

## **Molecular Dynamics**

Simulate a single particle in a three dimensional box. It should reflect off the walls in an elastic manner and its energy should remain unchanged for 10000 crossing time. [10%]

Simulate a system  $N$  non-interacting particles in a three dimensional box. Calculate pressure on each wall as a function of time. Compute the time over which pressure must be averaged for it to be constant within 0.1% as a function of the number of particles. Obtain a macroscopic equation of state for the system. [20%]

Simulate a single hard sphere of radius  $R$  in a cubical box of sides  $L$ , with  $L \gg R$ . The sphere should reflect off the walls and its energy should remain unchanged for 10000 crossing time. [30%]

Simulate a system of two hard spheres of radius  $R$  in a cubical box of sides  $L$ , with  $L \gg R$ . The spheres should reflect off the walls and collide in an elastic manner off each other. The total energy energy should remain unchanged for 10000 crossing time. [40%]

Generalise this to a system of  $N$  hard spheres of this type. Implement a method for searching for neighbours. Calculate pressure on each wall as a function of time. Compute the time over which pressure must be averaged for it to be constant within 0.1% as a function of the number of particles. Obtain a macroscopic equation of state for the system. [60%]

Study the effect of two body collisions when you start the system away from equilibrium. How long does it take for the distribution function to reach equilibrium in terms of crossing time? How does it depend on the total number of hard spheres? [70%]

Simulate a system of  $N$  particles in a box interacting via a short range force. Calculate pressure on each wall as a function of time. Compute the time over which pressure must be averaged for it to be constant within 0.1% as a function of the number of particles. Obtain a macroscopic equation of state for the system. [90%]

Study the effect of interactions when you start the system away from equilibrium. How long does it take for the distribution function to reach equilibrium in terms of crossing time? How does it depend on the total number of hard spheres? [100%]