Adaptive Brownian Dynamics

Benedict Leimkuhler, University of Edinburgh

Brownian/Langevin dynamics is among the most ubiquitous of models used in biology, chemistry and physics. In thermal equilibrium a fluctuation-dissipation relation regulates the temperature, but it is not always easy or even possible to parameterize the system a priori. I will describe the design of ``adaptive'' forms of Brownian and Langevin dynamics based in each case on an auxiliary control law, in the manner of a thermostat, as well as associated issues of ergodicity and numerical analysis. By extending the versatility of Brownian dynamics, the new formulations widen the range of potential applications in nonequilibrium and multiscale modelling. As an illustration, I will demonstrate the use of these methods for controlling flocking behavior in stochastic-dynamical particle models.