1 Random walks in one dimension

Discuss the scaling of a one-dimensional random walk: Universality, moments, probability densities, data-collapse, dimensionality.

2 Random walks in two dimensions

Discuss the scaling of a two-dimensional random walk: Universality, moments, probability densities, data-collapse, dimensionality.

3 Self-avoiding random walks in two dimensions

Discuss the scaling of a two-dimensional self-avoiding random walk: Algorithms, moments, probability densities, data-collapse, dimensionality, universality. Compare to high-dimensional behavior.

4 Self-avoiding random walks in three and higher dimensions

Discuss the scaling of a self-avoiding random walk: Algorithms, moments, probability densities, data-collapse, dimensionality, universality. Compare to two-dimensional behavior.

5 Molecular-dynamics algorithms

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

6 Molecular-dynamics in the micro-canonical ensemble

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

7 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?

8   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.

9   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? How is it related to percolation theory and probability densities for the random walk?

10   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?

11   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?

12   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?

13   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?

14   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?

15 Cluster size in 1-d percolation

Introduce the characteristic and average 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.

16 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?

17 The cluster number density

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

18 Scaling ansatz for cluster number density

Motivate and introduce the scaling ansatz for cluster number density. Sketch possible applications.

19 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?

20 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?

21 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?

22 Random walks in disordered system

Discuss the scaling theory for the distance $r^2(t)$ of a random walker dropped at a random occopied site on the percolation system.

23 Random walks in disordered system

Discuss the scaling theory for the distance $r^2(t)$ of a random walker dropped at a random site on the spanning cluster.