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Computational Physics II

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8.1. Molecular dynamics

Consider a system of N particles in the plane, interacting by repulsive potentials $V(r) = 1/r^n$ with $n = 2$. An external harmonic potential $V_h = (V_0/2)\sum_i \mathbf{x_1^2}$ keeps the particles in a finite volume.

Set up a molecular dynamics simulation that advances the particles in time using the Verlet algorithm. For the Initial conditions take zero velocity and Gaussian random distributions in position. For demonstration purposes, consider particles numbers in the range $N = 10 \ldots 20$.

Monitor the total energy as a measure of integration accuracy: how much does it change in the course of 10 time units?

The kinetic energy is a measure of the temperature of the system. How does it vary with time? Given that all velocities vanish initially, it will start from zero and then reach a statistically steady state. How long does it need to reach that state?

In order to realize different temperatures (i.e. different kinetic energies), reduce the kinetic energy by rescaling all velocities by the same amount, i.e. $v_i \to \lambda v_i$. How long does the system need to reach a new statistical equilibrium?

What changes do you see in the spatial arrangement of particles?

8.2. Directed percolation

Directed percolation is a non-equilibrium process that shows a phase transition from a decaying state to a persistent one as parameters are changed.

In order to obtain a space-time representation of the one-dimensional percolation process, consider a square lattice with space along the horizontal and time along the vertical and states $x(i, t)$.

The bottom row (time=0) is initialized with all sites in state 1. The next row $(t + 1)$ is obtained from from the preceeding one at t by the rule that the probability that a site i is in state 0 is given by $q = (1 - rx(t, i - 1))(1 - px(t, i))(1 - rx(t, i + 1))$, with the two parameters r and p. Consider a lattice with 100 sites and parameter $p = 0.7$ for increasing r.

Study the fraction f of sites in state 1 as a function of time by averaging over several realizations. Show that below a critical value in r the fraction falls off exponentially with t and that it reaches a constant value for larger r. How does the asymptotic value of f for large times vary with r?