Molecular dynamics

1 particles

A particle is implemented as a struct that contains the position,velocity and force(accelaration) of the particle in all dimensions. All particles in the system is represented as an array of such structs.

2 Initialization

The function *init* is called in the beginning of the program. It begins by putting the particles on an initial cubic lattice, this is done with the function *lattice_position*. The particles are then given an initial randomized velocity. Further, the velocities are scaled to obtain the desired temperature.

3 Forces

Forces on the particles are calculated with the $force$ function. The function enters a loop that calculates the distances between all particles, if the radial distance between two particles is larger than a certain $cutoff$ distance, the function *lennard_jones* is called. This function calculates the forces on the two particles based on the lennard jones potential. The lennard jones potential is formulated as:

$$V(r) = 4\epsilon\Big[\big(\frac{\sigma}{r}\big)^1 2 - \big(\frac{\sigma}{r}\big)^6\Big] \tag{1}$$

Where ϵ is the reduced unit of energy, and σ is the reduced unit of length. When taking the derivative of this function with respect to r the forces are obtained:

$$F(r) = \frac{\partial V}{\partial r} \tag{2}$$

4 Integration

Integration with respect to time to obtain the velocities and positions of the particles is done in the function *integrate*. This function implements the *velocity verlet algorithm*.

The velocity verlet algorithm is based on the following scheme: Accelerations are computed from the potential (lennard jones), this is then used to propagate the positions:

$$x(t + \Delta t) = x(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2 \tag{3}$$

New accelerations (forces) are then computed using the new positions. The old accelerations are then stored and are used along with the new values to get the velocities of the particles:

$$v(t + \Delta t) = v(t) + \frac{a(t) + a(t + \Delta t}{2}\Delta t \tag{4}$$

5 MD-loop

The function integrate is called a certain number of timesteps in a for-loop to propagate the positions,velocities and forces of the particles. The kinetic energy can be determined from the velocities of the particles, the potential energy can be determined from the lennard-jones potential. The total energy is the sum of the kinetic and potential energy.