Mid term exams

Molecular Dynamics simulation and Application in Chemical Physics

Course Instructor: Dr. Jagannath Mondal

Date : 01-03-2025

Total time: 2.5 hrs

Full marks: 50

Part A (30 marks):

1. Derive the Verlet equation of motion that is required for carrying out Molecular Dynamics (MD) simulation. (5)
2. What is the purpose of implementation of periodic boundary conditions in Molecular Dynamics simulation? Write a short algorithm for implementation of periodic boundary conditions. (5)
3. What advantage does MD simulation provide that a wet-lab experiment might not be able to give? (5)
4. Why do one need a cut-off in non-bonding interactions in MD simulations? Please describe 'Shift and Cut-off" scheme and its benefit over other methods (5)
5.
    a. What are the units of distance, energy and time in GROMACS? (2)
    b. What are the two key GROMACS tools for carrying out Molecular Dynamics simulations? (2)
    c. Write the file formats which GROMACS uses for the following:
        i. The file which contains information regarding the system's interaction parameters. (1)
        ii. A file that informs GROMACS regarding the various parameters required for performing a MD simulation. (1)
    d. Write the equation for calculation of radius of gyration of a protein. (2)
    e. In a Lennard Jones potential, what does "sigma"(σ) and "epsilon" (ϵ) represent? Derive the expression of distance of minimum energy ($\mathbf{r}_{min}$) in terms of sigma. Demonstrate all these terms in a graph. (2)

Part B (20 marks):

In the provided MD code in python, complete the functions force and potential with their respective expressions provided below:

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{\alpha} - \left(\frac{\sigma}{r}\right)^{\beta}\right] \text{ and}$$

$$F(r) = 4\frac{\epsilon}{r}\left[\alpha\left(\frac{\sigma}{r}\right)^{\alpha} - \beta\left(\frac{\sigma}{r}\right)^{\beta}\right] \text{ (5)}$$

Run MD simulations using the following sets of α and β: (8, 2), (12, 6) and (24, 18). (5).

Calculate the radial distribution function (RDF) using gromacs for each set. (5)

In a single plot, plot the different RDFs. (5)