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Driven Langevin dynamics: heat, work and pseudo-work DAVID SIVAK, Lawrence Berkeley National Laboratory, JOHN CHODERA, University of California, Berkeley, GAVIN CROOKS, Lawrence Berkeley National Laboratory — Common algorithms for simulating Langevin dynamics are neither microscopically reversible, nor do they preserve the equilibrium distribution. Instead, even with a time-independent Hamiltonian, finite time step Langevin integrators model a driven, nonequilibrium dynamics that breaks time-reversal symmetry. Herein, we demonstrate that these problems can be resolved with a Langevin integrator that splits the dynamics into separate deterministic and stochastic substeps. This allows the total energy change of a driven system to be divided into heat, work, and pseudo-work – the work induced by the finite time step. The extent of time-symmetry breaking due to the finite time step can be measured and true equilibrium properties recovered. This interpretation of discrete time step Langevin dynamics as a driven process provides new insights into the practical use of stochastic integrators for molecular simulation.

David Sivak
Lawrence Berkeley National Laboratory

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