Session 2 Pre-Quiz

**1. Which of the following must be run before a simulation can be run to collect data?**

a) Energy minimisation

b) NVT equilibration

c) NPT equilibration

d) All of the above.

I feel this may be a bit misleading for the next sessions. I would say energy minim, then run the NPT and skip the first XX ns.

Can we change the Q?

Maybe make it focused on the MD theory?

e.g. (more Qs in quiz doc)

**What is classical molecular dynamics simulation?**

1. A method to predict molecular interactions using quantum mechanics
2. A technique that uses classical mechanics to simulate the motion of atoms and molecules over time
3. A computational approach to solve large systems of linear equations
4. A biological experiment to observe molecular behaviour in real-time

**2. During which phase is the system stabilised at a constant temperature?**

**a) Energy minimization**

**b) NPT equilibration**

**c) NVT equilibration**

**d) Production run**

**NPT also is const T,**

**Let’s rephrase to be something like:**

**Which ensemble simulates a system with a constant number of particles, constant temperature, and constant pressure?**

1. Microcanonical (NVE) ensemble
2. Canonical (NVT) ensemble
3. Isothermal-isobaric (NPT) ensemble
4. Grand Canonical (μVT) ensemble

**3. Which command allows you to view the last 10 lines of a file?**

a) head -l 10

b) tail -n 10

c) more -l 10

d) cat -n 10

**4. Why is it important to check the evolution of the potential energy during energy minimisation simulation?**

a) To validate the force field

b) To ensure stable molecular structure

c) To optimize pressure

d) To adjust box size

**5. Why is solvation important in protein simulations?**

a) It increases computational power

b) It mimics the protein’s natural environment

c) It stiffens the protein structure

d) It reduces molecular dynamics

**6. Which software is frequently used for visualizing molecular dynamics trajectories?**

a) Photoshop

b) VMD

c) Excel

d) AutoCAD

**7. What is the purpose of using a thermostat in protein simulations?**

a) To change the colour scheme

b) To apply harmonic restraints

c) To control system temperature

d) To remove periodic boundaries

**8. What components are typically included in molecular mechanics force fields?**

a) Bond lengths, angles, and torsions

b) Atom colours and sizes

c) Simulation speed and duration

d) Protein sequence and structure

**9. Which GROMACS command would you use to produce a plot of pressure evolution during the simulation?**

a) gmx calculate

b) gmx energy

c) gmx editconf

d) gmx pressure

**10. Which command solvates the protein in GROMACS?**

a) gmx insert-molecules

b) gmx solvate

c) gmx add-ion

d) gmx build