

# Proposal Summary

To be written soon.

## Project Description

### Current Work

The group I am researching with is studying simple fluids by using Monte-Carlo simulations to verify density functional theories.

Finding better ways to simulate simple fluids in homogeneous and non homogeneous configurations will allow us to study the fluids and predict how they may act without spending vast resources on actual experimental setups. For example, we as scientists have the capability of taking fluids down to very cold temperatures, but it takes large amounts of energy to do it. If we find a reliable simulation 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, and potentially, the time and space required to set up the simulations.

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. (possibly add graph-Look into and add)

(Hard sphere's used a lot, soft spheres are relatively new? Need to verify this.)-Verify and modify.

I am taking a Monte-Carlo program and modifying it to simulate a soft sphere theory. The data I take is being used to verify a density functional theory for soft spheres. (Density functional theory-What is it? Add info)

### Future Plans

Potentially the Monte-Carlo simulation can 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 somewhat clear line of pressure of which the number of sphere's below it should be in a loose flowing state, and the shperes that show pressure data above should be in a more crystalline shape.

## **References Cited**

(To be added later.)

## **Facilities, Equipment and Other Resources**

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