for a high-contrast structure and its application to randomly £lled composite

Berlyand L.V.[1] **and Kolpakov A.G.**[2]

[1] *Pennsylvania State University, State College, USA*
[2] *Siberian State University of Telecommunications and Informatics, Novosibirsk, Russia*
7-3832-665280, fax 7-3832-661039, e-mail agk@neic.nsk.su

We consider Laplas equation in the domain with the large number of small absolutely conducting randomly distributed £llers. It is a model of capacitor with composite layer £lled with particles having large dielectric constant. One the method to analyze such the problem is the reduction of the original problem to a ”net” model. The method proposed in [1] uses the continuum model of medium. In practice we usually deal with the mixtures formed from homogeneous components and it is impossible adopt the model [1] to describe such kind media.

Formulation of the problem. In the domain $P = [-1, 1] \times [-L, L]$ the disks $D_i, i = 1, ..., N$ of the radius R are distributed in a random way; $Q = P \setminus \cup Q_i$. Consider the problem

$\Delta u = 0$ in Q_P ; $u(x) = t_i$ on D_i ; $\int_{\partial D_i} undx = 0, i = 1, ..., N$; $u(x, \pm 1) = \pm 1, \partial u/\partial n(\pm L, x) = 0$.

The effective conductivity of the £lled medium is de£ned as $A = (1/2L) \int_{x=\pm 1} undx$.

The ”net” (£nite-dimensional) model. The ¤ux between the pair of disks ($i - th$ and $j - th$) is equal to $g_{ij}(t_i - t_j)$, where $\sqrt{R/\delta_{ij}}$, δ_{ij} is the distance between the disks [2]. We obtain the net $x_i, t_i, g_{ij}; i, j = 1, ..., N$, where x_i are the nodes (corresponding to the disks) and t_i are the potentials, which satisfy the equations (the ”net” model)

$\sum g_{ij}(t_i - t_j) = 0, i \in I; t_i = \pm 1, i \in S^{\pm}$ (I means the interior and $S^{\pm}$ means the boundary nodes).

Theorem. The effective conductivity A has the order of $\sqrt{R/\delta}$ as $\delta \to 0$, where $\delta = max\delta_{ij}$ and max is taken for the neighbor disks. The leading term is expressed through solution of the ”net” model in the form $A = 1/4 \sum g_{ij}(t_i - t_j)^2$.

The relation with the earlier models. In [2] a periodic structure of the conducting disks was analyzed and the order $\sqrt{R/\delta}$ was predicted for the effective conductivity.

The numerical investigation of the ”net” model. We use the discrete network to compute A numerically. We compute the dependence of A on the volume fraction of the inclusions V for monodispersed composites and obtained results which are consistent with the percolation theory predictions. For polydispersed composites (random inclusions of two different sizes) the dependence $A(V)$ is not simple and is determined by the relative volume fraction V_r of large and small particles. Some results will be published in [2].

References

1. Borcea, L., Papanicolaou G., Network approximation for transport properties of high contrast materials. SIAM J Appl Math, 58(2), pp.501-539 (1998).
2. Keller, J.B., Conductivity of a Medium Containing a Dense Array of Perfectly Conducting Spheres or Cylinders or Nonconducting cylinders. J. Appl. Phys., 34:4, pp 991-993 (1963).
3. Berlyand, L., Kolpakov, A. Network Approximation in the Limit of Small Interparticle Distance of the Effective Properties of a High Contrast Random Dispersed Composite. Arch. Rat. Mech. Anal. (in print)

Research of growth of crystall from melt by method molecular dynamics

Kotov Sergey Vladimirovich[1], **Khukhryanskiy Yuriy Pavlovich**[2]

[1]*Kotov Sergey Vladimirovich, VSTU, Moskovskiy pr.14, Voronezh, 394026, Russia*
[2]*Khukhryanskiy Yuriy Pavlovich, VSTU, Moskovskiy pr.14, Voronezh, 394026, Russia*

The microscopical model of phase equilibrium in a system a solution - melt Ga-P - solid phase is designed. The numerical analysis of model on a computer with use of a method of molecular dynamics is conducted. In the basis of the model there is a ¤uid system of 2500 atoms of gallium and 500 atoms of phosphorus placed in a cube with the size of an edge calculated from the real density of the system. The upper side of the cube is re¤ecting. On lateral sides the periodical conditions are used. The lower border represents a potential barrier with an altitude E1 on the side of a liquid and altitude E2 on the side of a crystal, and E2 $>$ E1. E1 and E2 are activation energies of surface atoms of the crystal.

The interaction between particles is described by a potential of Lennard-Jones. For calculation of forces between particles the Verlet algorithm based on the numerical solution of Newton equations was used. For optimization of calculation we de£ned a matrix of the nearest neighbours, which are taken into account during calculation of interparticle interactions. The matrix of the neighbours is renovated in each 15 time steps. One step is equal to 10-15 s. The surface diffusion was taken into account at simulation.

The dependence of quantity of desorbed atoms from the substrate on a potential well depth E2 and of adsorbed atoms on E1 on the liquid - crystal border is investigated. The exponential nature of the dependence of a desorption factor on a well depth E2 is established.

Further we intend to substitute the potential well on the lower liquid - crystal border for the atomic structure of a crystal GaP.

The spinodal of the overheated solid

Maxim N.Krivoguz

Moscow Institute of Physics and Technology, Institutskii per. 9, 141700, Dolgoprudnyi, Russia

e-mail: maximian@mail.ru

Considering the processes such as electrical explosion of the conductors, when the times of the energy input are much smaller then the characteristic times of thermal expansion, the solid can be overheated into the metastable region [1]. The overheating of the solids of different chemical compound was actually observed experimentally in pulsed mode [2, 3] in accordance with the theoretical views.

In analyzing the possibilities of overheating the information about the spinodal, i.e. the ultimate overheating is required. The spinodal is the locus in P-V-T coordinates, which corresponds to the limit of thermodynamic stability. The criteria of thermodynamic stability is $(\partial P/\partial V)_T < 0$. The points in which $(\partial P/\partial V)_T = 0$ form the spinodal.

The spinodal of the solid, like other physical or chemical properties of a macrosystem, can be obtained by using the methods of computer simulation proceeding from the intermolecular potentials. In this work the molecular dynamics method of computer simulations was used to obtain the curve of the spinodal. The solid was considered as a system of particles, which interact with each other by means of the pair potential of "soft spheres" $U = \epsilon(\sigma/r)^n$. The periodical boundary conditions were used to eliminate the surface effects. The uniformity of the potential as the function of distance allowed to carry out all the numerical calculations in the dimensionless variables $X = (N\sigma^3/\sqrt{2}V)(\epsilon/kT)^{3/n}, Z = PV/NkT$, regardless of the values of the parameters ϵ, σ of the potential of "soft spheres".

The equation of state of the solid in the far metastable region was obtained in the computer simulations. The spinodal was derived as the extrapolation of the numerical equation of state to the region of ultimate thermodynamic stability. The simulations were carried out for different powers of soft-sphere potential. The numerical values of the parameters of the potential, given in [4], allowed to build the curve of the spinodal for some solid metals in P-V-T coordinates and to plot it to the real phase diagram. Also the results of simulation and the results of [5] for the ¤uid-solid transition gave ultimate overheating of some solid metals, which are in accordance with the experiment.

References

1. Valuyev A.A., Norman G.E., JETP, 1999, V.116, No 6(12), p.2176-2181.
2. Chemezova L.I., Mesyats G.A., Sedoi V.S., Semin B.N., Valevich V.V., Proc.XVIII Int. Simp. Disch. and El. Insul. in Vacuum. (Eindhoven, 1998), p. 48-51.
3. Baikov A.P., Shestak A.F., Letters to JTP, 1979, V.5, No 7, p. 1335-1339.
4. Levashev P.R., Preprint UIHT RAS, No 1-446, 2000, 29 p.
5. Hoover W.G., Gray S.G., Johnson K.W., J.Chem.Phys., 1971, V.55, No3, p.1128-1136.

Constructing isotropic polycrystal materials via molecular dynamics

A. M. Krivtsov

St. Petersburg State Technical University, Dep. of Theoretical Mechanics,
Politechnicheskaya Street 29, 195251 St.-Petersburg, Russia

Phone: +7-812-5504208, Fax: +7-812-3214771
Email: krivtsov@AK5744.spb.edu

One of the main challenges in use of molecular dynamics technique for simulating macroscopic behaviour of materials is that all regular particles packings produce computer materials with anisotropic mechanical properties. If generally it is possible to choose interparticle potentials to obtain isotropic conditions for elastic moduli, there is no way to satisfy isotropic conditions for inelastic and strength properties of the materials. This can be the reason why molecular dynamics, which is very successful in modeling crystalline materials [1], still has limited applications in the case of homogeneous isotropic solids.

There are several approaches allowing bypass this problem. Use of particles mixture with various sizes and potentials allows obtaining isotropic materials. Unfortunately this technique can not be used as a general panacea since the nonhomogeneity of the material does not disappear for high temperatures. That is why such materials behave like glasses without clear difference between solid and liquid phases. Another approach is to construct polycrystal particle packings with random distribution of the monocrystal grains orientations. This method can produce isotropic computer materials, which can satisfy to very wide range of mechanical, thermodynamic and physical properties. Obviously this technique requires much more computer resources, since the elementary volume is now the monocrystal grain, containing itself hundreds of particles at least. Therefore the full-scale use the polycrystal computer materials was started only recently, following the sharp increase in the power of the modern computers. The interest to the simulation of the polycrystals was increased also by the recent discoveries that the materials with the crystal grains of the nanometer scale range possess unique mechanical and physical properties. These results stimulated molecular dynamics aided research in the area of nanocrystal materials [2].

In the presented paper computer constructing of polycrystal materials via molecular dynamics is considered. Two different techniques for obtaining computer polycrystals are presented, namely melting or compression techniques. In the melting method the initial con£guration of the particles (could be some monocrystal packing) is subjected to strong heating. Here the heating means that a random component is added to the velocities of all particles, and these additional velocities are high enough to break the crystal structure of the material, so that melting of the solid structure can be observed. Afterwards the material is subjected to a slow cooling (the energy is removed from the system by means of weak dissipation forces), resulting in polycrystal material packing. The second technique for polycrystal creation is compression of the mixture of monocrystal grains, obtained beforehand from the condensation of vaporized media. Mechanical properties of the polycrystals obtained by these two techniques are compared using various computer experiments including strong compression and impact loading. The results are also compared with the similar computer experiments performed for regular particles packings [3], [4].

References

1. M. Parrinello, A. Rahman. *J. Appl. Phys.*, 1981, 52(12), 7182–7190.
2. J. Schiotz, T. Vegge, F. D. Di Tolla, K. W. Jacobsen. *Physical Review B*, 1999, 60(17), 11971-11983.
3. A. M. Krivtsov. *Interna-tional Journal of Impact Engineering*, 1999, 23, 466-476.
4. A. M. Krivtsov, Y. I. Mescheryakov. *Proceedings of SPIE*, 1999, 3687, 205-212.

Density-functional study of multielectron ionization of sodium clusters by strong femtosecond laser pulses

L.I. Kurkina

Institute of Thermophysics SB RAS, Acad. Lavrentyev ave.,1, Novosibirsk 630090, Russia

tel: 7-3832-343094, fax: 7-3832-343480, e-mail: kurkina@itp.nsc.ru

In recent years, new experimental techniques have opened the very interesting regime of strong electronic excitations in clusters which are induced by intensive short laser pulses. One of the most powerful approaches to describe the interaction of atomic clusters with electromagnetic £elds is the time-dependent density-functional theory[1], the highly ef£cient linearized version of which is widely used for weak perturbations. However, the density-functional formalism in itself is a nonlinear nonperturbative approach suitable for studying strong electronic excitations, too. This report presents density-functional calculations of the valence electron emission from sodium clusters containing 8, 20, and 40 atoms under strong laser pulses with peak intensities of $10^{12} - 10^{14} W/cm^2$, time duration of 10 - 200 fs, and photon energies of 1.0 - 3.5 eV (with the mesh width of 0.05 eV). The computations were performed by direct numerical solution of the time-dependent Kohn-Sham equation with the local exchange-correlation potential. The clusters are simulated by jellium spheres. The initial state is borrowed from the self-consistent density-functional calculation of the ground-state problem. The spherical symmetry is retained in the time-dependent study via the average of the effective potential over angular variables. The spherical model limits the investigation to single-particle excitations separating them from the dipole surface plasmon (which is also excited in the visible part of the optical spectrum and can cause the electronic autoionization). The emission is evaluated through the number of valence electrons escaping from a sphere of radius $1.5R$ (R denotes the cluster radius) around the cluster. A heavy dependence of the electron response on cluster size, intensity and time duration of light pulses is obtained. The electron emission markedly decreases when the light intensity is reduced even though the pulse energy is conserved through the respective increasing of the pulse duration. By this is meant that the ef£ciency of the cluster-laser interaction is essentially dictated by the pulse intensity instead of the pulse energy. The dependence of the electron emission on the pulse length is signi£cantly weaker than on the pulse intensity. With increasing cluster size, the electron emission rises. The emission spectra for different clusters under the same light pulses come close together if the spectra are normalized to cluster radii squared. The strongest electron escape occurs in the region between 2 and 3 eV. With increasing intensity and/or time duration of laser pulses, the main peaks in the electron emission spectra are enhanced, blue-shifted, and complicated. The blue-shift is connected with the coupling of the over-the-barrier ionization to the single photon resonant absorption. During the cluster-pulse interaction the over-the-barrier ionization starts prior to the resonant one and leads to the depression of one-electron energy levels as well as to the increase of the distance between the levels, as a result of which the resonant absorption comes about at higher photon energies than it follows from the ground-state energy spectrum. The complication of electron emission spectra with increasing laser intensity may be caused by the enhancement of the multiphoton ionization. A great increase in the kinetic energy of electrons keeping in the clusters is also detected (that can involve the subsequent thermal electron emission).

This work was supported by RFBR (Grants No.99-15-96028, 00-03-33043).

References

1. E.K.U.Gross, W.Kohn, Adv. Quant. Chem. 21 (1990), 255.

Stability of sodium nanoclusters and phase transition

H.B. Liu[1]**,J.A.Ascencio**[1] **and M.J.Yacaman**[2]

[1]*Instituto Nacional de Investigaciones Nucleares,*
Amsterdam 46-202, Hipódromo Condesa, 06100 México, D.F., México
[2]*Center for Nano and Molecular Technology,*
Texas materials Institute and Department of chemical Engineering,
The University of Texas at Austin, Of£ce Number CPE-5-404,
Austin, Texas 78712-1062
52-53297342, 52-53297245, h_b_liu@yahoo.com

Nanotechnology has become one of the most important goals of the material sciences application, the stability of systems and the possibility to change their con£gurations are involved in the manipulation methods for new devices, since the pioneering work of Wheeten[1], Andres[2] and Ijima, who have obtained well de£ned systems using passivating agent to control the size and morphology in order to use the resulting self-assembled arrays and the particular nanostructure properties in nanoelectronics and nanophotonics. The structures and structural evolutions as well as their related behaviors and properties have fascinated scientist for many years. Marks (1994)[3] and Wang (1998)[4] contributed an incisive and comprehensive reviews elucidating the progress in these £elds, the latter paid much attention to passivated clusters. Much progress has been made either in the unexpected discovery of noncrystallographic structure types (multiply twinned particles (MTPs): icosahedra and the so-called Ino and Marks decahedra), or in structural transitions (shape ¤uctuations, quasimelting, melting[5].

In our study we stress the following factors: typical simple metal,intermediate size, multitwined structure, and thermodynamic properties as well as dynamic behavior. We consider that our work will be of help for the research in thin £lm growth, cluster-assembling materials and other fundamental studies for the development of nanotechnologies.

The MD simulations were performed using XMD developed by Prof. J.Riffkin, Centers for Simulation, University of Connecticut. Gupta-like potential was used to describe the interatomic interaction among sodium atoms. In all the simulations reported here, a time step of 5×10^{-16} second was used, which is a fairly small value as considering the temperature of 0K. It is rather necessary to ensure the accuracy of energy calculation due to small energy difference among different isomers. Meanwhile, long runs, usually 2×10^{6} time steps, are adopted in order to obtain fully relaxed con£gurations, after that the equilibrated nanoclusters were heated at the heating rate of 5×10^{12} K/s. This order of heating rate is too large from the point of view of experiment, but it will not cause a large amount of overheating in computer simulations according to our previous research work.

The molecular dynamics simulation results show relative stability order among cuboctahethedron, icosahedron, decahedron, Marks decahedron, deeply trancated decahedron, rounded bcc cluster from small size to intermediate size. Some rounded bcc clusters was found quasimelting at ground state. Melting behaviors of different clusters was featured, some relationship on multiscale from small clusters to the intermediate-sized all the way to the bulk were attempted to establish.

References

1. R.L.Whetten, J.T.Khoury et al., Adv.Mater. **8**,428(1996).
2. T.G.Schaaff, M.N.Sha£gullin et al., J.Phys. Chem. B **101**, 7885(1997).
3. L.D.Marks, Rep.Prog.Phys. **57**, 603(1994).
4. Z.L.Wang, Adv.Mater. **10**,1(1998).
5. Furio Ercolessi, Wanda Andreoni et al., Phys.Rev.Lett. **66**,911(1991).

Percolation in a $1+1$ ballistic deposition model

N. I. Lebovka and N. V. Vygornitskii

Biocolloid Chemistry Institute named after F.D. Ovcharenko, = NASU, 42, Vernadskii av., 04142, Kyiv, Ukraine and
University of Kiev Mogyla Academy, 2, Scovorody Str., 04070, = Kyiv, Ukraine

Formation of thin £lms in the process of deposition and aggregation of particles on a substrate is of great importance from fundamental and engineering points of view [1]. A large amount of work dealing = with dynamical scaling of surface evolution has been already done, but there = also exist large interest in studying morphology of deposits, their fractal, percolating and hydrodynamical properties and electrical conductivity = [2, 3].

The aim of this work is to study the percolation, scaling and fractal properties of the discontinuous £lms formed in one-dimensional lattice model simulating ballistic deposition of conducting particles. The problem of percolation is well studied for random percolation in = lattice and non-lattice systems [4]. But the main feature of the model under consideration is in introduction of the directed growth into percolation problem.

The model is based on the standard $1+1$ dimensional ballistic = deposition model [1]. All the particles are assumed to be conducting. Particles are randomly deposited and aggregate upon £rst contact with clusters in the sites of a square lattice. A substrate length L vary = from 40 to 1000. The planar and nonplanar substrates with initial = roughness were studied. The initial roughness is assumed to be Gaussian and characterized by a value of height dispersion σ for nonplanar = case. The results were averaged over the 1000 different con£gurations. The clusters were labeled using Hoshen-Kopelman algorithm with periodic = boundary condition in lateral direction.

The analysis of the percolative structure of deposits was done for = different values of σ and L. The percolation concentration p_c = follows the usual scaling relation $p_c = 3Dp_c^{\infty} + aL^{-1/\nu}$, where = p_c^{∞} is a percolation threshold for an in£nite ($L \to \infty$) system, a is a constant and ν is a scaling exponent. For a planar case ($\sigma = 3D0$) we have obtained $p_c^{\infty} = 3D0491 \pm 0.001$ and $\nu = 3D1.74 \pm 0.02$. The obtained value of the correlation length of the scaling exponent is $\nu = 3D1.74 \pm 0.08$, which differs substantially from the known values for random and directed percolation [4]. It was shown that the width of the percolation deposit grows with the system size increase, approximately, following the logarithmic law $h_p \propto \ln(L)$. The effect of the initial substrate nonplanarily is also discussed. We have observed increase of ν and decrease of p_c^{∞} with increase of the initial roughness. In a general case, the percolation cluster is not an isotropic fractal, but a scaling relation between the mass and the size of a cluster was observed in the longitudinal direction of the cluster with the effective fractal dimension $D = 3D1.44 \pm 0.02$.

So, the percolative, scaling and fractal properties of conducting deposits for $1+1$ ballistic model were studied. It was assumed that this model belongs to a new class of universality of the directed deposition percolation.

References

1. A.L.Barabasi, H.E. Stanley, Fractal Concepts in Surface Growth, Cambridge University Press, Cambridge, 1995.
2. F. Family, Physica A266 (1999) 173.
3. S. Tarafdar, S. Roy, Physica, B254 (1998) 28. sedimentary rocks, Physica B254,N
4. D. Staufer, A. Aharony, Introduction to Percolation = Theory, Tailor & Francis, London, 1992.

Atomistic study of structural correlations at a model liquid-solid interface

Adham Hashibon[1], Joan Adler[1], Michael W. Finnis[2], and Wayne D. Kaplan[3]

[1] *Department of Physics, Technion, Haifa, ISRAEL*
[2] *Atomistic Simulation Group, School of Mathematics and Physics,* The Queen's University of Belfast, Belfast BT7 1NN
[3] *Department of Materials Engineering, Technion, Haifa, ISRAEL*
Tel: 972-4829-2043, Fax:972-4822-1514, phadham@aluf.technion.ac.il

Metal-ceramic interfaces play a prominent role in a variety of technological applications that range from electronic devices to protective coatings and high-temperature structural components. The functionality of these systems depends crucially on their macroscopic properties such as fracture, yield, and electrical conductivity. These properties are strongly correlated with microscopic details of the metal-ceramic interface, such as bonding, chemistry, diffusion, and structure. Correlating macroscopic properties to the structure and chemistry of interfaces is one of the most intriguing topics in materials science.

Atomistic simulations, such as Molecular Dynamics or Monte Carlo permit the controlled study of these systems at the atomistic level for a large number of atoms and for large structures. However, the main limitation to such simulations is the lack of appropriate interatomic potential schemes which can model both metallic and ionic bonding across the interface. Nevertheless, simpli£ed models can be used to obtain basic qualitative insights into the problem.

In this study we explore structural correlations at a metal-ceramic interface with Molecular Dynamics simulations of a model aluminium system with the Ercolessi-Adams potential and up to 4320 atoms. Several rows of substrate atoms are pinned to equilibrium crystalline positions to mimic a rigid ceramic substrate, and the remaining aluminium atoms form a liquid metal whose atoms are free to move. The density pro£le and inplane structure at the interface are investigated for different interface crystallographic orientations and temperatures. An exponential decay of the density pro£le was observed, $\rho(x) \sim \mathrm{e}^{-\kappa \mathrm{x}}$, leading to the de£nition of κ as a quantitative measure of the ordering at the liquid-solid interface. We £nd a direct correlation between the amount of ordering in the liquid phase and the underlying substrate structure.

Computational study of structures of amorphous carbon

Anastassia Sorkin and Joan Adler

Department of Physics, Technion, 32000, Haifa, Israel

972-4-8292043, e-mail:anastasy@techunix.technion.ac.il

Amorphous structures are characterized by the high degree of short range order and the absence of long range order. In amorphous structures, the bond length, the number of nearest neighbour atoms, and the angle betweeen adjacent bonds are close to those in crystalline structures.

There are various methods to obtain amorphous carbon from diamond or from graphite. Two speci£c amorphous forms of carbon may be obtained: the diamondlike amorphous carbon, which will be denoted by *ta-C*, and graphitelike amorphous carbon named *a-C*. These two structures can be distinguished clearly by their macroscopic and microscopic properties. The former is a hard and dense material, mostly made of distorted sp^3 sites, while the latter has a less dense structure and mainly consists of sp^2 sites.

We apply a tight-binding molecular dynamics method to investigate the characteristics of *ta-C* and *a-C* solids. The method incorporates electronic structure calculations in the molecular dynamics through an empirical tight-binding Hamiltonian, and bridges the gap between *ab initio* molecular dynamics and simulations using empirical classical potentials.

The *ta-C* and *a-C* networks are obtained by quenching or annealing of liquids of various densities. The £rst peak of the radial distribution function is very sensitive to the relative concentration of *sp*, sp^2 and sp^3 bonding; that is in good agreement with work of Wang and Ho [1].

Doping by ion implantation in diamond may result in graphitization and give rise to the onset of electrical conductvity, due to the ability of carbon atoms to form the two types of bonds. Inrease of electrical conductivity associated with the creation of graphitelike pathways, i.e., with transformation of sp^3 to sp^2 bonds, was observed by Prawer and Kalish [2] and investigated in computer simulations by Saada [3].

The purpose of this study is to understand the conditions of graphitization of diamond at the surface between a crystal diamond layer and an amorphous carbon layer. The radial and angle distribution functions, the statistics of threefold and fourfold bonds, as well as the depth of the bandgap are studied.

References

1. C.Z. Wang, K.M. Ho, Phys. Rev. B **50**, 12429 (1994)
2. S. Prawer, R. Kalish, Phys. Rev.B **51**, 15711 (1995)
3. D. Saada, J.Adler, R.Kalish, Phys. Rev. B **59**, 6650 (1999)

In¤uence of point defects on the shear elastic coef£cients and on the melting temperature of vanadium

V. Sorkin, J. Adler and E. Polturak

Dept. of Physics, Technion Institute of Technology, 320000 Haifa, Israel

Tel:+972 4 829 3651 e-mail: phsorkin@tx.technion.ac.il

Melting is the fundamental process in which a crystal undergoes a phase change from a solid to a melt. Understanding this process is still a challenge, despite its common occurrence. For instance, most theoretical models do not taken into account the effects of lattice defects [1]. It is not feasible experimentially to directly observe the melting process on the atomic level. In contrast, the role of vacancies and interstitials in crystal melting can well be studied by means of simulations.

The in¤uence of point defects on the shear elastic coef£cients of fcc metal copper was examined by means of MD simulations[2]. A phase diagram of the melting temperature as a function of the density of point defects was established. It is turned out, that crystal containing no free surface undergoes mechanical melting as a result of the vanishing of $C' = (C_{11} - C_{12})/2$, when its speci£c volume reaches a critical value equal to the volume of the liquid phase. This volume can be attained either by heating of the crystal or by increasing the number of its point defects at constant temperature.

In the example of the copper fcc crystal with a free surface, the melting process starts to nucleate at the surface at thermodynamic melting temperature (which is always below the mechanical melting temperature). It was proposed that the mechanism of melting at the surface is the same as in the bulk. The difference between the surface melting temperature and the bulk melting temperature is explained by the higher local density of the point defects at the surface.

It was not clear if those results were speci£c to the fcc structure of copper. Therefore, in the present project, the melting of the vanadium bcc crystal was studied using molecular dynamics. An EAM potential for vanadium, proposed by Adams and Foiles [3], was applied to investigate the bulk solids under various temperature and pressure conditions. A canonical ensemble was simulated by means of the Nose-Hoover algorithm. The Parinello Rahman algorithm [4] has been used to simulate an isothermal-isotensial ensemble, which describes a system under constant stress.

References

1. S. R. Phillpot, S. Yip, D. Wolf, Computers in Physics **3**, 20 (1989).
2. A. Kanigel, J.Adler and E. Polturac, submitted
3. J. B. Adams, S. M. Foiles, Phys. Rev. B **41**, 3316 (1990).
4. M. Parinello, A. Rahman, Phys. Rev. Lett. **45**, 1196 (1980).

Sequence design of protein-like copolymers using time evolution of the system

A.V. Chertovich, V.A. Ivanov and A.R. Khokhlov

Physics Department, Moscow State University, 117234 Moscow, Russia

+7 095 9394756, +7 095 9397988, chertov@polly.phys.msu.su

Some years ago in work [1] a new method for sequence design of copolymers with special functional properties was proposed - the so called conformation-dependent sequence design. That method was realized in computer simulations for several problems: design of sequences for protein-like AB-copolymers (i.e. copolymers, for which favorable globular state shows microsegregation in dense core of A-units and shell of B-units), for AB-copolymers tuned to adsorption on a plan surface, for ABC-globules with compact center of C-units, etc. (see [2]-[3]). Being prepared according to this scheme copolymers are able afterwards demonstrate some features of parent conformation. Nowadays a theoretical description of that method is under construction.

In this work we propose further investigation of this approach and offer sequence design method taking into account time evolution of the system. Thus we suggest more realistic algorithm for conformation-dependent synthesis, which can be compared with analogous laboratory experiments. Furthermore, we announce a new computer algorithm for optimization of copolymer systems. Such algorithm can be considered as a rough model for a biomolecular evolution process, caused by simple mutagenesis (amino asid substitution in DNA).

We use Monte-Carlo method end bond ¤uctuation model [4]. We perform simulations on linear AB-copolymers with length N = 256 and 1024 monomer units. As the value for characterization statistical properties of our sequence we use the dispersion of the number of given type units in the window of variable length. For characterization of properties of obtained copolymers we use coil-globule transition temperature, gyration radius, etc.

It occurs that taking into account time evolution during conformation-dependent sequence design we observe signi£cant changes both in statistical properties of the sequences and in structural properties of the globules. Analogous changes take place during optimization procedure as well and bring us (hopefully) to few optimum sequences with best properties.

Financial support from INTAS, NATO and RFBR is appreciated.

References

1. A.R. Khokhlov, P.G. Khalatur, Physica A, 1998, v.249, p.253; Phys. Rev. Lett., 1999, v.82, p.3456
2. E.A. Zheligovskaya, P.G. Khalatur, A.R. Khokhlov, Phys.Rev.E, 1999, v.59, p.3071
3. V.A. Ivanov, A.V. Chertovich, A.A. Lazutin, N.P. Shusharina, P.G. Khalatur, A.R. Khokhlov, Macromol. Symposia, 1999, v.146, p.259
4. I. Carmesin, K. Kremer, Macromolecules, 1988, v.21, p.2819

A simple model for the DNA denaturation transition

Maria Serena Causo[1], **Barbara Coluzzi**[2], **and Peter Grassberger**[3]

[1]*INFM and Scuola Normale Superiore, I-56100 Pisa, Italy*
[2]*INFN and Universita di Roma "La Sapienza", I-00185 Roma, Italy*
[3]*NIC - Forschungszentrum Jülich, D-52425 Jülich, Germany*
causo@penelope.sns.it

The study of the nature of the DNA denaturation is a long standing open problem. Experimentally a multistep behaviour in light absorption as a function of the temperature was observed already in the £fties [1]. This suggested a scenario which reminds the cooperative melting behaviour at a discontinuous £rst order transition, in which the system changes suddenly its state from a double strand to two molten single-stranded chains.

The early Ising-like models which were used to study the denaturation transition could not even reproduce a phase transition behaviour, but only a continuous crossover between double stranded and denaturated state. A £rst re£nement consisted in taking into account the different entropic weights of opened bubbles, modeled as self-avoiding loops, and double stranded parts, modeled as single self-avoiding walks [3]. In this model the self avoidance between bases within the same loop was taken into account, but the other mutual excluded volume effects were completely neglected and a smooth second order transition in two and three dimensions was found.

We consider a simpli£ed model where many important features of DNA, as heterogeneity in the sequence, the effect of supercoiling, which can give rise to structures with writhes, or the possibility of mismatch in base pairings are totally disregarded, but excluded volume interactions are fully taken into account [2]. Our model consists of two interacting self-avoiding walks, corresponding to the two single strands, with the same origin on a 3d cubic lattice. Each monomer corresponds to a base and is supposed to have its complementary at the same position in the other chain. Two monomers with different positions in the two chains are not allowed to occupy the same lattice site, whereas the overlap of monomers at the same position is favored by an energetic gain ϵ that represents the binding energy. Base-pair misalignments are forbidden. We consider the homogeneous case, where all the binding energies are equal.

We study the denaturation transition in this model using Monte Carlo simulations based on the pruned-enriched Rosenbluth method (PERM) with markovian anticipation [4] , which is particularly effective to simulate interacting polymers. Our simulations indicate that the transition is of £rst order (the energy density is discontinuous), but the analog of the surface tension vanishes and the scaling laws near the transition point are exactly those of a second order transition with crossover exponent $\phi = 1$. Numerical and exact analytic results show that the transition becomes second order if the the self-avoidance constrain is relaxed or completely neglected.

References

1. R.M. Wartell and A.S. Benight, Phys. Rep. **126**, 67 (1985)
2. M.S. Causo, B. Coluzzi, and P. Grassberger, Phys. Rev. **62**, 3958 (2000).
3. D. Poland and H.A. Sheraga, J. Chem. Phys. **45**, 1456, 1464 (1966).
4. P. Grassberger, Phys. Rev. **E 56**, 3682 (1997).

Solvation of molecular complexes. A combined self-consistent-£eld and integral equation study

Chuev G.N.[1,2]**,Tikhonov D.A.**[2]

[1] *Institute of Mathematical Problems of Biology,* [2] *Institute of Theoretical and Experimental Biophysics, Russian Academy of Sciences, Pushchino, Moscow Region, 142290, Russia*

The study of solvation processes is of considerable interest to computational chemistry since most of the chemical reactions are observed in solution. A large number of problems on solvation of molecular, macromolecular and colloidal complexes has been investigated by the integral equation theory (IET) during last two decades [1]–[3]. The main goal of this report to present possibilities of the IET for modeling solvation effects in various molecular and macromolecular systems. A special attention is gained for solvation of molecular complexes. The proposed method takes account for the relations between quantum chemical and solvent thermodynamic properties. This method is based on a hybrid approach including quantum chemical calculations and the integral equation theory.

We suppose that the electronic and the solvent distributions are coupled through the electrostatic interactions between the interaction sites assigned to solute and solvent. We apply reference-interaction-site-model (RISM) to treat molecular aspects of solvent within a reasonable cost of computation. The latter version of integral equation method is widely used to investigate a wide variety of processes in liquids, in particular, to calculate the local microstructure of solvent around a solvated molecular complex. The RISM allows us to calculate site-site correlation functions and £nd distribution of solvent molecules around the solvated complex. These solvent molecules induce an electrostatic potential, which can be calculated via the site-site correlation functions. The above potential can be considered as external £eld acting on the electronic structure of solvated complex. Therefore, we can use conventional quantum-chemical methods to calculate the electronic structure of the solvated complex subjected to the external £eld. The evaluation of the electrostatic potential and electronic structure is to be optimized in a self-consistent manner resulting in microscopic self-consistent £eld (SCF) calculations of combined RISM-SCF equations. We have applied the method to calculate energetic and structural characteristics of solvated positronium, positron and electron and compared the obtained results with the experimental data. The results obtained by us indicate that although the absolute values of energies of solvated electron and positronium, found by the RISM-SCF method, can be quantitatively differ from the experimental values, such calculations are very promising for evaluation of structural parameters of solvated complexes.

References

1. Rossky P J *Annu. Rev. Phys. Chem.* **l36** 321 (1985)
2. Hirata F *Bull. Chem. Soc. Jpn.* **71** 1483 (1998)
3. Schweizer K S, Curro J G *Adv. Chem. Phys.* **98** 1 (1997)

A diffusion-collision model uses the thermodynamic information extracted by a neural network to predict the folding times of all-α proteins

M. Compiani[1,2], **E. Capriotti**[2,3] **and R. Casadio**[2,4]

[1] *Department of Chemical Sciences, University of Camerino, Camerino, Italy. Via S. Agostino 1, 62032 Camerino MC, Italy*
[2] *CIRB, Centro Interdipartimentale per la Ricerca Biotecnologica, University of Bologna, Bologna, Italy*
[3] *Department of Physics, University of Bologna, Bologna, Italy*
[4] *Department of Biology, University of Bologna, Bologna, Italy*
compiani@camserv.unicam.it

Protein folding poses one of the most challenging problems in molecular biology and the physics of complex systems [1]. The diffusion-collision model [2] (DC model) depicts the folding of proteins as a series of stochastic encounters among structured portions of the protein (microdomains) that aggregate to form the native structure. The focus of the present work is on proteins that have secondary structures of helical type. Here we propose to equate the microdomains with stretches of α-helices that are formed in the early stages of folding [3]. A crucial parameter of the theory is the probability that the colliding microdomains are correctly folded for the collision to be successful. This means that the helices must have suf£ciently grown in order to form a stable aggregate. We split the overall folding dynamics in two concurrent dynamical processes. Local dynamics take into account the processes of nucleation and elongation of the helices, whereas global dynamics are described in terms of the DC model. In this investigation we make an innovative use of a feedforward neural network that is originally designed to predict the secondary structure from the sequence of proteins [4]. The output of the network is used to locate the microdomains within the residue sequence of the protein and to model the kinetics of formation of helical structures. This allows us to gather the missing pieces of information as to the local dynamics and to eventually evaluate the probability of a favourable collision.

Our simulations show that the DC model complemented by our neural network-based procedure is an effective tool for the prediction of folding times starting from the sequence of proteins. Our model is also sensitive to point mutations that substantially alter the kinetics of folding of the protein under study.

References

1. Frauenfelder, H. & Wolynes, P.G. (February 1985), *Physics Today*, 58-64.
2. Karplus, M. & Weaver, D.L. (1994), *Protein Sci.* **3**, 650-668.
3. Compiani, M., Fariselli, P., Martelli, P-L. & Casadio R. (1998), *Proc. Natnl. Acad. Sci. USA* **95**, 9290-9294.
4. Casadio, R., Compiani, M., Fariselli, P., Jacoboni, I. & Martelli, P.L. (2000), *SAR QSAR Environm. Res.* **11**, 149-182.

Adaptive numerical method for Poisson-Boltzmann equation and its applications

Pavel Dyshlovenko

Department of Physics, Ul'yanovsk State Technical University, 32 Severny Venets St., Ul'yanovsk 432027, Russia

Tel.: +7-842-2439095, E-mail: pavel@ulstu.ru

The nonlinear Poisson-Boltzmann equation describes, in some approximation, the electric potential and charge distribution in colloidal systems. The detailed information on the free energy and the forces of interaction which can be obtained from the solutions of the equation plays an important role in studying stability of colloidal dispersions, formation of colloidal crystals, membrane separation processes and other £elds. One of the most intriguing phenomenon is metastable superheated crystalline structures formed by charged latex spheres in water. The structure and dynamics of these metastable colloidal crystals seems to be accounted for by the long-range attraction between the like-charged spherical particles [1].

Owing to the nonlinearity, Poisson-Boltzmann equation is mostly solved numerically. A £nite-element method with dynamical error estimation and adaptive mesh re£nement is developed with the aim of investigating the particle-particle and particle-surface interaction in colloidal systems.

The standard Galerkin £nite-element approach is used for solving the equation on a cylindrical domain. Due to the axial symmetry, the problem can be reduced to two dimensions. Other two-dimensional geometry and boundary conditions are also possible. Electrical neutrality of the system is taken into account. Quadratic approximation and six-noded triangular elements are used. The mesh is a Delaunay triangulation in each step of the adaptive process. The system of nonlinear algebraic equations arising from the £nite-element discretisation of the initial differential equation is solved by means of quasi-Newton method with analytical evaluation of Jacobian. The sparse matrix technique is used to reduce the memory requirement. The results of testing calculations for the force between two identical spherical colloidal particles in a bulk solution for the case of constant electric potential on their surface are in accord with known results.

Interaction between a charged sphere and a plain was investigated. Calculations show that a charged wall can attract a like-charged spherical particle for some values of the problem's parameters although repulsion is a common situation.

Computer experiments with a geometrically con£ned pair of spheres concern the widely discussed phenomenon of the attraction of two like-charged spherical particles in a con£ned geometry [1]. Attraction was observed in the numerical experiments within the framework of the Poisson-Boltzmann theory in [2]. Rigorous theoretical analysis predicts pure repulsive interaction of the particles [3, 4]. Method of the present work demonstrates the repulsive interaction in a cylindrical domain under any circumstances which is in agreement with theoretical predictions. A satisfactory explanation of the phenomenon remains an unresolved problem.

References

1. A. E. Larsen and D. G. Grier, *Nature* **385**, 230-233 (1997).
2. W. R. Bowen and A. O. Sharif, *Nature* **393**, 663-665 (1998).
3. J. C. Neu, *Phys. Rev. Lett.* **82**, 1072-1074 (1999).
4. J. E. Sader and D. Y. C. Chan, *J. Colloid Interface Sci.* **213**, 268-269 (1999).

Rigid-body formalism for simulating the macromolecules

M.R. Ejtehadi, R. Everaers, L. Delle Site, K. Kremer

Max-Planck Institute for Polymer research, Ackermannweg 10,
55128 Mainz, Germany

Macromolecules exhibit interesting dynamical and conformational properties on a wide range of length and time scales which are dif£cult to study within a single model. In the case of DNA, local can be studied in all atoms simulations while large scale conformational properties are accessible within continuum models such as elastic rod model of DNA, do not care about the compositional details of these molecules. The dif£culty with this approach is that phenomena on these widely different length scales are not always independent. For example, torsional strain can either lead to super-coiling or to local denaturation.

Regards to our informations about the con£gurational ¤uctuations of atoms [1] or geometry of chemical links between them [2], we introduce a new schema for coarse graining of the macromolecules. In this picture more rigid parts of macromolecules consider as rigid ellipsoid objects which are connected with some ¤exible arms to neighboring ellipsoids . Any arm is £xed to its ellipsoid and is recognized with its constant coordinate system in its ellipsoid frame. For the non-bonded interactions we use a variant of the Gay-Berne potential, while the bonded interactions are split into an orientational part and a harmonic potential. Three orthonormal vectors of arm's frame (tangent, normal and binormal) let us to introduce the orientational potential for the arms connections. Moreover, we consider a link point for any arm to introduce the bond ¤uctuation potential too. The shape, number of arms and position of arm link points depend on the geometry, topology and chemical structure of macromolecules as well as their rigid parts themselves. The potential energies can be expressed in terms of three dimensional vectors and rotation matrices. This form is suitable for Monte Carlo simulations. Singularity free representation of forces and torques can most conveniently be achieved in a quaternion representation which is suitable for molecular dynamics simulations. In our model there is not any restriction on the number of arms for ellipsoids. Thus the model could be used for any kind of macromolecules, from simple chains to highly condensed systems.

Finally we consider the inverse problem how to £nd the our potential parameters from equilibrium ¤uctuations in all atoms simulations of selected parts of macromolecules.

References

1. N. Bruant *et all.*, Biophysics Journal **77**, 2366-2376 (1999)
2. M.F. Thorpe *et all.*, Journal of Molecular Graphics and Modeling **19**, 60-69 (2001)

Computer simulation study of irreversible adsorption: coverage ¤uctuations

Jordi Faraudo and Javier Bafaluy

Grup de Fisica Estadistica, Facultat de Ciencies
Universitat Autonoma de Barcelona E-08193 Bellaterra (Spain)
Tel: +34 935812878 Fax: +34 935812155 E-mail: Jordi.Faraudo@uab.es

The irreversible adsorption of colloidal particles from ¤uid suspensions to solid surfaces is a complex phenomenon of great interest. Much effort has been devoted to the study of the effect of transport mechanisms on the adsorption kinetics and on the structure of the adsorbed monolayer [1]. Recently, both experimental [2, 3] and theoretical [4] studies have analysed the density ¤uctuations of the adsorbed monolayer. It is expected that the behaviour of density ¤uctuations reveals valuable information about the adsorption process. In adsorption driven by diffusion, the experimental results obtained by different researchers lead to very different conclusions about the behaviour of the reduced variance $\sigma^2/\langle n\rangle$ of the number of adsorbed particles [2, 3]. In addition, existing theoretical results are not applicable to the diffusion dominated case [4]. In this contribution we perform a computer simulation study of density ¤uctuations in diffusion driven adsorption. Also, we extend the mean £eld analysis of Ref [4] to analyze the simulation results. In order to obtain good statistics for $\sigma^2/\langle n\rangle$ we develop cellular automata simulations which are less time consuming than Brownian dynamics simulations. The simulation cell consists of an adsorbing surface with $N_x \times N_y$ adsorbing sites at $z = 0$ and a bulk phase discretized in a cubic lattice of $N_x \times N_y \times N_z$ sites. Each site can allocate only one particle. At each time step, all diffusing particles randomly select an adjacent free node and jump to it. When a particle reaches a site at the adsorbing surface, it is irreversibly adsorbed and remains immobilized at this site. When all the sites at the adsorbing surface are occupied, the simulation ends. We consider two kinds of boundary conditions at $z = N_z$. The £rst kind of boundary conditions is chosen to mimic open cell experiments. In this situation, a constant number of particles n_B is maintained at $z = N_z$ at each time step by removing or adding particles if necessary. Also the positions of particles at $z = N_z$ are randomized at each time step, so the surface $z = N_z$ behaves as an equilibrium reservoir with £xed concentration. The second kind of boundary conditions corresponds to closed cell experiments. At $t = 0$, n_0 particles are randomly distributed within the bulk and no more particles are added to the system during the simulation. In this case, an impenetrable barrier is placed at $z = N_z$ so particles arriving at this plane are re¤ected down.

The results in the case of open boundary conditions show that the behaviour of $\sigma^2/\langle n\rangle$ as a function of the density of adsorbed particles is in agreement with the extension to the diffusion driven situation of the mean-£eld theory presented in [4]. In the case of closed boundary conditions it is observed that $\sigma^2/\langle n\rangle = 1$ (which correspond to a Poisson process) for low surface densities ρ. When ρ increases, $\sigma^2/\langle n\rangle$ deviates from 1 depending on the size of the subsystems considered. As the size of the subsistems increases, the deviation from 1 decreases. These results are in qualitative agreement with the experiments described in [2] and can explain the differences between the results of different experimental setups. Therefore, our simulations clearly show that, in the diffusion dominated case, ¤uctuations in the density of adsorbed particles are strongly affected by the macroscopic boundary conditions imposed to the diffusion process.

References

1. J. Faraudo and J. Bafaluy, J. Chem. Phys. **112**, 2003 (2000).
2. Lavalle *et al*, Proc. Natl. Acad. Sci. USA **96**, 11101 (1999).
3. Z. Adamczyk *et al*, J. Chem. Phys. **113**, 11336 (2000).
4. J. Bafaluy *et al*, J. Chem. Phys **107**, 2089 (1997).

Molecular dynamics study of structure formation of a polymer chain in solution

Susumu Fujiwara[1] **and Tetsuya Sato**

Theory and Computer Simulation Center, National Institute for Fusion Science, 322-6 Oroshi-cho, Toki 509-5292, Japan

[1]*Corresponding author. Tel: 81-572-58-2382, Fax: 81-572-58-2626, e-mail: fujiwara@toki.theory.nifs.ac.jp*

Computer simulation of structure formation of polymer systems has recently become the focus of attention in physics, chemistry, biology and materials science. Although numerous computer simulation studies have thus been made on structure formation of isolated chain-molecule systems [1, 2, 3], little is known about the detailed mechanisms of structure formation of polymer chains in solution *at the molecular level*. With a view to investigating structure formation of polymer solution systems at the molecular level, we carry out the molecular dynamics simulations of a polymer chain in solution and analyze the formation process of the orientationally ordered structure of a polymer chain.

The polymer chain consists of 500 methylene groups and the solvent molecules consist of 3747 short chain molecules, each of which consists of six methylene groups. The atomic force £eld used here is the DREIDING potential [4]. At £rst, we provide a randomly distributed con£guration of a polymer chain in solution at high temperature (550 K). The system is then quenched to several lower temperatures (300, 350 and 400 K).

Our simulations show that (1) at higher quenching temperature (400 K), a toroidal structure is formed and (2) at lower quenching temperature (350 and 300 K), a toroidal structure is formed £rst, and then it changes into a folded orientationally-ordered structure (Fig. 1).

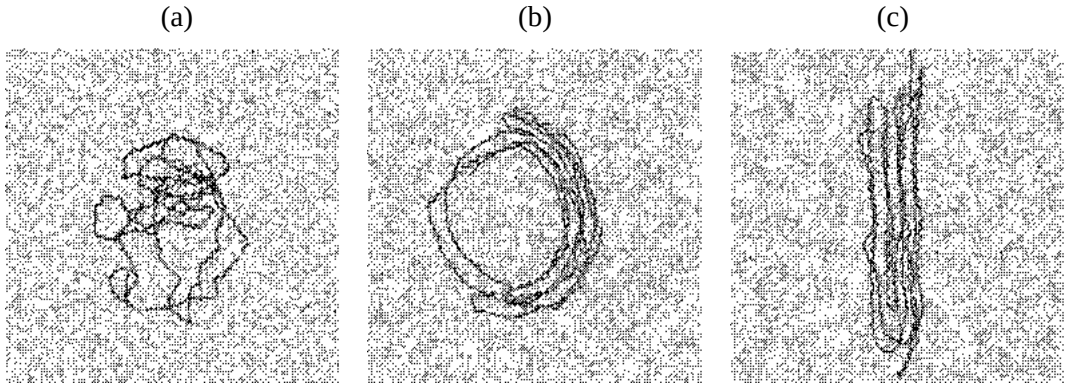


Fig. 1. Chain con£guration of a single polymer chain in solution for $T = 350$ K: (a) at $t = 0.0$ ns, (b) at $t = 2.5$ ns and (c) at $t = 6.0$ ns. Black and grey denote a polymer chain and solvent molecules, respectively.

References

1. S. Fujiwara and T. Sato, J. Chem. Phys. **107**, 613 (1997).
2. S. Fujiwara and T. Sato, Phys. Rev. Lett. **80**, 991 (1998).
3. S. Fujiwara and T. Sato, J. Chem. Phys. **110**, 9757 (1999).
4. S.L. Mayo, B.D. Olafson, and W.A. Goddard III, J. Phys. Chem. **94**, 8897 (1990).

Dynamics of orientationally ordered domains in a short chain-molecule system: size dependence of domain oscillation

Hiroaki Nakamura, Susumu Fujiwara and Tetsuya Sato

Theory and Computer Simulation Center,
National Institute for Fusion Science,
Oroshi-cho, Toki, GIFU, 509-5292, Japan

PHONE:+81-572-58-2356, Fax:+81-572-58-2626, mailto:nakamura@tcsc.nifs.ac.jp

As the fundamental process of structure formation for short chain molecules[1, 2, 3], the coalescence of two orientationally ordered domains were investigated by numerical simulation[4]. It was also demonstrated[4] that domains move collectively as if they were rigid bodies in spite of the non-bonded short-range interaction potential (Lennard-Jones potential) among chain molecules. In this paper, dynamics of domain is investigated for several domain size. Average angle θ for right or left domains is plotted for (61+61) and (61+29) chain-molecule system in Fig. 1. From this £gure, inertia of domain depends on its size. This property is not surprising, because the ordinal rigid body has this property. However, we £nd that the two cases in Fig. 1 have the same periods of the domain's oscillation. This fact is not observed in motions of the ordinary rigid body.

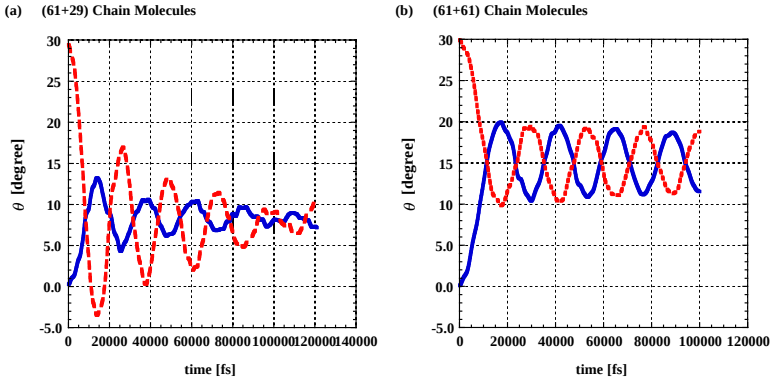


Fig. 1. Time evolution of angles θ for (a) (61+29) chain-molecule system and (b) (61+61) chain-molecule system.

References

1. S. Fujiwara and T. Sato, Phys. Rev. Lett. **80,** 991 (1998).
2. S. Fujiwara and T. Sato, Molecular Simulation **21,** 271 (1999).
3. S. Fujiwara and T. Sato, J. Chem. Phys. **110,** 9757 (1999).
4. H. Nakamura, S. Fujiwara and T. Sato, J. Phys. Soc. Jpn. ,**70** (2001) (in press).

Molecular process of slippage of macromolecular chain in highoriented linear polyethylene

Ulmas Gafurov

Institute of Nuclear Physics, Tashkent, Ulugbek 702132,Uzbekistan

(email: ulmas@suninp.tashkent.su)

An oriented crystalline polymer with homogeneous chemical structure of type of linear polyethylene is examined. Models of the thermoactivated slippages of stressed macromolecules and of the relaxation of local loads on amorphous parts of these molecules are presented. The crystalline polymer is considered as two-phasic one with interchanging amorphous and crystalline regions in a micro£brille. For calculations Frenkel-Kontorova's soliton model is used. In dependence on external load and amorphous region length two cases are realized. The £rst case takes place when the load is moderate. In this case the load on the amorphous section of a slipped out chain are completely relaxed and this section could change its conformation state. In the second case slipped out amorphous part of a macromolecule is in strained state but its strain is less than one of the macromolecule before its slipping out. The energy activation dependencies on molecular parameters and the local load are different for the two cases.

Simulation of diffusion in multi-protein-systems

C. Gorba and V. Helms

Max-Planck-Institute of Biophysics, Kennedyallee 70, D-60596 Frankfurt

Tel.:+49-69-6303-254, Fax:+49-69-6303-251,

E-mail:Christian.Gorba@mpibp-frankfurt.mpg.de

Photosynthesis and respiration are fundamental processes in molecular bioenergetics that are the basis for life on earth. The whole machinery includes photoexcitation, transfer of electrons and protons, and various chemical reactions. All these steps take place in several large integral membrane proteins, characterized over the past 15 years by X–ray and electron diffraction. In this work I focus on the diffusion of cytochrome c, a soluble electron carrier protein, between the bacterial reaction centre and the cytochrome bc_1 complex. The simpli£ed process can be described as follows: cytochrome c starts by picking up one electron at the bc_1 complex and diffuses in solution to the reaction centre to deliver its electron. A real system contains a large number of cytochrome c and membrane molecules and therefore is a many-particle system[1].

This project will concentrate on studying diffusional aspects of such a system. An essential question is: what is the rate of contacts between cytochrome c's and membrane proteins, i.e., how often is an electron picked up and delivered to the reaction centre? Thus, in contrast to often done detailed atomistic treatments of only a few molecules, I want to simulate macromolecular diffusion by modelling the system in a more abstract way, as a collection of spherical particles or particles composed of several spheres that move in the potential £eld of the membrane with the embedded, immobile, membrane proteins, the organization of which can be modelled using the experimental results in[2]. Then it should be possible to learn about the 'global' behaviour of a photosynthetic sytem.

The Brownian dynamics simulation method I use is based on the Langevin equation. This equation gives a statistical description on typical Brownian time scales of 100 ps. The basic iteration algorithm which solves the Langevin equation numerically on that time scale was developed in [3]. It includes calculation of the electrostatic and hydrodynamic interaction between the participating particles on each time step. The most time consuming part is the computation of the hydrodynamic tensor involved. Furthermore, to £nd values for the diffusion tensor elements, it might be necessary to include explicit Molecular dynamics simulations because of the more complicated hydrodynamic interaction if the proteins are very close to the membrane surface[4]. Thus, I want to develop a parallel algorithm for a Linux Cluster which has recently been setup in our group. Since it is planned to use the program as a module for a large simulation package in the future, I chose an object oriented approach.

The serial code developed so far is able to simulate test systems in a box containing about 100 charged spherical particles attracted by a charged surface.

Whereas the photosynthetic process is well understood on a molecular level, there is a lack of information concerning the interplay of several parts of a 'big' system. The aim of this project is to give a contribution to the understanding of a photosynthetic apparatus as a whole.

References

1. 'Stochastic Dynamics Simulations of Macromolecular Diffusion in a Model of the Cytoplasm of *Escherichia coli*', D.J. Bicout + M.J. Field, J. Phys. Chem. 1996, 100, 2489–2497.
2. 'Supramolecular organization of the photosynthetic apparatus of *Rhodobacter sphaeroides*', C. Jungas, J.-L. Ranck, J.-L. Rigaud, P. Joliot and A. Vermeglio, The EMBO journal Vol. 18 No.3 pp.534–542, 1999.
3. 'Brownian dynamics with hydrodynamic interactions', D.L Ermak, J.A. McCammon, J. Chem. Phys. 1978, 69, 1352–1360.
4. 'The Smoluchowski diffusion equation for structured macromolecules near structured surfaces', J. Chem. Phys., Vol. 112, No. 12, 22 March 2000.

Binding isotherms calculated for Cu2+ and Ca2+ ions interaction with DNA on its condensation in solution

E.Hackl, V.L. Galkin, and Yu.Blagoi

Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, 47 Lenin Ave., 61164 Kharkov, Ukraine
present address: Institute of Cell and Molecular Biology, University of Edinburgh, King's Buildings, May£eld Road, Edinburgh EH9 3JR, UK
ehackl@srv0.bio.ed.ac.uk

As it is well known, the DNA macromolecule is a polyelectrolyte. In a solution it exists in complexes with counterions, which, together with hydration surrounding, determine its structure. DNA may also be a target for a number of drugs interacting with nucleic acids due to intercalating or cation mechanism. Thus the problem of mathematical description of the DNA interaction with ligands is one of the most important both from the points of view of polymer physics and chemistry and molecular biology. In our previous works [1, 2] we have shown that under the action of Cu2+ and Ca2+ ions DNA is able to transit into the compact state in aqueous solution at 290C. DNA compactisation may be both of intra- and intermolecular character. This process is highly cooperative. DNA in the compact state remains in B-conformation limits [1, 2]. In the presence of alcohol DNA condensation occurs at a rather lower concentration of Me2+ ions than that of aqueous solution. In this case binding constants and cooperativity of the metal ion binding rise and binding isotherms (i.e. dependences of the binding degree r on the concentration of free metal ions Cf) take a nonmonotonous S-like character with metastable and nonstable parts characterised with the reverse dependence of r on Cf. Such isotherms for a stable process may be replaced with a dependence with a jump along r, that evidences a phase transition. Thus, the DNA transition into the compact state under the Cu2+ and Ca2+ ions action in aqueous-ethanol solutions may take the character of a phase transition. But when calculating binding isotherms in [2] we did not take into account the distribution of values along the assembly of DNA molecules. To obtain the more sequential thermodynamic description for the system of ions interacting with the biopolymers, in the present work we carried out calculations in terms of the macromolecule statistical sum. In this case binding isotherms are not nonmonotonous with any values of binding constants and cooperativity parameters. This is connected with the fact that the use of accurate expression for the statistical sum leads to the automatic ful£lment of all the thermodynamic inequalities. Thus, on the coil - globule transition single DNA molecules may undergo the £rst-kind phase transition while the transition of the assembly of DNA molecules is of sigma-like character typical of the cooperative and continuous transition.

References

1. E.V.Hackl, S.V.Kornilova, L.E.Kapinos, et.al., J. Mol. Struct. 408 / 409 (1997) 229-232.
2. S.Kornilova, E.Hackl, L.Kapinos et.al., Acta Biochim. Polon. 45 (1998) 107-117.

Ground state structures of polymers

J.Hauck and K.Mika

IFF, FZ Jülich, D–52425 Jülich

Two- and three-dimensional structures A_xB_y can be characterized by the numbers T_1 and T_2 of nearest and next-nearest neighbors of the same kind. A small number of structures at the border of the T_1, T_2 structure map is stabilized by enthalpy compared to an increased number of entropy stabilized structures. About 60 three-dimensional structures with T_1 = 2 nearest neighbors of all A atoms are suitable for in£nite chains of polymers like $(CH)_\infty$, $(CHCH_2)_\infty$ or $(CH_2)_\infty$ [1]. The size of the unit cell was increased in a systematic way and the A and B positions occupied to a maximum of 50% at r = y/x =1. The structures at higher A content are identical by exchange of A and B. The T_i values of all A atoms were averaged to the T_1 T_2 T_3 ; y/x values of the structure map. The present method will be outlined in some detail for the square net and the diamond lattice (adamantane structures). The structures T_1 T_2 T_3 ; y/x with T_1 = 2 nearest neighbors like 2 0 4 ; 1 or 2 0 2 ; 2 of the square net (with T_2 = 0 next-nearest and T_3 = 4 or 2 third neighbors; y/x = 1 or 2) can be considered for chains $(AB)_\infty$ or $(AB_2)_\infty$ of A atoms with covalent bonding between A atoms and one or two B atoms similar to polymeric $(CH)_\infty$ or $(CH_2)_\infty$ chains. Low T_1 and maximum T_2 values correspond to repulsive interactions, low T_2 values to attractive interactions. Most structures with M^i = 2 different values of A and B atoms are at corners of the structure map with maximum interactions. Few other structures like the homometric 2 2 0 ; 1a and b structures, which are not on the border of the structure map, do not show maximum interactions. The enthalpy is reduced because of decreased lattice energy. A large number of other structures, which are not on the border of the structure map, is stabilized by entropy at increased temperatures (disordered structures). Polymers with variable chain length and defects like dead ends or vacant positions are disordered. Some Monte Carlo simulations are approaching the border of the structure map.

The angle at C atoms in adamantane structures (β = 109^0) is more realistic than β = 90^0 (2 2 0 ; 1a/b) or 180^0 (2 0 4 ; 1 or 2 0 2 ; 2) in the square net. The various homometric structures can be described by different directions of the chain as one proceeds from the £rst C at projection height z = 0 ([100] square layers)

down,left,down,left,up,right,up,left	2 4 6 5 ; 1a ($P\bar{1}$)
up,right,down,left,up,right,up,left	2 4 6 5 ; 1b ($C\bar{2}$)
up,right,up,right,up,right,up,left	2 4 6 5 ; 1c ($P\bar{1}$)
down,left,up,right,up,right,down,right	2 4 6 5 ; 1d (C2)
down,left,up,left	2 4 6 4 ; 1 (C2/c)
up,left	2 4 6 6 ; 1a (Pmma)
up,right,down,left	2 4 6 6 ; 1b ($P4_122$)
up,left	2 2 2 ; 2a (Imma)
up,up′,up,right,up,left	2 2 2 ; 2b ($P3_112$).

The projection height z is decreased for the steps up′ of the last structure. The pathways are very complicated and can probably not be obtained by Monte Carlo methods. The listed directions must be continued periodically for pathways without voids or dead end. The homometric structures have all the same lattice energy but different space groups. The weak interactions between C atoms further apart and the complex pathway might give rise to disorder.

References

1. J. Hauck and K. Mika, Progr. Solid State Chem. 28(2000)1–200.

Direct pair correlation functions and elastic constants in liquid crystals: A computer simulation study

Nguyen Hoang Phuong, Guido Germano, Friederike Schmid

Theoretical Physics, University of Bielefeld, 33501 Bielefeld, Germany
Tel. +49-521-106 6197, fax +49-521-106 6455,
e-mail phuong@physik.uni-bielefeld.de

The direct correlation function is important in the statistical mechanics of ¤uids because it is the starting point of many density functional theories [1]. While its determination in computer simulations from pair distribution functions is well established in isotropic liquid crystals [2], corresponding studies of nematic liquid crystals have usually resorted to the approximation of ignoring the director orientation [3].

In the present work, we present a method to obtain the direct correlation function of a nematic liquid crystal from computer simulations without any approximations: the orientation of the director is taken fully into account.

As an application of the method, we compute the direct correlation functions in the isotropic and nematic states of an idealized model liquid crystal of soft ellipsoidal particles in molecular dynamics and Monte Carlo simulations. The results for the isotropic phase are compared with theoretical predictions. The results for the nematic phase are used to calculate the Frank elastic constants K_{11}, K_{22} and K_{33}; these values are in good agreement with those obtained from the same con£gurations by the established method of measuring the order ¤uctuations [4].

References

1. R. Evans, in *Liquids at Interfaces*, Les Houches Session XLVIII, J. Charvolin, J. F. Joanny, J. Zinn-Justin eds. (Elsevier, Amsterdam, 1988).
2. M. P. Allen, C. P. Mason, E. de Miguel, J. Stelzer, *Phys. Rev. E* **52**, R25 (1995).
3. J. Stelzer, L. Longa, H.-R. Trebin, *J. Chem. Phys.* **103**, 3098 (1995).
4. M. P. Allen, M. A. Warren, M. R. Wilson, A. Sauron, W. Smith, *J. Chem. Phys.* **105**, 2850 (1996).

New cellular automaton designed to simulate geometration in gel electrophoresis

M.J.Krawczyk, K.Kulakowski and A.Z.Maksymowicz

Faculty of Physics and Nuclear Techniques, University of Mining and Metallurgy, al.Mickiewicza 30, 30-059 Cracow, Poland

+(4812)6173539, fax(4812)6340010,kulakowski@novell.ftj.agh.edu.pl

Recent computer simulations on the gel electrophoresis show that at large electric £eld, the mobility collapses to zero [1]; this result is new and intriguing. Here we propose new kind of cellular automaton to simulate transportation of molecules of DNA through agarose gel. Two processes are taken into account: reptation at strong electric £eld E, described in the particle model [2], and geometration [3], i.e. subsequent hookings and releases of long molecules at and from gel £bres. The automaton rules are deterministic and they are designed as to describe both processes within one uni£ed approach. Thermal ¤uctuations are not taken into account. This approach is relevant for large E/T, where T is temperature. The number of simultaneous hookings is limited only by the molecule length. New features of the automaton are: i) the size of the cell neighbourhood for the automaton rule varies dynamically, from nearest neighbours to the entire molecule; ii) the length of the timestep is determined at each step according to dynamic rules. Calculations are made up to $N = 250$ reptons in a molecule. Two subsequent stages of the motion are found. During the £rst transient stage, initial set of random con£gurations of molecules is transformed into an ordered phase, where most molecules are elongated in parallel to the £eld direction. Such a reorientation is known to characterize the geometration effect [3]. During the second stage, which arises after some transient time, the mobility μ reaches a constant value. Then, it varies with N as $1/N$ for long molecules. The band dispersion varies with time t approximately as $\sqrt{t}$. Our results suggest, that the well-known plateau of the mobility μ vs N [4] does not hold for asymptotically large electric £eld.

References

1. A.van Heukelum and H.R.Beljaars, J.Chem.Phys. 113 (2000) 3909.
2. M.E.J.Newman and G.T.Barkema, Monte Carlo Methods in Statistical Physics, Clarendon Press, Oxford 1999, Chpt.12.
3. J.M.Deutsch, Science 240 (1988) 922.
4. J.-L.Viovy, Rev.Mod.Phys. 72 (2000) 813.

AB-copolymers mimicking some properties of membrane proteins: MC computer simulation

Lazutin A.A., Ivanov V.A., Khokhlov A.R.

Moscow State University, Physics Department
119899, Moscow, Vorobyevy Gory, Physics Department
tel: +7(095)939-4756, fax: +7(095)939-2988, e-mail:lazutin@polly.phys.msu.su

Present research is a further development of a so-called conformation dependent approach to sequence design of AB-copolymers proposed in [1, 2]. We study by means of Monte Carlo computer simulation the AB-copolymer chain with primary structure which was specially prepared on the basis of particular spatial conformation of a homopolymer globule: monomer units lying in thin cylindrical slice were assigned to be of B type (hydrophobic units), while others were assigned to be of A type (hydrophilic units) (Fig. 1). The idea of such ”coloring” procedure was to create a coarse model of synthetic AB-copolymer, which would mimick some basic properties of membrane protein. Properties of AB-copolymers with different primary sequences were compared.

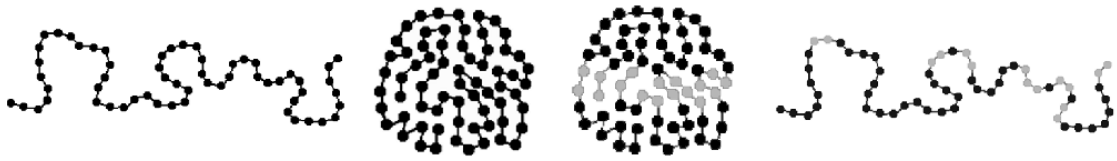


Fig. 1. Preparation of primary sequence of protein-like AB-copolymer modeling some properties of membrane protein.

The chain collapse from coil conformation was performed by simulated annealing method. Chains of 250 monomer units using interaction parameters $(\varepsilon_{AA}, \varepsilon_{AB}, \varepsilon_{BB}) = (-1, -1, -2)$ were examined.

The partial restoration of ”parent” conformation structure was revealed after the chain swelling into the coil conformation and collapsing back into the globular state. B units which were in one hemisphere in ”parent” globule stay close to each other and those from different hemispheres stay far from each other. So, we observed spatial segregation of monomer units identical from the viewpoint of interactions, i.e. segregation is caused by primary structure of copolymer chain.

Analyzing the sequences of considered chains we give a simple theoretical explanation of this effect. Using it we have improved the segregation effect by means of modifying the initial primary sequence of monomeric units.

We acknowledge the £nancial support from RFBR, from INTAS and from NATO.

References

1. A.R. Khokhlov, P.G. Khalatur, *Physica A*, 1998, **249**, 253.
2. A.R. Khokhlov, P.G. Khalatur, *Physical Review Letters*, 1999, **82**, 3456.

Orientational instability induced by light wave in waveguide with liquid crystal core

M.F.Lednei, I.P.Pinkevich

Kyiv National Taras Shevchenko University, Physics Faculty,
Prospect Glushkova 6, Kyiv, 03022, Ukraine

E-mail: lednei@phys.univ.kiev.ua, pink@phys.univ.kiev.ua

Let the monochromatic light wave propagates in nematic liquid crystal core of round cylindrical waveguide. The waveguide surface is assumed to be the metallic one. If the light wave is polarized perpendicular to nematic director and intensity of the light £eld exceeds some threshold value the so-called light-induced Frederiks transition (LIFT) takes place and nematic director changes its direction [1]. That leads to the change of conditions for the propagating light wave and as a result to the change of such its characteristics as wave vector value, dispersion law, group velocity and so on. We have studied numerically the dependence of LIFT threshold value on the type (TE and TM) of light wave and its frequency at the different (planar and homeotropic) boundary conditions on the waveguide surface as well as director anchoring energy with the surface. It is shown that LIFT threshold value increases with increasing of light wave frequency for all the types of light waves and boundary conditions except for the TM-wave at the planar boundary conditions for nematic director. In last case the LIFT takes place only when the light wave frequency exceeded some critical value. Both the single-mode and two-mode regimes for the light £eld in a waveguide were studied using a computer modelling. In this connection it was shown that LIFT threshold decreases with increasing of the portion of light power contained in the second (with less value of wave vector) light mode except for the already mentioned case of TM-mode at planar boundary conditions. We have also studied the possibility of waveguide blocking for the low-frequency light modes caused by LIFT in a waveguide.

References

1. B.Ya.Zel'dovich, N.V.Tabiryan, Yu.S.Chilingaryan, *ZhETP*, **81**, 72 (1981).

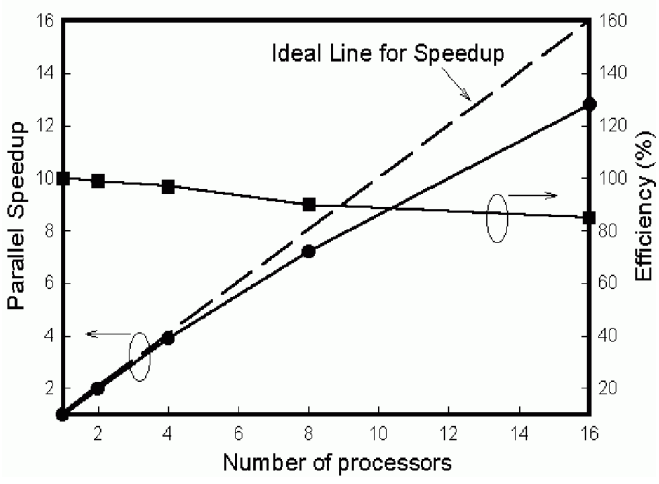
A novel parallel £nite volume solution of 3D nonlinear Poisson-Boltzmann equation in biophysics

Yiming Li, Hsiao-Mei Lu, and S. M. Sze

National Chiao Tung University, Hsinchu 300, Taiwan
Corresponding address: P.O. Box 25-178, Hsincu 300, Taiwan
Email: ymli.ee87g@nctu.edu.tw and Tel. 886-930330766

In biology, physics, and chemistry communities, the electrostatic properties for structures, binding phenomena, proteins, and complex molecules have been of great interests and studies in past years. Modelling and simulation for these interactions play an important role especially in biophysics. Just like various semiconductor device models, such as drift diffusion, hydrodynamic and Boltzmann transport equations require to solve the multi-dimensional Poisson equation for the potential distribution, a 3D linear or nonlinear Poisson-Boltzmann equation should be solved numerically for the behavior of electrostatic potential in molecure biophysics [1, 2].

In this paper, a three-dimensional nonlinear Poisson-Boltzmann equation is solved numerically with novel parallel £nite volume and monotone iterative methods [3, 4]. The proposed computational techniques have been successfully implemented on a PC-based Linux-cluster with message passing interface (MPI). First of all, the Poisson-Boltzmann equation is discretized with £nite volume (or called £nite box) method. This discretization leads to a system of nonlinear algebraic equations and it is directly solved with a global convergent monotone iterative algorithm. Based on the strong nonlinear property of Poisson-Boltzmann equation, the proposed new iterative method does not reqeuire accurate initial guess to start the solution procedure and it converges monotonically. Furthermore, by comparing with conventional Newton's iterative method, the new method is easy for implementation, relatively faster with much less computation time, and its algorithm is inherently parallel in large scale computing. The developed parallel nonlinear Poisson-Boltzmann solver has been tested on a variety of structure problems, such as acetemide and SOD enzyme to show the ef£ciency and robustness. Achieved parallel speedup as shown in the following £gure demonstrates the parallel performance of the method.



References

1. B. Honig, et al., Science, **26**, 1144 (1995); A Neumaier, SIAM Rev., **39**, 407 (1997).
2. MJ Kim, et al., J. Coll. Inter. Sci., **236**, 173 (2001); VK Misra, et al., J. Mol. Biol, **299**, 813 (2000).
3. Y. Li, et al., SIAM Proc. 10th Parall. Process. Sci. Comp., 685 (2001).
4. Y. Li, et al., Proc. Model. Simul. Microsys. 538 (2001).

Phase transitions in highly charged colloidal suspensions

Vladimir Lobaskin[1] **and Per Linse**[2]

[1] *Institute of Physics, University of Fribourg, 1700 Fribourg, Switzerland*
[2] *Physical Chemistry 1, Lund University, 22100 Lund, Sweden*

+41-26-3009116, +41-26-3009747, e-mail: Vladimir.Lobaskin@unifr.ch

Direct simulations of highly asymmetric electrolytes (such as charged colloids) meet signi£cant technical obstacles related to charge and size asymmetry of the components. Being often unfeasible by means of desktop computers, such simulations are however crucial for assessing accuracy of approximate theories of electrostatic screening and colloidal stability. Besides, due to extremely strong interparticle interactions involved, certain effects can be missed by approximate theories, which disregard correlations between small charged species. In this contribution we discuss recent developments in computer simulations of highly asymmetric electrolytes, which are based on application of the Ewald summation and various multiparticle moves within Metropolis Monte Carlo method.

We present our new results regarding attraction between like-charged macroions, which is induced by multivalent counterion correlations [1]. As it was shown recently by means of Monte Carlo simulation [2], this attraction can lead to macroion aggregation and even to phase separation in highly asymmetric electrolytes. The observed attraction is very short-range and is hardly affected by addition of a simple salt. However, our recent studies show that if a suf£cient amount of multivalent salt is added the macroions get overcharged and macroion aggregates can dissolve.

Another intriguing and counter intuitive phenomenon in the £eld of charged colloids is long range attraction between highly charged colloidal particles immensed in low stregth electrolyte [3, 4]. The possible mechanisms and even existence of this attraction and reentrant order-disorder transitions in colloidal suspensions has become a subject of controversy in literature for the last years. Using Monte Carlo simulations of electrolytes with charge asymmetry up to few thousand we demonstrate existence of the reentrant liquid phase in highly charged colloidal suspensions. The anomalous phase behaviour is related to inhomogeneous small ion distribution in the suspension and cannot be properly described in mean £eld theories of electrostatic screening.

References

1. V. Lobaskin, A. Lyubartsev, and P. Linse, Phys. Rev. **E 63**, 020401 (2001)
2. P. Linse and V. Lobaskin, Phys. Rev. Lett. **83**, 4208 (1999)
3. J. Yamanaka, H. Yoshida, T. Koga. N. Ise, and T. Hashimoto, Phys. Rev. Lett. **80**, 5806 (1998)
4. J.-P. Hansen and H. Löwen, Annu. Rev. Phys. Chem. **51**, 209 (2000)

Interface properties and the wetting transition of polymers at a wall

L. G. MacDowell and M. Müller

Institut für Physik, WA31, Johannes Gutenberg Universität, 55099 Mainz, Germany

49 6131 3923645, 49 6131 3925441, luis.macdowell@uni-mainz.de

Since the £rst theoretical studies [1], the nature of the wetting transition has attracted much interest. One challenging characteristic of this subject is that many of the theoretical predictions have preceeded experimental veri£cation [2]. It is precisely in this context were molecular simulations may become an exceptional tool. Yet, simulation of ¤uids at interfaces pose very many methodological dif£culties that are being surmounted but very recently, with the advent of con£gurational bias, histogram re-weighting, £nite size scaling, etc.

In this paper we report the application of a novel approach to the study of the wetting transition of a polymer melt at a wall. We show that the wetting transition may be readily calculated using an extended grand canonical ensemble, where the strength of the polymer-wall interaction is considered itself as a thermodynamic variable. This allows to calculate right away the free energy difference between liquid-wall and liquid-vapour interfaces as a function of the polymer-wall interaction strength. In accordance with Young's equation, the wetting transition is then located at that point where this free energy difference equals the liquid-vapour surface tension. We show that the surface tension may be calculated in the grand canonical ensemble with out the need to evaluate explicitly the pressure tensor. This is accomplished by measuring the activation barrier required for the system to tunnel from the vapour phase to the liquid phase. The pre-wetting line is then calculated by monitoring the probability distribution of the surface layer thickness. Above the wetting transition, two distinct peaks appear, and the actual pre-wetting line is located by the requirement that both peaks have equal area. The pre-wetting critical point is estimated using £nite size scaling [3].

We £nd that the proposed techniques are a very useful tool for the study of surface properties. The wetting transition is observed to be strongly £rst order. Evidence of a very weak £rst order drying transition is also observed, while the pre-wetting critical point seems to conform to the 2 dimensional Ising universality class. The density pro£les and other structural properties are compared with a recently proposed self consistent £eld theory, and good agreement is found. For the surface energies, on the contrary, only qualitative agreement is obtained [4].

References

1. J. W. Cahn, J.Chem.Phys. 3667, **66**, (1977).
2. M. Schick, in "liquids at Interfaces", Elsevier, Amsterdam, 1990.
3. K. Binder and D. P. Landau, "A Guide to Monte Carlo Simulations in Statistical Physics", Cambridge University Press, Cambridge, 2000.
4. M. Müller and L. G. MacDowell, Macromolecules, 3902, **33** (2000).

Critical properties of the bond-diluted Ising model in three dimensions

P.E. Berche[1], **C. Chatelain**[2], **B. Berche**[3] **and W. Janke**[2]

[1]*Groupe de Physique des Matériaux,*
Université de Rouen, F-76821 Mont Saint-Aignan Cédex
[2]*Institut für Theoretische Physik, Universität Leipzig, D-04109 Leipzig*
[3]*Laboratoire de Physique des Matériaux,*
Université Henri Poincaré, (Nancy I),
F-54506 Vandoeuvre-lès-Nancy Cédex
tel: (33) 2 35 14 70 38, fax: (33) 2 35 14 66 52,
e-mail: pierre.berche@univ-rouen.fr

We investigate by extensive Monte Carlo simulations the critical properties of the bond diluted 3D Ising model. From the Harris criterion, we expect a strong in¤uence of disorder since the speci£c heat exponent α, which plays the role of the scaling dimension of disorder, is positive for the pure system [1]. To date, only the Ising model with site dilution has been studied in 3D: a new universality class has been found but the question of its stability versus the the disorder concentration is not completely solved [2], [3]. In the case of the bond dilution, we have determined the phase diagram of the model and we have measured, for three different disorder concentrations, the critical exponents by Finite-Size-Scaling techniques and temperature behaviour [4]. It appears that the slight variation of the exponents with the concentration is due to the competition between the new disordered £xed point and the percolation one.

References

1. Harris A.B., *J. Phys. C* **7** (1974) 1671.
2. Ballesteros H. G., Ferńandez L. A., Martín-Mayor V., Muñoz Sudupe A., Parisi G. and Ruiz-Lorenzo J. J., *Phys. Rev. B* **58** (1998) 2740.
3. Folk R., Holovatch Y. and Yavors'kii T., *Phys. Rev. B* **61** (2000) 15114.
4. Berche P.E. , Chatelain C., Berche B. and Janke W., *in preparation*.

New results in the computation of large-order high-temperature expansions for observables of the Ising model

Butera Paolo [1] **and Marco Comi** [2]

[1] *Istituto Nazionale di Fisica Nucleare Dipartimento di Fisica, UniversitÁa di Milano-Bicocca*
Piazza della Scienza 3, 20126 Milano, Italy
[2] *Istituto Nazionale di Fisica Nucleare Dipartimento di Fisica, UniversitÁa di Milano-Bicocca*
Piazza della Scienza 3, 20126 Milano, Italy

[1] $Tel.: 0039-2-64482509$; $Fax: 0039-2-64482582$ *butera@mi.infn.it;*
[2] *Tel.:0039-2-64482510; Fax: 0039-2-64482582 comi@mi.infn.it*

The study of the Ising model has long been of a paradigmatic value for the study of the critical phenomena[1] and, more generally, for the description of a large variety of physical situations. Since the model is (partially) solved only in two dimensions and for very special choices of the interaction among the spins, it is customarily studied by a variety of approximate methods which could be described either as machine-labour intensive or as man-labour intensive and have both their virtues and limitations. Stochastic simulations are typical of the £rst class of approaches, whereas high-temperature expansions are probably the best example of the second. We shall present recent extensions and analyses of high-temperature expansions for several observables in various kinds of three-dimensional Ising models. Our work can be used in £rst place to improve the accuracy in the determination of the critical parameters and is a continuation and extension of that appeared in [2], as well as in previous papers[3], devoted to the more general N-vector lattice model. Presently, the state of the art is extremely advanced, so that a signi£cant addition to the data already in the literature must involve the computation of a huge number ($\approx 10^7$) of topologically inequivalent "renormalized" graphs. The codes which implement the calculation must be devised and organized with utmost care in order not just to barely accomplish their task, but also to contain the CPU time and the memory occupation, mainly to leave the possibility of further extensions open.

References

1. C. Domb, in *Phase Transitions and critical Phenomena*, edited by C. Domb and M.S. Green, (Academic, London, 1974),Vol. 3.
2. P. Butera and M. Comi, Phys. Rev. B **62**, 14837 (2000)
3. P. Butera and M.Comi, Phys. Rev. B **56**, 8212 (1997).

In¤uence of dilution on the strong £rst-order phase-transition of the 3D 4-state Potts model

C. Chatelain[1], **P-E. Berche**[2], **B. Berche**[3] **and W. Janke**[1]

[1] *Institute für Theoretische Physik, University of Leipzig, Germany*
[2] *Groupe de Métallurgie Physique, University of Rouen, France*
[3] *Laboratoire de Physique des Matériaux, University of Nancy, France*
phone : +49 (0)341 97 32438, e-mail : chatelai@itp.uni-leipzig.de

A perfectly pure experimental system does not exist, disorder being hardly avoidable (as for example isotopic composition of the sample). Systems undergoing a phase transition are particularly sensible to randomness. The transition temperature is shifted and it is well-known since the pioneering work of Harris that the universality class at a second-order phase transition may be changed under the in¤uence of randomness [1]. First-order phase transitions are softened by randomness and it was shown that they may be turned into continuous transitions for strong enough disorder. Aizenmann and Wehr [2] proved that an in£nitesimal amount of disorder is suf£cient in dimension $d = 2$ to clear any discontinuities. In higher dimensions, it may exist a tricritical point in the phase diagram separating the £rst-order transition line from the continuous one in the strong disorder regime. Such a tricritical point has been reported in the case of the diluted 3-dimensional 3-state Potts model, which undergoes a weak £rst-order phase transition in the pure case.

We investigate the phase diagram of the diluted 3-dimensional 4-state Potts model which undergoes a strong £rst-order phase transition in the pure case. We used standard large-scale Monte Carlo simulations with cluster algorithm coupled to multicanonical methods in the regime of low dilution where the transition is supposed to be £rst-order. We present strong numerical evidences for the existence of a tricritical point and we give an estimate for its location. Using a £nite-size scaling study, we estimate the critical exponents in the second order regime. We tried to take into account corrections to scaling which turned out to be important and we showed that they are due to cross-over effects with the percolation £xed point. In contradistinction which was observed for the 3-state Potts model, we report an estimate of the ν exponent clearly different from that of the Ising model.

References

1. A.B. Harris (1974) J. Phys. C **7**, 1671.
2. M. Aizenman et J. Wehr (1989) Phys. Rev. Lett. **62** 2503
3. H. G. Ballesteros, L. A. Fernandez, V. Martin-Mayor, A. Munoz Sudupe, G. Parisi and J. J. Ruiz-Lorenzo (2000) Phys. Rev. B **61** 3215

Critical behaviour of fully-frustrated Potts models

D. P. Foster, C. Gérard and I. Puha

Laboratoire de Physique Théorique et Modlélisation (CNRS ESA 8089)
Université de Cergy-Pontoise, 5 Mail Gay-Lussac
95035 Cergy-Pontoise Cedex, France

tel: +33 1 34 25 68 65, fax: +33 1 35 25 70 04, email:
Damien.Foster@ptm.u-cergy.fr

The phase diagrams and ground state properties of two three-state fully-frustrated Potts models are investigated using numerical transfer matrix calculations: The piled-up-domino and zig-zag models. In the piled-up-domino model the phase diagram shows a reentrant paramagnetic phase[1].

The piled-up-domino three-state Potts model is de£ned as a three-state Potts model on the square lattice with ferromagnetic interactions J_1 all vertical bonds and alternate rows of horizontal bonds. The remaining bonds are of strength J_2, which will be taken both ferro and antiferromagnetic. The zig-zag three-state Potts model is de£ned analogously, except that alternate columns of the lattice are displaced vertically one lattice spacing, giving a zig-zag pattern of J_2 bonds. We de£ne the ratio $\alpha = J_2/J_1$. These models are natural Potts extensions of the previously exactly solved Ising equivalents[2].

It is shown, using a mapping to a dimer model, that the ground-state entropy per spin is the same in zig-zag Ising and Potts models for all values of α, i.e. $s = 0$ for $\alpha > -1$, $s = 0.1615\cdots$ for $\alpha < -1$ and $s = G/\pi = 0.2916\cdots$ for $\alpha = -1$. The phase diagram calculated for the Potts model, using a phenomenological renormalisation group calculation, gives the same qualitative behaviour as the zig-zag Ising model: The ferromagnetic critical point found when $J_1 = J_2$ extends into a line of critical points. The critical temperature decreases as α is reduced, vanishing when $\alpha = -1$. There is no £nite temperature transition for $\alpha < -1$.

The ground-state entropy per spin is calculated for the piled-up-domino Potts model using transfer matrices, and is found to be substantially higher then for the Ising model case for $\alpha = -1$ and $\alpha < -1$. The phase diagram for the Potts model is qualitatively different from the Ising model: The Ising model phase diagram is made of two critical lines, in the Ising universality class, one for $\alpha > -1$ and the other $\alpha < -1$. The paramagnetic phase separates the ferromagnetic phase, $\alpha > -1$, from a partially ordered phase, $\alpha < -1$, and both transition lines meet at a multiphase point $\alpha = -1,\ T = 0$. In the piled-up-domino Potts model the $\alpha > -1$ transition line extends beyond $\alpha = -1$ before doubling back on itself and again the two transition lines meet at a multiphase point $\alpha = -1,\ T = 0$. The paramagnetic phase is now reentrant, but still separates the ferromagnetic and partially ordered phases. The transfer matrix calculations show the possibility of an additional partially ordered phase, though this is very speculative at this stage.

The disorder line for the piled-up-domino Potts model, de£ned as the lines on which the correlation length changes from monotonic to oscillatory, is also calculated using transfer matrices. It is found to be consistent with the existence of a reentrant paramagnetic phase.

References

1. Foster D P, Gérard C and Puha I 2001 *preprint submitted to J. Phys A*
2. André G, Bidaux R, Carton J -P and Conte R 1979 *J. Phys. (France)* **40** 479

Monte Carlo study of the critical phenomena in the double exchange systems using massive parallel computers

Nobuo Furukawa[1] **and Yukitoshi Motome**[2]

[1]*Department of Physics, Aoyama Gakuin University, Tokyo, Japan*
[2]*Institute of Matrials Science, University of Tsukuba, Japan*

Tel:+81-3-5384-6114, Fax:+81-3-5384-6100, e-mail:furukawa@phys.aoyama.ac.jp

Monte Carlo study of the double exchange model is performed on a massive parallel PC cluster systems [1]. This model, which has been introduced to explain ferromagnetism of colossal magnetoresistance manganites, deals strongly correlated electron systems. Until recently, it was quite dif£cult to take into account effects of critical spin ¤uctuations in a controlled manner. An improved Monte Carlo technique developed by the present Authors [2] made it possible to calculate the model at £nite size clusters which are large enough to obtain thermodynamic limits. Here we show the numerical results for the critical phenomena of the double exchange model, which is fundamental and challenging subject to this model. Using £nite-size scaling analysis as well as the Binder parameter plots, Curie temperature ($T_{\rm c}$) and critical exponents are estimated accurately. We discuss [3]: 1) $T_{\rm c}$ is substantially decreased from its mean-£eld estimate, which makes the model to explain the experimental values consistently. 2) Critical exponents are consistent with estimates from the neutron scattering measurements. These are inconsistent with d.c. and r.f. magnetization measurements which exhibit mean-£eld like exponents. 3) To the best of our knowledge, this is the £rst time that critical exponents of a metallic system in the strong coupling limit is precisely estimated.

References

1. `http://www.phys.aoyama.ac.jp/∼aoyama+/index-e.html`
2. Y. Motome and N. Furukawa, J. Phys. Soc. Jpn. **68** (1999) 3853.
3. Y. Motome and N. Furukawa, J.Phys. Soc. Jpn. **69** (2000) 3785.

Finite size critical behaviour of the driven lattice gas in two and three dimensions

Sergio Caracciolo[1], **Andrea Gambassi**[1], **Massimiliano Gubinelli**[2] **and Andrea Pelissetto**[3]

[1] *Scuola Normale Superiore and INFN – Sezione di Pisa, P.za dei Cavalieri, 56100 Pisa, Italy*

[2] *Dipartimento di Fisica and INFN – Sezione di Pisa, Universit£a degli Studi di Pisa, 56100 Pisa, Italy*

[3] *Dipartimento di Fisica and INFN – Sezione di Roma I,Universit£a degli Studi di Roma "La Sapienza", 00185 Roma, Italy*

tel.+39-050-509086, e-mail mgubi@cibs.sns.it

We report on a detailed Monte Carlo study of the high-temperature phase of the two and three dimensional driven lattice gas (DLG) at large driving £eld. This model is a kinetic Ising model on a periodic domain with Kawasaki dynamics and biased jump rates which mimic the action of an external force £eld. This perturbation drives the system into a non-equilibrium steady state which shows a £nite-temperature phase transition. For a review see [1]. Despite its simplicity, the DLG has not been solved exactly. Nonetheless, many results have been obtained by means of Monte Carlo (MC) simulations in two and three dimensions [2, 3] and by using £eld-theoretical methods. Our analysis of the MC data follows the method introduced in[4]. We de£ne a £nite-volume correlation length generalizing the de£nition of the second-moment correlation length that is used in equilibrium systems. Once de£ned a £nite-volume correlation length ξ we can use the method of Ref. [4] to determine in£nite-volume quantities. For the correlation length $\xi(\beta, L)$ and a generic observable $\mathcal{O}(\beta, L)$ measured at temperature β and on a system of (transverse) size L we assume an FSS ansatz of the form

$$\frac{\mathcal{O}(\beta, \alpha L)}{\mathcal{O}(\beta, L)} = F_{\mathcal{O}}\left(\frac{\xi(\beta, L)}{L}\right) \tag{1}$$

where $\alpha \geq 1$ is a scale factor (typically $\alpha = 2$). We simulate severals couples of systems of transverse sizes L and αL at the same temperature β. For each observable $\mathcal{O}$ we check the validity of the FSS ansatz (1) and extract the FSS functions $F_{\mathcal{O}}$. Then, using the functions F_ξ and $F_{\mathcal{O}}$ we can extrapolate the pairs $(\xi(\beta, L), \mathcal{O}(\beta, L))$ to obtain estimates $(\xi(\beta, \infty), \mathcal{O}(\beta, \infty))$ for their in£nite-volume values.

In two dimensions we apply this method to obtain the transverse correlation length ξ and the transverse susceptibility in in£nite-volume, then we determine the corresponding critical exponents ν and γ and the critical value of the temperature β_c. They turn out to partially con£rm the theoretical predictions [1]. We report also preliminary results on the three dimensional DLG.

References

1. B. Schmittmann and R. P. K. Zia, Statistical mechanics of driven diffusive systems, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz, Vol. 17 (Academic Press, London, 1995).
2. J. S. Wang, J. Stat. Phys. **82**, 1409 (1996).
3. K.-t. Leung and J. S. Wang, Int. J. Mod. Phys. C **10**, 853 (1999).
4. S. Caracciolo, R. G. Edwards, S. J. Ferreira, A. Pelissetto and A. D. Sokal, Phys. Rev. Lett. **74**, 2969 (1995), e-print hep-lat/9409004.

High temperature series expansions for d-dimensional disordered Potts models

Meik Hellmund and Wolfhard Janke
Institut für Theoretische Physik, Universität Leipzig
Meik.Hellmund@itp.uni-leipzig.de

Despite considerable efforts there are still many open problems in the physics of disordered systems. One alternative to large-scale numerical simulations are systematic series expansions. Such expansions for statistical models de£ned on a lattice are a well-known method to study phase transitions and critical phenomena [1]. The extension of this method to disordered systems [2, 3, 4] demands the development of new graph theoretical and algebraic algorithms.

We developed further the method of "star graph expansion" which allows to take the disorder average on the level of individual graphs. For the £rst time, we classi£ed all star graphs up to order 19 and calculated their embedding numbers for d-dimensional hypercubic lattices. These data are used to calculate e.g. free energies and susceptibilities for disordered q-state Potts models on d-dimensional hypercubic lattices. The probability distribution of couplings is parameterized by e.g. $P(J_{ij}) = p\delta(J_{ij} - J_0) + (1-p)\delta(J_{ij} - RJ_0)$ which includes spin glasses, diluted ferromagnets, random-bond models and transitions between them. The series allow the determination of the phase diagram, critical couplings and critical exponents in a large region of the (q,d,p,R) parameter space. The physical systems of interest which are studied this way include:

- Random-bond (RB) Ising model in 2D – logarithmic corrections to the pure £xed point
- RB Ising model in 3D – universality of a new random £xed point
- RB Ising model in 4D – corrections to mean-£eld behavior
- RB Potts model with $q = 3, 4$ in 2D – change of critical exponents due to disorder
- RB Potts model in 3D – softening of £rst-order phase transitions to second order
- Spin glasses in different dimensions

References

1. C. Domb and M. S. Green, eds., *Phase Transitions and Critical Phenomena*, Vol. 3 (Academic Press, New York, 1974).
2. R.R.P. Singh and S. Chakravarty, Phys. Rev. B **36**, 546 (1987).
3. B. Lobe, W. Janke, and K. Binder, Eur. Phys. J. B **7**, 283 (1999).
4. A. Roder, J. Adler, and W. Janke, Phys. Rev. Lett. **80**, 4697 (1998); Physica A **265**, 28 (1999).

Critical behavior of the two-dimensional dipolar in-plane Ising model

A. Hucht

Theoretische Physik and SFB 491,
Gerhard-Mercator-Universität, D-47048 Duisburg, Germany
Tel: +49-203-379-3486, Fax: +49-203-379-2965,
E-mail: fred@thp.Uni-Duisburg.de

We investigate the critical behavior of the two-dimensional Ising model with long range dipole interactions and in-plane spin axis. Ultra-thin magnetic £lms with an in-plane easy axis are expected to belong to this universality class [1], as the dipole interaction, albeit small, is always present in these systems. The Hamiltonian reads

$$\mathcal{H} = -\frac{J}{2}\sum_{\langle ij\rangle}\sigma_i\sigma_j + \frac{\omega}{2}\sum_{i\neq j}\frac{(r_{ij}^{\perp})^2 - 2(r_{ij}^{||})^2}{|\vec{r}_{ij}|^5}\sigma_i\sigma_j$$

with spin variables $\sigma = \pm 1$, ferromagnetic exchange interaction $J > 0$, and dipole constant $\omega = \mu_0\mu^2/4\pi a_{\mathrm{nn}}^3$ (here μ_0 is the vacuum permeability, μ is the magnetic moment of the spins, and a_{nn} is the nearest neighbor distance, which is set to one). $\vec{r}_{ij} = (r_{ij}^{||}, r_{ij}^{\perp})$ is the distance between spin σ_i and σ_j, decomposed into contributions parallel and perpendicular to the spin axis, and $\langle\cdot\rangle$ denotes the sum over nearest neighbors.

We use the cluster Monte Carlo algorithm for long range systems introduced by Luijten *et al.* [2], extended to anisotropic interactions. Using this method, no approximation or cutoff of the long range dipole interaction need to be done. We £nd that for $\omega > 0$ the system shows *strong anisotropy*, i. e. the correlation length exponents $\nu_{||}$ parallel to the spin axis and $\nu_{\perp}$ perpendicular to the spin axis are different. This behavior is similar to the anisotropic next nearest neighbor Ising model (ANNNI model) at its uniaxial Lifshitz point [3]. However, due to its short range interactions the ANNNI model should belong to a different universality class.

Taking strong anisotropy into account we simulate systems of different linear sizes $L_{||}$ and $L_{\perp}$, keeping the ratio $L_{||}^{1/\nu_{||}}/L_{\perp}^{1/\nu_{\perp}}$ £xed [4]. We determine the critical exponents of the system using £nite size scaling analysis and histogram methods.

References

1. M. Bulenda, U.C. Täuber and F. Schwabl, *J Phys A: Math Gen* 33, 1 (2000)
2. E. Luijten and H.W.J. Blöte, *Int J Mod Phys* C 6, 359 (1995)
3. W. Selke, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. Lebowitz (Academic, London, 1992), Vol. 15
4. K. Binder, in *Finite Size Scaling and Numerical Simulation of Statistical Systems*, edited by V. Privman (World Scienti£c, Singapore, 1990)

Collective pattern of random expansion by pairs in moderate number of £nite systems

Wlodzimierz Kozlowski

Institute of Biocybernetics and Biomedical Engineering of The Polish Academy of Sciences, Trojdena 4, 02-109 Warsaw, Poland

tel.: +48 (22) 659-91-43 ext 118, fax.: +48 (22) 658-28-72

e-mail: wlodekak@ibbrain.ibb.waw.pl

This research concerns the situation when a moderate number M of complex systems of the same type evolve simultaneously under in¤uence of stochastic factors in the same ambient conditions to result in a collective effect that manifests itself for (in) a single receiver system. The systems are discrete and composed of £nite number of elements. The feature of being moderate in number M for the system ensemble means: The M is so large that ensemble is suf£ciently various to have a number of systems differing substantially from the others and the M is so small that these distinguished systems contribute signi£cantly to the collective effect.

One investigates the collective effect represented by the sequence of patterns having mean expected form of those resulting in each system of the ensemble from random covering sites of a hexagonal array within a half-plane from stright initial chain of sites covered. This covering is modelled as a random expansion process (REP) whose states at subsequent stages of its development are £nite random sets being multiplicity of sets-realizations that have evolved independently (in parallel) within the same spatial domain. This domain is £nite discrete space whose elements coincide with centers of hexagons of the array. The REP is simulated as Markov process of covering sites of the array so that information about covering a site is transmitted: between members of a pair of neighbour sites and due to conditional effective jump of this pair to a position close by, with preserving mutual situation of its elements on the array. Information about organization of two sites into a pair identi£es this effective displacement. Thus contribution of the £nite-size entities to the information transmission is simulated; this is generalization of the discrete displacement method (DDM) developed previously for modeling the £nite-size effects[1]. Accomplishment of the collective effect is revealed by sequence of patterns $RP(t)$ being mean expected forms of the M patterns characterizing all the various realizations at the respective stages t of the REP development.

Distribution of the number of sites covered $I_{RP}(t)$ that constitute the $RP(t)$ shows a number of discrete steps that is attributed to discretness and the M quality of being moderate. Structural characteristic of the RP has been designed and this enabled us to detect qualitative changes in the $RP(t)$ evolution whose occurrence can be attributed to the DDM-type modelling of the £nite-size effects: Starting from certain detectable step, the $RP(t)$ patterns are structuraly bi-stable. The stage at beginning of that step is important structural characteristic of the collective effect accomplishment.
One reports results of high performance computing (HPF, Cray T3E) that reveal certain regularity in variation of the $RP(t)$ evolution characteristics with changing of the REP parameters: forcing parameter P (formally this is probability of site covering) and degree $0 \leq \alpha \leq 1$ of the £nite array randomization. Variation of the number of realizations M in computations suggests way of determining the upper bound of the M being moderate. Some initial considerations and an applied aspect of this work have been revealed in [2].

References

1. W. Kozlowski Int.J.Num.Meth.Fluids vol 23, 105-124 (1996)
2. http://www.foresight.org/Conferences/MNT05/Papers/Kozlowski/index.html

Monte Carlo simulations of vector spin glasses at low temperatures

Helmut G. Katzgraber and A. P. Young

Department of Physics, University of California, Santa Cruz, CA 95064

+1-831-459-4762 (TEL), +1-831-459-3043 (FAX), dummkopf@physics.ucsc.edu

The ground state structure of spin glasses is poorly understood. While there has been considerable work on Ising-type spin glass systems, models with a vector order parameter symmetry have not yet been analyzed in much detail.

There are different theories[1] describing the spin glass phase: the “droplet picture” by Fisher and Huse and the replica symmetry breaking picture (RSB) by Parisi. According to the droplet picture, excitations that ¤ip a £nite cluster of spins cost an in£nite energy in the thermodynamic limit and have a fractal dimension less than the space dimension. By contrast, RSB predicts that these excitations cost a £nite amount of energy in the thermodynamic limit and are space £lling. Recently, work by Krzakala and Martin as well as Palassini and Young[2] for Ising-type systems (referred to as KMPY) that £nd an intermediate picture: while large scale excitations cost only a £nite amount of energy in the thermodynamic limit, their surface is fractal. These results have been backed up by Monte Carlo simulations at low temperatures for the Edwards-Anderson Ising spin glass in three and four dimensions[3].

Here we test which of the above predictions apply to the three dimensional gauge glass[4] as well as the four dimensional XY model by performing simulations down to low temperatures (to avoid effects of critical ¤uctuations) for a modest range of sizes using the parallel tempering Monte Carlo technique[5]. This method allows us to equilibrate frustrated systems much faster than conventional Monte Carlo, thus permitting us to simulate larger system sizes at lower temperatures.

Parallel tempering Monte Carlo allows us to better overcome large energy barriers present in frustrated systems, because several identical replicas of the system at different temperatures are simulated. Global moves are made such that the temperatures of two replicas (with adjacent temperatures) are exchanged in a way which obeys detailed balance.

From our simulations we £nd a scenario compatible with the KMPY picture: while excitations of the system cost a £nite energy in the thermodynamic limit, their surface appears to be fracxtal.

References

1. D. S. Fisher and D. A. Huse, J. Phys. A. **20** L997 (1987); G. Parisi, Phys. Rev. Lett. **43**, 1754 (1979).
2. F. Krzakala and O. C. Martin, Phys. Rev. Lett. **85**, 3013 (2000); M. Palassini and A. P. Young, Phys. Rev. Lett. **85**, 3017 (2000).
3. Helmut G. Katzgraber, M. Palassini and A. P. Young, Phys. Rev. B **63**, 184422, (2001).
4. Helmut G. Katzgraber and A. P. Young, submitted to Phys. Rev. B, (cond-mat/0105077).
5. K. Hukushima and K. Nemoto, J. Phys. Soc. Japan **65**, 1604 (1996); E. Marinari, *Advances in Computer Simulation*, edited by J. Kertész and I. Kondor (Springer-Verlag, Berlin 1998), p. 50, (cond-mat/9612010).

Density of partition function zeroes and phase transition strength

Wolfhard Janke[1] **and Ralph Kenna**[2]

[1] *Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany*

[2] *School of Mathematics Trinity College Dublin, Ireland*

Tel: +353 1 608 1699, Fax: +353 1 608 2282, e-mail: rak@maths.tcd.ie

In statistical physics, one is interested in the determination of the order and strength of phase transitions [1]. First order transitions involve the coexistence of two phases and a discontinuity in the £rst derivative of the free energy. The strength of such a transition is measured by the size of this discontinuity (the latent heat in the temperature driven case). In the second order scenario the appropriate second derivative of the free energy diverges, as does the correlation length. Here, the transition strength is characterised by critical exponents. In the temperature driven case the α exponent determines the nature of the speci£c heat divergence. Such non-analytic behaviour is only present in an in£nitely large system.

Monte Carlo simulations are, however, restricted to systems of £nite size. Finite-size scaling [FSS] is a method whereby ratios of critical exponents may be determined from measurements taken on systems of £nite extent. Application of FSS to thermodynamic functions such as the speci£c heat is a well established approach in statistical physics. An increasingly popular alternative is the use of the FSS behaviour of the zeroes of the partition function. These zeroes exist in the complex temperature or complex magnetic £eld planes.

In the second order temperature driven case, FSS of the £rst zero yields the correlation length critical exponent ν. Identi£cation of ν with $1/d$ in the £rst order case can be used to discriminate between the two types of transition (d being the dimensionality of the system). However, the *strength* of the transition has heretofore not been determined from properties of zeroes. Instead, direct measurement of latent heat or interface tension (in the £rst order case) or the ratio α/ν (in the second order case) has been used.

We present an alternative method to *directly* determine the strength of phase transitions from partition function zeroes. The method involves the *density* of zeroes - a quantity which is proportional to the latent heat in the £rst order case and which is characterised by α in the second order one. It has long been considered dif£cult if not impossible to extract the density of zeroes (a continuous function) from their (discrete) distribution for a £nite lattice [2].

Recently, however, there have been some attempts to extract the density from numerical studies. In view of the increasing importance attached to this approach, we wish to suggest an appropriate way this should be done [3]. The novel aspect is the consideration of the *cumulative* density of zeroes. This new and powerful technique allows to determine (i) the order and (ii) the strength of the transition directly. The method also elucidates crossover between £rst and second order transitions. Furthermore, the method leads to alternative insights into statistical physics and illuminates the origin of £nite-size scaling. Application to a number of models illustrates the ef£cacy of the density approach.

References

1. W. Janke, in: *Computer Simulations in Condensed Matter Physics VII*, eds. D.P. Landau, K.K. Mon and H.-B. Schüttler (Springer Verlag, Heidelberg, Berlin, 1994); p. 29.
2. P.P. Martin, Nucl. Phys. B **220** (1983) 366; *ibid* **225** (1983) 497.
3. W. Janke and R. Kenna, J. Stat. Phys. **102** (2001) 1211.

The program for calculation of pulsed magnetic £elds in the experimental device with a complex electrode structure

A. Chorniy and K. Nemchenko

Department of Physics and Technology
Karazin Kharkov National University, Kharkov, 61077, Ukraine
tel/fax 38-0572-35-27-22, e-mail: antonchorniy@hotmail.com

One of the leading places among the technologies used to generate nanosecond high-current ion beams belongs to magnetically insulated diodes (so called B_r -£eld diodes). Magnetic £eld in such diodes is formed by two ¤at coaxial coils that are fed with a pulse current from the battery of capacitors. This paper is devoted to the problem of calculation of the pulse magnetic £eld spatial distribution in the ion diode with allowance for the induced currents in metal elements of the diode construction.

The calculation technique consists in partitioning of the solid conductors into elementary ones so that the current density inside of each of them may be considered to be uniform. The currents induced in the elementary conductors are calculated from the equation system including coef£cients of self-inductance and those of the elementary conductors mutual inductance. The matrix of such system coef£cients is asymmetric which calls for the right and left eigenvectors to be introduced into it to diagonalize the matrix. The eigenvector-composed operators-projectors to sub-space of stable solutions allow one to avoid the instabilities which arise inevitably when the solid conductors are partitioned into separate elementary ones (non-existing in reality). Besides, to solve the problem some special methods allowing to avoid accumulation of the errors in the numerical calculations are applied. Generally such errors appear when the conductors are being partitioned into greater and greater number of elements.

One of the typical results supporting the reliability of the technique is the correctly determined depth of the pulsed magnetic £eld penetration into the conductors (skin value).

Orbital dynamics via multiresolution

Antonina N. Fedorova and Michael G. Zeitlin

Russian Academy of Sciences, Institute of Problems of Mechanical Engineering,
Mathematical Methods in Mechanics Group
V.O., Bolshoj pr., 61, 199178, St. Petersburg, Russia

tel: +7-812-3214776, fax: +7-812-3214771, E-mail: zeitlin@math.ipme.ru,
anton@math.ipme.ru
http://www.ipme.ru/zeitlin.html, http://www.ipme.nw.ru/zeitlin.html

We consider the applications of a new numerical-analytical technique which is based on the methods of local nonlinear harmonic analysis or wavelet analysis to the orbital motion in transverse plane for a single particle in a circular magnetic lattice in case when we take into account multipolar expansion up to an arbitrary £nite number and additional kick terms.

We reduce initial dynamical problem to the £nite number (equal to the number of n-poles) of standard algebraical problems and represent all dynamical variables as expansion in the bases of maximally localized in phase space functions (wavelet bases). Wavelet analysis is a relatively novel set of mathematical methods, which gives us a possibility to work with well-localized bases in functional spaces and gives for the general type of operators (differential, integral, pseudodifferential) in such bases the maximum sparse forms. Our approach is based on the generalization of variational-wavelet approach from [1]-[3], which allows us to consider not only polynomial but rational type of nonlinearities [4]. .

The solution corresponds to the full multiresolution expansion in all time scales and gives us expansion into a slow part and fast oscillating parts. So, we may move from coarse scales of resolution to the £nest one for obtaining more detailed information about our dynamical process. The £rst term corresponds on the global level of function space decomposition to resolution space and the second one to detail space. In this way we give contribution to our full solution from each scale of resolution or each time scale. The same is correct for the contribution to power spectral density (energy spectrum): we can take into account contributions from each level/scale of resolution.

Starting from Hamiltonian of orbital motion in magnetic lattice with additional kicks terms, we consider also variational formulation for dynamical system with rational nonlinearities and construct via multiresolution analysis explicit representation for all dynamical variables in the base of nonlinear high–localized eigenmodes (compactly supported wavelets and wavelet packets). Best convergence properties and minimal cost of algorithms led to saving CPU time and hdd space.

References

1. Wavelets in Optimization and Approximations, *Math. and Comp. in Simulation*, **46**, 527-534, 1998.
2. Variational Approach in Wavelet Framework to Polynomial Approximations of Nonlinear Accelerator Problems, American Institute of Physics , Conf. Proc., vol. 468, Nonlinear and Collective Phenomena in Beam Physics, pp. 48-68, 1999.
3. Symmetry, Hamiltonian Problems and Wavelets in Accelerator Physics, American Institute of Physics , Conf. Proc., vol. 468, Nonlinear and Collective Phenomena in Beam Physics, pp.69-93, 1999.
4. Variational-Wavelet Approach to RMS Envelope Equations, Proc. 2nd Advanced Accelerator Workshop on The Physics of High Brightness Beams pp.235–254, World Scienti£c, 2000

Simulation of Coulomb interacting particles in a potential well

G. Bassi, A. Bazzani and G. Turchetti

Dipartimento di Fisica – UniversitÁ di Bologna

+39 0512091004, +39 051247244, turchetti@bo.infn.it

The collective effects in high intensity beams at low or medium energies have a strong in¤uence on the transport properties, the beam stability and the halo formation[1]. Indeed the resonances between the collective motion of the beam and the liner or non linear betatronic motion may excite new resonances and create chaotic motion. The particle in core models[2] and the PIC solution of Poisson-Vlasov equations have been used to investigate the dynamical behavior of a test particle in 2D and 3D geometries[3][4]. We analyze here the possible effects of collisions by introducing a noise in the particle in core and Poisson-Vlasov equations. A reference model is a set isotropic harmonic uncoupled oscillators with a repulsive Coulomb interaction, which describes a coasting beam in a constant focusing lattice. The effect of nonlinearities in the external £eld are examined.

References

1. G. Franchetti, I. Hofmann, G. Turchetti *A symplectic map approach to the space charge problem* Proceedings of the Luneburg workshop “Non;linear and stochastic beam-dynamics. A challenge to theoretical and computational Physics” . (DESY 97-161) DESY Proceedings 1998-03
2. A. Bazzani, M. Communian, A. Pisent *Frequency map analysis of an intense mismatched beam in a FODO cell* Part. Accel. **63** (1999) 79.
3. G. Turchetti, S. Rambaldi, A. Bazzani, M. Communian, A. Pisent *3D solutions of the Poisson-Vlasov equation for a line of FODO cells* Phys. Rev. Special Topics - Accelerators and Beams (2001) in press
4. I. Hofmann, G. Turchetti, G. Franchetti *Frequency map analysis of resonances in a nonlinear lattice with space charge* Nuc. Instr. Meth. (2001) in press

New numerical tools to study waves and instabilities of ¤owing plasmas

A.J.C. Belien, M.A. Botchev, J.P. Goedbloed, B. van der Holst

FOM-institute for Plasma Physics, Association Euratom-FOM
P.O.Box 1207, 3430 BE Nieuwegein, the Netherlands.
tel.: +3130 6096 953, fax: +3130 6031 204, botchev@rijnh.nl

Studying plasma waves and instabilities is an indispensable part of present thermonuclear-fusion and astrophysical magnetohydrodynamics (MHD). Up till recently, spectral analysis was mostly restricted to static plasmas. However, the assumption of a static plasma is unrealistic not only for astrophysical but also for modern fusion research. Plasmas with ¤ow have been shown to have spectra essentially different from those of static plasmas [1].

We present two new numerical tools for spectral studies of plasmas with ¤ow. The £rst one, a program called FINESSE (FINite Element Solver for Stationary Equilibria), computes equilibria of non-static plasmas for a variety of fusion and astrophysical con£gurations (tokamaks, solar loops, solar winds, etc.). FINESSE can handle axisymmetric ideal plasmas with toroidal and/or poloidal ¤ows in three different ¤ow regimes: sub-slow, sub-Alfvénic (slow) and super Alfvénic (fast).

In FINESSE, MHD equilibria are not found by the standard time stepping to reach a steady state but by a direct solution of the nonlinear stationary MHD equations. The new solution algorithm involves analytical reformulation of the problem in an equivalent form suitable for ef£cient numerical solution by a special inner-outer iterative procedure. The transformed MHD equations are discretized by isoparametric bicubic Hermite £nite elements providing quartic convergence which is practically observed. The FINESSE algorithm is computationally ef£cient and its main attraction is that the computed equilibria are very accurate. This is crucial for subsequent spectral studies.

Ideal and resistive spectra of the computed equilibria are studied with another tool, a program called PHOENIX. The linearized MHD equations are discretized by quadratic or cubic Hermite £nite elements in the radial direction and by a Fourier spectral method in the poloidal direction. This leads to a large-scale generalized eigenvalue problem

$$Ax = \lambda Bx,$$

that is solved by the recently proposed iterative Jacobi-Davidson method [2]. This method is of the Krylov subspace type. It allows to £nd eigenvalues in a region of interest and the corresponding eigenvectors fast and with unprecedented accuracy. The implementation of the Jacobi-Davidson method for PHOENIX is parallel.

Our numerical examples show how FINESSE and PHOENIX can be used to study the effect of the poloidal ¤ows on Toroidal Alfvén Eigenmodes.

References

1. B. van der Holst, A.J.C. Belien, J.P. Goedbloed, New Alfvén continuum gaps and global modes induced by toroidal ¤ow, Phys. Rev. Lett., 84:2865–2868, 2000.
2. G.L.G. Sleijpen and H.A. van der Vorst, A Jacobi-Davidson iteration method for linear eigenvalue problems, SIAM J. Matrix Anal. Appl., 17:401–425, 1996.

Modelling of black holes in the string Einstein-Born-Infeld gravity with massive dilaton

T.L. Boyadjiev[1] **and S. Yazadjiev**[2]

[1]*Faculty of Mathematics and Computer Science, University of So£a "St. Kliment Ohridski", So£a, Bulgaria.*

[2]*Faculty of Physics, University of So£a "St. Kliment Ohridski", So£a, Bulgaria.*

todorlb@fmi.uni-so£a.bg; yazad@phys.uni-so£a.bg

We investigate numerically a model of spherically symmetric black holes in the string theory inspired Einstein-Born-Infeld gravity with a massive dilaton. Within the framework of this model the main system of differential equations can be rewritten in the form

$$f' + (f-1)/r + rf\varphi'^2 + r\gamma^2 V(\varphi) - Q(r,\varphi) = 0,$$

$$f\left(\varphi'' + 2\varphi'/r\right) + \left[(1-f)/r + Q(r,\varphi) - rW(\varphi)\right]\varphi' + 2\,\alpha Q(r,\varphi)/r - \gamma^2 V'(\varphi)/2 = 0,$$

on the interval $r \in [R_h, \infty)$ with following boundary conditions

$$f(R_h) = 0, \quad \left[1/r - Q(r,\varphi) - r\gamma^2 V(\varphi)\right]\varphi' + \alpha Q(r,\varphi)/r - \gamma^2 V'(\varphi)/2\big|_{r=R_h} = 0,$$

$$\varphi(r) \xrightarrow[r\to\infty]{} 0.$$

Here the function $f(r)$ describes the metric, $\varphi(r)$ is the dilaton £eld, the quantity R_h is the unknown horizon of the black hole, and $Q(r,\varphi) \equiv 2e^{2\alpha\varphi}\left(r^2 - \sqrt{(r^4+q_e^2)}\right)/r$.

The last condition needed to close the system is the mass equation

$$M + \int_{R_h}^{\infty} e^{-\delta}\left[2e^{2\alpha\varphi}\left(r^2/\sqrt{r^4+q_e^2} - 1\right) + \gamma^2 V(\varphi)\right] r^2 dr - 2\pi R_h^2 T = 0,$$

where M is the given mass of the black hole, the metric function $\delta(r)$ satis£es the equations

$$\delta' + r\varphi'^2 = 0, \quad \delta(\infty) = 0,$$

and the temperature T is calculated via the formula

$$4\pi T = e^{-\delta(R_h)} f'(R_h).$$

The continuous analog of Newton method [1] is used to solve the above formulated free-boundary problem.

We prove, that the presence of the dilaton potential $V(\varphi)$ leads to black holes with much more complicated causal structure than the case of massless dilaton [2]. The extremal black solutions ($f'(R_h) = 0$) are also studied. We show that, depending of mass M, charge q_e, the dilaton mass γ, and the dilaton potential $V(\varphi)$ it is possible that black holes with more than one horizon exists. The dependence of the black hole structure on the form of the dilaton potential $V(\varphi)$ is examined too.

References

1. I. V. Puzynin et al, in *Physics of Elementary Particles and Atomic Nuclei*, **30**, No 1, 87 (1999).
2. T. Tamaki, T. Torii, Phys. Rev. **D62**, 061501R (2000); gr-qc/0101083.

ASTROMD. A data analysis and visualization tool for astrophysics

Fulvio Buonomo[1]**, Claudio Gheller**[1] **and Ugo Becciani**[2]

[1]*CINECA, Via Magnanelli 6/3, Casalecchio di Reno, Bologna, Italy*
[2]*Astrophysical Observatory of Catania, Via S.So£a 78, Catania, Italy*
f.buonomo@cineca.it, c.gheller@cineca.it, ube@sunct.ct.astro.it

Since the beginning of modern astronomy, the scienti£c community expressed a great interest in scienti£c visualisation tools, and today image processing tools are of fundamental importance in astronomy. We present a new data visualization/analysis software, AstroMD [1] speci£cally projected to deal with astrophysical data. The software gives a 3D graphic representation of the data exploiting all the available information and making use of the immersive visualization techniques. These, converting huge amounts of digital data into a clear graphical representation, enhance the human skill in recognizing interesting features in complex data structures. AstroMD is developed using the Visualization Toolkit (VTK) by Kitware [2], a freely available software portable on several platforms which range from the PC to the most powerful visualization systems.

VTK supports a wide variety of visualization algorithms, it supports stereo-graphic rendering and can be used for virtual reality visualization. Furthermore VTK allows the user to implement speci£c data analysis modules.

The development of AstroMD is the aim of the Cosmo.Lab project, £nanced by the European Community in the Fifth Framework. It is developed according to the requirements proposed by several astrophysical research £elds:

- data coming from cosmological simulations [3]
- data coming from observational catalogues (VIRMOS)
- observational data of extragalactic radio sources

AstroMD can manage different physical quantities. It can £nd structures having a not well de£ned shape or symmetries, and performs quantitative calculations on a selected region or structure. The display of data gives the illusion of a surrounding medium into which the user is immersed. The result is that the user has the impression of travelling through a computer-based multi-dimensional model which could be directly hand-manipulated. In this sense, the virtual reality is a progressive lowering of the barrier which separates users from their data [4].

AstroMD is developed by the Visual Information Technology laboratory at CINECA in collaboration with the Astrophysical Observatory of Catania. AstroMD is an open source completely free code which is freely available (http://www.cineca.it/astromd).

References

1. U. Becciani, V. Antonuccio-Delogu, C. Gheller, L. Calori, F. Buonomo, S. Imboden ”AstroMD. A multi-dimensional data analysis tool for astrophysical simulations”, astro-ph/0006402
2. Schroeder, W., Ken, M. , Lorensen, B., ”The Visualization Toolkit”, *Prentice Hall*, 1999.
3. U. Becciani, V. Antonuccio-Delogu, F. Buonomo, C. Gheller, ”An Integrated Procedure for Tree-Nbody Simulations: FLY and AstroMD”, astro-ph/0101447
4. Earnshaw, R.A., Watson, D., ”Animation and Scienti£c Visualization”, *Academic Press ltd.* 1993

Jet ¤ows in the astrophysical environment

M. Camenzind, M. Krause, M. Thiele

Landessternwarte Königstuhl,
D-69117 Heidelberg, Germany

Jets are supersonic, or supermagnetosonic collimated ¤ows encountered in various astrophysical objects. Highly collimated out¤ows are generated by young stellar objects, known as Herbig–Haro objects in molecular clouds, as well as by rapidly rotating supermassive Black Holes in the centers of massive elliptical galaxies. Since these jets propagate on the background of an ambient medium with £nite density and pressure, matter in the bow shock will be constantly heated to high temperature and cool down by various emission mechanisms. Depending on the astrophysical environment, the cooling time can be much shorter than the typical propagation time. While traditional jet simulations are based on time–explicit methods involving an adiabatic equation of state, cooling has to be implemented on the basis of time–implicit schemes. For that purpose we enlarged the magnetohydrodynamic C–code NIRVANA (originally developed by Udo Ziegler) to include cooling processes. We present various simulations in 2 and 3 spatial dimensions of magnetized Herbig–Haro jet ¤ows including line emission and extragalactic jets in a high density environment. The latter case is particularly interesting in view of recent observations by the Chandra satellite of Bremsstrahlung emission from extragalactic radio jets embedded into a cluster medium.

Automatization of calculations for analysis and visualization of magnetic £eld and space plasma data (ADO)

Gilberto Casillas Pérez and Xochitl Blanco Cano

Departamento de Física Espacial, Instituto de Geofísica, UNAM, Coyoacán D.F., CP 04510, México

(52)5622-4142, (52)5550-2486, gacp@£s-esp.igeofcu.unam.mx

A plasma is a ionized gas as a result of its high temperature, nevertheless the plasma as a whole still remains electrically neutral. The Universe is constituted almost totally of plasma and its study is very important to learn how plasmas work. The expanding atmosphere of the Sun, is a plasma that extends beyond Pluto's orbit. This expanding atmosphere is known as the solar wind. The study of solar wind and space plasmas is very important in Space Physics because of the processes and phenomena that take place there. Among these phenomena, the study of waves and instabilities in the interplanetary medium are of interest since waves play an important role in the dissipation processes and heating of plasmas, via particle-wave interactions. One of the means used for the study of solar wind and interplanetary plasmas is the analysis of registered observations made by spacecrafts in different regions of space. This analysis uses enormous amounts of data which require the use of computational techniques to carry out the analysis.

In the present work the ADO (Análisis de Datos Observados) system is described. ADO is a system developed with the purpose of automating data analysis and data visualization calculations of solar wind and space plasmas observed by the ISEE1, ISEE2 and AMPTE-UKS spacescrafts. The types of analysis included in the system are: Fourier analysis, minimum variance analysis, estimates of some wave identi£ers and averages of some physical variables. These analysis allow the determination of some wave properties like the direction and angle of propagation, the sense of polarization, the mean polarization rate, the magnetic compression, the magnetic polarization and the noncoplanar ratio. ADO is a support tool for the study of waves and instabilities in the interplanetary medium, and it will be used by scientists and students at the Departamento de Física Espacial, of the Instituto de Geofísica, at UNAM. Results obtained with ADO have been compared with those reported in scienti£c papers [1] [2] and the results are found to be consistent.

References

1. Reference No 1. Blanco Cano X. and Schwartz S.J., "Identi£cation of low-frecuency Kinetic wave modes in the Earth's ion foreshock", Ann. Geophysicae 15, 273-278 (1999).
2. Reference No 2. Blanco Cano X., Russell C.T. and Le G., "Identi£cation of foreshockwaves with 3-s periods", Journal of Geophysical Research, Vol. 104, No. A3, pages 4643-4656, March 1, 1999.

Separation of muons in the giant air showers by the geomagnetic £eld

E.E.Antonov[1], L.G.Dedenko[1], G.F.Fedorova[2], A.V.Glushkov[3], V.A.Kolosov[3], M.I.Pravdin[3], Yu.P.Pyt'ev[1], T.M.Roganova[2], I.E.Sleptsov[3]

[1] *Department of Physics, M.V.Lomonosov Moscow State University, 119899 Moscow, Russia*

[2] *Scienti£c and Research Institute of Nuclear Physics, M.V.Lomonosov Moscow State University, 119899 Moscow, Russia*

[3] *Institute of Space Physics and Aeronomy, Siberian Branch of the Russian Academy of Sciences, 677891 Yakutsk, Russia*

telephone: (095)939-14-89, fax: (095)939-14-89, e-mail:ddn@dec1.npi.msu.su

The observation of giant air showers with energies above $\sim 10^{20}$ eV is extremely interesting for elementary particle physics and astrophysics. This energy range lies beyond the Greisen-Zatsepin- Kuz'min "cutoff" of the cosmic ray energy spectrum on account of the interaction of protons (or nuclei) with the relic microwave photons. The giant air shower is a cascade of secondary particles generated in the atmosphere by an ultra high energy ($\geq 10^{19}$ eV) primary cosmic ray particle. Billions of electrons and muons produced in interactions with atomic nuclei and decay processes pass through the atmosphere diverging in space and time to strike the Earth surface. The density of electrons and muons at £xed distance from the shower axis (primary particle direction of motion) is usually used as an shower energy estimator. Shower arrival direction is estimated with the help of shower time front [1] of muons detected.

It was shown [2] that de¤ections of muons by the geomagnetic £eld is noticeable. It is here demonstrated that this de¤ection perturb not only the energy estimator [3] but also time delays of muons detected. Billions of muons diverging from the shower axis are de¤ected by the geomagnetic £eld. Because muons are produced at different depths in the atmosphere and with various energies and directions of motion it is a problem to simulate their trajectories. Calculations were carried out in terms of the quark-gluon string model for primary protons and observation level of 1020 g/cm^2 for inclined showers. The Landau-Pomeranchuk-Migdal effect and interactions of neutral pions with nuclei in the atmosphere at ultra high energies were taken into accunt.

The interactions of the primary particle with the nuclei in the atmosphere were simulated by the Monte Carlo method. The passing of secondary hadrons was treated with the help of the cascade equations. Muons were grouped into blocks with some differences in depth production, zenith and azimuthal angles and energy. For every "block" of muons equation of motion was solved as for a single muon with average energy, height production and zenith and azimuthal angles in each bin (a method of "group" particle). At last equations of motion for these groups were solved. The calculated lateral distribution of muons displays noticeable assymetry at all distances from the shower axis and particullary the energy estimator changes by a factor of 1.5. Due to de¤ection in the geomagnetic £eld arrival time of muons detected increases disturbing shower time front. Thus the discussed examples show an importantce to treat experimental data on giant air showers taking into account the geomagnetic £eld.

References

1. A.M.Anokhina, L.G.Dedenko, G.F.Fedorova, V.I.Galkin et al., Phys. Rev. D **60** 033004 (1999).
2. E.E.Antonov, L.G.Dedenko, Yu.P.Pyt'ev, A.V.Glushkov et al., JETP Lett. **68**, 185 (1998).
3. E.E.Antonov, L.G.Dedenko, Yu.P.Pyt'ev, A.V.Glushkov et al., JETP Lett. **69**, 614 (1999).

Numerical simulations of the global baroclinic instability in accretion disks

Hubert Klahr[1] **and Peter Bodenheimer**[2]

[1] *Computational Physics, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany*

[2] *UCO/Lick Observatory, University of California, Santa Cruz, CA 9506*

phone: +49-(0)7071-29 77682, fax: +49-(0)7071-29 5094,

Email: klahr@tat.physik.uni-tuebingen.de

Protoplanetary disks appear to be a common feature around young stars. They are thought to provide the material and the environment for the formation of planets. Thus one needs to know the internal properties of such disks, such as the density, temperature and turbulence, in order to estimate the time scales of the formation process [1].

We present the global baroclinic instability as a source for vigorous turbulence leading to angular momentum transport in Keplerian accretion disks. Instead of relying on Magneto Hydrodynamical Turbulence with the known dif£culties of the low ionisation values in Protoplanetary Accretion Disks [2] we performed numerical simulations of a purely hydrodynamical instability that works in accretion disks, namely the famous baroclinic instability, which is also responsible for turbulent patterns on planets, for example, Jupiter's red spot and the weather patterns of cyclones and anti-cyclones on earth. Baroclinic instabilities arise in rotating ¤uids when surfaces of constant density are inclined with respect to the surfaces of constant pressure. Vortensity, de£ned as vorticity per unit surface density, is not conserved as is the case in barotropic two-dimensional ¤ows, and vortices can be generated.

We show by analytical considerations and three-dimensional radiation hydro simulations using the TRAMP code [3] that, in particular, protoplanetary disks have a negative radial entropy gradient, which makes them baroclinic. Two-dimensional numerical simulations show that this baroclinic ¤ow is unstable and produces turbulence. These £ndings are tested for numerical effects by performing barotropic simulations which show that imposed turbulence rapidly decays. The turbulence in baroclinic disks draws energy from the background shear, transports angular momentum outward and creates a radially inward bound accretion of matter, thus forming a self consistent process. Gravitational energy is transformed into turbulent kinetic energy, which is then dissipated, as in the classical accretion paradigm. [3]

We measure accretion rates in 2D and 3D simulations of $\dot{M} = -10^{-9} \text{ to } -10^{-7}$ $M_\odot$ yr^{-1} and viscosity parameters of $\alpha = 10^{-4} - 10^{-2}$, which £t perfectly together and agree reasonably with observations. The turbulence creates pressure waves, Rossby waves, and vortices in the $(R - \phi)$ plane of the disk. We demonstrate in a global simulation that these vortices tend to form out of little background noise and to be long-lasting features, which have already been suggested to lead to the formation of planets [4].

References

1. Lissauer, J.J. 1993, Annual Review of Astronomy and Astrophysics, 31, 129
2. Sano, T., Miyama, S.M., Umebayashi, T. & Nakano, T. 2000, Astrophysical Journal, 543, 486
3. Klahr, H.H., Henning, Th., & Kley, W. 1999, Astrophysical Journal, 514, 325
4. Klahr, H.H., & Bodenheimer, P. 2001, Astrophysical Journal, submitted,
   see $http://www.tat.physik.uni-tuebingen.de/\sim klahr/baro.ps.gz$

Maartje: Three–dimensional astrophysical gasdynamics and radiative transfer

Garrelt Mellema[1] **and Andrew Lim**[2]

[1] *Sterrewacht Leiden, Postbus 9513, NL-2300 RA Leiden, the Netherlands*
[2] *Dept. of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK*

Phone: +31 71 527 5738, Fax: +31 71 527 5819, Email: mellema@strw.leidenuniv.nl

In astrophysics three–dimensional gas dynamic calculations are still quite rare, at least with grid based codes. Because of this, even less work has been done on including the effects of the additional physical processes which are taking place in interstellar or intergalactic gas clouds. One very important process is the interaction of light and matter, for which the paths of the photons through the gas need to be followed. This combination of radiative transfer and 3D hydrodynamics will prove to be invaluable for studying the birth and death of stars, as well as the development of structures in the universe (see [1] for an example).

We are developing a code which combines a 3D hydrodynamic calculation on an adaptive grid, with radiative transfer on the same grid. The working name of this code is *Maartje*. It is written in C++, and we aim to keep it modular, so that one has the choice to include certain features or not. The adaptive grid is regular and of the nested type. The Euler equations are currently solved using van Leer's ¤ux vector splitting method, but we are working on a module based on Roe's approximate Riemann solver to offer a choice of solvers. The radiative transfer is calculated using a 'short characteristics' type method (but a 'long characteristics' module is also available).

We use the *Maartje* code to study the progression of an ionization front through an inhomogenous medium. This generic problem is relevant for the emergence of HII regions around massive stars, and the formation of Planetary Nebulae around lower mass stars, and has not been studied numerically before. It also provides a good testing ground for the new code.

To represent the radiation effects on the gas, we include the ionization and recombination of hydrogen due to photons and collisions with electrons, and the heating through photo–ionization. The radiative cooling is implemented through a typical interstellar cooling curve. This is a simpli£ed version of the *DORIC* module described in [2] and [3]. The *DORIC* module calculates the non–equilibrium cooling and ionization for astrophysically important elements (currently H, He, C, N, O, Ne and S), and will in the future be incorporated in *Maartje*.

On the poster we present the £rst results from this code.

References

1. T. Abel, G. L. Bryan, M. L. Norman, 2000, Astroph. J. 540, 39
2. A.C. Raga, G. Mellema, P. Lundqvist, 1997, Astrophysical Journal Supplement 109, 517
3. G. Mellema, A.C. Raga, J. Cantó, P.L. Lundqvist, B. Balick, A. Noriega–Crespo, W. Steffen, 1998, Astronomy & Astrophysics 331, 335

Direct n-body integration with variational equations and close encounters multi-regularization: The *NNEWTON* package

Ana Nunes[1] **and Nuno Pereira**[2]

[1] *Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, Campo Grande, Edifício C8, 1749-016 Lisboa, Portugal.*

[2] *Área Departamental de Matemática, ESTIG/IPB, Rua Afonso III, nº 1, 7800-050 Beja, Portugal.*

Phone: +351 284311540, Fax: +351 284311542, email: nuno.pereira@estig.ipbeja.pt

Direct integration methods have been widely used for the study of self-gravitational N-body systems, namely in modeling star clusters. Hermite integration and two-body regularization are now considered standard approaches [1].

In this work we present a software package for N-body simulations based on a new direct integration method including close encounters treatment with a new regularization algorithm [2]. The package includes N-body integrators (the *NNEWTON* programs) initial conditions genera-tors (the *NN*-VIRIAL program) and data analysis applications (the *NN*-ETL and PROCVAR programs).

Our work have a two fold purpose: the development of N-body integrators capable of dealing with the numerical problems induced by close encounters and, the study of the growth of perturbations on the initial conditions of the system. In particular, we are interested in measuring the time scale of the exponential instability. The system is described by a set of $6N$ £rst order differential equations – the Newton equations of motion – plus $6N$ £rst order variational equations of motion, for the study of the evolution of variations (perturbations) on initial conditions.

We have developed a direct integration scheme based on a Runge-Kutta variable step method, in which we have implemented standard Kustaanheimo-Stiefel binary regularization and a new regularization method: the *InOut* algorithm [3]. This algorithm was generalized to the case of multiple encounters using an heuristic procedure.

The *NNEWTON* programs show good performance in simulations of systems in which close encounters play an important role in the dynamics. The algorithm is capable of dealing with simultaneous binary encounters and high order encounters (triple or more). Our £rst results of the study of perturbations on initial conditions show an exponential growth with a time scale in good agreement with the the time scale presented in [4] for similar simulations.

The simple regularization procedures implemented in these programs proved to be ef£cient in preventing the growth of numerical errors in the presence of close encounters. The package is adequate for the study and simulation of N-body systems and the measurement of the time scale of the exponential instability.

References

1. Aarseth , S. J. (1999): *Star Cluster Simulations: The State of the Art.* Accepted by Cel. Mech. Dyn. Astron. (URL: http://babbage.sissa.it/astro-ph/9901069).
2. Pereira, N. S. A. (2001): *Master's Thesis.* Faculty of Sciences, University of Lisbon, Portugal.
3. Simó, C., Lacomba, E. A. (1992): *Regularization of Simultaneous Binary Collisions in the n-Body Problem.* Journal of Differential Equations, Vol. 98, No. 2, August.
4. Goodman, J., Heggie, D. C., Hut, P. (1993): *On the Exponential Instability of N-Body Systems.* The Astrophysical Journal, **415**:715-733.

Spiral arms in astrophysical discs

S. Pfalzner

I. Physikalisches Institut, Zülpicherstr.77, Albertus-Magnus-Universität zu Köln, Germany

pfalzner@ph1.uni-koeln.d

Flattened disc-shaped objects are a common feature in the cosmos - for example spiral galaxies as well as protoplanetary discs around early stars display such features. These objects often show characteristic spiral patterns, which consist in the mayority of cases of two more or less tightly wound spiral arms.

During the last 15 years it became possible to simulate such structures with many body methods. Due to the long-range nature of the often dominating gravitational forces and the necessary large number of simulation particles ef£cient algorithms are essential. Hierarchical tree codes [1][2] in combination with smoothed particle hydrodynamics methods [3] are a very useful tool to tackle such problems. There have been many simulations of single galaxies as well as encounters between two and more galaxies (the same can be said for protoplanetary discs). These simulations proved very useful to explain the general dynamics of such systems.

Here it will be shown how such techniques can be employed to study the actual reason for the formation of spirals as well in galaxies as in accretion discs. In encounters between such discs a gravitational is introduced. The £rst spiral arm develops due to the actual encounter and resulting shock wave. The second spiral arm is caused by the fact that the geometrical center of the disc and its center of mass are no longer identical. Moreover, after some time the £rst spiral arm decays. However, the center of mass of the system oscillates, so that a new spiral arm is created. So that most of the time the system appears as a two-armed spiral structure.

In addition, the mass loss due to such encounters will be studied. It will be shown that the mass distribution within the disc steepens in such encounters.

References

1. J. Barnes, P. Hut, Nature 324, 446–449, (1986)
2. S.Pfalzner, P.Gibbon, *Many-Body Tree Methods in Physics*, Cambridge University Press (1996)
3. J.J. Monaghan, Ann. Rev. Astron. Astrophys. 30, 543–574, (1988)

Jump processes in option pricing theory

Claudio Albanese[1], **Joe Campolieti**[2], **Sebastian Jaimungal**[1] **and Dmitri Rubisov**[3]

[1] *Department of Mathematics, University of Toronto, 100 St George Street, M5S 3G3, Toronto, Ontario, Canada*

[2] *Mathematical Finance Program, New College, University of Toronto, First Classic Av., M5S 3G3, Toronto, Ontario, Canada*

[3] *Bank of Montreal, First Canadian Place, Toronto, M5X 1A1, Ontario, Canada*

albanese@math.utoronto.ca, (416) 567 1351 (cell), (416) 978 5237 (of£ce)

My name is Claudio Albanese and work as Professor of Mathematics at the University of Toronto, where I mostly teach Mathematical Financ and occasionally Mathematical Physics. My PhD is in Theoretical Physics from ETH Zuerich. My industrial experience includes one year on Wall Street as VP for research at Morgan Stanley Dean Witter. My collaborators hold junior positions at the University and all of them have a PhD in Physics. I would propose to make a presentation describing topics in computational £nance which are at the center of the attention in £nancial institutions and to which a physicists audience can easily relate to. The presentation would cover the content of a series of articles, in part published and in part submitted for publication.

In [1], Sebastian Jaimungal, Dmitri Rubisov and I propose a model of lines to price derivative claims assuming the underlying obeys a jump process of the variance-gamma (VG) type. The model is based on the method of lines and involves the solution of ordinary differential equations and a Richardson extrapolation method. We describe the method in the context of equity options and show how to price Bermudan and barrier options with VG jumps.

In [2], Joe Campolieti and I introduce a canonical transformation method to £nd exact solutions to pricing problems. The method is systematic and allows one to re-derive in a simple, uni£ed framework exact solutions in the pricing theory literature such as af£ne, quadratic and root models, and to identify new families of solvable models based on the Bessel proccess.

In [3], a new binomial volatility model with variance-gamma jumps is introduced and developed by Jaimungal, Rubisov and myself. The model is based on the assumption that the volatility can switch at random between two pre-assigned values at pre-assigned times. In the case of European style options, explicit analytical solutions can be obtained. The above mentioned method of lines, can also be implemented in this framework, making it possible to study path-dependent options as well. In the case of American and Bermudan we £nd that the exercise boundary consists of a double boundary, one for each volatility level.

Finally, in [4], Jaimungal and I introduce a general class of multi-variate diffusion models for forward LIBOR rates which extend the Brace-Gatarek-Musiela model and also includes the Hull-White and other models as particular cases. This class can be extended further to include variance-gamma jumps and leads to closed form, exact pricing formulas for caplets. Pricing formulas and the no-arbitrage drift condition in the presence of jumps are both obtained by using the method of canonical transformations. We use the method of lines to price path dependent options and derive approximate pricing formulas for swaptions.

References

1. C.A., S. Jaimungal, D.Rubisov, “Jumping in Line”, Risk Magazine, forthcoming in February 2001.
2. C.A., J. Campolieti, “A New Family of Integrable Diffusions”, submitted to the Annals of Probability.
3. C.A., S. Jaimungal, D.Rubisov, “Binomial Volatility Models with Variance-gamma Jumps”, submitted to the Journal of Derivatives.
4. ‘C.A., S. Jaimungal, ‘Jump-LIBOR Models”, in preparation.

Learning from examples by PCA

C. Bunzmann, M. Biehl and R. Urbanczik

Institut für Theoretische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg

telephone 0049 931 888 5146, fax 0049 931 888 5141,
bunzmann@physik.uni-wuerzburg.de

Supervised learning from examples aims at designing a student neural network that matches given pairs of example inputs and teacher network outputs. To date, the method of choice for training large multilayer neural networks has been stochastic gradient descent and its variations. It is computationally cheap, as each update of the weight vectors is based on the presentation of a single example. One £nds that inevitable symmetries slow down the convergence of the method drastically [1, 2]. In the case where every example is used only once for an update, its learning dynamics can be analyzed in the limit of large input dimension N [2], yielding that far more than KN examples are needed for good performance, where K is the number of hidden units in the system.

Committee machines de£ne a rule $\tau(\boldsymbol{\xi}) = g\left(\sum_{i=1}^{K} f\left(\boldsymbol{B}_i^T \boldsymbol{\xi}\right)\right)$ via K weight vectors $\boldsymbol{B}_i$. We propose and analyze a new approach to the supervised learning of Committee machines, which is based on the Principal Component Analysis (PCA) of a covariance matrix build up using the examples with their respective teacher output [3]. For an isotropic distribution of inputs, a K dimensional space constructed from the principal components is shown to approximate the space spanned by the unknown weigth vectors of the rule. In a second step, the optimal weight vectors of the student are chosen within this space. Since the dimensionality of the space to be searched is reduced drastically from N large to a £nite K, this step needs far less than KN examples.

Simulations for large but £nite N show, that our algorithm is an ef£cient tool to estimate the weight vectors of the teacher on the basis of given examples. We use our algorithm for both Soft-Committee machines with sigmoidal activation functions f and a linear output unit, and Hard-Committee machines with threshold units in both layers. For the Soft-Committee machine with $K = 3$, it is possible to give a good approximation to the teacher space after using as few as $8.7\ KN$ examples. For large K (while $K \ll N$), the number of examples needed for a good approximation scales for the Soft-Committee machine as $1.96\ K^2 N$. In the case of Hard-Committee machines, our algorithm is compared with simulations of stochastic training procedures found in the literature [4]. Our algorithm yields a good approximation of the rule using a 20 times smaller number of examples.

For anisotropic input distributions, an estimator of the covariance matrix of the distribution of the example components is constructed, which is used to whiten the matrix used for the PCA.

As our simulation results prove to be far better than all available simulations of stochastic gradient descent methods, our method can be considered as an interesting candidate for the development of a new class of algorithms for learning from examples.

References

1. H. Schwarze and J. Hertz. *Europhys. Lett.*, 21:785, 1993.
2. D. Saad and S. Solla. *Phys. Rev. Lett.*, 74:4337, 1995.
3. C. Bunzmann M. Biehl and R. Urbanczik. *Phys. Rev. Lett.*, 86:2166-2169, 2001.
4. J. Kim and H. Sompolinsky. *Phys. Rev. E*, 58:2348, 1998.

A computational ef£cient solution technique for traf£c netwok O/D matrix estimation

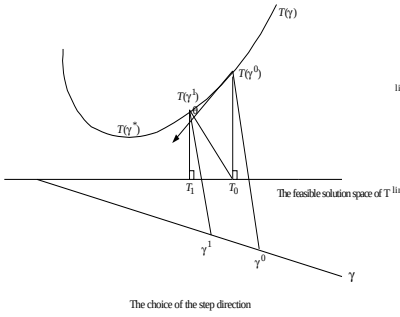
Hsun-Jung Cho[1], Cheng-Hsiang Chen[2], Pei-Wei Lin[2], and Ian-Lam Ng[2]

[1] *Professor, Dept. Tran. Tech. Mang., Nat'l Chiao Tung Univ., Taiwan*
[2] *Master, Dept Tran. Tech. Mang, Nat'l Chiao Tung Univ., Taiwan*
Corresponding address: Department of Transportation Technology and Management, National Chiao Tung University, Hsincu 300, Taiwan
Email: hjcho@cc.nctu.edu.tw and Tel.(Fax) 886-35710657

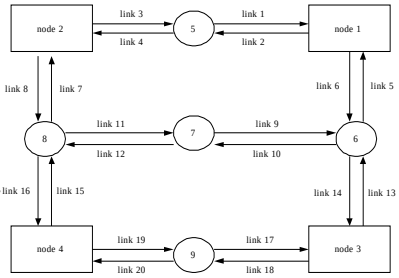
It′s necessary to collecting the data of travel distribution (O/D matrix) in the transportation planning process. But it takes huge cost. Under the assumption of the user equilibrium behavior principle, many authors [1], [2] and [3] proposed the methods to consistent arc ¤ow from traf£c counts for the estimate model to be feasible.

In this paper, based on use of the Moore-Penrose generalized inverse [4], a new method estimating the reasonable travel distribution matrix. The assumption of the travel behavior includes user equilibrium principle of the traf£c assignment and the travel distribution presented by Entropy model. The developed simulator based on Jacobian iterative method, Frank-Wolf method, network traf£c ¤ow sensitivity information has been developed. Due to the robust features of the method, the proposed sensitivity information provide a accurate searching direction.

In the £rst £gure, the sensitivity information provides an accurate searching direction, we can estimate the O/D matrix by arc ¤ow that detected or observed. The second £gure is the network example and the table shows us the estimated O/D matrix.



The choice of the step direction



Network

Estimating T_{ij}

	1	2	3	4	O_i
1	0	82.165	126.944	32.891	242
2	47.995	0	36.056	36.949	121
3	131.005	69.835	0	50.160	251
4	5.0	6.0	70.0	0	81
D_j	184	158	233	120	695

References

1. M. Florian and Y. Chen, The **7th** IFAC/IFORS Sysposium on Transp. System, 1029-1034 (1985).
2. J. Oh, Math. in Transport Planning and Control, 35-44 (1992).
3. H. Yang etc. Transportation Research, **26B**, 417-434 (1992).
4. H-J. Cho and S.C. Lo, Transportation Research Record, **1667**, 96-106 (1999).

Series solutions of the anharmonic motion equations

A. Raouf Chouikha
University of Paris-Nord
Institut Galilee
LAGA,CNRS UMR 7539
Villetaneuse F-93430
Chouikha@math.univ-paris13.fr

Consider the class of non linear oscillators of the form

$$\begin{cases} \frac{d^2u}{dt^2}+f(u)=\epsilon g(t) \\ \\ u(0)=a_0 \\ u'(0)=0 \end{cases}$$

where $g(t)$ is a $2T-$periodic function, f is a function only dependent on u and ϵ is a small parameter. We are interested in the periodic solutions with minimal period $2T$, when the restoring term f and g satisfy suitable conditions.
By using methods of trigonometric series for solving differential equations we prove the existence of a periodic solution of this perturbed Duf£ng equation.
These results develop and extend a previous ones [1].

References

1. R. Chouikha *Remark on Periodic solutions of Non Linear Oscillators* To appear in Applied Math. Letters , 2001

Quantifying coexistence of collectivity and noise in complex systems

S. Drożdż[1], F. Grümmer[2], J. Kwapień[1], M. Sawa[1], J. Speth[2] and M. Wójcik[1]

[1] *Institute of Nuclear Physics, Radzikowskiego 152, 31–342 Kraków, Poland*
[2] *Institute für Kernphysik, Forschungszentrum Jülich, D–52425 Jülich, Germany*
(+4812)6370222ext220, (+4812)6375441, stanislaw.drozdz@ifj.edu.pl

Studying complex systems is typically based on analysing large, multivariate data representing both, the space and the time variability. The related principal characteristics of complexity is coexistence of collectivity and noise. One possible framework to quantify such effects is in terms of several variants of the correlation matrices. It allows to make use of the random matrix theory as a null hypothesis and to identify correlations as deviations. The related useful characteristics involve the structure of eigenspectrum and the distribution of matrix elements. They can be used to identify certain system-speci£c, non-random properties of the system.

When addressing this sort of questions we perform a systematic study of the £nancial empirical correlation matrices accounting for correlations among different companies comprised by a single stock market (based on the Deutsche Aktienindex) [1], between two different, geographically distant stock markets (DAX versus Dow Jones) [2] and, based on high-frequency recordings, even between consecutive trading days [3]. An interdisciplinary potential of the corresponding methodology is illustrated by its application to other complex natural systems such as the human brain [4] (studied using the multichannel magnetoencephalography recordings obtained from the human cortex in response to sensory stimulations) and the strongly interacting Fermi systems [5].

The results document utility of our methodology in quantifying deterministic aspects, such as collectivity and memory effects in the dynamics of complex systems, as well as its noise content. Furthermore, several system speci£c novel empirical facts about dynamics of the systems mentioned above have been identi£ed. Some of such facts have already been presented in the literature cited below. Several others are to be presented.

References

1. S. Drożdż, F. Grümmer, A.Z. Górski, F. Ruf, and J. Speth, Physica A **287** (2000) 440
2. S. Drożdż, F. Grümmer, F. Ruf, and J. Speth, arXiv:cond-mat/0011488, Physica A, in press
3. S. Drożdż, J. Kwapień, F. Grümmer, F. Ruf, and J. Speth, arXiv:cond-mat/0102402
4. J. Kwapień, S. Drożdż, and A.A. Ioannides, Phys. Rev. E **62** (2000) 5557
5. S. Drożdż and M. Wójcik, arXiv:nucl-th/0007045

Fast and reliable techniques for using Racah's algebra in many–particle physics

S. Fritzsche[1], **B. Fricke**[1], **G. Gaigalas**[2], **T. Jacob**[1], **and M. Tomaselli**[3]

[1] *Fachbereich Physik, Universität Kassel, Heinrich–Plett–Str. 40, D–34132 Kassel, Germany.*
[2] *Institute of Theoretical Physics and Astronomy, A. Goštauto 12, 2600, Vilnius, Lithuania.*
[3] *Institut für Kernphysik, Universität Darmstadt, D–64289 Darmstadt, Germany.*

s.fritzsche@physik.uni-kassel.de; phone: ++49–(0)561–804–4128;
FAX: ++49–(0)561–804–4006

The theories of angular momentum and irreducible tensor operators are two fundamental concepts in studying (classical and quantum) many–particle systems. They are therefore widely applied in many different fields of physics including, for example, £eld theory, atomic and molecular physics, quantum chemistry, solid state physics, quantum optics, and others. The applications of these concepts does not only concern *isolated* many–particle systems but also various (quantitative) investigations on molecular and nuclear reactions, collision processes, or even the modelling of living cells. By applying group–theoretical methods, in particular, most of the mathematical techniques of these theories were developed by Racah [1] and Wigner [2] about 50 years ago. Today, these techniques are often briefly refered to as Racah algebra techniques.

The main power of Racah's algebra for practical computations is that it enables one to carry out the integration over the angular coordinates of a (complex) many–particle system analytically. The proper choice of coordinates and the use of the rotational symmetries of the system then often allows to reduced the number of independent variables considerably. In practical applications, Racah algebra techniques typically lead to expression which are written in terms of generalized Clebsch–Gordan coefficients, Wigner $n-j$ symbols, (tensor) spherical harmonics and/or rotation matrices. While, in principle at least, the evaluation and simpli£cation of such expressions is rather straightforward, in practise this step often becomes very laborious and prone to making errors.

Over the years, different *paths* have been developed to overcome these dif£culties. They include both, the explicit knowledge of sum rules (as been found in the literatur, see Ref. [3]) as well as graphical methods to recognize possible simpli£cations. — Today, a more reliable alternative is however provided by symbolic manipulations. To facilitate the application of the theory of angular momentum to a larger variety of many–particle systems, we developed the RACAH program [4] which, in the framework of MAPLE V, facilitates both the simpli£cation of complex expression as well as numerical computations. This new (symbolic) tool is designed to be ¤exible and powerful enough for most practical applications. Although it is meanwhile based on a rather large number of individual procedures, the knowledge of about 15 of these *commands* is still suf£cient to deal with most cases. In this contribution, we explain the symbolic techniques which have beeen developed for this package; several examples, moreover, will show how it can be utilized in (atomic and nuclear) many–particle physics.

References

1. G. Racah, Phys. Rev. **61**, 186 (1941); Phys. Rev. **62**, 438 (1942); Phys. Rev. **63**, 367 (1943).
2. E. P. Wigner, *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra* (Academic Press, New York, 1959).
3. D. A. Varshalovich , A. N. Moskalev and V. K. Khersonskii, *Quantum Theory of Angular Momentum* (World Scientific, Singapore a.o., 1988).
4. S. Fritzsche et al., Comput. Phys. Commun. **103**, 51 (1997); Comput. Phys. Commun. **111**, 167 (1998); Comput. Phys. Commun., in print (2001).

Numerical calculation of space charge distribution for dust grains in a plasma sheath equilibrium

L. G. Garcia and J. Goedert

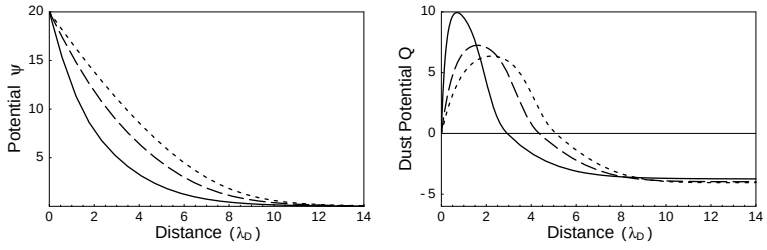
Centro de Ciências Exatas e Tecnológicas, UNISINOS, Av. Unisinos, 950, 93022-000
São Leopoldo, RS, Brazil

goedert@exatas.unisinos.br, Tel (51) 590 3333, Fax (51) 590 8162.

The interest for detailed information on dusty plasmas has increased considerably in the last decades. This is explained by its relevant applications, both in space plasmas and in laboratory or technology. In all of these systems, the interaction of a dusty plasma and a solid surface is a serious concern [1, 2]. One of the interests related to this problem is the grain charging process in the sheath region and their in¤uence in the sheath potential.

In order to verify the effects of the dust particle concentration in the dust charging process, we consider a one-dimensional stationary dusty plasma constituted of thermal electrons, cold ions and an uniform, immobile background of heavy dust grains. The dusty plasma is in contact with a plane cathode negatively biased where the incidence of ions produces a beam of energetic electrons which are also considered in the present model. Our setup is based on a model by Wang *et al.* [3]. However, no secondary emissions of electrons by dust particles are considered here. Poisson's equation and the balance of the electron, ion and beam currents entering the grain [3] form a complete set of nonlinear ordinary differential equations for the dust-plasma sheath problem. These equations are numerically integrated in a fully self consistent manner, yielding the electric potential ϕ and the dust charge q_d in the sheath region. The effect of secondary emission of electrons will be analyzed in a future, more detailed, paper.

In our simulations, we considered an argon plasma with an electron temperature $T_e = 2$ eV and an unperturbed electron density $n_{e0} = 6 \times 10^{15}$ m^{-3}. The normalized potential in the cathode was $\psi = -e\phi/T_e = 20$, the dust particle radius $a = 5$ μm and the Mach number $M = \sqrt{2}$. The numerical results show that when the concentration of dust particles is relatively small, e.g., $N_d = n_{d0}/n_{e0} \sim 10^{-9}$, the dust particles do not affect the sheath potential and the charging process as considered in [3]. However, at increasing values of dust concentrations, a signi£cant in¤uence of the charged dust particles is clearly observed. In the £gure, we show the in¤uence of the dust concentration in the sheath potential ψ (left side) and in the normalized dust potential $Q = -eq_d/aT_e$ (right side). The sequence of dotted, dashed and full curves represent increasing values of dust densities, with $N_d \sim 10^{-9}$, $N_d \sim 10^{-6}$ and $N_d \sim 10^{-5}$, respectively.



References

1. Jin-Xiu Ma, and M. Y. Yu, Phys. Plasmas **2**, 1343 (1995).
2. V. N. Tsytovich, S. V. Vladimirov, and S. Benkadda, Phys. Plasmas **6**, 2972 (1999).
3. D. Wang, D. Liu, and J. Liu, J. Appl. Phys. **88**, 1276 (2000).

Universal scaling functions for bond percolation on planar random and square lattices with multiple percolating clusters

Hsiao-Ping Hsu[1], **Simon C. Lin**[1,2] **and Chin-Kun Hu**[2,3]

[1]*Computing Centre, Academia Sinica, Nankang, Taipei 11529, Taiwan*
[2]*Institute of Physics, Academia Sinica, Nankang, Taipei 11529, Taiwan*
[3]*Department of Physics, National Dong Hwa University, Hualien 97401, Taiwan*

Tel: 886-2-2789-8008, Fax: 886-2-2788-5259,
E-mail: hphsu@gate.sinica.edu.tw

Percolation is related to many interesting phenomena in sciences. In recent years percolation problems with multiple percolating clusters have attracted much attention. Most of the simulational studies of such problems have been restricted to percolation on lattices. However, many physical systems with multiple percolating clusters such as Carbino disks used in the study of quantum Hall effects or oil £eld considered in oil drill problem do not have underlined regular lattice structures. Thus it is of interest to know the relationship between the quantities for percolation on regular lattices and the quantities for percolation on not regular lattices, such as random lattices. In the present paper [1], we use Monte Carlo simulations to study the bond percolation on $L_1 \times L_2$ planar random lattices, duals of random lattices, and square lattices with free and periodic boundary conditions in the vertical and horizontal directions, respectively as in [2], and with various aspect ratio L_1/L_2. We calculate the probability for the appearance of n percolating clusters, W_n, the percolating probabilities, P, the average fraction of lattice bonds (sites) in the percolating clusters, $< c^b >_n$ ($< c^s >_n$), and the probability distribution function for the fraction c of lattice bonds (sites) in percolating clusters of subgraphs with n percolating clusters, $f_n(c^b)$ ($f_n(c^s)$).

The random lattices are generated by the algorithm of Christ, Friedberg, and Lee [3]. In 1999 Hsu and Huang [4] determined the percolation thresholds, critical exponents, and demonstrated explicitly that the ideas of universal critical exponents and universal scaling function with nonuniversal metric factors can be extended to bond percolation on $L \times L$ periodic planar random lattices, duals of random lattices, and square lattices for the existence probability, the percolating probability, and the mean cluster size. In this paper, the results are extended to different boundary conditions with various aspect rations. Using a small number of nonuniversal metric factors, we £nd that W_n, P, $< c^b >_n$ ($< c^s >_n$), and $f_n(c^b)$ ($f_n(c^s)$) for random lattices, duals of random lattices, and square lattices have the same universal £nite-size scaling functions. We also £nd that nonuniversal metric factors are independent of boundary conditions and aspect ratios.

Many interesting problems are related to properties of multiple percolating clusters. It is of interest to extend the study of the present paper to higher spacial dimensions. In particular, the study of multiple percolating clusters in three dimensions could be related to oil drill problem.

References

1. H. P. Hsu, S. C. Lin and C. K. Hu, Phys. Rev. E, 2001 (submitted), cond-mat/0101112.
2. C. K. Hu and C. Y. Lin, Phys. Rev. Lett **77**, 8 (1996).
3. N. H. Christ, R. Friedberg, and T. D. Lee, Nucl. Phys. B **202**, 89 (1982); Nucl. Phys. B **210**, 310 (1982); **210**, 337 (1982).
4. H. P. Hsu and M. C. Huang, Phys. Rev. E **60**, 6361 (1999).

The evolution of nonlinear spatial economic models

S. V. Bulanov[1], **E. Yu. Echkina**[2], **I. N. Inovenkov**[2]

[1] *Institute of General Physics, Russian Academy of Sciences, Moscow, Russia,*
[2] *Moscow State University, Moscow, Russia*

bulanov@plasma.fpl.gpi.ru, ejane@cs.msu.su, inov@cs.msu.su

The economical activity corresponds with the certain time and place therefore the consideration of the spatial dependence has an important role during simulation of the nonlinear economic models' evolution. Slow processes of the city formation can be connected with irregular and regular temporary oscillations of some spatial system. The centralization of cities was observed as in advanced and developing countries but now we can see the opposite processes of decentralization in some leading states. Such different cities as New York, Stockholm, Paris and Tokyo which we can name "parent state" or "metropolis" represent the examples of complex urban forms [1].

Many models of cities formation in present and future time are suggested in the economical geography. One of the most interesting and promising models is a spatial dynamic approach allowing to us to investigate evolution of cities' internal structure.

In this paper we present results of the computer simulation of the dynamic market model [2]

$$\frac{\partial \lambda}{\partial t} + div(\chi(\lambda)\nabla\lambda) = -z(\lambda), \tag{1}$$

where $\lambda > 0$ is the local cost of goods, $z(\lambda) = \lambda(1-\lambda)$ is the local surplus of the offer, $\chi(\lambda)$ is an arbitrary positive scalar function of λ and the computer region is a regular hexagon.

The boundary conditions correspond to optimal trade conditions between market regions. We consider the structure of the spatial economics (potential function λ) which is structurally unstable. The potential function is given by the following expression

$$\lambda = x_1^3 - 3x_1x_2^2 + \alpha x_1 + \beta x_2, \tag{2}$$

where α is the cost of the fuel and β represents the volume of the transportations of the goods. We investigated two cases: the £rst is when $\alpha = 0, \beta = 0$ and the second corresponds to $\alpha = 0, \beta \neq 0$.

In the £rst case a self-consistent evolution of a con£guration with one centre leads to the con£guration with three centres.

In the second case we consider the con£guration with two connected centers. During the temporary evolution this system transforms into the con£guration with two but disconnected centres. For example such cities as Kanzas-city and Bolonga have the similar structure.

References

1. *W.-B. Zang.* Synergetic Economics. Springer-Verlag Berlin Heidelberg. 1991.
2. *S.V.Bulanov, E.Yu.Echkina, I.N.Inovenkov.* Transformation of structurally unstable con£gurations in Beckmann's model. Abstract. Applications of Physics in Financial Analysis -2. Volume - 24E.

Monte Carlo simulation of biomolecular systems with BIOMCSIM

H. Kamberaj[1] **and V. Helms**[2]

[1]*H. Kamberaj MPI Kennedyallee 70, 60596, Frankfurt, Germany*
[2]*V. Helms MPI Kennedyallee 70, 60596, Frankfurt, Germany*
0049 069 6303 371, 0049 069 6303 256, kamberaj@mpibp-frankfurt-mpg.de

A Monte Carlo program, BIOMCSIM, has been developed for simulating the biomolecular systems.

The computational complexity when simulating systems of high density like solvated proteins is enormous. The BIOMCSIM program seeks to provide these desirable features.

BIOMCSIM implements several biasing techniques to increase the convergence of simulations. As an example of its capabilities we will present results on hydrating an internal water cavity in BPTI. The calculated structural and thermodynamic properties of hydration waters are in excellent agreement with experimental data [1]. Using cavity bias [2] and a novel orientation biasing technique proved to be essential.

The program is modularly organized and implemented using an ANSI C dialect. Current state-of-the-art techniques are implemented for treating long-range forces like Ewald sum [3]. Short-ranged forces are handled using the spherical cutoff.

A parallel version of the program utilizes spatial decomposition of the molecular system and interprocessor communication is implemented by the MPI protocol. Periodic local balancing enables one to make most ef£cient use of the available computer power. The parallel performance will be presented in benchmark applications for molecular systems of variable size.

References

1. Denisov, V. P.; Veny, K.; Peters, J.; Horlein, H. D.; Halle, B. *J. Phys. Chem.* B **1997**, 101, 9380-9389.
2. M. Mezei, *Molecular Physics* **1987**, *Vol.* 61, *No.* 3, 565-582.
3. M. P. Allen, D. J. Tildesley, *Computer simulation of liquids*, Clarendon Press, Oxford, **1987**.

Phase dynamics in current driven Josephson junction networks

Takaaki Kawaguchi

Department of Technology, Faculty of Education, Shimane University
1060 Nishikawatsu, Shimane 690-8504, Japan

+81-852-32-6355, +81-852-32-6355, kawaguch@edu.shimane-u.ac.jp

Josephson junction networks (JJN) are arti£cially fabricated systems in which structures and some physical parameters can be controlled. Furthermore, some kinds of disorder can be arti£cially introduced to JJN using mesoscopic fabrication techniques. Physical properties of JJN have been attracting much attention not only in condensed matter physics but also in the nonlinear science. In particular, in the presence of driving currents, pinned and plastic or elastic ¤ow states of superconducting phases (or vortices) have important effects on several physical properties of JJN. Concerning the nonlinear dynamics and inhomogeneity of the plastic ¤ow state, however, there exist several unsolved complicated problems.

In this study, we investigate the nonlinear dynamics of phases of JJN in magnetic £elds, with emphases on a scaling behavior of plastic ¤ow and geometrical effects of arrays. To describe the dynamics of phases, the resistively shunted junction model is employed, and then the time evolution of phases is calculated using a molecular dynamical method at zero or £nite temperature. Two kinds of network structure are considered, i.e., a one-dimensional ladder (Josephson junction ladder) and a two-dimensional lattice (Josephson junction array), and then positional disorder of superconducting islands is introduced to them.

We evaluate two threshold currents that characterize the boundaries of the plastic ¤ow regime, and analyze them on the basis of the scaling theory of pinning due to random potentials. It is found that, for both structures, the two threshold currents show scaling behaviors characterized by certain scaling exponents. Furthermore, from the analyses of the current-voltage characteristics and the spatial distribution of vortex excitations, it is also found that there exists a close relationship between the inhomogeneity and nonlinearity of the plastic state. Several peculiar features of phase dynamics of JJN are discussed, compared with other related models.[1, 2, 3].

References

1. T. Kawaguchi, Phys. Letters A 251, p. 73 (1999).
2. T. Kawaguchi and H. Matsukawa, Phys. Rev. B **56**, 4261 (1997); *ibid.* **56**, 13932 (1997); *ibid.* **58**, 15877 (1998); *ibid.* **61**, R16366 (2000).
3. T. Kawaguchi and H. Matsukawa, in *Slow Dynamics in Complex Systems*, edited by M. Tokuyama and I. Oppenheim, 699 (AIP, 1999). Prog. Theor. Phys. Suppl. **138**, 580 (2000).

Nonlinear plastic behavior of phase-phase correlations in Josephson junction systems

Takaaki Kawaguchi

Department of Technology, Faculty of Education, Shimane University
1060 Nishikawatsu, Shimane 690-8504, Japan

+81-852-32-6355, +81-852-32-6355, kawaguch@edu.shimane-u.ac.jp

In several condensed matter systems such as vortex lattices in Josephson junction networks (JJN) and charge density waves in low-dimensional conductors, essential features can be described using phase variables. Then it is found that plasticity appears in the phase-phase correlations and plays important roles to determine several static and dynamical properties of these systems.

In this study, by employing two phase models concerning JJN, i.e., the resistively shunted junction model and the random £eld XY model, we investigate nonlinear plastic behaviors of phase-phase correlations. Using numerical simulations based on a molecular dynamics method, we calculate the time evolution of phases and then the phase correlations in the presence of driving force or current. We focus on two plastic effects: plastic depinning and plastic ¤ow. Effects of many degrees of freedom of systems and collective coupling between phases lead to complicated nonlinear behaviors in the plastic depinning and ¤ow. Using some theoretical concepts of phase transitions and scaling analyses, we clarify the relationship between the nonlinearity and the plasticity of phase-phase correlations in JJN and discuss also the relationship with the dynamics of other related phase and particle models.

References

1. T. Kawaguchi, Phys. Letters A 251, p. 73 (1999).
2. T. Kawaguchi and H. Matsukawa, Phys. Rev. B **56**, 4261 (1997); *ibid.* **56**, 13932 (1997); *ibid.* **58**, 15877 (1998); *ibid.* **61**, R16366 (2000).
3. T. Kawaguchi and H. Matsukawa, Prog. Theor. Phys. Suppl. **138**, 580 (2000).

Statistical mechanics of the three-state neural network: From the mutual information to the hamiltonian

Elka Korutcheva[1] **and David Dominguez**[2]

[1]*Dep. Fisica Fundamental, UNED, c/Senda del Rey No 9, 28080 Madrid, Spain*
[2] *Fac. of Informatics, UNiversidad Complutense de Madrid, 28040 Madrid, Spain*
tel. 0034-1-398-7143, fax number 0034-91-398-6697, e-mail address: elka@£sfun.uned.es

In the present work we propose a new method, based on the direct calculation of the mutual information I in the mean-£eld approximation, to obtain a Hamiltonian which maximizes I within a large range of values for the activity of the three-state neural network. The last is de£ned by the use of a set of $\mu = 1, ..., p\ ternary$ patterns, $\{\xi_i^\mu \in \{0, \pm 1\},\ i = 1, ..., N\}$, which are independent random variables given by the probability distribution $p(\xi_i^\mu) = a\delta(|\xi_i^\mu|^2 - 1) + (1 - a)\delta(\xi_i^\mu)$, a being the $activity$ of the patterns. The neuron states are also three-state variables, $\sigma_i \in \{0, \pm 1\},\ i = 1, ..., N$ and they are coupled to the other neurons through synaptic interaction, the speci£c form of which are of the Hebbian type.

It has been noted[1] that the order parameters, needed to calculate the mutual information, are the thermodynamic limits of the standard overlap of the μth pattern with the neuron-state, the neural activity, and the so called $activity$-$overlap$, which is a measure of the sites where the patterns and the neurons are both active. An expansion of I on the overlap and the activity-overlap around their values for the case of neurons almost independent on the patterns, gives an expression for a Hamiltonian which optimizes the retrieval properties of this system. This Hamiltonian has the form of a disordered Blume-Emery-Grif£ths model [2].

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j - \frac{1}{2}\sum_{i,j} K_{ij}\sigma_i^2\sigma_j^2 \tag{1}$$

with random interactions $J_{ij} = \frac{1}{a^2 N}\sum_{\mu=1}^{p} \xi_i^\mu \xi_j^\mu$ and $K_{ij} = \frac{1}{N}\sum_{\mu=1}^{p} \eta_i^\mu \eta_j^\mu$.

The dynamics corresponding to this Hamiltonian in the extreme diluted version is analyzed [3]. As a special characteristic of such network, we see that information can survive even if no overlap is present. Hence the basin of attraction of the patterns and the retrieval capacity is much larger than for the Hop£eld network and the phase diagram shows a very complex behavior. The comparison with the Self-Control Neural Network model (SCNN)[1] permits to obtain the main characteristics of the present model: when the activity is near $a = 2/3$, corresponding to the case of uniform ternary patterns, the model improves the information, compared with the SCNN model, while for small activities, ($a \sim .03$), it performs worst, giving a smaller value for the information. Improvement of the information content by increasing the noise, effect similar to the stochastic resonance, is also observed for activities $a < 2/3$, which is in agreement with results for real neurons.

References

1. D.Dominguez and D.Bollé, Phys. Rev. Lett. **80**, 2961 (1998).
2. M.Blume, V.J.Emery and R.B.Grif£th, Phys.Rev.A, **4**, 1071 (1971).
3. B. Derrida, E. Gardner, and A. Zippelius, Europhys. Lett. **4**, 167 (1987).

Friction mechanisms between polymer bearing surfaces

T. Kreer, M. H. Müser, and K. Binder

Institut für Physik, WA 331; Johannes Gutenberg-Universität
55099 Mainz; Germany
Tel: [++49] 6131 392-3643, Fax: [++49] 6131 392-5441, e-mail:
tkreer@plato.physik.uni-mainz.de

Polymers con£ned by surfaces modify friction forces between these surfaces and thus have important applications as lubricants. We focus on the aspects important for nanotribology [1], and are particularly interested in understanding the implications of boundary conditions such as grafting [2] and solvent quality on frictional properties. This is done by means of classical molecular dynamics simulations.

By simple modi£cations of the interactions between the polymer endgroups and the walls, we are able to anchor the polymers at the walls. This allows us to study the differences in the tribological behaviour between adsorbed and grafted polymers without changing the chemical nature of the polymer. Furthermore, it is possible to vary the solvent quality. Solvent molecules are not treated explicitely but indirectly in terms of a Langevin thermostat. The quality of the solvent is taken into account by changing the effective interactions between monomers [4]. In addition, we vary quantities like shear velocity, distance between the walls, grafting density, and solvent viscosity. No study has appeared as yet which addresses systematically the in¤uence of grafted vs. adsorbed and good solvent vs. poor solvent on the tribological properties of polymer bearing surfaces.

In the good solvent case, shear thinning is observed that can be attributed to an orientation of the radius of gyration along the sliding direction. This effect is particularly large for grafted polymers, resulting in small friction coef£cients at large sliding velocities. In this case, the shear stresses are mainly determined by the degree of interpenetration of the brushes. For adsorbed chains, the dissipation can be described in terms of a Navier-Stokes equation. Both, adsorbed and grafted polymers show a proportionality between shear stress and normal pressure. The proportionality constant increases with increasing velocity for adsorbed chains and decreases in the case of grafted chains.

References

1. M. O. Robbins and M. H. Müser, *Computer Simulations of friction, lubrication and wear*, in *Modern Tribology Handbook I*, pp. 717-765, Ed. B. Bhushan (CRC Press, Boca Raton, FL, 2001); cond-mat/0001056.
2. J. Klein, Annu. Rev. Mater. Sci. **26**, 581 (1996)
3. G.S. Grest, Phys. Rev. Lett. **76**, 4979 (1996)
4. G.S. Grest, M. Murat, *Computer Simulations of tethered chains*, in *Monte Carlo and Molecular Dynamics Simulations in Polymer Science*, pp. 476-578, Ed. K. Binder (Oxford University Press, NY, 1995)

A Monte Carlo simulation for multi-dimensional traf£c dispersion model

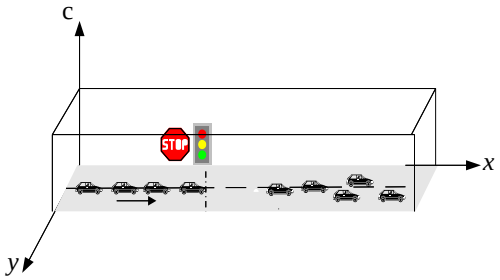
Hsun-Jung Cho, Fang-Yu Lai, and Hsiao-Mei Lu

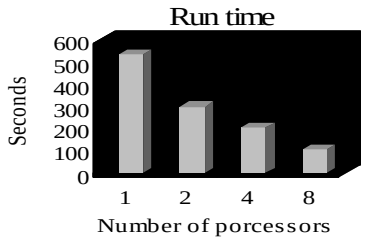
Dept. of Transportation Engineering and Management,
National Chiao Tung University, Hsinchu, Taiwan
Corresponding address: P. O. Box 25-90, Hsincu 300, Taiwan
Email: fylai.tem89g@nctu.edu.tw and Tel. 886-3-5712121 ext: 57237

A traf£c dispersion model for congested road was proposed by Baker [1]; however, this model is a two-dimensional model without source density. It has limits more than single lane for traf£c phenomena. In order to apply more realistic road, a novel three-dimensional traf£c dispersion model is presented here. In general, traf£c phenomena of speci£c region where need be analysed and studied, for example, intersection, ramp, and peak road etc. Compared with £nite difference method, Monte Carlo method [2] can calculate the solution of a speci£c point or region without completing all domain computation. Therefore, it is more suitable for these traf£c problems. Since the Monte Carlo method is a time consuming methodology. With this new model, traf£c ¤ow simulations using a message passing interface is implemented. As a result, the run time is reduced signi£cantly.

In this work we adapted vector £eld methodology to analyse the traf£c ¤ow property, and to establish a model for traf£c ¤ow motion behavior using divergence theorem. Furthermore, using the potential theory studies by Sheppard [3], the relationship between traf£c potential and traf£c ¤ow was well constructed. Then, a novel traf£c dispersion model, as $\frac{\partial^2 \phi}{\partial t^2} + \nabla^2 \phi = k(x, y, c, t)$, where x, y are spatial dependent variables, t is time, c is traf£c capacity, k is traf£c density, and ϕ is traf£c potential, is presented (Left Fig.). We £nd out the numerical solution of traf£c dispersion model by the parallel Monte Carlo method [4]. This method is ef£ciently and accurately demonstrated in speci£c traf£c phenomena or regions.

Considering a simple two-dimensional model problem which is a mixed type problem, we simulated by a parallel Monte Carlo method. In the process of computing, we execute the proposed model with one, two, four, and eight computers respectively. The right Fig. as below shows the comparison results. It is conducive to analyze real time traf£c information. Therefore, the simulation of three-dimensional traf£c dispersion model by parallel Monte Carlo method should be done in the futher work. An ef£cient Monte Carlo method for speci£c traf£c region is proposed in this work.





References

1. Baker, Robert G. V., Trans. Res. B **15** 319 (1981).
2. Matthew N. O. S., Ajose S. O., and Zhibao F., IEEE Trans. Micro. Theo. Tech. **42** 661 (1994).
3. Sheppard, E. S., Ann. Assoc. Amer. Geog. **69** 438 (1979).
4. Johnston, C. M. and Chronopoulos, A. T., Parallel and Distributed Processing 688 (1999).

Parallel traf£c ¤ow simulation using semi-viscous model

Fang-Yu Lai[1], **Hsiao-Mei Lu**[1], **Shui Sheng Lin**[2], **and Hsun-Jung Cho**[1]

[1] *Department of Transportation Engineering and Management, National Chiao Tung University, Hsinchu 300, Taiwan*

[2] *Department of Applied Mathematics, National Chiao Tung University, Hsinchu 300, Taiwan*

Corresponding address: P. O. Box 25-90, Hsincu 300, Taiwan; Email: fylai.tem89g@nctu.edu.tw and Tel. 886-3-5712121 ext: 57237

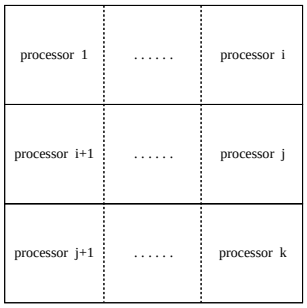
Macroscopic traf£c ¤ow continuum models based on ¤ow, density and speed have been used in studying the behavior of the roadway. These models involve partial differential equation with suitable boundary conditions, which describe various traf£c phenomena and road conditions. And many numerical methods have been developed to compute the solution of traf£c ¤ow continuum models. In this work, we solve high-order continuum traf£c ¤ow continuum models coupling with momentum equation on a cluster computing environment. This model is a semi-viscous model (SVM) [1, 2]. It considers acceleration and inertia effects and describes accurately non-equilibrium traf£c ¤ow dynamics.

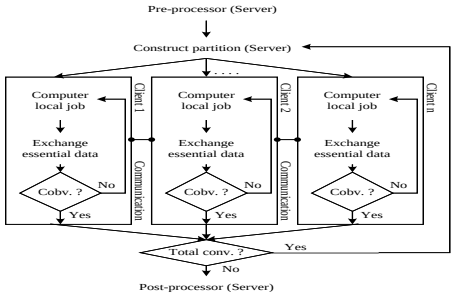
$$\frac{du}{dt} = \frac{1}{T}\left[u_f(x) - u\right] - \nu k^{\beta}\frac{\partial k}{\partial x} \qquad (1)$$

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} \qquad (2)$$

$$T = t_0\left(1 + \frac{rk}{k_j - rk}\right) \qquad (3)$$

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{E}}{\partial x} = \vec{Z} \qquad (4)$$





Firstly, we apply an implicit method to discretize the PDE (1)-(4). The implicit Euler method applied to the nonlinear PDEs generates a nonlinear system of algebraic equations. This nonlinear system is then linearized with Newton's method. This procedure leads to a linear system to be solved. Therefore, we solve the linear system follows a parallel approach proposed by Li, et al. [3, 4]. A geometric static graph partitioning method in x-y axis (see middle Fig.) is applied to partition the domain and the number of vertices are also assigned to each processor. The right Fig. is the parallel program organization [4]. The pre-processor performs several tasks, and one of the tasks is to prepare the input data required one of the tasks is to prepare the input data required for each parallel processor. The applied approach here has been implemented and test for various traf£c ¤ow successfully.

References

1. Chronopoulos, A. T., and Wang, G., Paral. Comp. **22** 1965 (1997).
2. Mathews, H., Numerical methods for computer science, engineering, and mathematics, Prentice-Hall (1987).
3. Li, Y., SIAM Proc. 10th Paral. Proces. Sci. Comp., 685 (2001).
4. Mastorakis N., Recent Advances in Applied and Theoretical Mathematics, WSES Press. (2000).

Numerical methods for multilane traf£c ¤ow simulation

Hsun-Jung Cho and Chi-Wei Lin

Dept. of Transportation Engineering and Management,
National Chiao Tung University, Hsinchu, Taiwan
Corresponding address: Dept. of Transportation Engineering and Management,
1001 Ta Hsueh Road, Hsincu 300, Taiwan
Email: cwlin.tem89g@nctu.edu.tw and Tel. 886-3-5712121 ext: 57237

The traf£c ¤ow models are conferred by the LWR model in general, but the LWR model can just be use to analyze the traf£c conditions on a single lane road of freeways. The LWR model assumed that following vehicles react instantaneously as leading vehicles change their behavior, but it can't describe the diffusion and overtaking of crowed traf£c ¤ow, and clearly this is not conformed to actuality traf£c situation. Therefore, this paper extends the traf£c ¤ow analysis model to analyze traf£c phenomena, such as multilane conditions and diffusion behaviors of crowed traf£c.

The model developed in this paper is based on the assumption of conservation law of vehicles on one-dimension with interchange between road lanes. The proposed model is a system one-dimensional PDE, so as to describe a multilane freeway. In addition, several numerical examples are employed to illustrate our model. Also, the comparison of the LWR model and our model is made herein.

The model of we want to describe is as following

$$\begin{aligned} \frac{\partial u_1}{\partial t} + \frac{\partial u_1}{\partial x} + f1(u_1, u_2) &= 0 \\ \frac{\partial u_2}{\partial t} + \frac{\partial u_2}{\partial x} + f2(u_1, u_2) &= 0 \end{aligned}$$

Based on the model above, we use £nite volume method [1][2]to compute the numerical solutions we want to know. Besides, we use parallel computing to compute our problem[2, 3], and the initial result we get is shown that the result is conformed to real traf£c condition, and the compute time is much shorter than normal computation.

This paper tries to develop a physical based traf£c ¤ow model, which can describe a multilane freeway with entrances and exits. The average and diffusion behavior are considered in the model. The model can be applied to predict and control traf£c ¤ow on freeway, such as providing real-time traf£c information and ramp metering, it can be a fundamental research of developing ITS.

References

1. Greenshields, C. J.; Weller, H. G.; Computer Modeling & Simulation in Engineering, Aug99, Vol. 4 Issue 3, p213-p219
2. Liu, Guoqing; Lyrintzis, Anastasios S.; Journal of Transportation Engineering, Nov/Dec97, Vol. 123 Issue 6, p503-p14
3. Hillis, W. Daniels; Bopghosian, Bruce M.; Science, 8/13/93, Vol. 261 Issue 5123, p856-p864

Numerical analysis of a self-consistent dynamic traf£c ¤ow model

Hsun-Jung Cho[1] **and Shih-Ching Lo**[2]

[12]*Department of Transportation Engineering and Management, National Chiao Tung University, 30010, Hsinchu, Taiwan*

[1]*Phone/Fax: +886-3-5710657, hjcho@cc.nctu.edu.tw*

Dynamic traf£c ¤ow theory is a new science, especially in the worldwide trend of intelligent transportation system (ITS), forecasting and controlling dynamic traf£c phenomena becomes more important. This study proposes a macroscopic dynamic traf£c ¤ow model which is based on the LWR model [1], car-following theory[2] and the second-order kinetic model[3]. The combination of three kinds of model improves the macroscopic models, which can hardly analyze the interaction between vehicular behavior. Thus a self-consistent model, which includes microscopic and macroscopic behaviors is proposed herein. In this study, we discuss the steady state case. Thus, our model is illustrated as follows:

$$\nabla_x \cdot (-k\mu\nabla_x\phi - v\nabla_x k) = 0 \tag{1}$$

$$div \cdot (grad\phi) = -\frac{k}{\epsilon} \tag{2}$$

$$k = \frac{K_0}{\Theta_e}\left[\zeta \exp\left(\frac{-\phi}{\Theta_e}\right)\right] \tag{3}$$

Eq.(1) is the steady state LWR model which couple with steady steady state motion equation, where k is ¤ow density and u is velocity. μ denotes $\frac{\lambda}{\tau_m}$, where τ_m denotes relaxation time of velocity and λ denotes interaction parameter. v is diffusion coef£cient, which denotes $\mu\Theta_e$. Eq.(2) is derived from car-following theory describes the interaction between vehicles, where ϵ is an adjust parameter and $grad\phi$ denotes traf£c £eld. Eq.(3) is a state equation, which is derived from the equilibrium state. Θ_e denotes the equilibrium velocity variance, ζ denotes the boundary condition and K_0.denotes the essential ¤ow density. The model is derived by Cho and Lo[4].

Since the model presented herein is a nonlinear model, we introduce a monotone iterative method to solve it. The existence and uniqueness of the solution has been proven in [4]. The monotone iterative method we applied here can converge £rst than other £nite difference method combined with the Newton's method. Also, the method can converge whatever initial guess is chosen. The advantages of th enumerical method may make real-time computing of dynamical traf£c ¤ow model possible. Another importance in this study is discussing traf£c ¤ow in two-dimensional space, which can describe the diffusion effect on traf£c without complicated behaviorial analysis.

This study proposes a self-consistent model, which prevents the inconsistency of assumptions in a macroscopic model. Also, in our macroscopic model described more traf£c behavior and can be extened unsteady model or advanced models. The theoritical discussion of unsteady state numerical method and the existence and uniqueness are left for further resarches.

References

1. Lighthill, M. J., and G. B Whitham, On Kinematics Waves II. A Theory of Traf£c Flow on Long Crowded Road , London, Proceedings Royal Society, A229, pp.317-345, (1955).
2. Gazis, D. C., R. Herman, and R. W. Rothery, Nonlinear Follow-The-Leader Models Of Traf£c Flow, Operations Research, Vol. 9, pp.545-567,(1960).
3. Payne, H. J, FREFLO: A Macroscopic Simulation Model of Freeway Traf£c. Transportation Research Record 722, pp. 68-77, (1979).
4. Cho, H. J., and S. C. Lo, A self-consistent dynamic traf£c ¤ow model part I: modeling and analysis, (temporary accepted in Urban Transport 2001, Lemnos, Greece, 2001).

Modeling and comparison of different vehicular ¤ow processes

Hsun-Jung Cho[1] **and Shih-Ching Lo**[2]

[12]*Department of Transportation Engineering and Management, National Chiao Tung University, 30010, Hsinchu, Taiwan*

[1]*Phone/Fax: +886-3-5710657, hjcho@cc.nctu.edu.tw*

In the trend of developing intelligent transportation system(ITS), the requirement of traf£c ¤ow theory evolves from static to dynamic so as to forecast and control dynamic traf£c phenomena. However, discussing dynamic vehicular traf£c in detail complicated behavior are found. This study analyzes different ¤ow processes £rst and derives mathematical models of them.The vehicular ¤ow processes consider herein includes (1) velocity variance of a vehicle is larger enough to pass through a platoon, (2) velocity variance of a vehicles is not so large but it has chance to pass through a platoon, (3) a vehicle catches a platoon and is recombined by the platoon. To model these phenomena, drift, pass, and diffusion processes are discussed. By these processes, different formula of ¤ow are obtained.

After deriving ¤ow equations, we couple these equations with a macroscopic dynamic traf£c ¤ow system, which is based on the LWR model [1], car-following theory [2] and the second-order kinetic model [3]. The system chosen herein includes microscopic and macroscopic behaviors . In this study, we discuss the steady state cases. Let the ¤ow equations denote by $Q(k(x,t),u)$. Thus, our model is illustrated as follows:

$$\nabla_x \cdot (Q) = 0 \tag{1}$$

$$div \cdot (grad\phi) = -\frac{k}{\epsilon} \tag{2}$$

$$k = K_0 \left[\zeta \exp\left(\frac{-\phi}{\Theta_e}\right)\right] \tag{3}$$

Eq.(1) is the steady state LWR model which couple with steady steady state motion equation, where k is ¤ow density and u is velocity. Eq.(2) is derived from car-following theory describes the interaction between vehicles, where ϵ is an adjust parameter and $grad\phi$ denotes traf£c £eld. Eq.(3) is a state equation, which is derived from the equilibrium state. Θ_e denotes the equilibrium velocity variance, ζ denotes the boundary condition and K_0.denotes the essential ¤ow density. The model is derived by Cho and Lo [4]. By numerical analyses, the results of different ¤ow types are shown and compared. Also, what kind of traf£c condition is described by each ¤ow equation is mentioned so as to make dynamic ¤ow simulation system more realized.

This study proposes a family of ¤ow equation and couples them with a dynamic traf£c ¤ow system to construct a consistent model. By the numerical comparison, there exists difference between ¤ow equations. Therefore, a different ¤ow equation should be considered as traf£c ¤ow condition is different.

References

1. Lighthill, M. J., and G. B Whitham, On Kinematics Waves II. A Theory of Traf£c Flow on Long Crowded Road , London, Proceedings Royal Society, A229, pp.317-345, (1955).
2. Gazis, D. et. al., Nonlinear Follow-The-Leader Models Of Traf£c Flow, Operations Research, Vol. 9, pp.545-567,(1960).
3. Payne, H. J, FREFLO: A Macroscopic Simulation Model of Freeway Traf£c. Transportation Research Record 722, pp. 68-77, (1979).
4. Cho, H. J., and S. C. Lo, A self-consistent dynamic traf£c ¤ow model part I: modeling and analysis, will present in Urban Transport 2001, Lemnos, Greece, 2001.

Effect of time slowing in biological ageing

M.S.Magdoń-Maksymowicz[1], M.Sitarz[2], M.Bubak[3,4], A.Z.Maksymowicz[2] and J.Szewczyk[1]

[1]*Department Mathematical Statistics, Agricultural University, al.Mickiewicza 21, 31-120 Cracow, Poland*

[2]*Faculty of Physics and Nuclear Techniques, University of Mining and Metallurgy, al.Mickiewicza 30, 30-059 Cracow, Poland*

[3]*Institute of Computer Science, University of Mining and Metallurgy, al.Mickiewicza 30, 30-059 Cracow, Poland*

[4]*Academic Computer Centre CYFRONET, ul.Nawojki 11, 30-950 Cracow, Poland*

+(4812)6321620, extn.261 fax(4812)6336265, rrmagdon@cyf-kr.edu.pl

The essence of the Penna model [1], applied in our simulations, of the population evolution is the fact that it also accounts for the possible death due to too many active 'bad' mutations μ, above a threshold value T. In the Penna model, mutations are essentially inherited from parents', yet only a fraction becomes activated at age a of an individual. The idea is that we scan the individual's genome string, inherited at birth, bit by bit, and count the bad mutations (if bit is one '1') up to position proportional to age a. The Penna model is easy for modi£cations for its very much open structure, and may withstand many possible and sensible modi£cations of the life game rules which are greatly simpli£ed in the standard version. In¤uence of age on fertility and birth rate [2, 3] is one of the great many already explored versions, fully discussed in [4]. This presentation is another attempt to improve classical model for which, when time goes on, proportional to the time fraction of genome is read out and the encoded bad mutations become activated. However, it is claimed that the biological clock runs faster when we are young. In this paper we consider suitable modi£cation of the model rules. We assume faster rate of genome learning at £rst, 4 bits read in per 'year', slowing down at mature age (2bits which is an average applied to the classical Penna model, for reference), and further slowing down to 1bit/year when becoming old. Main conclusion from the simulation is that the overall age a structure of the populations $n(a)$ is merely affected, yet there is a serious change in the distribution of active mutations for any age a group $n(\mu, a)$, $\mu = 0..T-1$. Therefore we may expect that the statistics of the health condition in society for different age a groups may help to con£rm or deny the tendency clearly seen in the simulation: assumed slowing down rhythm of the biological clock results in healthier young population as compared with classical Penna model, and for middle age and older population the two approaches seem to reproduce similar distribution. Before any attempt is made to compare simulation against real population distribution, we must extract from the overall statistics the genetic death which is the subject of the model. Simulations were done on HP EXEMPLAR machine at the Academic Computer Centre CYFRONET on population of about $n = 10^6$.

References

1. T. J. P. Penna, A Bit-String Model for Biological Ageing, *J. Stat. Phys.* **78** (1995) 1629.
2. R. C. Desai, F. James and E. Lui, Biological Ageing: a Bit-string Model with Fertility and Fecundity, *Theory in Biosciences* **118** (1999) 98.
3. M. S. Magdoń, A. Z. Maksymowicz and K. Kułakowski, Biological Ageing with Birth Rate Controlled by Mutations in the Penna Model, *Theory in Biosciences* **119** (2000) 139.
4. S. Moss de Oliveira, P. M. C. de Oliveira and D. Stauffer, *Evolution, Money, War and Computers*, Teubner, Stuttgart-Leipzig, 1999.

Shear stress in lattice Boltzmann simulations

A. M. Artoli[1], D. Kandhai[2], H. G. Hoefsloot[3], A. G. Hoekstra[1] and P. M. A. Sloot[1]

[1] *Section Computational Science, Institute Informatica, Faculty of Science, University of Amsterdam , The Netherlands*

[2] *Kramers Laboratorium voor Fysische Technologie, Faculty of Applied Sciences, Delft, The Netherlands*

[3] *Department of Chemical Engineering, Faculty of Science, University of Amsterdam, Amsterdam, The Netherlands*

Email: artoli@science.uva.nl

Shear stress plays a dominant role in biomedical diseases related to blood ¤ow problems. Conventionally, it is calculated from the gradients of the velocity pro£les obtained from experimental or simulation models. Recently, the lattice-Boltzmann method (LBM) has attracted much attention in simulation of complex ¤uid ¤ow problems (such as multiphase ¤ows and ¤ow in complex geometry) as an alternative computational method to study transport phenomena in ¤uids [1]. It also offers inherent parallelism and straightforward implementation. Furthermore, with LBM it is possible to compute the local components of the stress tensor of moving ¤uids without a need to estimate the velocity gradients from the velocity pro£les. The momentum rate tensor, which is related to the shear stress, is computed during the collision process from the non-equilibrium part of the distribution functions [2].

Here, the theory of obtaining the hydrodynamic stress tensor components from the lattice Boltzmann Method is revisited and validated with numerical simulations for three two-dimensional benchmarks: a channel ¤ow, a Couette ¤ow with injection and a symmetric bifurcation, for a range of Reynolds numbers using the bounce-back boundary condition, the equilibrium distributions boundary conditions and the velocity boundary conditions proposed by Zou and He [3]. The simulation results are compared to theory for the £rst two benchmarks and to a similar £nite volume method (FVM) simulation for the symmetric bifurcation, all showing excellent agreement. The accuracy of obtaining the stress tensor from the LBM follows the accuracy of the boundary condition. We have compared the results with the analytic solution derived from the analytic lattice BGK solution for the velocity £eld as obtained by He *et. al.*[4] and the Navier-Stokes solution for the shear stress in the Couette ¤ow with injection. In the case of the symmetric bifurcation, we £nd excellent agreement between the LBM and FVM results. To conclude, the method proved to be successful in accurately computing the stress tensor in complex geometry.

References

1. S. Hou, Q. Zou, S. Chen, G. Doolen and A. C. Cogley. Simulation of cavity ¤ow by the lattice-Boltzmann method, *J.Comp. Phys.* **118**, 118 (1995).
2. A. J. C. Ladd, Numerical simulations of particulate suspensions via a discretized Boltzmann equation. Part I. Theoretical foundation, *J. Fluid Mech.* **271** 285 (1994).
3. Q. Zou and X. He, On pressure and velocity boundary conditions for the lattice Boltzmann BGK model, *Phys. Fluids* **9**, 1591 (1997).
4. X. He, Q. Zou, L. S. Luo, and M. Dembo. Analytical solutions of simple ¤ow and analysis of non-slip boundary conditions for the lattice Boltzmann BGK model, *J. of Stat. Phys.*, **87**, 115 (1996).

Computing sensitivities of the electrostatic potential by automatic differentiation

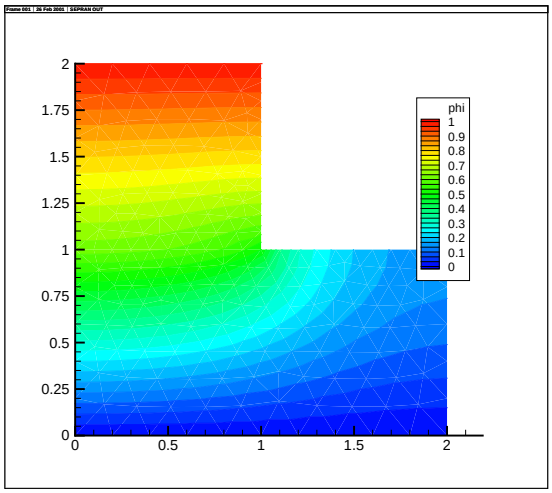
C. H. Bischof, H. M. Bücker, A. Rasch, and J. W. Risch

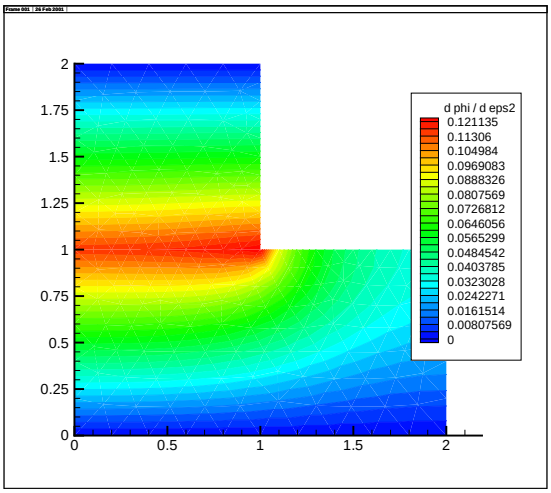
Institute for Scienti£c Computing, Aachen University of Technology,
D–52056 Aachen, Germany

phone: +49-241-804913, fax: +49-241-8888241, buecker@sc.rwth-aachen.de

To determine pro£table avenues for improving a design of a computer model, it is useful to assess the rate of change of the model output that is implied by changing certain model inputs. Derivatives are one way to implement such a sensitivity analysis. Traditionally, divided differences are employed in this context to approximate derivatives, leading to results of dubious quality at often great computational expense. Automatic differentiation [1], in contrast, is an alternative for the evaluation of derivatives providing guaranteed accuracy, ease of use, and computational ef£ciency.

We consider the solution of an electrostatic potential problem in an L-shaped region consisting of two regions with media of dielectric permeability ϵ_1 and ϵ_2. Given a computer program to numerically compute the electrostatic potential ϕ, we are interested in obtaining derivatives of ϕ with respect to ϵ_1 and ϵ_2. Using an actual implementation based on the general purpose £nite element package SEPRAN [2] developed at Delft University of Technology, we compute the sensitivities $\partial\phi/\partial\epsilon_i$ using automatic differentiation. The potential ϕ and its sensitivities $\partial\phi/\partial\epsilon_2$ are given as follows:





The ADIFOR tool [3] is used to transform the original SEPRAN code, consisting of approximately 400,000 lines of Fortran 77, into a new code containing additional statements for the computation of the sensitivities. Comparisons with a divided difference approach are reported demonstrating not only the improved performance of automatic differentiation but also its superior numerical accuracy. We also point out that, beyond this particular application from electrostatics, the functionality of automatic differentiation allows the sensitivity analysis of a wide range of potential applications from computational physics in a similarly easy fashion.

References

1. A. Griewank. *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation.* SIAM, Philadelphia, 2000.
2. G. Segal. *SEPRAN Users Manual.* Ingenieursbureau Sepra, Leidschendam, NL, 1993.
3. C. Bischof, A. Carle, P. Khademi, and A. Mauer. ADIFOR 2.0: Automatic differentiation of Fortran 77 programs. *IEEE Computational Science & Engineering*, 3(3):18–32, 1996.

Mapping cellular automata applications into cellular automata networks ones

C.R. Calidonna[1], **S. di Gregorio**[2], **M. Mango Furnari**[1]

[1]*Istit. di Cibernetica (CNR), Via Toiano 6, I–80072,Arco Felice (NA) Italy*
[2]*Dep. of Mathematics,Univ. of Calabria,Arcavacata,I–87036 Rende(CS)Italy*

tel.+39/+818534227, fax+39/+815267654, {C.Calidonna,mf}@cib.na.cnr.it
tel. +39/+984930010, fax+39/+984401186, toti.dig@unical.it

Cellular Automata (*CA*) proved to be a suitable model to simulate complex phenomena, especially when involving the composition of processes of different nature, e.g. physical, chemical, biological [1]. CA are based on a regular spatial grid of cells, each one embedding an identical *Finite Automata* (*FA*), whose input is the states of neighboring cells; FA have an identical transition function applied simultaneously to each cell. The neighboring is de£ned in terms of a spatial pattern, invariant in time and space. At the time $t = 0$, FA are in an arbitrary state and the CA evolves changing the state of all the FA simultaneously at discrete time steps, according to the FA transition function. Several programming environment and CA programming models were proposed and their descriptions are reported in [2]. The CA model proposed in this paper, called the *Cellular Automata Network* (*CAN*) model [3], extends the classical CA model. A CAN application can be derived applying a reduction process in constructing models for several complex physical phenomena. In a such reduction process, the overall phenomenon is decomposed in phenomenological components; each component has to be speci£ed by a proper computational procedure and interactions among the components (information exchange and composition) must be de£ned. The CAN approach consists on substituting the single automaton into the cell with a network (an acyclic oriented graph) of automata, where a phenomenological component is computed by a node of the graph. The CAN model provides the possibility to simulate a two–level evolutionary process in which the local cellular interaction rules evolve together with cellular automata connections. We stress some points concerning the previously described methodological approach to model or to transform CA applications into CAN model components. These aspects hold especially on dealing with macroscopic phenomena characterised by transfers of ¤ows from a cell to its neighbouring. The state of the cell can be individuated as a set of subtates (a substate individuates usually a physical characteristics of space portion corresponding to a cell); in the CAN model, each substate is updated in a node of the automata network; When a good precision level must be reached, the ¤ow computation can be time wasting in standard CA, as each cell must compute not only own out¤ows, but also the in¤ows (that are out¤ows of neighbouring cells); while in the CAN context this problem is solved easily because all the information can be opportunely transferred to the node where the £nal computation will be performed. Furthermore, some bene£ts can derive form this new point of view, because some computational advantages arise in individuate coupled and uncoupled components. In fact, for a class of geological and ¤uid dynamics problems, more speci£cally for the Sarno landslide simulation [4], we obtained a signi£cant drop of the computational costs on expressing them in terms of CAN model. In this paper we describe some advantages arise on applying CAN model to a class of geological and ¤uid dynamics problems. We expect that a similar computational gain happens also for models involving mixed phenomena of biological, physical, chemical nature [1].

References

1. Di Gregorio, S., Serra, R.: An empirical method for modelling and simulating some complex macroscopic phenomena by cellular automata, Future Generation Computer Systems 16, pp. 259–271, 1999.
2. Worsch, T.: Programming Environments for Cellular Automata, Proc. of ACRI '96, Springer, pp. 3–12
3. Carotenuto, L., Mele, F., Mango Furnari, M., Napolitano, R.: PECANS: A Parallel Environment for Cellular Automata Modeling. Complex Systems 10, Complex Systems Publications 1996, pp. 23–41
4. D'Ambrosio, D., Di Gregorio, S., Iovine, G., Lupiano, V., Rongo, R., Spataro, W.: First simulations of the sarno debris ¤ows through cellular automata modelling, to appear in Geomorphology after revision.

An ef£cient data compression method for the Davidson subspace diagonalization scheme - New possibilities in computational science

Holger Dachsel

John von Neumann Institute for Computing
Central Institute for Applied Mathematics, Research Centre Jülich
(+49) 2461 61 6569, (+49) 2461 61 6656, h.dachsel@fz-juelich.de

The Davidson Subspace Diagonalization Scheme [1, 2, 3] is an important method to compute the lowest eigenvalues and the corresponding eigenvectors for high dimensional diagonal dominant matrices. It became a standard method in computational physics and chemistry. The idea is to approximate the eigenvectors by linear combinations of expansion vectors. The processing of large amounts of data which arise in high dimensional sparse eigenvalue problems has always been a severe bottleneck for the Davidson method. On the other hand the expansion and product vectors contain information which does not contribute to the requested accuracy of the eigenvalues and eigenvectors.
A highly ¤exible and very ef£cient data compression method [4] for both, expansion and product vectors is presented within the Davidson diagonalization method. The data compression method is based on an error analysis of the eigenvalues in terms of the expansion and product vectors and on compression schemes for representing ¤oating point numbers with a variable length of the mantissa.
Depending on the sparsity of the eigenvalue matrix saving factors between 10 and 100 can be achieved. Because the data is always processed in compressed form the interprocess communication and the access to secondary storage is dramatically reduced.
This new approach allows to solve diagonal dominant eigenvalue problems with a dimension up to 10^{11} on massively parallel architectures.

References

1. E. R. Davidson, J. Comp. Phys. **17**, 84 (1975).
2. R. Shepard, J. Comp. Chem. **11**, 45 (1990).
3. R. J. Harrison, and N. C. Handy, Chem. Phys. Letters **96**, 386 (1983).
4. H. Dachsel, and H. Lischka, Theor. Chim. Acta **92**, 339 (1995).

Analytical Hartree-Fock gradients for periodic systems

Klaus Doll
Institut fuer Mathematische Physik, TU Braunschweig, Mendelssohnstrasse 3,
D-38106 Braunschweig
k.doll@tu-bs.de

Electronic structure calculations for molecules and solids are nowadays routinely done with a wide variety of codes and methods. One of the main targets is the determination of the equilibrium structure. This can be greatly facilitated with the availability of analytical gradients. As a rule of thumb, the numerical effort can be reduced by a factor N proportional to the number of parameters to be optimized.

Gaussian basis sets have become the standard tool in quantum chemistry and nearly all molecular codes rely on this choice of basis sets. These basis functions are centered at the positions of the nuclei. All the contributions to the total energy such as kinetic energy, nuclear attraction and electron-electron repulsion depend on integrals over the basis functions. Therefore, when computing forces on the nuclei, additional derivatives have to be computed because of this dependence of the basis functions on the nuclear coordinates. These contributions to the gradients are the Pulay forces [1].

Most codes for solids are based on plane-wave basis sets. In contrast to these codes, the CRYSTAL [2] code uses Gaussian basis sets in close analogy to molecular codes. The total energy part has been optimized over two decades and the present code is able to compute total energy, band structure etc for systems with any periodicity (i.e. molecules, polymers, slabs and solids). This can be done at the Hartree-Fock or density functional level, and also hybrid functionals which have recently become fashionable (such as B3LYP, for example) can be used.

As the total energy part has become numerically stable and reliable, the lack of analytical gradients has become one of the bottlenecks of this code. The target of this contribution is therefore to summarize the £rst implementation of analytical gradients in the CRYSTAL code.

The £rst step has been the generation of all the derivatives of the integrals, in close analogy to the molecular case. The integrals are evaluated with the McMurchie-Davidson algorithm[3], and new recursion relations have been implemented to generate the derivatives. The second step is the mixing of the derivatives with the density matrix and the calculation of the energy-weighted density matrix, again similar to the molecular case. Finally, the forces are obtained and a comparison with numerical derivatives demonstrates that a high accuracy (typically 7 digits for molecules and 4 digits for periodic systems) is possible [4]. This is to the best of our knowledge the £rst implementation of analytical Hartree-Fock gradients for systems periodic in two and three dimensions.
Further development of the code has now become feasible: the implementation of density functional gradients will in great parts rely on Hartree-Fock gradients, and tools for structural optimization can now use analytical gradients.

References

1. P. Pulay, Mol. Phys. **17**, 197 (1969).
2. V. R. Saunders, R. Dovesi, C. Roetti, M. CausÁ, N. M. Harrison, R. Orlando, C. M. Zicovich-Wilson CRYSTAL 98 User's Manual, Theoretical Chemistry Group, University of Torino (1998).
3. L. E. McMurchie and E. R. Davidson, J. Comput. Phys. **26**, 218 (1978).
4. K. Doll, V. R. Saunders and N. M. Harrison, accepted by Int. J. Quantum Chem.

New representation of the Ising model and new cluster method for £nite and in£nite size systems

H.G. Evertz, H.M. Erkinger, and W. von der Linden

Inst. f. Theor. Physik, TU Graz, 8010 Graz, Austria

Tel. +43-316-873-8196, Fax -8677, evertz@itp.tu-graz.ac.at

The Fortuin-Kasteleyn (FK) representation [1] of the Ising model has led to great progress both on the analytical side with the random cluster representation of the Ising model, and on the numerical side by implying the Swendsen-Wang [2] cluster algorithm. Here we introduce a new representation for the Ising model, which extends the FK representation to contain also the bonds of the *high-temperature representation*, in addition to the FK bond variables and spins. All previous representations in terms of spins, FK-bonds and/or high temperature bonds follow easily by marginalization. Speci£cally, by summing over spins, a new representation in terms of FK bonds and high-temperature bonds results. Contrary to the FK representation, a magnetic £eld can be included naturally here, in terms of two sets of source-variables. As a new exact result, clusters of high-temperature bonds turn out to be strictly contained within FK clusters, explaining, e.g., a recent connection found by Caselle and Gliozzi [3]. We point out resulting consequences for the critical exponents of clusters and new geometric representations of observables. In the same way that the FK representation leads to the Swendsen-Wang algorithm, our representation provides a cluster algorithm, which is now also applicable to models with £nite magnetic £elds. Its scaling properties will be shown. The approach leading to the new representation also gives a generic formalism for "tentative updates" and for treating models with constraints.

We will then show how a simple modi£cation of this and other cluster algorithms allows us to perform simulations directly on *in£nite size* systems [4], completely overcoming £nite size effects. These simulations use single-cluster updates, but always start clusters at the same lattice point, thereby equilibrating a region of spins which grows as simulation time increases. Since two-point functions in cluster representation ("improved estimators") have support on single clusters, all two-point functions can be obtained, including dynamical information in the quantum case. Results can be used by themselves, and also as additional data for the asymptotic limit of £nite size scaling. The method is restricted to the non-percolating phase, i.e. T smaller than (but right up to) T_c. For quantum models, simulations can also be performed at $\beta = \infty$, i.e. directly at zero temperature. When the number of iterations is increased, correlation functions at larger distances become available. Limits $q \to 0$ and $\omega \to 0$ can be approached directly. As examples we calculate spectra for the d=2 Ising model at $L \equiv \infty$ and for Heisenberg quantum spin ladders with 2 and 4 legs at $L \equiv \infty,\ T \equiv 0$.

References

1. P.W. Kasteleyn and C.M. Fortuin, J. Phys. Soc. Jpn 26 (Suppl.) 11 (1969); C.M. Fortuin and P.W. Kasteleyn, Physica 57,536 (1972).
2. R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. 58, 86 (1987).
3. M.Caselle and F.Gliozzi, J. Phys. A33, 2333 (2000).
4. Cond-mat/0008072.

Variable high order £nite difference algorithms and important domain sampling for solving the Schrödinger equation in molecular dynamics

Stavros C. Farantos

Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, and
Department of Chemistry, University of Crete, Iraklion 711 10, Crete, Greece
+30-81-391813, +30-81-391305, farantos@iesl.forth.gr

Classical Molecular Dynamics are the most popular theories to study the time evolution of molecular systems especially of large size. However, in cases where quantum effects are important, such as tunneling or when detailed vibrational spectroscopy of excited states is available, one must solve the Schrödinger equation for the pertinent degrees of freedom. When the number of degrees of freedom is more than three this becomes a formidable task for Pseudospectral (PS) methods which require the representation of the wave function in the complete grid space.

Recently we have explored Finite Differences (FD) methods for solving the time dependent and time independent Schrödinger equation. The view of considering global Pseudospectral methods (Sinc and Fourier) as the in£nite order limit of local Finite Difference methods, and vice versa, Finite Difference as a certain sum acceleration of the Pseudospectral methods has been exploited to investigate high order Finite Difference algorithms for solving the Schrödinger equation in Molecular Dynamics [1, 2]. Radial and angular variables are treated on the same ground with centered equi-spaced grids as well as non uniform Legendre and Chebyshev grids [3].

Investigating highly excited vibrational states we have found that the construction of the continuation/bifurcation diagrams of classical periodic orbits reveals the con£guration domains where eigenstates are localized [4]. This information is then used to select the grid subspace for the representation of a family of eigenstates which is localized in these domains, thus reducing the dimensionality problem in solving the time dependent Schrödinger equation.

Results from 1D to 5D systems will be presented which demonstrate the stability and accuracy of High Order Finite Difference approximations of wave functions compared to global Pseudospectral techniques. Furthermore, we shall show the signi£cance of important domain sampling.

References

1. R. Guantes and S. C. Farantos, J. Chem. Phys., , **111** 10827, 1999.
2. R. Guantes, A. Nezis and S. C. Farantos, J. Chem. Phys. **111**, 10836, 1999.
3. R. Guantes and S. C. Farantos, J. Chem. Phys., **113** 10429, 2000.
4. H. Ishikawa, R. W. Field, S. C. Farantos, M. Joyeux, J. Koput, C. Beck and R. Schinke, Annual Review of Physical Chemistry, **50**, 443, 1999.

Numerical solution of an inverse problem for the hydraulic properties of porous media

Afet Golayoglu Fatullayev

Baskent University, School of Applied Sciences, Ankara, Turkey

A nonlinear parabolic equation arising in modeling ¤ow in homogeneous and isotropic porous media is considered in which coef£cients representing water capacity and hydraulic conductivity are unknown and to be determined from overspeci£ed data measured on the boundary. The problem is described by the following inverse problem of simultaneously determining $u(x,t)$ and unknown coef£cients $c(u)$ and $k(u)$ which satisfy

$$c(u(x,t))\frac{\partial u(x,t)}{\partial t} = \frac{\partial}{\partial x}(k(u(x,t))\frac{\partial u(x,t)}{\partial x}), \qquad (x,t) \in Q_0 = (0,1)\times(0,T) \tag{1}$$

$$u(x,0) = u_0, \qquad x \in (0,1), \tag{2}$$

$$\frac{\partial u}{\partial x}|_{x=0} = 0, \qquad t \in (0,T), \tag{3}$$

$$u(1,t) = f(t), \qquad t \in (0,T), \tag{4}$$

subject to the overspeci£cations

$$h(t) = u(0,t), \tag{5}$$

$$g(t) = k(u)\frac{\partial u}{\partial x}|_{x=1}. \tag{6}$$

Such problems arise, for example, in modeling ¤ow in homogeneous and isotropic porous media. If we interpret $u(x,t)$ as pressure head, then $c(u)$ and $k(u)$ may be interpreted, respectively as water capacity and hydraulic conductivity for porous medium[1].

One approach to solve this problem referred to in the literature as the method of output least squares is to assume that the unknown coef£cients are a speci£c functional form depending on some parameters and then seek to determine optimal parameter values so as to minimize an error functional based on the overspeci£ed data. The approach of method presented in this paper is not of this type. The strategy used here is to approximate unknown coef£cients by polygons and eliminate their in the equation, using over-speci£ed data measured on the boundary. In so doing, the problem can be transformed into the standard nonlinear initial boundary value problem in which coef£cients are functions depending on the values of unknown solution and theirs derivatives. Such problem can be solved by the £nite difference method and the unknown coef£cients can be determined from the numerically obtained solution. In other articles [2,3] by using this approach we have considered the problems of determining single unknown coef£-cient in a nonlinear parabolic equation. Here we develop this approach for the case of simultaneously determining of two unknown coef£cients in equation (1).

References

1. J. Bear, Dynamics of Fluids in Porous Media, Elsevier, New York, 1975.
2. A.Fatullayev, Determination of unknown coef£cient in nonlinear diffusion equation, Nonlinear Analysis, Theory, Methods & Applications, 44 (2001) 337-344
3. A. Fatullayev, E.Can, Numerical procedure for identi£cation of water capacity of porous media, Mathematics and Computers in Simulation, 52 (2000) 113-120

A new lattice Boltzmann approach to the mechanical properties and microstructure of the pattern formation in magnetic ¤uids

Miki Hirabayashi[1], **Yu Chen**[2], **and Hirotada Ohashi**[3]

Department of Quantum Engineering and Systems Science, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

tel:+81-3-5841-6991, fax: +81-3-5800-6857, e-mail:
[1]*hirabayashi@crimson.q.t.u-tokyo.ac.jp,* [2]*chen@crimson.q.t.u-tokyo.ac.jp, and*
[3]*ohashi@q.t.u-tokyo.ac.jp*

The structural pattern formation at the interface between a magnetic ¤uid and another immiscible non-magnetic liquid in a thin horizontal Hele-Shaw cell made from two transparent plates is studied using a powerful new lattice Boltzmann model for magnetic ¤uids.

Magnetic ¤uids are arti£cial colloidal suspensions of small ferromagnetic particles. The magnetic £eld can serve as an effective means to exercise control over magnetic ¤uids. Several lattice Boltzmann studies have ever tried to simulate the magnetic moments carried by particles in such ¤uids [1]. We applied a new type of two-dimensional lattice Boltzmann model for a magnetic ¤uid, which we have already developed by the appropriate extension of the lattice Boltzmann scheme for magnetohydrodynamics [2], to the simulation of the structural formation of a magnetic ¤uid which includes the effect of the internal angular momentum and the magnetic interaction [3]. This new model deals with a magnetic ¤uid as a single-phase ¤uid and can deal with the internal angular momentum caused by the magnetic dipole moment more ef£ciently than previous models, because it deals with magnetic ¤uids with a single component.

We applied this new type of lattice Boltzmann model for magnetic ¤uids to the problem of pattern formation with two components, which are a magnetic ¤uid and another immiscible non-magnetic liquid, on 2D triangular lattice. Several interesting morphologies in the pattern formation at the interface between these two kinds of liquids have been obtained experimentally by the alternating magnetic £eld or by changing the control parameters [4].

Our numerical results show that labyrinthine, stripe and bubble patterns are induced by a static perpendicular magnetic £eld, and the cellular structure, the non-magnetic bubble lattice and the ring structure are formed by an alternating £eld. It is thought that these equilibrium structures are due to the delicate balance between van der Waals attractive interactions and long range magnetic dipolar repulsion, which minimizes the energy of the system.

These results are relevant to understand the mechanism and conditions for the formations of patterns experimentally observed in magnetic ¤uids. Possiblity of providing control over the structure of a magnetizable media has great sciecnti£c importance. The lattice Boltzmann procedure is convenient to study the mechanical properties of these complex phenomena numerically. It is suitable to describe such complex hydrodynamics, because details about the short range behavior of a ¤uid are given up in exchange for complex interactions in ¤uids.

References

1. V. Sofonea, Europhys. Lett., 25 (5), pp. 385-390 (1994).
2. D. O. Martinez, S. Chen, and W. H. Matthaeus, Phys. Plasmas, 1(6) pp. 1850-1866 (1994).
3. J.-C.Bacri, F. Elias, C. Flament, ”Pattern Formation in Magnetic ¤uid”, Proc. of the 5th Japanese-French Seminar on Magnetic Fluids, pp. 1-2 (1998).
4. M. Hirabayashi, Y. Chen, and H. Ohashi, New Lattice Boltzmann Model for Magnetic Fluids, to be submitted.

Generalized evolutionary programming with Lévy-type mutation

Masao Iwamatsu
Department of Information & Computer Engineering
Kisarazu National College of Technology
Kisarazu City, Chiba 292-0041, Japan
Tel:+81-438-30-4132, Fax:+81-438-98-5717, e-mail:iwamatsu@j.kisarazu.ac.jp

Evolutionary algorithms [1], such as genetic algorithms, evolutionary strategies, and evolutionary programming of numerical optimization are population-based parallel search methods inspired by the biological genetics. Recently, the present author [2] has shown that the evolutionary programming can be successfully used to £nd the lowest energy structure of atomic and molecular clusters [2]. In the traditional evolutionary programming, the continuous variables are perturbed by the random numbers called "mutation", which follows the Gaussian distribution $p(x)$ [1, 2]:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-(x/\sigma)^2\right) \tag{1}$$

and the "strategy parameter" σ is self-adapted during the evolution of the population. Therefore, neither the cumbersome planning of cooling schedule in simulated annealing nor the local optimization by gradient in genetic algorithm is necessary in evolutionary programming.

In this paper, we propose a new generalized evolutionary programming algorithm based on the mutation which follows Lévy-type distribution:

$$p(x) = \frac{N_q}{\left(1+(q-1)(x/\sigma)^2\right)^{1/(q-1)}} \tag{2}$$

instead of Gaussian (1), where N_q is the normalization constant and q is the parameter characterizing the power-law distribution. This Lévy-type distribution is know to reproduce Gaussian, Cauchy, and Student's t-distributions when q is some rational numbers. Generally, however, q can be fractal, and this distribution can be derived from the Tsallis generalized statistical mechanics [3]. This Lévy-type distribution is characterized by the so-called fat-tail when $q > 1$, so that occasional long jumps occur, which make the spatial search more effective than the intensive search by the traditional narrow Gaussian distribution. We have modi£ed the evolutionary programming algorithm compiled by previous researchers [4] by replacing the Gaussian mutation with the Lévy mutation. We have tested our new algorithms using several hard test functions with numerous local minima. We found that the performance of our new evolutionary programming algorithm using the fat-tailed Lévy mutation with $q > 2$ surpasses the performance of the traditional algorithm for hard problems.

References

1. T. Bäck and H.-P. Schwefel, Evol. Comp. **1** (1993) 1.
2. M. Iwamatsu, "Applying Evolutionary Programming to Structural Optimization of Atomic Clusters", CCP2000 (2000).
3. A. M. C. de Souza and C. Tsallis, Physica A **236** (1997) 52.
4. X. Yao, Y. Liu, and G. Lin, IEEE Trans. Evol. Comp. **3** (1999) 82.

Rapid transit system origin-destination pattern calculation with statistical Gibbs sampling and Kalman £lter techniques

Yow-Jen Jou

Assoc. Prof., Institute of Statistics, Nat'l Chiao Tung Univ., Taiwan
Corresponding address: Institute of Statistics, National Chiao Tung University, Hsincu 300, Taiwan
Email: yjjou@stat.nctu.edu.tw and Tel.(Fax) 886-35710657

Origin-Destination matrices (O-D matrices) representing trip demands from one place (origin) to another (destination) are the most essential input data to many transportation and traf£c engineering analysis[1]. Traditionally, O-D data are mainly used in transportation planning, deciding the location of a station and scheduling the frequency of the transit for an urban network.

Due to the facts that the numbers of passengers from a certain origin or to a certain destination, denoted by y, are easy to obtain and the path ¤ows, denoted by x, are not directly observable, we formulate the interrelation between x and y and the dynamics of x by a state space model with unknown transition matrix. Conventionally, Chang and Wu [2] use extended Kalman £lter or impose assumptions to modify the model to estimate O-D ¤ow matrix [3][4].

In this paper, we develop a Markov chain Monte Carlo algorithm to estimate the O-D matrix and predict future ¤ows for our nonlinear, hence non-Gaussion, state-space model. The methodology is applied to the data of Taipei rapid transit system in the table which gives £ve-minute counts of passenger whose destination is Taipei main station. In the £gure, the estimated data pattern is similar to the real data pattern.

References

1. C. Tebaldi and M. West, J. Amer. Stat. Assoc. **93**, 557-576 (1998).
2. G.L. Chang and J. Wu, Transportation Research **28B**, 141-160 (1994).
3. C.K. Cater and R. Kohn, Biometrika **83(3),** 589-601 (1996).
4. J. Durbin and S.J. Koopman, Biometrika **84(3)**, 669-684 (1997).

New integrator for molecular dynamics simulations

Z. M. Khakimov
Institute of Nuclear Physics of Uzbekistan Academy of Sciences
998-712-605694, 998-712-642590, khakimov@suninp.tashkent.su

Thanks to a great progress in power of computers and simulation approaches, molecular dynamics (MD) simulations [1] of multi-atomic systems (solids, surfaces, polymers etc.) have now become possible even using sophisticated inter-atomic potentials [2] and £rst principles force calculations [3]. Ef£ciency and reliability of these simulations also strongly depend on availability of algorithms that provide an acceptable accuracy in the energy conservation at high time steps δt for integration of Newtonian equations of motion. Unfortunately, all more or less complicated integration algorithms have in fact no preference over simple 3th-order velocity Verlet algorithm (VVA) at $\delta t \geq 10^{-15}$ s.

This paper presents a few new algorithms that, unlike other ones, provide one or two order of magnitude improvement in prediction of particle positions and energy conservation as compared to VVA at high-time steps. These algorithms explicitly account for a local curvature of potential relief, the £rst derivatives of forces (accelerations), for particles. Note that Gear predictor-corrector algorithm (GPCA), which is the most accurate among other algorithms, uses one ore more additional force calculations to improve results. At £rst sight, from the viewpoint of ef£ciency of simulations, additional force calculations in GPCA and calculations of force derivatives in our algorithms seems all the same. However, the later actually consumes considerably less time than the former, because force derivatives can be calculated simultaneously with forces at the same force calculation loop and using the same quantities (exponents, square roots, etc) evaluated for the forces. Note it is possible to avoid calculation of force derivatives, storing one more memory word for accelerations.

In the one of proposed algorithms the positions, R, and velocities, v, of particles are advanced using following equations

$$R_{t+\delta t} = \left[1 - \frac{1}{12}\frac{da_t}{dR_t}\delta t^2\right]^{-1}\left[R_t + v_t\delta t + \frac{1}{12}(7a_t - a_{t-\delta t})\delta t^2\right], \tag{1}$$

$$v_{t+\delta t} = v_t + \frac{1}{12}\left[8a_t + 5a_{t+\delta t} - a_{t-\delta t}\right]\delta t\,, \tag{2}$$

where a_t is particle's accelaration; da_t/dR_t is its derivative with respect to particle's position R.

The algorithms are tested in both the simplest model systems and silicon clusters using the self-consistent semiempirical tight-binding method [4] for the force calculations. It was shown that the proposed algorithms could provide, besides a signi£cant improvement in the energy conservation, 5-10 times speedup of typical MD simulations.

References

1. M. P. Allen and D. J. Tildesley, Computer simulation of liquids (Clarendon Press, Oxford, 1987).
2. A. E. Carlsson, Solid State Physics: Advances in Research and Applications, Eds. D. Turnbull, H. Ehrenreich (Academic Press, New York, 1990), p.1.
3. M. C. Payne, M. P. Teter, D. C. Allan, T. A. Arias, and J. D. Joannopoulos, Rev. Modern Phys., **64**, 1045 (1992).
4. Z. M. Khakimov, Comput. Mater. Sci., **3**, 95 (1994).

Feature extraction and classi£cation with cellular spaces

Christian Kuhn
Technical University of Ilmenau, D-98684 Ilmenau, Germany,
Faculty of Computer Science and Automation,
Department of Automation and System Engineering,
Division of System Analysis
Phone: +49-(0)-3677-69-1467, Fax: +49-(0)-3677-69-1434,
email: christian.kuhn@rz.tu-ilmenau.de

Methods of automatic classi£cation are established in many £elds of various techniques, so for instance in image and speech processing or pattern recognition. In the automatic control engineering £elds of applications are especially the fault diagonsis, process monitoring and problems of prognosis. Classi£ers are used in special kinds of controls to select approximated subprocesses which describe a whole nonlinear process. Here the classi£er has the task to detect the actual process situation.

We have to solve three subproblems in most cases. These three subproblems are *signal preprocessing, feature generation* and *classi£cation.* The *signal preprocessing* supports the preparation of the data for the further numeric processing in a computer. The *feature generation* follows the signal preprocessing. The situation vector with measured data is transformed in a feature vector and a suitable feature space. Here the algorithms of feature extraction analyse the feature spaces and select suitable features. The *classi£er* executes the assignment of an object or an actual process situation to a class. The classi£cation is based on the selected features. A high quality for the decisions needs a careful feature selection.

Another way to design a classi£cation system don't use these subcomponents, because the disadvantage of this design process is the inhomogeneous way. Now we have three levels which allow the design and training of a classi£cation system with a dynamic structure. Each level of the classi£cation system interacts with another levels of this system. The *data level* includes all signal processing routines, so the measurement of process data, signal preprocessing and signal transformations. The *feature level* is necessary for the investigation of the feature space. Last not least we need the *decision level* for the aggregation of multiple decisions and the analysis of the £tness of the whole system.

In this article we want to discuss the feature level especially. A new tool for the analysis of the feature space — the *cellular space* — is shown. Additional this article introduces a mathematical model to describe the relations of between data objects of a learning sample. The cellular space is the result of the discretization process of a part of the feature space. The orthogonal area of the feature space $\mathcal{M}$ including the whole learning sample is called as *analysis space* $\mathcal{A}$, which we want to rasterize in subspaces $\mathcal{R}$.

Now we need mathematical models for working with this cellular space. This article describes two models: the *density model* and the *£eld model*. Both models have advantages, but disadvantages, too. The models are developed for various conditions: the density model leads to good results with large sets of objects, it is recommended for investigations of heterogeneity and feature extraction. The £eld model leads to smooth object descriptions in the analysis space. It's advantage is the possibility of the extrapolation im empty, new areas im the feature space. The favourite application £eld is the clustering of data. Two simulations calculated with these models are discussed.

Validation of the Lowe-Frenkel tracer dispersion method in the lattice Boltzmann method

R. M. H. Merks, A. G. Hoeksta and P. M. A. Sloot

Section of Computational Science
University of Amsterdam,
Kruislaan 403, 1098 SJ Amsterdam, The Netherlands
Tel. (+31) 20 525 7582, Fax. (+31) 20 525 7490, roel@science.uva.nl

In many ¤uid dynamics applications one is interested in the dispersion of a solute in a ¤uid. An example of such a convection-diffusion problem is the transport of nutrients towards a growing coral colony [2].

Apart from numeric solutions of the convection-diffusion equation, several methods have been developed to solve convection-diffusion by releasing tracer particles in lattice Boltzmann simulations. One of these methods is the Lowe-Frenkel method [3] that we aim to validate in this paper. In this method a single scalar per lattice Boltzmann site for each tracer species is propagated. The direction of propagation is biased by the velocity £eld.

We are unaware of any attempts to numerically validate the Lowe-Frenkel method against analytic benchmarks. We undertake such validation by comparing the Lowe-Frenkel method against the analytic Taylor-Aris result of tracer dispersion in two- and three-dimensional tubes [1].

The Taylor-Aris theory predicts the dispersion of solute in a tube ¤ow about a point moving with the mean ¤ow velocity $\bar{u}$. Aris has shown that the dispersion coef£cient K is the sum of the molecular diffusion coef£cient D_m and a contribution by convection, $K = D_m + \kappa\alpha^2\bar{u}^2/D_m$, where $\kappa = \frac{1}{210}$ for a 2D and $\kappa = \frac{1}{48}$ for a 3D Poiseuille ¤ow; α is the tube cross section for a 2D ¤ow and the tube radius for a 3D ¤ow.

We track the dispersion of an initial point pulse of tracer in the middle of the tube, by measuring the £rst (σ_x) and second (σ_{xx}^2) order moments. After an initial transient, approximately the time needed for the solute to reach the wall of the tube by diffusion, the variance of tracer $V = \sigma_{xx}^2 - (\sigma_x)^2$ increases linearly with the dispersion coef£cient $K = \frac{1}{2}\frac{\partial V}{\partial t}$. This linear dependence no longer holds if a fraction of tracer has reached the end of the tube and reenters the tube over the periodic boundary.

We have measured the dispersion coef£cient in 2D and 3D Poiseuille ¤ows for Péclet numbers between 0 and 55 and for Reynolds numbers between 0 and 55. Lattice Péclet numbers range from 0.0 to 0.55. The measured dispersion coef£cients for the 2D and 3D ¤ows agree well with the theoretical prediction; in all experiments, even for the highest velocity, we measure dispersion coef£cients of at most 5% below the theoretical value.

Relative to other methods for solving convection-diffusion, the Lowe-Frenkel is ef£cient and requires few memory. Within the range of Péclet-numbers we have measured, the method gives good results for the Taylor-Aris problem. We conclude that the Lowe-Frenkel method is a valuable and valid computational tool for the simulation of convection-diffusion processes.

References

1. ARIS, R. On the dispersion of a solute in a ¤uid through a tube. *Proceedings of the Royal Society London A 235* (1956), 67–77.
2. KAANDORP, J. A., LOWE, C. P., FRENKEL, D., AND SLOOT, P. M. A. Effect of nutrient diffusion and ¤ow on coral morphology. *Phys. Rev. Lett. 77* (1996), 2328–2331.
3. LOWE, C. P., AND FRENKEL, D. The super long-time decay of velocity ¤uctuations in a two-dimensional ¤uid. *Physica A 220* (1995), 251–260.

Dynamical memory time in molecular dynamic simulations

I.V. Morozov[1], **G.E. Norman**[2] **and A.A. Valuev**[2]

[1]*Department of Physics, Lomonosov Moscow State University, Vorob'evy Gory, 119899, Moscow, Russia*
[2] *Department of Molecular Physics, Moscow Institute of Physics and Technology, Institutskii per. 9, 141700, Dolgoprudnyi, Russia,*
e-mail: bogous@orc.ru

The problem of the accuracy of molecular dynamic simulations is discussed in the context of the Lyapunov trajectories instability. The problem is important when computing correlation functions for the systems of collective degrees of freedom comparable to unity. The time t_m, during which the behavior of a dynamic system can be predicted from initial conditions and deterministic equations of motion, is called the dynamical memory time. After t_m the correlations become stochastic due to the Lyapunov instability and a small numerical error. The dynamical memory time depends on a simulation scheme and stochastic properties of the system are investigated such as the Lyapunov exponent (Krylov-Kolmogorov entropy) K. These properties were calculated for neutral particles in [1, 2] and for one-component strongly coupled plasmas in [3].

We consider two-component strongly coupled plasmas in equilibrium and non-equilibrium states. The values of K and t_m are calculated for both, electrons and ions with mass ratios $10 - 10^5$. The details of the computation method is presented in [4]. The Lyapunov exponent turns out to be independent of the initial displacement and is the same for the divergence of coordinates and velocities. It is found that at the initial stage of trajectories divergence, the values of K for electrons and ions coincide. At $t = t_m$ the divergence of electrons reaches its saturation level. Therefore at $t > t_m$ only ion trajectories continue to diverge exponentially with another value of K depending on the mass ratio. The dependence of K and t_m on the number of particles, the nonideality parameter and the form of the interaction potential, are investigated. In the nonequilibrium case, the K value is found to be closely related to the rate of the kinetic energy growth.

A universal relation between Kt_m and the ¤uctuation of the total energy of the system is obtained. This relation does not depend on a numerical integration scheme, temperature, density, and the interparticle interaction potential, so that it may be applied to arbitrary dynamic systems. The transition from the dynamical to the stochastic regime is investigated in the electron and ion velocity correlation factors as well as in the Langmuir and ion-sound plasma wave dynamic structure factors. The dependence of t_m on the numerical noise level is logarithmic, thus using a very small value of integration step does not increase t_m signi£cantly. It constitutes a problem when computing long wavelength regions of both Langmuir and ion-sound plasma waves or the the autocorrelation function tail.

References

1. W. G. Hoover, *Time Reversibility, Computer Simulation and Chaos* (World Scienti£c, Singapore, 1999).
2. G. E. Norman and V. V. Stegailov, Zh. Eksp. Theor. Phys. **119**, No.5, (2001)
3. D. M. Barnett, T. Tajima and Y. Ueshima, Phys. Rev. Lett **83**, 2677 (1999).
4. I. V. Morozov, G. E. Norman, A. A. Valuev, Phys. Rev. E **63**, March 2001.

Poster Session B

Calculation of induced electron states in three dimensional semiconductor arti£cial molecules

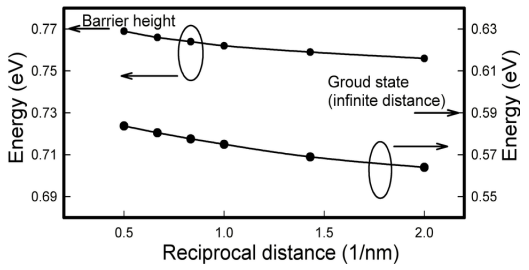
Yiming Li[1], **O.Voskoboynikov**[1,2], **C. P. Lee**[1], **and S. M. Sze**[1]

[1] *Institute of Electronics, National Chiao Tung University, Hsinchu, Taiwan*
[2] *Kiev Taras Shevchenko University, 252030, Kiev, Ukraine*
Corresponding address: P.O. Box 25-178, Hsincu 300, Taiwan
Email: ymli.ee87g@nctu.edu.tw and Tel. 886-930-330766

Semiconductor quantum dots are now under an extensive study because they demonstrate rich properties of ”arti£cial atoms”. Unlike for ”natural atoms”, the quantum dot properties can be controlled technologically [1]. Recent advances in semiconductor nano technology make it possible to consider systems of coupled quantum dots ”arti£cial molecule”). The main future in this system is an effect of the electronic structure tunability by dot-to-dot electronic entanglement and charge transfer [2]. This considerably enhances physical and practical interest to arti£cial semiconductor molecules [2, 3]. Most of theoretical studies of those systems have been done within a two dimensional (lateral) geometry and two dimensional con£nement potential models [2]. In the same time, the real three dimensional approach can allow us to enhance suf£ciently the system tunability range.

In this work we compute the ground state energy and wave function of electrons con£ned in small three dimensional coupled quantum $In_{1-x}Ga_xAs$ dots embedded into GaAs matrix. The dots have the disk shapes and are separated (in the disk symmetry axis direction) by a certain distance. We treat the problem with an effective one electronic band Hamiltonian, energy and position dependent electron effective mass approximation and Ben Daniel-Duke boundary conditions. A hard-wall (of £nite height) tree dimensional con£nement potential is used. To solve three dimensional Schrödinger equation we employ full numerical solution using £nite difference method and balanced QR algorithm [4]. In the case when dots have a big difference in x parameter we can consider a situation when one of separated (very large interdot distance) dots has one well bound state and another one does not. Then, the distance decreasing leads to an induction of an ”additional” weak bound electron energy state.

The £gure demonstrates both the £rst bound energy state (lower line) and the induced energy state (upper line) as function of the interdot distance. Both dot have the same radius (7.5 nm) and heights (1.5 nm). For the £rst dot we choose $x = 0$ and for the second $x = 0.2$.



References

1. D. Bimberg, M. Grundmann, F. Heirichdorff, et al., Thin Solid Films **367** 235 (2000).
2. X. Hu and S. Das Sarma, Phys. Rev. A **61** 062301(2000).
3. P. Yu, W. Langbein, K. Leosson, et al., Phys. Rev. B **60** 16 680 (1999).
4. I. C. F. Ipsen, SIAM Rev. **39** 254 (1997).

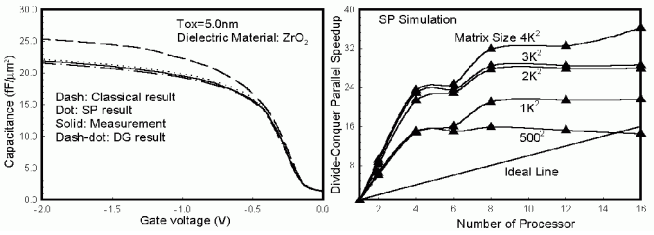
Numerical simulation of quantum effects in high-k gate dielectrics MOS structures using quantum mechanical models

Yiming Li[1], Jam-Wem Lee[1], Ting-Wei Tang[2], Tien-Sheng Chao[1], Tan-Fu Lei[1], and S. M. Sze[1]

[1] *Institute of Electronics, National Chiao Tung University, Hsinchu, Taiwan*
[2] *Dept. Elec. & Comp. Engr., Univ. Mass., Amherst, MA 01003, USA*
Corresponding address: P.O. Box 25-178, Hsincu 300, Taiwan
Email: ymli.ee87g@nctu.edu.tw and Tel. 886-930-330766

The operation of deep submicron MOSFET's is now entering a regime in which quantum con£nement effects (QCE) become noticeable and classical transport theory is no longer suf£cient for accurate modeling of operating characteristics. Development of metal gate and high-k dielectric materials, such as $(B_a, S_r)T_iO_3$, T_iO_2, or Z_rO_2 is a novel alternative to fabricate devices with reliable and high quality characteristics. One of the most obvious QCE is that the inversion layer charge density calculated using quantum mechanics approach is smaller than that calculated classically for a given applied gate voltage, thus affecting the shift of the C-V curves. Simulation models for QCE, e.g., Van Dort, Hansch, MLDA, density gradient (DG), and Schrodinger-Poisson (SP) models have been received many interests and applied to thin S_iO_2 studies in MOS structures [1, 2].

In this paper, a self-consistent SP and a DG are applied to study the QCE numerically. The C-V characteristic of MOS structure with high dielectric constant oxides, Z_rO_2, is then investigated by means of the developed simulators. The quantum transport results are found to compare quite well with experimental data. Comparisons are also made with results obtained using classical simulations and these approaches as well (see left Fig.). In order to solve the models ef£ciently, a parallel divide-conquer method is applied to solve SP model and a monotone £nite volume scheme [3] is derived for DG model, respectively. The £rst algorithm proposed here is given for fast calculating the carrier wave function and energy levels of a large sparse band matrix of discretized Schordinger equation. It's stable and for a large class of matrices it is, asymptotically, faster by an order of magnitude than the conventional method. The discretized DG model leads to a system of nonlinear algebraic equations that is then solved by monotone upper and lower iterative method instead of conventional Newton's iterative method. Both of this two simulations have been implemented successfully and test for various applications in high-k gate dielectrics and ultra thin oxides MOS structures. Some parallel benchmarks are also given to show a good computational ef£ciency (right Fig.).



References

1. M. G. Ancona, IEEE J. TCAD, 1 (1998); S.-H. Lo, et al., IBM J. Res. Dev., 327 (1999).
2. C. A. Richter, IEEE EDL, 35 (2001).
3. Y. Li, et al., Proc. Model. Simul. Microsys. 538 (2001).

A novel simulation approach for the numerical solution of heterojunction bipolar transistors

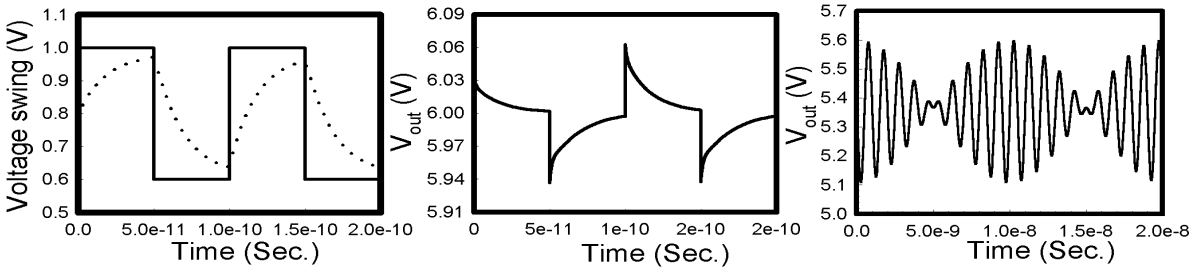
Yiming Li, Kuen-Yu Huang, C. P. Lee, and S. M. Sze

Deaprtment of Electronics Engineering and Institute of Electronics, National Chiao Tung University, Hsinchu 300, Taiwan
Corresponding address: P.O. Box 25-178, Hsincu 300, Taiwan
Email: ymli.ee87g@nctu.edu.tw and Tel. 886-930-330766

Due to the unusually high linearity of heterojunction bipolar transistors (HBTs) at high frequences, these device structures have been of great interests for wireless applications in recent years [1, 2]. A standard approach to analyse the physical behaviors for an HBT circuit is to solve a set of equivalent circuit ordinary differential equations (ODEs) in frequency domain (FD). The harmonic balanced method is a way for the solution of the HBT ODEs in FD. The discretized ODEs in circuit simulation are then solved with the Newton's iterative (NI) method traditionally. However, NI method is a local method, in general, it converges quadratically in a suf£ciently small neighborhood of the exact solution.

In this paper, a novel simulation method for HBT physical characteristics calculations in large-scale time domain (TD) is proposed. This approach is mainly using the monotone iterative (MI) method instead of the NI method to solve the ODEs. The MI method has been successfully developed and applied to semiconductor device simulation by us earlier [3, 4]. Based on waveform relaxation (WR) and MI methods, the HBT circuit ODEs are solved in TD. Compared with the NI method, this method converges globally and is inherently parallel. First of all, a set of ODEs are decoupled with WR method. Each decoupled nonlinear ODE is then solved directly with MI technique. The proposed computational approach has been successfully implemented on a PC-based cluster with message passing interface. The primary parallel results show that a well-designed parallel algorithm can reduce the execution time up to an order of magnitude. As shown in Figs, the left 2 Figs show the TD results of V_{in} (solid), V_b (dotted) and V_{out} with a square wave input signal and the right Fig show the TD result with a two-tone input signal.

In a short conclusion, a novel circuit simulation that based on the WR and MI methods is proposed. With this approach, high frequency physical characteristics for an HBT circuit is directly analysed from TD results. Numerical results on a realistic HBT are also presented to show the accuracy and ef£ciency of the method.



References

1. N. Guofu, et al., Proc. Bipolar/BiCMOS Circuits and Technology Meeting, 50, (1999).
2. S. Sheu, et al., IEEE Trans. Electron Devices, **45**, 326 (1998).
3. N. Mastorakis, Recent Advances in Applied and Theoretical Mathematics, World Scienti£c, (2000).
4. Y. Li, et al., Proc. CCP, 138, (2000).

Calculation of the electronic structure and disordering effects in $La_{0.5}Li_{0.5}TiO_3$ compound

L.V.Tymoshevska[1], B.Z.Yanchitskii[1] and A.G.Belous[2]

[1] *Institute of Magnetism, 36-B Vernadsky St., 03680 Kiev, Ukraine*
[2] *Institute of General and Inorganic Chemistry, 03680, Kiev, Ukraine*
+380/44 444 1014, +380/44 452 1811, liliya@ukron.kiev.ua

Solid electrolytes, possessing an ionic lithium conductivity, are very interesting subjects due to the two main reasons: £rstly, for fundamental studying of the transport mechanisms, and, secondly, due to their speci£c industrial applications as a high power batteries, chemical sensors and separators. Phenomenon of the lithium ionic conductivity occurs through the peculiar interaction of the lithium ion with the TiO_3 sub-lattice and, as the result, it depends on the ordering of La and Li atoms in the perovskite lattice. Therefore, studying the electronic structure of the $La_{\frac{2}{3}x}Li_{3x}TiO_3$ oxides seems to be important from the both above points of view. At present, there are no theoretical investigations of the atomic and electronic structure of lanthanum-lithium titanates. These investigations are necessary step for understanding the nature of the super-ionic conductivity phenomenon.

In the present work, we have carried out the theoretical and experimental investigations of peculiarities of the electronic structure of the $La_{0.5}Li_{0.5}TiO_3$ compound and tried to clarify the in¤uence of the La and Li atoms ordering on the energy spectrum of valence electrons. Now there is no the one opinion as to the crystal structure of the $La_{0.5}Li_{0.5}TiO_3$ compound. We have prepared the samples using the different methods, and this resulted in a different ordering of the La and Li atoms in this compound. As the objects, we have chosen three structures with the different La and Li atoms ordering. In order to determine cell parameters and atomic coordinates for each structure, we have carried out the set of the total energy calculations for the different positions of atoms.

Using the highly accurate ab-initio Full Potential LAPW method [1] of the band structure calculations, we have calculated the lattice parameter and the electronic structure of the compounds with a good accuracy. Experimentally, the electronic structure of the samples was studied by the X-ray emission spectroscopy. The O Kα emission spectra of the $La_{0.5}Li_{0.5}TiO_3$ compound were obtained.

From our studies we can conclude that among those three investigated crystal structures, modeling the atomic structure of the $La_{0.5}Li_{0.5}TiO_3$ compound and corresponding to the different La and Li atoms ordering, the most advantageous is the structure with the alternating La and Li layers. For this structure we have reached a good agreement between the experimental and calculated Kα spectra of the oxygen atoms. This is due to the presence of the different types of nonequivalent oxygen atoms situated at the different inter-atomic distances from the titanium atom.

References

1. P.Blaha, K.Schwarz, and J.Luitz, WIEN97, Technical University of Vienna 1997. (Improved and updated Unix version of the original copyrighted WIEN-code, which was published by P.Blaha, K.Schwarz, P.Sorantin, and S.B.Trickey, in Comput. Phys. Commun. 59, 399 (1990)).

Simulation of liquid solution doping from gas phase by the method of molecular dynamics

A.R. Lyutikov, Yu.P. Khukhryansky

Voronezh State Technical University
Department of Solid State Physics
e-mail: larsoft@mail.ru

We have used the method of molecular dynamics for computer simulation of a two-phase two-component system gas - nonvolatile liquid.

Two spatial regions were considered. These are volume of a liquid phase and surface layer of a gas phase. It was supposed that a nonvolatile component exists only in a liquid phase as monoatomic molecules, and a volatile component exists in a gas phase as diatomic molecules while in a condensed phase as mono and diatomic molecules. That corresponds to solutions of element B^{V} in A^{III}(such as Ga-P, InP). Association and dissociation of volatile component diatomic molecules occurs mainly in a surface layer of the liquid phase. The Lennard-Jones (6-12) potential was selected as a potential of molecular interaction. Potential parameters for a case of GaP system simulation were taken from [1], [2]. Coordinates and velocities of the volatile component molecules, both in a liquid and in a gas phase, were determined through solution of the equations of motion. The in¤uence of molecules of the non-volatile component was taken into account via calculation of stochastic force. Coordinates of non-volatile component molecules were assigned randomly in sphere around of each molecule of the volatile component. Such approximation supposes that the nearest environment of each molecule of the volatile component changes completely on each iteration. In this connexion the value of an integration step was selected equal to average time of molecules free run in a liquid phase.

This model enables to simulate systems containing more than 10^{6} particles at time of simulation about 10^{-8} seconds. Application this model to the system Ga-P allows evaluate energy of molecules P_2 association, energy of interphase potential barrier and ¤ux density of molecules P_2 at T=1000 K.

References

1. Calculation of potentials of gallium and phosphorus atoms pair interaction. D.V. Ryazanov, V.A. Skripnikov, Yu. P. Khukhryansky. Physics. 1999. V 1. p 95-99.
2. Thermodynamic and thermalphysic characteristics of combustion products. V.1. Methods of calculation. Moscow. 1971.

Dynamic structure of liquid germanium studied by a £rst-principles and a classical molecular-dynamics simulations

Shuji Munejiri[1], **Fuyuki Shimojo**[2], **Kozo Hoshino**[2]
and Toshio Itami[1,3]

[1]*National Space Development Agency of Japan, Tsukuba 305-8505, Japan*
[2]*Hiroshima University, Higashi-Hiroshima 739-8521, Japan*
[3]*Hokkaido University, Sapporo 060-0810, Japan*
munejiri@minerva.ias.hiroshima-u.ac.jp

It is known that structure factor $S(Q)$ of liquid germanium has a clear shoulder on the high-Q side of the £rst peak, which is related to a complex local structure originating from some kinds of chemical bonds. However, it is not understood how these chemical bonds affect dynamic structure. In this paper, to investigate dynamic properties of the liquid germanium at 1253 K, £rst-principles and classical molecular-dynamics (MD) simulations are carried out.

Our method of the calculation for the electronic structure is based on the density functional theory with the generalized-gradient approximation (GGA). A norm-conserving pseudopotential is employed for the interaction between the valence and the core electrons. The electronic wavefunctions are expanded by a plane-wave basis set with the cutoff energy of 11 Ryd. The Kohn-Sham energy functional is minimized by the preconditioned conjugate-gradient method. The simulations are performed in the cubic supercells of 64 and 128 atoms for over 10000 steps with the time step of 3 fs.

The calculated structure factor is in good agreement with the experimental data. The three-body angle distribution functions show a peak around 100°. For dynamic properties, it is found that an atom diffuses quickly not only when its coordination number becomes smaller but also when surrounding atoms are not positioned at angle of around 100°. This results show that an atomic diffusion process in liquid germanium is strongly in¤uenced by the presence of a chemical bond. Dynamic structure factor $S(Q,\omega)$ is also calculated. The result shows *de Gennes* narrowing and agrees with the recent x-ray inelastic experimental data [1].

To study a dynamic property for a long-wavelength region, a classical MD simulation is still useful, since a large-scale simulation is easily performed. However, it is dif£cult to obtain a reliable interatomic potential for the liquid germanium whose structure is much complex. In the present study, the interatomic interaction is derived by an inverse method [2], in which an effective pair potential $\phi(r)$ is calculated from an experimental structure factor $S(Q)$. Though, thus obtained $\phi(r)$ can reproduce the experimental static structure factor $S(Q)$, it is not obvious that this effective pair potential can also be used to investigate the dynamic structure. We performed a large and long time scale MD simulation with $\phi(r)$ to calculate the dynamic structure factors $S(Q,\omega)$ accurately. We show that the experimental $S(Q,\omega)$ [1] is well reproduced by the MD simulation with $\phi(r)$. The velocity of sound was also calculated from the gradient of the dispersion relation in the small Q-region and the result was in good agreement with the experiment.

References

1. S. Hosokawa *et al., Phys. Rev.* B **63** (2001) 134205.
2. S. Munejiri *et al., J. Phys. Soc. Jpn.* **64** (1995) 344.

Computation of the thermodynamic criterion for migrating grain boundary pinning during recrystallization processes in the dispersion-hardened alloys

L. A. Marvina, V. B. Marvin, V. R. Karibyants, and I. V. Neupokoeva

Astrakhan State Technical University, 16, Tatishcheva str., Astrakhan, 414025, Russia
tel: 7-(8512)-381239, fax: 7-(8512)-256427, e-mail: marvin@astu.astranet.ru

Development of adequate physical models of the processes taking place in dispersion-hardened alloys (DHA) at increased temperatures is one of the important tasks of the modern physical materials technology in studies of their structural and mechanical properties. So, it is known, that the stability of a DHA grain structure can be broken at high temperatures owing to recrystallyzation by means of the detachment of second phase particles from the migrating grain boundary (GB) or through the joint migration of the GB and mobile particles [1-3]. Conditions of the GB structure stability in the case of unmovable particles have been considered in the paper [1]. In this work the following thermodynamic criterion of the DHA grain structure stability is derived by way of calculation of the system free energy increment in the process of the GB migration with the account of work expend on the second phase particles movement:

$$NMf_Z^2 dt + \gamma dS_b - Gd\Omega \geq 0 \qquad (1)$$

where N is the number of particles per GB area, M is the particles mobility, f_Z is the Zener pinning force [2, 3], dt is the migration time, γ is the GB surface tension, dS_b is the GB area increment [1], G is the migration driving pressure, and $d\Omega$ is the volume sweeping by migrating GB in the time dt. The criterion (1) is common for all types of recrystallization and makes it possible to predict the particular mechanism of the DHA grain structure stability breaking.

A condition of the migrating GB pinnig for the case of the secondary recrystallization built upon the general criterion (1) is derived within the framework of the "¤at" boundary model (where the boundary is presumed to be curved around particles and ¤at between them). Three regions of the grain boundary stability depending on the ratio between particle and GB mobilities and G value are set apart for speci£c alloys. Results of computation carried out with the use of the obtained criteria for a $Ni - HfO_2$ alloy and a $Fe-Cr$ alloy with $NbCN, TiCN$ particles are in agreement with experiment (where GB pinning at $G/Nf_Z \gg 1$ and increase of the maximum possible G/Nf_Z value with decrease of the particles volume fraction have been observed), on the one hand, and contradict to predictions of the DHA grain structure stability based on the traditional force criterion of the grain structure stability $G/Nf_Z \leq 1$ and its modi£cations [2, 3], on the other.

References

1. Marvina L. A., Marvin V. B., Fizika metallov i metallovedenie, **88**, 5, 11 (1999).
2. Marvina L. A., Marvin V. B., Diffusive processes and structure degradation in metals, Dalnauka, Vladivostok - Blagoveshchensk (1996).
3. Gottstein G., Shvindlerman L. S., Acta metall., **41**, 3267 (1993).

Simulating stochastic geometries: Topological and morphological phase transitions of overlapping grains

Uwe Brodatzki[1] **and Klaus R. Mecke**[2,3]

[1]*Fachbereich Physik, Bergische Universität, 42097 Wuppertal, Germany*
[2]*Max-Planck-Institut für Metallforschung, Heisenbergstr. 1,*
[3]*Institut für Theoretische und Angewandte Physik, Universität Stuttgart,*
Pfaffenwaldring 57, D-70569 Stuttgart, Germany
+49-202/4392863,+49-202/4392635, mecke@theorie.physik.uni-wuppertal.de

The effective modeling of spatial structures becomes more and more important in statistical physics, particularly on mesoscopic scales in order to bridge different length and time scales. For instance, overlapping discs and spheres serve as standard models of stochastic geometries for many physical applications, e.g., for porous media, complex ¤uids, or for the large-scale structure in the universe [1]. The morphology, i.e., the shape and connectivity (topology) of random structures is relevant for the determination of physical properties such as transport properties in porous media. Integral geometry furnishes a suitable family of morphological descriptors, known as Minkowski functionals which are related to curvature integrals [2]. Despite the conceptual importance of morphological measures to characterize mesoscopic systems, the numerical evaluation of such measures has not been completely successful yet. Here, we present an algorithm for the exact calculation of Minkowski functionals for overlapping grains each with arbitrary location, orientation and shape (Boolean model). The method is numerically robust even for large samples, independent of statistical assumptions, and yields global as well as local morphological information. We illustrate the method by applying it to several stochastic processes and determine the statistics of Minkowski functionals for Poisson distributed grains and hard disks.

Under rather natural assumptions a general expression for the Hamiltonian of overlapping grains can be given including energy contributions related to the volume, surface area, mean curvature, and Euler characteristic of the mesoscopic spatial domains. This Hamiltonian extends the Widom-Rowlinson model as well as the model of hard spheres to partially penetrable shapes. The complex structure leads to multi-particle interactions, so that the computational cost to evaluate the energy of a con£guration is enormous and ef£cient algorithms have to be invented in order to make Monte-Carlo simulations feasible. In two dimensions this has been done for the parallel machine CM5 using the SIMD technique. Several new phase transitions in the morphology and topology of the spatial structures can be observed which are directly related to the inherent many-particle interactions of the morphological Hamiltonian. These results can be applied to the phase behavior of colloidal particles embedded in a binary ¤uid indicating the existence of re-melting solid phases and new topology-stabilized ¤uid phases. Applications to wetting and capillary condensation of ¤uids in porous media show evidence of a second critical point. Lattice approximations of the Minkowski functionals allow the study of the morphology during spinodal decomposition by Lattice-Boltzmann [3] and of microemulsions by Monte-Carlo techniques on cubic lattices [4].

References

1. K. R. Mecke and D. Stoyan (Eds.), *Statistical Physics and Spatial Statistics - The Art of Analyzing and Modeling Spatial Structures and Pattern Formation*, Lecture Notes in Physics, Vol. 554, Springer, 2000.
2. L. A. Santal Áo, *Integral Geometry and Geometric Probability* (Addison - Wesley, Reading, MA, 1976).
3. V. Sofonea and K. R. Mecke, European Physical Journal B **8**, 99-112 (1999).
4. C. N. Likos, K. R. Mecke, and H. Wagner, J. Chem. Phys. **102**, 9350-9361 (1995).

Classical and ab initio molecular dynamic simulation of a silica surface

C.Mischler[1], **W.Kob**[2] **and K. Binder**[1]

[1]*Institut für Physik, WA 331; Johannes Gutenberg-Universität*
55099 Mainz; Germany
[2]*Laboratoire des Verres, Universite Montpellier II*
34000 Montpellier; France
Tel: [++49] 6131 392-3643, Fax: [++49] 6131 392-5441
e-mail: mischler@plato.physik.uni-mainz.de

We present both classical molecular dynamic simulation and *ab initio* molecular dynamic simulation of silica surfaces. In the case of the classical Molecular Dynamic Simulation we use the so called BKS-potential which was developed by van Beest, Kramer and van Santen [1]. First we checked, if it is possible to simulate a silica surface by using a sandwich-geometry [2]. Such a geometry consists of the normal system and a variable empty space in one direction (e.g in z-direction). Furthermore we assume periodic boundary conditions (pbc) in three dimensions. The advantage of such a geometry is, that the calculation of the long range coloumb interaction is much faster for systems with pbc in three dimensions than for systems with pbc in only two dimensions. In order to restrict the size of the simulation box we have made some further simpli£cations. First we have cut the system perpendicular to the z-direction and have saturated the free oxygen atoms by hydrogen atoms. At the end of this procedure we have a system of 91 oxygen, 43 silicon and 10 hydrogen atoms in a simulation box with $L_x = L_y = 11.51$ Å. In the z-direction the dimension is approximately 18 Å. By using the sandwich-geometry we add in the z-direction an empty space between 4 Å and 10 Å. In our case a classical MD-Simulation of a system with pbc in three dimension is nearly six times faster than for the same system with pbc in two dimensions. Also the CPU time hardly depends on the size of the empty space. The test of static properties (e.g. pair-correlation-functions, angles distributions, coordination-defects and ring-length) shows, that for an empty space around 6 Å the static properties of the systems with pbc in three dimensions (sandwich-geometry) are in good agreement to those with pbc in two dimensions.
The BKS-potential, which we use for our classical MD-simulations has been shown to be very reliable for bulk-systems. However, it is not clear, if this effective potential takes into account the different charge density on the surface. To test this question we have compared the static properties of our system by using classical molecular simulation with Car-Parrinello-Simulation [3] results. It turns out, that the classical MD-results are in some case different from the *ab initio* MD-Simulation results, but this effects do not affect the bulk region. Concluding we can say, that it is possible to simulate a silica surface by using a sandwich-geometry and that the BKS-potential does not consider the different charge density on a surface, so that we have to use ab initio MD-simulation to study the surface properties exactly.

References

1. B.W.H.van Beest, G.J.Kramer and R.A.van Santen, Phys.Rev.Lett. **64**, 1955 (1990)
2. B.P.Feuston and S.H.Garofalini, J.Chem.Phys. **91**, 564 (1989)
3. R.Car, M.Parrinello, Phys.Rev.Lett. **55**, 2471 (1985)

A kinetic Monte Carlo method for the simulation of heteroepitaxial growth

F. Much, M. Ahr, M. Biehl, W. Kinzel

Julius-Maximilians-Universität Würzburg, Institut für Theoretische Physik und Astrophysik, Am Hubland 97074 Würzburg, Germany

+49 931 888 5139, +49 931 888 5141, much@physik.uni-wuerzburg.de

Common methods for the simulation of heteroepitaxial growth, like molecular dynamics, consume a lot of computer time and are therefore only practicable for rather small system sizes. On the other hand a lot of parameters are needed to include stress in faster methods like Kinetic Monte Carlo simulations (KMC) with a £xed lattice.

Here a simulation algorithm similar to [1] is introduced which allows the off-lattice simulation of various phenomena observed in heteroepitaxial growth (see e.g. [2]) like a *critical layer thickness* for the appearance of mis£t dislocations, or *self-assembled* island formation. The only parameters of the model are deposition ¤ux, simulation temperature and an interaction potential between the particles of the system.

Growth is simulated in $1+1$ dimensions using a rejection free KMC algorithm. The rate R_i for a diffusion event i is given by $R_i \propto exp\left[-E_{A,i}/\left(k_B T\right)\right]$, where $E_{A,i}$ is the activation barrier for this diffusion step and T the simulation temperature. The particles of the system interact pairwise via a *Lennard-Jones* potential with a characteristic length σ. Because of the isotropy of this interaction the particles arrange in a triangular lattice with a lattice constant proportional to σ. For that reason different values σ_S and σ_A denote different kinds of particles e.g. substrate and adsorbate. The activation barrier $E_{A,i}$ is then determined by calculating the binding and transition energy of a particle interacting with all other particles of the system within a certain range. To consider the elastic deformation of the crystal after each microscopic event (diffusion or deposition) the total potential energy of the system is minimized under variation of the particle coordinates. Using this algorithm we are able to simulate heteroepitaxial growth for a mis£t $-15\% \leq \varepsilon = (\sigma_A - \sigma_S)/\sigma_S \leq 15\%$.

We are able to determine the dependence of the *critical layer thickness* for the appearance of mis£t dislocations on the mis£t ε. Our results complement those of a molecular dynamics simulation study [3] which was done for a rather small system size and only a few different values of ε and are compared with theoretical treatments of the problem.

In the early stages of growth we £nd a *2D-3D transition* at the formation of islands depending on mis£t ε and temperature T. This transition is identi£ed with the self-assembled island formation in heteroepitaxial growth (see e.g. [4]).We observe that this transition takes place at a distinct 2D island size and discuss the dependence of this transition size on the mis£t ε. Furthermore we investigate the 3D island size distribution after the transition.

References

1. A. Schindler. Theoretical aspects of growth on one an two dimensional strained crystal surfaces. Dissertation, Duisburg, 1999.
2. P. Politi, G. Grenet, A. Marty, A. Ponchet, J. Villain. Instabilities in crystal growth by atomic or molecular beams. Phys. Rep. **324**, 271-404, 2000.
3. L. Dong, J. Schnitker, R.W. Smith, D.J. Srolovitz. Stress relaxation and mis£t dislocation nucleation in the growth of mis£tting £lms: A molecular dynamic simulation study. J. Appl. Phys. **83**, 217-227, 1998
4. A. Barabasi. Self-assembled island formation in heteroepitaxial growth. Appl. Phys. Lett. **70**, 2566, 1997.

Electronic structure of oxidized and oxygen de£cient SnO_2(110) surfaces

Matti A. Mäki-Jaskari and Tapio T. Rantala

Institute of Physics, Tampere University of Technology, P.O. Box 692, FIN-33101 Tampere, Finland

matti.maki-jaskari@tut.£

The surface properties of polycrystalline tin oxide and related metal oxide materials have a huge importance technologically. In the present state of research, accurate experimental determination of the surface structure and properties is hampered due to dependence of preparation conditions of the samples and due to need of nonconventional measurement techniques [1]. Therefore, theoretical and especially *ab-initio* methods can give an insight to the surface structure and properties in this connection

We study, using £rst principles density functional and plane wave - pseudopotential methods [2, 3], ideal and defected (110) surfaces of tin dioxide [4]. The densities of states of the surface systems are evaluated and compared. Also, ultraviolet optical constants are determined, and compared to experiments.

In case of the stoichiometric surface, the bridging oxygens contribute to occupied states near the top of the bulk valence band. In case of oxygen de£cient surfaces, £lled states appear higher in the band gap, and are associated with weakly localized electron density of the rehybridized tin Sn^{2+} ions, depending on the oxygen de£ciency. In agreement with other density functional calculations our results with different pseudopotentials, predict similar surface relaxation.

The ultraviolet optical properties based on the calculation of dipole transition matrix elements with a scissor correction, allows relatively accurate predictions to be made for the absorption. The surface contributes to the optical spectra by shifting the absorption edge to lower energy (below 4eV) due to band gap states. A signi£cant low energy absorption peak appears below the bulk absorption edge of SnO_2 and it is pronounced in a case of oxygen de£ciency.

References

1. V.E.Henrich and P.A.Cox, *The surface science of metal oxides*, (Cambridge Cambridge University Press 1994).
2. D.Vanderbilt, Phys. Rev.B **41**, 7892 (1990).
3. M.Teter, Phys.Rev.B **48**, 5031 (1993).
4. M.A.Mäki-Jaskari and T.T.Rantala, submitted.

Theoretical calculations of the energy dissipation in complex luminescence centers in ion-covalent oxide crystals

Nedilko S.G.

Physics Faculty, Taras Shevcheenko National Kyiv University 6, acad. Hlushkov Ave., 03680 Kyiv, Ukraine

+380 44 2664036, +380 44 2664036, nedelko@ups.kiev.ua

Study of absorption and emission processes in local centers formed by molecular anions in dielectric crystals allowed to establish their structure and common properties. The recent results have shown that total combination of formed centers is very complicated. It contains, besides isolated centers, also centers of complex structures containing molecular anion, as a core of the center, and a defect. Complex character of structure of luminescent center leads essential deformations of crystal matrix those cause strong static and dynamic gradient of crystal £eld close to local center. The last factor can change rate of non-radiation relaxation of energy of excited states and therefore changes characteristics of kinetic and temperature quenching of luminescence.

Parameters which characterize processes of electron energy dissipation in the several emission centers were founded from experimental investigations. We have proposed physical model of luminescence participation of two or more excited levels in the emission, one of which is metastable. The second is caused by existence of two minimums in the excited state potential. Such feature of excited state of complex centers is revealed in speci£c dependencies of intensity and decay time was versus temperature. Experimental data have been £tted to theoretical calculations which were also performed in assumption about spin-lattice relaxation processes between excited levels. Inasmuch as theoretical model requires consideration of a many factors, then a number of computer simulation procedures was necessary for correlation with experimental data and dependencies.

Phase-£eld modelling of multi-phase solidi£cation

Britta Nestler

Giesserei-Institut, RWTH Aachen, Intzestrasse 5, D–52072 Aachen, Germany

Phone: +49 241 804067, fax number, Fax: +49 241 8888 276,

e-mail: b.nestler@gi.rwth-aachen.de

The phase-£eld methodology has achieved considerable importance in modelling and numerically simulating a range of phase transitions and complex growth structures that occur during solidi£cation. In particular, they offer the promise of a formulation particularly suitable for the numerical simulation of the temporal evolution of complex interface shapes associated with realistic features of solidi£cation of alloys. In recent years, the phase-£eld methodology has been extended to describe the evolution of multiple interfaces. The phase-£eld model discussed in this paper is based on an ad hoc model formulation for binary three phase systems originally proposed in [1]. This model was further developed to include anisotropy, to describe binary eutectics [2] and its sharp interface asymptotic limit was studied in [3] and [4].

A new phase-£eld model for a general class of multi-component multi-phase metallic alloys is now proposed which describes both, multi-phase solidi£cation phenomena as well as polycrystalline grain structures. The model serves as a computational method to simulate the motion and kinetics of multiple phase boundaries and enables the visualization of the diffusion processes and of the phase transformations in multi-component multi-phase systems. In the asymptotic limit of vanishing interfacial thickness, the diffuse interface (phase-£eld) model can be related to classical sharp interface models. This analysis ensures that the phase-£eld model recovers physical laws at phase boundaries and multiple junctions. Numerical simulations are presented which illustrate the capability of the phase-£eld model to recover a variety of complex experimental growth structures. In particular, the phase-£eld model is used to simulate phase transformations and microstructure evolutions in eutectic, peritectic and monotectic alloys. Within this context, £rst application of the model to multi-component (ternary) multi-phase systems will be shown. In addition, polycrystalline grain structures with effects such as wetting, grain growth, coarsening, symmetry properties of adjacent triple junctions in thin £lm samples and stability criteria at multiple junctions are described by phase-£eld simulations. Based on these twodimensional results, simulations in three dimensions and the incorporation of convection and elasticity into the phase-£eld model are planned for future developments.

References

1. I. Steinbach, F. Pezzolla, B. Nestler, M. Seesselberg, R. Prieler, G. J. Schmitz and J. L. L. Rezende, 1996, Physica D, **94**, 135–147
2. B. Nestler and A. A. Wheeler, Physica D, **138**, 114-133 (2000)
3. H. Garcke, B. Nestler and B. Stoth, 1998, Physica D **115**, 87 - 108
4. B. Nestler and A. A. Wheeler, 1998, Phys. Rev. E **57**, No. 3, 2602 - 2609

Band structure of the orthorhombic indium chloride

M.I. Kolinko and A.H. Nevidomskyy

Physics Faculty, Ivan Franko National University of Lviv,
1 Universytetska str., Lviv 79602, Ukraine

tel: +380 322 744127, fax: +380 322 727981, e-mail:kolinko@franko.lviv.ua

The layered InCl single crystals belong to the A^3B^7 family of compounds and their high temperature, red phase, which is actual above the point of the £rst-order phase transitions (120°C), crystallizes in orthorhombic structure of TlI-type (space group Cmcm). Its band structure has not been yet reported, thus the £rst-principle calculations are required to investigate the properties of this semiconducting compound.

For the £rst time the band dispersion in $\mathbf{k}$-space has been obtained and the fundamental optical properties of the high-temperature modi£cation of InCl have been analyzed in this work. This is the more actual if one takes into account a very small amount of experimental papers on this compound. The results that we have obtained can help to settle some principle issues of chemical bonding and structural peculiarities of InCl crystals.

In order to get the precise band structure and electron charge density distribution $\rho(\mathbf{r})$ the ab-initio self-consistent calculations in the local density approximation (LDA) have been performed using the non-local norm-conserving pseudopotentials from [1]. To obtain the band diagram $E(\mathbf{k})$ after self-consistent potential determination, the energies have been tabulated at 535 points localized at edges and high-symmetry lines in the irreducible part of the Brillouin zone. In the calculation of density of states the tetrahedron integration method was used. The theoretical framework and main approximations used are presented elsewhere (see e.g. [2],[3]).

The smallest interband intervals of the forbidden gap are formed far from the Γ point. This typical gaps location peculiarity at the periphery of the Brillouin zone arises immediately from the electronic con£guration of these compounds with their surplus cation s-electron pair. The smallest direct gap is located at the Σ line and amounts to 2.49 eV ($\Sigma_{4,v} \rightarrow \Sigma_{1,c}$ for $\mathbf{E} \parallel \mathbf{b}$ polarization). However, the bottom of the conduction band at 2.39 eV is localized at the Σ^* point (and at the equivalent C^* point). In such a way, rhombic InCl is an indirect semiconductor. Although usually band gaps are underestimated seriously in the LDA, in the case of InCl it turns out a good agreement with experiment ($\sim$ 2.4 eV). The contour lines of $\rho(\mathbf{r})$ obtained demonstrate the simultaneous coexistence of covalent and ionic types of chemical bonding. The fact that an excess charge accumulates between In atoms of different layers and forms a weak interlayer bond is of interest. It can explain unusually short distances between cations in this crystal, that were reported. The genetic origin of certain bands was determined as well on the basis of their partial contributions into the total charge density distribution. The role of certain groups of electrons in bonding interactions has been shown. The density of states of InCl has been calculated as well. The appearance in the future of the experimental data of x-ray photoemission spectroscopy will make it possible to associate them with the calculated density of states.

For the £rst time the results were presented for the valence and conduction band energies, density of states and charge density distribution of red modi£cation of InCl single crystals.

References

1. G.B. Bachelet, D.R. Hamann, M. Schlüter, Phys. Rev. B. **26**, 4199 (1982)
2. P.E. Van Camp, V.E. Van Doren and J.T. Devreese, Phys. Status Solidi b **146**, 573 (1988)
3. M.I. Kolinko, J. Phys.: Condens. Matter **6**, 183 (1994)

Kinetics of ordering during codeposition

Jun Ni and Binglin Gu

Department of Physics, Tsinghua University,
Beijing 100084, P.R.China

fax:(8610)62781604, email:junni@mail.tsinghua.edu.cn

Nonequilibrium kinetics of materials plays an important role in materials growth. In recent years, new experimental methods such as rapid quenching, laser processing, ion beam bombardment and various epitaxial processes have been used to prepare materials that are in nonequilibrium state thermodynamically. The long-range ordering in metal alloys and ternary III-V semiconductor alloys has been observed during epitaxial growth and extensively studied. In the epitaxial growth the layer-by-layer stacking process is a kinetic processes involving the adsorption, evaporation, and surface diffusion.[1, 2, 3] .The ordering-disordering processes of the surface for the epitaxial growth on a (001) substrate of system such as CuAu alloy, ternary III-V semiconductor alloys is a kinetic process of the system on the square lattice. In the present work, we study the kinetics of ordering in alloys during codeposition. We consider monolayer codeposition of two atomic species onto an fcc (001) crystal surface. The system is descibed by the stochastic lattice gas model with nearest neighbor and next nearest neighbor interactions. In epitaxial growth, the surface kinetic processes comprises the relaxation processes such as the adsorption and the evaporation, and the surface diffusion processes. The adsorption and the evaporation are described by the single-site relaxation processes[1, 2] The kinetics of ordering is described by the micro-master equation method in the pair approximation.[4, 5] In order to describe the ordering of the system with the nearest-neighbor and next-nearest-neighbor interactions, we divide the square lattice into four sublattices. There are 22 independent pair distribution functions which are characterized by 10 long-range order parameters and 12 short-range order parameters. The differential equations describing the kinetics of the system are integrated numerically using the Gear's method appropriate to the stiff differential equations. There are three kinds of ordered phases in equilibrium state. The evolutions of the long-range order and short-range order parameters during codeposition are calculated. There are different types of the kinetic path depending on the interaction and relaxation parameters. The kinetics of the system is controlled by three charateristic times, the adsorption rate and the jumping rates of two atomic species. It is found that there are transient ordered states during the codeposition. The occurrence of the transient states depend on both the adsorption rate and the atomic jumping rates. The kinetic path involves various stages of relaxation. The transient ordered states make the evolutions to exhibit distinct features for different equilibrium phase regions. The correlation also has signi£cant effects on the evolutions It is found that the short-range order relaxes gradually in the ordering stage of transient ordered state in contrast to the fast change of the short-range order in the ordering stage of the equilibrium phase. This property of short-range order for the transient ordered state is also different with that of long-range order which has a very fast initial change for both the transient ordered state and equilibrium phase.

References

1. Y.Saito and H.Mueller-Krumbhaar J.Chem.Phys. **70**, 1078 (1979).
2. R. Venkatasubramanian, J. Mater. Res. **7**, 1023 (1992).
3. Jr.J.R.Smith and A. Zangwill, Phys.Rev.Lett. **76**, 2097 (1996).
4. L.Q.Chen and J.A.Simmons, Acta Metall. Mater. **42**, 2943 (1994).
5. J.Ni and B.L.Gu, J.Chem.Phys. **113**, 10272 (2000).

Stochastic dynamics for switching between the metastable state and the ground state in photoinduced phase transition

Masamichi Nishino and Seiji Miyashita

Department of Applied Physics, Graduate School of Engineering,
The University of Tokyo, Bunkyo-ku, Tokyo, Japan

+81-3-5841-6865, +81-3-5841-6849, nishino@spin.t.u-tokyo.ac.jp

Photoinduced phase transition (PIPT) has become one of topics in the condensed matter physics [1, 2]. PIPT is accompanied by a structural phase transition as observed in TTF-CA [2] or by a magnetic phase transition as observed in Co-Fe complex [1]. Because the energy level of the low spin state of such a complex gets cross to that of the high spin state, the spin state can be changed between these states by stimulus due to changes of temperature, pressure, photoexcitation, etc.

We have been studying such dynamics of the phase transition from the viewpoint of statistical physics [3, 4]. We adopt a stochastic dynamics using the master equation. There can be several factors which dominate the switching dynamics. Her we adopt the following two cases.
(I)the distortional energy is important to induce the phase transition. In several experiments, the lattice constant changes after illumination. Here we assume that when a site in the high spin state neighbors a site in the low spin state, the lattice distortional energy becomes larger than in the other cases. Then, we can express the effect of illumination by a £eld that causes the symmetry breaking. In this case we can show the switching between the low spin state and the high spin state.

(II)the magnetic interaction is important to induce the phase transition.
We consider switching between the stable nonmagnetic state and the metastable ferromagnetic state. Switching from the stable nonmagnetic state to the metastable magnetic state con¤icts with the thermodynamic stability and it is considered to be dif£cult to realize as far as we apply only symmetric disturbance, e.g., illumination. We consider how the two-way switching is realized in a symmetric applied £eld. Here we adopt a stochastic dynamics with multi-time scales. For this purpose, we will extend the Glauber dynamics to introduce a more complicated relaxation process. We demonstrate that the switching can be realized.

References

1. O.Sato, T.Iyoda, A. Fujishima, and K. Hashimoto, Science **272**, 704 (1996).
2. S. Koshihara, Y. Takahashi, H. Sakai, Y. Tokura, and T. Luty, J. Phys. Chem. B 103, 2592 (1999).
3. M. Nishino, K. Yamaguchi, and S. Miyashita, Phys. Rev. B **58**, 9303 (1998).
4. M. Nishino and S. Miyashita, Phys. Rev. B **63**, 174404-1 (2001).

Image analysis of composite £lms

S. Novák[1], R. Hrach[2,1] and M. Sobotka[2]

[1] *Faculty of Education, J. E. Purkyně University, České mládeže 8, 400 96 Ústí nad Labem, Czech Republic*

[2] *Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, 180 00 Prague 8, Czech Republic*

+420 47 5214417, +420 47 5212053, novaks@pf.ujep.cz

Composite metal/dielectric £lms consisting of metal particles embedded into an oxide or polymer matrix have received more and more attention in last few years - e.g. [1], [2], due to their interesting optical and electrical properties. These properties are also determined by £lm morphology - by the form of metal objects, by their concentration and by their distribution in dielectric matrix, therefore the morphological analysis of these £lms is very important. The algorithms for the image analysis of the micrographs of two-dimensional (2D) metal £lms based on the theory of mathematical morphology are well suited for the morphological description of these £lms. However, the methods for quantitative characterisation of composite £lm morphology are being invented. If the micrographs, i.e. projections, of composite £lms from the transmission electron microscopes are used as a main source of morphological information, part of information is lost and the complete reconstruction of 3D arrangement of objects cannot be performed. Contrary to computer tomography, where sets of projections made under various angles are used, in the image analysis of composite £lms the combination of a projection and one or more sections must be used. First attempts to perform such analysis were made a long ago - e.g. [3], however, only present computational methods and resources can give satisfactory results.

The complete goal of the image analysis of composite £lms is to derive spatial characteristics as the object concentration, the distribution function of the characteristic dimensions of objects (or at least the mean dimension), and the distribution of objects in 3D. The basic morphological analysis of such £lms can be performed analytically for the structures with low metal volume fraction and supposing metal particles are spherical and randomly distributed in the dielectric matrix. However, in more complex cases the analysis with the help of computer models is much more convenient [4]. Although under some experimental conditions, e.g. in plasmachemical technologies, the composite £lms with randomly distributed spherical particles can be prepared, much more probable are £lms with either spherical particles of various diameters, or even particles with non-spherical forms. Moreover, these particles can be placed with some spatial distribution - either isotropic or with some preferred orientation - in a matrix.

In our contribution, we studied the unfolding problems arising from the image analysis of composite £lms with non-uniform structure. Our two main tasks were to gain information about the size distribution of spherical objects and about the 3D spatial distribution of objects in isotropic systems. A modi£ed hard-disk model of composite £lm was prepared for the analysis of in¤uence of £lm parameters on various morphological algorithms. This method enabled us to select the convenient algorithms as well as to derive their sensitivity for various types of composite £lms. The £rst ideas of the morphological analysis of the most general composite £lms (irregular objects, non-isotropic £lms) are presented in the last part of our contribution.

References

1. Ichinohe T. et al., Thin Solid Films 343-344 (1999), 119.
2. Biederman H. et al., Thin Solid Films 351 (1999), 151.
3. Wicksell S. D., Biometrika 17 (1925), 84.
4. Novák S., Hrach R., Thin Solid Films 373 (2000), 203.

Incommensurate phases in adsorbed monolayers: structure and energy of domain-walls

A. Patrykiejew[1] **S. Sokołowski**[1] **K. Binder**[2]

[1]*Faculty of Chemistry, MCS University, 20031 Lublin, Poland.*
[2]*Institut für Physik, Johannes-Gutenberg-Universität Mainz, 55099 Mainz, Germany.*
tel. +48 81 537 56 87, fax +48 81 533 33 48, e-mail andrzej@miki.umcs.lublin.pl

In our recent paper [1], possible ground state structures of monolayer £lms adsorbed on the (100) plane of fcc crystals have been discussed. Monte Carlo simulation method has been used to investigate the formation of various incommensurate structures in the £lms of different density and subjected to the surface potential of different strength. It has been demonstrated that incommensurate phases with well developed domain-wall structures may appear in adsorbed £lms, even when the corrugation of the surface potential is strong. The particles which belong to the walls exhibit rather large in-plane ($\Delta x, \Delta y$) and out of plane (Δz) displacements from the registry positions.

The problem that has not been discussed in [1] is the estimation of the domain-wall energies and the interaction between walls [2, 3]. Another question concerns the conditions under which the domain-walls are localized (delocalized). In the case of localized walls only the particles right in the core of the wall show deviations from the commensurate lattice positions. On the other hand, when the wall is delocalized then the displacement £eld ($\Delta x, \Delta y, \Delta z$) is expected to be a slowly decaying function of a distance from the wall core.

The above two problems are the subject of the present work. First, we consider the effects of the surface potential properties (its strength and corrugation) on the structure and energy of domain walls. Different types of incommensurate phases with stripe-like domains separated by parallel walls as well as with rectangular domains separated by crossing walls are discussed. Then, we concentrate on the changes of the structure and properties of domain walls resulting from the changes in the mis£t between the adsorbate and the surface lattice.

We estimate wall energies, energy contributions due to wall crossings and discuss the interaction between walls. Also, we address the problem of the stability of incommensurate structures in £lms formed on surfaces characterized by a strong corrugation potential.

References

1. A. Patrykiejew, S. Sokołowski, K. Binder, J. Chem. Phys. (submitted)
2. J. M. Houlrik, D. P. Landau, Phys. Rev. B 44 (1991) 8962.
3. M. E. Fisher, A. M. Szpilka, Phys. Rev. B 36 (1987) 644.

Hybrid computer modelling of plasma oxidation process

R. Hrach[1,2], M. Vicher[1,2] and J. Pavlík[2]

[1]*Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, 180 00 Prague 8, Czech Republic*
[2]*Faculty of Education, J. E. Purkyně University, České mládeže 8, 400 96 Ústi nad Labem, Czech Republic*
+420 47 5214417, +420 47 5212053, pavlikj@pf.ujep.cz

In plasma chemistry the oxidation of metals belongs to one of the most important technologies [1], therefore it is necessary to obtain full information about physical and chemical mechanisms taking part during the interaction of oxygen plasma with substrates. However, the plasma oxidation represents a complex process consisting of several stages - activation of oxygen in the discharge, transport of charged particles from the undisturbed plasma to metal substrate immersed into plasma, surface processes on the substrate and the transport of both oxygen and metal ions through the growing oxide layer.

For the analysis and optimisation of the plasma oxidation process the combination of experiments (based on rather sophisticated diagnostic methods) and computer modelling is typically used. The complete computer experiment, which ought to describe the oxidation process in full extent, cannot be created by one program only - it must be formed by several individual programs based on various computational methods. Our computer experiment describing the plasma oxidation of aluminium in the oxygen/argon glow discharge consisted of:

- model of physical and chemical processes in the bulk of oxygen/argon plasma (more than one hundred reactions between neutral, charged and excited particles of oxygen, argon and mixture oxygen-argon) - based on a macroscopic kinetic approach, e.g. [2]

- transport of charged species from undisturbed plasma through the boundary layer, sheath and presheath, in the vicinity of metal substrate - based on the particle modelling technique (PIC-MC method), e.g. [3]

- model of plasma-solid interaction including basic processes on the substrate (impingement of charged particles, their absorption, re¤ection and secondary emission) and processes in the growing oxide £lm (diffusion of negative oxide ions and positive aluminium ions through the oxide layer under the in¤uence of voltage bias applied to metal substrate) - these models are based on the combination of particle and ¤uid approaches.

Our main attention was devoted both to evaluation of the in¤uence of individual reactions and scattering processes in the sheath region of plasma on the quality of the oxidation process and to various techniques of computational physics used during the computer experiment. While the individual techniques are known enough, the combination of such different approaches brings problems into the computer experiment. Therefore the coordination of these procedures is discussed in detail.

References

1. Siejka J., Perriere J., Plasma Oxidation. In Physics of Thin Films, Vol. 14, Academic Press Inc., Boston (1989), p. 81.
2. Legrand J.-C. et al., Vacuum 48 (1997), 671.
3. Birdsall C. K., Langdon A. B., Plasma Physics via Computer Simulation. Adam Hilger, Bristol (1991).

Surface effects in GaN growth

C. A. Pignedoli[1], R. Di Felice[1] and C. M. Bertoni[1]

[1]*INFM Unitá di Modena and Dipartimento di Fisica, Universitá di Modena e Reggio Emilia, via Campi 213 A 41100 Modena Italy*

0039-059-2055283, 0039-059-367488, pigna@unimo.it

Group-III nitrides are suitable semiconductors to build electronic and optoelectronic devices due to their stability at high temperatures, to the high carrier mobility, and to their outstanding optical properties. Alloys based on III-V nitrides are used to fabricate materials with electronic band-gaps ranging from $1.9\,eV$ to $6.2\,eV$ [1]. GaN can also be employed to fabricate high power transistors. The dif£culty of growing good quality £lms represents a limitation in the development of GaN-based technology. To improve material quality, it is helpful to understand the mechanisms governing the growth, and a tool to pursue such investigation is given by ab-initio simulations. The use of NH_3 as the nitrogen precursor and of H_2 as the carrier gas in MOCVD, and the strong dependence of the growth ef£ciency on the temperature and on the interactions between H and NH_2 groups adsorbed at the surface, suggested to study mechanisms for the chemisorption of NH_3 at the GaN(0001) surfaces as indicative for the growth process, consistently with previous works on NH_2 and H adsorption on GaN$(10\bar{1}0)$ [2] and GaN$(000\bar{1})$ [3].

We performed ab-initio calculations of the equilibrium structure for several GaN(0001) surfaces containing NH_2 groups and H atoms bonded to both Ga and N atoms. The total energy was obtained in the frame of Density Functional Theory in the Local Density Approximation. The ions were described by pseudopotentials, and Non Local Core Corrections were included for the Ga species. By minimizing the energy with respect to the atomic positions and the electronic wavefunctions, using plane wave expansions with a cutoff of 60 Ry, we obtained several metastable con£gurations. We used repeated supercells with 2×2 surface periodicity containing 8 GaN layers, 1 layer of pseudo-hydrogen atoms to saturate the N bonds at the $(000\bar{1})$ bottom surface, 13 Å of vacuum hosting the adsorbed species.

We studied the following cases: clean surface with a Ga adatom and clean surface with a N adatom [4], *hydrogenated* surface with $\frac{3}{4}$ ML of H adsorbed on topmost Ga atoms, *nitridated* surfaces with one NH_2 group adsorbed on a surface Ga and zero, one, and three hydrogen atoms surrounding a surface Ga vacancy. The relative formation energy of the different samples, with respect to a stable clean surface, was calculated as a function of the chemical potential of Ga, N and H. Our results reveal that growth of GaN under N-rich conditions may result in a defective £lm: in fact, *nitridated* surfaces result stable inducing subsurface hydrogen incorporation. We suggest Ga and H rich condition for the growth of good-quality £lms: in this case, the *hydrogenated* surface is favored, with a ¤at 1×1 like geometry.

We £nally performed dynamical simulations for a NH_3 molecule impinging on an ideal Ga-terminated GaN(0001) surface and on a 2×2 GaN(0001) surface with a Ga vacancy. The observed dissociation of the molecule into NH_2 and H and the evolution of the system supported the results of the static investigation.

This work was supported by INFM under the PRA 1MESS.

References

1. F. A. Ponce and D. P. Bour, Nature **386**, (1997) 351-359.
2. J. E. Northrup and R. Di Felice, Jörg Neugebauer, *Phys. Rev. B* **56**, R4325 (1997).
3. J. Fritsch, O. F. Sankey, K. E. Schmidt, J. B. Page, *Surf. Sci.* **427 428**, 298-303 (1999).
4. A. R. Smith, R. M. Feenstra, D. W. Greve, J. Neugebauer, and J. E. Northrup, Phys. Rev. Lett. **79,** (1997) 3934-3937.

Charge dependence of temperature-driven phase transitions of molecular nanoclusters: molecular dynamics simulation

S. Pisov and A. Proykova

University of So£a, Faculty of Physics, 5 James Bourchier Blvd., So£a-1126, Bulgaria

tel: (+359 2) 688176, fax: (+359 2) 9625276, anap@phys.uni-so£a.bg

Small free clusters of atoms or molecules exhibit solid-like or liquid-like properties that differ from the properties of their bulk counterpart. It has been realized that the cluster structure (microcrystalline or amorphous), [1, 2] depends on the production method. Some of the microcrystalline states coexist dynamically [3] in a given temperature interval and those, which are only locally stable phases, disappear when the temperature increases as it was con£rmed both experimentally [1] and theoretically [3]. Those states correspond to a partial order of the molecular axes of symmetry. The system becomes completely ordered at very low temperatures. The transition rate between the ordered and disordered states can be retrieved from the potential energy surface (PES) of the system, [4]. It has been shown in [3] that clusters of the same numbers of molecules, having the same symmetry but different size exhibit different dynamics.

In the present study we explore the changes of the cluster PES due to the changes of the charge distribution in a single molecule. Our hypothesis is that the molecular polarization is changed by using different production methods. In order to £nd out the in¤uence of the charge changes on orientational order-disorder phase transitions we have simulated the temperature behavior of molecular clusters with the help of a constant energy molecular dynamics. The intermolecular potential is a sum of atom-atom interaction (¤uorine-¤uorine, tellurium-tellurium, ¤uorine-tellurium) :

$$U_{pw}(i,j) = \sum_{\alpha,\beta=1}^{7} \left[4\,\epsilon_{\alpha\beta} \left[\left(\frac{\sigma_{\alpha\beta}}{r_{ij}^{\alpha\beta}} \right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r_{ij}^{\alpha\beta}} \right)^{6} \right] + \frac{q_{i\alpha} q_{j\beta}}{4\pi\epsilon_0 r_{ij}^{\alpha\beta}} \right]$$

$$U_{pot} = \sum_{i,j=1\,(i<j)}^{n} U_{pw}(i,j)$$

The parameters $\sigma_{\alpha\beta}$ and $\epsilon_{\alpha\beta}$ are chosen to £t the experimental diffraction results, [2].

The Coulomb term takes into account the small negative charge q_F assigned to the ¤uorine atoms. Here we compare the temperature-driven transitions for the case of $q_F = 0.1e$ and $q_F = 0.25e$, where e is the electron charge.

Our results show that the charge increase shifts the transitions temperature towards higher values and some of the meta-stable states disappear. This con£rms our understanding that the repulsive interaction maintains the order in molecular systems.

References

1. E. Lefterova, I. Dragieva, V. Tchanev, D. Mehandjiev, M. Mikhov, Journal of Magn. and Magn. Mat. 140-144 (1995) 457-458
2. L.S. Bartell and Shimin Xu, J. Phys. Chem. **95** 8939 (1991).
3. S. Pisov and A. Proykova, in Proc. of the Meeting of Young Researchers in Physics, Heron Press 2001
4. K.D. Ball, R.S. Berry, R.E. Kunz, F.Y. Li, A. Proykova, D. Wales, Science Vol.271 877-1024 (1996) 963-965

Parallel J-W Monte Carlo simulations of thermal phase changes in £nite-size systems

R. Radev and A. Proykova

Department of Atomic Physics, University of So£a, So£a-1126, 5 J. Bourchier Blv.
tel:+359-2-688176, fax: +359-2-9625276, anap@phys.uni-so£a.bg

The interest in temperature driven phase transitions in £nite systems is two-fold: £rst, bulk properties of the material can be simulated if the system is studied under periodic boundary conditions [1] and a proper account for rounding and shifting of the measurable quantities is taken in the analysis. Second, free £nite systems, such as molecular clusters, are of interest due to their peculiar properties, which are not observed in bulk systems of the same substance [2].

The results obtained with the help of MD calculations point out that the system is frequently trapped in a local minimum on the potential energy surface for times longer than any realistic computational times. This would cause incomplete spanning of the phase space in the simulations if a special care is not taken.

One way to overcome the problem of a poor sampling in the case of rugged PES is to use the jump-walking technique [3].

In practice, J-walking technique can be implemented in two ways. The £rst approach is to write the con£gurations from the simulation at the J-walking temperature to an external £le and access these con£gurations randomly £le while carrying out a simulation at the lower temperature. It is necessary to access the external £les randomly to avoid correlation errors. The large storage requirements limit the application of the method only to small systems. The second approach uses tandem walkers, one at a high temperature where Metropolis sampling is ergodic, and multiple walkers at lower temperatures.

The best features of these two approaches can be combined into a single J-walking algorithm with the use of multiple processors and the Message Passing Interface (MPI) library. We incorporate MPI functions into MC code to send and receive con£guration geometries and potential energies of the clusters. Instead of generating external distributions and storing them before the actual simulation, we generate the required distributions during simulation and pass them to the lower-temperature walkers.

The computer code has been ported, tested and optimized on SUN 3500 and CRAY-T3E machines. In our program has been implemented dynamic memory management for optimal usage of the memory. We £nd that memory and performance requirement make CRAY-T3E more suitable for such computations. In our runs we use 64 processors each with 64 MB RAM. Each run of 6.10^5 steps takes approximate 11h per CPU.

Using the parallel code described in the previous section we make set of production runs for 59 molecules clusters. A quantity examined is the heat capacity from the ¤uctuations of potential energy to characterize the phase transition. The result reveals a two-step transition as it was predicted by the MD calculation [4].

References

1. *Monte Carlo Methods in statistical physics*, edited by K. Binder (Springer - Berlin 1979).
2. A. Proykova and R. S. Berry, Z. Phys D. **40**, 215 (1997).
3. D.D. Frantz, D.L. Freeman, J.D. Doll, J. Chem. Phys. **93**, 2769 (1990)..
4. A. Proykova, R. Radev, Feng-Yin Li, R.S. Berry, J. Chem. Phys. **110**, 3887 (1999).

Computer modeling of processes of second harmonic generation and methods of their optimization in one-dimensional photonic bandgap structures

A.D. Pryamikov and V.A. Bushuev

Post-graduate student, M.V.Lomonosov Moscow State University, physical department, 119899 Moscow, Russia
Professor, M.V.Lomonosov Moscow State University, physical department, 119899 Moscow, Russia
(7-095)939-1226, fax (7-095) 939-0247, vab@runar.phys.msu.su

The study of one-, two- and three-dimensional periodic, dielectric structures – the so-called photonic band-gap (PBG) structures has developed successfully in the past few years. The essential property of these structures is an allowed and forbidden frequency bands and gaps, in analogy to the allowed and forbidden energy bands and gaps of semiconductors. We have concentrated our attention on study of one-dimensional nonlinear PBG structures having a great signi£cance for making new types of nonlinear-optical devices such as nonlinear optical diode, limiter, photonic band-edge laser.

For the £rst time phenomena of second harmonic (SH) generation and its enhancement in PBG structures was suggested in [1], then it was predicted in some works speci£cally in [2] that a strong enhancement of SH generation took place near the band-edge of a £nite one-dimensional PBG structure. In recent papers it were revealed two general mechanisms that had a decisive in¤uence on effectiveness of SH generation in nonlinear PBG structures. First of them is related to a strong concentration of electromagnetic energy of fundamental wave near the band-edge [3]. Second mechanism is due to so called phase-matching that is a condition of equality of phase velocities at frequencies of SH and fundamental wave. It was established that under these conditions the SH generation may be enhanced by several orders of magnitude compared to SH generation from a bulk sample of similar length.

A general purpose of our investigation was to develop further new calculation methods and techniques that are related to modeling of processes taking place in such one-dimensional PBG structures. Our £rst approach was based on optical transfer matrix techniques suggested in [4], the second one was a new in this £eld and it was derived from recurrent alignments used in theory of X-rays diffraction. Using these methods it was constructed a theory of SH generation and propagation in one-dimensional PBG structures and it was carried out a broad analysis of all mechanisms in¤uencing on effectiveness of SH generation. Moreover with the aid of this theory we found out some interesting special features of this phenomena concerning a strong enhancement of SH generation under different con£guration of PBG structure. One of the main point of our investigation was also a searching for optimization regimes of SH generation in PBG structures. Basing on our results it can be reached some optimization regimes and with the aid of them to increase suf£ciently an effectiveness of SH generation in PBG structures. In conclusion we can note that our results are in a good agreement with experimental data received in our University.

References

1. N. Bloembergen,A.J. Sievers Appl. Phys. Lett. 17, 483 (1970).
2. M. Scalora, M.J. Bloemer, A.S. Manka et al. Phys. Rev. A56, 3166 (1997).
3. A.V. Balakin, V.A. Bushuev, N.I. Koroteev et al. Optics Letters 24, 793 (1999).
4. D.S. Bethune J. Opt. Soc. Am. B6, 910 (1989).

Simulation of thermodynamic variables ¤uctuations in ¤uids by the molecular dynamics method

Rudyak V.Ya. and Kharlamov G.V.

Novosibirsk State University of Civil Engineering, Leningradskaya, 113, 630008, Novosibirsk, Russia

(3832)668014, fax: (3832)161107, rudyak@ngasu.nsk.su

The problem of the mathematical description of transport processes in high-dispersed ¤uids and colloids is connected with the study of the density, momentum and energy ¤uctuations in small volumes of ¤uid medium. A. Einstein's thermodynamic ¤uctuation theory, based on the Taylor expansion of the entropy variation, connected with the ¤uctuation, leads to the Gauss distribution of thermodynamic variables. This theory is invalid for small ¤uid volumes medium with a small number of molecules.

In present paper the results of the simulation of the statistical distributions of the density, momentum and energy ¤uctuation in small volumes of ¤uid, as well as modeling of the density, momentum and energy ¤uctuation relaxation are presented. We used the molecular dynamics method. The systematic study of the ¤uctuations in small volumes, including 5, 25, 100, 200, 300, 500 molecules with different density of the systems (α = 1.5; 2.0; 4.8. $\alpha = V/V_0$, V - volume of the cell, V_0 - close-packed speci£c volume) has been ful£lled. The whole number of the hard spheres in the modeled cell was equal $10^3 \div 5 \cdot 10^3$. Periodic boundary conditions has been used. It was shown that the molecules density ¤uctuations in small volumes follow the Gauss distribution. However the dispersion of this distribution is essentially differed from the value predicted by the classical theory. The results of simulation coincide with data of this theory only for large $< N >$ ($< N >$ is the particles number in studied subsystem).

The statistical distribution of the total momentum in a small volume of the ¤uid molecular systems also obeys the Gauss distribution. The distribution dispersion can be described by the following expression: $\sqrt{< p^2 >} = \sqrt{< N > kT}$ (T is the temperature of a system), which accords with the well-known physical ideas about hydrodynamic ¤uctuations.

The energy statistical distribution in the small ¤uid volume is not the Gauss one and has asymmetrical form. Nevertheless, if $< N >$ is growing, the distribution becomes more symmetrical and closer to the Gauss distribution. Thus, in present, the peculiarities have been discovered, of the density and energy statistical distribution in the small ¤uid volumes which can not be explained by the Einstein's thermodynamic theory.

The simple theory of simulated ¤uctuations is presented in the last part of the paper. Then we give the data of the investigation of the density, momentum and energy ¤uctuation relaxation in the small ¤uid volumes.

This work was supported by the Russian Foundation for Basic Researches (grants No. 00-15-96164).

Applications of cluster computing for the Anderson model of localization

P. Cain, F. Milde, R.A. Römer, and M. Schreiber

Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

+49 371 531 3146, +49 371 531 3151, r.roemer@physik.tu-chemnitz.de

Disordered systems represent a major challenge for modern computational methods. Due to their ubiquitous nature and their many applications, there is an ever growing need to understand the physics that governs their behavior [1]. Unfortunately, it is exactly their disordered nature that also makes any analytical approach and thus a simple mathematically tractable solution so very hard to come by. Nevertheless, in recent years a vast and extensive body of knowledge has been collected mainly based on extensive use of high-performance computing [1].

In the present paper, we will consider modern numerical approaches to the so-called Anderson model of localization [2], a paradigmatic quantum system of disordered electrons. For a simple cubic lattice with $N \times N \times N$ sites, we have to solve the Schrödinger equation, which is given in site representation as

$$\psi_{i-1,j,k} + \psi_{i+1,j,k} + \psi_{i,j-1,k} + \psi_{i,j+1,k} + \psi_{i,j,k-1} + \psi_{i,j,k+1} + \varepsilon_{i,j,k}\psi_{i,j,k} \;=\; E\psi_{i,j,k} \qquad (1)$$

with i, j, k denoting the Cartesian coordinates of a site and E an eigenvalue with wave vector $\vec{\psi}$. The disorder is encoded in the random potential site energies $\varepsilon_{i,j,k}$.

In this work, we review recent efforts in constructing algorithms that work on modern day computer systems using scalable distributed memory and cluster architectures [3]. The application of these methods has enabled us to compute localization properties and electronic wave functions with highest accuracy and for extremely large system sizes of up to 1367631 sites.

We consider parallelization strategies for the two most important algorithms used in numerical investigations of the Anderson model of localization. After a brief review of the physics of Anderson localization, we outline the Cullum-Willoughby implementation of the Lanczos diagonalization scheme (P-CWI) and the transfer-matrix method (P-TMM) used for the numerical characterization of localization properties. For applications of these algorithms to massively parallel cluster architectures, we develop and test various parallelization strategies. Both algorithms rely on fast matrix-vector multiplications and this part of the algorithms is ideally suited for a massively parallel approach. On the other hand, the ef£ciency of P-CWI is reduced due to the increasing communication between different sections of the matrix. Also, the ef£ciency of P-TMM is limited due to the required orthogonalization of all vectors with each other which necessarily implies a large communication effort.

Our results show that the application of parallel methods to the Anderson problem is useful when large system sizes have to be reached, *e.g.* for a special set of parameters such as $E = 0$ and $W_c = 16.5$ that characterize the MIT. There, we have been able to investigate hitherto unreached system sizes [4].

References

1. B. Kramer and A. MacKinnon, Rep. Prog. Phys. **56**, 1469 (1993).
2. P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
3. U. Elsner *et al.*, SIAM J. Sci. Comp. **20**, 2089 (1999), physics/9802009.
4. F. Milde, (2000), Dissertationsschrift, Technische Universität Chemnitz.

The dynamics of supercooled liquids in con£nement

Peter Scheidler[1], **Walter Kob**[2], **and Kurt Binder**[1]

[1] *Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, 55099 Mainz, Germany*

[2] *Laboratoire des Verres, Universite Montpellier II, 34000 Montpellier, France*

tel: +49-(0)6131-3925158, fax: +49-(0)6131-3925441, email: peter.scheidler@uni-mainz.de

Most liquids show upon cooling a strong increase of their relaxation times. At a certain temperature this time is so large that the system falls out of equilibrium and forms a glass. The investigation of this glass transition is currently a very active £eld of research since glasses are not only interesting from a scienti£c point of view but also from the one of application. One theoretical approach to describe this transition involves the existence of a diverging length scale. Hence in the past many investigations were done to identify such an increasing length scale. One type of approach was to study the dynamics of the glass forming liquid in con£ned geometries, such as narrow pores or thin £lms. The idea was to see how the £nite system size affects this dynamics and thus to be able to draw a conclusion for the existence of a growing length scale. The results obtained so far are rather mixed due to two problems which are experimentally dif£cult to control. One is the interaction of the liquid with the con£ning material since this interaction is usually not known. In addition there is the problem of the geometry of the con£nement since it is dif£cult to control this size with high precision. Since in computer simulations one can avoid both problems we have done extensive simulations to investigate the dynamics of liquids in con£nement.

In this work we present the results of a large scale computer simulation of a binary mixture of particles interacting via a Lennard-Jones (LJ) potential. Since we are mainly interested in the dynamics of the system we use molecular dynamics simulations, i.e. we solve the equations of motion for an N-particle system, to determine the relaxation properties of the liquid. In order to avoid that the structure of the con£ned liquid differs from the one in the bulk, we chose a wall which has the structure of the bulk liquid but whose particles do not move anymore. The geometries studied are tubes with various diameters and thin £lms. In both cases we observe a dramatic slowing down of the structural relaxation in terms of the decay of density ¤uctuations in the intermediate scattering function $F_{\mathrm{s}}(q,t)$ close to the wall. From this we can de£ne a characteristic relaxation time τ which shows a strong dependence on the distance from the wall. We £nd that for extended systems this z-dependence is a function of the distance only, i.e. does not depend on temperature, and depends only weakly on the type of con£nement. $\tau(z)$ is decribed empirically in two different ways, both of them leading to growing dynamical length scales in the supercooled liquid.

Structure of steps and small islands on Si(111):As

A. Antons, R. Berger, S. Blügel and K. Schroeder

Institut für Festkörperphysik, Forschungszentrum Jülich, D-52425 Jülich, Germany

02461-61-4068, fax number, K.Schroeder@fz-juelich.de

The energetically preferred structures of steps and small Si island on As covered Si(111) are studied using £rst-principles total energy calculations. On As covered Si(111) only doublelayer steps with 1×1 structure of the terraces are experimentally observed during growth[2]. One goal of our investigation of cluster evolution during Si homoepitaxy on Si(111):As is to obtain evidence for the transition from mono- to doublelayer growth during Si homoepitaxy on Si(111). Our investigations show that the reduction of the surface free-energy due to the surfactant leads to a vanishing critical island nucleation-size. A cluster of three Si atoms shows a trimer of As atoms on top of the Si atoms. A fourth Si atom added to the trimer replaces one of the As corner atoms pushing it to a second layer position where it binds to both As and Si. This leads to a transition from mono- to doublelayer growth with the addition of the fourth Si atom.

In difference to Si homoepitaxy, Ge adatoms diffuse far across the surface [3]. Thus the step-edge structure has a decisive in¤uence on the growth mode of Ge on Si(111):As. Ge will grow by step-¤ow mode if Ge is easily incorporated at the step edges or by island nucleation on the terrace otherwise[1]. Our investigations of the step edges show that the energetically preferred structure is obtained by replacing the second layer Si atoms at the exposed step edge-positions by As. This leads to a naturally three fold coordinated position of As at the $(11\bar{2})$ step edge and a two fold coordinated position of As with a formation of As dimers at the $(\bar{1}\bar{1}2)$ step edge. Since the As atoms at the step edges are in similar positions as on the terrace the step edges are passivated and Ge will likely show the same behaviour as on the terrace, i.e. Ge will not be easily incorporated at the step edges.

All calculations are carried out in the local density approximation with norm conserving, separable pseudopotentials and a plane wave basis set using our parallelized `EStCoMPP`-code on a Cray-T3E parallelcomputer[3].

References

1. D. Kandel and E. Kaxiras, Phys. Rev. Lett., 75, 175 (1996)
2. B. Voigtländer *et al.*, Phys. Rev. B, 51, 7583 (1995)
3. R. Berger *et al.*, NIC-Workshop ”Molecular Dynamics on parallel Computers”, Jülich, 08.-10. Februar 1999 (World Scienti£c 2000)

Fluctuations of steps on crystal surfaces

Walter Selke[1], **Ferenc Szalma**[2], **and Johannes Hager**[1]

[1] *Institut für Theoretische Physik, Technische Hochschule, D-52056 Aachen, Germany*

[2] *Institute for Theoretical Physics, Szeged University, H-6720 Szeged, Hungary*

+49-241-807029, +49-241-8888188, selke@physik.rwth-aachen.de

The dynamics of steps on crystal surfaces has attracted much interest in recent years, both experimentally and theoretically [1]. In our contribution, we shall present results of Monte Carlo simulations and random walk analyses studying the step ¤uctuations mainly in the framework of solid–on–solid (SOS) models. Characteristic asymptotic time laws depend on the microscopic mechanism for detachment and attachment of atoms at the steps. We shall consider the three limiting cases of step–edge diffusion, evaporation–condensation, and terrace diffusion. In particular, we study the dynamics of isolated steps of monoatomic height as well as pairs of non–crossing steps.

Exact enumeration of random walks provides the basis of our analysis of terrace diffusion, including the possibility of interactions between the diffusing adatom and the step as well as re¤ecting or adsorbing quenched obstacles on the terrace. We calculate the probability distribution of an atom to return to the step at a given distance from the detachment site. That distribution determines the time law governing the step ¤uctuations, as seen in related Monte Carlo simulations [2]. New results of extending the simulations to pairs of ascending steps will be presented as well, analyzing especially the time dependence of the separation of the two steps due to the competition between the entropic repulsion and the effective attraction due the exchange of atoms between the steps.

In the case of step–edge diffusion and evaporation–condensation kinetics, we performed Monte Carlo simulations on SOS models [3]. Among others, time–dependent correlation functions along steps and between steps have been computed, checking and extending predictions of a recent continuum theory [4]. In particular, the long–time behaviour is found to be describable by the classical theory of Mullins on the ¤attening of surface corrugations above roughening [3]. We also present new results on isolated steps with a £xed number of kinks, discussing resulting pro£les along the step and characteristic scaling properties, using random walk considerations as well as Monte Carlo techniques.

We should like to thank especially M. Bisani and S. Fischer for enjoyable cooperation, as well as the Deutsche Forschungsgemeinschaft and the Hungarian Scienti£c Research Fund for £nancial support.

References

1. H. C. Jeong and E. D. Williams, Surf. Sci. Rep. 34, 175 (1999).
2. M. Bisani and W. Selke, Surf. Sci. 437, 137 (1999).
3. F. Szalma, W. Selke, and S. Fischer, Physica A, in print (2001).
4. B. Blagojevic and P. M. Duxbury, Phys. Rev. E 60, 1279 (1999).

Non-unique universal distributions of largest cluster size at the percolation threshold

Parongama Sen

Department of Physics, University of Calcutta, 92 A. P. C. Road, Calcutta 700009, India.

paro@cucc.ernet.in, paro@cmp.saha.ernet.in

Universal distribution functions for clusters in dilute lattices are known to exist for the spanning cluster as well as for smaller clusters [1, 2] at the percolation threshold p_c. These distributions are in general non-Gaussian.

The distributions for spanning clusters at p_c and for the largest cluster below p_c [3, 4] are well-studied. We study the distribution of largest cluster sizes for two, three and four dimensional hypercubic lattices at p_c in an extensive numerical simulation. The study of the largest cluster size is an example of extreme value statistics, relevant to several physical problems. Our special interest is in the cases when the lattice does not span at p_c. We use the Hoshen-Kopelman algorithm for generating clusters and impose open boundary condition in general.

At the percolation threshold, a lattice is spanned with a certain probability $R(p_c)$ usually less than unity. We £nd that the universal distribution function P_{sp} of the largest cluster size and that of the spanning cluster size coincide for all practical purposes at p_c when the lattice spans. For the lattices which do not span at p_c, the largest cluster size distribution P_{ns} has an entirely different universal function, which cannot be obtained from P_{sp} using any trivial transformation. This is a counterintuitive phenomena observed for the £rst time. P_{ns} is also distinct from the distribution for the largest cluster sizes below p_c [3, 4]. Both P_{ns} and P_{sp}, however, can be £t to a conventional double exponential form[1] $f(x) = a\exp(-b/x^c)\exp(-dx^e)$ with different values of the exponents. For example, e for $P_{sp} \sim 10.8$ and for $P_{ns} \sim 3.0$ and $c \sim 1.5$ for P_{sp} and ~ 2.5 for P_{ns} in two dimensions. In higher dimensions, values of c and e are closer.

The total distribution, P_{tot} can be independently computed and is given by

$$P_{tot} = R(p_c)P_{sp} + (1 - R(p_c))P_{ns}.$$

This distribution has a non-conventional form and is not a simple analytical function in two dimensions. In three and four dimensions, it can again be £t to the double exponential form. This is again a novel feature as the total distributions in two and in higher dimensions have different characteristic behaviour. In fact, P_{tot} in higher dimensions bears no signature of being generated from two independent functions in contrast to the two dimensional case. The novel feature of P_{tot} in two dimenions is also present in the distribution of the second largest cluster in a lesser extent.

A detailed analysis of the ratio of the cumulants show that the non-conventional form of P_{tot} in two dimensions is consistent with the fact that the widths of P_{sp} and P_{ns} are comparable. In two dimensions, we repeat the study with helical boundary conditions, which shows similar features indicating that the results are not boundary condition dependent.

References

1. A. U. Neumann and S. Havlin, J. Stat Phys **52** 203 (1988).
2. P. Sen, J. Phys. A **32** 1623 (1999).
3. P. M. Duxbury and P. L. Leath, J. Phys. A **20** L411 (1987).
4. M. I. Zeifman and D. Ingman, J. App. Phys. **88** 76 (2000); M. Bazant, Phys. Rev. E **62** 1660 (2000).

Interlayer atomic diffusion as the reason for self-assembled quantum dots formation

D. V. Brunev, I. G. Neizvestny, N. L. Shwartz, Z. Sh. Yanovitskaya

Institute of Semiconductor Physics RAS SB, 13 pr.Lavrenteva, Novosibirsk, 630090, Russia

phone +7 3832 332961 e-mail: natasha@spy.isp.nsc.ru

Self-assembled quantum dots formation during heteroepitaxial growth has been attracting much attention in past decade. One of the possible kinetic mechanisms of 3D island formation during heteroepitaxy is considered. In¤uence of step energy barriers E_{st} (Schwoebel barriers) on surface relief formation during epitaxy was investigated by kinetic Monte Carlo model [1]. Diffusion hop probability to cross the step is changed by the factor $P = exp(-E_{st}/kT)$ as compared with diffusion hops at the same atomic level. Factor P_{up} changes probability of atom hops to the upper layers, and P_{down} — to the lower ones. Increase of nucleation rate of islands in the second monolayer was associated in [2] with such asymmetry of Schwoebel barriers in SiGe system. Phase diagram in coordinates P_{up} — P_{down} indicating different growth modes: 2D, Stransky-Krastanov and 3D was obtained. The change from 2D to 3D mode is determined only by the parameter $\chi = P_{up}/P_{down}$ and not by the absolute values P_{up}, P_{down}. For 3D island formation without wetting layer condition $\chi > 1$ is necessary.

Critical 2D nucleus size i^* was obtained for different growth regimes. The critical size of island i_{cr} when nucleation of new layer starts was of interest. Dependencies i^* and i_{cr} on χ show that as χ increases these sizes decrease approaching 1. From some χ, $i^* = i_{cr}$, that means 3D nucleation from the initial phase of growth. Dependence of expectation time for appearance of the nucleus of the second monolaeyr on 2D islands versus χ was exponential one.

3D islands without wetting layer demonstrate rather sharp size distribution. That is due to dependence of hops up to hops down ratio N_{up}/N_{down} on boundary length of islands. Such N_{up}/N_{down} variation is due to decrease of atoms capable to attach into descending island boundary because of their attachment to the island of upper layer. It is precisely this fact leads to 2D to 3D growth mode transformation during deposition process for χ value close to Stransky-Krastanov regime. Step density oscillations and their disappearance with time con£rm such transformation.

This work were supported by the Russian Foundation for Basic Research (N 99–02–16742) and the Federal Target-Orientated Program “Investigation and development of prospective science and technology lines for civil purposes”.

References

1. I. G. Neizvestny, L. N. Safronov, N. L. Shwartz, Z. Sh. Yanovitskaya, A. V. Zverev. Proceedings of the 8^{th} International Symposium Nanostructures: Physics and technology. St.Peterburg, Russia, June 19-23, 2000, P.129.
2. M. Kummer, B. Vogeli, T. Meyer, H. Kanel, Phys.Rev.Lett. 84 (2000) 107.

Usage of adaptive grids for Fokker-Planck model of rari£ed gas ionization in ECR plasma source

A. P. Smirnov and A. B. Shmelev
Moscow State University faculty of Computation Mathematics and Cybernetics, Russia
sap@cs.msu.su, shmelev@cs.msu.su

Recently the research of the plasma sources has been very popular. This can be explained by a wide variety of their technological applications. Different approches were used for the discharge investigation. Fokker-Plank approach for rari£ed gas ionization modelling allows computation of many important discharge characteristics. Comparatively to the hydrodynamics models it provides better accuracy as it allows taking into account real distribution function, which in many cases differs from the Maxwell distribution signiicantly. In our work [1] we observe such a model for Electron Energy Distribution Function (EEDF) for rari£ed gas ionization in plasma source. It takes into account the following effects: ECR heating in quasilinear approximation, energy losses and angular scatter due non elastic electron-atom collisionsionization and excitation of the gas atoms, electron angular scatter due to elastic collisions with the atoms, appearance of electrons due to ionization, electron-electron and electron-ion collisions and electron trapping with magnetic £eld and self-consistent ambipolar potential.

The problem is averaged over the space and from the mathematical point of view this is a two dimensional nonlinear parabolic equation with self consistent boundary (see [1] for details). Part of the boundary has a EEDF equal to zero boundary condition and part has a ¤ow through the bundary equal to zero condition.

Ambipolar potential in¤uences the cone of losses, which is re¤ected in the model by a moving boundary. During numerical solution this movement should be calculated very accurately as this is a critical parameter which de£nes many other important discharge characteristics, such as density and temperature. The problem is that the EEDF has an exponential behavior and small variations of the cone of losses position can have big impact. There can be two approaches to the solution of this problem the £rst is to take a larger grid for the numerical solution. The other one is two use adaptive grids.

In this work we examine both (larger grid and adaptive grids) possibilities, using this problem [1] as a testing model for comparison. We show that in some cases usage of adaptive grids can signi£cantly reduce the demands for the grid sizes for the same accuracy of the solution. Though the grid sizes for the two dimensional problems are not so big and can be easely used on modern computers without adaptive grids technology, for three dimensional problems, or problems with higher computational costs, the adaptive grids approach can simetimes be the only acceptable choice.

References

1. Reference No 1. A.P. Smirnov, N.V. Suetin and A.B. Shmelev Two-dimensional bounce-averaged Fokker-Planck modelling of an electron cyclotron resonance plasma source. J. Plasma Physics (1998) vol. 59, part 2.

Numerical solution of three-dimensional Poisson equation for electric £eld potential in the presence of set of conductors

A. P. Smirnov[1], **J. J. Oh**[2], **E. A. Sheina**[1], **J. K. Shin**[2] **and A. B. Shmelev**[1]

[1] *Moscow State University, faculty of Computation Mathematics and Cybernetics, Russia*

[2] *Samsung Advanced Institute of Technology, Computational Science and Engineering Laboratory, Korea*

sap@cs.msu.su

This work is devoted to the numerical solution of a 3D Poisson equation for the electric £eld potential with the additional condition on the conductor boundary in the integral form. This additional condition re¤ects conductor total charge. The equation is solved in the domain with a lot of insulators with different permittivity and conductors .

The solution of his problem can be used for the electron devices construction. In our work the effective algorithm that determines the electric potential inside the domain and the potential on the conductor surface is presented.

First the algorithm removes the additional integral condition by reducing the task to two primary Poisson equations without the integral condition. This approach gives us the opportunity to solve this problem corresponding to different values of charge on the insulators and conductor by one step. The second step is to construct the algebraic system of the equations with the second order approximation both for the Poisson equation and the boundary conditions. The essential feature of this algorithm is the arbitrary permissible form of the insulators and conductors. It allows to £nd the coef£cients of numerical Laplace operator across the permittivity thresholds and bounds of used main domain by the uniform algorithm. The conjugated gradient method [1] was chosen for the solution of the given algebraic system.

On the base of the proposed algorithms Fortran 3D Poisson solver was created for the numerical solution of the (3D) Poisson equation. A set of testing calculations was made to verify the code.

This work was supported by Samsung Advanced Institute of Technology.

References

1. Reference No 1. Hockney R.W., Eastwood J.W. Computer Simulation Using Particles, Moscow, (1987)

Numerical modelling of soliton formation and transients in dense resonant media

A.A.Afanas'ev,[1] **R.A.Vlasov,**[1] **O.K.Khasanov,**[2] **T.V.Smirnova,**[2] **and O.M.Fedotova**[2]

[1]*Institute of Physics, NAS, 68 F.Scaryna Ave., 220072 Minsk , Belarus*
[2]*Institute of Physics of Solids and Semiconductors, NAS, 17 P.Brovki Str.; 220072 Minsk, Belarus*
khasanov@ifttp.bas-net.by; tel.: +375 172 841117; fax: +375 172 840888

This report is concerned with study of the nonstationary interaction of laser radiation with dense resonant media when the local-£eld effects associated with the near dipole-dipole (NDD) interaction between atoms are essential. The soliton formation and transients under such conditions are considered. Two soliton regimes: "coherent" and "incoherent" are to be distinqiuished. The former takes place when the pulse duration is much shorter than the lateral and longitudinal relaxation times, and the latter occurs when the pulse duration falls between the times. The incoherent regime is of most interest because the very soliton existence is ensured by the NDD interaction that allows the dephasing process to be suppressed. Its realization is hindered by the rather large necessary NDD interaction constant [1]. These restrictions are facilitated when the group velocity dispersion is large quit or by making use of the tilted pulse technique, taking account of the diffraction. Characteristic properties of spontaneous responses such as echo signals and free polarization decay are analyzed. The transients can markedly be in¤uenced by the upconversion. In the present work the system of Maxwell-Bloch equations is solved numerically , and the results of computer simulations are compared with the analytical ones. In solving system an ef£cient numerical algorithm was used. The primary features of the computational procedure are the following: discrete approximations of second-order approximation are constructed using £nite-difference methods; a fully implicit scheme is used to solve the grid equations; the implementation of the nonlinear difference scheme at every time-level is carried out by means of the iterative process. This integration method permitted us to test soliton solutions for the stability and study the possibility of one- and two-soliton solutions in a general case.The questions of interest is a parameter region of soliton existence. First, we have analyzed numerically the power pulse £ssion into separate solitons and also pulse transmission through dense media under bistable behaviour of population difference. Second, the peculiarities of transients are considered for both coherent and incoherent propagation. As shown , echo responses can arise even in the absence of the inhomogeneous broadening, unlike the usual echo formation.

References

1. A.A.Afanas'ev, R.A.Vlasov, A.G.Tcherstvyi, J. Exp. Ther. Phys. **90**, 428 (2000)

Structure and surface tension of interfaces between demixing liquids con£ned in porous materials

A. Patrykiejew, W. R£ysko and S. Sokołowski

Faculty of Chemistry, Maria Curie-Skłodowska University, 20031 Lublin, Poland
tel. +48 81 537 56 76, fax +48 81 533 33 48, e-mail stefan@zool.umcs.lublin.pl

The structure of interfaces between two coexisting immicsible Lennard-Jones (12,6) ¤uids, con£ned by porous materials exhbiting large porosity is studied by using integral equations. We use two theoretical approaches to calculate the interfacial pro£les and the surface tension. The £rst theory is based on the solution of a set of equations involving the modi£ed Born-Green-Yvon type equation and the Replica Ornstein-Zernike equation, supplemented by closure equations between two-particle correlation functions. This theory is a modi£cation of the approach developed to study liquid-vapor interfaces between two phases coexisting in a porous medium [1]. In the second approach [2], we follow the method introduced by Iatsevich and Forstmann to study interfacial properties of bulk systems, and replace the BGY eqaution by the Lovett-Mou-Buff-Wertheim relation. In both cases the concept of averaged density is invoked to approximate inhomogeneous two-particle correlation functions by the corresponding functions, evaluated for uniform systems. We also compare the results of the theoretical predictions with Monte Carlo simulation data and also present a version of a density-functional theory to investigate the coexistence between two immicsible phases in con£ned lattice ¤uids.

References

1. A. Trokhymchuk, S. Sokolowski, J. Chem. Phys., **109**, 5044 (1998).
2. S. Iatsevitch, F. Forstmann, J. Chem. Phys. **107**, 6925 (1997).

Decomposition of multicomponent experimental ESEEM signals measured at low temperatures

A. A. Stanislavsky[1], **W. Hilczer**[2], **K. Weron**[3]

[1]*Institute of Radio Astronomy*
4 Chervonopraporna St., Kharkov 61002, Ukraine
[2]*Institute of Molecular Physics PAN*
ul. Mariana Smoluchowskiego 17, 60-179 Poznan, Poland
[3]*Institute of Physics, Wroclaw University of Technology*
Wyb. Wyspianskiego 27, Wroclaw 50-370, Poland
alexstan@ira.kharkov.ua

Electron Spin Echo Envelope Modulation (ESEEM) is one of methods used to study the hyper£ne interaction between electron spins and nuclear spins. There are cases when this only techniques can be employed and there are situations where complementary results are obtained from ESEEM and Pulsed ENDOR (Electron Nuclear Double Resonance). ESEEM can yield detailed information about the electronic and microstructural properties of materials [1]. Therefore, the ESEEM signals have been subject to intensive analysis with regard to their signi£cance in the context of investigating material properties. However, for a given experimental ESEEM signals, the determination of the unknown parameters, which is an ”inverse problem”, is not always a simple problem. The corresponding theoretical analysis has proved to be very complicated, and, if realistic theoretical models are used, it requires involved calculations on computers. Very often such computer simulations reveal properties of studied systems which are not at all obvious from just looking at the experimental data. All this requires the comprehensive analysis of experimental ESEEM signals.

A visual inspection of the experimental ESEEM signals shows that they re¤ect the superposition of relaxation, oscillation and noise processes, i. e. such signals are enough complicated. The aim of the work is to determine a numerical iterative procedure in decomposing the signals and determining the values of the signal parameters for which the calculated signal best matches the observed signal. Nonlinear least squares optimization is the tool preferable for this purpose [2]. We have chosen the Levenberg-Marquardt algorithm, which has the advantage of converging rapidly. We start with crude estimates of the unknown parameters which enter our model of the signals. Then the nonlinear least squares £t is applied to get the best values of these parameters. This allows us to extract more information from the available experimental data. It should be noted that the procedure of the signal decomposition was distinctive for different parts of the signal. This adjustment is necessary, since we observed that the experimental signals are transformed in time from the almost determinate response (in the start of time series) to a noise-like signal (in the end of time series) at low temperatures. The analysis gives £ne information about the energy exchange between spins and lattice in reference to the kinetics of relaxation, in particular to the nonexponential spin-lattice relaxation.

Using the experimental data, we have investigated the in¤uence of temperature on the spin-lattice and spin-spin relaxation times, as well as on the spectrum of modulation. The obtained results are in agreement with other independent experimental data and validate the approach [3]. As a result, we suggest the robust numerical algorithm for the ESEEM signal processing.

References

1. S. A. Dikanov, Yu. D. Tsvetkov, *Electron Spin Echo Envelope Modulation (ESEEM) Spectroscopy* (CRC Press, 1992).
2. C. Chachaty, E. J. Soulié, J. Phys. III France **5**, 1927(1995).
3. S. K. Hoffmann, J. Goslar, W. Hilczer, Mol. Phys. Rep. **18/19**, 39(1997).

Dynamical memory time in molecular systems

Vladimir V. Stegailov

Moscow Institute of Physics and Technology, Institutskii per. 9, 141700, Dolgoprudnyi, Russia

e-mail: stega@nu.jinr.ru

In this work a classical many-particle system of neutral atoms interacting via Lennard-Johnes potential is considered. The in¤uence of stochasticity on the system's dynamics is investigated by molecular dynamics method (MDM). Stochastic properties of the system are determined by exponential instability (Lyapunov instability) that is peculiar feature of this type of dynamical systems. It means that system's trajectory in the phase space is very sensitive to the initial conditions. Two initially close phase points diverge exponentially with time. The average rate of the divergence is determined by the Krylov-Kolmogorov entropy (K entropy, the Lyapunov exponent).

The instability is the reason that the time interval during which the behavior of the system can be predicted is £nite. During the calculation process the system completely loses the initial state information after the time t_m, which is called $the\ dynamical\ memory\ time$. After this moment the system being calculated has nothing in common with the original one.

The dynamical memory time and K entropy of the Lennard-Johnes system were calculated with use of MDM. Classical equations of motion were solved numerically with periodic boundary conditions. The schemes applied were of second and fourth order of approximation. The number of particles in the main cell was taken $N = 16 - 216$. Initial state corresponds to equilibrium con£guration [1].

Numerical integration realizes the coarse graining of the system's phase space and causes unnatural ¤uctuations of the total energy $< \Delta E^2 >$. The instability results in that MDM-trajectory deviate from right newtonian one very quickly, in fact exponentially [2]. Trajectories diverge completely to the moment of t_m when the distance between them is of the same order as the system's size.

The logarithmic dependence of t_m on $< \Delta E^2 >$ was obtained. The higher is the accuracy of numerical integration (and less $< \Delta E^2 >$), the longer is time t_m. This dependence was shown to be a universal one and it can be applied to different systems and numerical schemes (results for plasma see in [3]).

The values of t_m obtained in this work were determined by the noise resulting from numerical errors. However, the fact that the dependence of the dynamical memory time upon the noise level is logarithmic, i.e. quite weak, allows one to extend the qualitative conclusions to the real molecular systems. In this case $finite$ values of dynamical memory time are determined by $the\ quantum\ uncertainty$ [4] and have to be in the picosecond range.

The further development of the introduced ideas leads to the conclusion that reversibility does not take place in the real processes, e.g. chemical reactions, and irreversibility (because of swift loss of initial state information) is an inherent property of molecular motion.

References

1. G.N.Norman, V.V.Stegailov, JETP, 119, 1 (2001).
2. Y.Ueshima $et\ al.$, Phys. Rev. E 55, 3439 (1997).
3. I.V.Morozov, G.N.Norman, and A.A.Valuev, Phys. Rev. E 63 (2001).
4. A.S.Kaklugin and G.E.Norman, J. Moscow Phys. Soc. (Allerton Press, USA) 5, 223 (1995).

Parallel computing in superradiation spin dynamics

C.L.Davis[1] **V.K.Henner**[1,2] **A.V.Tchernatinsky**[1,2]

[1]*Department of Physics, University of Louisville, Louisville, Kentucky 40292, USA*
[2]*Perm State University, Russia*

[1]*C.L.Davis@louisville.edu*

Superradiation phenomena are characterized by a quadratic dependence of the radiation intensity on the number of radiators, N. The properties of such coherent effects in optics, for example, super¤uorescence, superluminescence, collective induction and photon echo, have been extensively studied. However, it was not until 1977 that the £rst successful experiment to observe radiofrequency superradiation was performed [1]. This phenomenon occurs, when a highly polarized system of spins, placed in a strong magnetic £eld whose direction opposes the direction of polarization, interacts with a passive external coil. The motion of the spins induces a current in the coil, creating a varying magnetic £eld, which itself interacts with the spins. This interaction leads to a collective motion of the spins resulting in the emission of coherent radiation known as superradiation.

The computer modeling of the system of spins is based on the microscopic approach developed in [2]. In a constant magnetic £eld, the behavior of the system is highly dependent on the initial polarization and the distribution of spins leading to that polarization. To generate a spin system with a particular polarization, corresponding to a given temperature, we use an algorithm similar to that of Metropolis [3]. Using this procedure, both analytically and numerically, gives an initial spin distribution almost identical to the equilibrium distribution.

In the microscopic approach, the time dependence of the system is obtained from the solution of a system of ordinary, nonlinear, differential equations. We consider the solution of these equations via the ”predictor-corrector” method and the Runge-Kutta method. The £rst method can be adapted to make use of parallel algorithms. However, we £nd that the precision and stability of the calculations are compromised. The Runge-Kutta method cannot easily be adapted to make use of parallel architecture. The behaviour of the spin system depends critically on the initial spin distribution, but meaningful results for a particular polarization are obtained by averaging over many systems with the same initial polarization with different initial spin distributions. This can be achieved by allocating a different initial distribution of spins to each available processor. Each processor performs its own task independently. The use of parallel computing architecture is achieved with no alteration of the basic computational algorithms.

The results of our numerical simulation are presented when dipole- dipole interactions can and cannot be neglected. If dipole- dipole interactions can be neglected we also presnt a comparative theoretical analysis. The use of multiple processors allows us to investigate the thermodynamically averaged behaviour of relatively large spin systems. We also present a comparison of the behavior of such a spin system over a long time-scale, with that predicted by a phenomenological model based on Bloch-type equations. The phenomenological approach is in good qualitative agreement with our microscopic model, allowing the possibility of determining the Bloch relaxation time T_2. An X-class, HP/Convex Exemplar computer was used throughout this analysis.

References

1. P.Bosiger, E.Brun and D.Meier, Phys. Rev. Lett. **38**, 602, (1977)., Kiselev et al, JETP **94**, 344, (1988).
2. T.S.Belozerova, C.L.Davis, V.K.Henner, Phys.Rev. **B 58**, 3111, (1998).
3. N. Metropolis et al., J. Chem. Phys. **21**, 1087, (1953).

Short-range order and hyper£ne interactions in the fcc Fe-N alloys

A.N.Timoshevskii[1], B.Z.Yanchitskii[1] and V.A.Timoshevskii[2]

[1] *Institute of Magnetism, 36-B Vernadsky St., 03680 Kiev, Ukraine*
[2] *Materiaux Universite Claude Bernard-Lyon 1, Lyon, France*
+380/44 452 9654, +380/44 452 1811, tim@ukron.kiev.ua

Nitrogen austenites are distinguished for their mechanical properties, such as a strength, fracture toughness, wear resistance, as well as thermal stability. A controlling mechanism of the low temperature strengthening of austenite due to the nitrogen doping is still not clari£ed. It is obviously interesting to study the in¤uence of nitrogen on the electronic structure and physical properties of fcc iron. Carrying out the calculations of the structural and thermodynamic properties of materials allows resolving numerous practical tasks related to the development of the new alloys and interpreting the experimental data obtained from a high-precision methods, for example, Mössbauer spectroscopy. Our approach is based on a widely known full-potential band structure method (FLAPW) that is used for the calculation of the electronic structure, total energy and optimization of the lattice geometry of alloys, having the interstitial impurities. According to this approach, the calculations of the total electron energy of alloy for the set of a fully ordered structures are carried out. Total energy minimization procedures are performed for obtaining the equilibrium positions of atoms. Then, the system of linear algebraic equations over the energy parameters of con£gurational Izing model of alloy is composed. Structural and thermodynamic properties of alloys at the different temperature and concentration conditions are simulated using the Monte-Carlo (MC) method. In our previous work [1] we have simulated the Fe-C and Fe-N austenites by the ordered fcc Fe_8C and Fe_8N structures and have made the £rst attempt to clarify the difference between the electronic structures of the nitrogen and carbon austenites. In the present paper, we have studied in details the in¤uence of nitrogen on the atomic and electronic structure of fcc iron. In order to determine the pair potential of the N-N inter-atomic interaction for fcc Fe in the six coordination spheres, we have optimized the geometry and calculated the total energy for the ten fcc Fe structures, having the nitrogen atoms, as follows: three Fe_8N structures and three Fe_4N structures with a different distribution of the nitrogen atoms, Fe_3N, Fe_2N, Fe_4N_3 and FeN. Based on the pair potentials received, we have carried out the set of the MC calculations, allowing us calculating the short range order parameters for a wide temperature range. It is shown that when the temperature decreases, an appearance of the ordered N-Fe-N chains in the fcc lattice becomes energetically advantageous. For the comparison with the experimental Mössbauer data, we have studied in details the electronic structure and hyper£ne interactions in the three Fe_8N - type structures with a different distribution of the nitrogen atoms: the £rst structure does not include the N-Fe-N chains; the second structure includes non-intersecting chains and the third one - intersecting metal-nitrogen chains. The calculations have shown that the third structure is the most advantageous energetically. We have calculated a quadrupole splitting and isomer shifts for the Fe atoms in the three Fe_8N structures. Performing the calculations for the different energy ranges of the valence band, we could eliminated the contribution into the quadrupole splitting, which is due to the nitrogen atoms. Based on our calculations, we have carried on the detailed interpretation of the experimental Mössbauer spectra of the Fe-N austenite.

References

1. A.N.Timoshevskii, V.A.Timoshevskii, B.Z.Yanchitskii. J. Phys.: Condens. Matter 13 No 5 (2001) 1051-1061.

Molecular polarizability of semiconductor clusters and nanostructures

Francisco Torrens

Institut Universitari de CiÁncia Molecular, Universitat de ValÁncia, Dr. Moliner 50, E-46100 Burjassot (ValÁncia), Spain

Francisco.Torrens@uv.es

The role of *size* in modifying the properties of a material has not been exploited until recently. On the basis of interatomic potentials, the structure of some clusters are special. Nanocrystalline powders can be used to synthesize materials with physical processing such as sintering.

In previous papers, fullerenes, Sc clusters, Sc-cluster endohedral fullerenes [1], graphite models and Sc *hexagonal close packing* were studied [2]. Here, the following semimetallic clusters have been calculated: Si/Ge/GaAs.

The interacting induced dipoles polarization model implemented in program PAPID [3] is used for the calculation of the molecular dipole-dipole polarizability $\overline{\overline{\alpha}}$. The method is tested with Si_n, Ge_n ($n \leq 10$) and Ga_nAs_m ($n, m \leq 4$) small clusters.

Program PAPID has been used for the calculation of the dipole-dipole polarizability $\overline{\overline{\alpha}}$, with the interacting-induced-dipoles polarization model that calculates tensor effective anisotropic point polarizabilities [1,2] by the method of Applequist *et al.*. The bulk limit for the polarizability is estimated from the Clausius-Mossotti relationship.

The results for the polarizability are in agreement with reference calculations from J. R. Chelikowsky carried out within the density functional theory [4]. The clusters are all more polarizable than what one might have inferred from the bulk polarizability. Previous experimental work have yielded the opposite trend for somewhat larger clusters.

On varying the number of atoms, the clusters show numbers indicative of particularly polarizable structures. The polarizability trend for these clusters as a function of size is different from what one might have expected. The high polarizability of small clusters is attributed to arise from dangling bonds at the surface of the cluster.

References

1. F. Torrens, Microelectron. Eng. 51-52 (2000) 613.
2. F. Torrens, Molecules, submitted for publication.
3. C. Voisin, A. Cartier and J.-L. Rivail, J. Phys. Chem. 96 (1992) 7966.
4. J. R. Chelikowsky, The electronic and structural properties of semiconductor clusters and nanostructures, Res. Rep. UMSI 97/132, University of Minnesota Supercomputing Institute, 1997.

Mathematical simulation of photoacoustic microscopy with piezoelectric registration

Olena Vertsanova
National Technical University of Ukraine
tempus@webber.net.ua

The photoacoustic non-destructive control of solids is a powerful technology, which is applied to diagnostics of products and materials of electronics. The photoacoustic microscopy (PAM) enables to receive the images of the sub-surface structure, which cannot be found out by the traditional NDE-methods. The PAM is used for detection and analysis of the sub-surface heterogeneities, such as defects, cracks, inclusion, delaminations. This method allows to investigate a product during the manufacture without in¤uence on properties, quality and parameters of a product.

The principle of the PAM is based on the phenomenon of generation and distribution both thermal and acoustic waves excited by modulated on intensity laser radiation. The acoustic ¤uctuations in object are detected by the piezosensor and converted by it into electrical signal. The photoacoustic signal (PAS) is a sinusoidal voltage on electrodes of the piezosensor, the phase and amplitude of which carry the useful information about local sample properties. The computer processing of this signal by scanning a laser beam along the sample surface enables to receive the photoacoustic image of internal structure of a researched material.

For interpretation and decoding of the photoacoustic images it is necessary to establish connection between parameters of the PAS and a sub-surface structures. For this purpose the one-dimensional mathematical model of photoacoustic effect with piezoelectric registration in thermal thick and optical opaque sample was developed.

This model allows to restore the information about physical properties of researched object under the experimentally received amplitude and phase characteristics, estimate a minimal size and a maximal depth of defect and choose optimum modulation frequency for deep pro£ling of researched object.

Legitimacies, which were obtained as a result of mathematical simulation of a photoacoustic microscopy with piezoelectric registration, have allowed to investigate the production of electronic industry, including the integrated circuits, the microwelded connections, the thin-£lm covers, the multi-layer structures, and to evaluate their quality on the contrast of the photoacoustic images.

References

1. Vertsanova, O., *The investigation of piezosenser for PAM* // Electronics and communications **6**. – Kiev (Ukraine). - 1999. - P. 280-285.
2. Vertsanova O., Yakimenko Y., Selivanov S. *Nondestructive control of sub-surface defects by using PAM with bending bimorph piezoceramic sensor* // Proc. Ninth International Symposium on Nondestructive Characterization of Materials. – Sydney (Australia). – 1999. – P. 497-501.
3. Vertsanova O. *The contrast of the photoacoustic images of solids* // Electronics and communications **9**. – Kiev (Ukraine). - 2000. -P. 43-46.

The computer investigation of the super¤uid Bose-liquid with paired interaction and with coherent condensate of the boson pair as model quantum liquid ^4He.

E.A.Pashytskiy[1] **S.I.Vilchynskyy** [2]

[1] *Institute of Physics, 03650, Ukraine, Kiev*
[2] *Kiev Shevchenko University, 03127,Ukraine, Kiev*
+380 (044)2664567, +380 (044)2664507, e-mail: sivil@phys.univ.kiev.ua

The analysis of experimental and theoretical publication indicates that investigations of the unique phenomenon of super¤uidity of liquid helium are far from being completed. A number of discrepancies between the theoretical and experimental results include, for example, the 1.5-2 orders of magnitude difference between the theoretical value of critical velocity $v_{cr} \simeq 60m/s$ calculated on the basis of the Landau super¤uidity criterion from the value of the gap Δ_r near the rotonic minimum in the elementary excitation spectrum reconstructed from the scattering of slow neutrons on the one hand and the experimentally measured values of v_c on the other hand as well as the discrepansy between the theoretical density of the Bose-Einstein condensate, which is indenti£ed with the density ρ_s of the super¤uid component in He-II, and the experimentally measured (from the scattering of fast neutrons) fraction of ^4He atoms (1-3 percent) in the state with zero momentum at $T \simeq 1$ K [1]–[3].

We formulate a computer model of the quantum liquid ^4He on the bases of the approach to the description of the super¤uid state in a Bose-liquid on the bases of the concept of ”paired” effective condensates of free particles. On the basic of the Brueckner-Sawada approximation ”solid sphere” [4], we computer calculated the Fourier component of the effective potential of the regularize paired interaction between the bosons with taking acount the many-particle processes. The computer calculation show that the effective strong attraction in the wide region of the momentum spase, constrained with quantum diffraction of the particle one on another, can ensure of the necessary and suf£cient condition of the existence of the coherent pair condensate (CPC) bound pair of bosons. Such a strong CPC completely suppress the weak single- particle Bose condensate (SPBC). On the basic of the realize computer analysis and solution of the Dyson-Belyaev integrate equations we show that spectrum of the quasi-particle $\epsilon(p)$ is acoustic near the small momentum – $\epsilon(p) \simeq p\tilde{u}$, where the velocity $\tilde{u}$ does not coincide with the velocity c of hydrodynamic sound in liquid helium ($u << c$) and is determined by the pair order parametr $\tilde{\Psi}(p)$ for $p = 0$. This spectrum $\epsilon(p)$ may have a minimum in the region maximum attraction and determines the critical velocity.

References

1. A.F.G. Wyatt. Nature, 391, N 6662, p.56 (1998).
2. E.F.Tabbot, H.R.Glyde, W.G.Stirling, E.C.Swenson Phys.Rev.B38, 11229 (1988).
3. H.R.Glyde, W.G.Stirling Phys.Rev.B42, 4224 (1990).
4. K.A.Brueckner, K.Sawada. Phys.Rev. 106, 1117, 1128 (1957).

Monte-Carlo simulations of the quantum phase transition in disordered itinerant antiferromagnets

Thomas Vojta[1,2]**, Smaine Bekhechi**[1]**, and Michael Schreiber**[1]

[1]*Institut für Physik, TU Chemnitz, D-09107 Chemnitz, Germany*
[2]*Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, UK*
vojta@physik.tu-chemnitz.de, phone +49 371 531 3142, fax +49 371 531 3143

The in¤uence of quenched disorder on zero-temperature or quantum phase transitions is a topical problem in condensed matter physics. Using an asymptotically exact real-space renormalization group Fisher [1] investigated the one-dimensional disordered transverse £eld Ising model. The quantum phase transition in this model shows very unusual scaling behavior, it is controlled by an in£nite disorder £xed point. Similar behavior was also found numerically in one and two dimensions [2] In three dimensions and in the case of a continuous order parameter the situation is less clear.

A particularly interesting case is the quantum phase transition of dirty itinerant electrons from a paramagnet to an antiferromagnet. A perturbative renormalization group analysis [3] predicts a conventional critical point, at least at some intermediate disorder strength. However, non-perturbative effects due to rare ¤uctuations destroy this behavior. They appear to lead to runaway ¤ow to large disorder strength [4].

In order to investigate the ultimate fate of this quantum phase transition we calculate thermodynamic properties close to the critical point using Monte-Carlo simulations of the order parameter £eld theory of itinerant quantum antiferromagnets. This is equivalent to simulating a £ve-dimensional classical Ising or Heisenberg magnet with anisotropic disorder. Using £nite-size scaling we calculate the critical behavior at the transition, in particular we determine whether the critical point is characterized by conventional power law behavior or more exotic phenomena like activated scaling.

References

1. D. S. Fisher, Phys. Rev. B **51**, 6411 (1995).
2. J. Kisker and A.P. Young, Phys. Rev. B **58**, 14397 (1998); C. Pich, A. P. Young, H. Rieger, and N. Kawashima, Phys. Rev. Lett. **81**, 5916 (1998).
3. T.R. Kirkpatrick and D. Belitz, Phys. Rev. Lett. **76**, 2571 (1996); *ibid.* **78**, 1197 (1997).
4. R. Narayanan, T. Vojta, D. Belitz, and T. R. Kirkpatrick, Phys. Rev. Lett. **82**, 5132 (1999); Phys. Rev. B **60**, 10150 (1999).

Effects of anisotropy at semiconductor surfaces

T. Volkmann, M. Ahr, M. Biehl and W. Kinzel

Julius-Maximilians-Universität Würzburg, Institut für Theoretische Physik und Astrophysik, Am Hubland, 97074 Würzburg, Germany

+49 931 888 5139, +49 931 888 5141, volkmann@physik.uni-wuerzburg.de

The quality of semiconductor crystals grown in an MBE environment depends substantially on the surface structure of the underlying substrate. In this context surface reconstructions and associated phase transitions play a crucial role. Here we investigate a two-dimensional lattice gas model of metal-terminated II-VI(001) semiconductor surfaces [1]. Important properties of this class of materials are reproduced by the particular choice of anisotropic pairwise interactions. In our study we focus on the effects of this anisotropy.

The surface is modelled by a square array of sites $\{n_{xy}\}$ either being occupied $(n_{xy} = 1)$ or empty $(n_{xy} = 0)$. While a hard core repulsion excludes the simultaneous occupation of nearest neighbor (NN) sites in the y-direction, attractive interactions ϵ_x and ϵ_d between NN in x-direction and next nearest neighbors (NNN), respectively, lead to a competition of two vacancy structures. At low temperatures T, a $c(2\times2)$ ordered phase coexists with a low density disordered phase, whereas for higher temperatures the system becomes globally disordered or $c(2 \times 2)$ ordered depending on the coverage θ. In the disordered regime the local environment of an atom is dominated by (2×1) rows. Within the framework of this model the transition from a dominant $c(2 \times 2)$ ordering of the CdTe(001) surface to a local (2×1) arrangement of Cd atoms which is observed experimentally can therefore be explained as a concomitant phenomenon of an order-disorder phase transition in thermal equilibrium.

The investigation of the model is done by means of Monte Carlo simulations (MC) and transfer matrix (TM) calculations, examining the behavior of appropriate quantities: pair correlations c_x and c_d measure the probability of £nding an occupied NN pair or NNN pair respectively, i.e. the contribution of (2×1)- or $c(2 \times 2)$-dominated regions in the system, whereas $m_{c(2\times2)}$ measures the overlap with one of the two sublattices and therefore indicates long range order. In order to determine the phase boundaries in the $T - \theta$ diagram via MC simulations temperature intervals $[T_1, T_2]$ are scanned for £xed values of the coverage θ. We apply a non-local dynamics which proves signi£cantly better than the standard Kawasaki algorithm [2]. As another characteristic feature of the system we determine the line $\hat{T}(\theta)$ where $c_x = c_d$ which separates the regimes of local $c(2\times2)$ or (2×1)-dominance. Within the TM formalism correlations are obtained from proper derivatives of $\ln\mathcal{Z}_L$ where $\mathcal{Z}_L$ is the partition sum of a system with $M = N \times L$ sites (strip of width L) in the limit $N \to \infty$. Additionally the phase boundaries are calculated following the prescription outlined in [3]. By choosing two different strip orientations we are also able to calculate the anisotropic correlation lengths in x- and y-direction in the disordered regime.

The Monte Carlo algorithm mentioned above allows studying the equilibrium shape (ECS) of isolated islands of atoms and its temperature dependence. At low temperatures we £nd square clusters with facets oriented along the diagonals in accordance with experimental observations at CdTe(001) [4]. For higher temperatures the islands take on an ellipsoidal shape with the long half axis parallel to the x-axis and the degree of anisotropy depending on the NN interaction.

References

1. M. Biehl, M. Ahr, W. Kinzel, M. Sokolowski, T. Volkmann. Europhys. Lett. **53**(3), 169 (2000)
2. M.J. Newman, G.T. Barkema. *Monte Carlo Methods in Statistical Physics*. Clarendon Press, Oxford, 1999.
3. N.C. Bartelt, T.L. Einstein, and L.D. Roelofs. Phys. Rev. B **34**, 1616 (1986).
4. D. Martrou, J. Eymery, P. Gentile, N. Magnea. J. Crys. Growth **184/185**, 203 (1998).

Finite temperature properties of small quantum systems: Analytical and computer treatment

P.N.Vorontsov-Velyaminov and R.I.Gorbunov

Faculty of physics, St.Petersburg State University, 198504, St.Petersburg, Russia

+7-812-4284555, voron.wgroup@pobox.spbu.ru

For a system of N noninteracting identical particles the canonical partition function at the inverse temperature $\beta = T^{-1}$, $Z_N^{(A,S)}(\beta)$, can be expressed through a single particle canonical partition function, $Z_1(\beta)$, at an increasing set of values: $\beta, 2\beta,$ etc. So in the absence of interaction the problem is reduced to calculations for a single quantum particle in an external £eld. Unfortunately with the increase of N the expressions for $Z_N^{(A,S)}$ through Z_1 become more and more cumbersome. Even with the specially designed computer programmes we could generate these formulas for N not exceeding ≈ 100. Meanwhile insertion of $Z_N^{(A,S)}$ into the great canonical partition function and using of the so called cyclic decomposition allows us to construct expressions for potential Ω in the form of a one dimensional Feynman-type cycle series which converge at negative values of the chemical potential μ. The relevant thermodynamical properties are then derived allowing us to make fast numerical calculations for N ranging up to 10^8. The results were obtained for paricles of both statistics with the spin in a harmonic and other £elds with or without applied homogeneous magnetic £eld [1, 2].

For systems of interacting particles the above approach is inapplicable, so we had to implement path integral Monte Carlo (PIMC) method. To make PIMC method more effective a combined, bead-Fourier (BF), PIMC simulation scheme was introduced [3] with its extreme cases corresponding to the ordinary bead approximation and Fourier PIMC method. Optimal choice of the number of beads and of Fourier harmonics provides reliable test results for the ground state energy and electron density in H-atom as well as for the harmonic oscillator.

In applying BF method to systems of identical particles a scheme of simultaneous account for all classes of permutations suggested earlier [4] was used with symmetrization of the exchange factor in the weight function. A procedure of random walk in the spin space provides calculation of spin dependent averages [3].

Systems of $N = 2 \div 5$ fermions as well as up to 10 bosons in a harmonic £eld with no interaction and with Coulomb repulsion were threated. For systems with no interaction exact curves for energy and the square of the total spin, $< S(S+1) >$, vs T were reproduced in a considerable temperature range. Swithching on of the interpartical repulsion results in gradual cease of the exchange effects. Some few electron systems such as He, H_2, Li were also simulated. For fermions at low T the error increases considerably due to the sign problem. To weaken its in¤uence we applied several measures – "umbrella sampling", "gates", "non-negative average sign random walk". Study of distributions for the exchange factor W helps us to understand features of the simulation procedure for fermionic systems at low T. In order to overcome ergodicity problems at low T we implement 'V-type' steps which proved to be very helpful in works of other authors.

References

1. P.N.Vorontsov-Velyaminov, S.D.Ivanov, R.I.Gorbunov, Phys.Rev., **E** 55 (1999) 168.
2. P.N.Vorontsov-Velyaminov, R.I.Gorbunov, S.D.Ivanov, J.Phys., **A** 33 (2000) 1857.
3. P.N.Vorontsov-Velyaminov, M.O.Nesvit, R.I.Gorbunov, Phys.Rev., **E** 55 (1997) 1979.
4. A.P.Lyubartsev, P.N.Vorontsov-Velyaminov, Phys.Rev., **A** 48 (1993) 4075.

Agglomeration in charged suspensions

J. Werth[1*], Z. Farkas[1,3], S. Dammer[1], H. Hinrichsen[1,2] and D.E. Wolf[1]

[1] *Theoretical Physics, FB 10, University of Duisburg, 47048 Duisburg, Germany*
[2] *Theoretical Physics, FB 8, University of Wuppertal, 42097 Wuppertal, Germany*
[3] *Department of Biological Physics, Eötvös University, Budapest, Pázmány P. Stny 1A, 1117 Hungary*

[*] *phone: +49 203 379 4227, fax: +49 203 379 1681, e-mail: werth@comphys.uni-duisburg.de*

Granular materials play an important role in a large variety of industrial applications where solids are processed in form of granulates and powders. In particular, the controlled use of nanopowders is increasingly relevant for various technological applications, ranging from the fabrication of inhalable pharmaceutical products to the painting of cars without solvents. However, many open problems still need to be solved. In particular, it is not yet known, to what extent electric charges in¤uence the physical properties of granular materials. Moreover, the process of charging granular powders is not fully understood.

The aim of our work is to understand agglomeration of bipolarly charged powders suspended in nonpolar ¤uids. The concerted in¤uence of electromagnetic, hydrodynamic, thermal and van der Waals forces as well as Brownian forces leads to complex agglomeration behavior which depends on numerous parameters, e.g., the ratios of charges, sizes, temperature and concentrations of the particles.

The present theoretical investigation of the problem is based on molecular dynamics simulations. In order to keep the simulation time as small as possible, the surrounding liquid is not simulated as a whole. Instead we model the hydrodynamic forces between the particles by means of effective long range interactions, employing the so-called Stokeslet approximation [1]. This approximation gives the pair interaction of particles, assuming the particle movement is guided by their surrounding electrical £eld. However, the longranged hydrodynamic interaction and the unscreened Coulomb forces lead to a N^2 problem in computational effort. The other forces, i.e. van der Waals, lubrication and Brownian forces, are short ranged and thus computationally less expensive. In order to simulate larger systems, we parallelized the numerical integration, using so-called hypersystolic algorithms [2].

First results for particles which all carry the same charge show the existence of a typical cluster size due to the competition of Brownian motion and Coulomb repulsion [3]. If the thermal energy is higher than the effective Coulomb barrier, the particles agglomerate until the bigger charge and reduced mobility of the clusters prevent a further agglomeration. In all cases we assume that at contact the van der Waals attraction between particles exeeds the Coulomb repulsion, thus all established contacts between particles are conserved for all times.

References

1. I.M. Janosi, T. T'el, D.E. Wolf, J.A.C. Gallas, Phys.Rev. E **56**, 2858 (1997).
2. Th. Lippert, H. Hoeber, G. Ritzenhöfer, K. Schilling, *Hyper-Systolic Processing on APE100/Quadrics N^2-Loop Computations*, HLRZ 95-45, WUB 95-21 (1995).
3. Z. Farkas, J. Werth, S. Dammer, H. Hinrichsen, D.E. Wolf, *Stability of Charged Granular Matter in Suspension,* preprint.

Molecular dynamics study of heavy metal atoms (Pb, Bi, Sb) clustering in hydrogen reduced silicate glasses

Agnieszka Witkowska[1], **Jaroslaw Rybicki**[1],
Giorgio Mancini [2] **and Sandro Feliziani**[2]

[1] *Faculty of Technical Physics and Applied Mathematics and TASK Computer Centre, Technical University of Gdansk, Narutowicza 11/12, 80-952 Gdansk, Poland*
[2] *Istituto di Matematica e Fisica, Universita di Camerino, via Madonna delle Carceri, Camerino (MC), Italia*
Phone: 0048 58 347 18 32, fax: 0048 58 347 28 21, e-mail: agnieszka@mif.pg.gda.pl

Binary silicate glasses containing heavy metal oxides, such as PbO, Bi_2O_3 or Sb_2O_3, show many interesting and useful properties, £nding applications as low-loss wave-guide materials which operate at wavelength $> 3\mu$m, and as the active medium of Raman-active £bre optical ampli£ers and oscillators [1, 2]. These glasses, submitted to the reduction process (*e.g.* in hydrogen atmosphere or proton bombardment), undergo dramatic changes in their optical properties, and electrical surface conductivity [3]. Reduced glasses contain metallic granules and/or neutral
Pb/Bi/Sb atoms [4], reveal a very high secondary emission coef£cient, and £nd application in the production of electron channel multipliers.

In the contribution we report on the results of extensive molecular dynamics (MD) simulations of the structure of reduced lead-, bismuth-, and antimony-silicate glasses of composition xMe $(1-x)SiO_2$, Me = Pb, Bi, Sb, $0 \leq x \leq 0.5$. The classical Andersen algorithm for isobaric-isoenthalpic (NpH) ensemble has been used. The atoms interacted by a two-body Born-Meyer-Huggins interaction potential with full ionic charges Si^{+4} and O^{-2}. The metal atoms were neutral. In dependence on the glass stoichiometry the simulation box contained usually $2 - 3 \cdot 10^3$ atoms. Several 20000-atom simulations have been also performed. For each composition a homogeneous melt was prepared, and then slowly cooled down to 300 K. The room-temperature systems were sampled over 20000 fs time-steps. For all the considered glasses a strong tendency to the agglomeration of heavy metal atoms was observed. We compare the distributions of Pb, Bi, and Sb granules, their sizes and connectivity. We also discuss the granules melting temperatures, and the temperature dependence of the heavy atoms mobilities. In addition we discuss the in¤uence of the metallic inclusions on the medium-range structure of silica.

The calculations have been performed at the TASK Computer Centre in Gdansk.

References

1. Nassau K, Chadwick D L and Miller A E 1987 *J. Non-Cryst. Solids* **93** 115
2. Lin C 1983 *J. Opt. Commun.* **4** 2
3. Trzebiatowski K, Witkowska A and Chybicki M 1998 *Ceramics* **57** 157
4. Witkowska A, Rybicki J, Trzebiatowski K, Di Cicco A and Minicucci M 2000 *J. Non-Cryst. Solids* **276** 19

Auxetics and their microscopic mechanisms

K. W. Wojciechowski

Institute of Molecular Physics, Polish Academy of Sciences,
M. Smoluchowskiego 17, 60-179 Poznań, Poland

kww@man.poznan.pl

Auxetics are isotropic systems of anomalous (negative) Poisson's ratio: they expand (contract) transversely when stretched (pulled) longitudinally [1].

Various models and mechanisms have been proposed for auxetic behaviour. Amongst them a few theoretical mechanisms have been suggested which can be applied on microscopic level [2, 3, 4].

In this communication results of computer simulations testing the theoretical predictions are reported.

References

1. R. Lakes, Science **235**, 1038 (1987).
2. K. W. Wojciechowski, Phys. Lett. **A137**, 60 (1989).
3. K. W. Wojciechowski, Mol. Phys. Reports **10**, 129 (1995).
4. V. V. Novikov, K. W. Wojciechowski, Physics of the Solid State **41**, 1970 (1999).

A new algorithm of analyzing the metal-insulator transition of the Anderson model

Junko Yamasaki and Naomichi Hatano

Department of Physics, Aoyama Gakuin University
Chitosedai, Setagaya, Tokyo 157-8572, Japan
Phone: +81-3-5384-6582; Fax: +81-3-5384-6100;
e-mail: yamasaki@phys.aoyama.ac.jp

Upon increasing the impurity concentration, a metal undergoes a phase transition to an insulator owing to the Anderson localization. The aim of the present study is to analyze the metal-insulator transition numerically, using the one-electron Anderson model

$$\mathcal{H} = \frac{\vec{p}^2}{2m} + V(\vec{x}) = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{x}), \tag{1}$$

where $V(\vec{x})$ is a random potential. When a wave function of (1) has the form $\psi(\vec{x}) \sim e^{-\kappa|\vec{x}-\vec{x}_0|}$, its localization length around the localization center $\vec{x}_0$ is given by κ^{-1}. The electron is delocalized if $\kappa = 0$ and hence represents a metal, whereas it is localized if $\kappa > 0$ and represents an insulator. Our purpose is to compute κ.

We develop a new numerical algorithm of computing the localization length κ. New features of our algorithm are: it is suitable for treating huge sparse matrices; the code is fully parallelized.

It was recently shown [1] that the eigenvalue spectrum of the non-Hermitian generalization

$$\mathcal{H} = \frac{\vec{p}^2 + i\vec{g}}{2m} + V(\vec{x}) = -\frac{1}{2m}(\hbar\vec{\nabla} - \vec{g})^2 + V(\vec{x}) \tag{2}$$

yields κ of the Hermitian Hamiltonian (1). This method of computing the localization length is of recent interest as a very different method from the conventional one; In the conventional method, κ is calculated directly from $\psi(\vec{x}) \sim e^{-\kappa|\vec{x}-\vec{x}_0|}$ after computing the wave function.

It is easier to compute the pseudo-spectrum [2] of non-Hermitian Hamiltonian matrices than the spectrum itself. The pseudo-spectrum is the contour plot of the minimum singular value of the non-Hermitian matrix $z - \mathcal{H}$ in the complex energy plain (Fig. 1). Our new algorithm produces the contour plot by computing the maximum eigenvalue of the Hermitian matrix $(z - \mathcal{H})^\dagger(z - \mathcal{H})$.

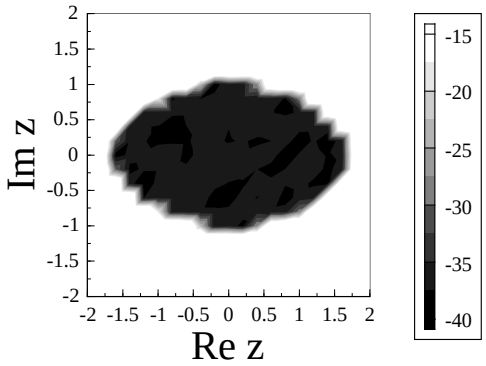


Fig. 1: The pseudo-spectrum of the non-Hermitian Hamiltonian (2) in one dimension with $g = 1.0$. This contour plot indicates that the eigenstates in the energy range $-1.6 < \varepsilon < 1.6$ are delocalized.

References

1. N. Hatano and D.R. Nelson: Phys. Rev. Lett. 77, 570 (1996); Phys. Rev. B 56, 8651 (1997); Phys. Rev. B 58, 8384 (1998). N. Hatano: Physica A 254, 317 (1998).
2. L.N. Trefthen: Acta Numerica, 217 (1999).

Mesoscopic phase transitions and their critical behavior of nano structured materials

Yoshitake Yamazaki[1,2], Herbert Gleiter[2], Yutaka Abe[1], Keiichiro Nakamura[1], Haruyasu Mizoguchi[1], Tomohiro Irie[1] , Dai Ito[1] and Masahiro Watanabe[1]

[1]*Institute of Fluid Science, Tohoku University, 2-1-1, Katahira, Aoba-ku, Sendai, 980-8577, Japan*

[2]*Institute of Nanotechnology, Karlsruhe Research Center, D-76021, Karlsruhe, Germany*

yamazaki@ifs.tohoku.ac.jp

Mesoscopic phase transitions and their critical behavior of nano structured materials are summarized [1, 2, 3].

The systems studied are as follows: (1) three-dimensional systems of spinless particles starting from the grains in the fcc or hcp structure as the initial con£guration, (2) two-dimensional spin systems interacting with both the magnetic and elastic interactions, and (3) two-dimensional, generalized q-states Potts spin systems with both the Potts spin and elastic interactions (here q = 3, 4 were chosen). The pair-particle interactions, for simplicity, is chosen in the type of Lennard-Jones.

Novelty of the paper is to establish how to investigate the nano structured materials and what to compute as their metastable behavior and to construct the computer simulation systems for them.

The problems of the nano sturctured materials are concerned with dominant contributions coming from nonequilibrium and local characteristics of grains and interfaces formed in lower dimensionality.

The computational methods used are of Metropolis Monte Carlo and renormalization methods generalized. The methods are improved to be able to evaluate the local, metastable properties of the systems.

The results obtained are summarized: (1) The similarity and difference in the nano structured properties derived in the type of the fcc or hcp structure as the initial con£guration, are discussed. (2) Together with the typical bulk magnetic and structural phase transitions, many local, magnetic and structural mesoscopic phase transitions are found, which have the characteristic functions coming from the characteristic structures and are controlled by the external £elds. (3) The order of the magnetic and structural phase transition temperatures is found to change according to the magnitude ratio of the magnetic and elastic interactions of the systems. (4) The magnetic and/or elastic grains are found in various, characteristic mesoscopic phases. (5) The concepts of the bulk, ordered and disordered phases magnetic and/or elastic are completely corrected in the mesoscopic phases. (6) The mesoscopic critical behaviors of N-component nanosystems are found.

The conclusions are summarized. We could construct the computer-simulation systems for typical nano structured systems and derive main characteristics for them. Further detailed characteristics are being computed.

References

1. Y. Yamazaki, et al., ”Fundamental Study and Application of Intelligent Nano and Mesoscopic Structured Materials by Field Control” ed. by Chonan, et al., (2000), 140
2. Y. Yamazaki, et al., ”Statistical Physics”, World Scienti£c, (1998), 139.
3. H. Gleiter, *Acta Materia*, **48**, (2000), 1.

Adenine tautomer complexes with closed- and open-shell copper ions. *Ab initio* examination

Rubina A.Yu.[1,2], **Rubin Yu.V.**[1], **Sorokin V.A.**[1],
Shukla M.K.[2], **Leszczynski J.**[2]

[1]*Molecular Biophysics Department, Institute for Low Temperature Physics and Engineering, National Academy of Science, Lenin ave.47, Kharkov, 61164, Ukraine*
[2]*Computational Center for Molecular Structure and Interaction, Jackson State University,1400 J.R.Lynch.str, Jackson, Mississippi, 39217-0510, USA*
+38-0572-30-85-58, +38-0572-33-55-93, rubina@ilt.kharkov.ua

Adenine is one of the fundamental structural components of the DNA molecule. The ability of its analogs and complexes to incorporate into DNA opens wide prospects for developing new drugs. On the other hand, the same its properties can lead to mutagenous consequences for organism when formation of complexes takes place, for example, with heavy and transition metal ions [1]. A great number of works both theoretical [2] and experimental [3] is devoted to investigation of structure and physical characteristics of such complexes. There are con¤icting experimental data in literature now about sites of binding of metal ions to adenine molecule. N1, N3, N7 positions and N of aminogroup are proposed by authors as binding centers depending on the method of preparation of samples [4]. We £rst studied tautomer stabilities of adenine complexes with Cu(I) and Cu(II) ions by the help of theoretical methods. The total energies, molecular geometry optimizations and excited state energy calculations were performed for two tautomers of adenine (Ade) and their complexes with closed-shell Cu (I) ion and open-shell Cu (II) ion using Gaussian98. N1, N3, N7, N9 binding sites were considered. The ground state geometry optimization was carried out on the (U)HF/6-31+G** (for open-shell metal ions), total energies were obtained on (U)MP2/6-31+G** levels of theory, while transition energies were calculated using the con£guration interaction involving singles excited con£gurations (CIS method). The effect of bulk aqueous solvation was studied applying the polarized continuum model (PCM) of the self-consistent reaction £eld (SCRF) theory. The aminogroup rotation problem is being discussed too. An xperimental UV-spectrum of adenine complexes with Cu (II) in water solution has been obtained. This spectrum has a low-frequency shift approximately 1000 cm-1 in comparison with ones of adenine. Analysis of the values obtained for total energies in cases of Cu(I) and Cu(II) showed that preference of one tautomer in the gas phase can be change with including of the continuum model (PCM). Thus, the most probable binding site of Cu(I) ion in gas phase is the N7 atom of the adenine N9H tautomer, while in the solvation model the site in question is N1 or N3. Analysis of energies calculated for the £rst electronic singlet $\pi - \pi^*$ transitions showed that the metal ion binding to the adenine N1 or N7 atoms must result in the red shift of the UV spectrum (0-0 transition) of complexes studied while the N9 site binding leads to the blue shift.

References

1. Andronikashvili E.L.// Bio£zika,1987,23, 782-794.
2. Burda J., Sponer J., Hobza P. //J. Phys.Chem.1996,100,N17, 7250-7255.
3. Rodgers M., Armentrout P. //J. Am. Chem. Soc.,2000, 122, 8548-8558.
4. Swaminathan V., Sundaralingam M.// CRC Crit. Rev. Biochem,1979, 6, 245-336.

FTBF: A new software package for the analysis of extended X-ray absorption £ne structure (EXAFS) spectra

Zhuchkov K.N. and Gnezdilov A.V.

Department of Physics, Rostov University, Zorge str., 5, Rostov-on-Don, 344090, Russia

secontrol@aaanet.ru

Analysis of EXAFS data obtained from time resolved experiment can become an extremely time consuming and inconvenient due to the large number of the consecutive absorption spectra. The number of spectra measured during one single experiment can easily amount to several hundred investigations demand data reduction software prepared to cope with large data sets. FTBF is a new package combining a user friendly graphical environment with collection of numerical algorithms. The numerical library implemented in FTBF contains the most common and useful algorithms [1] such as a derivative, integration, least square re£nement of a large variety of pro£le functions, Forward and Inverse Fourier transform, nonlinear £tting procedure. Necessary steps for conventional EXAFS data treatment [2] can be carried out (such as background subtraction, Fourier transform). The optimization procedure permits to £t experimental spectra to model calculation using phase and amplitudes of single scattering computed in spherical wave formalism by ©XAFSS code or ©FEFF code [3].

The package also includes the program of deglitching worked out on basis procedure proposed in [4]. It permits to easily locate and to eliminate from the EXAFS spectra the additional signals originated from the Bragg scattering by crystalline samples or artifacts by the single crystal monochromator.

The analysis from 1-st shell Fourier transform EXAFS is not enough informative because it doesn't permits to estimate tilts of the 1-st shell atoms group (for example, oxygen octahedra rotations in perovskite crystals) or displacements of atoms in the neighbouring cells (phase transitions in a ferroelectrics). The program for analysis the multiple scattering processes on chains and £tting procedure with effective phases and amplitudes of scattering depended from angles also included in FTBF package. The effective amplitudes and phases can be produced by ©XAFSS .

The package is tested on the EXAFS spectra of Cu, $KNbO_3$ and $NaNbO_3$ crystals.

References

1. Press W.H., Teukolsky S.A., Vetterling W.T., Flannery B.P. (1996) Numerical Recipes in C Cambridge: Cambridge University Press.; Stoer J. and Bulirsch R. (1990) Introduction to Numerical Analysis New York: Springer-Verlag
2. Teo B.K. (1986) EXAFS: Basic Principles and Data Analysis New York: Springer-Verlag
3. Bugaev L., Ildefonse Ph, Flank A.-M., Sokolenko A., Dmitrienko H. (1998) J. Phys. C., 10, p. 5463; Rehr J.J., Albers R.C., Zabinsky S.I. (1992) Phys. Rev. Lett., 69, p. 3397
4. Zhuchkov K.N., Shuvaeva V.A., Yagi K., Terauchi H. (2001) J. Synchrotron Rad., 8, p. 302

Epitaxial growth on porous $\{111\}$ and $\{100\}$ Si surfaces

A. V. Chemakin, N. L. Shwartz, Z. Sh. Yanovitskaya, A. V. Zverev

Institute of Semiconductor Physics RAS SB, pr.Lavrenteva 13, 630090 Novosibirsk, Russia

natasha@spy.isp.nsc.ru

Recently porous silicon was demonstrated to be promising compliant substrate for heteroepitaxial growth [1]. Number of deposited layers necessary for complete pores sealing is of great importance for high-quality heteroepytaxial growth on porous substrates. This value could be estimated using Monte Carlo simulation. Kossel crystal model based on "solid on solid" principle forbids voids formation. Being more complicated and needing large computer resources, 3D models for diamond type crystals are vastly less evolved. 3D Monte Carlo model of epitaxial growth and sublimation process on $\{100\}$ and $\{111\}$ surfaces of diamond like crystals permiting atom diffusion along walls in any direction was developed. Using original rapid algorithm we could simulate crystal fragments with hundreds atomic layers in the depth. One monolayer could contain up to 10^5 atoms. The model permits voids and overhanging formation. This model was applied for simulation of homoepitaxy on (111) and (100) porous silicon surfaces. Simulation of homoepitaxy process on porous Si surfaces was carried out giving estimation of necessary dose for complete pores sealing of different sizes, porosity and deposition rate.

Simulations were carried out in the ranges of substrate parameters and regime of growth according to experimental works [1, 2, 3]: substrate temperature during epitaxy $T = 1073$ K, deposition rate $V = 0 - 0.1$ nm/s, porosity $P = 28$ %, pores diameter $d = 3 - 40$ atomic sites (a.s.) for Si(111) and $d = 3 - 20$ a.s. for Si(100). Deposition rate $V = 0$ nm/s corresponds to annealing process. High temperature annealing was carried out at temperature $T_a = 1400$ K.

Essentially different character of surface relief evolution during annealing and epitaxy processes on (111) and (100) surfaces has been found. During epitaxy on (111) surface at £rst pores sealing is observed and only then roughness of the surface is evolved. On (100) surface roughening starts at the initial stages of growth. Pores on Si(100) surface provoke relief evolution in growing layer. Deposited dose one order of magnitude greater than on Si(111) surface is necessary for pores sealing of the same diameter leading to later pores sealing on Si(100). Distinct facetting is observed on these two surfaces: on Si(111) pores walls facetting by highindex planes was observed and on Si(100) pyramidal pits evolving in growing layer over pores were restricted by (111) surfaces. Analogues differences during annealing process was observed as well. During prolonged annealing fragmentation of narrow pores was observed. Created voids approach equilibrium shape as annealing time increase.

This work was supported by the RFBR (No. 99–02–16742) and the Federal Target-Orientated Program "Investigation and development of prospective science and technology lines for civil purposes".

References

1. S. I. Romanov, V. I. Mashanov, L. V. Sokolov, A. Gutakovski, O. P. Pchelyakov. *Appl. Phys. Lett.* **75**, 4118 (1999).
2. T. Ito, T. Yasumatsu, A. Hiraki, *Appl. Surf. Sci.* **44**, 97 (1990).
3. Y. Yasumatsu, T. Ito, H. Nishizawa, A. Hiraki, *Appl. Surf. Sci.* **48/49**, 414 (1991).

Tight binding modeling of bonding and electronic properties of heterostructures

Hilmi Ünlü

Department of Physics, Istanbul Technical University
Maslak 80626 Istanbul, Turkey

Tel: 90 (212) 285 3201, Fax: 90 (212) 285 6386, email:hunlu@itu.edu.tr

Predictive process and performance simulation of semiconductor heterojunction devices requires analytic models which are qualitatively consistent with the laws of solid state physics and quantitatively accurate[1]. One of the most important issues is the understanding the formation and determining the magnitude of conduction and valence band offsets at heterointerfaces which dominate various device properties such as injection ef£ciency in heterojunction bipolar transistors (HBT) and carrier con£nement in the modulation doped FETs (MODFETs)[2]. In this article, an extended sp^3 tight binding model is shown to be highly succesful in the qualitative and quantitative treatment of heterojunction band offsets and Schottky barriers at any temperature, strain, pressure, and alloy composition. The presented model includes the overlapping of hybrids at neighboring bonds and anti-bonds such that it cannot simply be absorbed into a re-scaling of other parameters to £nd the valence band energies which are screened by the optical dielectric constants of constituents[3].

In £nding the heterojunction band offsets an average internal reference level, called tight binding midgap (TBM), at which the bandgap states are equally bonding (valencelike) and antibonding (conductionlike), is de£ned at a special point within the Brillouin zone of constituent semiconductors. By aligning the average TBM levels at the heterointerface, the band offsets are £rst obtained at zero temperature and 1 bar of pressure. The nonlinear effects of temperature, strain, pressure, and alloy composition on the band offsets are then obtained using the two universal statistical thermodynamic postulates: (i) the free electrons and holes are electrically charged weakly interacting quasi-chemical particles and (ii) the electron-hole pairs are generated by the charge transfer from the bonding (valencelike) states to antibonding (conductionlike) states.

The model is applied to AlGaAs/GaAs and HgCdTe/CdTe heterostructures, with normal and inverted interfaces, to determine the bonding properties and band offsets as a function of temperature, strain, pressure and alloy composition. The model predicts a crossover between $E_{g\Gamma}$ and E_{gX} at about P=46 Kbar for GaAs, in agreement with measurements of Goni et al., Phys. Rev. **B 36**, 1581 (1987)) and the fundamental bandgap of HgTe increases with pressure and becomes £nite at about P = 25 and 15 Kbar for T = 75, 150 and 300 K. Pressure moves up the energy of Γ_{6c} antibonding states above the energy of bonding Γ_{8v} states and HgTe becomes a diamond type above these pressures. The band alignment at the HgTe/CdTe interface transforms from type III to type I at pressures above 20 Kbar. The calculated pressure effects on the valence band offsets are found in good agreement with measurements of Woldorf et al. (J. Vac. Sci. and Tech., **B 4**, 1043 (1986)) for (Al,Ga)As/GaAs and Lambkin et al. (Phys. Rev. **39**, 5546 (1989)) for AlAs/GaAs quantum wells for pressures below 60 Kbar. Proposed model compares well with experiment for the band offsets of many heterostructures.

References

1. H. Ünlü, Book of Programme and Abstracts, pp-32-33, 2nd Int. Workshop on Challenges in Predictive Process Simulation, Wandlitz, Germany, 15-18 May 2000 ChiPPS'2000.
2. H. Morkoç, H.Ünlü, and G. Ji, *Principles and Technology of MODFETs*, **Vols. 1, 2**, Wiley (1991).
3. H. Ünlü, *Phys. Stat. Sol.* **(b) 223** (2001) 194-205.

Folding in lattice models with sidechains

Mai Suan Li
Institute of Physics, Al. Lotnikow 32/46, 02-668 Warsaw, Poland
masli@ifpan.edu.pl

Lattice models with sidechains are more realistic for proteins than those without sidechains. The sidechains would make the folding problem much more, however, involved computationally. In this contribution we examine the ef£ciency of three different move sets [1] for studying the folding of model proteins with sidechains. Move set I includes only single monomer moves. Single and double bead moves are allowed in move set II. Finally, set III involves one-, two- and three-monomer moves. We have studied the scaling of folding times, t_f, under optimal folding conditions for three-dimensional Go models with sidechains. t_f was found to grow with the chain length, N, by power law with exponent λ [2]. We obtained $\lambda \approx 7,4$ and 4 for set I, II and III, respectively. These values are higher than $\lambda \approx 3$ for Go models without sidechains [3]. Our results show that the sidechains slow down the folding process remarkably.

References

1. M. R. Betancourt, J. Chem. Phys. **109**, 1545 (1998).
2. D. Thirumalai, J. Physique I **5**, 1457 (1995).
3. A. M. Gutin, V. I. Abkevich, and E. I. Shaokhnovich, Phys. Rev. Lett. **77**, 5433 (1996); M. Cieplak, T. X. Hoang and Mai Suan Li, Phys. Rev. Lett. **83**, 1684 (1999).

Effects of geometric anisotropy on local £eld in composite media

C. K. Lo, Jones T. K. Wan and K. W. Yu

Department of Physics, The Chinese University of Hong Kong
Shatin, New Territories, Hong Kong, China

Corresponding author: Chi-keung Lo
Phone: (852) 2609 6339 Fax: (852) 2603 5204
Email: cklo1@phy.cuhk.edu.hk

Field-induced structure changes are most pronounced in the case of periodic composites. In a recent work [1], we have applied the Ewald-Kornfeld formulation to study the effects of geometric anisotropy on the local distribution for a tetragonal lattice of point dipoles numerically. In this work, we apply the Lekner formulation [2, 3] to yield an analytic expression of the local £eld in terms of geometric anisotropy. In both cases, the results show that the geometric anisotropy has signi£cant impact on the local £eld distribution. In this regard, we have also studied the geometric anisotropic effects on the piezoelectric coef£cient in both two-dimensional rectangular lattice of line dipoles and three-dimensional tetragonal lattice of point dipoles.

In actual computation, as an alternative to the Ewald summation, the Lekner summation technique is applied in two-dimensional periodic lattices so as to avoid the use of an arbitrary convergence parameter. Firstly, the Lekner sum yields a single, exponentially convergent series in the real space. Secondly, the resulting local £eld expression is analytic in the geometric anisotropy, thus allowing us to derive analytic expression for the piezoelectric coef£cient from the local £eld. In computing the piezoelectric coef£cient in three-dimensional tetragonal lattices by using the Ewald-Kornfeld formulation for different values of the adjustable parameter η of the sums, no plateau value can be found for all range of η although we thought that the Ewald-Kornfeld summation should be independent of the arbitrary convergence parameter. So we use spherical summation region instead of tetragonal region to obtain better convergence. Due to the fact that the derivative of the local £eld behaves even worse than the conditionally convergent summation of the local £eld, the reciprocal lattice sum will diverge as η increases. Nevertheless, our result shows that the values of piezoelectric coef£cient by applying Ewald-Kornfeld formulation agree with those obtained by a simple numerical differentiation of the local £eld expression with respect to the geometric anisotropy.

In summary, the results show that the geometric anisotropy has a signi£cant impact on the local £eld distribution and the piezoelectric coef£cient, in both two-dimensional and three-dimensional periodic lattices. We check that the piezoelectric coef£cient obtained by applying the Ewald-Kornfeld formulation agree with those obtained by a simple numerical differentiation of the local £eld distribution with respect to the geometric anisotropy. The results offer potential applications as arti£cial piezoelectric materials as one can change the degree of anisotropy easily in a suspension.

References

1. C. K. Lo, Jones T. K. Wan and K. W. Yu, J. Phys. : Condensed Matter **13**, 1315 (2001).
2. J. Lekner, Physica A **176**, 485 (1991)
3. N. Gronbech-Jensen, Int. J. Mod. Phys. C **7**, 873 (1996)

Computer modelling of light scattering in £lled liquid crystals

M.F.Lednei, I.P.Pinkevich, V.Yu.Reshetnyak, T.J.Sluckin*

Kyiv National Taras Shevchenko University, Physics Faculty,
Prospect Glushkova 6, Kyiv, 03022, Ukraine
** University of Southampton, Faculty of Mathematical Studies, Southampton, SO17 1BJ, UK*
E-mail: lednei@phys.univ.kiev.ua, pink@phys.univ.kiev.ua

Macroscopic particles embedded in liquid crystal (LC) cause the multiple defects in alignment of LC director that results in a strong Rayleigh light scattering. The transformation and disappearance of a part of them under the electric £eld action as well as the turn of LC molecules along the electric £eld cause a media enlightenment. Due to this the LCs £lled with particles of micron size are very perspective for using in display technologies and are intensively studied in last time. We report the results of investigation of the angular dependence of the Raleigh light scattering intensity in LCs which contain the particles of spherical or cylindrical form using the computer modelling. It was studied the in¤uence of particle size, form and aspect ratio, director anchoring strength on the particle surface, light polarisation, and external electric £eld. The concentration of particles is assumed to be small so the interaction between them via nematic media is negligible. For some cases we have found the director spatial distributions near the particles and investigated the in¤uence of external electric £eld on the director texture. To study light scattering in the case of $kR \leq 1$, where k is a wave vector of light, R is a size of director inhomogeneity area, we used Rayleigh-Gans approximation. If a size of the particles in LC is approximately $\geq 0.1\mu m$ or the director anchoring on the particles surface is strongly rigid one can use the anomalous-diffraction approach. In this approach we have calculated the total light scattering cross sections by £lled LCs assuming the director anchoring on the particles surface in£nitely rigid so the disclinations appear in the director £eld near the particles. Finally the in¤uence of LC ¤exoelectricity on the Rayleigh light scattering cross-section in external electric £eld was studied as well.

Work supported by INTAS grant 97-1315

First-order scaling near a second-order phase transition: Tricritical polymer collapse

Thomas Prellberg[1] **and Aleksander L. Owczarek**[2]

[1]*Institut für Theoretische Physik, Technische Universität Clausthal, Arnold-Sommerfeld Straße 6, D-38678 Clausthal-Zellerfeld, Germany*
[2]*Department of Mathematics and Statistics, University of Melbourne, Parkville, Vic 3052, Australia*
Tel: +49-5323-72 2085, FAX: +49-5323-72-3799, Email: thomas.prellberg@tu-clausthal.de

The coil-globule transition of an isolated polymer has been well established to be a second-order phase transition described by a standard tricritical O(0) £eld theory. We provide compelling evidence from Monte Carlo simulations in four dimensions, where mean-£eld theory should apply, that the approach to this (tri)critical point is dominated by the build-up of £rst-order-like singularities masking the second-order nature of the coil-globule transition. As indicated in Figure 1, the distribution of the internal energy has two clear peaks that become more distinct and sharp as the tricritical point is approached. However, the distance between the peaks slowly decays to zero. The evidence shows that the position of this (pseudo) £rst-order transition is shifted by an amount from the tricritical point that is asymptotically much larger than the width of the transition region [1, 2].

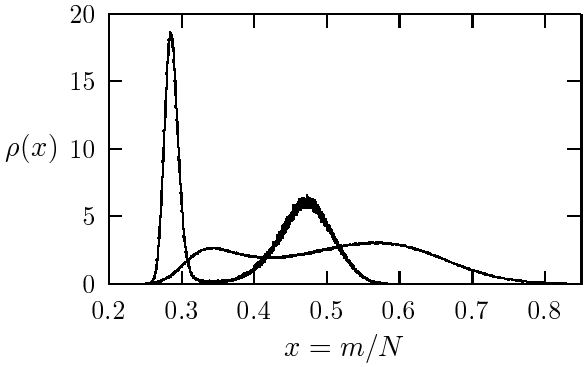


Fig. 1. *Internal energy density distributions for lengths* $N = 2048$ *and* 16384*, each at their respective transition temperatures. The more highly peaked distribution is associated with length* 16384.

The Monte Carlo simulations are based on a new stochastic enumeration algorithm, known as PERM, which has been recently developed by Grassberger [3]. This is essentially a kinetic growth strategy that adds clever enhancements to simultaneously allow a wide range of temperatures to be accessed and for the attrition of samples through trapping to be lessened.

References

1. A. L. Owczarek and T. Prellberg, Europhysics Lett. **51** (2000), 602.
2. T. Prellberg and A. L. Owczarek, Phys. Rev. E **62** (2000), 3780.
3. P. Grassberger, Phys. Rev. E **56**, 3682 (1997).

Mathematical model of biosensor with multilayer charged membrane

V.Rossokhaty and N.Rossokhata

Kiev National University, P.O.Box 262, 02222 Kiev - 222, Ukraine

tel. (+038 044) 545 17 30, E-mail: ross@nv.kiev.ua

Biosensors combining the basic principals of microelectronics, chemistry and biotechnology attract considerable attention in such £elds as medicine, environmental monitoring, pharmaceutic and food quality control. Now the most important problem for manufacture is to develop the inexpensive, commercially available, reliable devices with high operation performances. The latter can be achieved in particular by employment of multilayer charged enzyme membranes [1]-[2]. The prediction of response of such type of sensor requires detail analysis of the reaction-diffusion-drift phenomena occurring in the multilayer membrane which is complicated by necessity to take into account interaction between charged species of a test solution and charge encapsulated in some layer(s) of the membrane.

In this work a mathematical model of a glucose biosensor with multilayer charged membrane is developed. A solid-state transducer covered by the membrane linearly transforms a value of proton concentration near membrane-transducer interface into electrical signal. Multilayer membrane contains at least one enzyme layer with uniformly distributed immobilized enzyme molecules of a given concentration and other layers involving (if necessary) encapsulated charge of constant concentration. Test solution is considered to be in£nite source of £ve types of species: glucose, oxygen, protons, buffer and its conjugate base. The Michaelis-Menten theory is used to describe reaction kinetics. The model is reduced to one-dimensional transmission problem for the system of nonlinear evolution equations describing diffusion-drift transport of reaction components and products in membrane as well as Poisson equation for electrostatic potential.

To £nd approximate solution, we used implicit difference scheme with automatic selection of time step and constructed irregulal space grid with automatic adaptation of grid points to physical data of the model. In numerical experiment the developed model of the biosensor was adopted to the real experimental sample of the glucose biosensor 2-layer charged membrane [1]-[2]. We considered the inner layer to be enzyme one while the second (charged) layer contains the uniformly distributed negative or positive charge, and the outer (neutral) layer plays role of a spacer in which species concentrations change from their values in the charged layer to those in bulk of a buffer. As a result of computer simulation, the transient and position dependencies of all species concentrations and potential, time dependencies of output signal and calibration curves of glucose biosensor were obtained. Numerical experiment shows that i) potential barrier at the membrane-solution interface (or within the membrane) can cause a tremendous changes in proton pro£le within the membrane and hence, in sensor performances and ii) dependencies of sensor sensitivity on charged layer thickness can be strongly non-monotone with substantial difference between maximal and minimal values.

Thus, the developed model and algorithm give an opportunity to predict and optimize enzyme potentiometric biosensor performances by varying combination of physical and biochemical parameters of the membrane layers as well as create a basis for development of sensor with electrically controlled performances.

References

1. A.Soldatkin, A.El’skaya et al. Anal. Chim. Acta, **283**(1993), pp.695-701.
2. V.Volotovsky, A.Soldatkin, V.Rossokhaty et al. Anal. Chim. Acta, **322**(1996), pp.77-81.

Calculation of the condensate fraction in liquid Helium-4

A. A. Rovenchak and I. O. Vakarchuk

Department for Theoretical Physics, Ivan Franko Lviv National University, 12 Draghomanov Str., Lviv, Ukraine, UA–79005

+380 322 979443, andrij@ktf.franko.lviv.ua

The problem of the condensate fraction in liquid helium-4 was £rst considered in the classical paper by Penrose and Onsager. The authors used a very rough approximation of hard spheres and calculated this quantity f as approximately 0.08 or 8 per cent. Since that time there were a lot of different theoretical estimations and experimental measurements for f. All of them do not differ much from the £rst estimation and vary from about 4 to 20 per cent.

In this work, we propose a simple method for the calculation of the condensed fraction using formulae obtained earlier in [1]:

$$f = N_0/N = \exp\left(I_{1A} + \Delta_1 J + \ldots\right), \tag{1}$$
$$I_{1A} = -\frac{1}{4N}\sum_{\mathbf{q}\neq 0}(\alpha_q - 1)^2/\alpha_q, \quad \Delta_1 J = \rho\int d\mathbf{R}\left[2h^*(R) - h(R) + h^2(R)/4\right]$$
$$h(R) = F_2(R) - 1, \qquad h^*(R) = \sqrt{F_2(R)} - 1,$$

dots denote terms having more than one integration over wave vector or coordinate, $F_2(R)$ is the pair distribution function, N is the number of atoms, and

$$\alpha_q = \sqrt{1 + 2\varrho\nu_q \Big/ \frac{\hbar^2 q^2}{2m}}, \tag{2}$$

$varrho$ is helium density, $\varrho = 0.02185$ Å^{-3}, m is the mass of helium atom, $m = 4.0026$ a. m. u., q is the wave vector. These expressions contain ν_q being the Fourier image of the interatomic potential in helium that has an effective nature. It is obtained from the £rst principles using the collective variables formalism in the Schrödinger equation, as described in [2]. The only quantity we need to know for it is the static structure factor of helium at zero temperature. It is the advantage comparing to those methods that involve such quantities as the dynamic structure factor, measurements on the high-energy scattering [3], phenomenological assumptions [4], etc.

We have calculated the condensate fraction at zero temperature using two different models for the short-range repulsive part of the potential. In the £rst one, we do not take it into account directly and in the second one this repulsion is modeled by Meyer's function $e^{(A/R)^n} - 1$, R is the radius-vector. We choosed $A = 2.1$ Å and $n = 12$.

The calculated values of f are 13.2 per cent and 11.2 per cent respectively. We expect the real value being about 10–30 per cent less than calculated due to the contribution of the higher-order terms, as described in [1]. But in the £rst approximation we consider it to be a good accuracy for such a hardly-measurable quantity as condensate fraction in helium.

References

1. I. O. Vakarchuk, Ukr. Fiz. Zhurn. **35**, 1261 (1990).
2. I. O. Vakarchuk, V. V. Babin, A. A. Rovenchak, J. Phys. Stud. **4**, 16 (2000); available in PS-format at `http://www.ktf.franko.lviv.ua/JPS/2000/1/ps/16_22.ps.gz`
3. J. Mayers, C. Andreani, D. Colognesi, J. Phys.: Condens. Matter, **9** 10639 (1997).
4. J. Mayers, Rutherford Appleton Laboratory Technical Report RAL–TR–96–031 (1996).

Non-equilibrium molecular dynamics simulation of block copolymers in selective solvents

Igor Rychkov, K. Yoshikawa

Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

e-mail: rych@chem.scphys.kyoto-u.ac.jp

Block copolymers, which are macromolecules with immiscible parts, are attracting considerable attention due to their ability to self-assemble into various ordered structures. While block copolymer melts are fairly well studied [1], research on block copolymers in selective solutions stay rather limited, as the addition of low molecular weight solution, which is both a diluent and a medium favorable for one of blocks, makes the phase behavior of the system more complicated due to the extra degrees of freedom. Yet recently a phase diagram of some structures in block copolymer solutions was presented using a self-consistent mean-£eld theory [2].

We present a Non-Equilibrium Molecular Dynamics (NEMD) simulation study of symmetric diblock copolymers in selective solvents. Fixing all the parameters that ensure immiscibility and the quality of solvent being favorable to one block and therefore causing collapse of the other block, we vary the concentration of block copolymers in the wide range, starting from the critical concentration of micelle formation up to dense solutions. With the increasing of the concentration the emerging of various structures as well as transitions between them are anticipated, namely, disordered phase, spherical micelles, cylindrical structures, bicontinuous (gyroid) structures and lamellar phase.

For each of the structures we study the structural properties as well as the rheological behavior in shear ¤ows using SLLOD+NEMD [3] simulation technique, with SLLOD equation of motions, and exploiting recent advanced symplectic numerical integrator [4]. Our interest here is twofold. Rheology is a useful tool for locating phase transitions, and block copolymers are promising systems for £nding non-standard rheological behavior. Our studies mainly result in the presentation of the various structures emerging and the dependency of viscosity on the concentration and the shear rate.

References

1. Block Copolymer Thermodynamics: Theory And Experiment, F.S.Bates, and G.H. Fredrickson, Thermoplastic Elastomers, 2nd Ed, Hanser Publishers, NY. (1996).
2. Self-consistent calculations of block copolymer solution phase behavior, Huang CI, Lodge TP, Macromolecules 31 (11), 3556-3565 (1998).
3. Statistical Mechanics of NonEquilibrium Liquids, Denis J. Evans and Gary P. Morriss, Academic Press, London (1990).
4. Reversible multiple time scale molecular dynamics, M. Tuckerman and B. J. Berne G. J. Martyna, The Journal of Chemical Physics, 97, 3, 1990-2001 (1992)

Kinetic theory of mechanical strength of carbon nanotubes

Guram G. Samsonidze[1] **and Georgii G. Samsonidze**[2]

[1] *Institute of Applied Physics, Corrensstraße 2–4, D–48149 Münster, Germany*
[2] *Department of Mechanical Engineering and Materials Science, Rice University, Houston, Texas 77005, USA*
samsonid@nwz.uni-muenster.de

Promising materials for many areas of science and technology, carbon nanotubes (CNT) are investigated intensively for the last decade. Among other intriguing properties, they demonstrate enormous mechanical strength. Studies of the strength limits involve survey of non-plastic mechanical relaxation processes in the material. On initial steps these processes are built up of diatomic interchanges, known as a Stone-Wales defects (SWD) in fullerene science. Detailed computer simulations performed [1] con£rm the mechanism of initial strain release through SWD generation. While the thermodynamics of SWD formation in CNT is discussed elsewhere [2], the kinetic aspects of such a process still present an open problem for science, in spite of the importance of the activation barriers and transition states (TS) in the exploration of CNT mechanical failure mechanisms. Two different atomic con£gurations of TS have been detected earlier [3, 4] in quantum *ab initio* studies of fullerenes, with some uncertainty due to the differences in the methods. Note that the imposed constraints on the atoms [3], which is equivalent to the inclusion of virtual forces in the system, can somewhat distort the resulting S structure.

Present study reveals several modes of TS corresponding to different positions of the rotating SWD bond atoms with respect to the graphite plane. Multiple computations, augmented by the analytical formulas for the second derivatives of the Tersoff-Brenner multibody empirical interatomic potential, allow us to compare the activation barriers for the competing TS modes. Our method does not involve any force-constraints and therefore allows £nding the exact free TS modes, within the classical potential limitations only. Our calculations demonstrate that both disputable TS modes [3, 4] exist and can be preferable in the CNT of different diameters and chiral symmetries and under variable strain levels. It is shown in the present paper that different branches of activation energy (i.e., energy barriers of different TS modes) are the most favorable for variable CNT chiralities, diameters, and strain levels, leading to TS mode competition in stretched CNT. The lower envelope of the activation energy branches as a function of CNT chirality, which de£nes the relative strength of CNT of different symmetries, is found to differ signi£cantly from the formation energy.

In conclusion, the paper presents a complex description of non-plastic mechanical relaxation channels based on SWD generation processes in CNT. It is shown that the kinetic behavior of a single SWD differs in principle from the thermodynamic one. Actually, from the kinetic point of view, the common thermodynamic conceptions of CNT mechanical yield are turned upside down. Some problems, such as correlation effects and curvature in¤uence, are not covered by the present paper and are subjects for future work.

References

1. M. B. Nardelli, B. I. Yakobson, and J. Bernholc, *Phys. Rev.* **B 57**, 4277 (1998).
2. B. I. Yakobson, Ge. G. Samsonidze, and G. G. Samsonidze, *Carbon* **38**, 1675 (2000).
3. C. D. Latham, M. I. Heggie, R. Jones, and P. R. Briddon, in *Recent Advances in the Chemistry and Physics of Fullerenes* (The Electrochemical Society, Pennington, 1995).
4. R. L. Murry, D. L. Strout, G. K. Odom, and G. E. Scuseria, *Nature* **366**, 665 (1993).

Representation of a network of £ller particles in polymeric composites as a mass multifractal

G.V. Kozlov, G.B. Shustov, I.V. Dolbin

Kabardino-Balkarian State University,
360004, Nalchik, Chernishevsky st., 173, KBR, Russia
E-mail: deanchem@ns.kbsu.ru

The computer program for quantitative description of a network of £ller particles as mass multifractal has been designed. For this purpose with the help of the pictorial editor Photo Editor the contours of £ller particles in an microphotograph of fracture surface were de£ned and on image the grid with square boxes with the size δ was superimposed. After that each particle was colored and moment M_q for each box in a microphotograph by the size L was calculated:

$$M_q \sim \left(\frac{L}{\delta}\right)^{D_q(1-q)}, \tag{1}$$

where D_q is dimension Renji, q – index.

Designed this diagrams $D_q(q)$ have the ”classical” S-shaped picture in an interval q= -40÷+40. It means that the network of £ller particles in polymeric composites is multifractal. The checkout of the method is carried out with the help of the inequality:

$$\frac{D_1}{|q|+1} \le D_q \le \frac{d|q|+D_1}{|q|+1} < d, \tag{2}$$

where d is dimension of Euclidean space, in which multifractal (in our case d=2) is considered. This checkout has con£rmed the correctness of the proposed procedure.

The estimation of £ller particles network structure with the help of the multifractal characteristics showed that increase of the £ller volumetric content φ_f gives an increase of Hausdorff dimension D_0 (at q=0) and increase of ”latent ordering” of a network Δ_{40}, de£ned as D_1-D_{40} (at q=1 and 40, accordingly). Besides the increase φ_f gives an increase of extremal dimension D_{-40} and D_{40}, describing most concentrated and most rare£ed sets in the system. The simultaneous increase D_{-40} and D_{40} in accordance with the increase φ_f means raise of £ller particles aggregation. It also supposed observed increase of correlation dimension D_2 (at q=2), describing probability of £nding in one box of points of set, in accordance with the increase φ_f.

Adsorption of polymer chains with variable stiffness onto a surface: Molecular dynamics simulations

V.A. Sorkin[1], **E.Yu. Kramarenko**[2], **P.G. Khalatur**[2], **and A.R. Khokhlov**[2]

[1] *Dept. of Physics, Technion Institute of Technology,320000 Haifa, Israel*
[2] *Dept. of Physics, Moscow State University, 117324 Moscow,Russia*
Tel:+972 4 829 3651 e-mail: phsorkin@tx.technion.ac.il

Adsorption of macromolecules onto a surface is one of the fascinating problems in polymer physics. Recently, the problem has been studied intensively due to its scienti£c importance and numerous technical applications [1, 2]. Despite of the signi£cant progress in this £eld, many questions still remain open [3, 4].

Up to now the main attention has been paid to adsorption of ¤exible polymer chains on a ¤at attractive surface, while the special features of stiff polymer chains adsorption were essentially not investigated. We propose that the rigidity of macromolecules in¤uences considerably the character of their interaction with an attractive surface.

In the present work, the impact of the chain stiffness upon its adsorption from a semi-dilute solution has been investigated. In addition, the appearance of liquid-crystalline ordering of the macromolecules in the vicinity of the attractive surface was studied.

We perform isothermal molecular dynamics simulations of polymer chains with excluded volume near an impenetrable attractive surface. The in¤uence of adsorption energy, chain stiffness, and concentrations of the chains in the system has been examined.

The morphology of the adsorbed chains has been studied in detail. In particular, quantities such as average length of the adsorbed and of the loop sections, the monomer density pro£le, and the segment orientation were calculated. We show that the average length of adsorbed sections increases with enlargement of adsorption energy as well as chain stiffness, and decreases with increasing chain concentration. In contrast, the average length of loops decreases with increasing adsorption energy and chain stiffness, and enlarges with increasing concentration of the chains in the system.

Orientation ordering of stiff polymer chains in the course of their adsorption from the semi-dilute solution onto a plane surface was also examined. We £nd that orientation ordering of polymer chains on the attractive surface increases with increase of adsorption energy, and so does the orientation ordering of polymer chains in the bulk. An enlarging of the number of polymer chains in the system leads to disappearance of orientation ordering of macromolecules on the attractive surface.

References

1. E. Yu. Kramarenko *et al.*, J. Chem. Phys. **104**, 12 (1996).
2. A. Miller, K. Binder, Macromolecules **29**, 343 (1996).
3. P. Y. Lai, J. Chem. Phys. **103**, 5742 (1995).
4. A. Yu. Grosberg, A. R. Khokhlov, Statistical Physics of Macromolecules. Am. Inst. of Physics, NY, 1994.

One-particle diffusional model to mimic some properties of glass transition

Sorkin A.V.[1] **and Ivanov V.A.**[2]

[1]*Department of Physics, Technion, Israel*

[2]*Department of physics, Moscow State University, Moscow, Russia*

anastasy@techunix.technion.ac.il

ivanov@polly.phys.msu.su

In recent time many properties of glass transitions have been investigated intensively. The phenomenon of glass transition has a considerable technologic importance. In particular the transition temperature is a most important charateristic in the technical use of amorphous polymers.

In spite of many theoretical, experimental and computer simulation works devoted to this theme, some physical properties of the glass transition are still not clear. There is no theory describing satisfactorily all the diversity of characteristics connected with the transition.

The most interesting question that cannot be answered on the base of available experimental facts is whether the glass state is a new phase state, or simply an unequilibrium state with freezed kinetical degrees of freedom.

All simulations describing the glass state are separated in two main methods. The £rst method is associated with realistic polymers or other glass systems under conditions corresponding to real physical conditions. The second investigates abstract models that may diverge far from real materials, but mimic correctly the behavior of real glass systems. The models of the second class are simpler are faster and enable to investigate extensively the in¤uence of various physical factors on the glass transition characteristics.

The purpose of this work is to investigate one of these abstract models that exhibits a transition between two regimes of behavior, similar to a glass transition. In this one-dimensional continuum model, a Brownian particle diffuses whithin a speci£c set of obstacles. The obstacles have a given lifetime. At the end of its lifetime, the obstacle disappears and emerges in another location. The particle cannot penetrate throuth the obstacle. Its diffusion cof£cient D is connected with the lifetime τ of obstacles in a self-consistent way, $D\tau = K$, where K is a constant. “Freezing” occurs at a suf£ciently large concentration of obstacles; the system is athermal. The model is based on a model proposed recently by Ivanov [1], in which “old” and “new” coordinates of obstacles were uncorrelated. We improved the model by introducing Gaussian correlations (characterized by a distribution width σ) between locations of obstacles.

The dependence of the diffusion cof£cient D was measured as a function of obstacle concentration c, correlation of obstacle positions, rate of successful moves of particle, and of the combination $\sigma\sqrt{K}$. Comparison between the previous and the improved model shows that the previous model is approximated by the new one in the limit $\sigma c \to \infty$.

References

1. V.A.Ivanov, B.Jung, A.N.Semanov, I.A.Nyrkova,A.R.Khokhlov, J.Chem.Phys. **104**(11), 4214 (1996)

Phase transitions of hard- and soft- disks in external periodic potentials: A Monte Carlo study

W. Strepp[1], **S. Sengupta**[2], **M. Lohrer**[1], **P. Nielaba**[1]

[1] *Physics Department, University of Konstanz, Fach M 691, 78457 Konstanz, Germany*

[2] *S.N. Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Calcutta 700098, India*

++49 (0)7531 883747, ++49 (0)7531 884462, strepp@hamilton.physik.uni-konstanz.de

The nature of the melting transition for a system of hard disks with translational degrees of freedom in two spatial dimensions has been analyzed [1] by a novel £nite size scaling technique for the computation of the crystals elastic properties [2] close to the melting transition. The behavior of the system is consistent with the predictions of the Kosterlitz-Thouless-Halperin-Nelson-Young theory.

Hard and soft disks in external periodic potentials show rich phase diagrams including freezing and melting transitions when the density of the system is varied. Here the phase diagrams of such systems in a spatially periodic external potential is studied using extensive Monte Carlo simulations. Detailed £nite size scaling analyses of various thermodynamic quantities like the order parameter, its cumulants etc. are used to map the phase diagram of the system for various values of the density and the amplitude of the external potential. For hard disks we £nd [3] clear indication of a re -entrant liquid phase over a signi£cant region of the parameter space. Our simulations therefore show that the system of hard disks behaves in a fashion similar to charge stabilized colloids which are known [4] to undergo an initial freezing, followed by a re -melting transition as the amplitude of the imposed, modulating £eld produced by crossed laser beams is steadily increased. Detailed analysis of our data shows several features consistent with a recent dislocation unbinding theory of laser induced melting [5]. The differences and similarities in systems with soft potentials (screened Coulomb, $1/r^n$, n=12) is discussed.

References

1. S. Sengupta, P. Nielaba, K. Binder, Phys. Rev. **E 61**, 6294 (2000).
2. S. Sengupta, P. Nielaba, M. Rao and K. Binder, Phys. Rev. **E 61**, 1072 (2000).
3. W. Strepp, S. Sengupta, P. Nielaba, Phys. Rev. **E** (2001) (in press).
4. C. Bechinger, M. Brunner, P. Leiderer, Phys. Rev. Lett **86**, 930 (2001).
5. E. Frey, D.R. Nelson, L. Radzihovsky, Phys. Rev. Lett. **83**, 2977 (1999).

Different structures of stiff-chain macromolecules: A Monte Carlo simulation

M. R. Stukan,[1] **V. A. Ivanov,**[1] **W. Paul,**[2] **K. Binder**[2]

[1]*Physics Department, Moscow State University, Moscow 117234, Russia*
[2]*Institut für Physik, Johannes Gutenberg Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany*

+007 (095) 939-4756, +007 (095) 939-2988, stukan@polly.phys.msu.su

Using a coarse-grained model of a semi¤exible macromolecule, the equilibrium shapes of the chain have been studied varying both the temperature and the chain stiffness. We have applied Monte Carlo techniques using the bond ¤uctuation model. Chains consisting of 40, 80, 160, 200 and 240 monomer units have been studied. We have used in our model two different types of interactions: a potential depending on the angle between successive bonds along the chain to control the chain stiffness, and an attractive interaction between non-bonded effective monomers to model variable solvent quality [1]. In a diagram of states for £xed chain length where chain stiffness and inverse temperature are used as variables, we £nd regions where the chain exists as coil, as spherical globule, and as toroidal globule, respectively (Fig. 1). This regions are not limited by sharply de£ned boundaries, but rather wide two-state coexistence regions occur in between them, where also intermediate metastable structures (such as rods and disks) occur. It was found that the transitions between coil and toroidal globule and between toroidal globule and spherical globule which take place at rather high values of stiffness are of the rounded £rst order type [2]. Using a new order parameter, we have found that the transition between toroidal globule and the spherical one for short chains occurs via the intermediate state of liquid-crystalline globule.

It was theoretically estimated [3] that the dependence of toroid radius on chain length should scale as $R \sim N^{1/5}$. In order to check this prediction we have investigated toroidal globules formed by chains of 40, 80, 160 and 240 monomers. According to our simulations we have found this dependence to be $R \sim N^{0.23\pm0.03}$ (Fig. 2) what is in good agreement with theory.

Fig. 1. Diagram of states for semi¤exible polymer chain with $N = 80$ in variables stiffness (b) vs. inverse temperature ($1/T$).

Fig. 2. Dependence of toroid radius on chain length.

References

1. V. A. Ivanov, W. Paul, K. Binder, *J. Chem. Phys.* **1998,** *109,* 5659.
2. V. A. Ivanov, M. R. Stukan, V. V. Vasilevskaya, W. Paul, K. Binder, *Macromol. Theory Simul.* **2000,** *9,* 488.
3. A. Yu. Grosberg, private communication.

Friction in atomistic Brownian systems

G. Sutmann and B. Steffen
Central Institute for Applied Mathematics, Research Centre Jülich
(+49) 2461 61 6746, (+49) 2461 61 6656, g.sutmann@fz-juelich.de

The calculation of the friction coef£cient, ζ, of a Brownian particle dissolved in a liquid is a delicate problem in a molecular dynamics simulation. Within the framework of linear response theory, ζ may be calculated via

$$\zeta = \frac{\beta}{3} \lim_{t\to\infty} \int_0^t d\tau \, \text{limth}\langle \mathcal{F}(\tau)\mathcal{F}(0)\rangle \tag{1}$$

where $\mathcal{F}$ is a *projected* random force acting on the Brownian particle, β the inverse thermal energy and *limth* denotes the thermodynamic limit ($N \to \infty$, $V \to \infty$, $N/V = const$). In the limit of an in£nitely heavy Brownian particle, $\mathcal{F} = F$, where F is the force on the Brownian particle due to the ¤uid. It was shown in Refs.[1, 3] that $\zeta = 0$ if one does not take into account the thermodynamic limit before taking $t \to \infty$. The reason for this behavior is the fact that the momentum of the ¤uid gained by collisions with the £xed particle cannot be carried off to in£nity [2], i.e. it is con£ned within the simulation box.

We propose here a simple but effective way to calculate friction coef£cients in systems with a £nite number of particles to which periodic boundary conditions are applied. The idea is to £x a Brownian particle in the center of the simulation box and to randomize the momentum of those particles which leave the simulation box on the one side and enter into it on the other side so that there are no dynamic correlations beyond the box boundaries. In that way the momentum of the ¤uid is randomized across the boundaries or one can say that it is carried off to in£nity.

The randomization of the ¤uid particles is done in a way that the statistics of the velocity distribution function in the system is not altered, i.e. the system is neither heated up nor cooled down. This may be achieved by the choice of new velocities across the boundaries $v_{new} = \alpha v_{old} + \sqrt{1-\alpha^2} v_{ran}$, where v_{ran} is a randomly chosen velocity from a distribution with the same mean and variance as v_{old}, and α is varied between 0 and 1. (choosing v_{ran} corresponding to a temperature T, our technique may also be applied as a thermostat).

We show that it is possible to obtain a £nite value of ζ in Eq.1 already for a small number of particles. We present calculations for ζ for a Brownian particle, modeled by a modi£ed Lennard-Jones potential, £xed at the origin of the simulation box and immersed in a Lennard-Jones ¤uid consisting of $N = 256$, 2048 and 16384 particles.

References

1. L. Bocquet, J. P. Hansen, and J. Piasecki. On the Brownian motion of a massive sphere suspended in a hard sphere ¤uid. II. molecular dynamics estimates of the friction coef£cient. *J. Stat. Phys.*, 76:527, 1994.
2. L. Bocquet, J. P. Hansen, and J. Piasecki. Friction tensor for a pair of Brownian particles: Spurious £nite size effects and molecular dynamics estimates. *J. Stat. Phys.*, 89:321, 1997.
3. P. Español and I. Zúñiga. Force autocorrelation function in Brownian motion theory. *J. Chem. Phys.*, 98:574, 1993.

Electrostatic effects in colloidal systems : Monte Carlo simulations

Takamichi Terao and Tsuneyoshi Nakayama

Department of Applied Physics, Hokkaido University, Sapporo 060-8628, Japan

Tel.*: +81-11-706-6622*, Fax*: +81-11-716-6175*,
e-mail*: terao@eng.hokudai.ac.jp*

Electrostatic interaction plays an important role in aqueous solutions of colloids and polyelectrolytes [1-3]. While the bare Coulomb interaction between charged colloidal particles is purely repulsive, the problem is nontrivial by the presence of the microscopic counterions, which are dispersed in an aqueous solution and screen the direct Coulomb repulsion. For weak Coulomb interaction or high dilution of the macroions, the linearized screening theory of Debye and Hückel always leads to an effective pure-repulsive interaction between macroions. This phenomena is described by the Derjaguin-Landau-Verwey-Overbeek(DLVO) theory, which predicts the screened Coulomb repulsion between charged colloidal particles in an aqueous solution. In the DLVO theory, the effective interaction between particles $U_{\mathrm{DLVO}}(r)$ is given by

$$U_{\mathrm{DLVO}}(r) = \frac{Z^2 e^2}{4\pi\epsilon}\left(\frac{\mathrm{e}^{\kappa a}}{1+\kappa a}\right)^2 \frac{\mathrm{e}^{-\kappa r}}{r} \quad , \tag{1}$$

where Z, e, κ, a, ϵ and r denote the surface charge of colloidal particles(macroions), the elementary charge of an electron, the inverse of Debye-Hückel screening length, a radius of colloidal particles, the dielectric coef£cient of the medium, and the center-to-center distance between two colloidal particles, respectively.

Recently, a lot of works are devoted to clarify the counterion condensation and the attractive interaction between charged colloids, which are inconsistent with the DLVO theory. In this paper, nonlinear screening effect of charged colloids and their *non-DLVO* behavior are numerically investigated. We perform "ion-counting" analysis by Monte Carlo simulation and clarify microion density pro£les on a charged colloidal particle. With multivalent salt ions, the calculated results on the electric double layer obey the drastically different pro£le from that described by the Gouy-Chapman theory. We also con£rm that the charge inversion phenomena becomes enhanced with increasing concentrations of multivalent salt ions.

References

1. S. Alexander, P. M. Chaikin, P. Grant, G. J. Morales, P. Pincus, and D. Hone, J. Chem. Phys. **80**, 5776 (1984).
2. T. Terao and T. Nakayama, Phys. Rev. E **60**, 7157 (1999).
3. T. Terao and T. Nakayama, J. Phys.: Condens. Matter **12**, 5169 (2000).

Glass transition in polymer £lms: A molecular dynamics study

Fathollah Varnik[1], **Jörg Baschnagel**[2], **Kurt Binder**[1]

[1]*Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, D–55099 Mainz, Germany*

[2]*Institut Charles Sadron, ULP, 67083 Strasbourg, France*

Tel: ++49 6131 3925158, Fax: ++49 6131 3925441, e-mail: varnik@mail.uni-mainz.de

Understanding the glassy state of condensed matter and in particular the transition that leads from a supercooled ¤uid to the amorphous solid is one of the greatest challenges of our time. A particularly controversial concept is the idea of a characteristic "correlation length" ξ that grows as the glass transition is approached. This length is supposed to measure the size of the regions over which cooperative structural rearrangements need to occur to allow the system to relax [1]. If such a growing length scale exists, the glass transition temperature, Tg, should depend on the system size, L, for $L \leq \xi$. The investigation of the glass transition in thin polymer £lms provides an attractive way for the study of the size dependence of Tg. Although there have been many experiments on polymer £lms [see for example Refs. 2 and 3] many details are still unclear. An intriguing feature clearly is that for long entangled chains the motion near a surface may differ from the one in the bulk [4]. Therefore, we study, via computer simulations, the glass transition of short polymer chains that are not entangled. The con£nement is realized by two completely smooth and repulsive walls acting via a $U_{wall} = |z_{\mathrm{particle}} - z_{\mathrm{wall}}|^{-9}$ potential. The in¤uence of this con£nement on the dynamic behavior of the melt is studied for various £lm thicknesses, i.e., wall-to-wall separations, ranging from about 3 to about 12 times the bulk radius of gyration. A comparison of the dynamic quantities like the mean square displacements or the incoherent scattering function for the £lm and for the bulk clearly shows an acceleration of the dynamics due to the presence of the (smooth) walls. The effect of the walls is more pronounced at low temperatures and small £lm thicknesses. We observe that some aspects of the dynamic behavior of the con£ned system can be described by the so called mode coupling theory (MCT). In particular, the α-relaxation time obeys a power law $\tau^{\alpha}(D,T) \propto |T - \mathrm{Tc}(D)|^{-\gamma(D)}$. Using this power law we obtain the D-dependence of the mode coupling critical temperature, $\mathrm{Tc}(D)$, which decreases for smaller D. This result is in qualitative agreement with that of the glass transition temperature observed in some experiments on supported poly mer £lms [2]. As for the critical exponent $\gamma(D)$, the observed D-dependence is rather weak. This motivates us to compare the time dependence of the mean sqaure displacements for various £lm thicknesses and for the bulk at temperatures with the same distance from the corresponding critical temperature. For intermediate times, all curves can be well described by a unique master curve. This remarkable propertiy of the dynamics at intermediate times, is also observed for the intermediate scattering function.

References

1. E. Donth, *Relaxation and Thermodynamics of Polymers: Glass Transition* (Akademie-Verlag, Berlin, 1992).
2. J.-L. Keddie, R. A. L. Jones, and R. A. Cory, Europhys. Lett. **27**, 59 (1994).
3. J. A Forrest and R. A. L. Jones in pp. 251-294 of *Polymer Surfaces, Interfaces and Thin Films*, Ed. A. Karim and S. Kumar (World Scienti£c, Singapore, 2000).
4. P. G. de Gennes, Eur. Phys. J. E **2**, 201 (2000).

Monte Carlo approach to double-stranded polymers

Yuri S. Velichko[1,2], **K. Yoshikawa**[1] **and A. R. Khokhlov**[2]

[1] *Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan*

[2] *Physics Department, Moscow State University, Moscow 117234, Russia*

e-mail: velichko@scphys.kyoto-u.ac.jp

Double-helix structure of DNA provides a suitable model system for studying equilibrium properties of macromolecule. In contrast to the models of linear polymers, the secondary structure as well as most interaction parameters, such as stiffness of molecules backbone or solvent quality can be introduced into the model. We present studies of double-stranded twisted circular polymer chain by mean of computer simulation. The attention was focused on the effect of polymer chain twisting and anisotropy of rigidity on the topology of macromolecule. As applications, we considered the effect of chain twisting on the conformation of polymer coil, macromolecules behavior on the surface and coil to globule transition.[1, 2] Anisotropy of rigidity, £nite chain length effect, and solution quality are investigated.

Polymer molecules provide some of most important examples of fractals in the nature. Scaling idea introduce index or fractal dimension, that can be used to describe structure of fractals. In case of a twisted chain, the formation of helical structures and loops affects a monomer units distribution. The number of loops increases with increase in the number of double helical turns, and as a result, the polymer chain becomes more compact. The same allocation of monomer units into helical or loops structures shows a plausible route for the chain compaction, which we observed in the dependence of the radius of gyration on the number of double helical turns. Chain size decreases slightly until number of double-helical turns is small enough. With father increase in the chain twisting, macromolecule forms supercoiled structures under in¤uence of torsional tension, which also growth up. Chain size decreases and mean square radius of gyration decays exponentially depending on the number of double helical turns. Bending and torsional energies also show exponential behavior. We propose that the linking number density affects the distribution of monomer units in the space and changes the scaling of the polymer chain.[1].

Behavior of double-stranded twisted polymers in coil state strongly depends on the number of double-helical turns. That affects not only the size or energies of macromolecule, but also the chain conformation. We have found that transition from coil state to the globule is accompanied with changes in the polymer chain topology. With increase in the number of double-helical turns, polymer chain obtains supercoiled structure and the number of intersections of chain axes (writhing number) grows with decrease in the temperature. Last one suppress contribution of the entropy of the chain and makes conformation of the molecule dependent on the interplay between parts of internal energy (bending and torsional energies), so becomes strongly dependent on the number of double-helical turns. We also found dependence of theta-temperature on the linking number. With increase in the twisting of the chain, theta-temperature becomes lower.

References

1. Y. S. Velichko, K. Yoshikawa and A. R. Khokhlov, J. Chem. Phys., **111**, 9424 (1999).
2. Y. S. Velichko, K. Yoshikawa and A. R. Khokhlov, Biomacromolecules, **1**, 459 (2000).

Phase diagrams of compressible polymer-solvent mixtures - A Monte Carlo investigation

Peter Virnau, Marcus Müller, Luis McDowell

Institut für Physik, WA331, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany

telephone number: +49 6131-3923683, fax number: +49 6131 39-25441 , e-mail address: Peter.Virnau@Uni-Mainz.de

Classical nucleation theory exhibits de£ciencies in describing the creation of bubbles in polymer foams [1] hereby inhibiting the design and development of new foams. A better microscopic understanding of the underlying processes is therefore desirable.

To examine the problem in more detail we simulate a hexadecane-CO_2 mixture with the help of a coarse-grained model: CO_2 is described by a single LJ-sphere and hexadecane by a chain of £ve LJ monomers with additional FENE-interactions. Interaction parameters are derived from the critical points of pure hexadecane and CO_2 using a modi£ed Lorentz-Berthelot mixing rule. A grand-canonical con£gurational bias algorithm allows for an ef£cient relaxation of density ¤uctuations, reptation and local MC steps additionally update the chain conformations. Data analysis is based on histogram-reweighting techniques which also enable a calculation of the interface tension. Up to now these methods were succesfully implemented to incompressible polymer mixtures [2], [3] but were only recently applied to compressible polymer-solvent mixtures [4].

Due to the extensive computational effort necessary only small parts of binary mixture phase-diagrams have been simulated so far [4]. Coarse-graining allows us to explore a substantially larger part of parameter space. Consequently we will be able to show a novel pressure-temperature projection of the polymer-solvent phase diagram with complete critical lines. In addition we will present pressure-composition projections, binodales of pure hexadecane and CO_2 as well as very recent investigations of the interfaces.

References

1. C.M. Stafford, T.P. Russell and T.J. McCarthy, Macromolecules 32, 7610 (1999).
2. H.P. Deutsch and K. Binder, Macromolecules, 25, 6214 (1992).
3. M. Müller and K. Binder, Macromolecules, 31, 8323 (1998).
4. J.J. Potoff, J.R. Errington and A.Z. Panagiotopoulos, Molecular Physics 97, 1073 (1999).

Constraints on clusters of colloidal particles by interactive molecular dynamics

Oliver Vormoor

Göttingen University, Institute for X-ray physics,
Geiststrasse 11, 37073 Göttingen, Germany
Tel.: ++49 551 39 9384, Fax.: ++49 551 39 9430, email: ovormoo@gwdg.de

While molecular dynamics techniques have been well established for studying matter in the last decades, the new branch of interactive molecular dynamics has grown up only during the last years [1]. Usually high end workstations or virtual reality systems [2] have been used for visualization of molecular dynamics simulations. Recently desktop PC's have reached a level of graphical power that allows rendering virtual universes in real time. This graphical power enables the usage of desktop computers for interactive molecular dynamics. Our project in interactive molecular dynamics is motivated by studying the cluster formation of colloidal particles, particles with a diameter $10nm \leq d \leq 1\mu m$, in aqueous solution. Under certain conditions of the environment cluster of these colloidal particles are formed. Their structure may be characterized by a fractal dimension and is directly visible when studying colloidal systems using X-ray microscopy techniques. But the clusters are exposed to some constraints resulting from the experimental setup. We are interested in the effects of these constraints on the structure of the clusters.

An interactive molecular dynamics package based on Java has been set up for studying the behavior of colloidal clusters under constraints. The Java3D API provides a high level access to the world of virtual reality in Java [4] and allows programming portable, dynamical virtual reality applications without relying on low level libraries like Direct3D or OpenGL and keeping focus on the actual problems. The software package called JIMD (= *Java Interactive Molecular Dynamics*) [5] is a quick and easy client software for interactive molecular dynamics that can be adapted to existing molecular dynamics software by a Java, C or C++ interface. It is not the aim of JIMD to be an interactive molecular dynamics package designed for optimum performance on high end workstations. Running on a common desktop PC it easy to use in order to upgrade existing molecular dynamics software to interactive molecular dynamics. Nevertheless JIMD is ¤exible enough for future extensions that may be necessary in certain problems. The current implementation allows tuning of parameters as well as a direct user interaction with the single particles of the simulated system in order to model constraints as introduced above. JIMD does not merge simulation and visualization, but allows a dynamical adaptation and detachment of the visualization. Measurements show that the performance of the simulations is only very slightly affected by an adapted visualization application. The visualization application of JIMD is able to visualize continuously ≈ 500 particles on a modern desktop PC. Future hardware will be able to handle larger systems. Since the development of JIMD has been £nished recently, only some performance measurement results have been presented at this point. Results of the constraint measurements will be available in the near future.

References

1. D. C. Rapaport, Physica A **240**, 247-254 (1997)
2. B. Bierwald in R. Esser, D. Mallmann (*eds.*), *Beiträge zum Wissenschaftlichen Rechnen*, p. 17-26, Forschungszentrum Jülich, Zentralinstitut für Angewandte Mathematik, 2000
3. A. Ruprecht, J. Thieme in W. Meyer-Ilse et al. (*eds.*), *X-ray microscopy*, p. 329-333, AIP Conference Proceedings, American Institute of Physics, 2000
4. H. A. Sowizra, M. F. Deering, IEEE Computer Graphics and Applications, 1999
5. O. Vormoor, submitted for publication

Effect of binary mixtures on the isotropic-nematic transition: A lattice model simulation study

Viktor V. Yarmolenko* **and Doug J. Cleaver**

Materials Research Institute, Shef£eld Hallam University, Pond Street, Shef£eld S1 1WB, United Kingdom

* *tel: +44 114 2253068, fax: +44 870 4064544, e-mail:viktor.yarmolenko@physics.org*

In this poster, we build upon our previous study [1] into the phase behaviour of two-component liquid crystal mixtures performed using a generalisation of the Lebwohl-Lasher lattice model [2]. The simplicity of this model has allowed us to survey the effects of changing both the relative concentration and the coupling constant ratio of the two components. Having mapped out the global phase behaviour, we now consider the effect that introducing another component has on the characteristics of the nematic-isotropic (N-I) transition as well as the behaviour associated with the various demixing transitions shown by the model. Our analysis includes use of the histogram technique to investigate the changing nature of the N-I transition, and comparison of the behaviour of short- and long-ranged correlation function data at various transitions.

References

1. V. V. Yarmolenko and D. J. Cleaver, in preparation.
2. P. A. Lebwohl and G. Lasher, *Phys. Rev. A*, 6, 426 (1972)

Field-induced structure transformation in ER solids: Beyond the point-dipole approximation

K. W. Yu, C. K. Lo, Jones T. K. Wan and Y. L. Siu

Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, China

phone: (852) 2609 6349; fax: (852) 2603 5204; kwyu@phy.cuhk.edu.hk

When a strong £eld is applied to a composite medium, the induced change of the medium can lead to spectacular behavior, both in electrical transport and in optical response [1]. If a strong electric £eld is applied to a suspension of particles, the induced dipole moments of the particles can order the suspended particles into a body-centered tetragonal (BCT) lattice [2], which is known as an electrorheological (ER) solid. Recently, Tao and coworkers [3] proposed that a structure transformation from the BCT ground state to some other lattices can occur when one applies a magnetic £eld perpendicular to the electric £eld and the polarized particles possess magnetic dipole moments. Sheng and coworkers [3] veri£ed the proposal experimentally and observed a structure transformation from the BCT to the face-centered cubic (FCC) lattices. Motivated by these studies, we propose an alternative structure transformation from the BCT to the FCC structure, with the application of electric £elds only.

Tao et. al. [2] adopted the point-dipole (PD) approximation to predict the ground state as well as the structure transformation. However, it is known the PD approximation errs considerably when the particles get close and touch. We have recently shown that a dipole-induced-dipole (DID) model, which takes into account the mutual polarization effect between touching particles, can drastically improve the accuracy towards the fully multipolar calculations [4]. It is thus instructive to re-examine the calculations.

Since the DID contribution becomes important for a small reduced separation $\sigma = d/2R < 1.1$ between the particles [4], we can simplify the calculations by considering touching particles only. Each particle is in contact with a £nite number of neighboring particles and the number of DID images dipoles is thus £nite. We have computed the electrostatic energy by incorporating the DID model into the Ewald-Kornfeld [5] formulation. The results show that the dipole moment of each particle increases by 25% in the BCT ground state, while there is no change in the FCC and the intermediate BCC lattices. The PD approximation thus yields qualitatively correct results.

The structure transformation can be realized in experiments by applying a rotating electric £eld in the plane perpendicular to the uniaxial electric £eld. In this £eld con£guration, both the time average value of the induced dipole moment and that of the rotating electric £eld itself vanish in the plane. However, the instantaneous dipole moment will induce an overall attractive force between the particles in the plane perpendicular to the uniaxial £eld. We should remark that the £eld con£guration is all electrical; no magnetic £eld and/or magnetic materials need to be used.

References

1. For recent work, see *Proceedings of the 5th International Conference on Electrical Transport and Optical Properties of Inhomogeneous Media*, Physica B **279**, (2000).
2. R. Tao and J. M. Sun, Phys. Rev. Lett. **67**, 398 (1991).
3. R. Tao and Q. Jiang, Phys. Rev. E **57**, 5761 (1998); P. Sheng et al, Physica B **279**, 168 (2000).
4. K. W. Yu and Jones T. K. Wan, in *Proceedings of the 8th International Conference on Discrete Simulation of Fluid Dynamics*, Comput. Phys. Comm. **129**, 177 (2000).
5. P. P. Ewald, Ann. Phys. (Leipzig) **64**, 253 (1921); H. Kornfeld, Z. Phys. **22**, 27 (1924).

Monte Carlo simulations of continuous phase transitions in the 3D Ashkin-Teller model

G. Musiał, G. Kamieniarz, L. Dębski

Institute of Physics, A. Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland

tel. (+48 61)8273071, fax (+48 61)8257758, e-mail: gjk@zawrat.amu.edu.pl

The three-dimensional (3D) Ising model was extensively investigated with the large-scale Monte Carlo (MC) simulations [1], in which the accurate estimates of critical exponents were obtained. The critical behaviour of the 3D Ashkin-Teller (AT) model was studied by Ditzian *et.al.* [2] using the MC and series expansions methods. However, the systems used in MC method by these authors were moderate and the series were rather short so that the phase diagram still deserves some more attention in the region of the continuous transitions and the tricritical point [3, 4].

The AT model can be expressed in terms of Ising spins, with two spins s_i and σ_i at each lattice site, and can be interpreted as two superimposed Ising models [2]. One of them is described in spin variables s_i and the other in variables σ_i and in both models there are exclusively two-spin interactions of a constant magnitude J_2 between the nearest neighbors only. Simultaneously, these two different models are coupled by four-spin interaction of a constant magnitude J_4, also only between couples of spins residing at the nearest neighboring lattice sites. Thus, the Hamiltonian of this model is $-\beta\mathcal{H} = H = \sum_{[i,j]}\{K_2(s_i s_j + \sigma_i\sigma_j) + K_4 s_i\sigma_i s_j\sigma_j\}$, where $\beta = (k_B T)^{-1}$, k_B is the Boltzmann's constant, T the temperature, $[i,j]$ denotes summation over nearest neighboring lattice sites and $K_i = -\beta J_i$, with $i = 2$ or 4.

In this paper we perform the simulations of Monte Carlo type that base on the invariance of the Binder cumulant Q, which is the ratio of the square of the second moment of the order parameter to its fourth moment, in the critical point [1, 5]. The phase transition point T_c was determined from the analysis of the cumulant Q_L of cubic samples of the size $L \times L \times L$ ($L \leq 30$).

In our simulations we use the order parameter $\langle\sigma\rangle$ for the phase boundaries between the Baxter phase and the ferromagnetic $s\sigma$ phase and the order parameter $\langle s\sigma\rangle$ for the phase boundaries between the paramagnetic phase and the ferromagnetic $s\sigma$ and the antiferromagnetic phases [2]. Here the symbol $\langle\ldots\rangle$ denotes the thermal average. We have applied the accurate estimates of critical exponents of the 3D Ising model [1] in the £nite-size-scaling analysis to calculate the locations of continuous phase transitions points on the (K_4, K_2) phase diagram of the 3D AT model.

Simulations have been performed on SGI Power Challenge XL nad L supercomputers using the 64-bit random number generator and thermalization of the initial con£gurations. Gibbs distribution was sampled using the Metropolis algorithm. One point on the phase diagram was calculated using 10^7 to 10^8 MCS. Owing to application of £nite-size-scaling analysis we not only allocated points on the phase diagram with precision of at least 3 decimal digits, but also we con£rmed the continuous character of phase transitions.

References

1. H.W.J. Blöte, E. Luijten, J.R. Heringa, J. Phys. A28 (1995) 6289.
2. R.V. Ditzian, J.R. Banavar, G.S. Grest, L.P. Kadanoff, Phys. Rev. B22 (1980) 2542.
3. P. Arnold, Y. Zhang, Nuclear Phys. B501 (1997) 803
4. L. Dębski, Acta Phys. Polon. A97 (2000) 859
5. G. Kamieniarz, H.W.J. Blöte, J. Phys. A26 (1993) 201

Statistical synchronization in Bose-Einstein condensation

R. Kutner and M. Regulski

Inst. of Experimental Physics, Warsaw University, Ho¢a 69, Pl-00681 Warsaw, Poland

phone/fax:+004822 8536980, e-mail address: erka@fuw.edu.pl

The purpose of this work is to answer to the open, commonly asked question: is there any signature of the Bose-Einstein condensation (BEC) on excited energy levels [1]? This question is important from the theoretical and experimental points of view since a positive answer would be, for example, an important step towards the study of BEC via excited levels which are much easier to observe in experiments than the ground level. To answer the above question we considered noninteracting bosons within the canonical ensemble which maps the £nal experimental conditions more accurately than the standard grand canonical one. As a typical example we considered the bosons placed in $3d$ isotropic harmonic oscillator (IHO) which is equivalent to the bosonic lattice gas [2] with proper transition rates and boundary conditions [3]. In this work we study numerically, by Monte Carlo (MC) simulations, and directly by using canonical partition functions (CPF), ground and excited levels occupancies and their ¤uctuations. In our earlier paper [3] we developed the MC algorithm which was able to mimic quantum indistinguishability. We proved that this algorithm was able to correctly reproduce the λ-transition. Moreover, we veri£ed this result by applying the recurrent algorithm [4] to calculate CPF and hence the desired statistical and thermodynamical quantities (such as mean ground state occupancy and speci£c heat). This work is a continuation of our previous studies [3]. We calculated by the above independent numerical methods both the equilibrium occupancies of £rst few excited levels as well as the dispersions (¤uctuations) of particle occupancies of these levels. We found that the mean occupancy of the £rst excited level vs. temperature has the same behaviour as dispersion of particles on the ground level and the second excited level; all these quantities have a characteristic λ-shape versus temperature. An analogous situation occurs for other excited levels. In this sense we can speak of statistical synchronization in BEC. Interpretation of this effect is straightforward since, when the number of bosons is £xed, the equilibrium occupancy of any level is determined by the exchange of bosons mainly with nearest levels, i.e., thanks to ¤uctuations of bosons on these levels. We have to deal in BEC within IHO mainly with one-component condensate and not with two-component "supercooled" and normal ones.

References

1. P. Navez, D. Bitouk, M. Gajda, Z. Idziaszek, and K. Rza¸¢ewski, Phys. Rev. Lett. **79** (1997) 1789.
2. R. Kutner, K. W. Kehr, W. Renz, and R. Przeniosło, J. Phys. A **28** (1995) 923.
3. R. Kutner and M. Regulski, Comp. Phys. Comm. **121-122** (1999) 586.
4. M. Wilkens, Ch. Weiss, J. Mod. Optics **44** (1997) 1801.

On non-Markovian quantum master equations

K. Lendi and A. Aissani

Institute of Physical Chemistry, University of Zürich, Winterthurerstr. 19, 8057 Zürich / Switzerland

carlen@pci.unizh.ch

Quantum dynamics of open systems is of particular importance in £elds of atomic and molecular spectroscopy where for modest time-scales mostly Markovian master equations have been used. For modern time-resolved experiments on very short time-scales more general dynamical equations of non-Markovian or, else, Nakajima-Zwanzig type are needed for which theoretical treatments have remained on a rather semiphenological level and are much less satisfactory than in the Markovian case [1, 2]. It is therefore urgent to try to improve the methods, mainly regarding quantum-theoretic and mathematical consistency. The main problems arise from perturbational treatments of integral kernels in integro-differential equations which are most likely to violate fundamental quantum-mechanical requirements on density operators such as the von Neumann conditions, particularly the indispensable positivity. Furthermore, the problem of entangled initial states which is of great importance in quantum information [3] has been disregarded in the past. We avoid those dif£culties by incorporating all requirements from the very outset as strict boundary conditions. In addition to a rigorous derivation of bounds on kernels we have tried to generalize time-independent positivity inequalities known from quantum dynamical semigroups to appropriate time-dependent versions. So far, open two-level systems have been treated since they are of primary importance in laser physics. In a coherence-vector representation of density operators there appear three coupled integro-differential equations of convolution Volterra type for real-valued functions for which the applied numerical treatments are either by Adams-Moulton or backward differentiation methods [4]. In this way, it is possible to work out sets of admissible parametrized kernel functions [5]. Further analytic and numerical results are in progress. They will help to assess suitability of memory functions which have been obtained by rather phenomenological physical reasoning as is frequently attempted in the literature.

References

1. R. Alicki and K. Lendi,*Quantum Dynamical Semigroups and Applications*, Springer, Berlin, LNP Vol. 286 (1987).
2. K. Lendi and A.J. van Wonderen, J.Phys.A:Math.Gen. **34**, in press (2001).
3. D. Bouwmeester, A. Ekert and A. Zeilinger (Eds.), *The Physics of Quantum Information*, Springer, Berlin (2000).
4. P.H.M. Wolkenfelt, IMA J.Numer.Anal. **2**: 131 (1982).
5. A. Aissani, *Sur la déformation d'un £l élastique et sur l'étude d'une équation intégro-différentielle*, PhD-thesis, University of Metz (2000).

Numerical study of complex quantum systems by a method of approximate integration in metric spaces

Yu.Yu.Lobanov

Lab. of Information Technologies, Joint Institute for Nuclear Research, 141980
Dubna, Moscow Region, Russia

tel.: +7 09621 64619, fax: +7 09621 65145, e-mail: lobanov@cv.jinr.ru

Numerical functional (path) integration is one of the most important methods for calculating the characteristics of complex systems in quantum and statistical physics. It is very useful when other methods such as perturbation expansion, semiclassical approximation, etc. cannot be applied. However, the existing approaches to path integrals in physics are not always quite correct in a mathematical sense and the usual Monte Carlo method of their computation gives the results only as probabilistic averages while requiring too much computer resources to obtain the good statistics.

Using the rigorous de£nition of an integral with respect to probability measure in complete separable metric space we elaborated the new method of computation of path integrals [1]. This method is based on our new approximations which satisfy the condition of being exact on a class of polynomial functionals of arbitrary given degree. They can be considered as quadratures in metric spaces. The method does not require preliminary discretisation of space and time, it allows to use the more preferable deterministic algorithms in computations and proves to be more effective than the other existing nonperturbative numerical methods especially in the case of high dimensions [2]. Theorems on the convergence of approximations to the exact value of the integral as well as on estimate of the remainder are proven. According to these theorems one can obtain numerical results with the guaranteed (not probabilistic) accuracy control. Practical computations show that the good accuracy (about 1 percent) can be reached using the low-dimensional (3-5) Riemann integrals in our approximations. We calculate them by the Tchebyshev quadratures or by the Korobov method.

We used our method in the solution of some problems of quantum and statistical mechanics and quantum £eld theory, including the study of tunneling phenomena and the many-particle problems in nuclear physics [3]. The method appeared to be convenient for studying the nonperturbative topological structure of vacuum in gauge theories, namely for computation of the topological charge, topological susceptibility, θ-vacua energy [4]. Now we are applying it to the study of the open quantum systems, i.e. systems interacting with their environment. Such an approach provides a natural framework for description of nonequilibrium irreversible processes accompanied by a dissipation of energy, which £nds a use in various areas of quantum physics and chemistry.

Description of the method, its applications and comparison of the numerical results with theoretical estimates and experimental data as well as with the values obtained by the other authors are presented.

References

1. Yu.Yu.Lobanov, *Comp. Phys. Comm.* **99** (1996) 59-72.
2. Yu.Yu.Lobanov et al., *J. Comput. Appl. Math.*, **70** (1996) 145-160.
3. Yu.Yu.Lobanov, *J. Phys. A: Math. & Gen*, **29** (1996) 6653-6669.
4. Yu.Yu.Lobanov, *Comp. Phys. Comm.* **121** (1999) 60-63.

The coordinated valence - force £eld and thermodynamic properties of organic sulphur molecules and radicals

[1]**Yu. Orlov,** [2]**V. Turovtsev**

[1] *Tver state university. 33 ul. Zhelyabova, Tver, 170000, Russian Federation*
[2] *Tver state medical academy. 4 ul. Soviet, Tver, 170000, Russian*
Fax: (082-2) 33-12-74. E-mail: Yurij.Orlov@tversu.ru

For the £rst time on the basis of the decision of a direct and inverse spectral problem and semiempirical relations linking the geometrical and the force characteristics of compounds is offered a coordinated valence - force £eld molecules and radicals containing sulphur. At the decision of a inverse spectral problem the following physical condition was imposed: force constants of the alkyl groups should correspond to constants of alkanes. The determined force £eld with satisfactory accuracy reproduce the vibration spectrums of the speci£ed substances. The calculations and assignments of vibration frequencies 40 molecules and 12 radicals containing divalent sulphur are produced. In an temperature interval 298 1500 the thermodynamic properties (enthalpy, entropy and heat capacity) indicated compounds are designed by methods of a statistical physics. The quantitative correlations ”structure - property” for the listed above characteristics and substances are explored within the framework of additive - group model. The appropriate parameterisation is produced. The comparison of results of calculations to the data of experiments is carried out and good consent is marked. Is shown, that the obtained data are applicable for an estimation of the thermodynamic characteristics alkanepolythiols. The prognosis of thermodynamic properties for a series of molecules alkanethiols, alkanedithiols, alkanepolythiols, alkanesul£des and sulphur radicals not described by the earlier relevant data is made.

High-precision estimates of critical parameters by means of improved hamiltonians

M. Campostrini,[1] **M. Hasenbusch,**[2] **A. Pelissetto,**[3]
P. Rossi,[1] **and E. Vicari**[1]

[1]*Dip. di Fisica dell'Universit¶a di Pisa and INFN, I-56100 Pisa, Italy*
[2]*Inst. für Physik, Humboldt Universität, D-10115 Berlin, Germany*
[3]*Dip. di Fisica dell'Universit¶a di Roma I and INFN, I-00185 Roma, Italy*

Presented by A. Pelissetto, tel. +39-06-4991-4536, e-mail: Andrea.Pelissetto@roma1.infn.it

We have studied [1, 2, 3, 4, 5, 6] the critical behavior of classical systems with an N-vector order parameter for $N = 1, 2, 3$. These universality classes describe many important physical systems: for instance, the case $N = 1$ corresponds to the liquid-vapor transition, the liquid-liquid transition in multicomponent ¤uids, and the magnetic transition in uniaxial materials; the case $N = 2$ describes the λ-transition in ^{4}He and the magnetic transition in easy-plane magnets; Heisenberg ferromagnets are systems with $N = 3$. Traditionally, numerical studies used the N-vector Hamiltonian

$$H = -\sum_{\langle xy \rangle} \sigma_x \cdot \sigma_y$$

where σ_x is an N-dimensional unit vector. However, it is much more advantageous to work with *improved* Hamiltonians. Such Hamiltonians are obtained by tuning a parameter and are such that the leading corrections to scaling vanish. In order to obtain high-precision estimates we employ the following strategy: (a) we consider a Hamiltonian that depends on an irrelevant parameter; (b) by means of £nite-size scaling Monte Carlo simulations we determine the value λ^* of the parameter that corresponds to an improved Hamiltonian, and $\beta_c(\lambda^*)$; (c) we consider high-temperature expansions for the improved Hamiltonian and determine the critical parameters by biasing the analyses with the Monte Carlo estimate of $\beta_c(\lambda^*)$. By using 20-th order series on the square lattice we obtain for the critical exponents γ and ν:

$N = 1:$	$\gamma = 1.2371(4)$	$\nu = 0.63002(23)$	Ref. [1]
$N = 2:$	$\gamma = 1.3177(5)$	$\nu = 0.67155(27)$	Ref. [5]
$N = 3:$	$\gamma = 1.3960(9)$	$\nu = 0.7112(5)$	Ref. [6]

Beside the critical exponents, we also compute the four-point zero-renormalized coupling and the £rst coef£cients of the expansion of the free energy in powers of the magnetization. By using these results and appropriate parametric representations we determine the equation of state in the whole (t, H) plane. This allows us to obtain an accurate determination of several amplitude ratios. We also study the behavior of the static structure factor for small momenta.

References

1. M. Campostrini, A. Pelissetto, P. Rossi, and E. Vicari, Phys. Rev. E **60**, 3526 (1999).
2. M. Hasenbusch, J. Phys. A **32**, 4851 (1999).
3. M. Hasenbusch and T. Török, J. Phys. A **32**, 6361 (1999).
4. M. Campostrini, A. Pelissetto, P. Rossi, and E. Vicari, Phys. Rev. B **61**, 5905 (2000); B **62**, 5843 (2000).
5. M. Campostrini, M. Hasenbusch, A. Pelissetto, P. Rossi, and E. Vicari, Phys. Rev. B **63**, 214503 (2001).
6. M. Campostrini, M. Hasenbusch, A. Pelissetto, P. Rossi, and E. Vicari, "The three-dimensional Heisenberg universality class," submitted to Phys. Rev. B (2001).

Microcanonical analysis of continuous phase transitions: ef£cient algorithm and critical exponents

Michel Pleimling and Alfred Hüller

Institut für Theoretische Physik I, Universität Erlangen-Nürnberg,
D – 91058 Erlangen, Germany

phone +49-9131-85-28451, fax +49-9131-85-28444,
pleim@theorie1.physik.uni-erlangen.de

The microcanonical analysis of discontinuous phase transitions has been very successful in several respects. It allows a clearcut distinction between continuous and discontinuous phase transitions and it yields excellent estimates of the transition temperature and of the latent heat. Compared to that, only moderate progress has been achieved for continuous phase transitions. On the one hand typical features of symmetry breaking as diverging susceptibilities or the abrupt inset of the order parameter turn up in the microcanonical analysis already for fairly small system sizes [1]. This is in contrast to the canonical ensemble where singularities appear exclusively in the thermodynamic limit. On the other hand, however, computation of critical exponents yielded mean £eld values for all £nite system sizes [1].

The aim of this contribution is twofold. First, we present a highly ef£cient algorithm, based on the Flat Histogram method [2], for the computation of the entropy $S_N(E, M)$ of £nite size systems. Here E is the energy and M is the magnetization of our £nite system. Using transition variables, this method allows a speedy and precise determination of the density of states for remarkably large system sizes [3]. In this contribution, this algorithm is used for the microcanonical analysis of the two and three dimensional Ising models with up to $N = 5 \cdot 10^5$ spins.

Secondly, we show how to obtain the in£nite lattice critical exponents by expanding the £nite system entropy at the critical point of the in£nite system [3]. As an example, we discuss the critical exponent of the order parameter (microcanonically de£ned as the maximum of $S_N(E, M)$ with respect to M for E £xed) for the Ising model in two and three dimensions. The values obtained for the critical exponents are in excellent agreement with the expected non classical critical exponents. Finite-size effects and corrections-to-scaling are also discussed from the microcanonical point of view.

The algorithm presented in this contribution rapidly builds up good estimates for the density of states. When this point is reached all macrostates are visited with the same frequency and the quality of the density of states is improved with the same rate over the whole parameter range considered. These characteristics make it a suitable tool for the analysis of complex systems in the future.

References

1. M. Kastner, M. Promberger, and A. Hüller, J. Stat. Phys. **99**, 1251 (2000).
2. J.-S. Wang, Eur. Phys. J. B **8**, 287 (1999).
3. A. Hüller and M. Pleimling, submitted.

Quantum chaos and its testing

A.K. Prykarpatsky[1,2]**, R. Basiura**[2] **and K. Prykarpatska**[1]

[1] *Dept. of Nonlinear Mathematical Analysis at the IAPMM of the NAS, Lviv, Ukraina*
[2] *Dept. of Applied Mathematics at the AGH, Krakow, Poland*

Since 1963 when V.K. Melnikov developed an analytical tool for testing the transition of classical weakly perturbed planar dynamical systems to homoclinic due to A. Poincare chaotic motion via the Birkhoff-Smale scenario, a lot of new results and generalizations were obtained by many researchers worldwide. Especially there were devised new techniquesfor studying the chaotic motion both in multidimensional and adiabatically (slowly) perturbed Hamiltonian systems. On the other hand a great deal of results both theoretical and computational were produced by mathematical physicists concerning the related problem of describing so called quantum chaos in £nite dimensional quantum dynamical systems, especially weakly perturbed . Our study here deals with developing some physically reasonable quantum analog of the above mentioned Melnikov theory and its application to studying transition to quantum chaotic motion in weakly perturbed quantum completely integrable Hamiltonian systems.Since 1963 when V.K. Melnikov [1] developed an analytical tool for testing the transition of classical weakly perturbed planar dynamical systems to homoclinic due to A. Poincare chaotic motion via the Birkhoff-Smale scenario, a lot of new results and generalizations were obtained by many researchers worldwide. Especially there were devised new techniques [2,3] for studying the chaotic motion both in multidimensional and adiabatically (slowly) perturbed Hamiltonian systems. On the other hand a great deal of results both theoretical and computational were produced by mathematical physicists concerning the related problem of describing so called quantum chaos in £nite dimensional quantum dynamical systems [4], especially weakly perturbed [3]. Our study here deals with developing some physically reasonable quantum analog of the above mentioned Melnikov theory and its application to studying transition to quantum chaotic motion in weakly perturbed quantum completely integrable [4]Hamiltonian systems.

References

1. Melnikov V.K. On the stability of the center for the time-periodic perturbations. Transactions of the Moscow Math. Soc., 1963, v.12, p.1-57
2. Samoylenko A.M., Tymchyshyn O.Ya., Prykarpatsky A.K. Geometric analysis of the Poincare-Melnikov transversal splitting of separatrix manifolds of slowly perturbed nonlinear dynamical systems. Ukr. Math. Zhurnal, 1993, v. 45, N12, p. 1668-1681
3. Wiggins S. Global bifurcations and Chaos- Analytical methods. N.Y. Springer, 1988
4. Steiner F. Quantum Chaos. DESY 94-013 P

Nucleation in the two-dimensional Ising model

S.B. Rutkevich

Institute of Solid State and Semiconductor Physics, P. Brovka str., 17, 220072 Minsk, Belarus

fax: (375-17) 2840-888 , e-mail: rut@mailaps.org

Nucleation of "bubbles" of the stable phase is a very common phenomenon which initiates relaxation of metastable states near the first order phase transition in many systems of the condense matter physics. The main quantity of interest for the theory and applications is the nucleation rate, which characterizes the rate of spontaneous generation of the so-called critical bubble in the metastable surrounding. The nucleation rate in the Ising model has been extensively studied in literature by use of different numerical schemes such as computer simulations under appropriate dynamics, and constrained transfer-matrix method (see e.g. [1, 2]). Results obtained this way are usually interpreted in terms of the classical nucleation theory, or in terms of its field-theoretical version proposed by Langer [3]. However, such interpretation has been severely hampered by the fact, that the Langer's theory of nucleation was developed not for the Ising, but for the Ginzburg-Landau model, which (unlike the Ising model) is continuous and isotropic. So, to provide correct interpretation of existing and future numerical results, one needs to extend the Langer's nucleation theory to the Ising model. Such an extension is the main subject of the present report. We develop the analytic transfer-matrix theory of nucleation in the two-dimensional Ising model and compare it with the results obtained by Günther, Rikvold and Novotny by use of the numerical constrained transfer-matrix method [2].

It is well-known, that the free energy $F(H)$ of the two-dimensional Ising model in the ferromagnetic phase $T<T_c$ has singularity at the origin $H = 0$. The phenomenological droplet theory claims that near the cut drawn from the singularity point along the negative real axis $H<0$, the free energy gains the imaginary part, which Langer proposed to identify (with some dynamical factor) with the nucleation rate of the metastable state characterized by positive magnetization in a small negative magnetic field. The phenomenological nucleation theory predicts the following structure for this imaginary part: $\mathrm{Im}F[\exp(\pm i\pi) \mid H \mid] = \pm B|H|\exp(-A \mid H \mid)$ for small $\mid H \mid$. Previously [4] we verified this prediction for the square lattice Ising model in the extreme anisotropic limit. Now we generalize the transfer matrix approach developed in [4] and verify analytically the phenomenological droplet theory predictions for the square lattice Ising model for all temperatures $0<T<T_c$ and arbitrary anisotropy ratio J_1/J_2. We obtain an expression for the constant A which coincides exactly with the prediction of the droplet theory. For the amplitude B we obtain $B = \pi M/18$, where M is the equilibrium spontaneous magnetization. Furthermore, we find the discrete-lattice corrections to the above mentioned phenomenological formula, which oscillate in H^{-1} with the period $\beta M/\langle\omega(\theta)\rangle$, where $\beta = 1/k_BT$ and $\langle\omega(\theta)\rangle$ is the one particle spectrum of the zero-field Ising model, averaged over the quasi-momentum θ. Such oscillations were observed by Günther *et al.* [2] in numerical constrained transfer matrix calculations of the imaginary part of the (constrained) free energy. The period of oscillations which we obtain agrees well with that reported by Günther *et al.* It is shown, that these discrete-lattice oscillations should be taken into account when interpreting numerical calculations of the nucleation rate in the Ising model at low temperatures.

References

1. S. Wonczak, R. Strey, and D. Stauffer, J. Chem. Phys. **113**:1976-1980 (2000).
2. C.C.A Günther, P.A. Rikvold, and M.A. Novotny, Phys. Rev. Lett. **71**:3898 (1993).
3. J.S. Langer, Ann. Phys. (N.Y.) **41**:108 (1967).
4. S.B. Rutkevich, Phys. Rev. B **60**:14525 (1999).

Molecular dynamics simulation study of N,N-dimethylformamide – water solutions

Antonios Koufou, Michalis Chalaris and Jannis Samios[1]

University of Athens, Department of Chemistry,
Laboratory of Physical Chemistry,
Panepistimiopolis 15771 Athens, Greece

[1] *isamios@cc.uoa.gr phone: +3017274751*

N, N-Dimethylformamide (DMF) is a simple amide compound with interesting properties. Note also that the DMF-water mixture is of particular importance due to its extensive use as a mixed solvent. Despite the research effort on this mixture, one may assert that a deep understanding of the behavior of the physicochemical properties of this molecular system has not yet been achieved.

As far as we know, molecular dynamics (MD) simulation studies for DMF-water mixtures have not been carried out so far. In this work, we present for the £rst time a MD simulation study of the mixture at ambient conditions (298K, 1bar). Thus, the mixture was studied over a wide range of DMF mole fractions (X_{DMF} = 0.07, 0.30, 0.49, 0.70) by using three available potential models for water (SPC, SPC/E, TIP4P) and the six site interaction potential CS2 [1] for liquid DMF.

The statistical mechanical ensemble employed to study this mixture was the microcanonical (NVE) one. The number of molecules used was 256. The results obtained may be summarized as follows:

A. The reliability of the DMF-water models was tested against available experimental data. Specifically, the SPC/CS2 mixture models are found to predict potential energy and pressure in quite satisfactory agreement with experiment. Also, the calculated diffusion coef£cients of the species in the mixture are found to follow the expected behavior in the whole range of DMF mole fractions.

B. The local intermolecular structure of the mixture has been studied in terms of the calculated center of mass (COM) and the site-site pair correlation functions (PCFs). The behavior of these functions at small correlation distances, indicate clearly the existence of hydrogen bonds between the DMF and the water molecules. In the present study, we have applied a capable criterion to investigate the hydrogen bonding network in the system, not only between the water-water molecules but also between the water and DMF molecules. Thus, it was possible to estimate the number of hydrogen bonds per molecule in the system.

C. It is found that a hydrogen bond among DMF and water, takes place between the oxygen atom of DMF and the hydrogen atom of water. Moreover, the mean intermolecular structure among the aggregate molecules (DMF-water) has been found to be in quite satisfactory agreement with results obtained from ab-initio calculations [2, 3].

References

1. M.Chalaris and J.Samios, *J.Chem. Phys.*, 112 (19), 8581 (2000)
2. J. Gao *J.Am.Chem.Soc.* 115 2930 (1993)
3. J.Samios G.Froudakis - Paper in Preparation (2000)

Solute-solvent interactions in in£nitely dilute supercritical mixtures: A molecular dynamics investigation

Zoe Cournia, Dimitris Dellis and Jannis Samios[1]

[1] *University of Athens,Department of Chemistry, Laboratory of Physical Chemistry, Panepistimiopolis, 15771, Athens, Greece*

+3017274751, isamios@cc.uoa.gr

Supercritical ¤uids (SCFs) have a broad range of applications in chemical syntheses, separation processes, and also in soil, water and waste treatment[1]. A SCF cannot be described neither as a liquid, nor as a gas and its properties differ from the ones observed in the liquid and gas states. The solvating properties of SCFs, may be widely varied from gaslike to liquidlike values by applying small changes in temperature and pressure of the ¤uid. The greatest variation of solvent density, ρ, is attained in the proximity of the solvent's critical point. So, in that case, small changes in pressure yield large changes in density. This region around the critical point is called the "compressible regime". Large ¤uctuations in local solvent density may occur, leading to regions of high and low densities, which results to inhomogeneities. Solvent and solute clustering disappears as we move away from the compressible regime (i.e. for $T/T_c \geq 1.10$). The observed inhomogeneities affect strongly the solvent's and solute's solvation dynamics and reaction. This may be easily studied through vibrational lifetimes as a function of solvent density. Close to the critical temperature, the vibrational relaxation lifetime of the solute, T_1, seems to be density independent and similar to that of glasses, suf£ciently different compared to the T_1 of liquids and gases. Experimental techniques (i.e. vibrational spectroscopy)[2], as well as two dimensional molecular dynamics (MD) simulation studies have been employed so far to explore the underlined molecular mechanisms which are responsible for the overall behavior of such systems[3]. In addition, theoretical studies based on the ¤uctuation theory, have been devoted to study the problem[4].

In the present work, a three-dimensional (3D) SC diluted mixture of reasonable size has been simulated to study the problem mentioned above. By using the MD simulation technique, we were able to calculate the vibrational relaxation lifetime of a diatomic solute (N_2) in a three-dimensional SC noble ¤uid (Xe), as a function of density. Our results ($T_1 = f(\rho)$) exhibit the same unexpected plateau behaviour as it has been experimentally observed for other real diluted systems[5]. The results obtained provide us with the opportunity of further exploration of the molecular mechanisms which are responsible for the behavior of such SC systems. It seems that this behavior for a SCF in its compressible regime is universal for such ¤uids and this remains to be experimentally veri£ed.

References

1. Charles A.Eckert et al., *Supercritical ¤uids as solvents for chemical and materials processing*, Nature, Vol.383, 1996, p.313
2. R.S.Urdahl et al., *Vibrational relaxation of polyatomic solute in a polyatomic SCF near the critical point*, J.Chem.Phys. 105, 19, 1996, 8973
3. G.Goodyear, S.C.Tucker, *Glass-like behavior in supercritical ¤uids: The effect of critical slowing down on solute dynamics*, J.Chem.Phys. 111, 21, 1999, 9673
4. R.Zwanzig, *Theory of vibrational relaxation in liquids*, J.Chem.Phys. 34, 1961, 6, 1931; S.C.Tucker et al., *The effect of solvent density inhomogeneities on solute dynamics in SCFs*, J.Phys.Chem., 1998B, 102, 2437
5. Z.Cournia, J.Samios (paper in preparation)

Ultrametric £eld theory and Random Energy Model (REM) statistical mechanics

D.B. Saakian
Yerevan Physics Instititute,
Yerevan 36,Armenia
3742-352649, 3742-350030,
saakian@jerewan1.yerphi.am

We propose to formulate 2d £eld theory on the ultrametric space (UM) with the free correlators identical to 2d correlators and the same potential. We construct UM space as a hierarchic tree with branching number close to 1. Here we have integration measure, diagonalized free £eld action and can mimicate perturbative section of a corresponding model in a real 2d space. The point is, that there is a way to investigate nonperturbatively bulk structure of theory putting the same model on the tree with large branching number.The considered ultrametric models may be naturally expressed via and Directed Polymer on Cayley tree and Random Energy Model. We believe, that at critical point statistical mechanical system misses memory about secondary details and model in UM space carries on some features of the original model in 2d space.For the case of 2d conformal models it is possible to derive exact results. There is a big area of numerical work to check this approach, which could be generalized in principle to high dimensions also.

References

1. B. Derrida, Phys. Rev. Lett. **45** (1980) 79.
2. H.E.Castillo et all,Phys.Rev. B.**56**(1997)10668
3. D.B.Saakian, PRevE, 61.(2000)6132

Common features of decon£ning and chiral critical points in QCD and the three state Potts model in an external £eld

F. Karsch, Ch. Schmidt and S. Stickan

Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld

Phone: +49 521/106-6130, Fax: +49 521/160-2961, stickan@physik.uni-bielefeld.de

The spontaneous breaking of global symmetries and their restoration at high temperature are common features of quantum £eld theories and statistical models. It is well known that universal properties at £nite temperature phase transitions in (3+1)-dimensional gauge theories are related to those in 3-dimensional spin models. In this paper we discuss the universal properties at the second order endpoint of a line of £rst order phase transitions. In QCD such critical points exist in a region of large quark masses as well as for light quarks[1]. The 3-dimensional 3-state Potts model has such a critical point at a certain strength of the external £eld.

In order to determine these critical points and their universality class we used a method original proposed to study the liquid-gas transition point[2]. Within this approach one considers the relevant ordering-£eld and energy-like operators as a linear combination of the energy and magnetization parts of the Hamiltonian. To £x the coef£cients for the energy-like operator it is assumed that the temperature-like direction is given by the £rst order phase transition line. For the ordering £eld coef£cient one demands uncorrelated energy-like and ordering-£eld like directions. In a £eld theory the situation is in general more complex. We extend the ansatz for both parameters appropriately in this case.

Once we have found the mapping between these operators, we use the intersection points of the fourth order cumulant of the ordering £eld to obtain a precise location of the critical point. The universality class is then identi£ed by the characteristic £ngerprint of the joint histograms of these new £elds.

Using this methods we show that the decon£ning critical point (large m_q) as well as the chiral critical point (small m_q) in 3-¤avour QCD belong to the universality class of the 3-dimensional Ising model. We furthermore use these techniques to analyze the critical point in a 3-d, 3-state Potts model in an external £eld and £nd the same result[3].

For the numerical investigation of the Potts model we used a Wolff cluster algorithm with a ghost spin to implement the external £eld. For the £nite size scaling analysis we used various lattice sizes ranging from 40^3 up to 70^3. For the simulations with the SU(3) gauge theory we used lattices of size $N_\sigma \times 4$ with $N_\sigma = 8, .., 24$. Simulations with staggered fermions have been performed with the Hybrid R Monte Carlo algorithm. All the data are analyzed with the Ferrenberg-Swendsen method[4].

References

1. S.Gavin, A. Gocksch, R.D.Pisarski, Rhys. Rev. D 49 (1994) 49.
2. N.B. Wilding, J. Phys.: Condens. Matter 9 (1997) 585.
3. F. Karsch, S. Stickan, Phys. Lett. B 488 (2000) 319.
4. A.M. Ferrenberg, R.H. Swendsen, Phys. Rev. Lett. 61 (1988) 2635.

Study of plasma-solid interaction in low-temperature plasma

M. Vicher, R. Hrach, M. Entlicher and R. Mareš

Faculty of Mathematics and Physics, Charles University,
V Holešovičkách 2, 180 00 Prague 8, Czech Republic

+420 2 21912343, +420 2 6885095, miroslav.vicher@mff.cuni.cz

Low-temperature plasmas are widely used in plasma-chemical technologies and the theoretical description and the understanding of mechanisms, which take part during plasma processing of materials, is very important. During their transport to substrates, active particles from plasma are crossing the transient region of disturbed plasma, so-called sheath and presheath. The plasma properties are changed due to the proximity of substrate; local electric £elds in the sheath change both the velocity distributions and concentrations of individual species in plasma. The magnitude of this £eld determines the ¤ux of charged particles and thus the kinetics of chemical reactions on the substrates. The second motivation for the study of plasma-solid interaction is the probe diagnostics. The interpretation of Langmuir probe characteristics is complicated as the probes perturb their local surroundings. Theoretical analysis brings successful results for limited set of probe geometries only and for low pressures, when scattering of charged particles during their transport through the sheath region can be either completely neglected or at least is non-important [1].

The computer simulation technique seems to be very promising tool to study the cases where the analytical methods cannot be used - substrates of complicated forms, higher pressures, plasma consisting of more types of particles including negative ions, chemically active plasma, etc. There are two basic techniques of the sheath simulation - ¤uid modelling and particle simulation techniques. Fluid models are much more effective, however their accuracy is typically very limited due to simpli£ed assumptions about processes in the sheath region and on the surface of solids immersed into plasma. On the contrary, self-consistent particle models can bring very precise results but the performance of standard algorithms is rather low.

In our contribution, we tried to compare the two approaches - particle simulation technique and ¤uid simulation technique, and combine their good features into one hybrid model. The main attention was devoted to the various aspects of the simulation - how to increase the performance of particle simulation models, how to handle various substrate or probe geometries, how to incorporate realistic physical assumptions into ¤uid models, etc. The basic techniques of both particle and ¤uid simulation methods were the standard ones:

- Particle simulation models are based on the combination of deterministic and stochastic approach - trajectories of charged particles between scattering events were calculated from the Newton's equations of motion and interactions were treated by the Monte Carlo technique. Forces acting on individual particles were calculated either by standard PIC method [2] or the in¤uence of all other particles was directly summed by several modern algorithms [3].

- Fluid model is based on the transport equation. Electrostatic £eld is obtained from the Poisson equation. Further modi£cation was done which re¤ects the effects of given electron energy distribution function.

References

1. Swift J. D., Schwar M. J. R., Electrical Probes for Plasma Diagnostics. Illife Books, London (1970).
2. Birdsall C. K., Langdon A. B., Plasma Physics via Computer Simulation. Adam Hilger, Bristol (1991).
3. Hrach R., Czech J. Phys. 49 (1999) 155.

Avalanches in the ground state of the 3d gaussian random £eld ising model driven by an external £eld

Carlos Frontera[1] **and Eduard Vives** [2]

[1] *Institut de CiÁncia de Materials de Barcelona, Consell Superior d'Investigacions Cientí£ques, Campus de la UAB, E-08193 Bellaterra, Catalonia,Spain.*

[2] *Departament d'Estructura i Constituents de la MatÁria, Universitat de Barcelona, Diagonal 647, Facultat de Física, E-08028 Barcelona, Catalonia,Spain*

phone: 34934021587, fax: 34934021174, e-mail: eduard@ecm.ub.es

We present a numerical study of the exact ground states of the 3d Gaussian Random Field Ising model (G-RFIM) with an applied external £eld B. We combine an standard max-¤ow min-cut algorithm with an optimal procedure for determining all the ground states when B is swept from $-\infty$ to ∞ [1]. The behaviour of different ground state properties is studied as a function of the degree of disorder in the system σ (standard deviation of the gaussian random £elds). A large number of different realizations of the random £elds ranging from 10^4 to 10^2 have been analyzed for systems with sizes up to $N = L^3 = 110592$. The evolution of the magnetization m when B is swept consists in a sequence of jumps or 'avalanches' with a certain size Δm. The statistical distribution of avalanche sizes $p(\Delta m)$ becomes a power law $p(\Delta m) \sim \Delta m^{\tau}$ for a certain degree of disorder $\sigma_c(L)$. The extrapolation of the results to $L \to \infty$ renders $\sigma_c \simeq 2.35 \pm 0.15$ and $\tau \simeq 1.8 \pm 0.1$. We compare the results with thermal equilibrium ($T > 0$) studies at $B = 0$ [2] and with numerical simulations at $T = 0$ of the 3d G-RFIM externally driven under metastable conditions [3].

References

1. C.Frontera and E.Vives, J. Comp. Phys. (2001), in press.
2. J.Machta, M.E.J.Newman and L.B.Chayes, Phys. Rev. E **62**, 8782 (2000).
3. O.Perkovic, K.A.Dahmen and J.P.Sethna, Phys. Rev. B 59, 6106 (1999), and references therein.

A model of internal waves mixing via numerical solution of Korteweg-de Vries system

A. A. Halim[1], **S.P. Kshevetskii**[2], **S.B. Leble**[3]

[1,3] *Technical University of Gdańsk, Gdańsk, Poland,*
[2] *Kaliningrad State University, Kaliningrad, Russia*
[3] *leble@mif.pg.gda.pl*

We study the initial value problem for a coupled KdV (cKdV) system that is obtained by projecting technique from Euler equations with a strati£ed background state that is valid for internal water waves. We simulate an initial stage of the McEwan experiment [1] for a tank of dimensions 50 in x by 25 cm in (vertical) z directions and salted water of the constant buoyancy frequency 1.23 s^{-1}. The solution of the problem we search in the waveguide mode representation [2] for the current function $\psi = \sum_{n=1}^{N} Z^n(z)\theta^n(x,t)$. Basic eigenfunctions $Z^n(z)$ describe a shape of the internal waves modes and satisfy Sturm-Liouville problem with zero boundary conditions for the variable z. Functions $\theta^n(x,t)$ are solutions of the cKdV system $\theta^n_t + c_n\theta^n_x + \sum_{m,k}^{N} g_{mkn}\theta^m\theta^k_x + \sum_{m}^{N} d_{nm}\theta^m_{xxx} = 0$, c_n are the modes linear velocities and the coef£cients of nonlinearity g_{mkn}, and dispersion d_{nm} are introduced in [2]. The table below presents the three-mode model coef£cients $d_{22} = 4\cdot 10^{-5}$, $d_{44} = 5\cdot 10^{-6}$, $d_{66} = 2\cdot 10^{-6}$, $c_2 = 5\cdot 10^{-2}$, $c_4 = 2.5\cdot 10^{-2}$, $c_6 = 1.6\cdot 10^{-2}$.

g_{mk2}

m\ k	2	4	6
2	0	72.3	0
4	28.9	0	202.4
6	0	130	0

g_{mk4}

m\k	2	4	6
2	28.9	0	57.8
4	0	0	0
6	0	0	0

g_{mk6}

m\k	2	4	6
2	0	33.7	0
4	48.2	0	0
6	0	0	0

The cKdV system is solved by the numerical scheme [3] which stability and convergency are established. The results combined with the solution of the Sturm-Liouville problem give the function ψ and internal wave pro£les. Due to symmetry the contour plots are made for the upper half of the tank.

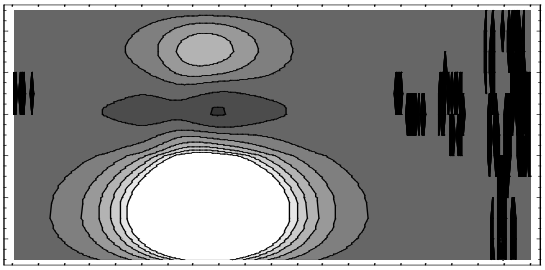


Fig.1

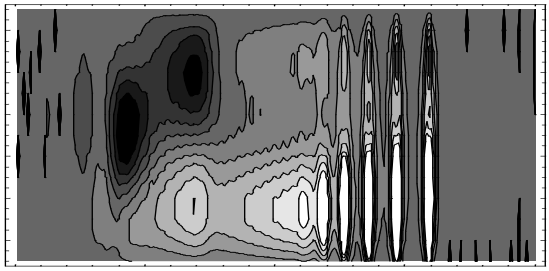


Fig.2

The three-mode contribution adopts about 80 % of the initial energy. A linear dispersion (Fig.1) is compared with nonlinear one and show a typical multisoliton-like contribution (Fig.2) with more than 5 solitons already appeared at the very early time 0.02 sec. Hence we expect effective internal waves mixing at a longer time with a £ne horizontal structure (and the vertical one if higher modes are accounted) that presumably should resemble results of [1].

References

1. A.D. McEwan, J. Fluid Mech. **128**, pp.47-57, pp.59-80, (1983).
2. S.B. Leble, Nonlinear waves in waveguides, Springer-Verlag, Berlin, Germany, 1991.
3. S.P. Kehevetskii, Nonlinear Processes in Geophysics **8**, pp.37-53, (2001).

Computational method for transition to chaos prediction of the forced oscillations

I.A. Bashkirtseva, L.B. Ryashko

Department of Mathematics,Ural State University,
pr.Lenina 51, 620083 Ekaterinburg, Russia
e-mail: irina.baskirtseva@usu.ru

Many nonlinear systems have periodic oscillations as an essence of its dynamics. Stochastic ¤uctuations of periodic processes play an important role for understanding of the corresponding phenomena for lasers, radiofrequency generators, chemical and biological systems. The various transitions (”bifurcations”) through periodic to more complicated regimes are a central problem in modern nonlinear dynamic theory. There are many papers devoted to a qualitative analysis of the forced oscillations .

We suggest a new computational techniques [1] for investigation of the local stochastic dynamics near limit cycles. This techniques is based on nonequilibrium quasipotential [2]. An approximation of quasipotential is expressed by some scalar function. This function (sensitivity function) is introduced as a base tool of a quantitative description for a system response on the external disturbances.

The new cycle numerical characteristics (sensitivity factor, parameter of stiffness) are suggested. The possibilities of sensitivity function to predict some peculiarities of dynamics for stochastically and periodically forced oscillators are shown.

From this analysis the critical value of Brusselator parameter is found. The dynamic of forced Brusselator for this critical value is investigated. For small stochastic disturbances, the burst of response amplitude is shown. For small periodic disturbances, the period doubling regime of the transition to chaos scenario is demonstrated.

Thus, the function of sensitivity is the effective computational tool for a prediction of singular responses of a non-linear system both to stochastic and to periodic disturbances.

This work is supported by RFBR grant (N00-01-00076).

References

1. Bashkirtseva I.A., Isakova M.G., Ryashko L.B. Quasipotential in stochastic stability analysis of the nonlinear oscillator orbits. *J. Neural, Parallel & Scienti£c Computations,* **7**, 299-310, 1999.
2. Graham, R., Tel, T. Nonequilibrium potential for coexisting attractors. *Physical Review A,* **33**, 1322-1337, 1986.
3. Bashkirtseva I.A., Ryashko L.B. Sensitivity analysis of the stochastically and periodically forced Brusselator.*Physica A,* **278**, 126-239, 2000.

Localization and coherent structures in wave dynamics via multiscales

Antonina N. Fedorova and Michael G. Zeitlin

Russian Academy of Sciences, Institute of Problems of Mechanical Engineering,
Mathematical Methods in Mechanics Group
V.O., Bolshoj pr., 61, 199178, St. Petersburg, Russia

tel: +7-812-3214776, fax: +7-812-3214771, E-mail: zeitlin@math.ipme.ru,
anton@math.ipme.ru
http://www.ipme.ru/zeitlin.html, http://www.ipme.nw.ru/zeitlin.html

We consider the applications of a new numerical-analytical technique which is based on the methods of local nonlinear harmonic analysis or wavelet analysis to the wave motion/turbulence problems described by some nonlinear differential equations. Such approach may be useful in all models in which it is possible and reasonable to reduce all complicated problems related with statistical/stochastic distributions to the problems described by systems of nonlinear ordinary/partial differential equations with or without some (functional)constraints. Wavelet analysis gives us the possibility to work with well-localized bases in functional spaces and gives for the general type of operators (differential, integral, pseudodifferential) in such bases the maximum sparse forms.

In our variational-wavelet approach [1]–[4] we can consider polynomial and rational type of nonlinearities. The solution has the multiscale/multiresolution decomposition via nonlinear high-localized eigenmodes which corresponds to the full multiresolution expansion in all time/space scales. This gives us expansion into the slow part and fast oscillating parts. So, we may move from coarse scales of resolution to the £nest one for obtaining more detailed information about our dynamical process. The £rst term corresponds on the global level of function space decomposition to resolution space and the second one to detail space. In this way we give contribution to our full solution from each scale of resolution or each time/space scale or from each nonlinear eigenmode. The same is correct for the contribution to power spectral density (energy spectrum): we can take into account contributions from each level/scale of resolution.

Our functional space decomposition corresponds to exact nonlinear eigenmodes decompositions. It should be noted that such representations give the best possible localization properties in the corresponding (phase)space/time coordinates. In contrast with different approaches we do not use perturbation technique or linearization procedures and represent dynamics via generalized nonlinear localized eigenmodes expansion with the best possible convergence properties. So, by using wavelet bases with their good (phase)space/time localization properties we can modelling the dynamics of high-localized coherent structures in spatially-extended stochastic/turbulent systems with collective behaviour. In all these models numerical modelling demonstrates the appearence of coherent high-localized structures and stable patterns formation.

References

1. Wavelets in Optimization and Approximations, *Math. and Comp. in Simulation*, **46**, 527-534, 1998.
2. Wavelet Approach to Mechanical Problems. Symplectic Group, Symplectic Topology and Symplectic Scales, *New Applications of Nonlinear and Chaotic Dynamics in Mechanics*, 31-40, (Kluwer, 1999).
3. Wavelet Approach to Polynomial Mechanical Problems. *New Applications of Nonlinear and Chaotic Dynamics in Mechanics*, 101-108 (Kluwer, 1999).
4. Variational Approach in Wavelet Framework to Polynomial Approximations of Nonlinear Accelerator Problems, American Institute of Physics , Conf. Proc., vol. 468, Nonlinear and Collective Phenomena in Beam Physics, pp. 48-68, 1999.

Numerical simulation ¤uid ¤ow with a obstacle on a channel wall: Quasi - oscillation regime

A.Ya. Gorbatchevski [1], **A.G. Churbanov**[2]

[1] *Lomonosov Moscow State University, Chemical Dept., Vorob'evy Gory, Moscow 119899, Russia,*

[2] *Institute for Mathematical Modeling RAS, 4 Miusskaya Square, Moscow 125047, Russia*

Phone (095) 9393207, Fax: (095) 9328846, E-mail: gorba@radio.chem.msu.ru

In the present work there is studied numerically ¤ow with crystals on a channel wall. Flows in channels with obstructions on their walls are of great practical importance for industrial applications, including heat transfer enhancement by rib roughness, cooling of electronic components and equipment, cooling towers etc. Transient mixing phenomena induced by bluff bodies result in increasing (or, in opposite, decreasing) some essential parameters of the process. In this study a roughness element under consideration is a single immobile crystal of square cross-section located on a rigid reactor wall. Its in¤uence on heat and ¤uid ¤ow in the surrounding and in the bulk of the channel is investigated for laminar steady-state and oscillatory regimes in the 2D planar formulation.

A general-purpose CFD tool has been used to conduct analysis of this problem. The algorithm employed to solve numerically the incompressible Navier-Stokes equations is based on the £nite difference approach and the primitive variable formulation of the governing equations. It presents a development of the well-known SIMPLE-like (pressure-based) approaches to solve the incompressible and slightly-compressible Navier-Stokes equations. The up-to-date theoretical achievements in CFD were used, selection of the most ef£cient variant of algorithm was performed via a lot of practical calculations. To validate possibilities of the numerical method for studying transient ¤ow problems of the considered class, a ¤ow over a square cylinder has been investigated as a test [1]. Predicted vortex shedding structures for the Reynolds number in the range from 100 up to 1000 have indicated a good agreement with available numerical and experimental data both in the Strouhal number and average drag / lift coef£cients. It is well-known that at approaching a bluff body to a rigid wall transient behaviour of the ¤ow becomes more complicated in compare with the freestream case. Peculiarities of the limiting case of a square roughness element placed on a channel wall is studied here with application to chemical reactors with crystallization processes [2].

Peculiarities of convective transport were analyzed for Re in the range from 5 up to 500 at the assumption of 2D ¤ow downstream of the square body. The critical value of Reynolds number at which transition from steady-state ¤ow regime to oscillatory vortex shedding takes place has been estimated from numerical experiments. A parametrical study on in¤uence of Re on the Strouhal number and average drag coef£cient has been conducted and has indicated signi£cant differences from the freestream case. Dependence of the overall time- and surface-averaged Nusselt numbers on ¤ow regimes was examined.

References

1. A.G.Churbanov, A.N.Pavlov, P.N.Vabishchevich. Operator-splitting methods for the incompressible Navier-Stokes... Part 1: First-order schemes. Int. J. Numer. Methods Fluids 21, 617-640 (1995).
2. Kutepov A.M., Melikhov I.V., Gorbatchevski A.Ya., Churbanov A.G. Deposition growth in a wall... In: Theoretical Foundation of Chemical Engineering 2000, Vol. 34, No. 6, pp. 537–546.

Convection instability in a small Rayleigh-Bénard system

Manabu Hasegawa

Institute of Engineering Mechanics and Systems, University of Tsukuba, Tsukuba 305-8573, Japan

hasegawa@esys.tsukuba.ac.jp

Molecular dynamics study on the Rayleigh-Bénard system was explored by Mareschal *et al.* [1, 3] and by Rapaport [2] in the middle of 1980's. The former researchers demonstrated that fully developed convective rolls could be observed even in a small system made up of a few thousands of molecules. In our previous [4] and present studies, the dynamical behavior of a small Rayleigh-Bénard system of a hard disk ¤uid con£ned in a square box is reexamined. Our interest lies in an unstable motion of convective roll observed near the conventional bifurcation point, especially in a similarity to another critical phenomena with bifurcation.

A series of experiments is performed by changing various physical conditions, namely the number of disks and the boundary condition and so forth, as well as the temperature gradient. The temperatures of the top and the bottom walls are kept constant in each run and a gravitational £eld is introduced so that a disk moving between these two walls experiences a zero net energy change. Initially, the disks are uniformly spaced and their velocities are sampled from the Maxwellian distributions with linearly interpolated temperatures between the two thermal walls. The disks are assumed to be re¤ected specularly on the walls; however, thermal effect is taken into account to the velocity departing from the top and the bottom walls in conventional ways. In addition to the macroscopic ¤ow £elds, variation of angular momentum of the system around the center of the box is examined because the stabilization of a convective ¤ow coincides with the state in which the direction of this momentum is kept unchanged.

Our £ndings are summarized as follows. When the temperature difference, ΔT, is small, no ¤ow can be observed: only heat conduction occurs. As ΔT increases, spontaneous single-roll structure emerges after the initial transient state. At £rst, both clockwise and counterclockwise convections are observed irregularly; however, the average lifetime of a convective roll pattern is prolonged with progression of ΔT. In most of the cases examined, this tendency continues to the largest temperature gradient imposed in our experiment. For the stabilization of a convective roll pattern, it is necessary for the system to contain an enough number of disks and to be run under the stress-free (slip) type boundary condition. In any case, there is no distinct critical point between no-roll and fully developed single-roll states in the present small system.

References

1. M. Mareschal and E. Kestemont, Nature **329**, (1987) 427.
2. D. C. Rapaport, Phys. Rev. Lett., **60**, (1988) 2480.
3. M. Mareschal, M. Malek Mansour, A. Puhl, and E. Kestemont, Phys. Rev. Lett., **61**, (1988) 2550; A. Puhl, M. Malek Mansour, and M. Mareschal, Phys. Rev. A **40**, (1989) 1999.
4. M. Hasegawa, Prog. Theor. Phys. Suppl., **138**, (2000) 604.

Interaction of dissipative quasi-particles: Scattering, formation of bound states, generation and annihilation

Andreas W. Liehr[1] **and Mathias Bode** [1,2] **and Hans–Georg Purwins**[1]

[1] *Institut für Angewandte Physik, Corrensstraße 2/4, D-48149 Münster, Germany*
[2] *Cortologic-AG, Ostendstr. 25, D-12459 Berlin, Germany*
http://www.uni-muenster.de/physik/ap/purwins/struktur

Excitable media show a broad range of structure formation processes which are investigated in biological, chemical and physical systems with experimental, theoretical and computational methods [1]. A special type of structures observed in excitable media are so called dissipative quasi-particles, which are stationary or moving localized high-amplitude structures surrounded by a homogeneous background states. In order to model phenomenologically the quasi-particle phenomena of a dc-gas-discharge-system [2] a three-component reaction-diffusion system of 1-activator-2-inhibitor type is investigated. Near the drift-bifurcation the in£nite degrees of freedom of the partial differential equations can be reduced to ordinary differential equations describing the interaction of moving quasi-particles in terms of their position and their drift [3]. In this approach one inhibitor acts as a nonlocal feedback to the activator and stabilizes the structure, while the other inhibitor determines the equilibrium velocity of the quasi-particle, which can be controlled by the time-constant of his temporal evolution. Depending on this control parameter the quasi-particle interaction can lead to the formation of bound states like moving or rotating quasi-particle-molecules [4], if the tails of the quasi-particles decay exponentially to the homogenous background state.

In order to check the interval of the control parameter where the reduced dynamics formalism is valid, we are solving the partial differential equations of the reaction-diffusion system numerically on two-dimensional domains. For small control parameters and thus small drift-velocities the simulations reproduce the predictions of the reduced dynamics formalism. Increasing the control parameter above some threshold value leads to the appearance of further interaction phenomena like generation or annihilation of quasi-particles. This shows that the well known interaction phenomena of dissipative quasi-particles like scattering, formation of molecules, generation and annihilation attribute to only one control parameter determining the drift-velocity of the quasi-particle. Previous to the appearance of generation and annihilation effects the reduced dynamics formalism is an important tool to investigate many particle dynamics in reaction-diffusion systems.

References

1. ENGEL, H. ; NIEDERNOSTHEIDE, F.-J. ; PURWINS, H.-G. ; SCHÖLL, E.: *Self-Organization in Activator-Inhibitor-Systems: Semiconductors, Gas-Discharge and Chemical Media.* Wissenschaft- und Technik-Verlag, 1996
2. PURWINS, H.-G. ; ASTROV, Yu. ; BRAUER, I.: Self-Organized Quasi Particles and Other Patterns in Planar Gas-Discharge Systems. In: DING, Mingzhou (Hrsg.) ; DITTO, William L. (Hrsg.) ; PECORA, Louis M. (Hrsg.) ; SPANO, Mark L. (Hrsg.): *The 5th Experimental Chaos Conference. Orlando, Florida, USA 28 June - 1 July 1999*, World Scienti£c, 2001
3. BODE, M. ; LIEHR, A. W. ; SCHENK, C. P. ; PURWINS, H.-G.: *Interaction of Two- and Threedimensional Moving Localized Solutions in a Three-Component Reaction-Diffusion-Model: A Particle Approach.* 2001. – resubmitted to Physica D
4. LIEHR, A. W. ; MOSKALENKO, A. ; SCHENK, C. P. ; BODE, M. ; PURWINS, H.-G.: *Localized Solutions with Two Axis of Symmetry in Reaction-Diffusion-Systems: The Rotational Degree of Freedom.* 2001. – in preparation

Computation of a diverging LX-17 detonation

Liu Eryan* Liu Bangdi and Wang Yuanshu

Institute of Applied Physics and Computational Mathematics
Beijing, P.R. China 100088
**telephone number: 86-10-62378793*
fax number: 86-10-62010108
e-mail: clqm@cb.col.com.cn

The reaction zone of a detonation wave is very small compared to the hydrodynamic length scale for a typical application. Consequently, it is impractical for numerical calculations to £nely rasolve the reaction zone. The Bukiet's modi£ed Hugoniot jump relations characterize the curvature effect of detonation wave. They express the conservation laws and are not sensitive to the detailed reaction dynamics.

As known, underdriven diverging detonation wave decouple from the ¤ow behind, and the wave front can be correctly propagated with detonation shock dynamics (DSD). From the knowledge of the local radius of curvature (which is a vailable since the fronts are sharp), the state quantities behind the front may be algebraically obtained from the modi£ed Hugoniot jump relations which include £ve parameters: the reaction zone width and the volume averages over the reaction zone of the pressure and of the mass, momentum and energy densities, they may be obtained from the planar wave for LX-17 using £nely zoned (50 zones per millimeter) ZND reactive ¤ow calculation. We use JWL equations of state for both the unreacted explosive and its reaction products and Lee-Tarver ignition and growth reaction rate.

The detonation wave motion and the state immediately behind the wave may be found after calculating the local curvature at each point along the front such that the detonation wave front and the hydrodynamic front are propagated consistently and then the ¤ow behind the front may be computed using JWL equation of state for detonation products. The method is known as Detonation Front Tracking Method (DFTM) which eliminates the need to resolve the reaction zone and allows us coarsen the entire mesh thus yielding great saving in computational effort. These results are implemented in a hydrocode to model a spherically diverging detonation of the explosive LX-17.

As the detonation wave speed is only valid to £rst order in k, it is consistent with the accuracy of the approximation to use the volume averages obtained from the planar wave for small values of k to obtain the state behind the front. We see, whether pressure pro£le or state quantities behind the front, the DFTM calculations agrees very closely the reactive ¤ow calculation.

Computational analysis of the evolution of steep gravity waves on ¤uid of an arbitrary depth

Lukomsky V.P., Gandzha I.S.[1], Lukomsky D.V.[2], Tsekhmister Y.V.[3]

[1] *Institute of Physics of National Academy of Sciences of Ukraine*
[2] *Taras Shevchenko Kyiv National University, Ukraine*
[3] *Bohomoletz National Medical University, Ukraine*

phone 380442657994, fax 380442651589, e-mail lukom@iop.kiev.ua

For proper understanding of air-sea interaction and of the generation and development of a wave £eld, the knowledge of the form and the dynamics of gravity water waves is highly essential. Dynamics of two-dimensional steep gravity waves on a surface of ideal incompressible ¤uid of an arbitrary depth is investigated. The wave evolution is described by the Laplace equation in the ¤ow domain for the velocity potential Φ and the dynamical and kinematic boundary conditions on the free water surface [1]. Up to this time, completely different methods are used to study wave propagation on the surface of deep and shallow water. To consider waves of arbitrary steepness without assuming a non-linearity to be small and to build solutions in the physical plane $\{x,\, y\}$ valid for ¤uid of arbitrary depth h we use the method of harmonic balance (Galerkin's approximation)

$$\eta(\theta) = \sum_{n=-N}^{N} \eta_n\, e^{in\theta}; \quad \Phi(\theta, y) = \sum_{n=-N}^{N} \varphi_n \frac{\cosh \mid n \mid k(y+h)}{\cosh \mid n \mid kh}\, e^{in\theta}, \quad -h < y < \eta(x,t); \qquad (1)$$

where $\theta = kx - \omega t$; x and y are respectively horizontal and upward vertical axes; $y = \eta(x,t)$ is the elevation of the free surface under still water level $y = 0$; k and ω are respectively wave number and frequency.

The only approximation of the harmonic balance procedure is the truncation of the Fourier series. The greater number of harmonics N is taken into account the higher precision of the approximate solution is achieved. Using expansions (1), the set of non-linear algebraic equations for unknown harmonics η_n, φ_n and wave frequency ω was obtained for numerical computer calculations. The general recurrence and explicit formulas were received for calculating the Fourier harmonics of exponential functions. At that, higly ef£cient technique of numerical analysis of systems with polynomial non-linearity developed by authors was used.

The proposed technique of numerically-analytical analysis of the propagation of water waves allowed us to investigate the Stokes waves in deep water and cnoidal waves in shallow water as well as intermediate cases using the same highly ef£cient code. The new solutions were found possibly responsible for the breakdown of waves. The sequences of bifurcations with periods divisible by prime numbers 2, 3, 5 were revealed. The respective subharmonic stationary states were found with subsequent doubling of corresponding sequences $2, 2^2, 2^3, \ldots$; $3, 3^2, 3^3, \ldots$.

The method is generalized by authors for three-dimensional water waves, gravity-capillary waves as well as for two-layer ¤uid.

References

1. Reference No 1. Lukomsky V.P. Modulational instability of gravity waves in deep water with allowance for non-linear dispersion. – JETP, 1995, 81(2), 306-310.

Analysis of vortex structures in a compressible isotropic turbulence

Hideaki Miura

Theory and Computer Simulation Center,
National Institute for Fusion Science,
Oroshi 322-6, Toki, Gifu 509-5292, JAPAN

TEL: +81-572-58-2381, FAX: +81-572-58-2626,
e-mail:miura@toki.theory.nifs.ac.jp

A mechanism to suppress growth rate of the kinetic energy in mixing layers or other sheared turbulence has been extensively investigated for more than one decade. Although it was thought £rst that some terms in the equation of the kinetic energy which were intrinsic to compressible ¤uid should be important for this problem, Sarkar(1995) has shown that one of the most important contributions of compressibility to a turbulence was modi£cation of rotational components of the velocity rather than these terms. However, detailed physical mechanism on a point how the compressibility changes the rotational components of the velocity remains unclari£ed.

In order to understand this mechanism, we investigate how tubular vortex structures in a compressible turbulence are affected by the compressibility. A tubular vortex structure is one of representatives of ¤uid motions. Identi£cation of vortex structures has been a hot and tough problem of an incompressible turbulence, because of lack of consensus on de£nition of a vortex. (Refer to Kida and Miura[2] and references therein for a review of this problem.) In order to prepare an objective de£nition of a vortex, we have developed a scheme to identify central axes of vortices and core regions of vortices around axes.[3, 4] Now we extend our scheme to a compressible ¤uid to identify and analyze vortex structures.

In order to clarify how the compressibility affects to vortex structures, we execute direct numerical simulations of compressible and incompressible, decaying isotropic turbulence. We set initial velocity £eld and the Reynolds number the same between these two kinds of simulations. By using our vortex identi£cation scheme, we identify tubular vortex structures. Because of the same initial condition, we are able to compare vortices in compressible turbulence to those in incompressible turbulence one by one. While the energy and enstrophy does not differ each other so much between compressible and incompressible simulations, clear differences are observed in vortex structures. The total volume of vortex cores identi£ed in compressible turbulence becomes clearly smaller than the one in incompressible turbulence. Furthermore, vortices in compressible turbulence are relatively straight and less bent compared with vortices in incompressible turbulence.

At last, detailed analysis on vortex structures in turbulence, discussions on compressibility effects, roles of tubular vortices in mixing and/or transport problems of compressible ¤uids will be presented.

References

1. Sarkar, S. 1995, “The stabilizing effect of compressibility in turbulent shear ¤ow”, *J. Fluid Mech.*, Vol. 282, pp. 163-186.
2. Kida, S. and Miura, H., 1998a, “Identi£cation and Analysis of Vortical Structures”, *Euro. J. Mech. B/Fluids*, Vol. 17, pp. 471-488.
3. Miura, H. and Kida, S., 1997, “Identi£cation of Tubular Vortices in Turbulence”, *J. Phys. Soc. Japan*, Vol. 66, pp. 1331-1334.
4. Kida, S. and Miura, H., 1998b, “Swirl Condition on a Low-Pressure Vortices”, *J. Phys. Soc. Japan*, Vol. 67, pp. 2166-2169.

Numerical modeling of turbulent wakes dynamics in strati£ed medium

G. G. Chernykh[1] **and N. P. Moshkin**[2] **and O. F. Voropayeva**[1]

[1] *Institute of Computational Technologies, Siberian Division of Russian Academy of Sciences, 6 Lavrentjev Ave., Novosibirsk, 630090, Russia.*
[2] *Suranaree University of Technology, School of Mathematics, Institute of Science, Nakhon Ratchasima, 30000, Thailand.*
(66-44) 224382, (66-44) 224185, moshkin@math.sut.ac.th

Turbulent wakes behind bodies of revolution in strati£ed ¤uids have been considered in many publications. Analyzing these works we noted that the results of the numerical modeling of internal waves generated by turbulent wakes are incomplete. There are no data on comparison of characteristics of the internal waves generated by the wakes behind the self-propelled and towed bodies. In the present work an attempt is made at £lling these gaps.

To describe the ¤ow in a far turbulent wakes behind self-propelled and towed bodies in strati£ed medium the parabolized three-dimensional system of the averaged equations in the Oberbeck-Boussinesq approach is used. The modi£ed $e-\varepsilon$ model of turbulence is used for the system to be closed. The unknown values of Reynolds stresses are approximated by "isotropic" relationships [1]. The turbulent ¤uxes and the dispersion of the density ¤uctuations are replaced by locally equilibrium approximations. In order to determine the turbulence energy e and the rate of dissipation ε we use the corresponding differential transport equations. Marching variable x in the considered problem plays the role of time. Initial conditions at some $x = x_0$ were assigned in accordance with experimental data of Lin and Pao [2],[3]. The numerical algorithm is based on the application of an explicit splitting into physical processes to the system of equations for the motion and incompressibility. The other equations are solved using an implicit splitting into space variables.

The results of the numerical modeling of the internal waves generated by the wakes in strati£ed ¤uids have been presented. The computed phase pattern in the case of momentumless wake agrees suf£ciently well with Chashechkin's results of the laboratory measurements [4]. Some calculations of internal waves generated by turbulent wakes in the pycnocline have been illustrated. These results are in agreement with experimental data of [5]. Based on the analysis of behavior of the total energies of turbulence and internal waves in the wake cross-section, simpli£ed mathematical models for a far turbulent wake and the internal waves generated by it have been constructed. The results of calculations show that the drag wake generates internal waves of essentially greater amplitude.

References

1. W. Rodi: J. Geophys. Res., **92**, No.C5, 5305 (1987).
2. J.T. Lin, Y.H. Pao: Annu. Rev. Fluid Mech. **11**, 317 (1979).
3. S. Hassid: J. Hydronautics **14**, 25 (1980).
4. Chashechkin Yu.D., Internal waves, vortices and turbulence in a wake past a bluff body in a continuously strati£ed liquid. Preprints of the Fourth Int. Symp. on Strati£ed Flows, Grenoble Inst. of Nech., June 29 – July 2, 1994, edited by Hop£nger E., Voisin B., and Chavand G., Vol. 2, sess. B4, 29, 8 p.
5. H.E. Gilreath, A. Brandt: AIAA Paper **83-1704** (1983).

Generalized thermostatistics description of turbulent temperature ¤uctuations

Fernando M. Ramos, Reinaldo R. Rosa, Camilo Rodrigues Neto, Mauricio J. A. Bolzan and Leonardo D. Abreu Sá

Instituto Nacional de Pesquisas Espaciais, Caixa Postal 515, 12201-970, São José dos Campos, Brazil

Corresponding author: F.M.R., fernando@lac.inpe.br, phone: 55(12)3456534, fax: 55(12)3456375

Since it was £rst proposed in [1], the connection between Tsallis' generalized thermostatistics [2] and turbulence has been attracting a growing interest. In particular, with this formalism we obtained analytical formulas for probability density functions (PDFs) of velocity differences which were in very good agreement with experiments [3].

Tsallis' generalized thermostatistics introduces a family of non-extensive entropy functionals $S_q(p)$ with a single parameter q. These functionals reduce to the classical, Boltzmann-Gibbs form as $q \to 1$. Extremizing $S_q(p)$ subject to appropriate energy constraints, we obtain the generalized canonical ensemble probability distribution

$$p_q(\epsilon_i) = [1 - \beta(1-q)\epsilon_i]^{1/(1-q)}/Z_q \ . \tag{1}$$

where β is suitable inverse temperature, ϵ_i is i-th microstate energy level, and Z_q is the generalized partition function. In the limit of $q \to 1$, we recover the classical statistical mechanics expressions.

Traditionally, the properties of temperature ¤uctuations in turbulent ¤ows are studied from the statistics of temperature differences $T_r(x) = T(x) - T(x+r)$ at different scales r. In this paper we show that if we associate ϵ_i with the thermal energy corresponding to the temperature ¤uctuation T_r (i.e., $\epsilon_i \sim |T_r|$), Eq. (1) provides a simple and accurate model for describing statistical behavior of turbulent temperature ¤uctuations. A major advantage of using Eq. (1) is that all his moments can be analitically evaluated. Therefore, if we assume as usual a scaling of the moments $\langle T_r^n \rangle$ as r^{ξ_n}, the variation with scale of q and β can be completely determined.

We checked the above model with turbulence data measured in the atmospheric surface layer during the LBA (Large Scale Biosphere Atmosphere Experiment in Amazonia) wet season campaign [4]. Results were found to be in good agreement with experiment through spatial scales spanning three orders of magnitude.

This work was supported by FAPESP-Brazil, grants 97/13374-1 and 97/9926-9. FMR also acknowledges the support given by CNPq-Brazil through the research grant 300171/97-8.

References

1. F. M. Ramos, C. Rodrigues Neto, R. R. Rosa, preprint cond-mat/9907348; see also in C. Tsallis, *Braz. J. Phys.* **29** (1999) 1.
2. C. Tsallis, *J. Stat. Phys.* **52** (1988) 479.
3. F. M. Ramos, C. Rodrigues Neto, R. R. Neto, M. J. A. Bolzam, L. D. Abreu Sá and H. F. Campos Velho, *Physica A*, to appear.
4. M. J. A. Bolzan, F. M. Ramos, L. D. Abreu Sá, R. R. Rosa, C. Rodrigues Neto, *J. Geophys. Res.*, to appear.

Gastrulation as a self-organized symmetry breaking process

Alcides Castro-e-Silva[1] **and A. T. Bernardes**[2]

[1] *Departamento de Física, Universidade Federal de Minas Gerais, Caixa Postal 702, 30.123-970, Belo Horizonte-MG, Brazil*

[2]*Departamento de Física, Universidade Federal de Ouro Preto, Campus do Morro do Cruzeiro, 35400-000, Ouro Preto-MG, Brazil*

atb@iceb.ufop.br

Contrary to unicellular organisms, multicellular ones do not spring fully formed. These organisms reach their £nal shape under a relative slow process of changes, with a progressive increase on complexity. At most cases, the development of a multicellular living being starts with a single cell, the fertilized egg called zygote. After fertilization, the egg development undergo the following stages: (1) A series of extremely rapid mitotic divisions (cleavage) that £nishes with a hollow sphere known as blastula. (2) The blastula's invagination, forming the gastrula, a bilaterally symmetric three-layered structure. (3) Organogenesis: After the formation of the three layers, the cells interact with one another producing the organs. (4) The £nal stage is the growth and maturation. An important question for developmental biology is what leads to the breaking of symmetry?; or, why the living being does not have the same symmetry shown when it was a zygote?

In this work we introduce a model dealing with those questions. This model is based only in local interactions. The "medium" where the embryo grows is represented by a square lattice. To each site is associated a value S_i: $S_i = 0$ is a free cell site and $S_i = k$ ($k = 1...C$) means that cell type k occupies that site. In this version, $C = 2$. The £rst stage starts with the central site occupied by a type one cell ($S_i = 1$), representing the fecunded egg or zygote. The zygote now undergoes to a stage of successives mitotic divisions, thus £lling a "spherical" region of the lattice. The inner cells change to type 2, while the outer cells remains of type 1. After this *differentiation* the blastula appears now as a "skin" of type 1 sites, or the blastomeres, and an interior of type 2 sites, the blastocoel. The embryo is now ready to gastrulate due to the changes in the relative positions of the cells. These movements are done via a Monte Carlo dynamics, minimizing a Potts-like energy given by:

$$\mathcal{H} = -J_1 \sum_{i,j} \delta_{S_i,S_j} - J_2 M_i \quad , \tag{1}$$

where the £rst term represents the cell adhesion (the sum is performed over the eight nearest neighbours); and the second term represents the action of diffusible substances called *morphogens*. In the beginning of the second stage, the free cell sites have the same amount of morphogens and a blastomere tends to go inwards. If it succeeds in this movement, the concentration of morphogens increase on that region, leading to new movements that will creates the gastrula.

We performed simulations for different values of the interaction parameters, as well as the "temperature", which represents the ¤exibility of the system. The results can de organized in three groups: (i) the system is so rigid and we obtain only a hollow sphere; (ii) the system is so ¤exible that it can split in many parts; and (iii) we observe the formation of a gastrula. Hence, the symmetry breaking can be achieved without any kind of external agent. The information necessary to reduce the symmetry order lies in the dynamic of the system and only local rules are required; the gastrulation takes place as a spontaneous, robust and self-organized process.

Uni£ed information sharing system and computational physics

S. Itoh[1], T. Saito[2], S.Ohnishi[3], R.Takaki[4], and S.Ogawa[4]

[1] *TOSHIBA R&D Center, Kawasaki, Kanagawa, 212-8582, JAPAN*
[2] *Information and Mathematical Science Laboratory, Inc. Ikebukuro, Tokyo, 171-0014, JAPAN*
[3] *NEC Fundamental Research Laboratory, Tsukuba, Ibaraki, 305-0841, JAPAN*
[4] *National Aerospace Laboratory, Chofu, Tokyo, 182-8522, JAPAN*
+81-44-549-2113, +81-44-520-1801, satoshi.itoh@toshiba.co.jp

Quite recently, large scale simulations have been carried out in various £elds of computational physics. The softwares used for such simulations are available; some of them are used freely, and the others are provided commercially. For large scale simulations, use of database system, for example the database of atomic scale structures of protein molecules for its electronic structure calculations, is one of keys to success. These softwares and/or database including visualization tools are going to integrate via internet. However, there is a serious problem of interoperatability. In this paper, we present a platform for large scale simulations, and discuss the relationship between the knowledge sharing system based on this platform and computational physics.

The present platform consists of servers and clients, where programs , input/output data and other knowledges are dealt with as the same type of ”document” data, and the data are structurized by using the XML(eXtensible Markup Language) description. The data on the servers are controlled by object oriented database management system ”Object Store” and the Java applet is utilized for visualization, retrieve and authoring of the data at the clients. All of data, i.e. programs, numerical data, text documents and so on, are traceable, because of the use of XML tag sets. These tag sets should be de£ned as two sets with different categories; one is a common tag set, e.g. bibliographic information, physical constants, data types, and so on, the other is a £eld speci£c tag set e.g. atomic mass and unit cell structure for materials science, and identi£cation number of protein in the protein data bank (PDB) for bioscience.

We demonstrate the platform for the £eld of materials science. A typical simulation in this £eld is an electronic structure calculation, where the Kohn-Sham equation, in the framework of the density functional theory, is integrated numerically by using the atomic species and atomic positions as input data. Since total energy can be evaluated in this simulation, the most stable structure can be determined. In this case, simulation conditions such as convergent criteria, mesh interval for numerical integration and so on are treated as data together with programs and input/output data. These data are stored as XML structurized documents in the database on the servers, and can be referred freely via the platform.

Other implementation is concerning to the ¤uid dynamics. In this £eld, the Navier-Stokes equation is solved with £nite element method (FEM) or boundary element method (BEM), where mesh generation scheme is key for highly ef£cient simulations. Past numerical results and corresponding mesh information related each other are stored with XML tag in the database. These structurized data are utilized for the simulations with other simulation conditions, or referred by visualization tool on the clients.

Several applications of the platform to various £elds including bioscience and geophysics are in progress. The system presented here is a prototype of groupwares for a scienti£c community, and will contribute to construct an inter-community of researches globally.

Multifractality of cloud base height pro£les

K. Ivanova[1,2], N. Gospodinova[2], H.N. Shirer[1], T.P. Ackerman[3], M.A. Michalev[2], and M. Ausloos[4]

[1]*Department of Meteorology, Pennsylvania State University, University Park, PA 16802, USA*
[2]*Institute of Electronics, Bulgarian Academy of Sciences, 72 Tzarigradsko chaussee, So£a 1784, Bulgaria*
[3]*Paci£c Northwest National Laboratory, Richland, WA 99352, USA*
[4]*SUPRAS and GRASP, Institute of Physics, B5, University of Liège, B-4000 Liège, Belgium*

Tel: (814)-863-4722; Fax: (814)-865-3663; E-mail: kristy@essc.psu.edu

The cloud base height pro£les are known to have highly ¤uctuating, irregular structure. The dynamics of cloud base height evolution is determined by a variety of processes in the atmosphere, especially those in the planetary boundary layer [1]. This irregular structure of the signals is a benchmark for nonlinear dynamical processes. An assumption that this dynamics is due to the behavior of a complex system leads to a new concept in statistical investigation, as largely discussed in [2]. This concept is to predict the probability distribution of the system at large times, thereby giving its overall behavior. To do so requires use of specially designed methods of analysis for studies the temporal evolution of cloud base height records.

The data used in this study are the cloud base height sequences measured with a ground-based laser ceilometer having a temporal resolution of 30 seconds. The measurements were taken in June 1992 in the Azores Islands during the Atlantic Stratocumulus Transition Experiment (ASTEX) in June 1992.

The multifractal approach [3, 4] id used here to estimate the (q-th) order moments of the structure functions and the singular measures, as constructed from the data. The method seeks various scales of self-af£nity, and so searches for multi-af£nity. This approach leads to characterizing the nonstationarity and intermittency pertinent to such signals produced by nonlinear dynamical processes. Multifractality is the signature of the cloud base height pro£les as characterized by a hierarchy of exponents. The value of the roughness parameter H1 is consistent with the one obtained for the same data using different method of analysis. Moreover, the multifractal behavior of the cloud base height pro£les also is consistent with the multi-af£ne properties of other atmospheric data recorded simultaneously during the same £eld experiment [4].

Further work will be to relate these statistical parameters to the dynamical properties of the clouds, an important step toward understanding and predicting their dynamical behaviour.

References

1. J. R. Garratt, *The Atmospheric Boundary Layer,* Cambridge University Press, 1992.
2. G. Parisi, *Physica A,* **263,** 557, (1999).
3. A. Davis, A. Marshak, W. Wiscombe, R. Cahalan, *J. Geophys. Research*, **99**, 8055 (1994).
4. K. Ivanova and T. Ackerman, *Phys. Rev. E*, **59**, 2778 (1999).

Study of some laser signals emergent from nonlinear optical media

Mihaela Ghelmez[1] **C.Toma and P.E.Sterian**[2]
Mihaela (Dumitru) Ghelmez[1] **C.Toma and P.E.Sterian**[2]
[1]*Politehnica University of Bucharest,77 206, Bucharest, Romania*
[2]*Politehnica University of Bucharest,77 206, Bucharest, Romania*
tel: (+40 1)410 45 42, fax: (+40 1)410 44 88, e-mail: dem@physics.pub.ro

Liquid crystals are known as nonlinear optical media, even at low incident laser power. [1].

Our previous works showed that thin £lms of fatty acids and fatty acid-cholesterol mixtures behaved as liquid crystals, between some temperature values. [2].

Replace this text by the Text of your Summary. The paper presents an experimental and computer study of different type laser signals, emergent from some fatty acids - cholesterol mixtures samples, in presence of ¤uctuations. The purpose was to estimate as accurately as possible the cholesterol amount in any mixture sample. The optical emergent power at different incident optical powers and the pulse width in the time domain at different bias voltages were experimentally determined for different type c.w. and pulsed lasers, as for example helium-neon and Nd3+glass lasers, before and after passing through the samples. The results were correlated with the amount of cholesterol in mixtures and with their microscopic aspect and response in external electric £eld. These measurements are in all cases affected by ¤uctuations. Therefore we developed some computer based procedures, by using equations Runge-Kutta in MATLAB and the TableCurve3D from Jandel Scienti£c software for taking into account these ¤uctuations. As it is known, in averaging procedures the user is interested in the mean value of the received signal over a certain time interval. Since the investigated structures are very sensitive at random variations of the integration period (generated by the switching phenomena at the end of the integration) a multiplication of the received signal with a test-function is recommended. In this paper we present some invariance properties of differential equations, which can be used for generating a ”practical” test-function on this time interval. We were looking for ”truncated” test functions (functions which differ to zero only on a certain interval and with only some derivatives continuous on the real axis) and we presents also the properties of second order oscillating systems (considered as generating ”practical” test functions) in £ltering and sampling procedures. [3].

Numerical simulations were using Runge-Kutta equations of order 4-5 in MATLAB. TableCurve3D program was used to £t the experimental dependencies of the output signals on different input physical amounts. A good agreement between the experiment and computer results was found. A method to estimate the cholesterol percentage in a mixture with fatty acids was developed. Since fatty acids and cholesterol are important substances for the living matter and especially for the biological membranes, we consider this study important for elucidating some mechanism belonging to this domain.

References

1. 1.I.C.Khoo, Y.R.Shen, Optical Engin., 24, pp.4-25, 1985
2. M.Dumitru (Ghelmez), M. Honciuc, M.C.Piscureanu, C.Gheorghe, ”New Nonlinear Optical Materials for Optoelectronics”, Optical Engin. 35(5), pp.1372-1376, 1996
3. S.Gong,H.Hentzell,S.Peterson,H.Hesselbon,B.Lofstedt,M.Hause,”Techniques for Reducing Switching Noise in High-Speed Digital Systems” -Proc. 8th Annual Intl. ASIC Conference, 18-21 Sept. 1995

Fluctuations of WIG- the index of Warsaw stock exchange

Danuta Makowiec and Piotr Gnaciński
Institute of Theoretical Physics and Astrophysics, Gdańsk University, Poland
£zdm@univ.gda.pl

In the following we present results of investigations of the WIG index - the index of Warsaw Stock Exchange. (WIG is an abbreviation of the Polish name.) The WIG index is calculated as a total return of the weighted sum of market capitalization of all stocks from the main market once per trading day after each session. The Warsaw Stock Exchange is a young market— the £rst session took place on the 16th April of 1991 and £ve stocks were traded. Now, i.e. on 1 August 2000 the portfolio of the WIG index enumerates 120 stocks of the main market and 61 stocks are traded on the parallel market. We study a time series of returns of the WIG index for the period of 5 last years: from September 1995 to December 2000. Thus we observe the emerging market in its second phase of development.

The presentation is organized as follows:

After introducing time series considered and giving a de£nition for returns- one of the basic notions in a study of £nancial markets, we present tests to estimate strength and character of long-range correlation of Warsaw market. We show the strongly antypersistant random walk occurring in case of WIG -index in the time horizon longer than three months what result from every three months revision of the formula for WIG index.

Then we discuss properties of probability density functions of returns. We show that the central part of distribution of WIG index returns is well £tted by a Lévy distribution. Some time scaling is therefore provided. The asymptotic behavior of the distribution of returns shows faster decay than predicted by a Lévy distribution. Hence, our result con£rms Mantegna and Stanley proposition [1, 2] of a truncated Lévy distribution as a model for the distribution of returns. The exponential truncation ensures the existence of a £nite second moment what concludes, by limit theorems, that the asymptotic distribution of returns is a Gaussian distribution.

Finally we translate the time series of WIG index values into a text [3, 4]. The Zipf analysis results in the observation that non trivial correlation exist between successive daily ¤uctuations, so that some predictions are possible.

References

1. R. N. Mantegna and H. E. Stanley, Nature **376**, 46 (1995)
2. N. Mantegna and H. E. Stanley, *An Introduction to Econophysics. Correlations and Complexity in Finance* Cambridge University Press,Cambridge 2000.
3. N. Vandewalle and M. Ausloos, Physica A **268**, 240 (1999).
4. M. Ausloos, N. Vandewalle, Ph. Boveroux, A. Minguet and K. Ivanova, Physica A **274**, 229 (1999).

Neural networks in image analysis of complex systems

M. Malý[1,2], R. Hrach[2,1] and D. Novotný[1]

[1] *Faculty of Education, J. E. Purkyně University, České mládeže 8, 400 96 Ústí nad Labem, Czech Republic*

[2] *Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, 180 00 Prague 8, Czech Republic*

+420 47 5214417, +420 47 5212053, maly@pf.ujep.cz

In science - e.g. in astronomy, metallurgy, thin film physics, biology, etc. - complex systems consisting of a large number of individual objects are often studied. The image analysis of such systems gives information either about the size distribution of objects or about the spatial distribution of objects in two or three dimensions and in this way about important physical characteristics of studied systems, too. In thin film physics especially the deviation of the spatial distribution of objects from an equilibrium state is in a close connection with a nucleation processes taking part during initial stages of thin film growth.

For the image analysis in thin film physics the standard methods based on the theory of mathematical morphology [1] are often used. The sensitivity of these algorithms differs for discontinuous metal layers of various thickness and has limited accuracy for thicker discontinuous as well as semicontinous films. Therefore new techniques for the study of images of such structures must be suggested.

In this contribution a new approach to the image analysis of the systems consisting of a large number of individual objects based on neural networks [2] is presented. This technique can profoundly simplify the image analysis of more complicated systems, however in the present stage of computational technique for the successful application of neural network for image analysis an appropriate pre-processing method must be applied [3]. Therefore several algorithms are tested and their usefulness for the pre-processing of simulated micrographs of metal films with different thicknesses is compared. Two groups of algorithms for the pre-processing were studied: 1) classical morphological methods - radial distribution function, distribution of nearest neighbours and covariance; 2) new algorithms based on ideas of the travelling salesman problem and on the distribution of Wigner-Seitz cells. All algorithms were applied to model structures generated by means of the hard-disk model [4].

It was found that the image analysis performed with neural networks allow gaining some information hidden in classical morphological methods. While the new approach is tested on simulated hard-disk models, the results can be applied to the experimentally derived microphotographs of discontinuous and composite metal films. The quality of the performance of the trained networks for real images is a subject of further investigation.

References

1. Serra J., Image Analysis and Mathematical Morphology. Academic Press, London (1982).
2. Judd J. S.: Neural Network Design and Complexity of Leaning. MIT Press, Cambridge MA (1990).
3. Malý M., Hrach R., Novotný D., Vacuum 60 (2001), in print.
4. Hrach R., Novák S., Novotný D., Pavlík J., Thin Solid Films 317 (1998), 39.

Pressure measurements in NVE simulations: The case of lipid bilayers

G.La Penna[1], V.Minicozzi[2,*], S.Morante[2] and G.C.Rossi[3]

[1]*CNR, via De Marini, 6 Genova, Italy*
[2]*Physics Department University of Rome "Tor Vergata" and INFM Unitá di Roma2, Via della Ricerca Scienti£ca, 1 Roma, Italy*
[3]*Physics Department University of Rome "Tor Vergata" and INFN Sez.Roma II, Via della Ricerca Scienti£ca, 1 Roma, Italy*
+39 06 72594554, +39 06 2023507, velia.minicozzi@roma2.infn.it

We discuss how in NVE simulations the evaluation of pressure, which has long been considered a problem because of its wild instantaneous ¤uctuations, can indeed be kept under control, if the "Jackknife" method [1] is used to compute the statistical error affecting *ensemble* averages. We show that it is possible to exploit the dramatic dependence of pressure on force-£eld parameters to accurately tune them to their optimal values. As an example of application of these ideas, we present Molecular Dynamics simulations of three different samples of butane (C_4H_{10}), made up of 256, 512 and 2048 molecules in a cubic box with periodic boundary conditions. Simulations are carried out at room temperature at the experimental density of 0.583 gr/cm^3. In these conditions butane is in its liquid phase [2]. We study the in¤uence of the magnitude of the inter-molecular potential parameters on the pressure and control the impact of the modi£cation of the force-£eld on other thermodynamical quantities (like speci£c heat, latent heat, diffusion coef£cients, etc.). We £nd that, after reproducing the experimental behaviour of the system along the liquid-vapor coexistence curve, even minor changes of the coef£cients of the attractive part of the Lennard-Jones inter-molecular potential give rise to huge variations of the pressure without signi£cantly affecting anyone of the other thermodynamic properties of the system. It is precisely this critical behaviour which can in turn be exploited to tune force-£eld parameters with remarkable accuracy.

We have extended these considerations to the measurement of the stress-tensor, t_{ij}, of a model-membrane simulated as a bilayer composed of 2×32 and 2×256 *Dimyristoyl-methyl-glycerol* (DMMG) molecules in vacuum, in its crystal and gel phases. We have extracted the values of the surface tension, τ, of the bilayer, as function of the temperature, in both phases, using the standard formula $\tau = \langle L_z(\frac{t_{xx}+t_{yy}}{2} - p_z)\rangle$ valid for a system with £xed surface area and ¤uctuating transverse width. Evaluation of statistical errors by the Jacknife method allows a meaningful comparison with experimental and simulation data [3]. Despite the scaring, strong dependence of τ on the details of the inter-molecular potential, we £nd numbers which compare rather well with the expectations for a planar bilayer.

As a £nal remark, we note that all the simulations carried out for the largest of the different volumes of the two physical systems we have discussed here, have been performed with the help of the APE100 parallel platforms.

References

1. B. A. Berg, Comp. Phys. Commun. **69** (1992) 7; B. Efrom, The Jackknife, the Bootstrap and other Resampling Plans, SIAM, Philadelphia (1982)
2. G. La Penna, S. Letardi, V. Minicozzi, S. Morante, G. C. Rossi and G. Salina, sent for publication to European Journal of Physics E
3. R. M. Venable, B. R. Brooks and R. W. Pastor, J. Chem. Phys. **112** (2000) 4822; F. J. Nagle, Ann. Rev. Phys. Chem. **31** (1980) 157

Dynamical system's approach to the busy beaver problem

Etsushi Nameda[1], **Toru Ohira**[2] **and Takashi Ikegami**[1]

[1]*Institute of Physics, Graduate School of Arts and Sciences, University of Tokyo, 3-8-1 Komaba, Meguro, Tokyo 153-8904, Japan.*
[2]*Sony Computer Science Laboratory, 3-14-13 Higashi-gotanda, Shinagawa, Tokyo 141-0022, Japan.*

Tel: +81-3-5448-4379, Fax: +81-3-5448-6535,
E-mail: nameda@sacral.c.u-tokyo.ac.jp

The Busy Beaver problem is one of modi£cations of the Turing machine halting problem, and famous for its easy de£nition. When starting from an all-blanc tape, some machines will halt and some never halt. The Busy Beaver is the machine with a given state size that halts with the longest time. When one makes a function of the beaver's lifetime against its state size, this function turns out to be uncomputable[3]. Since this problem was £rst stated in 1962, many computational studies have performed to search Busy Beavers[1][4]. This paper reports distributions of halting probabilities with a focus on time-space patterns of machine motions.

In the Busy Beaver Problem, the halting probability is phrased as follows: If we run a random Turing machine of a de£ned state size, what is the probability of halting? Also, halting probability was known to be uncomputable[3][2].

Fig.1 shows examples of distributions of halting probabilities. Integrating these functions, we can calculate the halting probabilities of each state size. However, as distributions change smoothly from exponential to power, precise estimation of probabilities gradually become harder.

Distributions of halting probabilities suggest that machines with short lifetime halt at random, but the cause of halting of machines with longer lifetime is not clear. Also, short and long lifetime machines show different trails on a tape. The former shows random motions, but the latter leaves remarkable recursive features that we could classify in 3 types. Fig.2 show the populations of 5-state machine's moving patterns on a tape.

The detailed analysis is yet to be understand. We shall, however, present a relevant analysis in analogy with random walks.

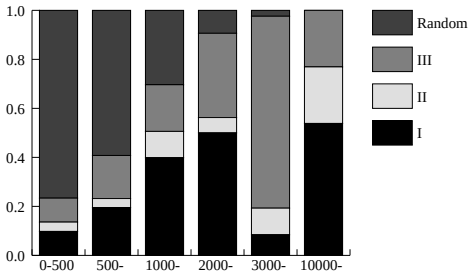


Fig.1 Fig.2

References

1. A. H. Brady, Mathematics of Computation, vol.40, 647 (1983).
2. G. J. Chaitin, Journal of the Association for Computing Machinery, vol.22, no.3, 329 (1975).
3. T. Rado, The Bell System Technical Jounal, vol.41, no.3, 877 (1962).
4. H. Marxen and J. Buntrock, Bulletin of the EATCS, vol.40, 247 (1990).

Characterisation of degree of arrangement in image analysis of complex systems

R. Hrach[1,2], D. Novotný[2], M. Sobotka[1], M. Vicher[1,2] and M. Kostern[1]

[1] *Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, 180 00 Prague 8, Czech Republic*

[2] *Faculty of Education, J. E. Purkyně University, České mládeže 8, 400 96 Ústí nad Labem, Czech Republic*

+420 47 5214417, +420 47 5212053, novotnyd@pf.ujep.cz

In some fields of physics as thin film physics, solid-state physics or in astronomy the systems consisting of a large number of objects are studied. During an image analysis of such complex systems various information can be derived: characteristics describing the whole image, size distribution of individual objects and the spatial distribution of objects. In image analysis in physics one of the most important tasks is the quantitative characterisation of the degree of the objects arrangement as the deviation of the studied system from the equilibrium random state can bring information about internal processes in the system. For the description of spatial distribution of objects in images several standard methods as the radial distribution function or distribution of nearest-neighbours are typically used [1]. However, the exact interpretation of derived morphological characteristics is often very difficult and the sensitivity of these methods differs for various studied systems.

In order to derive the proper interpretation of standard morphological characteristics and to test less known and new algorithms for the quantitative description of the degree of arrangement of objects in images a simple computer experiment was prepared. First, several types of simulated structures corresponding to various types of experimental data in physics were generated. The models were based on the hard-disk approach, on the regular structures with added Gaussian noise and on clustered structures. In all these models a parameter for the generation of various deviations from the equilibrium state was chosen. The degree of randomness of the sets of modelled structures was described by means of a Quadrat Counts method [2].

All generated structures were analysed by six both the well-known and the new algorithms: radial distribution function, distribution of nearest neighbours, covariance, chord-length distribution, Voronoi tessellations and Hartley integral transform - e.g. [3] [4].

The detailed analysis of obtained morphological characteristics of all used methods enabled us to divide tested algorithms into three groups: methods sensitive to small deviations from completely arranged systems, methods sensitive in the whole range of degrees of randomness and methods, the sensitivities of which can be adapted to the studied system. The results of sensitivity analysis of these algorithms are applied to the images of thin metal films grown on dielectric substrates.

References

1. Serra J., Image Analysis and Mathematical Morphology. Academic Press, London (1982).
2. Ripley B. D., Spatial Statistics, John Wiley, New York (1981).
3. Ebeling H, Wiedenmann G., Phys. Rev E 47 (1993), 704.
4. Hrach R., Novotný D., Novák S., Pavlík J., Vacuum 50 (1998), 175.

Stochastic three state model with delay

Naoya Sazuka[1] **and Toru Ohira**[2]

[1] *Department of Computational Intelligence and Systems Science, Interdisciplinary Graduate School of Science and Engineering, Tokyo Institute of Technology 4259 Nagatsuta, Midori-ku, Yokohama 226-8502, Japan*

[2] *Sony Computer Science Laboratory, 3-14-13 Higashi-gotanda, Shinagawa, Tokyo 141-0022, Japan*

Tel:+81-3-5448-4380, Fax:+81-3-5448-4273, E-mail:ohira@csl.sony.co.jp

Noise and time delay are two elements that are associated with many systems leading to complex dynamics. Understanding of such delayed stochastic systems is far from complete [1][2][3].

The main purpose of this paper is to investigate numerically and analytically a simple stochastic model with delay which shows a resonance phenomenon. From the point of view of stochastic resonance, this is a new type and one of the simplest models which is analytically tractable.

We here investigate the model which is a stochastic three state element, whose transition rate depends on its state at a £xed interval τ in the past. The main feature of the model is that much richer dynamical behavior can be obtained compared to the binary model[4]. We observe various rhythms, which are dynamics having some periodicity. Interestingly, as time step grows, the periodicity of rhythms becomes longer than delayed memory. A residence time histogram shows the peak and it can be considered stochastic resonance due to delay as in the case of binary state model.

The strength of this model is the property that the shape of such histograms can be derived analytically. Noting that it consists of statistically independent $\tau + 1$ Markov chains, one can exactly derive the analytical expression for histograms $h(u)$ using only P_i, the probability for the $i - th$ state in the stationary limit and w_{ii}, the transition probability which returns to itself. Further, a general expression extending to N state model can be obtained as well.

$$\begin{aligned} h_i(u) &= (P_i)^u(1-P_i)^2 \quad (1 \le u < \tau), & (1)\\ &= (P_i)^\tau\{(1-P_i) - P_i(1-w_{ii})\} \quad (u = \tau), & (2)\\ &= (P_i)^{\tau+1}(w_{ii})^{u-(\tau+1)}(1-w_{ii})^2 \quad (u > \tau). & (3) \end{aligned}$$

As an application of this model, we have studied yen-dollar currency exchange stochastic time series. We show that with a suitably chosen parameters in the model, some statistical feature of such dynamics can be well captured.

References

1. M.C. Mackey and L. Glass, Science **197**, 287 (1977).
2. J. Milton, A. Longtin, A. Beuter, M. C. Mackey, and L. Glass, J. Theor. Biol. **138**, 129 (1989).
3. T. ohira and T. Yamane, Phys. Rev. E. **61**, 1247 (2000).
4. T. ohira and Y. sato, Phys. Rev. Lett. **82**, 2811 (1999).

Synaptic polarities studied by the recurrent back-propagation

Kazumi Omata, Yuko Osana and Kiyoshi Kawamura

Faculty of Science and Technology, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama 223-8522, Japan

+81-45-563-1141, +81-45-563-1761, omata@rk.phys.keio.ac.jp

The information processing in neural systems has attracted much interests because the systems are regarded as typical complex systems, analogous with physical systems such as spin glasses, or important for application to computer science. While the past studies focused on development of algorithms in artiFcial neural networks, we deal with the neural network of the soil nematode *Caenorhabditis elegans* (*C. elegans*) to clarify the mechanism of the information processing in "real" neural systems. The *C. elegans* neural circuit has several advantages for investigations [1]: (1) all neurons are mapped; (2) the number of neurons is only 302 in an adult hermaphrodite; or (3) the connectivities between the neurons are almost identiFed. The purpose of the present work is to determine the synaptic polarities of the locomotion circuit, where a polarity is either positive or negative depending on whether the signal transmitted through the synapse is excitatory or inhibitory. Even though the polarity is a key factor for the functions of the circuit, the worm is so small (1 millimeter in length) that phsiological experiments cannot yet determine the polarities. The locomotion circuit consists of four classes of sensory neurons (ALM, AVM, PLM and PVM), Fve classes of interneurons (AVA, AVB, PVC, AVD and LUA), and two classes of motoneurons (A and B). These neurons control the locomotion of the worm [2].

Numerical calculations are carried out by use of the recurrent back-propagation algorithm [3]. The procedures are as follows. (1) A set of input signals is imposed on sensory neurons, and the steady-state output signals are measured. (2) For each motoneuron, the error deFned as the difference between the measured output signal and the required signal is calculated, and the errors are propagated reversely through synapses from the motoneurons to the sensory neurons. (3) The above procedures are repeated for several signal patterns until the errors come to be sufFciently small. (4) The set of the values in the synaptic connections, $\{w_{ij}\}$, are determined.

We have investigated 5000 samples, and derived frequency distributions of w_{ij}. For the synapses from the sensory neurons to the interneurons, and those from the interneurons to the motoneurons, the distributions have two peaks at a positive value and a negative value (there are a few exceptions). On the other hand, the distributions for the other synapses have only one peak at $w_{ij} = 0$. From these results, we have found that, when we choose a synaptic connection from a sensory neuron to an interneuron and use it as a Flter, the polarities of the other connections can be determined. For example, when w_{ij} of the connection PLM $\Rightarrow$ PVC is positive, the polarities of PVM $\Rightarrow$ PVC and PVC $\Rightarrow$ B is positive, and those of ALM $\Rightarrow$ PVC, AVM $\Rightarrow$ PVC and PVC $\Rightarrow$ A is negative. This result is consistent with the fact that PLM, PVM and B are neurons for forward movement, and ALM, AVM and A are neurons for backward movement. Although the polarities of the connections among internerons are not determined [4], our study can be developed in this direction and will lend support to future experiments.

References

1. D. L. Riddle, Ed., *C. elegans II* (Cold Spring Harbor Laboratory Press, New York, 1997).
2. M. ChalFe *et al.*, J. Neurosci. **5**, 956 (1985).
3. F. J. Pineda, Phys. Rev. Lett. **59**, 2229 (1987).
4. S. Gomi and Y. Iwasaki, private communication (2000).

On a £nite-dimensional reduction for a class of conservative dynamical systems and its applications

N.K. Prykarpatska, A.K. Prykarpatsky

Dept. of Applied Mathematics at the University of Mining and Metallurgy, Al. Mickiewicz 30, Krakow 30059 Poland

1. Introduction. We shall consider the following class of conservative ¤ows in one dimension:

$$d(u,h)^{\top}/dt = -\vartheta\, grad\, H[u,h] \tag{1.1}$$

where $(u,h) \in M \hookrightarrow H^{(\infty)}(\mathbf{R};\mathbf{R}^2),\ t \in \mathbf{R}$ is an evolution parameter, $\vartheta := antidiag(\partial/\partial x, \partial/\partial x)$ is the implectic operator on a functional manifold M and $H \in D(M)$ is a Hamiltonian function speci£ed properties of a ¤ow under consideration. The ¤ows (1.1) for special Hamiltonian functions are of interest in many applications. Below we will prove that all ¤ows (1.1) possess a uniform scalar Lax type representation

$$dl/dt = [p_H(l), l], \tag{1.2}$$

with the linear scalar differential operator

$$l := h^{-1}\partial/\partial x + u \tag{1.3}$$

in $L_2(\mathbf{R};\mathbf{C})$ and operators $p_H(l) :\ L_2(\mathbf{R};\mathbf{C}) \to L_2(\mathbf{R};\mathbf{C})$, depending only on the Hamiltonian functions $H \in D(M)$. This fact makes it possible evidently to apply modern Lie-algebraic tools [3-5] of treating equations like (1.2) thereby exhibiting their rich hidden internal sructure.

2. Lax type representation analysis and reduction scheme. The following lemma characterizes the ¤ow (1.1).

Lemma. Let $\tilde{l}[u,h;\lambda] : L_2(\mathbf{R};\mathbf{C}) \to L_2(\mathbf{R};\mathbf{C})$ denote the following differential operator

$$\tilde{l}[u,h;\lambda] := \partial/\partial x + (uh) + \lambda h, \tag{2.1}$$

where $\lambda \in \mathbf{C}$ is a spectral parameter. Then for any local functionals $a_H, b_H \in \Lambda^{(0)}(M)$ the dynamical system (1.1) is equivalent to the Lax type representation

$$d\tilde{l}/dt = [\tilde{p}_H(\tilde{l}), \tilde{l}], \tag{2.2}$$

where

$$\tilde{p}_H(\tilde{l}) := b_H + \lambda a_H. \tag{2.3}$$

We consider the £nite-dimensional reduction of the dynamical system (4.1) on the submanifold $M^{(N)} = \{(u,h) \in M :\ grad\mathcal{L}_N[u,h] = 0\}$ of critical points of the following Lagrangian function $\mathcal{L}_N \equiv \int_{x_0}^{x_0+2\pi} \mathcal{L}[u,h]dx = \sum_0^3 c_i H_i, \quad H_3 := H$, where H_i, $i = \overline{0,3}$, the corresponding to (1.1) four invariants, $N \in Z_+$ is an integer depending on the derivative degree of the Lagrangian function. The ¤ow (1.1) on $M^{(N)}$ is £nite dimensional and in some cases completely integrable by Liouville-Arnold procedure. Since the system (3.1) is a natural generalization of the well known Burgers ¤ow possessing both dissipative and soliton like solutions, the corresponding Cauchy data at which solutions are solitonic should be treated via the extended reduction method based on the well known Moser's mapping approach, devised in. This trend of our studying the system (3.1) is performed in detail.

Finite dimensional reductions of conservative dynamical systems and numerical analysis

A. K. Prykarpatsky[1], **N.K. Prykarpatsky**[2]

[1] *Department of Applied Mathematics at AGH, Krakow 30059 Poland*
[1] *Department of Nonlinear Mathematical Analysis of IAPMM of NAS, Lviv 290601 Ukraina*

The problem of £nding an appropriate set of initial conditions for the in£nite-dinensional Liouville-Lax integrable dynamical systems leading to such typical solutions as the travelling waves and solitons has been an important problem for numerical analysis of integrable equations. In this paper, we make an attempt to develop a regular method of £nding various types of initial conditions by employing the method of reductions [1, 2] of the in£nite-dimensional integrable systems on £nite-dimensional invariant submanifold. The reduced set of equations on a submanifold consists of a pair of Hamiltonian systems integrable in the classical Liouville sense. The £rst system is associated with the vector £eld d/dx on the £nite-dimensional submanifold and its solutions de£ne a set of initial conditions for the given in£nite-dimensional integrable equation. The other £nite-dimensional Hamiltonian system corresponds to the vector £eld d/dt on the submanifold and de£nes [3, 4] the time evolution of the initial data due to the dynamics of the in£nite-dimensional system. The phase portrait of the dynamical system corresponding to the vector £eld d/dx provides nesessary information for identifying the initial conditions for the solitons and travelling waves.

The method can be applied for the numerical analysis of not only the Liouville-Lax integrable dynamical systems but also to the conservative nonlinear dynamical systems possessing several conserved quantities.

The paper is organized as follows. We formulate the basic consepts of the method by Bogoyavlensky and Novikov of £nite-dimensional reductions of the Liouville-Lax integrable dynamical systems. These ideas are applied for the numerical study of the KdV equation. The £nite-dimensional reductions of the modi£ed nonlinear Schrödinegr equation (MNS) and the analysis of the corresponding Hamiltonian equations are presented. The applicability of these ideas to one hydrodynamical model possessing four conservative quantities is done in deatil.. We conclude with a discussion of our results and perspectives for the future work.

References

1. Bogoyavlensky O.I. and Novikov S.P. On connection of Hamiltonian formalisms of stationary and non-stationary problems, *Func. Anal. Appl.*, **10** (1976), 9–13. NovikovS.P. (ed.), *Theory of Solitons*, Consultants Bureau, New York - London, 1984.
2. Papageorgiou D., Tilley B. and Samulyak R. Potential ¤ow instabilities in a thin ¤uid sheet, *SIAM J. Appl. Math.* (submitted for publication).
3. Prykarpatsky A.K. and Mykytiuk I.V. *Algebraic Integrablity of Nonlinear Dynamical Systems on Manifolds*, Kluwer, Dordrecht, 1998.
4. Prykarpatsky A.K., Blackmore D.L., Strampp W., Sydorenko Yu. and Samulyak R., Some remarks on Lagrangian and Hamiltonian formalisms related to in£nite dimensional dynamical systems with symmetries, *Condensed Matter Phys.*, **6** (1995), 79–104.

A study on the form factors kernel function

Eric Zéghers and Christophe Renaud.

LLAIC : Laboratoire de Logique, Algorithmique et Informatique de Clermont-Ferrand 1

LIL : Laboratoire d'Informatique du Littoral

zeghers@iut.u-clermont1.fr, renaud@lil.univ-littoral.fr

Energy exchanges between object surfaces are characterized by geometrical quantities known as view factors or form factors. Computing these form factors is often the hearth of a lot of application code, both in terms of quality (a high accuracy is required for correctly taking into account energy exchanges) and in terms of quantity (their estimate generates a very high computationnal cost). A lot of domains are interested in computing those form factors, such heat transfer, lighting simulation , meteorology, remote sensing or plants growing simulation.

Previous researches about form factors estimate have been performed through the heat transfer theory. Due to the high complexity of their formula (double area integral), catalogs [1] have been proposed which list analytical expressions for some particular geometrical shapes. Form factors estimate for more complex problems are then generally extrapolated from those simplest environments. More recently researches have been performed in the £eld of computers graphics where form factors have to be computed for 3D scene illumination. Many speci£c form factors computation algorithms have been proposed (hemicube, hemiplane, disk-to-point ray tracing, Monte Carlo, etc) [2] providing an extended survey about these techniques. However all those methods suffer from a lack of accuracy when surfaces are closed from each other because of the inconstancy of their estimate. Furthermore their use sampling approaches for computing the form factors between distant surfaces, those approaches being prone to unaccuracy. Recent work [3] has provided a general analytical formula for the form factor computation between any two planar polygons. But this formula requires still to approximate some computation ans has a very high computationnal cost. Then it has not been designed to take into account partial visibility between the two polygons.

The study we present in this paper is centered about the characterization of the form factors kernel function. According to some distance criteria we have proved that this kernel function has a unique maximum and we are able to £nd it. Then it becomes possible to study and characterize some important parameters of this function : the relative orientation of the two polygons and their distance and the general form of the function. According to those results we compute the form factors between any two polygons by distinguishing the areas where the kernel has a smooth variation from the areas where it changes quickly. A £ne integration is thus performed for the more varying parts of the kernel whereas the other parts are computed more easily.

The accuracy of our approach is very closed to the results provided by the estimate of the analytical formula described in [3] but with a linear computation time speedup from 8 to 10. Furthermore the estimate error is always stable even for very closed polygons. Note that this stability is not ensured by any classical approache. An other interesting advantage of our approach is that it allows us to enclose the error obtained on the resulting energy exchanges. Finally it extends easily to partially occluded polygons with a low additionnal cost.

References

1. J. Howell. A catalog of radiation con£guration factors. McGraw-Hill, 1982
2. M. Cohen and J. Wallace. Radiosity and realistic image synthesis. Academic Press, 1993
3. P. Schroder and P. Hanrahan. On the form factor between two polygons. Proc. of SIGGRAPH 93, 1993

Least squares £tting of a polynomial of degree two to a set of data points

C.V.Sheth
Physics Department,
University of Zambia,
P.O.Box 32379, Lusaka, Zambia.
e-mail: csheth@natsci.unza.zm

Regression analysis is used extensively in astronomical research. The data often consists of pairs of observations, each member of the pair having random observational errors. The problem of £tting a function, usually a straight line $y = a + bx$ to a set of data which have errors in both coordinates x and y has been treated by a number of researchers , the list is too big and we refer to a sample of papers[1−3,7]. There have been some attempts in developing an algorithm for £tting the data to higher degree polynomials than the straight line[4−7].

We have considered problem of £tting the data to a polynomial of the form

$$y = a_0 + a_1 x + a_2 x^2$$
$$= \sum_{k=0}^{2} a_k X_k$$

where errors are present in both the coordinates, σ_{xi}^2 in x_i and σ_{yi}^2 in y_i for $i = 1....N$. Here N the number of data points.

To a £rst order approximation, we propose a maximum likelihood method with the function

$$\chi^2 = \sum_{i=1}^{N} \frac{(\ y_i \ - \sum_{k=0}^{2} a_k X_k \ )^2}{\sigma_{yi}^2 \ + \ a_1 \ \sigma_{xi}^2}$$

which is minimized w.r.t. the parameters a_k.

An algorithm to minimize χ^2 w.r.t. parameters a_k is given and hence the calculation of the parameters a_k. The algorithm is tested with data used earlier by previous researchers.The source code is available in Fortran-90. The calculations are compared with the existing methods[4−7]. The results are presented.

References

1. P.H.Borcherds and C.V.Sheth, Eur.J.Phys.16,204(1995).
2. C.V.Sheth,A.Ngwengwe and P.H.Borcherds, Eur.J.Phys.17,322(1996).
3. M.G.Akritas and M.A.Bershady, APJ 470,706(1996)
4. P.L.Jolivette,Computers in Phys. 7,208(1993).
5. M.O'Neill,I.G.Sinclair and F.J.Smith, Comput.J.12,52(1969).
6. M.Clutton-Brock, Technometrics 9,261(1967).
7. W.H.Press,B.P.Flannery,S.A.Tenkolsky and W.T.Vetterling, 'Numerical Recipes', (Cambridge U.P., Cambridge, N.Y.1986).

Pattern analysis for packing cells of wings of Pterygota

Mitsuhiro Seino[1]**, Yoshitaka Kakazu**[2] **and Dai Aoki**[3]

Faculty of Science, University of the Ryukyus, Okinawa 903-0129, japan

fwkh8023@mb.infoweb.ne.jp[1]*, akkun@cosmos.ne.jp*[2]*, cae05461@pop16.odn.ne.jp*[3]

Observing wing of Pterygota, we can watch hierarchical mode for the network formed by vein and cell. Its pattern formation is supposed to include fractal property. We note the polygonal cell in the cell pattern of the wing to measure for Odonata and Orthoptera. The cells are classi£ed into 6 or 7 kind of polygons, it is found that a great number of the pentagonal cells are distributed in all regions of wing. Then, its cell pattern is similar to voronoi polyhedron that is controlled coordinate of generatrices[1]. We assume that displacement of generatrices cause variation of the cells in an eclosion.

We note polygonal cell in the cell pattern of the wing to measure for Odonata.The means area distributions of polygonal cells are shown. According as the number of side increases, the means area of polygonal cells increase monotonously. The area frequency distributions are shown and those are similar to the generalized gamma distributions. As to *Crocothemis servilia*, *Orthetrum triangulare* and *Pantala ¤avesecens*, the values of correlation coef£cient between fore and hind wings of the area frequency distribution are determined as 0.95, 0.97 and 0.93, respectively.

We compare the cell pattern with the wing pattern that is reconstituted by voronoi tessellation and its voronoi diagrams are examined. For divided region of vein patterns with *Pantala ¤avescens*, deviation Δ from Voronoi Polyhedrons[2] for the fore and hind wing are determined as $0.46\sim0.61$ and $0.44\sim0.55$, respectively. The distance frequency distributions between neighboring Voronoi polyhedrons are shown and those are similar to the generalized gamma distributions. As to *Crocothemis servilia* and *Pantala ¤avesecens*, the value of correlation coef£cient between fore and hind wings of the distance frequency distributions between neighboring Voronoi polyhedrons are determined as 0.98 and 0.97, respectively.

References

1. M. Seino and Y. Kakazu, *Prog. Theor. Phys. Suppl.*, **138** (2000), 600.
2. H.Honda, *Intern. Rev.Cytol.*, **81** (1983), 191.

A model of urban mobility

A. Bazzani[1], **B. Giorgini**[1], **G. Servizi**[1] **and G. Turchetti**[1]

[1]*Dipartimento di Fisica – Universitá di Bologna*

+39 0512091004, +39 051247244, giorgini@bo.infn.it

In this communication we model the urban mobility[1] as a network of streets on which the individuals/citizens move randomly[2]. Moreover we include a deterministic public transportation[3] network and a set of chronotopoi which interact with the citizens, producing a biased diffusive motion similar to that of a gas in an external potential with several equilibrium states. The model is implemented as a computer code written in C++ object oriented programming language. In the absence of chronotopoi the mean £eld solutions have been computed and the analytical results are in good agreement with simulations[4].

References

1. B. Hutchinson, M. Batty eds: Advances in Urban Systems Modelling, North Holland, Amsterdam (1986).
2. E. Besussi, A. Cecchini eds.: Arti£cial World and Urban Studies, DAEST - Venezia, Italy (1996)
3. E. Cascetta, G. E. Cantarella: Modelling Dynamics in Transportation Networks: State of the Art and Future Developments, Journal of Simulation Practice and Theory I (1993)
4. A. Bazzani, B. Giorgini, G. Servizi, G. Turchetti: A computer implemented chronotopic model of mobility in urban spaces – preprint.

Application of parallel computations for the modelling of electromagnetic waves propagation in an anisotropic layer

N.M.Sharkova[1] **and I.V.Andronov**[1]

[1]*Dept. of Computational Physics, St.Petersburg University,*
1/1, Ulianovskaya Str., 198904 St.Petersburg, Russia
+7 (812) 4284343, +7 (812) 4287240, shark@mph.phys.spbu.ru

The novel technologies allow electromagnetic coatings with prescribed properties to be produced. In particular, such coatings may be anisotropic. The properties of electromagnetic £elds in such coatings is of interest in radio science. In some cases explicit formulae for the electromagnetic £eld in the form of Fourier or Fourier-Bessel integrals can be constructed. However due to complexity of the media these representations are cumbersome and dif£cult for the analysis [1].

In the presented paper the stationary moderate frequency electromagnetic £eld of a point dipole source in an anisotropic layer is computed. The distribution of the £eld in the near and far zones is described by asymptotic formulae. In the intermediate zone the £eld is represented in the form of Fourier-Bessel integral [2] (cylindrical coordinates ρ, ϕ, z are used)

$$\int_0^\infty H_0^{(1)}(\tau r) F(\tau, z) d\tau.$$

The function $F(\tau, z)$ has poles corresponding to waveguide modes in the layer. Some of these poles are on the real axis of τ and are avoided according to the limiting absorption principle. Two dif£culties appear when computing the above integral. The £rst problem is in the insuf£cient accuracy because of rapid oscillations of the integrated function. This problem is solved by means of appropriate deformation of the integration path into the complex plane of parameter τ. When performing this deformation the poles of function $F(\tau, z)$ may be crossed and the corresponding contributions of the residues are computed. That is careful numerical analysis of the function $F(\tau, z)$ in the complex domain of τ is required. The search of the poles is complicated by the indented character of the level curves of function $|F|$.

The following algorithms are used: 1. Modi£ed Newton iterations for the search of the poles. 2. Special quadrature formulae: a) near singularity of the function $H_0^{(1)}$, b) near the stationary phase points, c) near square root singularity of function $F(\tau, z)$.

The other problem is in the necessity to reduce the time of computations. Electromagnetic £elds are represented in the form of similar type integrals. This allows the code of the program to be parallelized on different hosts. The use of High Performance Fortan (HPF) directives [3] makes the. code easily portable. The achieved acceleration is almost proportional to the number of processors.

The developed algorithm allows generalization to the case of multiple layers in the coating and to more general cases of anisotropy.

References

1. L.B.Felsen, N.Marcuvitz *Radiation and Scattering of Waves* Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1973.
2. G.A.Korn, T.M.Korn *Mathematical Handbook for Scientists and Engineers*, McGraw-Hill Book Company, Inc., New York Toronto London, 1961.
3. Library of HPF at `http://www.psu.edu/dept/`

Energetics ef£ciency in homogeneous forced ratchets

T. Sintes[1] **and K. Sumithra**[2]

[1] *Dept. Fisica, Universitat de les Illes Balears, E-07071 Palma de Mallorca, Spain*
[2] *FG Theoretische Physik, FB Physik, Martin Luther Universitaet, D-06099 Halle-Wittenberg, Germany*

Phone: 971 17-2537, Fax: -3426, email: tomas@imedea.uib.es

Much of the recent interest in non-equilibrium induced transport processes is concentrated on stochastically driven ratchets. The development of this subject has been motivated by the challenge to explain unidirectional transport in biological systems. The novel synthesis of molecular devices, including molecules able to produce unidirectional rotary motion, has already been reported [1], and a clear understanding of the energetics of spatially homogeneous systems is required to de£ne optimal ratchet models. Kamegawa *et al.* [2], following the arguments developed by Sekimoto [3], formulated the energetics of the forced thermal ratchet concluding that the presence of thermal ¤uctuations cannot increase the ef£ciency of the energy transformation. This result was in contradiction with the claim made by Magnasco [4] and the later £ndings of Dan and coworkers [5] on inhomogeneous rocked systems with spatially varying friction coef£cient, that there is a region of the operating regime where the ef£ciency is optimized at a £nite temperature.

A forced thermal ratchet is described by the Langevin equation:

$$\dot{x} = -\partial_x V(x) + F(t) + \sqrt{2k_B T}\,\xi(t), \tag{1}$$

where $V(x)$ is the ratchet potential including an external load against global motion, and $F(t)$ an external ¤uctuating driving force. It is known that both the current and the ef£ciency do not admit analytical solutions for a general forcing and arbitrary potential. It is also known that the associated Fokker-Planck equation, under the assumption of the probability density to be periodic in time and space $P(x,t) = P(x+L,t) = P(x,t+\tau)$, can be analytically solved for a constant external driving force [4]. If we think with a slow forcing $F(t)$ compared to any other frequency in the problem, the average current can be de£ned by $J = \frac{1}{\tau}\int_0^\tau j(x,t)dt$, being $j(x,t)$ the probability current.The latter result was used by Kamegawa *et al.* to treat the case of a ¤uctuating $F(t)$ of square wave form of amplitude A and period τ.

By numerical integrating of the Langevin equation, we have computed the average current and ef£ciency of an overdamped Brownian particle moving in an asymmetric potential and subject to an external driving force. We found that there is a regime where the ef£ciency can be optimized at £nite temperatures, contradicting the results of Kamegawa *et al.*. This, in fact, proves that thermal ¤uctuations contribute to the ef£ciency. We also found the conditions for achieving maximum ¤ux and ef£ciency are different as claimed in previous investigations. The in¤uence of these quantities on the period of the external driving force is discussed and we show that the theoretical results are valid only in the limiting case of $\tau \to \infty$.

References

1. T. R. Kelly, H. De Silva, and R. A. Silva. Nature **401**, 150 (1999).
2. H. Kamegawa, T. Hondou, and F. Takagi. Phys. Rev. Lett.**80**, 5251 (1998).
3. K. Sekimoto. J. Phys. Soc. Japan, **66**, 1234 (1997).
4. M. O. Magnasco. Phys. Rev. Lett. **71**, 1477 (1993).
5. D. Dan, M. C. Mahato, and A. M. Jayannavar. Phys. Rev. E, **60**, 6421 (1999).

Networked virtual reality space for analyzing numerical simulation result

Yuichi Tamura, Akira Kageyama and Tetsuya Sato

Theory and Computer Simulation Center,
National Institute for Fusion Science,
322-6 Oroshi-cho, Toki, Gifu 509-5292, Japan

telephone number: +81-572-58-2357, fax number: +81-572-58-2626,
e-mail address: tamura@tcsc.nifs.ac.jp

One of the most practical bene£ts of utilizing a virtual reality system in science is to make it possible to percept a really tangled complex phenomenon in an intuitive way. We have developed a virtual reality system called “CompleXcope”. This CompleXcope is designed so that not only three-dimensional objects but also an auditory environment can be represented.

The CompleXcope is a projection-based VR system based on CAVE system [1] that is developed at Electronic Visualization Laboratory, University of Illinois at Chicago. This system has four screens whose size is 10 feet x 10feet. The screens are set up in a cube made of three rear-projection screens for walls and a down-projection screen for the ¤oor. This virtual reality system also has 3D-sound system. The 3D-sound system [2] is very powerful tool to represent more complex numerical simulation result.

This virtual reality system is very useful to represent and analyze complex physical simulation result. But it is dif£cult to communicate with other researchers about simulation results, since this system is very large and not portable. So it is very important issue to construct a multilateral communication network system where any researcher in any remote site (virtual reality space) can equally observe simulation result from any point, take an initiative action in controlling the display of the image in virtual space and the control is transmitted simultaneously to all sites. By this realization, collaboration among different sites becomes practical and realistic. The second issue is dif£culty of controlling the virtual objects (represented simulation data) with general input device. A voice control is very suitable to control in a virtual reality space.

In this study, we developed networked virtual reality system and speech recognition system to control virtual objects.

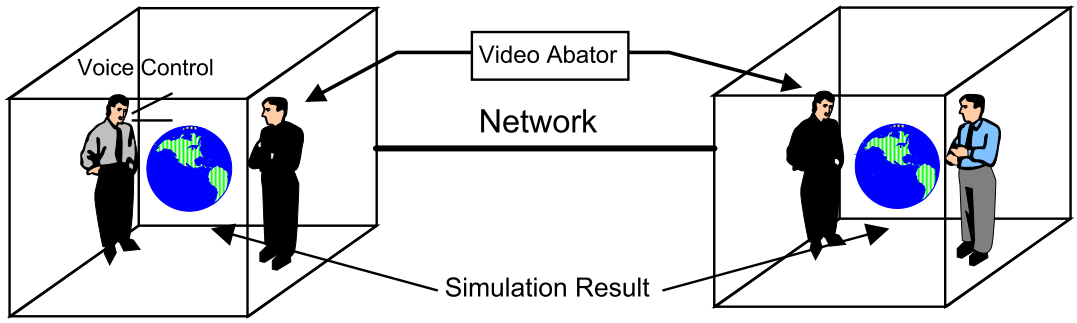


Fig. 1. Networked Virtual Reality Space

References

1. C.Cruz-Neira, D.J.Sandin, and T.A.DeFanti, Proc. of SIGGRAPH ’93 Comp. Graphics Conf. pp135(1993).
2. Y.Tamura, et.al, Proc. of CCP2000 (2001) in print.

Dynamical behavior of individual agents in Hogg-Huberman model

Masayoshi Inoue[1], **Toshijiro Tanaka**[2]
and Junko Shibata[2]

[1]*Department of Physics, Kagoshima University, Kagoshima 890-0084, Japan*
[2]*Department Information Science, Hiroshima Prefectural University Shobara, Hiroshima 727-0023, Japan*

81-8247-4-1736, tanaka@bus.hiroshima-pu.ac.jp

Recently, there has been done much efforts to study the dynamics of multi-agent systems. The dynamical resource allocation is an interesting subject in this £eld. In case of two resources, Hogg and Huberman [1] considered the dynamics of systems composed of interacting agents making decisions based on imperfect and delayed information. They proposed a reward mechanism to stabilize chaotic behavior of multi-agent systems. Ushio and Inamori [2] have extended this agent model to the case of a discrete time. In this paper we study the dynamical behavior of an individual agents in the discrete time Hogg-Huberman model. The probability $p(k+1)$ that an agent utilizes resource 1 at discrete time $(k+1)$ is assumed to be

$$p(k+1) = f_1(k) + \alpha\{\rho_1(k) - f_1(k)\}, \tag{1}$$

where $f_1(k)$ is the fraction of agents using resource 1 and is given by $f_1(k) = N_1(k)/N$. Here $N_1(k)$ is number of agents using resource 1 and N is total number of agents, and α denotes the ratio of agents reevaluating the choice of resources to all agents. The probability that agents will prefer resource 1 to resource 2 is expressed by

$$\rho_1(k) = \frac{1}{2}\left[1 + erf\left(\frac{G_1(f_1(k-\tau)) - G_2(f_2(k-\tau))}{\sqrt{2}\sigma}\right)\right], \tag{2}$$

where $erf(x)$ is error function, and σ is the uncertainty of information and τ is a time delay of information. The payoff functions are given by $G_1(f_1) = 4+7f_1-(16/3)f_1^2$ and $G_2(f_2) = 7-3f_2$. Eqs.(1) and (2) describe the dynamics of our system. Then we discuss effects of tiredness on the dynamical behavior of individual agents. We introduce "a Rule for Alternation of Resource Use" as follows; if an agent utilizes successively one of resources for a while, it must use unconditionally another resource after that time. We de£ne a parameter M_r as the number of times, which an agent is fed up with use of resource r $(r = 1, 2)$. We perform numerical simulations for this system. When there is a strong tiredness of agents described by $M_1 = 1, M_2 = 2$, the chaotic behavior of f_1 is suppressed. As the parameter values become larger in the system ($M_1 = 10, M_2 = 10$), it is seen that the behavior of individual agents is almost same as that of the conventional agent system without the tiredness effect. Finally, we conclude that the tiredness effect of individual agents can freeze out the chaotic behavior in the system.

References

1. T. Hogg and B. A. Huberman, IEEE Transaction on Systems, Man, and Cybernetics, Vol.21, No.6 (1991) 1325.
2. T. Ushio and T. Inamori, Proc. 36th IEEE CDC, San Diego, CA, (1997) 389.

Quantum spectral properties of a spin-1/2 particle in coupled quartic oscillator potential

Mitsuyoshi Tomiya[1] **and Naotaka Yoshinaga**[2]

[1]*Department of Applied Physics, Faculty of Engineering, Seikei University, Kichijyoji-Kitamachi 3-3-1, Musashinoshi, Tokyo 180-8633, Japan*
[2]*Department of Physics, Faculty of Science, Saitama University, Shimo-okubo 255, Urawashi, Saitama 338-0825, Japan*
tel +81-422-37-3787, fax +81-422-37-3871, tomiya@apm.seikei.ac.jp, yoshinaga@chaology.apt.seikei.ac.jp

The quantum spectral statistical properties, i.e. the nearest neighbor level spacing distribution(NNSD), the spectral rigidity etc. of a spin-1/2 particle in three-dimensional coupled quaritic oscillator potential are numerically studied. The Hamiltonian that we choose is

$$\begin{aligned} H = \frac{1}{2}\left(p_x^2 + p_y^2 + p_z^2\right) &+ x^4 + \frac{1}{2}y^4 + \frac{1}{10}z^4 \\ &+ 12x^2y^2 + 14x^2z^2 + 16y^2z^2 + r^2 z\left(ax + by\right) + crL \cdot S. \end{aligned} \tag{1}$$

where $r = \left(x^2 + y^2 + z^2\right)^{1/2}$, L and S represent angular momentum and spin operators. Note that we set dimensionless units: $\hbar = m = 1$, where m is the mass of the particle in the system. Changing coupling parameters: a, b and c, the system is continuously transformed from an integrable to chaotic ones. In the chaotic regime, selecting non-zero parameters, various kinds of ensembles: GOE, GUE and GSE can be achieved [1]. Especially the mode ¤uctuation distribution(MSD), the interpolation formulae of the Poissonian and the Wigner distribution for the NNSD and the alternate level spacing distribution(ASD), which is obtained by picking out every second level, are carefully investigated.

In order to have reliable statistics of quantum levels, it is necessary to evaluate thousands of energy levels from the ground state without missing. We compute the quantum energy levels by numerical diagonalization of the truncated matrix of the Hamiltonian(1) in the basis of harmonic oscillators. If there is no spin-orbit interaction term in (1), the calculation would be able to start with the system of the superposition of three truncated harmonic oscillators [2] [3]. In this work, however, the method has been developed to work with the spherical Bessel functions and the surface harmonics.

It is found that the MFD is more sensitive to the integrability of the system than the chaoticity. In spite of the lack of the physical meaning, the Brody distribution and its variation that we proposed work more properly as the interpolation formula than other distributions with some physical meanings. It is interesting that the ASD of GOE system becomes indistinguishable from the NNSD of GSE rather than the ASD that is made from the Wigner distribution [4]. The ASD can be also the useful interpolation formula as the Brody distribution is.

References

1. E. Caurier and B. Grammaticos, Phys. Lett. **A136** 387(1989).
2. M. Tomiya and N. Yoshinaga, Phys. Rev. **E58** 8017(1998).
3. M. Tomiya and N. Yoshinaga, J. Phys. Soc. Jpn. **69** 2786(2000).
4. M. L. Mehta, *Random Matrices, 2nd ed.* Academic Press, San Diego, 1991.

Optical soliton propagation in coupled systems with random perturbations

B.A.Umarov

Physical-Technical Institute of Uzbek Academy of Sciences, G. Mavlyanov Str. 2-b,
700084 Tashkent-84, Uzbekistan
umarov@physic.uzsci.net

Random imperfections introduced in the manufacturing process of optical waveguide, while they can be small, can create signi£cant effects in a £ber over long propagation distances. And, in fact, understanding the effects of uncertainty in £ber properties on light propagation has become crucial to the design of high capacity/low failure systems[1]. Our work in this direction entails the study of one particularly relevant and characteristic manifestation of random imperfections, namely those associated with the effect of index variations on stability of vector solitons. We tackle this problem through the implementation of perturbative method for Manakov system. The relevant equations, in dimensionless units read as [2]

$$iU_z + \frac{1}{2}U_{tt} + (|U|^2 + |V|^2)U = R_U, \tag{1}$$

$$iV_z + \frac{1}{2}V_{tt} + (|V|^2 + |U|^2)V = R_V. \tag{2}$$

Here U and V represent the complex envelopes of the two orthogonal polarization's of a transverse electromagnetic £eld in a cubic nonlinear medium, and R_U and R_V represent the random perturbation terms, which are assumed to be relatively small. Whenever $R_U = R_V = 0$, there are one soliton solution of Eqs.(1) and(2) [2]. The particular model which have been studied, is that of a vector soliton propagating in a weak disordered potential made up of many randomly placed copies of a basic scatterer, i.e.

$R_U = \varepsilon \sum_i \gamma_i \Psi(t - t_i)U, R_V = \varepsilon \sum_i \gamma_i \Psi(t - t_i)V$

where the locations t_i and the strengths γ_i are chosen randomly. This model was £rst studied in the work [3] for scalar NSE solitons. We propose the following way to consider the problem. Assuming that the scatterers are weak it is possible to use perturbation theory [4] to calculate the scattering of a soliton. This gives an expression for the parameters of the transmitted soliton in terms of the parameters of the incident soliton. Then, under the assumption that the average distance between scatterers is much greater than a soliton width, it is possible to derive the discrete dynamical system which relate the soliton parameters after nth scattering event to the soliton parameters after the $(n+1)$th scattering event. Taking the continuum limit of this system leads a set of ordinary differential equations for evolution of soliton parameters as a function of the number of scattering events. Analysis of these equations give the £nal state of soliton parameters after many scattering events. To verify the approximate theoretical results we perform extensive numerical experiments. When kinetic energy of the soliton is comparable to the height of the potential there arises the possibility of new phenomena, including capture of and total re¤ection of a soliton. We have observed similar phenomena in numerical simulations.

References

1. F.Kh.Abdullaev, B.A.Umarov, M.R.B.Wahiddin, D.V.Navotny, JOSA B, **17**, (2000) 1117
2. S.V.Manakov, Zh.Eksp.Teor.Fiz. **65**,(1973) 505 [Sov. Phys. JETP,**38**, 248, (1974)].
3. Yu.S.Kivshar, S.A.Gredeskul, A.Sanchez, L.Vazquez, Phys.Rev.Lett. **64** (15) (1990), 1693.
4. M.Midrio, S.Wabnitz, P.Franco, Phys.Rev.E **54**, (1996) 5743.

Modi£ed oscillator J-matrix method for scattering

W. Vanroose, J. Broeckhove, F. Arickx

Departement Wiskunde-informatica, Universiteit Antwerpen
Groenenborgerlaan 171, 2020 Antwerpen, Belgium
vanroose@ruca.ua.ac.be

The time-independent quantum scattering problem [1] consists in solving the radial Schrödinger equation, with kinetic energy T and potential V, at energy E and angular momentum l:

$$\begin{cases} (T+V)\psi = E\psi, & E = k^2/2m \\ \psi(r\to\infty) \to j_l(kr) + \tan\delta_l(k)\, n_l(kr). \end{cases} \tag{1}$$

The boundary condition requires the solution to behave asymptotically as a combination of the free-space j_l (Bessel) and n_l (Neumann) functions. The determination of the phaseshift $\delta_l(k)$ is the objective of the scattering calculation.

The J-matrix method [2] converts (1) by representing the solution in a harmonic or hydrogenic basis $\{\phi_{nl}\}_{n\epsilon I\!N}$

$$\begin{cases} \sum_{n=0}^{\infty} \langle\phi_{ml}|T+V|\phi_{nl}\rangle c_{nl} = E c_{ml} \\ c_{n\to\infty,l} \to c^j_{nl}(k) + \tan\delta_l(k) c^n_{nl} \end{cases} \tag{2}$$

The kinetic energy matrix has Jacobi-structure, i.e. is tri-diagonal, and the asymptotic boundary coef£cients can be determined in closed form [2]. Truncating the potential matrix to £nite dimension N allows one to solve the $N+1$ equations for the unknowns $(c_{0l}, c_{1l}, \ldots, c_{N-1l}, \tan\delta_l)$. We only consider the case of the oscillator basis.

The problem with this method is that full convergence often requires large dimension N of the matrix V. Calculation of the matrixelements contributes heavily to the cost of the method, making it scale as N^2.

We address this problem by introducing asymptotic approximations for the large n matrix elements, e.g. for the wavefunction

$$\langle\phi_{n\to\infty,l}|\psi_l\rangle \to \sqrt{2}b\sqrt{R_{nl}}\psi_l(R_{nl}) + (-1)^n\sqrt{2}b^{-1}\sqrt{K_{nl}}\tilde{\psi}_l(K_{nl}), \tag{3}$$

where $\tilde{\psi}_l$ is the Fourier transform, b the oscillator length and R_{nl} and K_{nl} the classical oscillator turning point in real and Fourier space. A similar approximation holds for the potential. Such approximations are derived from the strong oscillatory behaviour of the ϕ_{nl} as $n\to\infty$ [3]. The effect of the potential at large n can then be absorbed in the tri-diagonal structure of the matrix. The result is a matrix that is full at small n and tri-diagonal at large n. We solve (2) in a two-step procedure: the tri-diagonal matrix is solved as a three-term recurrence relation and matched to the remaining linear system. Thus only a £xed, small potential matrix needs to be calculated.

The result is a signi£cant speedup of the convergence in the modi£ed oscillator J-matrix method, which now scales linearly with N. A number of examples, both from molecular and nuclear scattering will be discussed.

References

1. H. Haken and H. C. Wolf, *Atomic and Quantum Physics*, Springer (1987).
2. E. J. Heller and H. A. Yamani, Phys. Rev. A, **9** 1201 (1974).
3. A. Erdélyi, *Asymptotic Expansions*, Dover New York (1956).

A numeric investigation of a vehicular traf£c ¤ow model based on a stochastic acceleration process

K. T. Waldeer

Department of Transportation and Traf£c, University of Applied Sciences
Braunschweig/Wolfenbüttel, Karl-Scharfenberg-Str.55, D-38229 Salzgitter, Germany
+49-5341-875-286, +49-5341-875-420, Th.Waldeer@fh-wolfenbuettel.de

The increasing traf£c density on roads in the last decades together with measurements showing characteristic ¤ow features, i.e. the fundamental diagram, induced a wide spread of theoretical models. Similar to physics these are roughly classi£ed as microscopic, mesoscopic and macroscopic. Where microscopic models are based on single car behavior using computer simulations analogous to molecular dynamics or particle hopping, macroscopic ¤ow models construct time development equations for the car density, mean velocity, etc. following the ideas of continuum mechanics. Between both mesoscopic models focus in the construction of equations for state probability functions of single cars or car clusters which are often of Boltzmann or Enskog type. Models based on single car states are called kinetic because the state is given by spatial and positive valued velocity coordinates. Like in gas kinetic theory the interaction is assumed to be a jump process in the velocity variable [1].

The mesoscopic model introduced here extends the state space by adding the acceleration variable because driver behavior controls the local ¤ow by changing the acceleration only. The durance of such a change is much shorter than any other kinematic timescale of the process. Therefore approximating the process by acceleration jumps seems to be applicable even at higher car densities. Assuming that the *leading* car pair distribution follows a Markov process, introducing a special vehicular chaos ansatz in single lane traf£c without overtaking, an Enskog like master equation for the single car state probability density is found. Details are shown in [2].

The standard test system of traf£c ¤ow models is a ring-road without any entrance or exit and a £xed number of vehicles on it. Here the behavior of the characteristic ¤ow variables in stochastic equilibrium (i.e. the fundamental diagram) are of special interest. Because this system is spatial symmetric, a homogeneous solution must exist. In this case the model equation simpli£es to a Boltzmann type equation which is only solvable analytically for academic interaction cases. It is widely accepted that in reality driver interaction behavior is threshold oriented. For the analysis presented here a distance threshold interaction is adopted from another kinetic model [3].

The numerical solution is done by using a modi£ed Nanbu direct simulation Monte Carlo algorithm from gas dynamics with step size control to the homogeneous case. For all calculations a commercial PC was used coding in FORTRAN 95 [4].

The resulting velocity and acceleration distributions as well as their mean values, variances and correlations together with their dependencies are discussed. They are found to be in good agreement with other models or measurements.

References

1. W. Leutzbach, Introduction to the Theory of Traf£c Flow, Springer Berlin Heidelberg 1988
2. K. T. Waldeer, A Vehicular Traf£c Flow Model based on a Stochastic Acceleration Process, submitted to Transp. Theory Stat. Phys. (2000)
3. A. Klar and R. D. Kühne and R. Wegener, Mathematical Models for Vehicular Traf£c, Surv. Math. Ind. **6**:(1996) 215
4. K. Nanbu, Direct Simulation Scheme Derived from the Boltzmann Equation, J. Phys. Soc. Japan **49**:(1980) 2042

Rotating dielectric sphere near a substrate interface

Jones T. K. Wan[1], G. Q. Gu[1,2] and K. W. Yu[1]

[1]*Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, China*
[2]*School of Computer Engineering, The University of Shanghai for Science and Technology, Shanghai, 200 093 China*

phone:(852) 2609 6339, fax:(852) 2603 5204, email: tkwan@phy.cuhk.edu.hk

The prediction of the strength of the electrorheological (ER) effect is a long-standing goal to achieve because of the implication of ER ¤uids in technological applications [1]. In deriving the induced interactions between polarized particles in ER ¤uids, existing theories assume that the particles are at rest. In realistic situations, the ¤uid ¤ow exerts force and torque on the particles, setting the particles in both translational and rotational motions. To gain some insight into the phenomenon, we have recently proposed a model, which describes the relaxation of polarization charges on the surface of a uniformly rotating particle [2]. We showed the rotational motion of the particles reduces the induced forces between the particles. In this work, we further consider a rotating spherical particle placed in front of a substrate interface. Again, the rotational motion leads to a redistribution of the polarization charge on the surface of the particle and hence changes the force between the particles and the substrate.

For a rotating dielectric sphere in an electric £eld, the rotational motion leads to a displacement of its polarization charges on the surface of sphere. As a result, there is a change of the dipole moment, described by $\vec{\omega} \times \vec{p}$, where $\vec{\omega}$ is the angular velocity and $\vec{p}$ is the dipole moment of the rotating sphere. The surface charges also suffer from relaxation of various kinds, and the rate of change of the dipole moment is described by $-(\vec{p} - \vec{p}_0)/\tau$, where τ is a relaxation time. The two effects have to be balanced against each other, resulting in a steady state dipole moment, which deviates from the equilibrium one $\vec{p}_0$. The deviation depends on the angular velocity of the particle. The interaction force is due to the mutual polarization between the particle and the substrate interface. The total polarization of the particle and the interface is calculated by a multiple images formula [3], which has been shown to be accurate by our integral formalism [4].

We show that the rotational motion of the particles generally reduces the force. The dependence of force on the angular velocity of rotation will be investigated. We will discuss the case of uniform rotation but the extension to a sinusoidal oscillatory shear motion is straight forward.

References

1. P. P. Phule and J. M. Ginder, MRS Bulletin, **23**, 19 (1998).
2. Jones T. K. Wan, K. W. Yu and G. Q. Gu, Phys. Rev. E **62**, 6846 (2000).
3. Jones T. K. Wan, G. Q. Gu and K. W. Yu, Phys. Rev. E, in press (2001).
4. Jones T. K. Wan, K. W. Yu and H. Sun, Physica B **279**, 75 (2000).

Quasiclassical calculations of Wigner functions in nonlinear dynamics via multiresolution

Antonina N. Fedorova and Michael G. Zeitlin

Russian Academy of Sciences, Institute of Problems of Mechanical Engineering,
Mathematical Methods in Mechanics Group
V.O., Bolshoj pr., 61, 199178, St. Petersburg, Russia

tel: +7-812-3214776, fax: +7-812-3214771, E-mail: zeitlin@math.ipme.ru,
http://www.ipme.ru/zeitlin.html, http://www.ipme.nw.ru/zeitlin.html

We present the application of variational-wavelet analysis to numerical calculations of Wigner functions in (nonlinear) quasiclassical dynamical problems. (Naive) deformation quantization and multiresolution representations are the key points.

We construct the representation via multiscale expansions in generalized coherent states or high-localized nonlinear eigenmodes in the base of compactly supported wavelets and wavelet packets.

Our approach is based on extension of our variational-wavelet approach [1]-[2]. Wavelet analysis is some set of mathematical methods, which gives us the possibility to work with well-localized bases in functional spaces and gives maximum sparse forms for the general type of operators (differential, integral, pseudodifferential) in such bases. These bases are natural generalization of standard coherent, squeezed, thermal squeezed states, which correspond to quadratical systems (pure linear dynamics) with Gaussian Wigner functions.

So, we try to calculate quantum corrections to classical dynamics described by polynomial nonlinear Hamiltonians such as orbital motion in storage rings, orbital dynamics in general multipolar £elds etc. from papers [1]-[3].

The common point for classical/quantum calculations is that any solution which comes from full multiresolution expansion in all space/time (or phase space) scales represents expansion into a slow part and fast oscillating parts. So, we may move from the coarse scales of resolution to the £nest one for obtaining more detailed information about our dynamical classical/quantum process. In this way we give contribution to our full solution from each scale of resolution. The same is correct for the contribution to power spectral density (energy spectrum): we can take into account contributions from each level/scale of resolution. Our (nonlinear) eigenmodes are more realistic for the modelling of nonlinear classical/quantum dynamical process than the corresponding linear gaussian–like coherent states. We mention only the best convergence properties of expansions based on wavelet packets, which realize the so called minimal Shannon entropy property, save CPU time and HDD space.

We present numerical calculations of Wigner functions as solutions of (non)stationary Wigner equations for a few models of beam/particle motions, which explicitly demonstrate quantum behaviour properties.

References

1. Symmetry, Hamiltonian Problems and Wavelets in Accelerator Physics, American Institute of Physics , Conf. Proc., vol. 468, Nonlinear and Collective Phenomena in Beam Physics, pp.69-93, 1999.
2. Variational-Wavelet Approach to RMS Envelope Equations, Proc. 2nd Advanced Accelerator Workshop on The Physics of High Brightness Beams pp.235–254, World Scienti£c, 2000
3. Quasiclassical Calculations for Wigner Functions via Multiresolution, Quantum Aspects of Beam Physics, World Scienti£c, 2001; Los Alamos preprint,physics/0101006.

Shifted contour auxiliary £eld Monte Carlo: Accurate electronic structure of molecules and extended model systems

Roi Baer[1] **and Daniel Neuhauser**[2]

[1]*Department of Physical Chemistry and the Lise Meitner Minerva center for quantum chemistry, The Hebrew University of Jerusalem, 91904 Jerusalem Israel*
[2]*Department of Chemistry and Biochemistry, University of California, Los Angeles CA 90095 USA.*
Tel: +927-2-6586114, Fax: +972-2-651-3742, Roi.Baer@huji.ac.il

Shifted contour (SC) auxiliary £eld Monte Carlo (AFMC) for electronic structure is a new method for accurate electronic structure computations in molecules[1-2]. We describe the method and give several applications that demonstrate the high accuracy achievable in molecular electronic structure, including force computation[3], excited states[4] using the recently developed correlated sampling and a multireference variational version of the method. The method is also applicable for treating Hubbard lattice models, without any restriction as to the range of the electron interaction. Applications for computing ground state energies for large lattices are shown.

References

1. Rom N., Charutz D. M., and Neuhauser D., Shifted-contour auxiliary-£eld Monte Carlo: Circumventing the sign dif£culty for electronic-structure calculations, *Chem. Phys. Lett.* **270** (1997) pp. 382-386.
2. Baer R., Head-Gordon M., and Neuhauser D., Shifted-contour auxiliary £eld Monte Carlo for ab initio electronic structure: Straddling the sign problem, *J. Chem. Phys.* **109** (1998) pp. 6219-6226.
3. Baer R., Ab initio computation of forces and molecular spectroscopic constants using plane waves based auxiliary £eld Monte Carlo with application to N-2, *J. Chem. Phys.* **113** (2000) pp. 473-476.
4. Baer R., Ab Initio computation of singlet-triplet molecular energy differences using Auxiliary Field Monte Carlo, Chem. Phys. Lett. submitted (2001).

A parallel Moore-Penrose generalized inverse algorithm for equilibrium network ¤ow sensitivity simulation

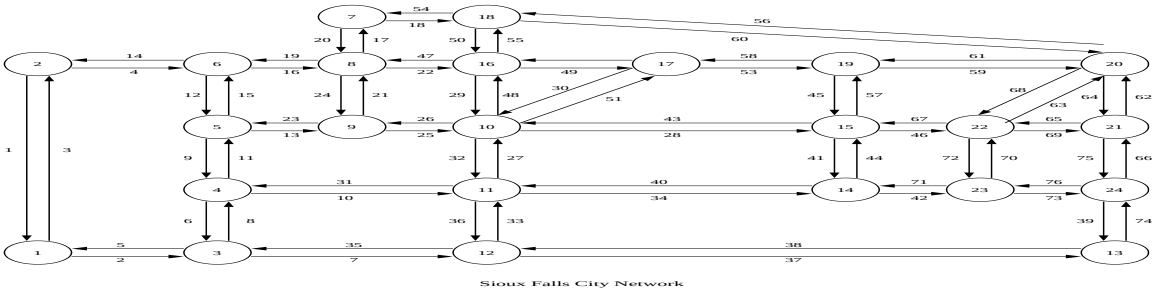
Hsun-Jung Cho[1], **Chih-Ku Fan**[2]

[1] *Professor, Dept. Tran. Tech. Mang., Nat'l Chiao Tung Univ., Taiwan*
[2] *Ph.D. Cand., Dept Tran. Tech. Mang, Nat'l Chiao Tung Univ., Taiwan*
Corresponding address: Department of Transportation Technology and Management, National Chiao Tung University, Hsincu 300, Taiwan
Email: hjcho@cc.nctu.edu.tw and Tel.(Fax) 886-35710657

Sensitivity methods direct application to the variational inequality formulation of the equilibrium network ¤ow problem is not feasible since its solutions do not typically satisfy the local uniqueness conditions required[1]. Tobin and Friesz [2] proposed an approach for the sensitivity analysis of equilibrium network ¤ow problems which restricts that the number of paths with positive ¤ow is less than or equals to the number of arcs plus the number of origin-destination pairs in the network of interest. Cho etc.[3] proposed a reduction method for local sensitivity analysis of network equilibrium arc ¤ows which allows standard sensitivity techniques for variational inequalities. Cho and Lo [4] proposed a Moore-Penrose generalized inverse method, in terms of arc variables and which satis£es the local uniqueness conditions.

In this paper, based on use of the Moore-Penrose generalized inverse, a new parallel simulation using the dynamic load balancing approach is presented and successfully applied to fast simulate the characteristics of the sensitivity of equilibrium network ¤ow. The developed simulator based on Jacobian iterative method, parallel process, Frank-Wolf method has been developed and implemented on a 16-processors Linux-cluster with message passing interface (MPI) library. Due to the robust features of the method, the proposed parallel domain decomposition algorithm reduces signi£cantly the execution time up to an order of magnitude.

The £gure shows the network of Sioux Falls City. We conclude that the generalized inverse method does provide a tractable means of overcoming the local uniqueness dif£culties which arise in applying sensitivity techniques to network problems. Furthermore, a domain partition approach to a parallel speedup and load balancing on a 16-CPUs Linux-cluster with MPI simulation of the sensitivity of equilibrium network ¤ow has been presented. Our achievement of parallel performance shows the computational ef£ciency and robustness of the method.



References

1. T.L. Friesz, Transportation Research **19A**, 413-427 (1985).
2. R.L. Tobin and T.L. Friesz, Transportation Science **22(4)**, 242-250 (1988).
3. H-J. Cho, T. Smith and T.L. Friesz, Transportation Research, **34B**, 31-51 (2000).
4. H-J. Cho and S.C. Lo, Transportation Research Record, **1667**, 96-106 (1999).

A fast way to optimize the design of an asymmetric dc–SQUID

C.R. Calidonna[1], **M. Mango Furnari**[1], **S. Pagano**[1], **E. Sarnelli**[1], **G. Testa**[1]

[1] *Istitute of Cibernetica (CNR), via Toiano 6 I–80072, Arco–Felice (NA) Italy*

tel. +39–081-8534227/229/196/141, fax +39–081-5267654,
{C.Calidonna,mf,S.Pagano,E.Sarnelli,G.Testa}@cib.na.cnr.it

The physics and applications of Josephson junctions is a very important £eld of the condensed matter physics[1]. The Superconducting QUantum Interference Device (SQUID) is one of the most successful devices based on Josephson junctions. It is very sentitive to the magnetic £eld, being limited only by the fundamental quanto–mechanical indetermination principle. Although SQUIDs have been largely investigated, a different con£guration involving asymmetric SQUIDs has recently attracted the interest of researchers for their potential advantages over the "traditional" ones[2]. In this work, we report on our steps towards the building of a fast simulation package, using a parallel architecture, to study the behaviour of asymmetric dc–SQUIDs in the presence of intrinsic thermal noise. The goal is to provide "quick & fast" information for the optimization of the SQUID design and fabrication process, and for the understanding of experimental results. The organization of the entire algorithm, and the use of a parallel architecture for the simulation, furnishes results in a comparatively short time with respect to that necessary on a sequential architecture. The iterative process of simulation can be extremely useful for the understanding and optimization of the characteristics of these devices, provided that the iteration time could be kept short enough. The simulation allows to obtain simultaneously the characteristic features of the device, the SQUID voltage and the low frequency power spectrum amplitude, for different parameter values. In order to optimize computational time, the SQUID voltage is averaged over the minimum time needed to obtain the single points of the overall voltage-¤ux characteristics. Moreover, only in the region of physical interest, the average time has been automatically increased of a factor of 100, increasing the output precision. In such a way, a strong reduction of the scattering of output data has been achieved. During the activity of setting up the code for the simulation, we have optimized the serial component of the algorithm, reducing of about 40% the computational time, by means of a compiler optimization level activation. [2]. Furthermore, by the natural independence of the points of the voltage–¤ux characteristics, it was possible exploiting the available resources, CPUs, obtaining a quasi–linear speedup in generating points. This kind of approach is promising for designing new devices characterized by high magnetic sensitivity. Results of simulation are obtained in very short time. Indeed, times necessary for the generation of the device characteristics were dramatically decreased, due both to code optimization and availability of multiple CPUs.

References

1. A.Barone and G.Paterno; Physics and Applications of the Josephson Effect, Wiley 1982
2. G. Testa, E. Sarnelli, S. Pagano, C.R. Calidonna, and M. Mango Furnari, Characteristics of Asymmetric Superconducting Quantum Iinteference Devices, to appear in Journal of Applied Physics, May 2001.

Non-relativistic electron transport in metals: A Monte Carlo approach

M. F. Rahimi and N. Ghal-eh
Physics Department, School of Sciences,
Ferdowsi University of Mashhad, Iran
Tel: +98-511-8432022, Fax: +98-511-8438032,
farhimi@science1.um.ac.ir

Monte Carlo methods can reproduce theoretically any process where the interaction probabilities can be expressed statistically, such as interaction of electrons with matter. Using ”random numbers”, computers are able to create a statistical history for the life of each particle. That is, an individual particle can experience several scattering interactions before absorption or leakage from the system. [1]

In this article, a simple Monte Carlo procedure is described for simulating the multiple scattering and absorption of electrons with the incident energy in the range 1-50 keV moving through a slab of uniformly distributed material of given atomic number, density and thickness. [2]

The simulation is based on a screened Rutherford cross-section and Bethe continuous energy-loss equation. [3]

A FORTRAN program is written to determine backscattering, transmission and absorption coef£cients, providing the user with a graphical output of the electron trajectories. The results of several simulations are presented by using various numbers of electrons, showing a good agreement with the experiment. The program is used to analyze the relation between the energy and the range of electron in the slab, the backscattering, absorption, transmission coef£cients and the angular distribution.

We can apply this technique to the transport properties of the electron through the body tissue as well. [4] Dividing media into several parts (three in our work) of different materials does this.

References

1. S. Weinzierl, hep-ph/0006269
2. W. Williamson, G. C. Duncan, Am.J.Phys, 54(3),1986
3. H. A. Bethe, Ann.Phys.5, 325, 1930
4. G. S. Sidhu, et al, Radiat.Prot.Dosim. 86(3), 1999

New cluster algorithm and its application to the S =1/2 XXZ chain

H. Otsuka

Department of Physics, Tokyo Metropolitan Univ., Tokyo 192-0397, Japan

Tel: +81-426-77-1111, Fax: +81-426-77-2483, otsuka@phys.metro-u.ac.jp

Recently, substantial developments have been achieved in methodological aspect of worldline quantum Monte Carlo (QMC) simulations [1]. Obviously, these innovations have been brought by natures of clusters constructed by the Fortuin-Kasteleyn (FK) mapping [2]. We propose one extension of the cluster algorithm, where a part of interactions is managed via the FK clusters and the rest via the so-called Hubbard-Stratonovich (HS) £elds [3]. These two kinds of auxiliary variables have been so far independently used in each context, while their aims are both in expanding interacting systems by some more preferable/tractable ones. Therefore, we give a £rst formulation of MC algorithm in the extended con£guration space including these variables.

To make the idea concrete, we consider the $S = \frac{1}{2}$ XXZ chain: $\mathcal{H} = \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \gamma S_i^z S_{i+1}^z \right)$. We separate the Hamiltonian into two parts, where the £rst (second) part is treated by the FK mapping (HS transformation). Speci£cally, here we set $\mathcal{H}_1 = \sum \mathbf{S}_i \cdot \mathbf{S}_{i+1}$ and $\mathcal{H}_2 = \lambda \sum S_i^z S_{i+1}^z$ with $\lambda := \gamma - 1$. Then, we obtain the path-integral representation of the partition function which is described by a sum in the extended con£guration space as $Z \simeq \sum_{S,G,U} \overline{W}_1(S,G)\overline{W}_2(S,U)$, where S, G, and U denote a set of spins on the space-time sites, graphs on the interacting plaquettes, and auxiliary £elds on the space-like bonds, respectively (see Fig. 1). For a given S, the ways to generate G and U are de£ned by $\overline{W}_1(S,G)$ and $\overline{W}_2(S,U)$. The spin con£guration is updated according to the dynamics of clusters in random £elds; we £nd that the Zeeman coupling between £elds and spins plays a central role in our algorithm.

We also clarify that our new algorithm possesses a computationally tractable continuous-time limit and maintains advantages of the original cluster algorithm. As a demonstration, simulations are performed for the $S = \frac{1}{2}$ XXZ chain, where the staggered component of the spin correlation function, $C(i)$, is calculated in the ground state. Figure 2 shows that the obtained data (marks) agree well with the exact results (dotted lines) in the asymptotic region ($i \to \infty$).

Our algorithm is applicable for Hubbard-type models which are relevant to the high-T_c superconductivity and further, it can be also applied to classical systems.

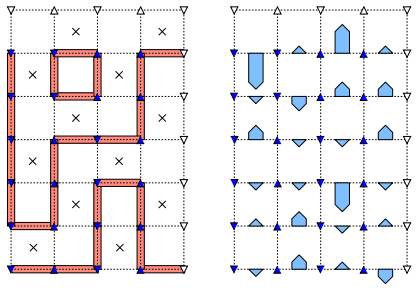


Fig.1 Schematic representation of S, G and U.

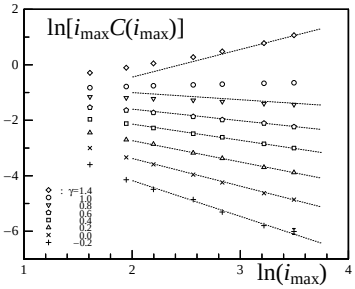


Fig.2 $C(i)$ in a log scale. Dotted lines show exact results.

References

1. For example, H.G. Evertz, in *Numerical Methods for Lattice Quantum Many-Body Problems*, ed. D.J. Scalapino, (Perseus books, Frontiers in Physics).
2. P.W. Kasteleyn and C.M. Fortuin, J. Phys. Soc. Jpn. **26**, (Suppl.) 11 (1969); C.M. Fortuin and P.W. Kasteleyn, Physica **57**, 536 (1972).
3. J. Hubbard, Phys. Rev. Lett. **3**, 77 (1959).

Contrasting models for the simulation of multi-particle collisions and dynamics in a one-dimensional space

J. A. Oyedele

Department of Physics, University of Namibia, Windhoek, Namibia.

E-mail: oyedelej@unam.na

There is increasing interest in the dynamics of one-dimensional systems of many colliding elastic particles. These systems are not only used to demonstrate the law of conservation of momentum but also have important technological applications such as to the proposed fail-safe pellet suspension reactors where the dynamics of many suspended and colliding fuel pellets affect the stability of the facility [1-3]. In studying the dynamics of these multi-particle systems, the motion of each of the several particles has to be known even as they move and collide repeatedly with each other. This could be done by computational simulation using an appropriate model.

In this work, the dynamics of a system of n = 100 particles moving and colliding elastically in a one-dimensional space or constrained to move and collide on a line bounded by elastic end walls is studied by computational simulation. The initial positions and velocities of the particles are assigned using two different random number generators. Two different models are used in the simulation. In one model, called the collisional model, the collision between particles is regarded as an exchange of momentum so that a given particle moves until it collides and exchanges momentum with one of its neighbours thereby changing its direction but never passing its neighbours. However, in the second but contrasting and simpler model, called the free model, the collision is interpreted as an exchange of position so that each particle effectively moves freely without collision throughout the one-dimensional space. The result obtained from each model is depicted as a tone-saturation function of coordinate and time. Also the particle current densities and relaxation times are calculated for the models. A comparison of the two sets of results obtained from the two models shows that they are very similar thus justifying and encouraging the use of the simpler free model for studying the dynamics of one-dimensional system of interacting multi-particle systems.

References

1. Dobrushin R. L. and Fritz J., ”Non-Equilibrium Dynamics of One-dimensional In£nite Particle Systems with a Hard-Core Interaction”, Commun. Math. Phys. 55, 275, 1977.
2. Harms A. A. and Kingdon D. R., ”Pasively Fail-Safe Fission Reactor Based On Pellet Suspension Technology”, Proc. Int. Joint Power Generation Conference, Kansas City, MO, USA, 17-21 Oct. 1993.
3. Giancoli D. C., Physics, Prentice Hall International Inc., London, 1998.

Dynamic Monte Carlo simulations with a phonon heat bath for a square-lattice ising ferromagnet

Kyungwha Park and M. A. Novotny

School of Computational Science and Information Technology,
Florida State University, Tallahassee, Florida 32306-4120, USA

1-850-644-7030, fax:1-850-644-0098, park@csit.fsu.edu

Dynamics of classical Ising spin systems have been studied extensively using the Glauber dynamic [1]. In a weak coupling limit, Martin [2] derived the Glauber dynamic starting with a quantum Hamiltonian that consists of a spin exchange term and a linear coupling term to a *fermionic* thermal heat bath attached to each spin. In this work, we derive explicitly the relationship between Monte Carlo time and physical time using a quantum Hamiltonian with a *phonon* heat bath interacting with a square-lattice nearest neighbor Ising ferromagnet. Since changing the microscopic dynamic can change the dynamics of the system but not the statics, we apply the calculated transition rates to the Ising ferromagnet, measure the lifetime of the metastable state, and compare this phonon dynamic with the Glauber dynamic as a function of temperature and magnetic £eld. In order to derive the transition rates, we consider that the phonon heat bath is attached to each spin and that the coupling between the heat bath and the spin system is linear. Assuming that the correlation time of the heat bath is much shorter than the time of interest, we integrate out all degrees of freedom of the heat bath. The transition rate from the l-th to the k-th eigenstates of the spin Hamiltonian with a two dimensional phonon heat bath is given by $W_{k,l}=\frac{\lambda^2}{2\rho\hbar^3 c^4}\left|\frac{(E_l-E_k)^2}{1-e^{-\beta(E_l-E_k)}}\right|$. Here λ is a coupling strength, ρ is a mass density of the unit cell consisting of one spin, c is the sound velocity, $\beta=1/k_BT$, and E_l is the energy eigenvalue of the l-th eigenstate of the spin Hamiltonian. This transition rate satis£es detailed balance and we obtain different transition rates depending on the dimensionality of the heat bath. The phonon dynamic has two major differences from the Glauber dynamic: (i) the energy difference in the numerator, (ii) the minus sign from the bosonic distribution in the denominator. To measure the lifetime of the metastable state, we perform dynamic Monte Carlo simulations using Absorbing Markov Chains (MCAMC) [3] with both the Glauber and phonon dynamics to simulate the long times required. Our MCAMC data show that the phonon dynamic gives £eld-dependent prefactors in the lifetimes at low temperatures different from the Glauber dynamic, which has piecewise £eld-independent prefactors. One striking effect of the phonon dynamic is that the lifetime prefactor diverges at low temperatures as $|H|\rightarrow 2J$ or $4J$, because certain kinds of spin-¤ips are not allowed. The addition of a small transverse £eld to the spin Hamiltonian prevents the lifetime prefactors from diverging near $|H|=2J$, $4J$.

References

1. R. J. Glauber: J. Math. Phys. **4**, 294 (1963)
2. Ph. A. Martin: J. Stat. Phys. **1**6, 149 (1977)
3. M. A. Novotny: 'A Tutorial on Advanced Dynamic Monte Carlo Methods for Systems with Discrete State Spaces'. In: *Annual Reviews of Computational Physics IX*, ed. by D. Stauffer (World Scienti£c, Singapore 2001) pp. 153-210

Path integral Monte Carlo study of a two dimensional polaron gas

J.T. Titantah, C. Pierleoni and S. Ciuchi

INFM, UdR L'Aquila and Physics Department, University of L'Aquila, via Vetoio, Coppito I-67100 L'Aquila

phone: +39 0862 433056, fax: +39 0862 433033, carlo.pierleoni@aquila.infn.it

Using a recently developed Path Integral Monte Carlo (PIMC) code that has been shown to reproduce accurately the energetic and con£gurational properties of the single Fröhlich polaron [1], we investigate the effect of Fröhlich like electron-phonon interactions on the properties of interacting coulomb systems. Of special interest to us is the mechanism of the melting of the polaron Wigner crystal which has been investigated theoretically[2] on the basis of the Feynman variational method. A qualitative and quantitative study of this mechanism could be relevant to understand the role of long range unscreened forces in the CuO plane of the high temperature superconductors ($HTSC$). Biased by the interesting properties of low dimensional cuprates[3], we embark in the study of two dimensional polaron gas.

We limit the preliminary study at densities low enough ($r_s > 60$) for Fermi statistics to be ignored so that we assume Boltzmann statistics in the liquid phase. In the absence of electron-phonon interactions, we £nd agreement with recent data for the melting temperature of the quantum two dimensional electron gas[4].

We have investigated Fröhlich type electron-phonon interactions with phonon frequency $\omega_{LO} = 27.2meV$, typical of low dimensional cuprates [2], at intermediate coupling $\alpha = 2.12$. At those low densities, the main effect of the electron-phonon interactions is the particle self-trapping while the interparticle effective attraction is a minor effect. In the intermediate coupling regime electron-phonon interaction enhances the structure of the liquid as if the particle mass was augmented. On the other hand we emphasize as the density effect (Coulomb coupling) provides a further increases of particle localization, by comparing single particle properties of the polaron gas (effective mass and charge-induced charge correlation function) with single polaron results at the same coupling. At low temperature ($T < \omega_{LO}$) coulomb coupling and electron-phonon self interaction are both relevant. With increasing temperature, the coulomb interactions are washed out by thermal effects much earlier than the self trapping due to phonon, and the polaron gas properties are dominated by the single polaron behaviour.

Extension of the present study to higher densities is interesting as Coulomb repulsion gets progressively screened by the Fermionic nature of the electron gas, and interparticle phonon-mediated attraction can become relevant. We are presently extending the code to simulate fermions in the framework of the Restricted Path Monte Carlo method[5].

References

1. J. T. Titantah, S. Ciuchi and C. Pierleoni, "*The Free energy of the Fröhlich polaron in two and three dimensions*", cond-mat/0010386; J. T. Titantah, S. Ciuchi and C. Pierleoni "*Path integral Monte Carlo study of the Fröhlich polaron problem*", in preparation.
2. S. Fratini and P. Quémerais, Eur. Phys. J. B **14**, 99 (2000).
3. Y. H. Kim, C. M. Foster *et al.*, Phys. Rev. B **38**, 6478 (1988); C. Taliani, R. Zambone, G. Raum *et al.*, Solid State Commun. **66**, 487 (1988); S. Lupi, P. Maselli, M. Capizzi *el al.*, Phys. Rev. Letts. **83**, 4852 (1999).
4. F. Douchen, L. Candido and D.M. Ceperley, unpublished.
5. D.M. Ceperley, in *Monte Carlo and Molecular Dynamics of Condensed Matter Systems*, Ed. K. Binder and G. Ciccotti, Editrice Compositori, Bologna, Italy, 1996.

Study of bifurcations and stability in Rayleigh-Bénard convection

D. Puigjaner[1], C. Simó[2] and F. Giralt[3]

[1] *Dept. Enginyeria InformÁatica i MatemÁatiques, ETSE, Univ. Rovira i Virgili, Ctra. de Salou s/n, 43006 Tarragona, Spain*

[2] *Dept. MatemÁatica Aplicada i AnÁalisi, Fac. MatemÁatiques, Univ. de Barcelona, Gran Via 585, Barcelona, Spain*

[3] *Dept. Enginyeria Química, ETSEQ, Univ. Rovira i Virgili, Ctra. de Salou s/n, 43006 Tarragona, Spain*

977559663, 977559710, dpuigja@etse.urv.es

Convection problems provide an appropriate physical situation to study order and chaos, and to understand the genesis and evolution of ¤ow patterns with Rayleigh numbers (Ra)[1]. The study of bifurcations and stability in convective ¤ows is usually carried out by time-forward integration of the nonstationary equations. This method involves CPU-time consuming calculations and is unable to follow unstable solutions which might become stable for values of Ra strictly greater than the critical ones. On the other hand, methods of weighted residuals, with properly chosen trial functions, need fewer modes than other methods using discretization of the ¤ow region.

A numerical study of bifurcations and stability of the stationary convective ¤ows in rectangular enclosures heated from below, has been carried out using a Galerkin spectral method. The complete set of trial functions used has been chosen so that each basis function satis£es the boundary conditions and the continuity equation. Pressure is eliminated and the study of stability of the steady ¤ow reduces to an eigenvalue problem [2]. A continuation algorithm, using a modi£ed Newton method [3], yields the stationary solutions of the non-linear governing equations for different values of Ra or the selected continuation parameter (aspect ratios, Prandtl number, etc.). Stationary solutions near a bifurcation point have been found by standard bifurcation analysis [3]. They are taken as the £rst step in the continuation method. Both, stable and unstable branches have been followed. The eigenvalue problem, associated with stability analysis of the non-linear stationary solutions along the bifurcated branches, has been solved using the QR algorithm.

The current numerical approach has been applied to the Rayleigh-Bénard ¤ow inside a cubical cavity heated from below with Ra as continuation parameter. For $Ra < 10^4$ four bifurcations from the conductive state are identi£ed. At the £rst transition an x–roll and a diagonal–roll are formed. While the former is stable, the latter is slightly unstable with instability increasing with Ra. The second bifurcation yields an unstable four–roll structure that becomes stable later on. The third and fourth bifurcations result in highly unstable structures. Other ¤ow structures showing up at all secondary bifurcations up to $Ra = 7 \times 10^4$ turn out to be unstable. These results agree with previous numerical and experimental results [4]. The effect of changing aspect ratios on the bifurcation Ra for rectangular cavities has also been studied. It shows that there is a continuous evolution towards multiple single–roll con£gurations as the cavity elongates.

References

1. A.V. Getling 1998, Rayleigh-Bénard convection: structures and dynamics. World Scienti£c Publishing.
2. D. Puigjaner, C. Simó, F. X. Grau, F. Giralt 2000, Stability analysis of the ¤ow in a cubical cavity heated from below. Phys. Fluids (submitted).
3. C. Simó 1990, Analytical and numerical computation of invariant manifolds. In D. Benest and C. Froeschlé, editors, Modern methods in celestial mechanics, 285-330, Editions FrontiÁeres, Paris.
4. J. PallarÁes, F.X. Grau, F. Giralt 1999, Flow transitions in laminar Rayleigh-Bénard convection in a cubical cavity at moderate Rayleigh numbers. Int. J. Heat Mass Transfer, 42, 753-769.

Kinetic theory for a ¤uctuating heat conduction equation

M. Ripoll and P. Español

Dpto Física Fundamental. Facultad de Ciencias, UNED. C/ Senda del Rey, 9 28040
Madrid, Spain

tfn:+34913987126, *fax:*+34913986697, *email:mripoll@£sfun.uned.es*

Dissipative Particle Dynamics (DPD) is a mesoscopic simulation technique that allows one to simulate complex ¤uids problems that deal with separate time and length scales. The method introduced originally as an hybrid between lattice gas and molecular dynamics simulations [1], has proven to be a ¤exible and powerful tool in the study of complex ¤uids as colloidal suspensions, ¤ow in porous media, polymer suspensions or multicomponent ¤ows. Moreover, an energy conserving generalization [2] has been introduced extending the range of applicability of this technique to non isothermal situations.

On the other hand, Smoothed Particle Hydrodynamics (SPH) is a well-known technique for the discretization of the hydrodynamic continuum equations. SPH has been recently generalized in order to include thermal ¤uctuations in a consistent way [3]. The method has been named Smoothed Dissipative Particle Dynamics (SDPD) since it captures the best of SPH (Navier-Stokes solver) and of DPD (hydrodynamic ¤uctuations).

In this work we restrict ourselves to the heat conduction problem, which has been treated recently with SPH [4] and with DPD [5]. We show that by including thermal ¤uctuations into the heat conduction equation it is possible to apply the methods of kinetic theory. In particular, we show that the wavevector dependent thermal conductivity can be computed explicitly. Therefore, we are able to quantify the effect of the discretization on perturbations of the same order of the interparticle distance.

References

1. P.J. Hoogerbrugge and J.M.V.A. Koelman, *Europhys. Lett.* **19**, 155 (1992).
2. P. Español, *Europhys. Lett.* **40**, 631 (1997).
3. P. Español, Preprint (2001).
4. P. W. Cleary and J. J. Monaghan, *J. Comp. Phys.* **148**, 227 (1999).
5. M. Ripoll, P. Español and M.H. Ernst, *Int. J. of Mod. Phys. C* **9** , 1329 (1998).

An alternative approach to the computation of critical properties with the renormalization group

Dorit Ron[1] **and Robert H. Swendsen**[2]

[1]*Department of Computer Science and Applied Mathematics, Weizmann Institute of Science, Rehovot 76100, Israel*

[2]*Physics Department, Carnegie Mellon University, Pittsburgh, PA 15213*

+972-8-9342141, +972-8-9342945, dron@wisdom.weizmann.ac.il

Several methods have been developed for the purpose of implementing a renormalization group analysis within the context of a Monte Carlo simulation [1]. These methods share a number of advantages, including great generality, ¤exibility, and a certain degree of control over both systematic and statistical errors. However, each method also has certain limitations that make it worthwhile to explore new approaches.

The two basic goals of such calculations are the determination of the renormalized couplings and the evaluation of the matrix of derivatives of the renormalized couplings with respect to the original couplings. The eigenvalues of the matrix of derivatives provide estimates for the critical exponents, while the determination of the renormalized couplings allows us to locate both the critical point of a model of interest and the £xed point of the renormalization group transformation.

We base our work on the Brandt-Ron [2] representation of the renormalized spin distribution. By measuring the probability distribution of a given spin conditional on the values of spins in its neighborhood, we are able to concentrate the computational effort on those con£gurations that provide the optimum information on properties of the renormalized Hamiltonian. This approach is particularly effective in determining the values of intermediate-range couplings that are normally dif£cult to compute accurately. We are able to compute both the renormalized trajectory and the location of the £xed point with higher accuracy than previously obtainable.

The determination of the renormalized couplings [3] is associated with multi-grid simulation techniques that greatly reduce the relaxation times of the simulation. We are even able to eliminate critical slowing down entirely for special cases.

By expressing the derivatives of the Brandt-Ron probabilities with respect to the coupling parameters, we are able to compute the matrix of derivatives that enables us to investigate the renormalization-group ¤ows near the £xed point.

Both the Brandt-Ron representation of the renormalization group and the analysis methods based on it are suf£ciently general to enable us to analyze a variety of systems non-Hamiltonian dynamics in addition.

References

1. Burkhardt Th. W. and Van Leeuwen J. M. J. eds., Real space renormalization, Vol. 30 (Springer, Berlin, 1982).
2. Brandt, A. and Ron, D., *J. Stat. Phys.* **102** (2001) 231-257.
3. Ron, D. and Robert H. Swendsen, submitted.

Local sensitivity computational analysis of stochastic 3D-cycles

L.B. Ryashko, I.A. Bashkirtseva

Department of Mathematics,Ural State University,
pr.Lenina 51, 620083 Ekaterinburg, Russia
e-mail: lev.ryashko@usu.ru

The problem of sensitivity of nonlinear system limit cycle with respect to small stochastic disturbances is considered. Kolmogorov-Fokker-Planck equation gives the most detailed description of such system probabilistic behavior. However, the direct using of this equation is very dif£cult even for the simplest situations. Important case when stochastic disturbances are small leads to famous problems of analysis of equations with small coef£cients near higher derivatives. A new asymptotic approach connected with using of quasipotential function in stochastic analysis is being actively developed [1],[2].

Due to some parametrization the construction of the £rst approximation (orbital quadratic form) of quasipotential is reduced to search for periodic function (sensitivity function). For the plane orbit case this function is scalar. Sensitivity function allows to compare the stability levels of the different pieces of orbit.

Stochastic sensitivity analysis for a plane cycle case is considered in [3] for Van-der-Pol oscillator. In [4] for Brusselator the capabilities of this method to predict the transition to chaos are demonstrated.

Expansion of this computational technique to sensitivity analysis of stochastic 3D- cycles is considered. The construction of a function of sensitivity is reduced to the solution of some singular boundary problem for a matrix differential Lyapunov equation. Probabilistic interpretation of this problem connected with linear stochastic system with periodic coef£cients is given. The iterated method for solution approximation is constructed. The conditions and degree of convergence are discussed.

The effectiveness of suggested computational technique of sensitivity analysis on the example of the Lorenz model cycles singularities is demonstrated.

This work is supported by RFBR grant (N00-01-00076).

References

1. Graham, R., Tel, T. Nonequilibrium potential for coexisting attractors. *Physical Review A*, **33**, 1322-1337, 1986.
2. Smelyanskiy, V.N., Dykman, M.I. and Maier, R.S. Topological features of large ¤uctuations to the interior of a limit cycle. *Physical Review E.*, **55**, 2369-2391, 1997.
3. Bashkirtseva I.A., Isakova M.G., Ryashko L.B. Quasipotential in stochastic stability analysis of the nonlinear oscillator orbits. *J. Neural, Parallel & Scienti£c Computations*, **7**, 299-310, 1999.
4. Bashkirtseva I.A., Ryashko L.B. Sensitivity analysis of the stochastically and periodically forced Brusselator.*Physica A*, **278**, 126-239, 2000.

Load-balancing of plasma particle-in-cell simulations

Josef Schüle[1], Carsten Othmer[2] and the EPCC team[3]

[1]*Rechenzentrum, Technische Universität Braunschweig, Hans-Sommer-Str. 65, 38106 Braunschweig, Germany*
[2]*Institut für Geophysik und Meteorologie, Technische Universität Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany*
[3]*Edinburgh Parallel Computing Centre, The University of Edinburgh, Edinburgh EH9 3JZ, UK*
Phone +49 531 391 5542, Fax +49 531 391 5549, j.schuele@tu-bs.de

Particle-in-cell (PIC) simulations have become a standard research tool in space plasma and laboratory plasma physics. Within this kind of simulation codes, the electromagnetic £eld is de£ned on a spatial grid, while the plasma itself is modeled as an ensemble of hundreds of thousands of particles that can move continuously through the simulation grid.

We have developed a three-dimensional electromagnetic PIC code for the simulation of ion thrusters. Electrons and ions are injected spatially localized on one side of the simulation box and then expand into the 3D computational volume. A straightforward parallelization of this code was realized by an equidistant, static decomposition of the physical simulation grid in up to three dimensions. Each processor is assigned one domain, and is responsible for the £eld update and the particles within that domain.

This equidistant decomposition scheme makes sure that the workload for the update of the grid-based electromagentic £eld is equally distributed over the PEs. The particles, however, cause a strong imbalance of work. As they are injected in a spatially very localized region, their distribution over the simulation volume is highly inhomogeneous. Processors, whose domains are very close to or even include the injection plane, are responsible for considerably more particles than those far off, which might not even get a single particle throughout the whole simulation run. This renders the parallel code very ineff£cient.

A cure for the workload imbalance associated with an inhomogeneous distribution of particles in plasma simulations was suggested by Liewer and Decyk [1]. In addition to the common primary equidistant domain decomposition, these authors introduced a secondary dynamic decomposition for the particles, which adjusts itself according to their momentary distribution. This method proved to be quite ef£cient for *slightly* inhomogeneous particle distributions [2]. For the high degree of inhomogeneity in our simulation, however, the method of Liewer and Decyk turned out to be inappropriate.

Based on the work of Carretti [3], we therefore developed another parallelization strategy, which successfully eliminates the particle associated imbalance of workload: All the particles of a domain are organized into smaller groups, which are then traded independently among the processors according to their individual workload. Processors with less or no particles in their domain take over some of the particles of busier processors without interrupting their work progress. The implementation of this strategy on the CRAY T3E of the Edinburgh Parallel Computing Centre and its effect on the scalability of the simulation will be demonstrated.

References

1. **Liewer, P. C., and V. K. Decyk,** A general concurrent algorithm for plasma particle-in-cell simulation codes, *J. Comput. Phys.*, **85**, 302, 1989.
2. **Wang, J., P. Liewer, and V. Decyk,** 3D electromagnetic plasma particle simulations on a MIMD parallel computer, *Comp. Phys. Comm.*, **87**, 35, 1995b.
3. **Carretti, E.,** Numerical simulations and power spectrum analysis of ESP redshift survey, PhD thesis, University of Bologna, Italy, 1998.

Semi-quantal simulations of hydrogen under extreme conditions

M. Knaup[1], **P.-G. Reinhard**[1], **C. Toepffer**[1], **and G. Zwicknagel**[1]

[1] *Institut für Theoretische Physik II, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany*

Tel.: ++49-9131/85-28461, Fax: ++49-9131/85-28907, email: toepffer@theorie2.physik.uni-erlangen.de

Classical molecular dynamics (MD) simulations are a well established tool to study equilibrium properties as well as the dynamics of manybody systems like strongly coupled plasmas. However, under extreme conditions of temperature and density quantum effects like the wave nature of the particles and their indistinguishability become important. A complete quantum treatment is an extremely demanding task as the $6N$ conjugate coordinates of the N-particle system have to be replaced by a full N-body quantum wavefunction. Here we employ an approximate quantum treatment which comes from the classical MD side, thus maintaining its simplicity as well as its correlation content. This is achieved by blowing up the classical point particles to a localized wave packet with a simple analytical form. Such a wave packet molecular dynamics (WPMD) based on the time-dependent variational principle is a good approximation if the width of the wave packet is smaller than the typical length scale of variation of the potential. The wave packet approach is able to reproduce many dynamical properties of many-body systems, e.g., the scattering of composite particles like atoms and molecules [1], heavy ion scattering [2] and Coulomb systems [3]. Usually Gaussian wave packets are employed reducing the time evolution of a complex wavefunction to the evolution of a few relevant parameters, as position, momentum and width of the wave packet. This reduces the amount of numerical work from the solution of a partial differential equation to the much simpler case of a set of ordinary differential equations. Nevertheless there remain formidable tasks like antisymmetrisation. However, expectation values of operators with Slater determinants can be calculated by matrix inversion which reduces the numerical expense from $O(N!)$ to $O(N^3)$, where N is the number of simulated particles. Within the wave packet formalism we use a force-bias Monte-Carlo algorithm to calculate the equation of state of hydrogen and deuterium at pressures between 40 and 500 GPa and solid state density. Recent shock wave experiments [4] showed a much larger compressibility of deuterium than the prediction of the Sesame tables [4]. In contrast to other “ab initio” theoretical approaches the WPMD reproduces the large compressibility very well.

References

1. E. J. Heller, J. Chem. Phys. **62** (1975) 1544
2. H. Feldmeier, Nucl. Phys. A **515** (1990) 147-172
3. D. Klakow, C. Toepffer, and P.-G. Reinhard, Phys. Lett. A **192** (1994) 55; J. Chem. Phys. **101** (1994) 10766
4. I. B. Da Silva et al., Phys. Rev. Lett. **78** (1997) 483

Non-Boltzmann sampling for percolation and the q-states Potts models

Martin Weigel

Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany

Tel.: +49-341-97-32450, Fax.: +49-341-97-32548, Email: weigel@itp.uni-leipzig.de

Monte-Carlo (MC) update algorithms based on the idea of generalized ensembles introduced with the multicanonical MC method [1] have found widespread application and proved very useful for the simulation of systems with large free energy barriers. Those occur for systems at a £rst order phase transition or, even worse, for disordered systems like spin-glasses and proteins and entail an exponentially strong slowing down of any local, canonical dynamics of the MC process. The idea of generalized ensembles copes with that problem by enhancing the otherwise exponentially small probability of visiting the suppressed regions of phase space, thus effectively eliminating the free energy barriers.

The q-states Potts models undergo £rst-order phase transitions for $q > 4$ in two dimensions and $q \geq 3$ in three dimensions, respectively; the strength of these transitions increases with the number of states q. Besides, they include the problem of (bond) percolation as the limiting case $q \to 1$. Making use of the *random-cluster* representation, they can be written as a bond-directed percolation model [2],

$$Z = \sum_{G' \subseteq G} p^{b(G')}(1-p)^{E-b(G')} q^{n(G')} \propto \sum_{b=0}^{E} \sum_{n=1}^{N} N_t(b,n)(e^K - 1)^b q^n, \tag{1}$$

where $N_t(b,n)$ denotes the number of possible con£gurations of b bonds on the lattice, decomposing it into n clusters. This quantity should be parallelled with the density of states $\Omega(E)$ in the case of the Ising model. Given an algorithm that samples $N_t(b,n)$ precisely, for the whole (b,n) region, the thermal averages of interest can be inferred from this representation for the whole range of the coupling K (i.e., temperature) and any, even non-integer, number of states q from one simulation.

We pick up the idea of *multi-bondic* simulations [3] that apply multicanonical weights $W(b)$ to the bond-con£gurations occurring in the cluster update of spin models and consider reweighting built into the update algorithm as a function of both, the number of bonds b and the number of clusters n. Since $N_t(b,n)$ is a purely geometrical quantity, we do not even have to consider a spin model, but only the percolation limit of a cluster decomposition of the lattice sites by setting and deleting bonds.

We suggest and compare different implementations of this basic idea including a multicanonical version using run-time extrapolation of the estimates, a generalization of the Wang-Landau algorithm [4] for this case and, £nally, a non-Markovian sampling scheme making use of the ef£ciency of union-£nd algorithms for the cluster decomposition problem.

References

1. B.A. Berg and T. Neuhaus, Phys. Rev. Lett. **68**, 9 (1992).
2. A. Coniglio and W. Klein, J. Phys. **A13**, 2775 (1980); C.-K. Hu, Physica **16A**, 265 (1982).
3. W. Janke and S. Kappler, Phys. Rev. Lett. **74**, 212 (1995).
4. F. Wang and D.P. Landau, preprint cond-mat/0011174.

A dynamic Monte Carlo study of random-bond Potts ferromagnet with trinary disorder distributions

H.P. Ying[1,2]**, D.R. Ji**[1]**, and L. Schülke**[2]

[1] *Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou 310027, PR China*

[2] *Fachbereich Physik, Universität Siegen, D-57068 Siegen, Germany*

0086-571-7951592. 0086-571-7951328(Fax), hpying@zimp.zju.edu.cn

The critical scaling and universality for the random-bond Potts ferromagnets (RBPF) are studied by Monte Carlo simulations in short-time dynamics (STD) [1, 2]. We introduced, for the £rst time, a trinary distribution of quenched disorders for the RBPF on the two-dimensional (2D) triangual lattices and applied the STD method to estimate the exponents θ, z and β/ν for several realizations of the quenched disorder distribution. The disorder strength is realized by the disorder amplitudes $\{r_1, r_2\}$. There are three types of such disordered systems of the trinary RBPF: (I) one-third bonds chosen randomly are strongly coupled with $\{r_1$=1, $r_2 > 1\}$, (II) two-third bonds coupled with different amplitudes $r_2 > r_1 > 1$ and (III) two-third bonds coupled with the same amplitude r_1=$r_2 > 1$. We consider the systems with the disorder amplitudes $r_1 \in (1, 12)$ and $r_2 \in (1, 12)$.

In the simulation the dynamic scaling behavior is veri£ed and the power-law dynamics is used to estimate both the dynamic and static exponents as a function of the disorder amplitudes. It is found the values of exponents θ and β/ν is variant continuously with the disorder amplitudes and violate the Ising -like universility. Further the measured values of the dynamic exponent z are found larger than that for the systems without disorders and increase with the strength of disorder amplitudes for the systems I: $r_1 = 1$, $r_2 > 1$ and III: r_1=$r_2 > 1$.

On the other hand, for the systems II where 2/3 bonds are strongly coupled with different amplitudes $1 < r_1 < r_2$, they seem to have been located at a “random” region where their values of the critical exponents β/ν and z are nearly independent of disorder amplitudes within the error bars, $z \sim 2.23$ and $\beta/\nu \sim 1.85$. By comparing these results to z=2.23(4) and β/ν=0.182(5) for the r_1=r_2=10 in III, we could argue that, after $r_1 = r_2 \geq 10$ (equivalent to r_1=1, $r_2 \leq 0.1$ in I) it will pass a “crossover” to the random region from other type, I or III, of the disordered systems, so that z and β/ν will be nearly constants.

In conclusion, our simulation veri£es that second order phase transitions are induced. Then the results show evidence that the dynamic universality class of the trinary RBPF should not belong to that of the Ising model, as inferred by Jacobsen and Cardy [3, 4]. Our critical scaling analysis strongly indicates that the bond randomness in¤uences the critical universality. From the work we £nd it rather encouraging to apply the dynamic MC to simulate the scaling and critical dynamics of disordered spin systems. We will pursue this £eld to explore the logarithmical slow dynamics [5].

References

1. H.-P. Ying and K. Harada, Phys. Rev. E**62**, 174 (2000).
2. B. Zheng, Int. J. Mod. Phys. B**12**, 1419 (1998).
3. J.L. Jacobsen and J. Cardy, Nucl. Phys. B**515[FS]**, 701(1998).
4. T. Olson and A. P. Young, Phys. Rev. B**60**, 3428 (1999).
5. J. Cardy, Physica A**263**, 215 (1999), and references there in.

Index of Authors

Already published:

Modern Methods and Algorithms of Quantum Chemistry - Proceedings
Johannes Grotendorst (Editor)
NIC Series Volume 1
Winterschool, 21 - 25 February 2000, Forschungszentrum Jülich
ISBN 3-00-005618-1, February 2000, 562 pages

Modern Methods and Algorithms of Quantum Chemistry - Poster Presentations
Johannes Grotendorst (Editor)
NIC Series Volume 2
Winterschool, 21 - 25 February 2000, Forschungszentrum Jülich
ISBN 3-00-005746-3, February 2000, 77 pages

Modern Methods and Algorithms of Quantum Chemistry - Proceedings, Second Edition
Johannes Grotendorst (Editor)
NIC Series Volume 3
Winterschool, 21 - 25 February 2000, Forschungszentrum Jülich
ISBN 3-00-005834-6, December 2000, 638 pages

Nichtlineare Analyse raum-zeitlicher Aspekte der hirnelektrischen Aktivität von Epilepsiepatienten
Jochen Arnold
NIC Series Volume 4
ISBN 3-00-006221-1, September 2000, 120 pages

Elektron-Elektron-Wechselwirkung in Halbleitern: Von hochkorrelierten kohärenten Anfangszuständen zu inkohärentem Transport
Reinhold Lövenich
NIC Series Volume 5
ISBN 3-00-006329-3, August 2000, 145 pages

Erkennung von Nichtlinearitäten und wechselseitigen Abhängigkeiten in Zeitreihen
Andreas Schmitz
NIC Series Volume 6
ISBN 3-00-007871-1, May 2001, 142 pages

Multiparadigm Programming with Object-Oriented Languages
Kei Davis, Yannis Smaragdakis, Jörg Striegnitz (Editors)
NIC Series Volume 7
Proceedings, Workshop MPOOL, 18 May 2001, Budapest
ISBN 3-00-007968-8, June 2001, 160 pages

All volumes are available online at http://www.fz-juelich.de/nic-series/.