

## Diffusion coefficient for liquid argon

The aim of this exercise is to familiarize with molecular dynamics (MD) simulations and get an insight on how to calculate macroscopic quantities starting from the atomic motion. You will generate molecular dynamics trajectories at two different temperatures for liquid argon and then use them to evaluate the diffusion coefficient.

This exercise is based on one of the first MD simulations performed by A. Rahman (see Physical Review, Vol.136, p. A405, 1964).

The MD program is available at the web page <http://boinc.gorlaeus.net/> (Leiden Classical) where you can also find a number of links for a basic introduction to Molecular Dynamics.

We have already prepared two input files with Cartesian coordinates for a system of 729 particles interacting with a Lennard-Jones potential already equilibrated at 94 K and 294 K, respectively.

1. Familiarize with the input file.
2. Starting from these two input files, you can run two MD simulations at 94 K and 294 K, respectively. The simulations should run for about 5 ps, with a time step  $\Delta t = 10^{-14}$  sec.

### QUESTIONS:

1. The Verlet algorithm is used to perform the numerical integration of the equation of motions. Give a short description of the algorithm.
2. How can you calculate the (average) temperature in a MD simulation?

### Calculation of Diffusion coefficient ( $D$ ):

The easiest way to calculate it from MD is by Einstein relation:

$$\langle \Delta r^2 \rangle = 6Dt$$

The trajectory, obtained in the MD run, gives the mean squared displacement  $\langle \Delta r^2 \rangle$  as a function of time  $t$ . The tangent of the linear fit gives the diffusion coefficient  $D$ .

### QUESTIONS:

3. Plot the mean squared displacement  $\langle \Delta r^2 \rangle$  as a function of time  $t$  for the two different temperatures.
4. Evaluate the diffusion coefficient by evaluating the slope of the curves.