High Performance Computing with Python

Final Report

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Contents

Abbreviations

BTE Boltzman Transport Equation

CI Continuous Integration

LBM Lattice Boltzman Method

SIMD Single Instruction Multiple Data

MPI Message Passing Interface

1

Introduction

The Lattice Boltzman Method (LBM) is a numerical parallelizable and efficient scheme for simulating fluid flows. In addition, the LBM can be extended with boundary conditions. The key property of the LBM is that it is a discrete kinetic theory approach featuring a mescoscale description of the microstructure of the fluid instead of discretizing macroscopic continuum equations. Other key advantages of the LBM include: efficient implementation by parallelization and the LBM can be applied to different kind of lattices.

All code is available at `https://github.com/infomon/lattice_boltzman_parallel_solver` under BSD license. We give the instructions how to reproduce the results of the experiments conducted in this report in the *README*.

Structure of report

The remainder of the report is organized as follows:

- **Chapter 2** describes the LBM. More specifically, we describe how we discretize the *Boltzman transport equation* resulting in the LBM. We also show how macroscopic quantities, e.g. density and velocity, can be calculated from the microscopic simulation. In addition, we describe several boundary conditions that can be applied in the LBM.
- **Chapter 3** describes how the LBM is implemented using *Python* as programming language. We also show how we parallelized the implementation and how we ensured software quality by unit testing.
- **Chapter 4** conducts extensive experiments showing the applicability and correctness of the implementation of the solver for the LBM.
- **Chapter 5** concludes this report.

2

Lattice boltzman method

2.1 Overview

In this chapter we describe the Lattice Boltzman Method (LBM). The main idea of the LBM is to *simulate a fluid density statistically on a lattice* instead of solving (and also discretizing) the Navier-Stokes equations.

2.2 Boltzman Transport Equation (BTE)

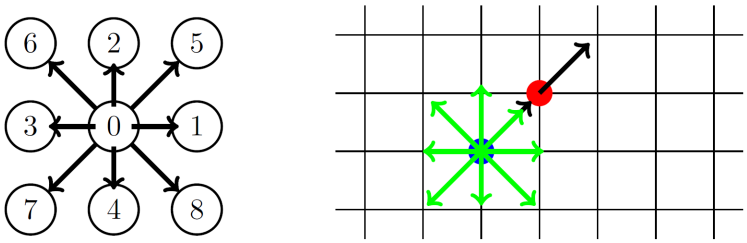
The boltzman transport equation $\frac{df}{dt}$ defines the fundamental differential equation of kinematic gas theory. It describes the evolution of the probability density function $f_(\mathbf{r}, \mathbf{v}, t)$ for finding a molecule with mass m and velocity $\mathbf{v}$ at position $\mathbf{r}$ over time t. Huang [1] shows that the BTE relaxes to the Maxwell velociy distribution function. Bhatnagar et al. [2] approximate the relaxation of f towards f^{eq} as follows:

$$\frac{df(\mathbf{r}, \mathbf{v}, t)}{dt} = -\frac{f(\mathbf{r}, \mathbf{v}, t) - f^{eq}(\mathbf{v}; \rho(\mathbf{r}, \mathbf{t}), \mathbf{u}(\mathbf{r}, t), T(\mathbf{x}, t))}{\tau} \tag{2.1}$$

where τ is the so-called characteristic time, ρ is the mass density, u is the average velocity at position $\mathbf{x}$ and T is the temperature (see section 2.3 for more details). The characteristic time determines how fast the fluid converges towards the equilibrium depending on the viscosity of the fluid. The higher the viscosity, the slower it converges towards the equilibrium. Note, that eq. 2.1 satisfies the Navier-Stokes equations.

Discretization of the BTE

The BTE of eq. 2.1 is defined in the continuous domain. In order to work with the BTE on the computer we have to discretize it in space, velocity and time. The space discretization can be done by just using a discrete lattice (e.g. two-dimensional array). To discretize the velocity and time we have to



(a) (b)

Figure 2.1: Discretization of BTE. (a) Discretization of the velocity space into nine discrete directions. The numbers $0, ..., 9$ uniquely identify the direction. (b) Spatial discretization for the two-dimensional lattice. The green arrows show the possible directions of the particle in the middle. For sake of simplicity, assume that the particle only moves in direction 5. In the next time step the particle is located at the red dot.

impose that the velocity multiplied with the time is equal to some integer, i.e. the particle can only travel on the given lattice and not in-between lattice nodes.

We discretize the velocity directions with the D2Q9 scheme (see fig. 2.1a), which is two-dimensional and consists of nine discrete velocity directions. The velocity directions point to each of its neighbors in the Moore neighborhood. Note, that at the central lattice node the particle is at rest. We define the velocity vectors as follows:

$$\mathbf{c_i} = \begin{pmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{pmatrix}. \tag{2.2}$$

Therefore, we discretize the probability density function $f(\mathbf{r}, \mathbf{v}, t)$ to obtain the discrete probability density function $f_i(\mathbf{x}, t)$, where the subscript i indicates the direction and $\mathbf{x}$ is the discrete lattice.

Finally, we get the discretized version of eq. 2.1:

$$\underbrace{f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - f_i(\mathbf{x})}_{streaming} = \underbrace{-\omega(f_i(\mathbf{x}) - f_i^{eq}(\mathbf{x}, t))}_{collision}, \tag{2.3}$$

where the *streaming* and *collision process* are the key steps in the LBM and $\omega = \frac{\Delta t}{\tau}$ is a relaxation parameter.

The equilibrium probability density function f_i^{eq} can be computed as follows:

$$f_i^{eq} = w_i \rho(x, t)(1 + 3\mathbf{c}_i \mathbf{u}(\mathbf{x}, t) + \frac{9}{2}(\mathbf{c}_i \mathbf{u}(\mathbf{x}, t))^2 - \frac{3}{2}\mathbf{u}^2(\mathbf{x}, t)), \tag{2.4}$$

where $w_i = \begin{cases} \frac{4}{9}, \ if \ i = 0 \\ \frac{1}{9}, \ if \ i = 1,2,3,4 \\ \frac{1}{36}, \ if \ i = 5,6,7,8 \end{cases}$. Fig. 2.1b gives a simplified example for eq. 2.3.

2.3 Moment update

In the LBM, the density ρ and velocity $\mathbf{u}$ are defined by the zeroth and first moments of the probability distribution function f, respectively:

$$\rho(\mathbf{x}, t) = \int f(\mathbf{x}, \mathbf{u}, t) \ d^3\mathbf{u}, \tag{2.5}$$

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho(\mathbf{x})} \int f(\mathbf{x}, \mathbf{u}, t) \cdot \mathbf{c}(\mathbf{u}) \ d^3\mathbf{u}. \tag{2.6}$$

The discretization of those equations yields

$$\rho(\mathbf{x}) = \sum_i f_i, \tag{2.7}$$

$$\mathbf{u}(\mathbf{x}) = \sum_i f_i \mathbf{c}_i. \tag{2.8}$$

2.4 Boundary conditions

The boundary condition describes how the fluid flow behaves during streaming at the boundaries. We define the boundary node $\mathbf{x}_b$ to have at least one link to a solid or fluid node. Note, that the boundary conditions have to be placed in the correct step inside the LBM (see algo. 1). For this reason we differentiate between the *pre-streaming* probability density function f_i^* and the *post-streaming* probability density function f_i. To apply boundary conditions the probability density function after the streaming f_i is modified at each boundary node $\mathbf{x}_b$ given the pre-streaming probability density function f_i^* in each time step:

$$f_i(\mathbf{x}_b + c_i \Delta t, t + \Delta t) = f_i^*(\mathbf{x}_b, t). \tag{2.9}$$

One question that arises is where the boundary nodes $\mathbf{x}_b$ are defined. We distinguish between so called *wet nodes* and *dry nodes* due to different domains, i.e. computational and physical domain. In the former, the computation and physical domain is the same (i.e. the boundaries are placed on the lattice nodes) but this comes with a increased difficulty for the implementation. In the latter the physical domain is half a cell away from the computational domain (i.e. the boundaries are located between the lattice nodes) retaining second order accuracy as long as the boundary is placed exactly in the middle of the lattice nodes.

Below we describe several boundary conditions. One key advantage of the LBM is its easy implementation of boundary conditions and in particular the arbitrary combination of boundary conditions as long as they do not contradict themselves.

Periodic boundary conditions

For a periodic boundary condition the flow leaving a boundary re-enters the domain on the opposite side of the domain

$$f_i(\mathbf{x}_1, t) = f_i(\mathbf{x}_N, t), \tag{2.10}$$

where $\mathbf{x}_1$ and $\mathbf{x}_N$ are the first and last node in the physical domain, respectively. Visually, we can imagine the bounce-back boundary conditions as if we have a cylindrical shape. Note, that therefore periodic boundary conditions conserve mass and momentum. The periodic boundary condition is implicitly implemented by the streaming function.

Periodic boundary conditions with pressure variation

The periodic boundary conditions with pressure variation add a density drop $\Delta\rho$ (or pressure drop Δp) between inlet and outlet. Note, that the pressure and density are related through the ideal gas of state $p = c_s^2\rho$, where c_s is the speed of sound. [3] Let's assume that we want to model a pressure drop in x-direction, then it holds $\forall y \in \{1, ..., l_y\}$ that $p(x_1, y, t) = p(x_N, y, t) + \Delta\rho$, where l_y denotes the diameter in y-direction and x_1 and x_N denote the left-most and right-most node in the LBM, respectively. Thus, we get $\rho_{out} = \frac{p_{out}}{c_s^2}$ and $\rho_{in} = \frac{p_{out}+\Delta p}{c_s^2}$, where the subscripts *in* and *out* denote the pressure values at the periodic boundaries. Note, that the velocity is the same at the periodic boundaries: $\mathbf{u}(x_1, y, t) = \mathbf{u}(x_N, y, t)$.

Let's now assume virtual nodes $\mathbf{x}_0$ and $\mathbf{x}_{N+1}$ at both ends of the periodic boundaries. Note, that the virtual nodes $\mathbf{x}_0$ and $\mathbf{x}_N$ correspond to $\mathbf{x}_N$ and $\mathbf{x}_1$, respectively. Visually we can imagine this like (infinitely) many pipes connected to each other. We decompose the probability density function into a equilibrium part f_i^{eq} and non-equilibrium part f_i^{neq}. The non-equilibrium probability density function is computed by $f_i^{neq} = f_i - f_i^{eq}$. Combining the correspondences of virtual nodes and nodes in the physical domain as well as the decomposition into (non)-equilibrium probability density function parts we obtain the inlet and outlet boundary condition, respectively

$$f_i(x_0, y, t) = f_i^{eq}(\rho_{in}, \mathbf{u_N}) + \underbrace{\{f_i^*(x_N, y, t) - f_i^{eq}(x_N, y, t)\}}_{f_i^{neq}(x_N, y, t)} \tag{2.11}$$

$$f_i(x_{N+1}, y, t) = f_i^{eq}(\rho_{out}, \mathbf{u_1}) + \underbrace{\{f_i^*(x_1, y, t) - f_i^{eq}(x_1, y, t)\}}_{f_i^{neq}(x_1, y, t)} \tag{2.12}$$

Bounce-back boundary

The bounce-back boundary condition applies a no-slip condition at the boundary. It simulates the interaction between the fluid with a non-moving wall without slip. It can also be applied to a stationary obstacle such as a plate.

$$f_{\bar{i}}(\mathbf{x}_b, t + \Delta t) = f_i^*(\mathbf{x}_b, t), \tag{2.13}$$

where the index $\bar{i}$ denotes the conjugate channel of i, e.g. the conjugate channel of 1 is equal to 3.

Moving wall

The moving wall extends the bounce-back boundary condition by taking into account the gain or lose of momentum of particles during interaction with the moving wall. Thus, we extend the bounce-back boundary condition with an extra term for the momentum change

$$f_{\bar{i}}(\mathbf{x}_b, t + \Delta t) = f_i^*(\mathbf{x}_b, t) - 2\omega_i \rho_w \frac{\mathbf{c}_i \cdot \mathbf{u}_w}{c_s^2}, \tag{2.14}$$

where c_s is the speed of sound, ρ_w and $\mathbf{u}_w$ are the density and velocity at the wall, respectively. The velocity at the wall $\mathbf{u}_w$ is equal to $\begin{pmatrix} U_w \\ 0 \end{pmatrix}$ for a tangentially moving wall in x-direction with wall velocity U_w. There are two main options for the estimation of the density at the wall ρ_w:

1. The density at the wall ρ_w is equal to the *average* density $\bar{\rho}$.
2. The density at the wall ρ_w is *extrapolated* from the densities ρ next to the wall. Depending on the order of the extrapolation, we use more or less nodes.

Open boundary

[4] describe open boundaries consist of inlets and outlets where the flow can either enter or leave the computation domain and where we typically *impose velocity or density profiles.* We implement the inlet as follows:

$$f_i(\mathbf{x}_b, t + \Delta t) = f_i^{eq}(\rho_{in}, \mathbf{u}_{in}) \; \forall i \in \{0, ..., 8\}, \tag{2.15}$$

where ρ_{in} and $\mathbf{u}_{in}$ are the density and velocity at the inlet, respectively.

For the outlet, we implement a first-order extrapolation scheme by using the information from the second last node $\mathbf{x}_{b_2} = \mathbf{x}_b - \Delta\mathbf{x}$

$$f_i(\mathbf{x}_b, t + \Delta t) = f_i(\mathbf{x}_{b_2}, t), \tag{2.16}$$

where i denotes the indices pointing into the domain.

3

Implementation

In this chapter we will describe how we implement the algorithm using *Python* as programming language.

3.1 Overview

Algo. 1 shows the pseudocode of the iteration loop of the LBM. As input we can specify the geometry of the physical domain, the boundary conditions (see section 2.4 for more details) as well as the initial conditions.

First we initialize the density ρ and velocity $\mathbf{u}$ and compute the initial value of the probability density function $f_i^{eq} = f_i$.

Then we iterate in a loop over several steps as long as the stopping criterion (e.g. maximum time steps) is not satisfied. Note, that there is some flexibility when to apply which step. [4, 5] The following order of steps corresponds to the order in the implementation of the LBM. We first compute the equilibrium function f_i^{eq} given the current density ρ and velocity $\mathbf{u}$. In the collision step we simulate the effects of collisions between particles (see section 2.2 for more details). After that, we simulate the streaming of f_i, i.e. we simulate the movement of particles to the nearest neighbour lattice nodes using the D2Q9 discretization. Then we apply potential boundary conditions on the probability density function f_i. Note, that we first apply the streaming operation at every node (including the boundary nodes $\mathbf{x}_b$) and then correct the boundary nodes $\mathbf{x}_f$ after the streaming. This has the advantage that the implementation of the streaming is easier. Lastly, we compute the density ρ and velocity $\mathbf{u}$ (see section 2.3 for details on the formulas on how to compute the macroscopic quantities).

After running the LBM we can obtain the density ρ and velocity $\mathbf{u}$ as macroscopic quantities.

Input: Geometry and parameters l, h, U, ν,...; boundary conditions; initial conditions
Output: Final density ρ and velocity $\mathbf{u}$
1 initialize ρ and $\mathbf{u}$
2 compute f_i and f_i^{eq}
3 **while** *stopping criterion is not satisfied***do**
4 | compute equilibrium function $\rho,\ \mathbf{u} \rightarrow f_i^{eq}$ ▷ `eq. 2.4`
5 | collision step $f_i^* = f_i(\mathbf{x},t) - \frac{\Delta t}{\tau}(f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t))$ ▷ `eq. 2.3`
6 | streaming $f_i(\mathbf{x} + c_i\Delta t, t + \Delta t) = f_i^*(\mathbf{x},t)$ ▷ `eq. 2.3`
7 | apply boundary conditions $f_i(\mathbf{x}_b + c_i\Delta t, t + \Delta t) = f_i^*(\mathbf{x}_b,t)$ ▷ `section 2.4`
8 | moment update $f_i \rightarrow \rho,\ \mathbf{u}$ ▷ `eq. 2.7 & 2.8`
9 **end**

Algorithm 1: Pseudocode of the iteration loop of the LBM.

3.2 Basic implementation in Python

In this section we show how we implemented the basic equations and data structures introduced in chapter 2. We use Python as programming language and use the python libraries *numpy* [6, 7] for array operations, *scipy* [8] for some more complex scientific computations and *matplotlib* [9] for visualizing the obtained results. And key advantage of numpy is to vectorize arrays, which lowers the computational time.

We represent the (discrete) probability density function $f_i(\mathbf{x})$ as a numpy array of size $l_x \times l_y \times 9$, where l_x and l_y are the size of the lattice in x- and y-direction, respectively. The last dimension (e.g. 9) of the numpy array corresponds to the discretized velocity direction. We represent the velocity directions $\mathbf{c}$ and the weights w_i as numpy arrays with size 9×2 and 9, respectively.

In steps 4 and 5 of algo. 1 we simulate the collision part of eq. 2.3. We implement the computation of the equilibrium probability density function f_i^{eq} of eq. 2.4 and the right-hand side of eq. 2.3 with vectorized numpy code. Algo. 2 shows the implementation of the collision step, separated into equilibrium probability density function computation and the collision.

In steps 6 of algo. 1 we simulate the streaming part of eq. 2.3. Algo. 3 shows the implementation using *np.roll*. The function rolls the the data in the direction specified by the *axis* argument. With the argument $shift$ we specify the number of places elements are shifted according to the discrete velocity directions $\mathbf{c}$. Note, that the function automatically implements the periodic boundary condition.

```
   Input: density ρ; velocity u, relaxation parameter omega ω
   Output: Probability density function before streaming f_i^*
1  w_i = np.array([4/9, 1/9, 1/9, 1/9, 1/9, 1/36, 1/36, 1/36, 1/36])
2  def f_eq(density:np.ndarray, velocity:np.ndarray)→np.ndarray:
3  |   w_i = w_i[np.newaxis, np.newaxis, ...]
4  |   ci_u = velocity @ c_i.T
5  |   uu = (np.linalg.norm(velocity, axis=-1) ** 2)[..., np.newaxis]
6  |   rho = density[..., np.newaxis]
7  |   return w_i * rho * (1 + 3 * ci_u + 9/2 * ci_u ** 2 - 3/2 * uu)
8  f_pre = f + (f_eq(density, velocity) - f) * omega
```

Algorithm 2: Python implementation of the collision step.

```
   Input: Probability density function before streaming f_i^*
   Output: Probability density function after streaming f_i
1  c_i = np.array([[0,0],[1,0],[0,1],[-1,0],[0,-1],[1,1],[-1,1],[-1,-1],[1,-1]])
2  def streaming(f_pre:np.ndarray)→np.ndarray:
3  |   f_post = np.zeros_like(f_pre)
4  |   for i in range (9):
5  |   |   f_post[..., i]=np.roll(f_pre[...,i], shift=c_i[i], axis=(0,1))
6  |   return f_post
```

Algorithm 3: Python implementation of the streaming step.

3.3 Parallelization

We parallelize the LBM using spatial domain decomposition and Message Passing Interface (MPI) [10, 11, 12]. MPI is a *communication protocol* for programming parallel computers, i.e. Single Instruction Multiple Data (SIMD) [13] by executing the same operation on multiple data points simultaneously.

3.4 Software quality

Static typing

Python is a dynamically typed language. That is that the Python interpreter does type checking only in runtime and the type of a variable is allowed to change. The opposite of dynamic typing is static typing. It is introduced by *PEP 484* in Python. In static typing, the types of the variables are checked before runtime and the change of types is generally not allowed. Note, as an exception type casting is a way to change the type of a variable in many languages.

Dynamic typing allows for rapid prototyping and thus it enables fast software development. On the other side static typing can help to catch errors due to type errors, document the code and help to build a cleaner software architecture. The last point in particular ensures that the programmer thinks about the types of the variables and uses the correct types. Thus, in any larger project typing is critical to build and maintain clean code.

Unit testing

One key component of every software project is extensive testing of the software. To this end, we implement several unit tests in order to validate the expected behavior of the implemented functions. We integrate the unit tests into Continuous Integration (CI) using *Travis CI* as build server so that the implementation and its potential unintentional modifications are validated for each commit to the repository.

4

Numerical results

To demonstrate the LBM we conduct several experiments with different combinations of boundary conditions.

4.1 Shear wave decay

To validate the implementation, we compare the simulated solutions with analytical solutions.

We choose the following simulation parameters for our experiments about the planar couette flow:

- lattice grid shape $= 50 \times 50$
- $\omega = 1.0$
- Sinusoidal density in x-direction $\rho(\mathbf{x}, 0) = \rho_0 + \epsilon_\rho \sin(\frac{2\pi x}{l_x})$
  - $\rho_0(\mathbf{x}) = 0.5$
  - $\epsilon_\rho = 0.08$
  - $\mathbf{u}_{initial}(\mathbf{x}) = 0.0$
- Sinusoidal velocity in y-direction $\mathbf{u}_x(\mathbf{x}, 0) = \epsilon_\mathbf{u} \sin(\frac{2\pi y}{l_y})$
  - $\rho_{initial}(\mathbf{x}) = 0.0$
  - $\epsilon_\mathbf{u} = 0.08$
- time steps $= 2000$

4.2 Planar couette flow

The planar couette flow is a steady, laminar flow between two infinitely long, parallel plates with a fixed distance. One of those plates moves tangentially

at a velocity of U relative to the other plate, which itself is stationary. The flow is caused by the viscous drag force acting on the fluid.

We choose the following simulation parameters for our experiments about the planar couette flow:

- lattice grid shape $= 20 \times 30$
- $\omega = 1.0$
- $U = 0.05$
- $\rho_{initial}(\mathbf{x}) = 1.0$
- $\mathbf{u}_{initial}(\mathbf{x}) = 0.0$
- time steps $= 4000$

We can see that the simulated solution almost exactly reproduces the analytical solution. This shows that the bounce-back boundary condition is first-order accurate. Furthermore, it is also second-order accurate, since the boundary values and its first-order derivative are reproduced exactly.

We can also observe that the solution is viscosity-independent.

4.3 Planar poiseuille flow

The planar poiseuille flow is a steady flow between two non-moving plates. The flow is caused by a constant pressure gradient $\frac{dp}{dx}$ in the axial direction, x, parallel to two infinitely long parallel plates, seperated by a distance h.

We choose the following simulation parameters for our experiments about the planar poiseuille flow:

- lattice grid shape $= 200 \times 30$
- $\omega = 1.5$
- $p_{out} = \frac{1}{3}$
- $\Delta p = 0.001111$
- $\rho_{initial}(\mathbf{x}) = 1.0$
- $\mathbf{u}_{initial}(\mathbf{x}) = 0.0$
- time steps $= 5000$

Some error can occure due to:

- Inaccuracy introduced by the bounce-back boundary condition. In particular, the error depends on the viscosity.[4]

In fig. xyz we can observe that the boundary velocity changes for different $\omega's$. This in turn shows that the poiseuille flow simulation is viscosity-dependent. This is called *numerical boundary slip*. [4]

4.4 Von Kármán's vortex street

4.5 Scaling tests

5

Conclusions

In this report we described the LBM and its implementation in Python. We also show several applications of the LBM to problems and compare the simulation results to analytical solutions if possible.

In chapter 2 we describe the LBM.

In chapter 3 we discussed the implementation and more specifically the parallelization of the LBM.

In chapter 4 we demonstrate in several applications the correctness of our LBM implementation. In addition, we demonstrate the speed-up that we obtain by parallelizing the LBM for the von Kármán's vortex street.

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