Antithetic Thermostat for Fast Computing Machines

Cristian Predescu, D. E. Shaw Research

Anton, a specialized supercomputer for performing molecular dynamics simulations, requires that particular attention be given to the implementation of integrators in which intensive variables, such as temperature, are controlled. Constant-temperature molecular dynamics methods are typically based on thermostats that minimally perturb classical dynamics. However, Anton, as well as certain other simulation codes and hardware platforms such as GPUs, store state information in reduced precision, which can cause numerical difficulties as intensive variables have vanishingly small fluctuations in the thermodynamic limit. Desirable thermostats for Anton and other fast computing machines must therefore be robust in dealing with reduced precision, must be fast enough to not impact overall speed, and must be faithful with respect to reproducing the canonical ensemble. These requirements led us to develop the antithetic thermostat, which is based on negatively correlating initial and thermostatted states. In this talk we will describe the thermostat's derivation and its features.