High Performance Computing with Python

Final Report

Jonas Bürgel

5500163

jonas.buergel@mail.de

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1

Introduction

2

Methods

2.1 Probability Density Function (PDF)

The Probability Density Function (PDF) is a concept that describes the probability of finding a particle at a certain position. In this project, the PDF is used to track the individual trajectories of particles in phase space. Usually this would require solving a very large number of equations. Because solving these equations would be too costly, only the averages over the volumes in the phase space are taken using the PDF. The PDF, denoted as $f(\mathbf{r}_i, \mathbf{v}_i, t)$, represents the probability density of finding a particle at a certain position $\mathbf{r_i}$ and velocity $\mathbf{v_i}$ at a given time t.

2.2 Boltzmann Transport Equation (BTE)

The equation formulates the evolution of motion for the PDF over time. The Boltzmann Transport Equation (BTE) consists of two parts. The first part is *streaming* and resembles only the moving of particles. The second part is called *collision* and deals with the interaction between particles while moving.

2.2.1 Streaming

The probability density of the PDF is able to move, which is described by the Boltzmann Transport Equation (BTE). BTE transports the probability density distributions at a specific velocity in real space. While transporting, the influence of the velocity and acceleration are considered. The combined effect of velocity and acceleration leads to the streaming of density.

The whole Boltzmann Transport Equation is denoted as

$$\frac{\partial f\left(\mathbf{r},\mathbf{v},t\right)}{\partial t} + \mathbf{v}\nabla_{\mathbf{r}} f\left(\mathbf{r},\mathbf{v},t\right) + \mathbf{a}\nabla_{\mathbf{v}} f\left(\mathbf{r},\mathbf{v},t\right) = C(f)\cdot \tag{2.1}$$

The l.h.s. of the equation denotes the streaming part that was just explained and the r.h.s. the collision, explained in the following part.

2.2.2 Collision

Only applying streaming resembles a probability of collision of 0%, which is not realistic. To account for collisions, an additional term is introduced into the equation to represent the collision process that occurs at each time step. In reality, collisions between particles result in an almost instantaneous exchange of energy and momentum. However, these collisions occur in extremely short time intervals on the order of femtoseconds (10^{-15} seconds), making it impractical to measure them directly in the model. Therefore, the collision process is approximated as an instantaneous process. Because of this instantaneous, it cannot be represented as a differential equation, which normally describes continuous changes. Instead, a probabilistic approach is taken to describe the effects of collisions.

In the previous section 2.2.1, the Boltzmann Transport Equation (BTE) was introduced (eq. (2.1)), where the right term represents the collision process. To simplify this collision term, a relaxation time approximation is commonly used. This approximation assumes that the probability density function (PDF) $f(\mathbf{r}, \mathbf{v}, t)$ relaxes towards a local equilibrium distribution, denoted as $f^{eq}(\mathbf{r}, \mathbf{v}, t)$. By interpreting the streaming term as the total time derivative of the PDF, the BTE can be reformulated as follows:

$$\frac{d}{dt} f(\mathbf{r}, \mathbf{v}, t) = -\frac{f(\mathbf{r}, \mathbf{v}, t) - f^{eq}(\mathbf{r}, \mathbf{v}, t)}{\tau}. \tag{2.2}$$

The included equilibirum function can is denoted as

$$f_i^{eq}(\rho(\mathbf{r}), \mathbf{u}(\mathbf{r})) = w_i \rho(\mathbf{r}) \left[1 + 3\mathbf{c}_i \cdot \mathbf{u}(\mathbf{r}) + \frac{9}{2}(\mathbf{c}_i \cdot \mathbf{u}(\mathbf{r}))^2 - \frac{3}{2}|\mathbf{u}(\mathbf{r})|^2\right]. \tag{2.3}$$

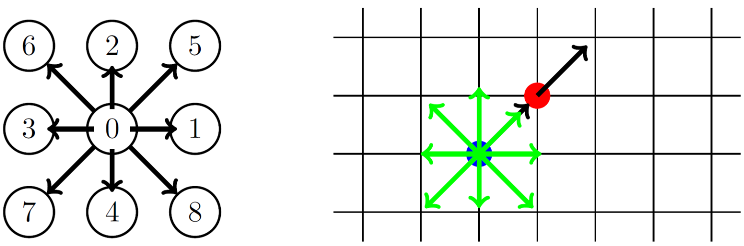
The equilibrium function introduces some additional quantities, namely the density $\rho(\mathbf{r})$, velocity $\mathbf{u}(\mathbf{r})$ and w_i. w_i is defined for a D2Q9 lattice as seen in eq. (2.4). The other two quantities can be calculated using the following formulas.

$$w_i = \left(\frac{4}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{36}, \frac{1}{36}, \frac{1}{36}, \frac{1}{36}\right) \tag{2.4}$$

$$\rho(\mathbf{r}) = \sum_i f_i \tag{2.5}$$

$$\mathbf{u}(\mathbf{r}) = \frac{1}{\rho(\mathbf{r})} \sum_i \mathbf{c}_i f_i(\mathbf{r}) \tag{2.6}$$

2.3 Lattice Bolzmann Scheme



(a) (b)

Figure 2.1: Visualization of the underlying grid including labled directions.
(a) directions with given labels
(b) streaming example of one particle

3

Implementation

4

Results

5

Conclusion

6

Chapter 1

This is an example of a citation [1]. The corresponding paper can be found in the bibliography section at the end of this document.

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Example of normal equation

$$f_i(\mathbf{x}_j + \mathbf{c}_i \cdot \Delta t, t + \Delta t) = f_i(\mathbf{x}_j, t) - \omega \left(f_i(\mathbf{x}_j, t) - f_i^{\mathrm{eq}}(\mathbf{x}_j, t) \right) \tag{6.1}$$

Example of aligned equation:

$$\rho(\mathbf{x}_j, t) = \sum_i f_i(\mathbf{x}_j, t) \tag{6.2}$$

$$\mathbf{u}(\mathbf{x}_j, t) = \frac{1}{\rho(\mathbf{x}_j, t)} \sum_i \mathbf{c}_i f_i(\mathbf{x}_j, t) \tag{6.3}$$

6.1 section title

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- Example of a list
- Example of a list
- Example of a list

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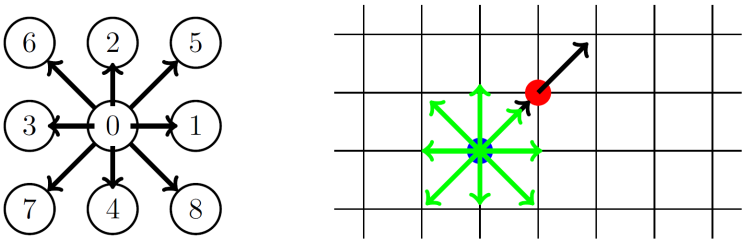
Chapter 2



(a) (b)

Figure 7.1: example figure

7.1 Section title

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Table 7.1: Sample table

S. No.	Column#1	Column#2	Column#3
1	50	837	970
2	47	877	230
3	31	25	415
4	35	144	2356
5	45	300	556

7.2 Code listing

here we provide a short example of code listing. For further information you can take look here:

https://www.overleaf.com/learn/latex/code_listing

This is just meant to used if you think that there is some relevant part of code to be shown. Please do not append your whole implementation in the report.

```
import numpy as np

def incmatrix(genl1,genl2):
    m = len(genl1)
    n = len(genl2)
    M = None # to become the incidence matrix
    VT = np.zeros((n*m,1), int)  # dummy variable
```

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Bibliography

[1] Krüger Timm, H Kusumaatmaja, A Kuzmin, O Shardt, G Silva, and E Viggen. *The lattice Boltzmann method: principles and practice.* Springer: Berlin, Germany, 2016.