Proposal Summary

(To be written after the paper)

Project Description

Why is it important?

Finding better ways to simulate simple homogeneous and inhomogeneous fluids will allow us to study the fluids and predict how they may act without spending vast resources on physical experimental setups. For example, scientists have the capability of taking fluids down to very cold temperatures, but it takes large amounts of energy to do so. If we find a reliable simultaion that can be used instead, computers can be tasked at running the simulations in many configurations. This will save the energy required to physically test the configuration.

Why Soft Spheres?

Currently hard sphere simulations are widely used (Verify) and can give decently accurate results, but are still not as accurate as we like. (melting point x2?-Verify and add) Hard sphere simulations are limited in capabilities. Hard spheres have either 0 or infinite potential interactions, they are either touching or not and are not allowed to overlap. One way to attempt to improve the model is to allow the spheres to overlap or soften their edges. By taking the basis of the hard sphere model, and applying a potential interaction to the spheres we hope to find a better more accurate model for fluids.

Current Focus

A Monte-Carlo program is being modified to simulate a soft sphere theory. The data will be used to verify a density functional theory for soft spheres. (Density functional theory-What is it? Add info)

Future Plans

The Monte-Carlo simulation could be used to test fluid transitional characteristics. By holding the temperature fixed and plotting pressure as a function of the number of spheres used, the phase transition of the simple fluid could be analyzed. The plot should show a line of pressure of which the number of spheres below it will be in a loose flowing state, and the shperes that show pressure data above will be in a more crystalline shape.

Timeline

Ongoing Tasks

- Debug code.
- Create code to plot and analyze data.

July 2013

- Run homogeneous soft sphere Monte-Carlo for low densities in order to calculate g(r) and compare with analytic low density equation.
- Run homogeneous soft sphere Monte-Carlo to obtain pressure data at various temperatures and densities.

August 2013

- Debug code.
- Compare pressure data to vivial expansion to verify correct theory.

September 2013

- Run inhomogeneous soft sphere Monte-Carlo near hard walls with different packing fractions and temperatures to find density equatioins n(z).

October 2013

- Run more inhomogeneous soft sphere Monte-Carlo near hard walls to figure out the number of spheres needed to obtain round number densities.

November 2013

- Run inhomogeneous soft sphere Monte-Carlo with a spherical inner wall.
- Compare Monte-Carlo resutls with the DFT results.

December 2013

- Alter soft sphere Monte-Carlo to handle soft walls and/or walls with attraction.

January 2014

- Begin studying DFT side of research.
- Run DFT code.

References Cited

(To be added later.)

Interesting DFT Resource, may or may not use

http://www.uam.es/personal_pdi/ciencias/jcuevas/Talks/JC-Cuevas-DFT.pdf

Facilities, Equipment and Other Resources

The similation programs and data are stored and executed from a secure redundant backup system.