Project 04

Verlet neighbor list for the calculation of particle-particle interactions

Keywords: Markov chain Monte Carlo, periodic boundary conditions, Lennard-Jones potential
Deadline: Please, hand in your report by **Tuesday, 29 July 2014**

1 Introduction

Consider a box of spherical particles which interact via a Lennard-Jones potential

$$V_{LJ}(r_{ij}) = 4\epsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] = \epsilon\left[\left(\frac{r_m}{r_{ij}}\right)^{12} - 2\left(\frac{r_m}{r_{ij}}\right)^{6}\right], \quad (1)$$

where r_{ij} is the distance between particle i and particle j, ϵ is the depth of the potential, σ is the distance at which the potential is zero, and r_m is the distance at which the potential reaches its minimum, i.e $V_{LJ}(r_{ij} = r_m) = \epsilon$. Even if the forces are truncated beyond a cut-off radius r_{LJ}, at each simulation step one still needs to find all pairs that fall within this cut-off radius. Hence, at each simulation step a loop over all $N(N-1)$ pairs of particles is required, and the simulation scale as $\mathcal{O}(N^2)$. Verlet (Ref. 2) introduced the concept of neighbor lists, in which the neighbors of each particle are stored, which reduces the computational effort. The neighbor list are typically update every 10 to 20 simulation steps. In this project, you will implement a molecular dynamics simulation program for a box of Lennard Jones particles which uses either the normal loop over all $N(N-1)$ pairs or a Verlet neighbor list

2 Outline of the project

1. Read and understand Chapter 5.3 of Ref. 3.
2. Implement a molecular dynamics simulation algorithm for a box of Lennard Jones particles using
   - Verlet integrator (see exercise 2)
   - periodic boundary conditions
   - constant volume
   - a fixed cutoff to calculate the forces

   Implement two alternatives to determine the pairs in within a cut-off radius
   - Loop over all $N(N-1)$ pairs in the system
   - Verlet neighbor list. (FORTRAN example code is available at Ref. 4.)

   Document the program.
3. Approximate the Lennard-Jones potential by a harmonic potential and choose the time step of your simulation as $\Delta = 0.1T$, where T is the period associated to the harmonic potential.
4. Plot the radial distribution function of the particles.
5. Plot snap shots of your simulation and the trajectory of a particular particle.
6. Compare the computational effort for a simulation of N_t time steps for the loop over all pairs and the Verlet neighbor list.
7. Increase the system size. How does this effect the computational effort?

3 Literature

1. Lecture notes and exercises.
2. L. Verlet, (1967). "Computer 'experiments' on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules". *Phys. Rev.* **159**, pp. 98Ð103 (1975).
3. M.P. Allen, D. J. Tildesley, "Computer simulations of liquids", Oxford University Press 1987.
4. http://www.ccl.net/pub/chemistry/software/SOURCES/FORTRAN/allen-tildesley-book/index.shtml
5. Chapter 13 in: T. Schlick, "Molecular Modeling and Simulation - an Interdisciplinary Guide", 2nd edition, Springer 2010.
6. Chapters 3 and 4 in: D. Frenkel, B. Smit, "Understanding Molecular Simulation - From Algorithms to Applications", Academic Press, Elsevier (USA) 2002.

Project requirements

- Describe the results of the your project in a report of 5 to 12 pages (font size 11 pt).
- The report should also contain a short description of the theory and the methods. If you implement an algorithm, briefly describe the algorithm.
- Hand in your program along with the report.
- You will present the results of your project in a 20-minute presentation, after which we will have about 10 minutes time for discussion.
- Besides questions which are directly related to the results of the project, the discussion will also cover the theory of the project and the course content which is relevant to the project.
- If you run into problems during the project or have questions, please contact us
  - Bettina Keller, bettina.keller@fu-berlin.de
  - Francesca Vitalini, francesca.vitalini11@gmail.com
- During the lecture hours (Thu, 2.15 - 3.45 pm) one of us will be in the library to answer questions.