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Uppsala University

Modeling Complex Systems - 10HP

Fluid Simulation with the Lattice Boltzmann Method

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Abstract

Solving the Navier-Stokes equations analytically is a difficult task due to its highly non-linear nature, particularly under complex boundary conditions. In this work, the Lattice Boltzmann Method (LBM) is implemented for simulating steady fluid flow around a cylinder and a parallelogram under varying Reynolds numbers (Re). The aim of this work is to reproduce the qualitative behavior of fluid flows, transitioning from laminar flow at low Re to turbulent flow at high Re. The results validate the effective use of LBM in these challenging contexts, offering a robust tool for modeling fluid flow in practical applications.

Contents

1 Introduction

The investigation of fluid flow around a cylinder is a significant topic in fluid dynamics, with widespread applications in engineering and science. Many practical scenarios, including vehicle design, pipeline systems, and building structures, involve understanding fluid interactions with cylindrical objects or similar sub-components.

Various complex phenomena characterize fluid flow around a cylinder, leading to different flow patterns based on fluid properties and the relative speed between the fluid and the cylinder. These patterns may be easily predictable when the flow is laminar, but more interesting patterns may emerge by varying the geometry and/or the value of the Re.

Analytical solutions for governing fluid flow equations, such as the Navier-Stokes equations, are challenging to obtain due to their nonlinearity, coupling, and complex boundary conditions. Consequently, computational methods have become indispensable tools for simulating fluid flow passing an obstacle, and other fluid dynamics problems.

The problem of fluid flow past a cylinder has been well-studied, providing a solid foundation to build upon. This "toy problem" serves as an excellent starting point for conducting more advanced research and exploring novel techniques or approaches in fluid dynamics simulations. As a result, it remains a valuable benchmark for evaluating the accuracy and performance of computational methods, such as the LBM, in simulating fluid flows.

The LBM is one computational method that has gained popularity for simulating fluid flow past a cylinder. The LBM is particularly well-suited for parallel computing and handling complex geometries, making it an effective tool for modeling and analyzing fluid flow in various applications. In this project, I will implement the LBM and use it to simulate fluid flow past a cylinder as well as a parallelogram for different Re. The content of the report will be completely based on [1] unless otherwise stated.

2 Background

2.1 Cellular Automata

Cellular Automata (CA) are discrete computational models that can be defined on a lattice, typically with a finite number of states. Mathematically, a CA can be represented as a map:

$$\mathrm{CA} : S^k \to S \tag{1}$$

where S is the set of states, and k is the number of neighboring cells considered. The function CA defines the update rule for each cell based on the states of cells in its neighborhood. The definition of which can significantly impact the resulting local and global behavior of the system. Various neighborhood configurations exist, each with distinct properties and associated phenomena.

The next state of a cell in the CA depends only on its current state and the states of its neighboring cells. This feature enables efficient parallelization, as the state of each cell can be updated simultaneously without the need for communication between cells that are not immediate neighbors. Consequently, CA can effectively utilize parallel computing architectures, such as multi-core CPUs and GPUs, for large-scale simulations.

Lattice gas cellular automata (LGCA) is a specialized type of cellular automata that models particle interactions on a grid. In LGCA, particles or cells are treated as lattices, e.g. cells in a grid, allowing for simplified representation and efficient computation of their interactions.

2.2 Fluid Dynamics

The continuity equation is derived from the principle of conservation of mass. In the context of an incompressible fluid, the continuity equation is given by

$$\nabla \cdot \mathbf{u} = 0, \tag{2}$$

where $\mathbf{u}$ represents the fluid velocity vector and depends on the spatial coordinates denoting with the positional vector $\mathbf{x}$ and the time t.

One can derive the Navier-Stokes equations by considering the principles of conservation of momentum and Newton's second law of motion, that is:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{F}, \tag{3}$$

where ρ represents the fluid density, p is the macroscopic pressure, μ is the dynamic viscosity, and $\mathbf{F} = \mathbf{0}$ is the external force acting on the fluid. The LBM that is implemented will assume incompressible fluid.

2.3 Non-dimensionalization of Navier-Stokes Equations

To analyze the Navier-Stokes equations more effectively, it is often useful to remove the units of the physical quantities involved. This can be achieved by defining dimensionless variables:

$$\mathbf{u}' = \frac{\mathbf{u}}{u_0}, \, \mathbf{x}' = \frac{\mathbf{x}}{L_0}, \, t' = \frac{t}{T_0}, \, p' = \frac{p}{p_0}, \, \mu' = \frac{\mu}{\rho u_0 L_0}$$

where u_0, L_0, T_0, and p_0 are characteristic velocity, length, time, and pressure scales, respectively. Substituting these dimensionless variables into the Navier-Stokes equations yields the unitless form:

$$\rho' \left(\frac{\partial \mathbf{u}'}{\partial t'} + \mathbf{u}' \cdot \nabla \mathbf{u}' \right) = -\nabla p' + \mu' \nabla^2 \mathbf{u}', \tag{4}$$

where ρ' and μ' are the dimensionless density and dynamic viscosity respectively[1].

2.3.1 Reynolds Number

An important dimensionless quantity in fluid dynamics is the Reynolds number, which characterizes the ratio of inertial forces to viscous forces in a fluid flow. It is defined as:

$$\mathrm{Re} = \frac{\rho u L}{\mu}, \tag{5}$$

The Reynolds number helps determine the flow regime, such as laminar or turbulent flow and influences the behavior of fluid flows in different situations.

2.4 Statistical Mechanics

In fluid simulations, modeling all the microscopic particle interactions can be challenging and often unnecessary, as the primary interest usually lies in the interpretable macroscopic phenomena. Statistical mechanics serves as a bridge between microscopic interactions and macroscopic behavior, allowing us to "smooth out" the fine-grained particle interactions by modeling them with a distribution.

Mean Field Theory (MFT) is an approximation method in statistical mechanics that simplifies particle interactions by considering the average effect of all other particles, reducing the

[1] To avoid clutter caused by the primes, the dimensionless parameters will from now, be denoted without the primes.

complexity of the original n-body problem for easier analysis and computation. Mathematically, given a system of particles with interaction potentials $\mathcal{H}^0$, MFT assumes an average field $\langle \mathcal{H}_i^{int} \rangle$ acting on each particle instead of considering the full interactions. The MFT Hamiltonian is written as:

$$\mathcal{H}_{\text{MFT}} = \sum_i \mathcal{H}_i^0 + \sum_i \langle \mathcal{H}_i^{int} \rangle, \tag{6}$$

where $\mathcal{H}_i^0$ represents the single-particle Hamiltonian for particle i. This approach streamlines the problem for more effective analysis and computation.

The Boltzmann equation, which can be derived using the MFT is given by:

$$\frac{\partial f}{\partial t} + \mathbf{u}\frac{\partial f}{\partial \mathbf{x}} + \frac{\mathbf{F}}{\rho}\frac{\partial f}{\partial \mathbf{u}} = \Omega(f). \tag{7}$$

In this equation, $f = f(\mathbf{x}, \mathbf{u}, t)$ [kgs^{3}m^{-6}] satisfying $\rho(\mathbf{x}, t) = \int f(\mathbf{x}, \mathbf{u}, t) d^3\mathbf{u}$ represents the velocity density distribution of the fluid in space $\mathbf{x}$ with velocity $\mathbf{u}$ at some time t. $\Omega(f)$ is the collision operator which contains the information on the interactions of f. The Boltzmann equation thus describes the evolution of a particle velocity distribution. This equation is related to the LBM through the lattice Boltzmann equation, which can be written as:

$$f_i(\mathbf{x} + \mathbf{u}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i(\mathbf{x}, t). \tag{8}$$

This equation describes how the velocity density distribution of the i:th particle f_i in a grid, will evolve after a small time interval Δt colliding with its neighbor particles.

2.5 Lattice Boltzmann Method - Origins and Evolution

The LBM evolved from the LGCA, which is a discrete model that represents particles as cells in a grid. The interactions in LGCA include:

- Collision rules: At each time step, particles at the same lattice node can collide and change their directions based on predefined collision rules, which have a stochastic nature. These probabilistic rules are weighted by the velocities and are designed to conserve mass and momentum locally, but they introduce randomness into the system, leading to statistical noise in the macroscopic fluid properties.
- Streaming step: After the collision step, particles move to their neighboring nodes following their updated directions. This movement, called streaming, is performed synchronously for all particles in the lattice, and it is during this step that the fluid flow emerges from the collective behavior of the particles.
- Boundary conditions: To simulate real-world scenarios, boundary conditions can be imposed on the lattice, such as solid walls, inflow, and outflow boundaries. These conditions affect the behavior of particles near the boundary, leading to phenomena such as reflections, absorption, or changes in particle directions.

Despite the simplicity of each rule, complex behaviors emerge in the form of fluid dynamics. However, LGCA has limitations, including statistical noise from collisions, global momentum conservation issues, and a binary approach where particles are either present in a cell or not, with no intermediate state possible.

The LBM addresses these limitations by employing continuous distribution functions that satisfy the Boltzmann equation, which allows for intermediate states of particles, resulting in a more accurate and smooth representation of fluid dynamics compared to LGCA's discrete particle model.

3 Methodology

3.1 Lattice Boltzmann Method - Algorithm and Implementation

The implementation of the Lattice Boltzmann Method (LBM) can be summarized in the following steps:

1. Initialize the particle distribution function f_i and set appropriate normalized constants for time, length, viscosity, and other relevant parameters.

2. Compute the macroscopic density $\rho(\mathbf{x}, t)$ by summing the particle distribution function over every lattice:

$$\rho(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t). \tag{9}$$

3. Calculate the macroscopic velocity by computing the first moment of f_i weighted by the directional lattice configuration $\mathbf{c}_i$ and dividing the resulting expression by the fluid density:

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho(\mathbf{x}, t)} \sum_i f_i(\mathbf{x}, t)\mathbf{c}_i. \tag{10}$$

4. Determine the equilibrium distribution function[2] for the chosen lattice structure using the formula:

$$f_i^{eq}(\mathbf{x}, t) = \rho(\mathbf{x}, t) \cdot w_i \left[1 + \frac{\mathbf{c}_i \cdot \mathbf{u}(\mathbf{x}, t)}{c_s^2} + \frac{(\mathbf{c}_i \cdot \mathbf{u}(\mathbf{x}, t))^2}{2c_s^4} - \frac{\mathbf{u}(\mathbf{x}, t) \cdot \mathbf{u}(\mathbf{x}, t)}{2c_s^2}\right] \tag{11}$$

   where w_i is the lattice weights corresponding to $\mathbf{c}_i$ and $c_s = \frac{1}{\sqrt{3}}$ is the unit-less quantity of the speed of sound.

5. The collision operator that is used is the Bhatnagar-Gross-Krook (BGK) model, which is given by:

$$\Omega_i(\mathbf{x}, t) = -\frac{1}{\tau}[f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)] \tag{12}$$

   where

$$\tau = \frac{\mu}{\rho c_s^2 \Delta t} + \frac{1}{2} \tag{13}$$

   is the dimensionless relaxation time[3].

6. Perform the streaming step, which updates the particle distribution function by streaming the particles to the neighbor lattices based on the lattice configuration coefficients $\mathbf{c}_i$:

$$f_i(\mathbf{x} + \mathbf{c}_i\Delta t, t + \Delta t) \leftarrow f_i(\mathbf{x}, t). \tag{14}$$

7. The no-slip bounce-back boundary condition is employed to manage the interaction between the particles and the obstacles in the simulation. This technique deals with the overlap of the particle distribution with an obstacle by causing the distribution function to alter its momentum. As a result, a "bounce-back" effect is created, effectively reflecting the particles upon contact with the obstacle. Furthermore, the no-slip condition ensures that the particle is at rest when it overlaps with the obstacle.

8. Repeat steps 3-7 for a desired number of time steps to simulate the fluid dynamics.

[2] This function describes the local state of the system at equilibrium.

[3] This parameter determines the duration of the collisions. We notice that a high density ρ means low τ. This makes intuitive sense since a higher-density fluid tends to collide more often. The same argument can be made for c_s which determines the velocity at which collisions transfer. Note also how τ is proportional to the dynamic viscosity μ.

3.2 Project Setups

In this simulation, I consider a fluid flow within a rectangular domain with the macroscopic velocity vector field given by $\mathbf{u}(x, y, t) = (u_x(t), u_y(t))$.
There is an incoming uniform horizontal flow from the left side with no vertical component. This phenomenon is modeled by the inhomogeneous Dirichlet boundary condition:

$$\mathbf{u}(\mathbf{x}_{\text{left boundary}}, t) = (u_0, 0) \tag{15}$$

for some unitless initial speed $u_0 > 0$. To compute the macroscopic density for the inflow, I consider the non-equilibrium bounce-back method and apply the equation 5.49 in the book [1], that is:

$$\rho = \frac{v}{v - u_x} \left[f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7) \right] \tag{16}$$

where f_i corresponds to the discrete lattice velocity distribution, see how the direction is defined in figure 3.2. Note that the speed $v = \frac{\Delta x}{\Delta t} = 1$ and $u_x < 1$ since unit-less quantities are considered.

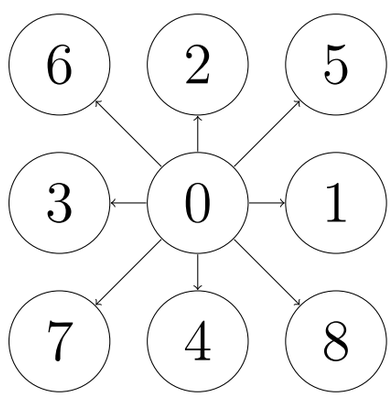
As the fluid flows past the cylinder, it exits the domain on the right side. This must occur in a way that the fluid dynamics inside the domain is unaffected as if the fluid continuously flows past the boundary. To model this effect, the homogeneous Neuman boundary condition is used:

$$\begin{cases} \nabla u_x \bullet \mathbf{n} = 0 \\ \nabla u_y \bullet \mathbf{n} = 0 \end{cases} \tag{17}$$

This is implemented by copying the second last vertical slice of the domain and then assigning the values to the last vertical slice. Since the velocity field does not change during this step, the normal components of the gradients are zero. The particles will interact with a cylinder placed inside the domain, and this interaction is modeled using the no-slip bounce-back boundary condition. The same method is applied to the top and bottom of the domain which are treated as walls, i.e. obstacles.

The lattice structure that is used is the D2Q9 scheme, which is a two-dimensional model (hence the name D2) that describes the local interactions of the particles in a 3 by 3 grid (hence the name Q9). The lattice indices specify the local relations of the discrete- velocities and densities.

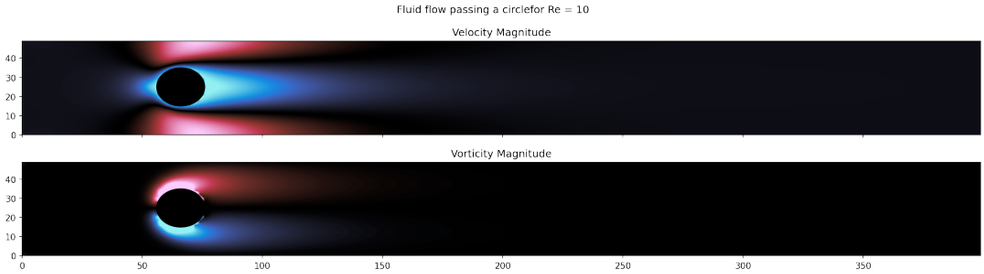
The lattice weights w_i have the following values: The center lattice velocity is weighted by $w_{\text{center}} = 4/9$, the north, east, south, and west lattice are weighted by $w_{\text{sides}} = 1/9$, finally, the corners are weighted by $w_{\text{corners}} = 1/36$. The weights sum up to 1. Below is an illustration of the D2Q9 lattice configuration.

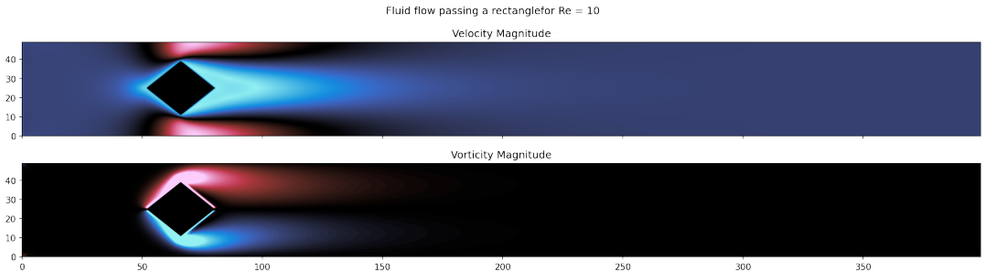


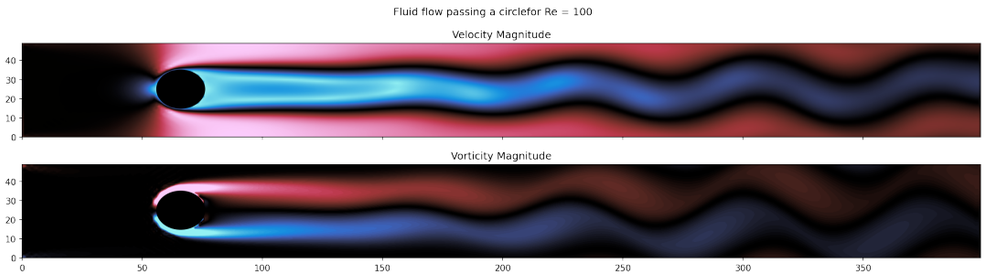
4 Results

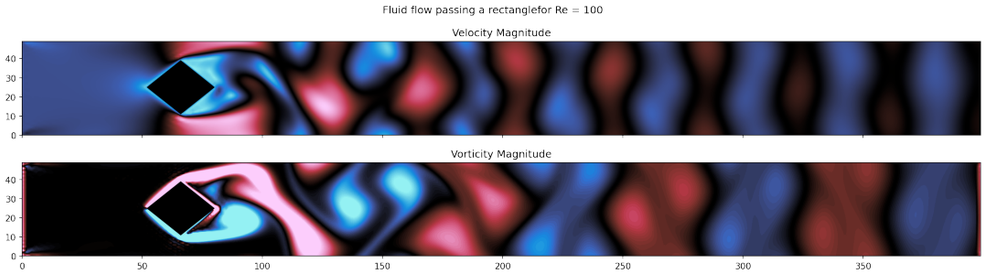
The figures below show the speed- and vorticity fields at the last step of the simulations for different Reynold's numbers. The animation displaying the system's time evolution can be

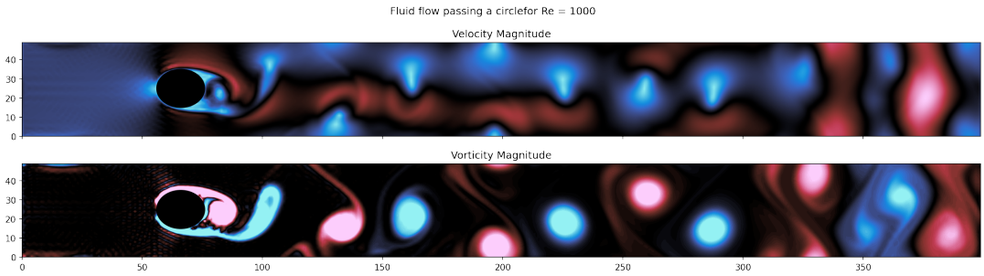
found at https://github.com/SunAndClouds/ComplexSystems.

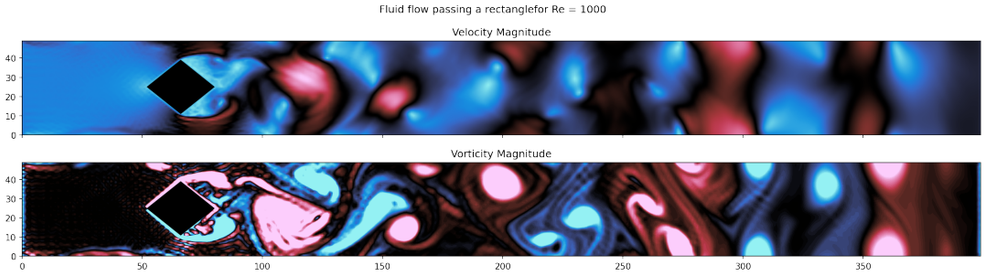












5 Discussion

There are some limitations of the LBM that needs to be addressed.

- The complete mesh of the simulation domain needs to be stored in memory at any given time to achieve the benefit of parallelization. This makes the LBM relatively memory expensive.
- The simulation is by nature a Markov process. This means that even for relatively simple simulations, such as steady-state laminar flow, the computational cost cannot be reduced.
- The LBM assumes that the fluid is incompressible, e.g., the macroscopic density of the fluid is constant. In the real world, fluids are more or less compressible. The incompressible fluid assumption will therefore introduce some additional errors to the simulation[4].
- The standard LBM does not consider temperature variations in the fluid[5].

6 Conclusions

In this work, the LBM was implemented for simulating the speed- and vorticity of a generic fluid flow passing:

1. A cylinder.
2. A Parallelogram.

The methodology managed to produce qualitatively correct behavior of the fluid for laminar flow when the value of Re is low, and turbulent flow for high valued Re.

[4]It is possible to consider a more advanced version of the LBM that better handles weakly compressible fluids. The theory and implementation are beyond this work.

[5]Again, it is possible to incorporate it in a more advanced model

References

[1] Krüger T. The Lattice Boltzmann Method Principles and Practice. 1st ed. Graduate Texts in Physics. Cham: Springer International Publishing; 2017.