Simulation of liquid-vapour phase separation on GPUs using Lattice Boltzmann models with off-lattice velocity sets

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We use a two-dimensional Lattice Boltzmann (LB) model to investigate the liquid-vapour phase separation in a van der Waals fluid. The model is based on the expansion of the distribution function up to the third order in terms of Hermite polynomials [1] . According to the Chapman-Enskog expansion, the third order expansion is required to ensure the necessary moments of the distribution function in order to retrieve the Navier-Stokes (mass and momentum) equations in an isothermal system when using the Bhatnagar-Gross-Krook collision operator [2, 3]. In two dimensions, the third order LB model based on the Gauss-Hermite quadrature is an off-lattice one and has 16 velocities. In our contribution, we discuss the numerical scheme used to evolve the corresponding distribution functions in the lattice nodes, as well as the implementation of this model on a nVIDIA Tesla M2090 Graphics Processing Unit (GPU). The resulted code, developed using the CUDA platform, allows one to follow the liquid-vapour phase separation on large lattices (up to 4096×4096 nodes).

To capture the behaviour of the liquid-vapour system, special attention should be paid to the body-force term that ensures the phase separation in the Lattice Boltzmann evolution equations. Here we considered the force term obtained by taking the derivative of the distribution function f with respect to the velocity vector and retaining the series expansion up to third order [1, 4]. This greatly improves the accuracy of the liquid-vapour phase diagram retrieved during computer simulations.

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