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A finite-volume method for fluctuating dynamical density functional theory

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Abstract-

We introduce a finite-volume numerical scheme for solving stochastic gradient flow equations. Such equations are of crucial importance within the framework of fluctuating hydrodynamics and dynamic density functional theory. Our proposed scheme deals with general free-energy functionals, including, for instance, external fields or interaction potentials. This allows us to simulate a range of physical phenomena where thermal fluctuations play a crucial role, such as nucleation and other energy-barrier crossing transitions. A positivity-preserving algorithm for the density is derived based on a hybrid space discretization of the deterministic and the stochastic terms and different implicit and explicit time integrators. We show through numerous applications that not only our scheme is able to accurately reproduce the statistical properties (structure factor and correlations) of physical systems, but also allows us to simulate energy barrier crossing dynamics, which cannot be captured by mean-field approaches.

Index Terms- Stochastic partial differential equation; Finite-volume; Fluctuating dynamical density functional theory

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