219a Accelerated Molecular Dynamics Methods

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A significant problem in the atomistic simulation of materials is that molecular dynamics simulations are limited to nanoseconds, while important reactions and diffusive events often occur on time scales of microseconds and longer. Although rate constants for slow events can be computed directly using transition state theory (with dynamical corrections, if desired, to give exact rates), this requires first knowing the transition state. Often, however, we cannot even guess what events will occur. For example, in vapor-deposited metallic surface growth, surprisingly complicated exchange events are pervasive. I will discuss recently developed methods (hyperdynamics, parallel replica dynamics, and temperature accelerated dynamics) for treating this problem of complex, infrequent-event processes. The idea is to directly accelerate the dynamics to achieve longer times without prior knowledge of the available reaction paths. I will present some recent applications, including metallic surface growth, deformation and dynamics of carbon nanotubes, and annealing after radiation damage events in MgO, and discuss future challenges in the development of these methods.