

Long time averaging for molecular dynamics simulations

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Many properties of chemical systems (such as the pressure inside a liquid, or radial distributions) are defined as phase space averages of functions depending on the state of the system. A common way to compute these averages is to use Molecular Dynamics and to compute time averages on long trajectories.

When considering systems at constant temperature, the problem amounts to finding a dynamics which is ergodic for the canonical (or Gibbs) measure. Many different methods have been proposed in this vein, some of them based on deterministic dynamics (Hamiltonian or not), some of them based on stochastic differential equations (such as the Langevin equation). We will review theoretical properties of some of these methods and compare their numerical efficiency on some simple examples.