Enhancing the stability of mollified multiple time stepping integrators

Jesus A Izaguirre
izaguirr@cse.nd.edu
University of Notre Dame, USA

This talk will present recent results in achieving long time steps using symplectic multiple time stepping integrators. Mollified variants of the Verlet-I/r-RESPA have consistently shown a 50% increase in the length of the maximum stable time step possible for comparable levels of accuracy over Verlet-I/r-RESPA. Mollified methods perturb the potential by evaluating the long range forces at time averaged positions, while the method remains symplectic by making the force a gradient of the perturbed potential. It is believed that long time steps at least an order of magnitude greater should be possible. However, stability remains the main limitation to the application of multiple time stepping methods that fully exploit the separation of time scales of biomolecular simulations, even the mollified variants of Verlet-I/r-RESPA. We will consider the effect on enhancing the stability, and thus lenghtening long time step of multiple time stepping methods through several improvements to current mollified methods: (i) the use of better averagings, which include more vibrations; (ii) the use of more stable forms of the innermost integrator, i.e., the position form of leapfrog instead of the velocity form. Recent work by Batcho and Schlick has shown analytically that the position form is more stable for long outer time steps; (iii) the use of more accurate integrators in the context of mollified methods, in particular Rowlands method. Some analytical and numerical results of stability, accuracy, and computational efficiency will be presented for simulations of solvent and solvated biomolecules. This describes work done in collaboration with Qun Ma and Robert Skeel.