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.

\[
M \ddot{V}(t) = F(x) = -\nabla E(X(t)) + \ldots \\
\dot{X}(t) = V(t)
\]
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 $E = k_B T/2$. 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.

\[ X_{n+1} = 2X_n - X_{n-1} + \Delta t^2 M^{-1} F_n \]
Minute Essay

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