Exam preperations FYS4460

Fredrik E Pettersen
f.e.pettersen@fys.uio.no

May 23, 2013

Contents

1 Molecular-dynamics algorithms

There are several different possibilities for "variation" when doing molecular dynamics. First of all one can use different potenitals according to what one would like to model. The simplest beeing the Lennard-Jones potential, which only includes two-particle interactions. The Lennard-Jones potential is typically pretty good for simulations of noble gasses. If we should want to study another material we will therefore need another potential. The weber-Stillinger potential includes both two- and three-particle interactions, and can model silicone (Si). Silicone will, in equilibrium, form 4-coordinated tetrahedral structures, which the Weber-Stillinger potential reproduces. The VKRE (Vashista, Kalia, Rino, and Ebbsjö) potiential is another potential which includes both two and three particle interactions, but this potential is made (specificly) to simulate SiO_2. The two-body part includes three terms, the Coulomb interaction, steric repulsion due to ionic sizes, and a charge-dipole interaction resulting from the large electronic polarizability of O_2^-. Yet another example of a possible potential is the reaxFF potential which also includes four-particle interactions. This potential lets us study water molecules in an SiO_2 matrix.
In our Lennard-Jones studies we used the Verlet algorithm for time-integration. It is a simple, yet quite good integrator which conserves energy very well. It can be viewed as an advanced Euler-Chromer method, where we first update the velocity of each particle at half the timestep, then the position is integrated one full timestep using the new velocity. When this is completed for all paritcles we calculate two-body forces using the new positions before we use the new forces to fully integrate the velocities.
All of the potentials mentiones above decrease in strength with the distance between atoms. For the Lennard-Jones potential, this is illustrated in figure 1. As we see from this figure, there is for all practical purposes no interaction between particles that are a certain length apart. This means that we can skip the calculations of forces (which is very expensive) between theese particles. As a practical measure we will therefore divide the system we are simulating into cells which are the same size as the cutoff length and only calculate forces between particles in neighbouring cells. In this way we are sure that no important calculations are left out

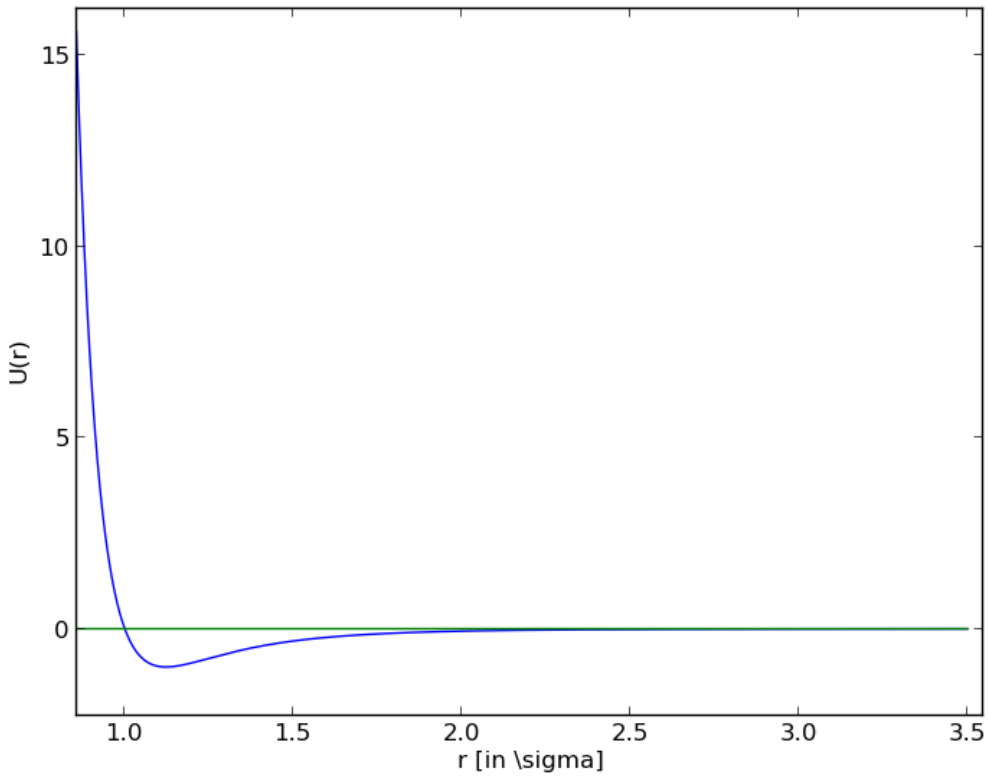

Figure 1: Strength of Lennard-Jones potential as a function of distance between atoms

2 Molecular-dynamics in the micro-canonical ensemble

3 Molecular-dynamics in the micro-canonical ensemble

4 Measuring the diffusion constant in molecular-dynamics simulations

5 Measuring the radial distribution function in molecular-dynamics simulations

6 Thermostats in molecular-dynamics simulations

7 Generating a nano-porous material

8 Diffusion in a nano-porous material

9 Flow in a nano-porous material

10 Algorithms for percolation systems

11 Percolation on small lattices

12 Cluster number density in 1-d percolation

13 Correlation length in 1-d percolation

14 Cluster size in 1-d percolation

15 Measurment and behavior of $P(p, L)$ and $\Pi(p, L)$

16 The cluster number density

17 Finite size scaling of $\Pi(p, L)$

18 Subsets of the spanning cluster

19 Random walks