Integrators and Ensembles

1/1/2009

Opening Discussion

- Do you have any questions?

Revisiting Verlet

- The preferred method of integrating MD simulations is using one of the Verlet integrators.
- These are all symplectic which is required given the number of time steps that have to be done.

$$X_{n+1} = 2\mathrm{X}_n - X_{n-1} + \Delta t^2 \tilde{F}_n$$

Leapfrog

- The leapfrog is actually a derivative of the Verlet algorithm.
- A proper leapfrog gets that name because it takes a half step, then has a kick, then takes a half step again.

$$V_{n+1/2} = V_{n-1/2} + \Delta t \tilde{F}_n$$
$$X_{n+1} = X_n + \Delta t V_{n+1/2}$$

Velocity Verlet

- This is another variation. This can be described by a set of equations that also described the leapfrog, but is often written in a different way.
- This version is commonly used because forces are only applied at ends of steps.

$$X_{n+1} = X_n + \Delta t\, V_n + \frac{\Delta t^2}{2} \tilde{F}_n$$

$$V_{n+1} = V_n + \frac{\Delta t^2}{2} (\tilde{F}_n + \tilde{F}_{n+1})$$

Position Verlet

- The last common derivative of the Verlet integrator is the position Verlet.
- This version apparently has some advantages for long time steps.

$$X_{n+1} = X_n + \Delta t V_n + \frac{\Delta t^2}{2} \tilde{F}_{n+1/2}$$

$$V_{n+1} = V_n + \Delta t \, \tilde{F}_{n+1/2}$$

Constrained Dynamics

- To increase time step lengths, methods have been developed where bond lengths are constrained to their minimum energy position.
- These require iterative solution after the normal integrator step, but allow significantly longer step sizes.
- Appears useful for bond lengths, but alters dynamics when used for bond angles.

Ensembles

- The methods discussed so far technically only work for systems with constant energies and volumes. Some systems of importance have other constraints such as constant temperatures.
- These need slightly modified approaches. They are still based on Verlet.

Potentials and Forces

- Because some of you might decide you want to do a simulation of a molecule, I figure we should spend a little time in class looking at potentials and deriving forces from them.
- Bond lengths aren't hard. The more challenging part is the bond angles and other potentials.

Minute Essay

- Questions?