Event driven simulation of a 2-dimensional gas

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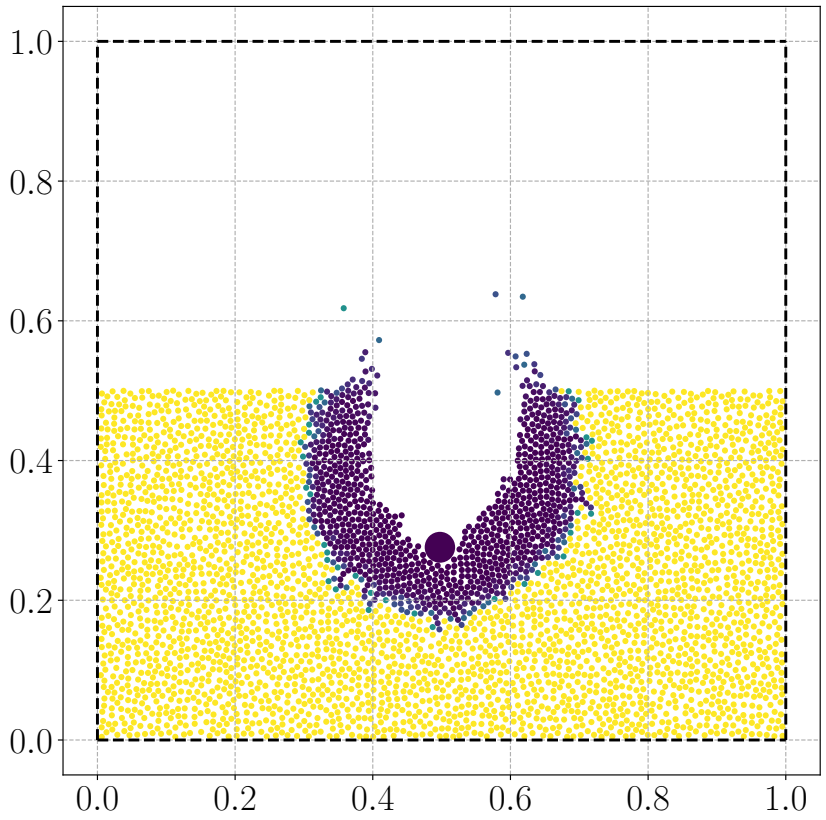
Abstract

An event driven approach is used to simulate a gas of hard discs in two dimensions. The framework built is used to study statistical properties of the gas at and towards equilibrium. The numerical results are compared with well known results from classical statistical mechanics. Towards the end, the formation of a crater from a projectile impact on a bed of particles is studied with the gas system.



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Introduction

1 Background

The central algorithm for event-driven simulations is the following [DTS05] [Nor21]:

```
Set velocities and positions of all particles in the gas;
Choose a stop criterion;
for each particle in gas do
    Calculate if and when the particle will collide with all the other particles and
     the walls;
    Store all the collision times;
end
while not reached stop criterion do
    Identify the earliest collision;
    if collision is valid then
        Move all particles in straight lines until the earliset collision;
        for each particle involved in collision do
            Change its velocity according to the equations given in section 2 in
             [Nor21] ;
            Calculate if and when the particle will collide with all the other
             particles and the walls;
            Store all the collision times;
        end
    else
        Discard collsion;
    end
end
```

Algorithm 1: Event driven simulation of a gas.

In the above algorithm, a collision is marked *valid* if the particle(s) involved in the collision has *not* collided since the time the collision time was stored. Equivalently — and more convenient when dealing with computations that *might* make the time between collisions *very* small — one can keep track of the number of collisions a particle has experienced and use this number to check whether the collision is valid.

The stop criterion mentioned in the while-loop will depend on the situation we are considering. To this end I have created a utility-class called `StopCriterion` which is an abstract class used for this purpose, with multiple children for stopping after reaching a specific number of collision, after reaching a specific time or after a certain amount of the initial energy has dissipated in collisions. This framework provides the option to easily extend to more such criterion, although requiring adding some modifications to the main simulation method.

2 Overview of code

In this section I briefly present how the algorithm is implemented and which considerations are put into the choices of data-structures. The code is written in `python`.

The main machinery of the code is collected in a class called `Gas` in `events.py`, which in essence is a collection of N `particles` and various methods to manipulate the coordinates of each particle to simulate the gas' time evolution according to the algorithm in section 1 and the more detailed equations for handling the changing velocities upon collisions given in [Nor21]. The easiest way to simulate the system is to initialise the gas by calling the constructor with the argument N giving the number of particles, setting the velocities by calling `gas.set_velocities(v)`, with `v` being an $2 \times N$-dimensional array, and subsequently `gas.simulate()`. The radius of the particles can also be set in the constructor as an optional argument. The particles are represented by their coordinates in the extended configuration space, that is their position and velocity. This is the member variable `particles` in the `Gas` class. Although the main algorithm presented in the introduction 1 invites to a fully object-oriented approach, I have chosen to restrain myself somewhat in that respect. For instance, I have chosen not to create an object representing each particle. The most prominent caveat preventing me from doing this is that it might affect the speed of the calculations. By choosing not to create a separate object representing each particle, I found it very simple to move the particles at each time step and also accessing them by ordinary slicing and indexing of arrays. Although it is possible to overload operators such that an array of self defined object can be added *like* `numpy`-arrays, I found this to be impractically slow. A quick test of adding the self-made particles compared to simply adding $4 \times N$ dimensional arrays establishes this observation quite firmly. The listings below shows the time spent on adding two arrays of 50 000 particles with each of the mentioned methods.

```
%time particles_array_1 += particles_array_2
```

```
CPU times:  user 443 µs, sys:  101 µs, total:  544 µs Wall time:  306 µs
```

```
%time particles_class_1 += particles_class_2
```

```
CPU times:  user 34.1 ms, sys:  87 µs, total:  34.2 ms Wall time:  33.2 ms
```

The issue of finding the earliest event for each time step is solved using a priority queue from the library `heapq` in `python`. This data structure allows for sorting any objects as long as they can be compared by the "less than"-operator. I have therefore chosen to make a class called `Event` to store the necessary information about each collision, and use these in the queue.

The code itself is well documented and should be easy to understand on its own. However, I would like to point out some solutions that I found to work particularly well. The part of the code that undoubtedly is the most computationally heavy is the one devoted to calculating if and when the particles will collide with all others. The naive approach would be to iterate over each particle and do the calculation for each of them separately. In `python`, these kind of nested loops will often become impractically slow. I found considerable improvements through vectorising this calculation.

By essentially replacing the piece of calculation in listing 1 by that in 2 I was able to reduce one of the loops over all of the particles.

```
for j in range(self.N):
  if i != j:
    delta_x = self.particles[:2,j] - self.particles[:2,i]
    delta_v = self.particles[2:,j] - self.particles[2:,i]
    R_ij    = self.radii[i] + self.radii[j]
    d       = (delta_x @ delta_v)**2 - (delta_v @ delta_v) * ((delta_x
   @ delta_x) - R_ij**2)

    if delta_v @ delta_x < 0 and d > 0:
      new_t =  - (delta_v @ delta_x + np.sqrt(d))/(delta_v @ delta_v)
      heapq.heappush(self.events, Event(new_t + t ,i,j,"pair",self.
   count[i], self.count[j]))
```

Listing 1: Loop over all particles.

```
T = np.full(self.N - 1, np.inf)
mask = np.arange(self.N-1)
mask[i:] += 1

r_ij = self.radii[mask] + self.radii[i]

delta_x = self.particles[:2,mask] - self.particles[:2,i][:,None]
delta_v = self.particles[2:,mask] - self.particles[2:,i][:,None]

vv = np.einsum('ij,ij->j',delta_v,delta_v)
vx = np.einsum('ij,ij->j',delta_v,delta_x)
xx = np.einsum('ij,ij->j',delta_x,delta_x)

d = vx ** 2 - vv * ( xx - r_ij**2 )

c_mask = (vx < 0 ) * (d > 0)

T[c_mask] = - ( vx[c_mask] + np.sqrt(d[c_mask]) )/(vv[c_mask])

T = T[c_mask]
J = mask[c_mask]

for j in range(np.size(T)):
  heapq.heappush(self.events,Event(T[j] + t ,i,J[j],"pair",self.count[i
   ], self.count[J[j]]))
```

Listing 2: Vectorized calculation.

Putting the central pieces[1] of each of these two calculations into two functions `loop()` and `vect()` and comparing the time spent shows that the latter is approximately 100 times faster than the former, when doing a test on 50 000 particles. It should be noted however that the latter also requires a separate loop for pushing the new events into the queue, whereas the former does not. The speed-up is probably somewhat smaller than shown here, but nonetheless it is a considerable improvement.

```
%timeit loop()
```

```
52.4 ms ± 260 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

[1]The *central* piece here is referring to line 1 through 6 in listing 1 and line 1 through 14 in listing 2.

```
%timeit vect()
```

```
429 μs ± 23.3 μs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

An explanation is probably appropriate for the somewhat cryptic `einsum`-function from `Numpy`. This function allows for writing sum operations on arrays using Einstein's summation convention. Once I have gotten used to the notation, I find it very readable. In addition it is very fast; the listed code in 3 below produces the following results:

```
u = np.random.random((2,50000))
v = np.random.random((2,50000))

%timeit np.einsum('ij,ij->j',u,v)
%timeit np.sum( u*v, axis = 0)
```

Listing 3: Timing einsum.

```
55.2 μs ± 364 ns per loop (mean ± std. dev. of 7 runs, 10000 loops each)
```

```
89.6 μs ± 4.78 μs per loop (mean ± std. dev. of 7 runs, 100000 loops each)
```

PART II

Results and discussion

In the following sections, I will present the results from the simulations in the problems. For a more detailed description of the problems consult the exercise sheet [Nor21].

3 Speed distribution at equilibrium

The first test is devoted to investigating the distribution of the velocities of the particles after sufficiently long time. From statistical mechanics, we know that the velocities of a 2-dimensional gas at equilibrium will distribute according to Maxwell-Boltzmann's velocity distribution:

$$p(v) = \frac{mv}{k_B T} \exp\left(-\frac{mv^2}{2k_B T}\right), \tag{1}$$

where k_B is Boltzmann's constant, T the absolute temperature, and m the mass of the particles. It is evident that the particles will have to have the same mass for comparing with the known distribution in equation 1. The case of dissimilar masses is considered in section 4 and 5.

We initialise a system of 32 000 particles[2] with velocities $\mathbf{v} = [v_0 \cos\theta, v_0 \sin\theta]$ with $\theta \sim \mathcal{U}[0, 2\pi]$. The initial distribution of the velocities is therefore $\delta(v - v_0)$. After simulating the system until equilibrium is reached, i.e. the the average number of particle collision is $\gg 1$, the distribution is as shown in figure 1. For this simulation, the stop criterion used was that the average number of collisions surpassed 50. To get a larger number of independent samples, I have used the speeds at different times in this simulation sampled such that all particles have collided between each sample. Specifically, here I have used every 10^{th} sample over the course of 250 time steps out of a total of 400 time samples. This should correspond to it being roughly 1.3 collisions per particle on average between each sample. Judging from the plot, the samples seem sufficiently independent as the distribution very well resembles the Maxwell-Boltzmann distribution.

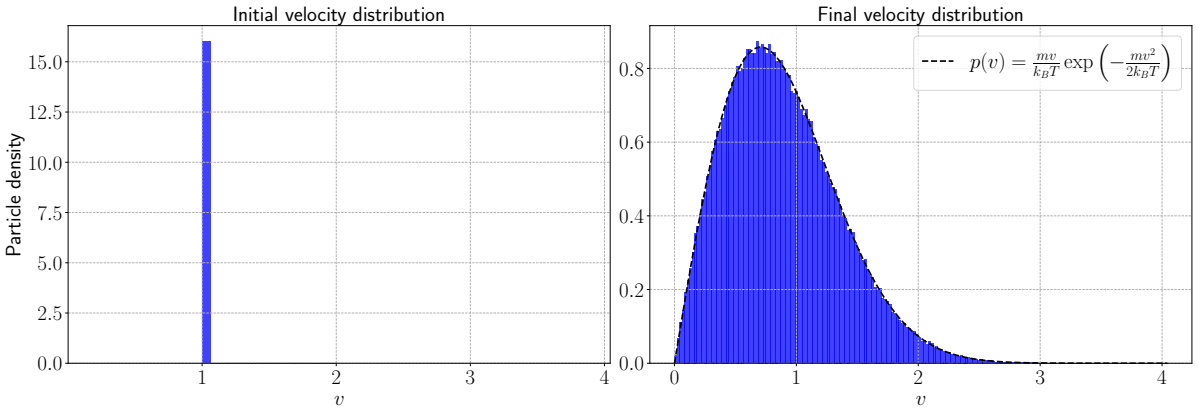

Figure 1: Distribution of velocities in a gas using 256 000 samples.

[2]That is, 8 ensembles of 4000 particles run in parallel.

To have a more quantitative measure of how good the fit is, divide the real line into k intervals and consider the normalized ℓ^1 and ℓ^2-norm of the difference at each interval

$$\texttt{err}_1 = \frac{1}{2}\sum_{j=1}^{k}|d_j - p_j| \quad \texttt{err}_2 = \sqrt{\frac{1}{2}\sum_{j=1}^{k}|d_j - p_j|^2}, \tag{2}$$

where d_j denotes the density of samples in interval I_j and

$$p_j \coloneqq \int_{I_j} p(v)\,\mathrm{d}v$$

is the probability that an observation falls into interval I_j[3]. For the distribution shown in figure 1 $\texttt{err}_1 \approx 0.007455$ and $\texttt{err}_2 \approx 0.001262$. This indicates a good fit with the known distribution.

4 Mixture of two gases

We repeat the exact same procedure as in section 3, except that we make half of the masses 4 times as big as the rest. The velocity distributions after equilibrium is reached is plotted in 2.

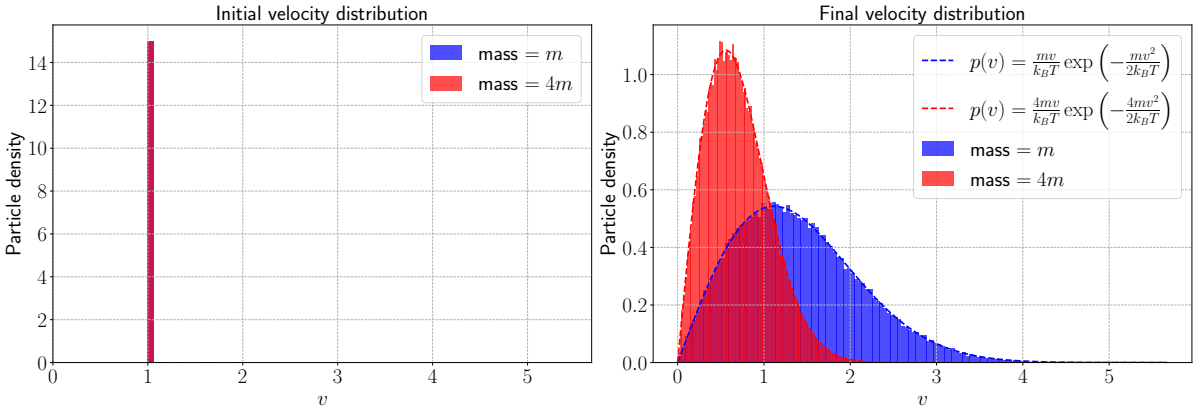

Figure 2: Distribution of velocities in a gas of 50000 particles, here using 112 00 samples for each distribution. The red distributions correspond to the heavy particles, while the blue correspond to the lighter particles.

The average speed and kinetic energy is shown in table 1. These results suggests that although the masses are different, the mixture of the gases eventually reach equilibrium. The fact that the two gases reaches equilibrium is however most easily seen by actually plotting the time evolution of the average kinetic energy. This is shown in section 5, where we also simulate situations where this is *not* the case.

[3]There are many approaches to constructing such a measure. These have the advantage that they range from 0 to 1, since the usual ℓ^1 and ℓ^2 norm of the differences is in the worst case 2 and $\sqrt{2}$ respectively if the support of the theoretical and measured distribution are disjoint. A disadvantage of $\texttt{err}_1$ is that it does not measure "closeness" in the usual *least-square* sense, as the ℓ^2 norm does.

Table 1: Average speed and kinetic energy for the light and heavy particles

Mass	**Average speed**	**Average kinetic energy**
m	1.400798	12.492590
$4m$	0.701439	12.507510

5 Mixing in the presence of energy dissipation

To investigate, at least visually, whether the gas mixture reaches equilibrium we plot the time evolution of the averages of the energy of each species. In addition, we include two similar cases with the restitution parameter ξ set to 0.9 and 0.8. This is shown in figure 3. By the very definition of thermal equilibrium, e.g. the one given in [Hua87, p. 3]

> Thermodynamic equilibrium prevails when the thermodynamic state of the system does not change with time.

it is clear that the system cannot reach equilibrium in the presence of energy dissipation.

The plot in figure 3 shows that the two different particle species reach equilibrium only in the case where the energy is conserved. Furthermore, it is seen that the heavy gas particles are always at higher temperature in the two latter cases. This is easily realised from the fact that the heavy particles start out at higher energy, as the speed of the molecules are the same initially. Even though energy will be transferred to the light particles as time evolves, the energy dissipation will eventually be larger than the gain, and so both types of particles will loose energy. As the total average is below the average of the heavy particles in the beginning, it will stay below for later times as well.

Although this fact is easily realised from elementary statistical mechanics, demonstrating it through these simulations is a good check that the correct physics is contained within the model made.

6 Crater formation from projectile impact

6.1 Distributing the discs randomly in $[0, 1] \times [0, 0.5]$

To distribute the particles randomly in the box defined by

$$\{(x, y) \in \mathbb{R}^2 : 0 < x < 1, 0 < y < 0.5\}$$

I use the following method.

To choose a suitable radius to have the particles fill up the available space with a packing fraction of $\rho \approx 1/2$ I solve for r in

$$N\pi r^2 = A(r)\rho = \frac{1}{2}A(r),$$

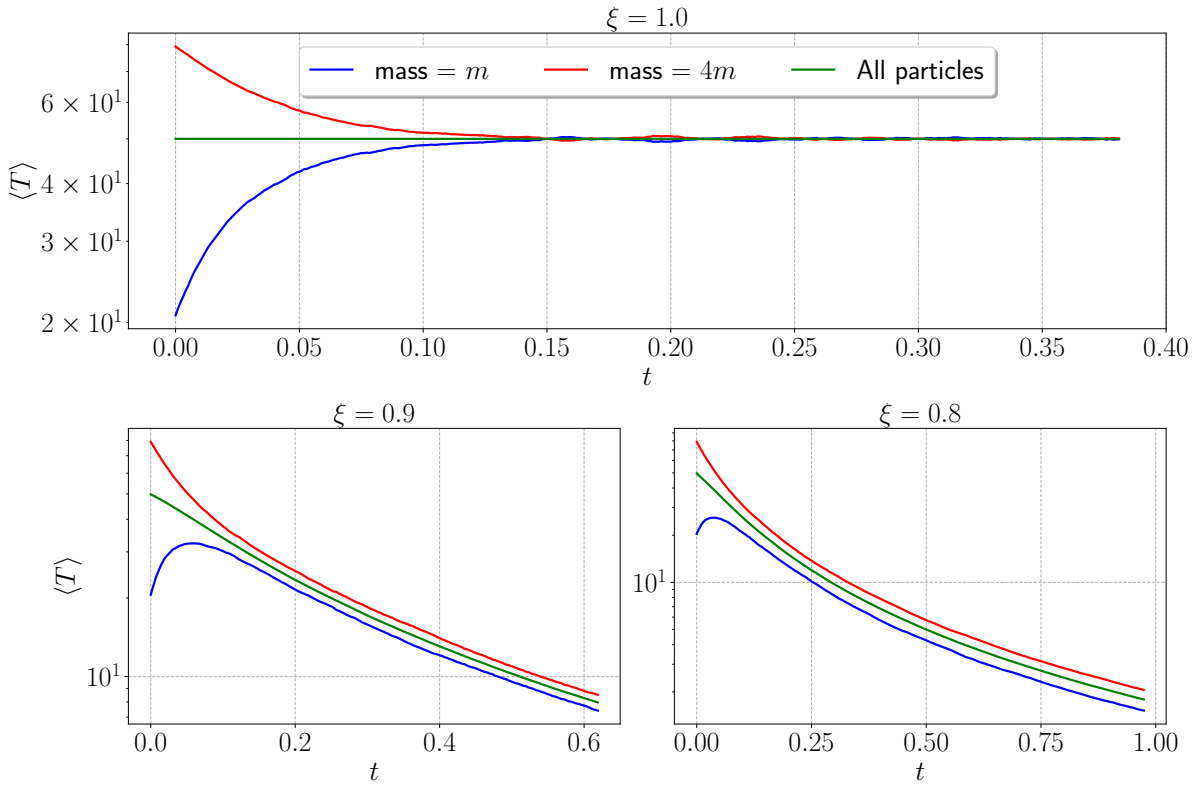

Figure 3: Time evolution of energy averages for restitution parameter $\xi = 1.0, 0.9, 0.8$. The data comes from an ensemble of 8 gases with 4000 particles each.

where, in order to avoid having particles outside the box, the area depends on r. If we clear a border of r on the boundary of the region facing the walls, we get r from solving

$$N\pi r^2 = \frac{1}{2}\left(1 - \frac{1}{2}r\right)(1-2r) \quad \Rightarrow \quad r = \frac{-1+\sqrt{N\pi}}{2(N\pi - 1)}. \tag{3}$$

To avoid having overlapping particles, I do the following

Choose number of particles N;
Find r corresponding to N from (3);
$\mathbf{x} \leftarrow [(0,0), \ldots, (0,0)]$;
Sample $x_i \sim \mathcal{U}_{[r,1-2r)}$ and $y_i \sim \mathcal{U}_{[r,0.5)}$;
$\mathbf{x}_1 \leftarrow (x_i, y_i)$;
for $i = 2 \ldots N$ **do**
  Sample $x_i \sim \mathcal{U}_{[r,1-2r)}$ and $y_i \sim \mathcal{U}_{[r,0.5)}$;
  $\mathbf{x}_i \leftarrow (x_i, y_i)$;
  while *Particle i does not overlap with particle* $1, \ldots, i-1$ **do**
    Sample $x_i \sim \mathcal{U}_{[r,1-2r)}$ and $y_i \sim \mathcal{U}_{[r,0.5)}$;
    $\mathbf{x}_i \leftarrow (x_i, y_i)$;
  end
end

Algorithm 2: Non-overlapping random placement of discs in rectangular region.

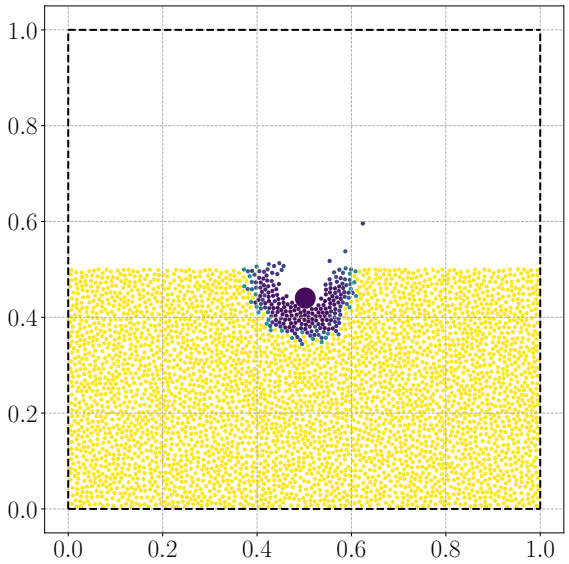

Figure 4: Example of crater formation using a projectile mass 5 times the mass of the remaining particles.

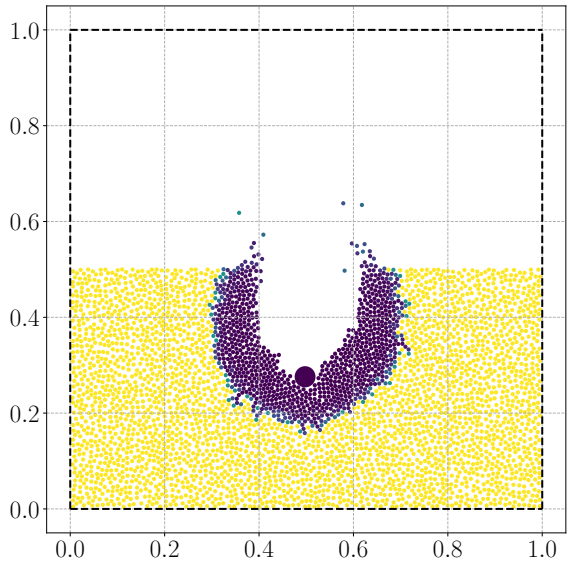

Figure 5: Example of crater formation using a projectile mass 25 times the mass of the remaining particles.

6.2 Illustration of crater formation

The plots in figures 4 and 5 shows the crater formed when the mass of the projectile is 5 and 25 times the mass of the particles in the bed, respectively. A video of the latter case can be seen here. The darker the colour of the particles, the more collisions they have been involved in. We define the *size of the crater*, $\mathcal{S}$, as the number of affected particles by the impact. That is, the number of particles moved during the impact. In the illustrations in figures 4 and 5 the size is the number of non-yellow particles.

6.3 Dependence on projectile mass

By simulating crater formation with projectile masses running from 1 to 25 times the mass of the remaining particles, the size of the crater is as shown in figure 6. The size of the crater $\mathcal{S}$ is simply the number of particles involved in the crater formation. The plot clearly shows that a larger projectile mass gives rise to a larger crater, as one intuitively would expect.

Interestingly, the size seems to scale approximately linearly with the projectile mass. A reasonable suspicion to make is that the size of the crater depends on the energy transferred to it. If this is the case, it would explain the linear dependence on the mass. Following this assumption, one should expect the size to scale quadratically with the initial velocity. However, when trying to demonstrate this I found no such relationship. In fact the crater size seems to be approximately invariant under changes in the projectile velocity. This may be explained through the fact that scaling the velocity amounts to scaling the time by the reciprocal factor due to the simple equations of motion only involving linear dependence on the velocity. This is also true for the collision times, since $\Delta t \sim \frac{1}{|\Delta v|}$ cf. [Nor21], for particle-particle collisions. When using as stop criterion that 90% of the energy is dissipated, the dependence on the velocity is ultimately insignificant.

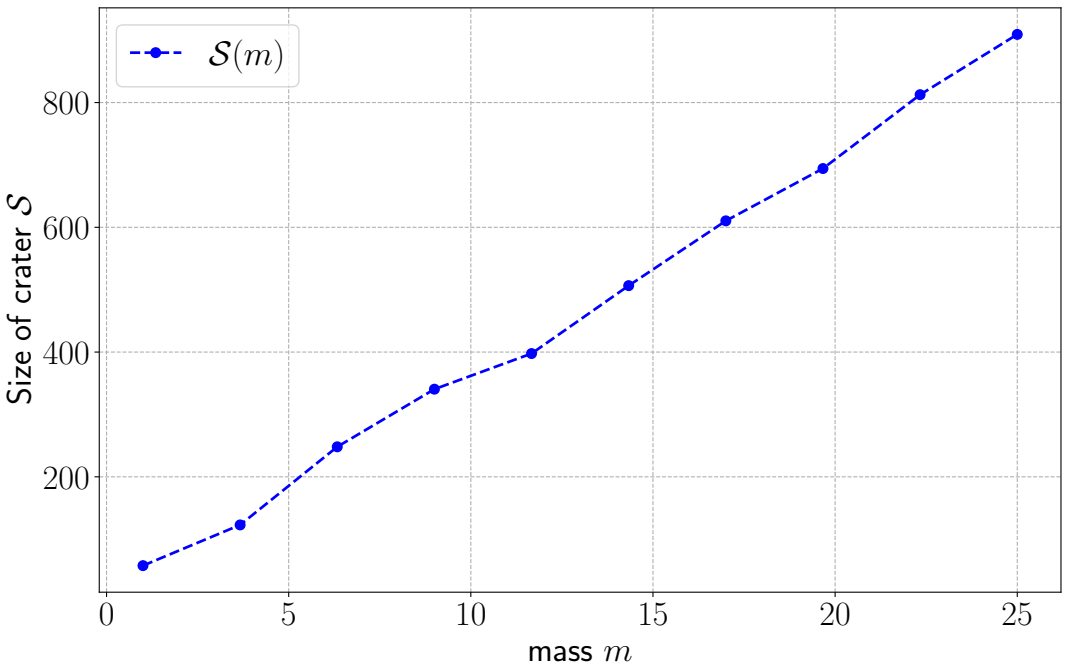

Figure 6: Size of crater as a function of projectile mass. The values are calculated from the mean of simulating projectile impact on 8 ensembles of a bed of 2000 particles.

To investigate the dependence on the velocity, one would therefore have to use another stop criterion.

PART III

Conclusion

We have used a event-driven procedure to simulate a 2-dimensional gas of colliding discs. As predicted by classical statistical mechanics, the distribution of speeds of the particles in this gas follows the Maxwell-Boltzmann distribution in equilibrium. In the presence of energy dissipation, a system consisting of heavy and light gas particles is demonstrated to *not* reach equilibrium. These demonstrations indicates that this simulation approach agrees with the more orthodox method of integrating the equations of motion. This fact is quite remarkable as the method used here only relies on the assumption that the particles undergo linear motion with constant velocity between the collisions, with no mention of any Hamiltonian nor Newtonian equation of motion.

References

[DTS05] Aleksandar Donev, Salvatore Torquato, and Frank H. Stillinger. Neighbor list collision-driven molecular dynamics simulation for nonspherical hard particles. i. algorithmic details. *Journal of Computational Physics*, 202(2):737 – 764, 2005.

[Hua87] Kerson Huang. *Statistical Mechanics*. John Wiley & Sons, 2 edition, 1987.

[Nor21] Tor Nordam. Exercise 1 - Computational physics TFY4235, 2021.