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

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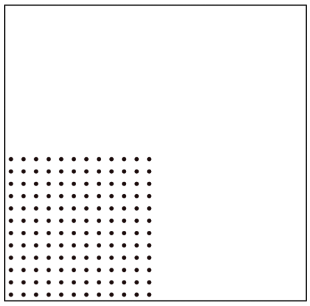
Abgabe bis 16:00 Uhr am 27.11.2018

Problem 6.1: **Time reversibility**

Let us consider the molecular dynamics simulation of a 2-dimensional system consisting of N particles inside a square box which initially arranged as shown in the figure.



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.

The number of particles is $N = 144$, the linear dimensions of the box are $L_x = L_y = L = 28\sigma$. All particles have a mass $m = 1$. The initial particle positions and velocities can be found on the website of the course ("initialization.dat").

a) With your implemented code for problem 5.1, compute the particle trajectories up to time $t = 1000\tau$ using an integration time step of $\delta t = 0.0005\tau$ starting from the configuration given in file `"initialization.dat"`. Plot the final configuration.

b) Check explicitly that the total energy E is conserved by plotting E as function of time.

c) Read the final configuration (coordinates and velocities) of a) and solve the equations of motion for 1000 time steps but now using $\delta t = -0.0005\tau$, i.e. now the time arrow is reversed, $\delta t \to -\delta t$. Display the final configuration.

d) Repeat a) to c) but propagate now the system over $10000, 20000, 40000$ integration time steps ($\delta t = \pm 0.0005\tau$). Explain your observation.

e) Are your observation in contradiction with the 2nd law of thermodynamics? Please discuss this in terms of Boltzmann's definition of entropy.

f) Modify your code to integrate the equations of motion using a symplectic Euler algorithm algorithm and repeat all the above steps. Explain your observations.