More MD

3/30/2009

Opening Discussion

- What did we talk about last time?

Integrating MD

- At its heart, MD uses the same types of techniques that we have talked about before for solving continuous systems.
- We have ODEs that we solve on the positions and velocities of the particles. In MD they tend to work with potential energy fields rather than directly with forces.

$$M\dot{V}(t) = F(x) = -\nabla E(X(t)) + \ldots$$
$$\dot{X}(t) = V(t)$$

Potentials

- Bond length potentials
  - To first order we can do Hook's law (quadratic potential) on bonded particles.
- Bond angle potentials
  - Bond angle potentials can be modeled as quadratic potentials or by trig functions on bond angles.
- Torsional potentials
- Non-bonded potentials
  - Van der Waals or Coulomb

Static vs. Dynamic

- It is possible to do static MD.
- This simply takes a configuration of atoms and uses an optimization technique to find the point of lowest energy.
- Dynamic simulation is typically more informative.

Range of Scales

- Spatial ranges
  - Atomic vibrations are much smaller than the size of full macromolecules.
- Timescale ranges
  - The real challenge is timescales.
  - Vibrations have fs timescales. Integrators need to take 0.1-1 fs timesteps.
  - 1e6 timesteps for just 1 ns.
  - Biological processes are on much linger timescales.

Initial Conditions

- Structure
  - Have to get atoms in the right places.
- Solvation
  - Typically surround with salt water.
- Velocity
  - Want $E=k_BT/2$. Pull from Gaussian distribution.
  - Subtract out average to get stationary center of mass.
- Equilibration

Computational Choices

- Chaos
  - These systems are chaotic so you aren't trying to predict exact behaviors.
  - Limited phase space means deviations saturate.
- Statistical view
  - Results should be taken from a statistical viewpoint. They describe rough behaviors.
  - Time averaging helps to give properties.

Computational Complexity

- Less work per step
  - Find ways to do less work in each timestep.
- Longer timesteps
  - Take longer timesteps. Runs into problems of resolving certain aspects of the system.
- Multiple-timestep (MTS) schemes
  - Use longer timesteps for types of interactions that don't need really fast interactions.

Verlet Integration

- MD systems must be integrated with symplectic methods because of the broad range of relevant timescales.
- The basic integrator they like to use is the Verlet integrator and derivatives of it.
- The formula below gives the position update Verlet algorithm which is fourth order accurate. The velocity is gotten with a central difference and is second order.

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

Minute Essay

- Any suggestions for what I should put on the last assignment?