

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Fluctuating lattice-Boltzmann model for complex fluids SANTTU OLLILA, Aalto University School of Science, COLIN DENNISTON, MIKKO KARTTUNEN, University of Western Ontario, TAPIO ALA-NISSILA, Aalto University School of Science — We develop, and test numerically, a lattice-Boltzmann (LB) model for non-ideal fluids that incorporates thermal fluctuations through a random component in the local stress tensor. The fluid model is a momentum-conserving thermostat, for which we demonstrate how the temperature can be made equal at all length scales present in the system by having noise both in the stress tensor of the fluid and by shaking the whole system in accord with the local temperature. The validity of the model is extended to a broad range of values of the sound velocity. Furthermore, our model features a consistent coupling scheme between the fluid and solid molecular dynamics objects, which allows us to use the LB fluid as a heat bath for solutes evolving in time *without* external Langevin noise added to the solute. This property expands the applicability of LB models to dense, strongly correlated systems with thermal fluctuations and potentially non-ideal equations of state. We benchmark our model by performing tests on the fluid itself and on the static and dynamic properties of a coarse-grained polymer chain under strong hydrodynamic interactions. We find that our model produces results for single-chain diffusion that are in quantitative agreement with theory

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Date submitted: 19 Nov 2010

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