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. What challenges do you expect? What can it be used for?

4. Measuring the diffusion constant in molecular-dynamics simulation

How to measure the diffusion constant in molecular dynamics simulations – limitations and challenges. Compare with methods and results from random walk modeling.

5. Measuring the radial distribution function in molecular dynamics simulations

How can you measure the radial distribution function in molecular dynamics simulations. What does it tell? What challenges will you face? Compare the measurement of the radial distribution function to the measurement of the probability densities for a random walk.

6. Thermostats in molecular-dynamics simulations

Discuss the micro-canonical vs the canonical ensamble in molecular-dynamics simulations: How can we obtains results from a canonical ensemble? Introduce two thermostats, and describe their behavior qualitatively. How can you use such a thermostat for rapid initialization of a micro-canonical simulation?

Advanced Molecular Dynamics

7. Generating a nanoporous material

Discuss how we prepare a nanoporous matrix with a given porosity. How do we characterize the structure of such a material and the dynamics of a fluid in such a material?

8. 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.

9. 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?

Percolation

10. 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?

11. 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?

12. 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?

13. Correlation length in 1-d percolation

Define the correlation length ξ for 1-d percolation. Discuss its behavior when $p \to p_c$. How is it related to cluster geometry and your results for two-dimensional percolation?

14. 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.

15. 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?

16. The cluster number density

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

17. 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?

18. 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?

19. Random walks / Flow in a disordered system

Either: Discuss the scaling theory for the distance $r^2(t)$ of a random walker dropped at a random occopied site on either (1) the percolation system or (2) the spanning cluster. (You can choose which case to discuss). Relate the results to diffusion in a bulk fluid and in a nanoporous system.

Or: How do you measure the conductivity of the spanning cluster? Discuss the scaling theory for the conductivity $\sigma(p, L)$ when $p > p_C$. Relate the results to permeability in a nanoporous system.