ISC 5935
Computational Materials Science
Fall 2013

Course Project

Due: Thursday, November 28

1 Overall

The course project may be done individually, or in teams of two. For teams, I set expectations at a correspondingly higher bar. It is advisable to form teams soon, so that you may be able to collectively brainstorm potential topics.

The project is worth 20% of the overall grade.

2 Submission

The project should be submitted as a single zipped folder to me via email (`sshanbhag@fsu.edu`) by midnight of the due date. The folder should contain a project report (in PDF format), and optionally, other miscellaneous files (programs, movies, etc.)

3 Project Topics

I am *very* open to potential topics. The only loose requirement is that it should have some element of "computation" (molecular dynamics, Monte Carlo, or density functional theory) and some element of "materials". Overlap with material covered in class is not necessarily required.

I suggest that you run your project idea by me to assess its suitability.

Your project can be:

(a) *Survey of methods for a particular class of materials*: For example, suppose you are interested in the mechanical properties of carbon nanotubes. You can survey the literature for the different computational methods used to study this system, and critically evaluate the advantages and disadvantages of different approaches.

(b) *Recalculation of a historically important paper*: You could critically survey a single historically important paper in MD, MC, or DFT, and write code to reproduce those results. A non-exhaustive list of such seminal papers may include:

- Metropolis, N., et al. "Equation of state calculations by fast computing machines." J. Chem. Phys. 21 (**1953**): 1087.
- Wang, J-S, and R. H. Swendsen. "Nonuniversal critical dynamics in Monte Carlo simulations." Phys. Rev. Lett. (**1987**): 86-88.
- Alder, B. J., and T. E. Wainwright. "Studies in molecular dynamics. I. General method." J. Chem. Phys. 31 (**1959**): 459.
- Rahman, A. "Correlations in Motion of Atoms in Liquid Argon." Phys. Rev. A 136(2A) (**1964**)

- McCammon, J. A., B. R. Gelin, et al. "Dynamics of Folded Proteins." Nature 267 (**1977**): 585-590.

(c) *A "novel" implementation*: You can implement many of the things we may have glossed over quickly in class. Examples include comparison of different integration algorithms for a particular system, different ensembles, order-N methods for autocorrelation functions, simulated tempering, building cell and neighbor lists etc.

(d) *Use software to solve a non-trivial problem*: Many open-source software can solve a wide variety of materials problems using MD and DFT problems. You could pick a problem that is of interest to you from a research point of view, and see if you can solve it.

(e) *Comparison of different software*: A wide variety of software for simulation and visualization are freely available. You could benchmark, and survey their strengths and weaknesses, and perhaps use them on a standard problem.

(f) *A good critique of an important scientific paper or method*: You don't have to implement the method necessarily.

The list above is not comprehensive.

4 Grading Rubric

I will use the following rubric to grade the project:

- topic/motivation/tool (30%),
- analysis/critical review (40%)
- clarity/quality of report (30%)

Note that there are no points for "quantity" of pages in the report. A good project report should not be a "core-dump" of random facts culled from the internet or scientific literature. You have to engage with the material critically, and present your findings and opinions in a cogent and analytical manner.