MSE 402: Computational Process Design

Sem I - AY 2024-25

28/08/2024

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 Sachin Tendulkar, please save the file as 'Sachin_Tendulkar.pdf'. File has to be uploaded on Google Classroom by the due date (and time). You need not attach any code.

Assignment 1: Molecular Dynamics Simulations using LAMMPS (Max score:100)
Due: 07/09/2024 by 11:55 PM

Q. No. 1: The first step you perform after creating your simulation box is Energy minimization. Why is Energy minimization required ? Is timestep required while performing Energy minimization. How is it different from time-integration ? **(20 Marks)**

Problems related to the simulation run:

Q. No. 2: Count the number of water molecules crossed through each membrane and plot their variation wrt time.**(20 Marks)**

Q. No. 3: Plot the variation of Temperature and Total Energy in each system wrt time during the final nvt run. Change the value of Tdamp (10, 100 and 1000) in one of the three systems (your choice) and plot its variation with time. Write down your observations ?**(20 Marks)**

Q. No. 4: Comment on the number of methane molecules that crossed through the membrane in three different systems. Based on this, which system would you consider most effective if the goal is to design it as a filtration membrane for methane?**(20 Marks)**

Q. No. 5: Design the same system for the filtration of Carbon dioxide molecules. Repeat the same analysis as conducted in Problem 4.**(20 Marks)**