

Summary Report (09), 7th Apr, 2014

Introduction to Statistical Mechanics

1. Review on last report

Last report was a summary on doing water molecular simulation and running MSCGFM.

2. Objectives of last week work

To install MSCGFM programs in our cluster and study some reading materials.

3. New progress/results/summary

3.1. About MSCGFM

- Installation of MSCGFM is recently the bottleneck of the project
- The "install" file still cannot be found and we are now contacting the original writer of this program for it.
- Simultaneously, I am trying my best to learn how to install it without that file.
- The bashrc file of the cluster has been studied.

3.2. About Reading Material

- To enhance my theoretical background for this MD simulation
- The following softcopies has be obtained from the internet and a big picture of them has been obtained:
 - i. Introduction to Modern Statistical Mechanics, David Chandler
 - ➔ Some of the content about MD simulation has been covered by the previous course that I have taken, AP6172 (Different ensembles, Monte Carlo Methods, $g(r)$, etc.)
 - ➔ Thermodynamics is my weakness and should be focused, since it's highly related to my project.
 - ➔ Some simple examples are listed to facilitate learning on abstract concepts.
 - ➔ Some content specifically about gas and solid simulation can be ignored.
 - ➔ I think the following chapters are to be intensively studied in the next week:

CH1, about thermodynamics
CH2, about equilibrium conditions
CH3, ensembles and the Gibbs Entropy Formula
CH7, more details on fluid
CH8, non-equilibrium system

- ii. Understanding Molecular Simulation, from algorithms to application, Daan frenkel et al.
- ➔ Some content is overlapped with the previous book but more detailed (Free energy, Gibbs Ensemble, Monte Carlo Methods, etc.)
 - ➔ Again, content about solid and gas can be ignored
 - ➔ Content about long-range interact isn't important (as CG usually ignores)
 - ➔ Not included in the previous book but important: Tackling time-scale problem, sampling methods and rare events
 - ➔ Study the previous book first

4. Objectives and plan for next week

- Finish MSCGFM installation
- Examine it and analyse the result
- Continuous reading on the mentioned reading materials

5. References

- *MSCGFM Codes, Lanyuan Lu et al.*
- *Introduction to Modern Statistical Mechanics, David Chandler*
- *Understanding Molecular Simulation, from algorithms to application, Daan frenkel et al.*
- *COMBO, Things You Need to Know*