MSE 402: Computational Process Design

Sem 1 - AY 2024-25

21/09/2024

General requirements:

Please label plots clearly, with appropriate units.
Answers are to be submitted in a single PDF file named 'first name_last name.pdf' generated using Latex (preferred) or any other word processing software. For e.g., if your name is Abdul Kalam, please save the file as 'Abdul_Kalam.pdf'. File has to be uploaded on Google Classroom by the due date (and time). You need not attach any code.

Assignment 2: Monte Carlo Simulations using LAMMPS and Cassandra
(Max score:100)
Due: 08/10/2024 by 11:59 PM

Q. No. 1: What are the key differences between Molecular dynamics and Monte Carlo simulations in terms of methodology and outcomes? How does the Metropolis algorithm function within the context of Monte Carlo simulations, and what role does it play in generating sample configurations? **(20 Marks)**

Problems based upon Simulation:

Q. No. 2: Two different types of Polymer beads or chains are considered. The task involves studying the miscibility of these two different polymer beads using Molecular dynamics with **Swap Monte carlo (SMC)** algorithm. A fix called "**mol/swap**" in LAMMPS is used to perform the Monte carlo swaps of one polymer bead with another. The system is modeled using Lennard-Jones potential by varying the values of "epsilon" for cross interaction (Interaction between type 1 and type 2).

a) Read about the "**mol/swap**" command in LAMMPS documentation and write down its application in molecular simulations. **(5 Marks)**

b) Run three different simulations with "epsilon = 0.1, 1.0 and 1.1" and write down your observation on the miscibility of two systems. Attach the visual representation of the last frame for all three different simulations. Plot the variation of the number of particles of Type1 and Type2 in all three simulations wrt time. **(15 Marks)**

Q. No. 3: The task involves studying the absorption of water molecules on amorphous silica using the **grand canonical monte carlo algorithm (gcmc)**. This is invoked in LAMMPS by using the fix "**gcmc**" command, which performs the grand canonical monte carlo simulations by exchanging the number of atoms or molecules with an ideal system/reservoir at a fixed temperature and chemical potential. The problem is divided into two parts. The first part is used to insert/delete water molecules using gcmc in a simple cubic box until it reaches a density of 1 gm/cm^3 and no more addition or deletion of water molecules is permitted. Second part is related to the adsorption of water in the siliia crack.

a) Plot the variation of density, number of hydrogens and number of oxygens wrt time. Attach the snapshot of the initial and final frame. **(10 Marks)**
b) Run the script that generates a crack in the amorphous silica. Attach the initial and final frame visualization. Following this, run the final script that executes water addition/deletion in the crack formed. Attach the final frame visualization. Plot and analyze the variation of energy and the number of water molecules absorbed in the crack wrt time. **(10 Marks)**

Q. No. 4: The **Ising model** is a mathematical representation of ferromagnetism that uses a lattice of discrete variables (spins), which can be in one of two states (+1 or -1/up or down). Each spin interacts with its neighbors, and the model captures how these interactions affect the spin alignment and phase transitions, particularly as the temperature changes.

a) Plot the variation of energy and magnetization as a function of temperature. Identify the critical temperature (Tc) point and discuss the influence of increasing temperature on the alignment of spins. Attach visualization of three different phases of Ising model: paramagnetic (T>>Tc), critical(T=Tc), and ferromagnetic (T < <Tc). **(15 Marks)**
b) Analyze the variation of energy fluctuations and magnetic fluctuations with temperature. Discuss the influence of magnetic fluctuations on the Ising model. **(5 Marks)**

Q. No. 5: Interaction of water with graphene is studied using **NVT Monte Carlo** method using the **Cassandra package**. A number of water molecules are placed randomly between the graphene sheets.

a) Conduct Monte Carlo simulations with Cassandra and plot variation of energy with Monte Carlo steps, analyzing system behavior. **(10 Marks)**
b) Attach visual representations of water distribution between graphene layers and analyze the simulation results of graphene-water interactions. **(10 Marks)**