

## Sample quiz questions IM/S: Molecular dynamics (MD 1-4)

The questions in the quiz will be a shorter. However, going through these questions will be a good preparation for the quiz and indicates what are the most important concepts.

### A. Analysis methods

1. What information does the radial distribution function give you? Look at the figure below and indicate which curve corresponds to a solid, liquid and gas. What do the peaks indicate?

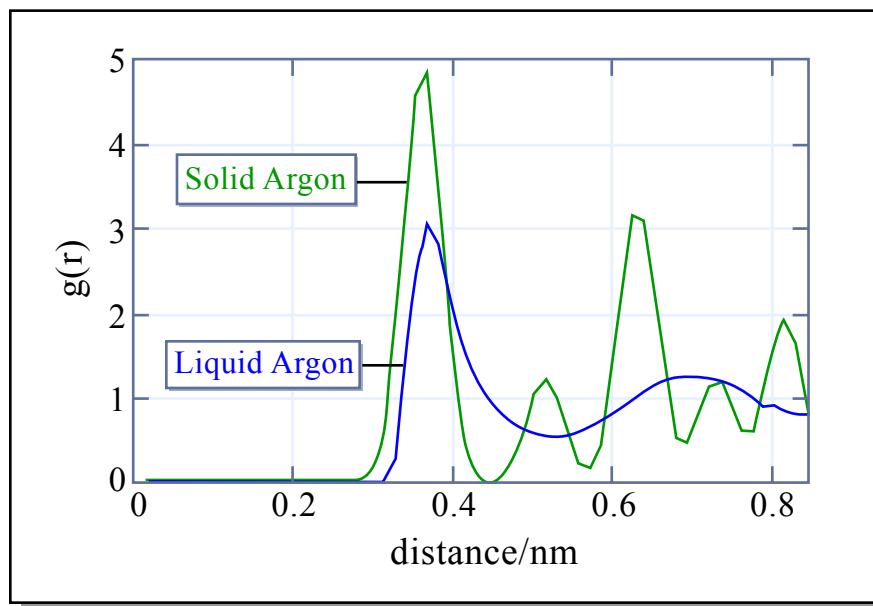


Figure by MIT OCW.

2. Assume you did an MD simulation with  $N=100,000$  atoms. You started with a solid, but you raised the temperature and you are not sure if the material is still in crystalline state. Without explicitly looking at the atomic positions, how could you distinguish a solid from a liquid using some analysis methods? Sketch some of the characteristic curves.

**Hint:** We presented two methods to distinguish a solid from a liquid, so there are two possible answers.

3. Assume you computed the mean square displacement (MSD) of a system of  $N$  particles. The MSD describes how far atoms have moved in average. How could you relate the diffusion coefficient  $D$  to the MSD? Give simple equations and visualize with a schematic plot of MSD over time how to determine  $D$  to the curve.

## B. Simulation schemes

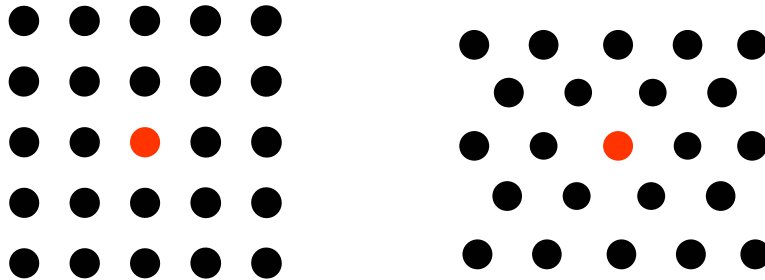
1. Summarize the key steps involved in the MD updating scheme. Draw a simple flowchart that depicts graphically how they interact with each other. Indicate the scaling behavior of the individual steps, with respect to the number of particles in the system, denoted by  $N$  (do this for force calculation and integration step).

How does the main integration loop scale with respect to the overall simulation time?

Express this scaling behavior in terms of discrete integration steps, with total number of  $n$  steps.

## C. Atomic interactions and failure mechanisms

1. The Lennard-Jones 12:6 potential is a widely used interatomic potential. Can you use a Lennard-Jones 12:6 potential (see lecture notes), within a classical MD scheme to predict the magnetization behavior? Motivate your answer with a few keywords.
2. In a pair potential approximation with nearest neighbors, do atomic bonds at a surface and in the bulk (that is, far away from surfaces) have the same bond strength?
3. For the two crystal lattices below, how many nearest neighbors does each atom have. Which of the two lattices is more stable, for a simple nearest neighbor pair potential, and why? Discuss the energetic driving forces and put it into context of the number of nearest neighbors.



4. We discussed some failure mechanisms in the lecture. Choose one of them, name it, and list some atomistic deformation mechanisms associated with it. Why is it recommended to use MD rather than MC to model failure mechanisms?

**Hint:** Equilibrium versus nonequilibrium processes.

5. Under which conditions is it recommended to periodic boundary conditions? Can you use this technique to simulate surfaces?

## Solution hints

A1 The radial distribution function (RDF) provides information about the atomistic microstructure. For example, it gives information about the crystal structure, preferred distances between atoms, or if the system is in solid, liquid or gas state. The peaks indicate preferred distances of atoms. The three curves correspond to a solid (many discrete peaks), liquid (several smooth peaks), gas (one peak).

A2. You could use either the RDF (see first question) or the velocity autocorrelation function (VAF). You could take advantage of the characteristic shape of the VAF for lattices versus liquids. For a lattice, the VAF shows oscillations (due to the characteristic vibrations of atoms backwards and forwards, reversing their velocity at the end of each oscillation) modulated with an exponential decay. A liquid will show a simple exponential decay (magnitude reduces gradually under the influence of weak forces since the velocity decorrelates with time; a specific atom 'forgets' what its initial velocity was).

A3. The diffusion coefficient relates to the slope of the MSD plot over time. Equations are given in the lecture notes;  $\lim_{t \rightarrow \infty} \frac{d}{dt} \langle \Delta r^2 \rangle = 2dD$ , where  $d = 3$  for a 3D system.

B1. Key steps: See lecture notes; including the flow chart. The force calculation scales  $\sim N^2$  without using neighbor tables or similar strategies, and  $\sim N$  with those (see homework problem). MD scales linearly with respect to the total simulation time, with time steps  $n$  the total simulation time is  $\sim n$ . The main integration loop is thus  $\sim N$  or  $\sim N^2$  and also  $\sim n$ , thus  $\sim nN$  or  $\sim nN^2$ .

C1. No, electronic properties can not be modeled using this approach, since the effect of individual electrons on the atomic interactions are condensed out into mathematical expressions such as the LJ potential that do not explicitly model the dynamics or interaction of individual electrons.

C2. All pairs of atoms have the same bond strength in this case, regardless whether they are at a surface or in bulk.

C3. Square lattice (left): 4 nearest neighbors; triangular lattice (right): 6 nearest neighbors. Thus, the triangular lattice has lower potential energy and is thus favored over the square lattice, since each bond contributes the identical potential energy to the total energy (provided that the bond length is always the equilibrium bond length). We expect that a square lattice will transform into a triangular lattice over time.

C4. Failure mechanisms: Ductile failure (dislocation motion, plastic bending, copper behaves like this), or brittle failure (formation of new surfaces by breaking of atomic bonds – glass behaves like this). Failure processes are nonequilibrium phenomena, and we are interested in how (in time) failure proceeds; thus MD methods are preferred over

MC. MC does not give dynamical information about how the system goes from one state to another. MD describes this dynamical transition.

C5. We use PBCs when we would like to model a bulk (infinitely large) system with a small number of particles. By turning off the PBCs in specific directions, we can model surfaces while retaining the “infinitely large” extension of the system in the other directions.