Multiple-Timestep/Particle-Mesh-Ewald Integrators for Biomolecular Dynamics

Tamar Schlick
schlick@nyu.edu
New York University and Howard Hughes Medical Institute, USA

Macromolecular simulations are increasingly demonstrating their value as a tool with which to study biomolecular structure and function. New algorithmic approaches are continuously needed to enhance the reliability of macromolecular simulations and increase their appeal and scope to experimentalists. Though a variety of simulation techniques are available, the molecular dynamics (MD) approach tops the list in popularity because of its physical appeal and biological connection. MD's popularity would be overwhelming if the technique's computational demands, and hence biological scope, were not so limited for large systems. This limitation stems from the numerical stability requirement, which restricts the timestep size used for integrating the equations of motion to a relatively small value (e.g., $\sim$1 fs). In my talk, I will present recent work on developing efficient long-timestep methods for MD applications that employ particle-mesh Ewald (PME) formulations for long-range electrostatic interactions. The apparent difficulty in optimizing multiple-timestep/PME combinations is that the reciprocal term — which should isolate long-range slow forces — contains significant force contributions from near-field particle interactions. Recent ideas based on alternative mathematical formulations, or a combination of distance and energy-component criteria for defining the force classes, will be presented, as recently incorporated into the AMBER modeling software package.