MD Implementation

4/3/2009

Opening Discussion

- What did we talk about last time?

- If you are doing something interesting for assignment #5 you can take extra time on it.

- Minute Essay comments

  - Was class good?

  - Would simulating an enzyme in solution be too much?

Gradient of Bond Angle Potential

- Last time we calculated the gradient of the bond length potential to get something that could be put into code.

- At the end of class we were discussing how a potential with cosines had a close relationship to the dot product.

- Let's try to take the gradient of that potential today.

Implementation

- I'd like to begin the process of writing an MD simulation. While Law is quick to remind us that simulation is not just an exercise in programming, we do have to be able to program it in order to get a simulation.

- I want to take an approach that is similar in many ways to what we did for the cloth mesh, but with additional capabilities.

Minute Essay

- Do you want to hear about integrator details next class or should we continue with our implementation and try to get something simple we can visualize?