Project 02

Markov chain Monte Carlo sampling of a Lennard-Jones fluid

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

1 Introduction

Spherical particles which interact via a Lennard Jones potentials are good models for ideal gases. The Lennard Jones potential between two particle i and j is given as

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

where 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 $V_{LJ}(r_{ij} = r_m) = \epsilon$. In this project, you will implement a Markov chain monte carlo sampling algorithm for a box of Lennard Jones particles.

2 Outline of the project

1. Implement a Markov chain Monte Carlo algorithm for a box of Lennard Jones particles using
   - periodic boundary conditions
   - constant volume
   - a fixed cutoff to calculate the forces
   - generating trial moves by drawing from a Gaussian distribution which is centered at the current position of the particle.

   Document the program.
2. Plot the radial distribution function of the particles.
3. Plot snap shots of your simulation and the trajectory of a particular particle.
4. Vary the way in which you generate proposal steps (e.g. change the width of the Gaussian, move several particles at the same time time...). What effect does this have on the acceptance ratio and the sampling speed?
5. Play around with other simulation parameters, e.g vary the density of the simulation box or the temperature. What do you observe?
6. Introduce particles which have a charge. (For simplicity, use a cut-off to truncate the Coulomb interactions at distance r_{Coulomb}. If you choose the charge small enough, you can use $r_{LJ} = r_{\text{Coulomb}}$). What do you observe?

3 Literature

- Lecture notes and exercises.
- Chapter 12 in: T. Schlick, "Molecular Modeling and Simulation - an Interdisciplinary Guide", 2nd edition, Springer 2010.

- 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.