

Algorithms for ensemble control

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I will discuss stochastic-dynamical formulations and numerical integrators for simulating model systems under various thermodynamic constraints. Models ranging from molecular dynamics to coarse-grained particle dynamics to macro-scale models in fluid dynamics may be endowed with a statistical-mechanical interpretation which allows for a more faithful match with prescribed environmental conditions (e.g. thermostats in molecular dynamics). Once the model formulation is established, there remains the important challenge of designing accurate, stable and robust discretization schemes which faithfully capture the features of the underlying system. Numerical methods for stochastic differential equations typically have their own invariant measures which is an approximation of that of the SDE itself. By carefully combining suitable modelling devices and discretization schemes it is possible to obtain high accuracy and excellent asymptotic properties, such as diffusion rate.