Weekly Report **Piyush Divyankar**
Dual Degree Project 2016-17
Prof. M.P. Gururajan Date: 26/09/2016

Problem Statement

Topic: Monte Carlo simulation of interfacial energy calculation in solid-solid systems
The topic is self explanatory. Apart form that, it is of note that I am currently working on Ni-Al systems. I am investigating the properties of system that statistically converge.

Model of the system

We are trying to model Ni-Al systems. It my underlying assumption that the crystal structure of the system is FCC at all temperatures and compositions. It should be this assumption is wildly inaccurate. However the code that I have written provides a possibility of accommodating different crystal structures, but it can't account for the transformation of structures yet.
The crystal consists of atoms that interact with each other, and they lead to a bond energy. This bond energy is modeled using embedded atom method. The embedded atom method is applied to up to 7 nearest neighbors to calculate bond energy of the atom. This i believe is overdoing it. If number of nearest neighbors can be reduced without sacrificing much accuracy due to the size of the unit cell. beyond a certain neighbor it makes little contribution, and eats away at the computation time.

Code base

EAM data model can be read and it is possible to calculate energies of all atoms. Crystal structure and other simulation inputs have been modeled and tested to be functional. Two phase equilibrium simulation seems has been written but it seems unable to run for larger systems. The system performs all operations that are subroutines of the simulation in constant time. It can be safely said that code is running in linear time.

New Ideas to Implement

The amount of RAM it takes to load a crystal structure information is an integer array, i.e $64 * sizeof(int)$. The information we load is binary, so we can store 64 atom information in one integer value. This will reduce the load on memory by 64 times. Making it possible to load larger systems efficiently. There is a chance that this method of doing things will make code run faster.

Ongoing activity

- Trying to make two phase equilibrium simulation to generate ensembles.
- Analysis code to be written(not sure what).
- Thermodynamic integration functions for the ensembles.

P.S

Disclaimer:Following are my personal opinions.
I would like to suggest a few things that we should do as a group, which I believe would create value in the long run.

- Documenting the code base, and an online method to host them. The objective of writing code is that nobody else has to rewrite it. This purpose can't be served if it isn't documented.
- GitHub organization of our lab. This make sharing code and tracking changes much more easier.
- Report be made in article format. Various organizations have long since stopped making presentations. I presentations believe are good for presenting your work, however terrible when you are revising. I believe that will increase our efficiency.