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Driven Langevin systems: fluctuation theorems and faithful dynamics DAVID SIVAK, University of California, San Francisco, JOHN CHODERA, Memorial-Sloan Kettering Cancer Center, GAVIN CROOKS, Lawrence Berkeley National Laboratory — Stochastic differential equations of motion (e.g., Langevin dynamics) provide a popular framework for simulating molecular systems. Any computational algorithm must discretize these equations, yet the resulting finite time step integration schemes suffer from several practical shortcomings. We show how any finite time step Langevin integrator can be thought of as a driven, nonequilibrium physical process. Amended by an appropriate work-like quantity (the shadow work), nonequilibrium fluctuation theorems can characterize or correct for the errors introduced by the use of finite time steps. We also quantify, for the first time, the magnitude of deviations between the sampled stationary distribution and the desired equilibrium distribution for equilibrium Langevin simulations of solvated systems of varying size. We further show that the incorporation of a novel time step rescaling in the deterministic updates of position and velocity can correct a number of dynamical defects in these integrators. Finally, we identify a particular splitting that has essentially universally appropriate properties for the simulation of Langevin dynamics for molecular systems in equilibrium, nonequilibrium, and path sampling contexts.

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