Heinrich–Heine–Universität Düsseldorf
Institut für Theoretische Physik II
Computational Physics
Wintersemester 2018/2019

Prof. Dr. J. Horbach
Dr. S. Ganguly
(saswati@thphy.uni-duesseldorf.de)
M. Eshraghi (Mojtaba.Eshraghi@hhu.de)
Blatt 5 vom 13.11.2018
Abgabe bis 16:00 Uhr am 20.11.2018

"Some people feel the rain. Others just get wet."

Roger Miller

Problem 5.1: **Molecular Dynamics simulation of a two-dimensional fluid**

In this exercise, we solve Newton's equations of motion for a two-dimensional system of $N = 144$ particles. The interactions between the particles are modelled via the pairwise-additive Weeks-Chandler-Andersen (WCA) potential. Here, the interaction between two particles, separated by a distance r, is given by

$$u(r) = \begin{cases} 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] + \varepsilon, & \text{if } r \leq 2^{1/6}\sigma \\ 0, & \text{if } r > 2^{1/6}\sigma \end{cases} \tag{1}$$

where the two parameters σ and ε have units of length and energy, respectively. Implement a molecular dynamics simulation for this system where you choose the mass, length and energy units such that $m = 1.0$, $\sigma = 1.0$, and $\varepsilon = 1.0$, respectively. The time t shall be given in units of $\tau = \sqrt{m\sigma^2/\varepsilon}$. The $N = 144$ particles are put into a quadratic simulation box with linear dimension $L = 14.0\sigma$.

In order to implement and run the molecular dynamics (MD) simulation, do the following steps:

a) Write a function to read in the initial position of particles and corresponding velocities from the files that you can download from our web page.

b) Write the function for the calculation of the force on each particle. To this end, first determine the functional form of the total force on a particle from the appropriate gradient of the total potential.

c) Implement the velocity Verlet algorithm (with a time step $\delta t = 0.0005\,\tau$), using periodic boundary conditions.

d) Run the MD programme and determine the temperature, the pressure, the potential energy, the kinetic energy, and the total energy as a function of time t.

e) Redo your simulation with the different time steps $\delta t = 0.05$, 0.01, 0.005, and 0.001 and discuss the time dependence of the total energy.