Molecular Dynamics

3/27/2009

Opening Discussion

- Do you have any questions about the quiz?
- Do you have any questions about anything?
- On the minute essay last time I was interested to see that the only things people are using are Excel and SwiftVis. Obviously, SwiftVis isn't widely used so that is just because people have worked with me some. I was expecting Matlab, Igor, IPL, or perhaps others to show up.

Movie of Cloth

- Before we go into molecular dynamics, I want to show a movie that I made of a 3-D rendering of that cloth simulation Chris showed us last time.

Molecular Dynamics

- The idea of molecular dynamics is simple and dates back to Laplace in the early 1800s.
- If you understand the force laws that govern particles you should be able to predict what they will go.
- Laplace's vision was tarnished by both the chaos discovered by Poincaré and later the non-determinism of quantum mechanics. However, the idea of simulating the basic pieces of matter lives on.

Basics of MD

- At its heart, MD is very similar to the cloth mesh. It is an N-body simulation of atoms.
- Standard MD uses Newtonian mechanics. It only considers the nuclear motions of the atoms.
- This causes limitations. To make sure everyone is on the same page here, let's go back over High School chemistry/physics and talk about the structure of matter.

Structure of Matter

- As far as chemists are concerned matter is made of atoms.
- Atoms have protons (positive charge) and neutrons (neutral charge) in the nucleus and are surrounded by a cloud of electrons (negative charge).
- The nucleus is much more massive that the electrons.
- Bonds.

Minute Essay

- How much of this stuff about how atoms work do you know? Any quantum mechanics?