# Project 03

## Molecular dynamics simulation of a Lennard-Jones fluid

**Keywords**: MD simulation, 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 $\epsilon$ is the depth of the potential, $\sigma$ 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 molecular dynamics simulation program for a box of Lennard Jones particles.

## 2 Outline of the project

1. 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

   Document the program.
2. 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.
3. Plot the radial distribution function of the particles.
4. Plot snap shots of your simulation and the trajectory of a particular particle.
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 $r_{\text{Coulomb}}$. 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 13 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.