Molecular Dynamics

1. Molecular-dynamics algorithms

Discuss the algorithms for molecular-dynamics modeling: Potentials, integration, cut-off, periodic boundary conditions, initialization, efficiency improvements.

2. Molecular-dynamics in the micro-canonical ensemble

Discuss initialization and initialization effects. Temperature measurements and fluctuations. Comment on use of thermostats for initialization.

3. Molecular-dynamics in the micro-canonical ensemble

How to measure macroscopic quantities such as temperature and pressure from a molecular-dynamics simulation. How is this done in your Lammps simluation? What challenges do you expect? What can it be used for? Provide examples from your own simulations.

4. Measuring the diffusion constant in molecular-dynamics simulation

How to measure the diffusion constant in molecular dynamics simulations – limitations, challenges and results. Compare with theoretical estimates for diffusive behavior. Discuss difference between the potential models you studied.

5. Interaction models in molecular-dynamics simulations

Introduce the three potential models you studied. Discuss similarities and differences in your results with particular emphasis on initialization, efficiency, $g(r)$ and $D(T)$. Provide examples from your own simulations.

Advanced Molecular Dynamics

6. Generating a nanoporous material

Discuss how we prepare a nanoporous matrix with a given porosity in Lammps. How do we characterize the structure of such a material and the dynamics of a fluid in such a material? Provide examples from your own simulations.

7. Diffusion in a nano-porous material

How can you measure the diffusion constant for a low-density fluid in a nanoporous system? Discuss what results you expect. Compare with diffusion in a bulk liquid and in a larger-scale porous medium. Provide examples from your own simulations.

8. Flow in a nano-porous material

Discuss how to induce flow in a nano-porous material. How can you check your model, calculate the fluid viscosity and measure the permeability? What challenges do you expect? Provide examples from your own simulations.

Percolation

9. Algorithms for percolation systems

How do we generate a percolation system for simulations? How to analyze and visualize the systems? How to find spanning clusters and measure the percolation probability?

10. Percolation on small lattices

Discuss the percolation problem on a 2×2 lattice. Sketch $P(p, L)$ and $\Pi(p, L)$ for small L. Relate to your simulations. How do you calculate these quantities and how do you measure them in simulations?

11. Cluster number density in 1-d percolation

Define the cluster number density for 1-d percolation, and show how it can be measured. Discuss the behavior when $p \to p_c$. How does it relate to your simulations in two-dimensional systems?

12. Cluster size in 1-d percolation

Introduce the characteristic cluster size for the 1-d percolation problem, and discuss their behavior when $p \to p_c$. Relate to your simuluations on two-dimensional percolation.

13. Measurement and behavior of $P(p, L)$ and $\Pi(p, L)$

Discuss the behavior of $P(p, L)$ and $\Pi(p, L)$ in a system with a finite system size L. How do you measure these quantities?

14. The cluster number density

Introduce the cluster number density and its applications: Definition, measurement, scaling and data-collapse.

15. Finite size scaling of $\Pi(p, L)$

Discuss the behavior of $\Pi(p, L)$ in a system with a finite system size L. How can we use this to find the scaling exponent ν, and the percolation threshold, p_c?

16. Effective percolation threshold

Define and discuss the effective percolation threshold in a system with a finite system size L. How can we measure it, and what consequences does it have that the effective percolation threshold is different from the actual percolation threshold?

17. Subsets of the spanning cluster

Introduce and discuss the scaling of subsets of the spanning cluster. How can we measure the singly-connected bonds, and how does it scale?