Accelerated Molecular Dynamics Methods

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Many important materials processes take place on time scales that vastly exceed the roughly one microsecond accessible to molecular dynamics simulation. This time scale problem is quite general, showing up in many areas of chemistry, physics, biology, etc. Over the past 15 years, we have developed an accelerated molecular dynamics (AMD) approach, in which we let the trajectory itself find an appropriate way to escape from each state, but we coax it into doing so more quickly. In this lecture, I will give an introduction to these AMD methods, hyperdynamics, parallel replica dynamics, and temperature accelerated dynamics.