5th problem set for Computer Simulations, 2024

Hand-in: see schedules for your group, linked in the TeachCenter.
Please upload/submit your program files in the TeachCenter *before* the conversation with the tutor.

Molecular Dynamics

Perform a Molecular Dynamics simulation for a gas of argon atoms. Use the Verlet algorithm, in e.g. the „Leap-Frog" variant.

Physical situation:

- N particles are located in a 2-dimensional box, infinitely high, with *hard, reflective* walls and bottom. You can choose N and the system size. (Minimum $N = 20$).
- The particles interact by the Lenard-Jones potential (with $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$)

$$U = 4\epsilon \sum_{i \neq j} \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right].$$

- In addition there is a gravitational force $F_y = -mg$.
- *Parameters:* Use reduced units. Look up approximate Lennard Jones values for argon. How large is the time scale $\sigma\sqrt{m/\epsilon}$ for argon, in seconds ? How large is $k_B T$ for room temperature (300K) in reduced units in case of argon ?
- *Gravity:* How large is the actual gravitational acceleration $g \simeq 10\frac{m}{s^2}$ in reduced units? How large is the gravitational energy mgh for heights h that may be reached in your system, compared to the Lennard Jones energy ϵ ?

  In order to actually see effects of gravity in your simulation, you will have to choose the parameter g much larger than $10\frac{m}{s^2}$. For your simulation, choose some plausible value such that the barometric height scale h_s (see last task) becomes reasonable, i.e. similar to the heights actually reached in the situation. If gravity appears to be far too strong (particles too much at the bottom or too much energy in the system) or far too weak (no effect of barometric equation visible) adjust g (details should not be important).

Simulation:

- *Initial state:* you can e.g. set the velocities at random. Be careful with initial positions, in order not to introduce too much potential energy (will also depend on g). It is advisable to place the particles onto a grid with a spacing of roughly the equilibrium distance ($\sim \sigma$).
- *Time step:* the time step τ must be small enough, so that during a time step the forces do not change too much. (One could introduce intermediate steps for particles at close distance, but you do not need to do this).

- *Boundaries:* You can implement the reflecting walls by switching the sign of the component of momentum which is perpendicular to the wall.
- *Computational effort:* How does it scale with N ? How much time might you save (roughly) by using one of the advanced strategies discussed in the lecture notes ? You do *not* need to implement such a strategy.
- *Energy:* During the simulation, check whether the total energy remains constant to within a few percent (time series). When τ is chosen very large, energy conservation is violated drastically (try it !). Why ?
- *Thermalisation:* After starting the simulation, wait for a time t_{therm}, so that the system becomes sufficiently independent of the initial conditions. Make sure that the particles typically move distances larger than the system size. (If they move only a little, then the time step or the total energy may be too small).
- *Measurements:* During the rest of the simulation, measure
(1) density as a function of height, and
(2) the distributions of velocities $|\vec{v}|$ of the individual particles.
- *Measurement time:* Conduct at least $n_{\text{meas}} = 1000$ measurements, each separated by n_{skip} (e.g. $O(100)$) time steps. Note that the total physical time $n_{meas} \cdot n_{\text{skip}} \cdot \tau$ needs to be sufficiently large so that the particles move a lot. When you choose τ very small, $n_{meas} \cdot n_{\text{skip}}$ must therefore be correspondingly large.

Visualize your simulation, after suitably chosen time intervals.

Analysis:

- Produce *histograms* (normalized) of the velocities $|\vec{v}|$ and of the height distribution.
- Fit (with plot) the two-dimensional *Maxwell distribution*
$$f(|\mathbf{v}|) = \frac{m}{k_B T}\,|\mathbf{v}|\ \exp\left(-\frac{m\,|\mathbf{v}|^2}{2k_B T}\right)$$
to the velocity histogram (`nlinfit`-command in MATLAB), and extract $k_B T/m$. Note that the Maxwell distribution is only valid in case no direction is preferred, and for vanishingly small particles. Compare with your actual distribution. What could cause differences ?
- Determine another estimate of $k_B T/m$ from the mean velocity
$$\langle |\mathbf{v}|^2 \rangle = \frac{2\,k_B T}{m},$$
where $\langle\ \ \rangle$ means an average over particles and time.
- How well is the *barometric height equation* reproduced ? Fit (with plot)
$$\rho(h) = \rho(0)\exp\left(-h/h_s\right)$$
to the measured histogram. Here $h_s = \frac{k_B T}{mg}$, which allows you to produce another estimate of $k_B T/m$. The barometric equation may not fit well, depending on your fit range and parameters. What could be the reason ? Does the barometric equation apply in a box ?
- Compare the results for $k_B T/m$. They might differ considerably.