

Exercise 1, TFY4235 Computational physics

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Introduction

The goal of this exercise is to simulate particles as flat, hard disks in a square, 2D container. This is done with a event-driven simulation, as described in the exercise [3]. This is implemented in Python, using the built-in library `heapq`. The simulation is used to first tested with scenarios we know the outcome of, then used to demonstrate the Maxwell-Boltzmann distribution and to investigate the effect of a large, heavy disk hitting a large number of small, inert particles.

Implementation

Though this implementation is largely based on the description in [3], some specific choices have been made, which this section aims to illuminate. It describes the overarching structure of the code and some of the main data structures. The most important function in the code is `run_loop()` in `utilities.py`. It instantiates the required objects, and executes a while loop containing the algorithm, as laid out in [3]. This simulations lends itself to simple parallelization, especially the last task where the same system with different parameters is simulated 20 times. This is handled by the `c1_arguments` functions, which allows for running the system from the command line in several instantiation, with different parameters.

The `run_loop` function can be given the argument `TC=True`. Then, it runs a TC-model, as described in [2]. This is done to avoid inelastic collapse. This is only needed when $\xi < 1$, and there are extremely many collisions in a short time step. Inelastic collapse were observed when the projectile created a wave, as Figure 2, and especially if it approach the bottom of the box. Good results were found with $t_c = 10^{-8}$. If the function is passed the argument `condition=func`, it will check the function `condition` at regular intervals. This makes it possible to exit the loop early. It is used to run the simulation until 10% of the energy is remaining, as described later in the report.

As the program runs, the priority queue `collision`, containing the collisions, becomes longer and longer as more than one collision is added each time one is removed. When it becomes too long, it is beneficiary to discard the `collision` heap, and start from scratch. This is handled by `run_check`. This function is called regularly in the main loop, at the same spot as `condition` as described in the paragraph above. If the time between each call is more than four times as long as it initially was, all collisions are discarded, and `collisions` are instantiated anew. This also decreases the risk of running out of RAM.

The `init` function depends on the situation that is being simulated. To place out particles randomly, in either the whole box or in a smaller part of the box, the `random_dist` function, located in `particle_init.py` is used. This function contains a loop that places a particle randomly within the desired bounds, and gives them velocity with a given magnitude, but uniformly distributed direction. Then, if the particle overlaps with any of the other particle already in the box, it is rejected. If too many particles in a row are rejected, There is a “emergency break”, and the codes throws an error. As this function only returns a numpy array, the just-in-time compilation library Numba is compatible with it. With 2 000 particles, of radius 0.008, the `@njit()`-decorator gives a speedup from 15.1 seconds to 0.8 seconds.

`profile.ipynb` shows the profiling of `run_loop`, and the subroutines that takes the most time. This shows that it is the loop that pushes the next collisions to the priority queue that is the bottle neck. A speedup of around 20 times, for 1 000 particles simulated over 10 000 steps was found by rewriting the function that finds

the collisions. The notebook `profile_old.ipynb` shows the time used by the old version of the function. It took as argument the index `i` of the particle in question, then found if and when it was to collide with all other particles, and returned this time as a list. The new version utilizes the fact that everything is contained in numpy-arrays. It does the same operations as the old function, only on arrays instead of single particles. This is done by using masks. An array of booleans can serve as indices, so `1st[np.arange(N) != i]` gives an array with all the elements of `1st`, except `1st[i]`. The profiling show that while most of the time went to the calculation of the next collision, it now goes to pushing to the `collisions`-heap.

To investigate the creation of craters by a projectile, a function that measures the size of crater is needed. This is done by laying a grid with a spacing Δx on top of the box, looping through each particles, and checking if it is inside the nearby grid cells. The process for checking if a disk is inside each square cell is illustrated in Figure 1. Then, the size of the crater is given by $m\Delta x^2$, where m is the number of unoccupied cells. This method relies on choosing a cell size Δx large enough so that only cells within the crater are marked as empty, while the cells around untouched particles are deemed full. This is done by inspecting the result, and comparing it to a plot of the crater as shown in Figure 2.

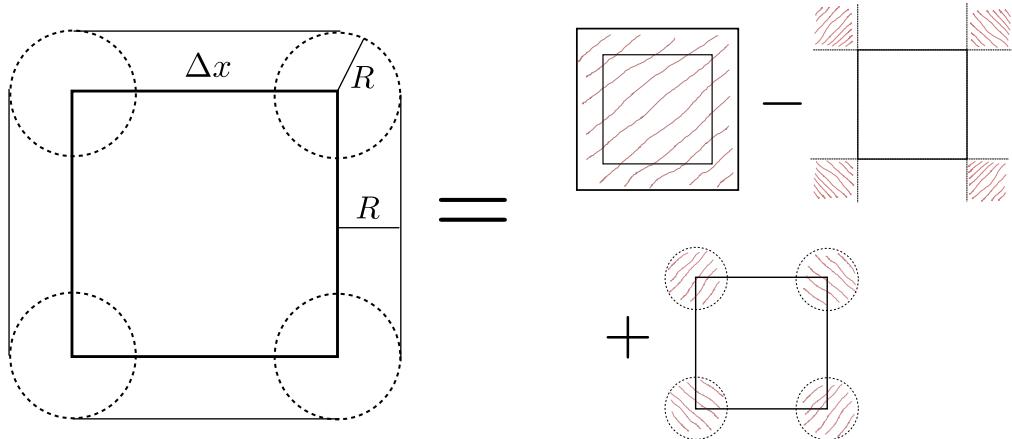


Figure 1: Checking if a disk of radius R is inside of a square of side length Δx , is equivalent to checking if the center of the disk is inside the shape on the left side. Thus, the task is reduced to checking if the center is inside the larger square of side lengths $2R + \Delta x$, but not at the corners, or inside one of the circles of radius R centered at the corners of the square.

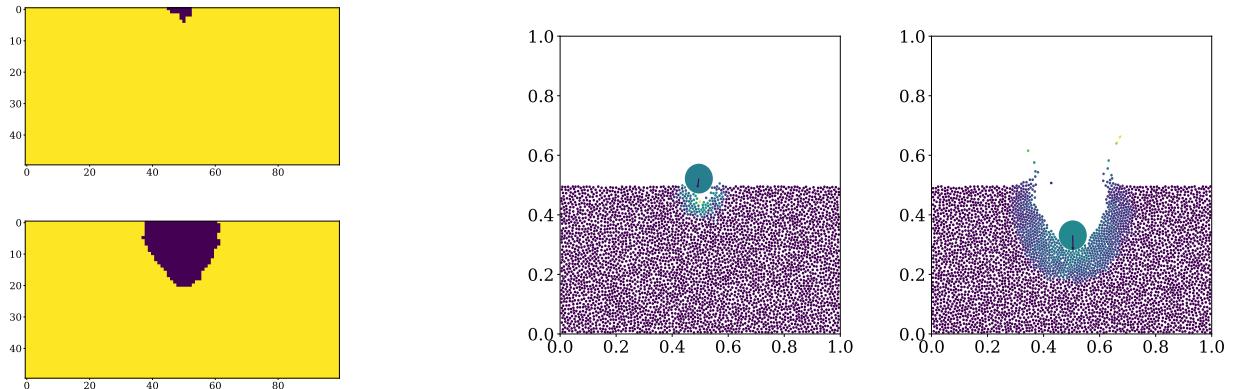
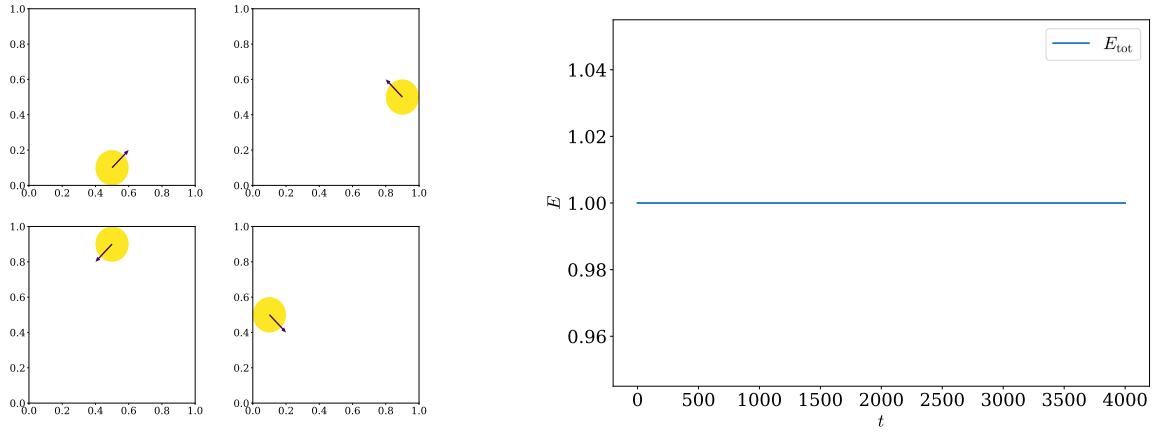


Figure 2: The grid cells with a particle inside is marked yellow, while the ones without a particle inside, i.e. those counted as making up the grid, are purple. The plot to the right shows the crater.

Tests

Several functions were developed to test the implementation for errors and bugs. First, one particle, starting at in the middle of the box all the way to the left with a velocity with at 45° to the x -axis, should move in a tilted rectangle. With $\xi = 1$ it should also conserve energy. Figure 3a shows that this is still the case after 10 000 events. Figure 3b shows that the energy of the system is conserved. A test of two particles bouncing of each other is shown in the video `video/test_case_two_particles.mp4`. This shows that two projectiles behave as expected, and follow a predictable pattern. After around 70 collisions, however, numerical errors accumulate such that the system is thrown into a chaotic state. This is expected behavior, and may even be argued is more realistic than perfectly predictable behavior, as this is not observed in nature. A video showcasing 10 000 particles over 100 000 collisions is found in `video/test_case_many_particles.mp4`

To test the validity of the particle collision, one small, light particle is sent towards a single, large and heavy particle, with varying impact parameter. The relationship between the impact parameter and the escape angle is $s(\theta) = a \cos(\theta/2)$, where a is the radius of the stationary particle [1]. The result is shown in Figure 4, and is in good agreement with the theory. The energy from a simulation of 10 000 particles over 100 000 events is shown in Figure 5, together with a snapshot of the particles. The energy is conserved, aside from negligible fluctuations. Lastly, a video showcasing one large particle crashing into a large mass of small, inert particles is available at `video/test_case_projectile.mp4`. This illustrates that the TC-simulation is working.



(a) After 10 000 steps, the disk still follows a regular pattern

(b) The energy of a single particle is constant.

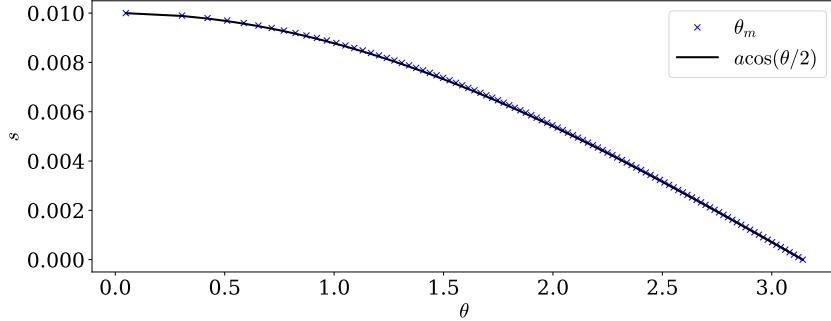


Figure 4: The impact parameter S , as a function of scattering angle. The dashed lines are the theoretical values, θ_m are the values from the simulation.

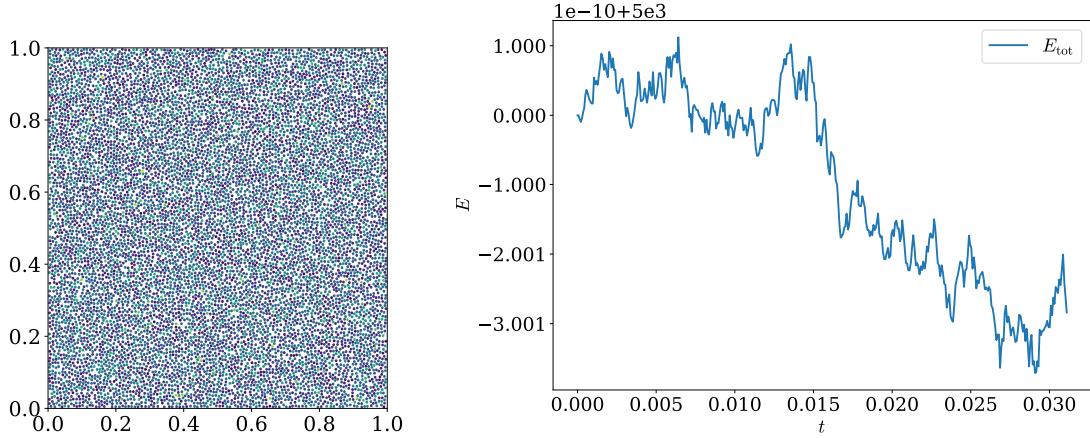


Figure 5: On the left is a snapshot of the particles. The arrows and colors represent the velocities. On the right, the energy is plotted as a function of events. The energy loss can be seen to be negligible.

Results

Velocity distribution

When the system is first initiated, all particles have the same magnitude of velocity. As the system equilibrates, it should reach the Maxwell-Boltzmann distribution, which in 2D is

$$f(v) = \frac{mv}{T} \exp\left(-\frac{mv^2}{2T}\right),$$

when using units in which $k_b = 1$. The equipartition theorem gives the temperature $T = E$ in 2D. Figure 6 shows the average velocity as a function of time. It is a indication of when the system has reached equilibrium, and was used to find a good point to start sampling. After that, the simulation is sampled every N event, where N is the number of particles. This ensures somewhat independent samples. Figure 7 shows the velocity distribution, compared to the Maxwell Boltzmann distribution.

Next, two different types of particles are simulated, one with a mass of 1, the other with a mass of 4. As the particles have the same magnitude of velocity, but different masses, they will have different energies, and thus have different temperatures. Figure 8 shows how the average speed evolves over time. After the system equilibrates, the both sets of particles should reach the Maxwell-Boltzmann distribution with a common temperature. The peak will nonetheless be at different velocities. This is, however, only the case when the restitution coefficient ξ is set to 1. For values less than one, the two sub systems approach each other in temperature, but does not come into equilibrium, as shown in Figure 10.

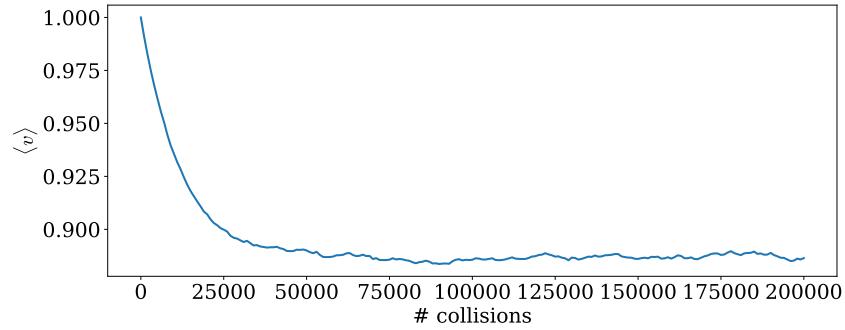


Figure 6: Average velocity, as a function of collisions. The distribution reaches equilibrium around 30 000 collisions, or $3N$

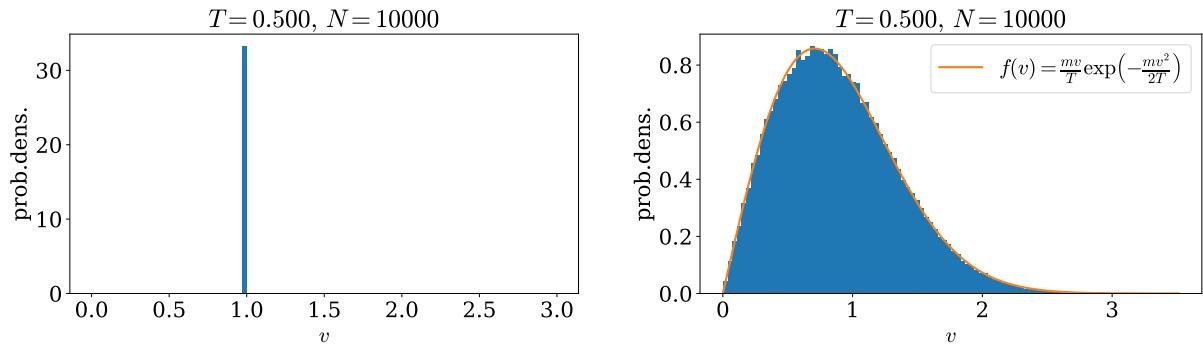


Figure 7: On the left, the initial velocity distribution of 10 000 particles is shown. The plot on the right uses from a total of 200 000 collisions, and shows a good fit with the Maxwell-Boltzmann distribution.

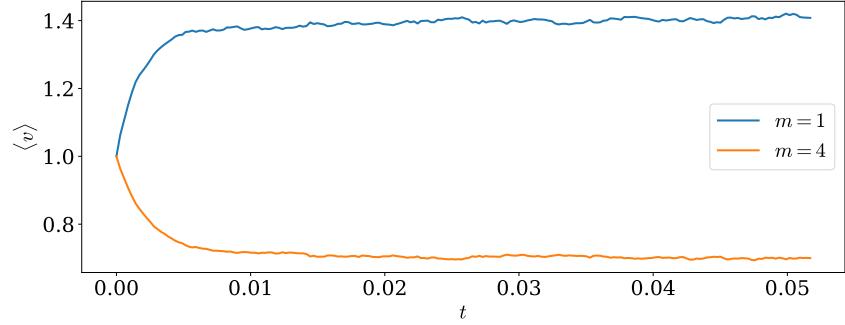


Figure 8: The velocity distribution of the particles with $m = 1$ and $m = 4$ is shown left and right, resp. and compared to the Maxwell-Boltzmann distribution.

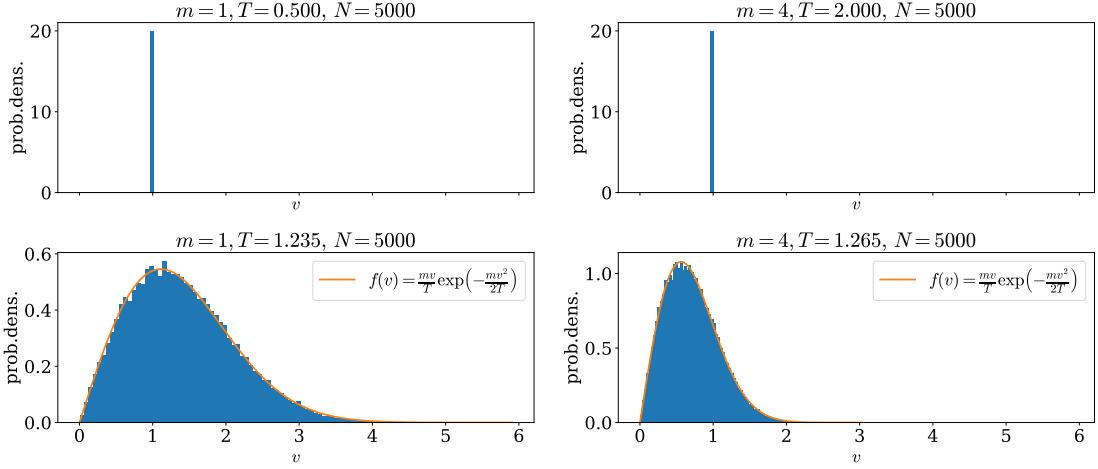


Figure 9: The velocity distribution of the particles with $m = 1$ and $m = 4$ is shown left and right resp., and compared to the Maxwell-Boltzmann distribution. The corresponding initial distribution is shown on top.

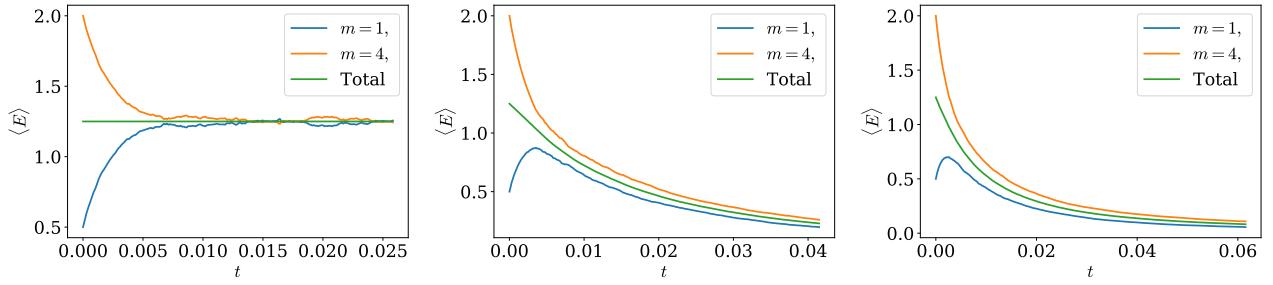


Figure 10: The average energy, as a function of time, of resp. $\xi = 1$, $\xi = 0.9$ and $\xi = 0.8$.

Projectile

To simulate the impact of a projectile, one particle is placed at $\vec{x} = (0.5, 0.75)$, and given a velocity of $v = (0, -10)$. The lower half of the square box is filled with small, light particles. As the large disk will create a crater. To investigate the effect of the size of projectile on the crater, the simulation is run 10 times, using projectiles with different radius. The crater is measured as described in the implementation section. The mass of the projectile is proportional to R^2 , so that the density is constant. The simulation uses the value $\xi = 0.5$, and it is run until the total energy of the system is 10% of the original value. There are placed out 4 000 particles, of radius $R = 0.0045$ and mass in the range $[0.02, 0.15]$. This means the packing fraction is $4000 \cdot \pi R^2 / 0.5 \approx 0.509$. Figure 11 shows the size of the crater, as a function of the radius of the projectile.

The relationship between the crater size and the mass of the projectile is close to linear, suggesting that the size of the crater might be proportional to either the initial energy or momentum. One would hope this hypothesis could be tested by simulating the projectile with different velocities, however even a large span in velocities leaves the crater nearly unchanged, not a very physically plausible result. This might be due to the criterion for stopping the simulation. It runs until the system has 10% of its initial energy, meaning high velocity projectiles still has a large velocity when the simulation is stopped. One plausible alternative is to stop the simulation when the projectile stops moving downwards, however this leads to unreasonably long simulations.

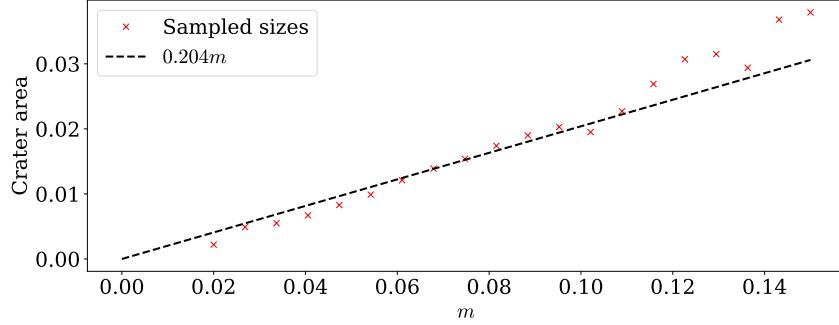


Figure 11: The size of the crater, as a function of the radius of the incoming projectile.

Discussion and conclusion

The simulation implemented yields accurate results. A good indication of this is how well the energy is conserved, as shown by Figure 5. The fluctuations here are mostly due to numerical inaccuracies, and negligible for the purposes of these simulations. Discrepancies between the histograms and the Maxwell-Boltzmann distribution comes from the fact that the simulated system is finite, and thus subject to stochastic fluctuations away from perfect equilibrium. The results from the simulation of a projectile are suggestive of a linear relationship between either momentum or energy, and the crater size. Further investigations, with a better cutoff criterion is needed to tease these apart.

When it comes to the thermodynamic properties, the most straight forward way to get better samples would be to simulate more particles, for longer periods of time. At this point, however, the simulation will become increasingly slow, even with the measures taken to speed it up. The largest bottleneck at this time is pushing the collisions to the priority queue. Some measures could be taken to limit this, for example given particle i , only push the next collision with, say j . Then, if j is involved in another collision, find particle i 's next collision. This, however, might lead to a large amount of tests reducing the possible gain.

References

- [1] Jaakko Akola and Martin Johnsrud. *Exercises classical mechanics, exercise 5*. 2020. URL: https://github.com/martkjoh/exercises_classical_mechanics.
- [2] Stefan Luding and Sean McNamara. “How to handle the inelastic collapse of a dissipative hard-sphere gas with the TC model”. In: *Granular Matter* 1 (1998), pp. 113–128. DOI: <https://doi.org/10.1007/s100350050017>.
- [3] NTNU, Institutt for Fysikk. *Exercise 1, TFY4235 Computational Physics*. 2021.