

From:

An Introduction to Computer Simulation Methods Third Edition (revised)

written by Harvey Gould, Jan Tobochnik, and Wolfgang Christian

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Project 12.14. Percolation in three dimensions

- a. The value of p_c for site percolation on the simple cubic lattice is approximately 0.3112. Do a simulation to verify this value. Compute ϕ_c , the volume fraction occupied at p_c , if a sphere with a diameter equal to the lattice spacing is placed at each occupied site.
- b. Consider continuum percolation in three dimensions where spheres of unit diameter are placed at random in a cubical box of linear dimension L . Two spheres that overlap are in the same cluster. The volume fraction occupied by the spheres is given by

$$\phi = 1 - e^{-\rho 4\pi r^3/3}, \quad (12.38)$$

where ρ is the number density of the spheres, and r is their radius. Write a program to simulate continuum percolation in three dimensions and find the percolation threshold ρ_c . Use the Monte Carlo procedure discussed in Problem 12.4 to estimate ϕ_c and compare its value with the value determined from (12.38). How does ϕ_c for continuum percolation compare with the value of ϕ_c found for site percolation in part (a)? Which do you expect to be larger and why?

- c. In the Swiss cheese model in three dimensions, we are concerned with the percolation of the space between the spheres. This model is appropriate for porous rock with the spheres representing solid material and the space between the spheres representing the pores. Because we need to compute the connectivity properties of the space between the spheres, we superimpose a regular grid with lattice spacing equal to $0.1r$ on the system, where r is the radius of the spheres. If a point on the grid is not within any sphere, it is “occupied.” The use of the grid allows us to determine the connectivity between different regions of the pore space. Use a cluster labeling algorithm to label the clusters, and determine $\tilde{\phi}_c$, the volume fraction occupied by the pores at threshold. You might be surprised to find that $\tilde{\phi}_c$ is relatively small. If time permits, use a finer grid and repeat the calculation to improve the accuracy of your results.
- d.* Use finite size scaling to estimate the critical percolation exponents for the three models presented in parts (a)–(c). Are they the same within the accuracy of your calculation?

(* is more difficult and optional)