Project Assignment Number One

In homework assignments 1 and 2, you have performed classical molecular simulations to reproduce results of a liquid and solid respectively. In this project, you face a similar task. However, you must identify your own system of interest to simulate.

Ideally, your choice will provide a first step toward a more sophisticated simulation, which is new to science, to be performed in project two. Hopefully, both projects are related to your graduate research. You are encouraged to consult your advisor.

Four items must be turned in. The first item is a project statement and is due before you begin any simulations. The last three items are due at the end of the project.

Due at Beginning of Project

1. Project Statement (please keep to one page)

- Identify system to be simulated.
- Identify published reference paper containing the simulation results that will be reproduced.
- Identify the number of atoms to be simulated.
- Identify the duration of the simulation.
- Note any special features required.

Due at End of Project

2. Brief Report

The report must contain the following sections.

- abstract
- Brief introduction and motivation to problem
- Simulation Methodology
- Results and Discussion (including comparison with literature)
- Conclusion
- Reference(s)

Target length. Brevity is fine. I estimate, this could be done in 10 to 12 paragraphs.
Append your LAMMPS input files.
There is no need to attach lengthy output.
Submit the report as a pdf file electronically through the blackboard system.
Please do not submit a paper copy of this report.

3. Mini-Poster

We will have an in class poster competition. Students will evaluate posters. Top three student-chosen winners will received an automatic "A" for the poster component of the project. Students can choose their own poster template or use the one provided on the course website.

4. Web page

Using the template provided on the project website, provide a customized HTML file and an interactive xyz file.

Submission Requirements

Bundle report (pdf), poster (pdf) and html and xyz file into a zip file and submit through blackboard.

Grade Distribution

- Project Statement 10%
- Report 40%
- Poster 40%
- Webpage 10%