6c Accelerated Molecular Dynamics

Kristen A. Fichthorn

A continuing challenge in chemical, materials, and biological simulation is to reach long time and large length scales, while accurately retaining atomic-scale detail. Molecular-dynamics (MD) simulations can provide accurate details at the atomic scale. However, MD is not practical for simulating times or distances far beyond the nano scale. In many systems (e.g., thin-film growth, catalysis at surfaces, protein folding), dynamical evolution occurs through a series of "rare events", in which the system spends a long time in one free-energy minimum before escaping and moving on to another. Since the localized motion in the free-energy minima is not important for many applications, dynamical evolution can be simulated as a series of jumps between minima. Simulations based on this strategy, such as kinetic Monte Carlo (KMC), can reach macroscopic times while, in principle, still retaining atomic scale accuracy. A significant challenge in simulating rare-event dynamics is to find the relevant free-energy minima and to catalog all possible jumps between them. While this has traditionally been done in the framework of transition-state theory (TST), none of the TST algorithms developed to date can ensure that all of the relevant rate processes will be found in a given system. Thus, research efforts have focused on the development of accelerated MD methods, which retain the accuracy of MD and are capable of reaching long times, comparable to those achieved in KMC simulations. In this talk, I will review the foundations of accelerated MD, including hyperdynamics, parallel replica dynamics, and temperature-accelerated dynamics. I will discuss problems presented by "stiff" systems and how these are dealt with in the framework of hyperdynamics. I will discuss the application of these methods to thin-film growth and future challenges in the development and application of these methods to problems in materials and biology.