Event driven simulation of a 2-dimensional gas

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Contents

1 Introduction and background

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The central algorithm for event-driven simulations is the following [1]:

```
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
            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 *valid* if the particle(s) involved in the collision has *not* collided since the time the collision time was stored.

2 Overview of code

In this section we briefly present how the algorithm is implemented and which considerations are put into the choices of data-structures.

2.1 Remarks on performance

3 Results

3.1 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's velocity distribution:

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

where k_B is Boltzmann's constant, T the absolute temperature, and m the mass of the particles. It is essential that the all the particles have the same mass m, as will become apparent in section 3.2 and 3.3.

We initialise an system of particles 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 $C\delta(v - v_0)$. 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. Judging from the plot, it seems to be sufficient for equilibrium to be reached.

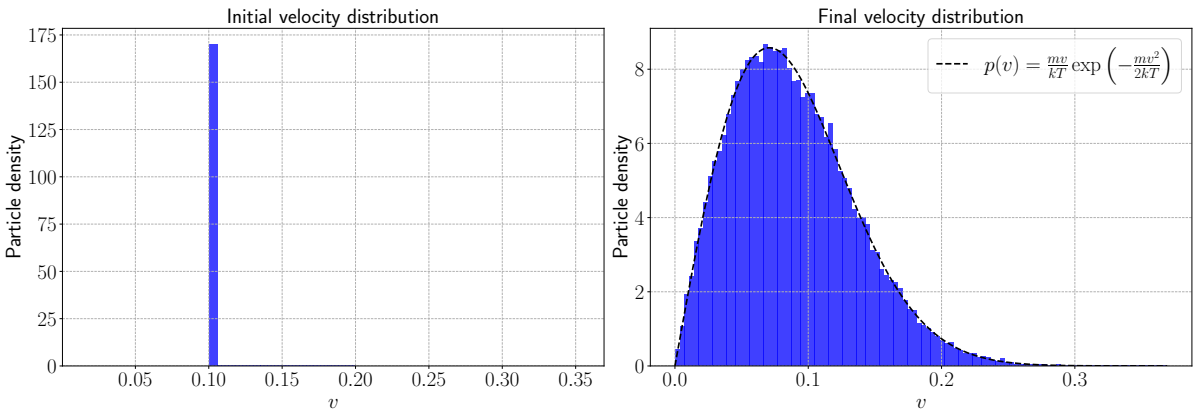

Figure 1: Distribution of velocities in a gas of 50000 particles.

To make the comparison more quantitative, we plot the difference between the Gaussian kernel density estimation of the final distribution and the Maxwell distribution.

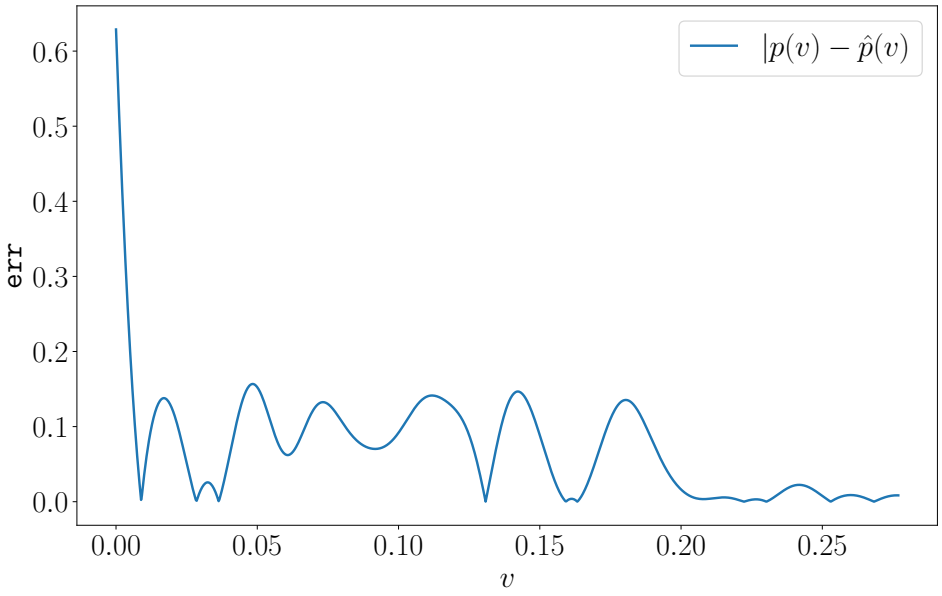

Figure 2: Deviation between Gaussian kernel density estimation of the velocity distribution, $\hat{p}(v)$ and the Maxwell-distribution $p(v)$.

3.2 Mixture of two gases

3.3 Mixing in the presence of energy dissipation

3.4 Crater formation from projectile impact

References

[1] 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.