Monte-Carlo Simulations of Interfacial free energy in γ/γ' interfaces in Nickel-Aluminium Alloy

DDP Phase 1 Presentation

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Outline

Nickel Aluminium alloys

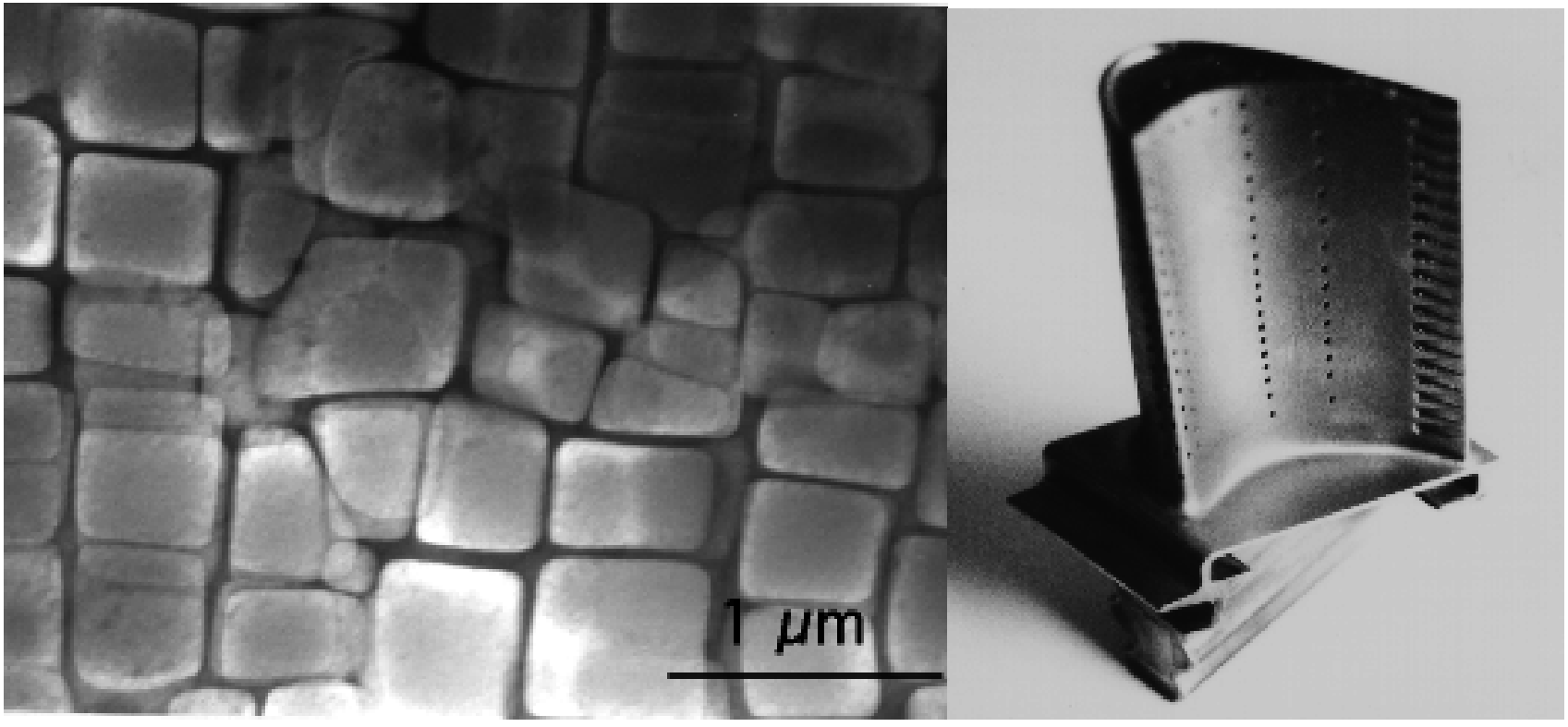

Figure: On the left we a microstructural image that is representative of situation in Ni-Al Superalloys. On right we see a practical application of this Technology, the turbine blade.

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How Do we look at Interfaces?

Capillary Wave Model

This is a model to explain behaviour of interfaces at a microscopic scale. At microscopic state systems can't be have fault free interfaces. This model tries to describe rough interfaces at microscopic scales[2].

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Lemma

The surface energy as a function of angle is given by Taylor Series expansion[2].

$$\sigma(\theta) = \sigma(0) + \sigma'(0)\frac{d\sigma}{d\theta} + \kappa\sigma''(0)\frac{d^2\sigma}{d\theta^2}\ldots \tag{1}$$

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Method of computation

Monte Carlo Method

Principle of Ergodicity

This is a core assumption is statistical physics. This states that given enough time a system will visit all the possible states in the ensemble[1].

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Key points about MC algorithm.

- Statistical sampling technique.
- Good at computing stationary distributions.
- Computation resource enables solving very complex problems.
- Importance Sampling

Outline

Appropriate representations of the system

Properties of the solid-solid alloy systems.

- Precipitate of γ' in γ matrix.
- We wish to study small angle fluctuations of this interface.
- We define that there is a constant temperature.
- Stability of interfaces means that we need to have constant 'μ' across interface.
- Volume is also assumed to be constant(practically not true).
- A reservoir constraint.

Putting This together Mathematically

Gaussian Ensemble Distribution

$$P = A \exp\left[-\frac{E - \mu N}{k_B T_0} - R(N - N_0)^2 \right] \tag{2}$$

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Explanation

What do various terms account for?

- $A \rightarrow$ normalization constant
- $E \rightarrow$ internal energy or bond energy.
- $\mu \rightarrow$ chemical potential.
- $\mu N \rightarrow$ energy due to chemical potential difference.
- $R(N - N_0)^2 \rightarrow$ reservoir constraint. Controls how far system can deviate form a fixed value.

Outline

Atomic Potential

Embedded Atom Method

This is a type of bond order potential. This takes into account along with pairwise repulsion of nuclie, the screening effect of the electron cloud.

$$E_{tot} = \frac{1}{2}\sum_{i,j}\phi_{ij}(r_{ij}) + \sum_{i}F_i(\bar{\rho}_i) \tag{4}$$

$$\bar{\rho}_i = \sum_{i \neq j}\rho_i \tag{5}$$

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Finnis-Sinclair Potentials[3]

These are called as such. We are using a model that was developed for solid-solid systems, known as Embedded Atom Method.

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System Specs

We currently are testing and developing the software environment. Following are the specs of the code base.

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- Programming Language: GNU-C
- Plotting: GNUPLOT, Octave
- Version Control: GitHub.
- Libraries: Standard C library, GNU Scientific Library.

Most of simulation code and related functions were independently developed.

Outline

Relevant Information

There is a need to organize data in computer systems for efficient storage and access. First we identify relevant information.

- Atoms modelled as a Ising type solid[4].
- Potential energy in tabulated form
- Simulation parameters in organized structure.
- Relative translations for neighbour coordinates.
- Some universal constants

Atoms

We store atom type as a binary state in a linear array.

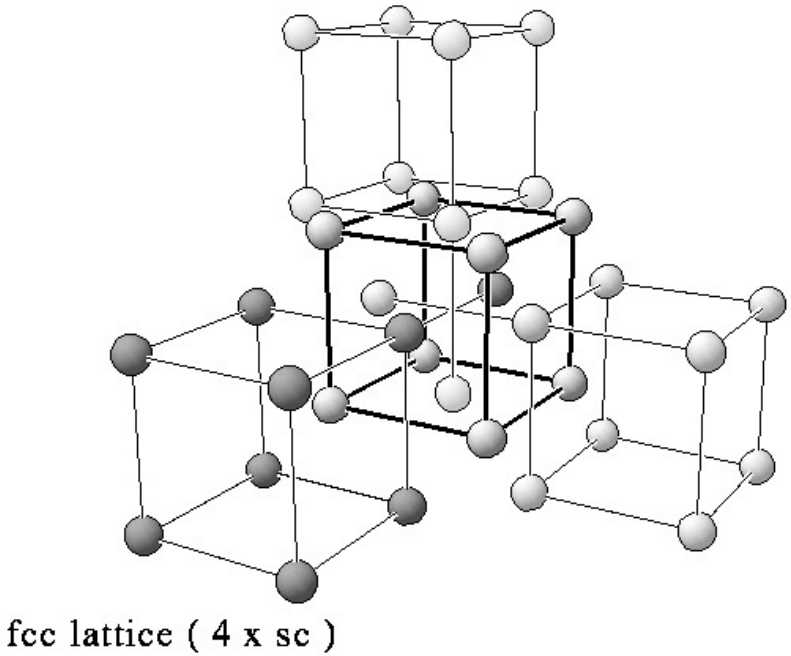

Figure: An FCC can be seen as 4 inter-penetrating cubic lattices.

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- Space for storage
- Efficient Methods used
  - Creation of energy tables.
  - Avoiding repeatative calculations.

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- Lattice parameter.
- Type of lattice.
- Temperature
- Pressure.
- Concentration.
- Reservoir parameter.

Constants are trivially stored as constant identifiers.

Outline

Implementation of Monte-Carlo

Algorithm

Following describes in general all Monte Carlo simulations

- Make a random change is current configuration.
- Calculate energy change for this change as ΔE.
- Accept the new configuration with probability.

$$P = min\{1, \exp(-\Delta E / k_B T)\} \tag{8}$$

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$$P = min\{1, \exp(-\Delta E / k_B T)\} \tag{9}$$

The algorithm described above is essentially **Metropolis Sampling**[5]. In this we can change the form of energy to obtain a reliable sampling of thermodynamic ensemble.

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Relative Neighbour Coordinates

In a solid lattice the neighbourhood of an atom determines its energy. It happened to be necessary to have relative coordinates of neighbours.

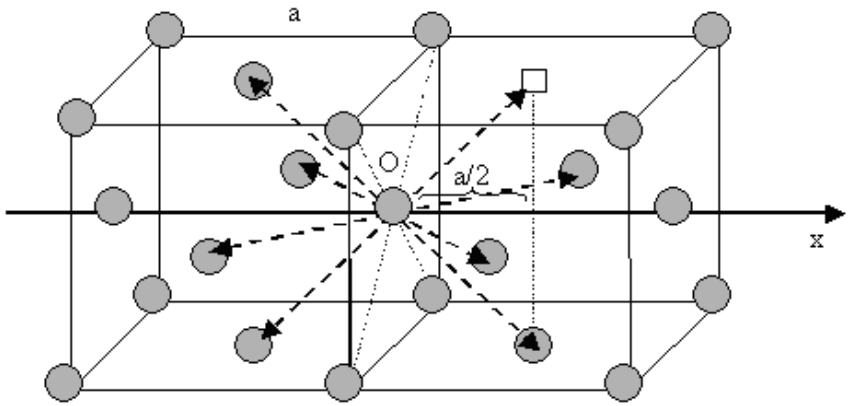

Figure: Here we can see 12 nearest and 6 second nearest neighbours.

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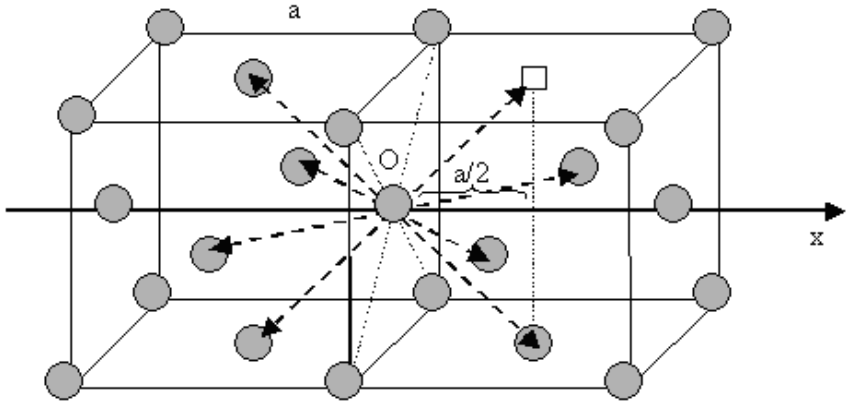

Figure: Here we can see 12 nearest and 6 second nearest neighbours.

We have calculated relative coordinates for nearest neighbours for upto 7th nearest neighbours. We store these as an array of form triple doubles (x, y, z). These represent points or vectors in 3D space.

Outline

Energy Calculation

Methodology

- Obtain type of atom at current site.
- Transform array index to global coordinates.
- Iterate over nearest neighbours
  - Compute global coordinate of neighbour.
  - Transform 3D coordinate to array index to see atom at that site.
  - Compute pairwise energies.
  - Compute electron density due to neighbour.
- Use electron density to compute Embedding Energy.
- Total energy is sum of embedded energy and pairwise energies.

Energy Tabulation

Observations

- An atom in the system can have only some fixed energies.
- This is given by neighbourhood of atom.
- We state that it only depends on number of atoms of each type at different distances.
- We have a lattice, so these values won't change.

Energy Table Advantages

- Fast simulation.
- Energies computed a only once.
- Better ensemble average.

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- **Purpose of benchmarking is to ensure that we are using correct data that model natural processes to a defined degree of acurracy.**

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Lattice Parameter Simulation

We tried to calculate the lattice parameter for Ni-FCC crystal.

Methodology

This was done by calculating energy of one atom using its 3rd nearest neighbours.

1. Making a random change in a set range $(-\Delta a, \Delta a)$ to the lattice parameter.
2. Calculating energy for the change.
3. Using Metropolis algorithm in 3.3 we determine whether to accept that change.

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Hypothesis

If the potential is good representation of internal energies then we should get lattice parameter close to the benchmark values[6].

Plot for Ni-FCC

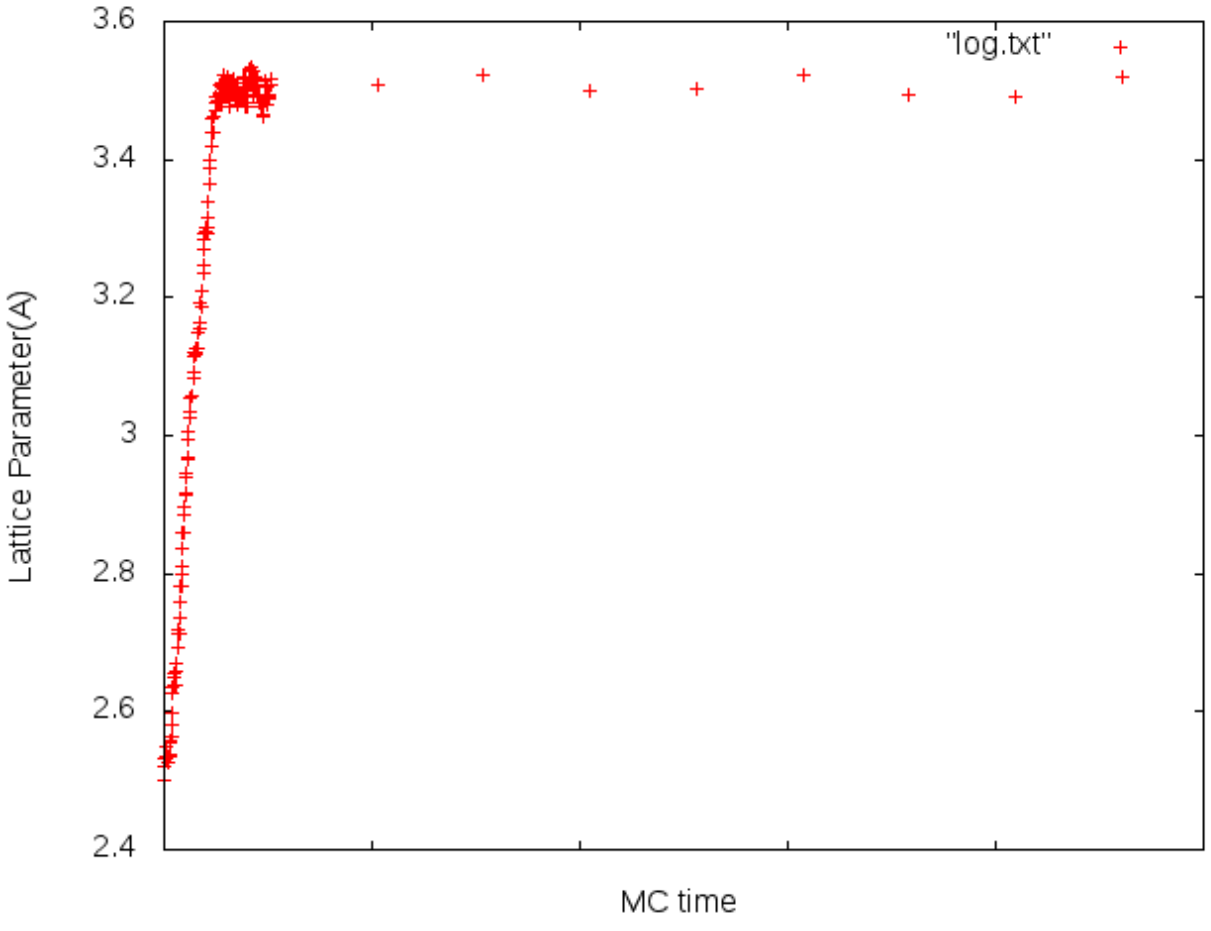

Figure: This shows convergence of Lattice parameter with increasing sample size.

Plot for Al-FCC

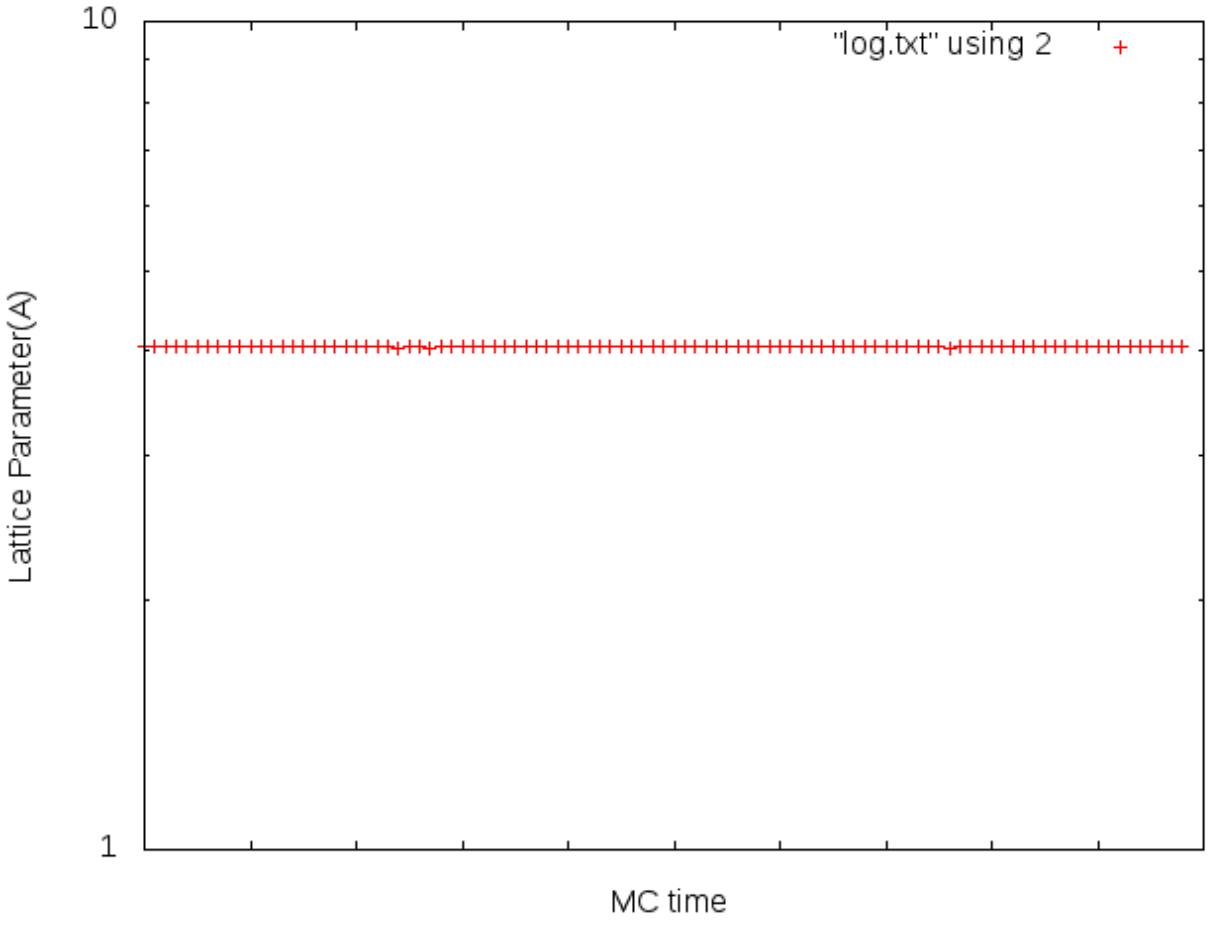

Figure: This shows convergence of Lattice parameter with increasing sample size.

Agreement with standard benchmark

The simulation was run at 3 different seed random numbers and their results are tabulated. For comparison are results availble with the used potential for benchmarking[6].

Computer Values	Variance	Benchmark Values
3.5204	0.0014971	3.519
3.5211	0.0015782	3.52
3.5199	0.0014812	3.521

Table: Table for Ni-FCC(All values in Angstrom($10^{-10}\mathrm{m}$))

Computer Values	Variance	Benchmark Values
4.0498	0.015209	4.045
4.0410	5.7e-06	4.05
4.041	5.7e-6	4.055

Table: Table for Al-FCC(All values in Angstrom($10^{-10}\mathrm{m}$))

We have excluded the discussion of **Random Numbers** that are very essential to functioning of Monte Carlo Code.
We have used GNU-GSL random number generator. This has a **period of** 10^{134} and very low autocorelation, covariance etc.
Hence, this is a good random number generator.

Future Work

In future we would like to do following things

- Test and benchmark *Gaussian Ensemble*
- Evaluate the equilibrium concentration profiles around interfaces.
- Use these concentrations to compute curvature of the interface.
- Extend this model to other coherent systems interfaces.
- Using interfacial energies to look at phase transformations in Ni-Al systems

Future Work

We would also like to make following improvements to our software

- Storing probability transition matrix for the state space.
- Parallel threading to increase computation power to sample larger part of ensemble.
- Storing atomic matrix in form bit instead of integers.
- More benchmarking for other phases.
- Trying to incorporate lattice parameter mismatch in energy calculations.
- Determination of defect energies in these systems.

Objectives for Future Work

- We have currently developed the basic software and analysis tools. This will help us focus more on physics part of the problem.
- We intend to explore possible uses and extensions of this method.
- Reducing error in our calculations is a key objective.
- We intend to explore different sampling techniques to better approximate our system.

Summary

- The Ni-Al Superalloys are of great importance to industry. Improvement in understanding of underpinning thermodynamics can lead to improvement in design and fabrication of these alloys.
- The Monte Carlo Method is used to study these systems. This is reliable model for computation, although, it isn't a good model for physical world.
- I have discussed most of code development process and the understanding that went into it.
- I have shown the benchmarking results and compared them to published ones.
- Finally, I have discussed future plans and vision for the project.

For Further Reading I


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