Simple computational Lennard-Jones fluid driven out-of-equilibrium.

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As in equilibrium, lattice models are fundamental in the study of criticality and nonequilibrium phase transitions (NPT). Despite its simplicity, they capture the essential features of real systems near the critical points and help us to understand the complex behavior behind ionic conductors, traffic jams, origins of life, granular matter, and many others fields[1]. However, a well known disadvantage concerning the usefulness of lattice models is that they are to crude to be compared directly with experiments. In fact, in order to obtain a precise phase diagram one often should employ more detailed models. This work is a new effort towards better understanding NPT. We here present a model for driven systems in which spatial coordinates vary continuously. Our aim is to provide a realistic model for Monte–Carlo (MC) types of computer simulations of anisotropic fluids. This leads us to discuss on the continuous limit[5] of the driven lattice gas (DLG[2] or KLS[3] due to its inventors), which is the prototype for anisotropic NPT, which sheds new light on its nature.

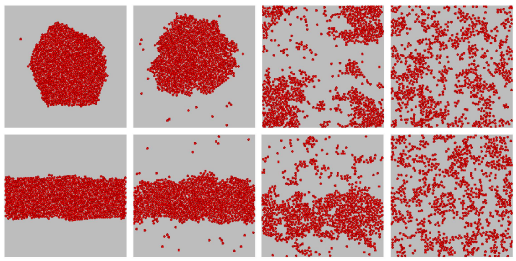

FIG. 1. Comparison of typical MC steady state configurations for the DLJF for 900 particles, number density[6] $\rho = 0.30$, $\epsilon = 0$, *i.e.* equilibrium, (upper row) and $\epsilon = 1.0$ (lower row) for temperatures (from left to right) $T = 0.25$, 0.35, 0.45, 0.55[6]. The field is oriented horizontally.

Our proposed model consists of a driven out-of-equilibrium two-dimensional Lennard-Jones fluid (DLJF)[4] with the particles hopping preferentially along one direction, say $\hat{x}$, under periodic boundary conditions. This is induced by an external drive, ϵ, *e.g.*, an applied electric field assuming the particles are positive ions. The preferential particle hopping is implemented in terms of a biased Metropolis rule by adding the drive $\epsilon\hat{x}\cdot\vec{\delta}$ to the familiar balance between potential (H) and thermal energy (k_BT), namely $-\Delta H/k_BT + \epsilon\hat{x}\cdot\vec{\delta}$ where $\vec{\delta}$ is the vector displacement of a MC trial move. In this work, we report the first results for a MC study in the 'canonical' ensemble, focusing on its structural quatities and its phase diagram including a detailed study of the coexistence curve.

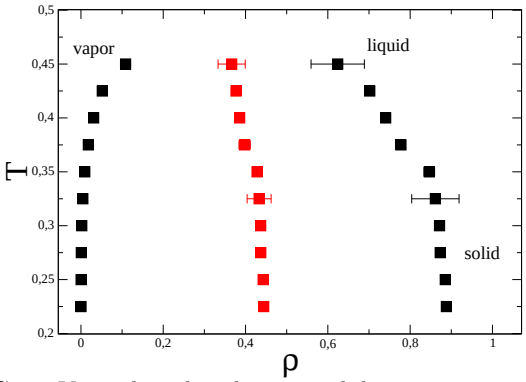

FIG. 2. Vapor-liquid and vapor-solid coexistence curve in the density-temperature plane for the DLJF (black squares). The middle points (red squares) are useful for estimate the critical point.

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[5] *i.e.*, a continuum analog with the same symmetries and possibly criticality.

[6] In rescaled units.