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ALGORITHMS FOR THE STOCHASTIC SIMULATION OF STEADY NONEQUILIBRIUM FLOW

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Nonequilibrium molecular dynamics (NEMD) are widely employed in the simulation of molecular fluids under steady, homogeneous flow to understand the rheological properties of complex fluids. Since the system is not a standard equilibrium statistical ensemble specialized dynamics and algorithms are necessary for the simulation.

We will discuss the derivation and implementation of the Nonequilibrium Langevin Dynamics, a stochastic dynamics for sampling a molecular system with a homogeneous flow field $\nabla \mathbf{u} = A$. Following and adapting a construction of Durr, Goldstein, and Lebowitz [1], where a single large particle interacts with a deterministic heat bath, we perform an upscaling from a microscopic bath model. The equations of motion are the limit of a family of mechanical systems containing a single large particle immersed in an infinite bath of small atoms that have a consistent mean velocity gradient and random initial conditions. The large particle interacts with the bath atoms via elastic collisions and feels no other external forces. In the limit as the mass of the individual bath atoms approaches zero, we find that the large particle evolves according to a stochastic dynamics.

We will discuss algorithmic aspects of the dynamics as well, in particular the implementation of efficient boundary conditions. In such a simulation the unit cell moves with the flow, and we describe particular boundary conditions that allow for long-time simulation by avoiding extreme deformation of the unit cell. We also describe extensions of molecular dynamics algorithms such as cell list techniques to the case of deforming boundary conditions.

REFERENCES

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