The Lattice Boltzmann Method

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Abstract

The Lattice-Boltzmann Method (LBM) in computational fluid dynamics (CFD) is a method for simulating fluid-flow by making assumptions to simplify and discretize the partial differential equations that govern these systems. The LBM is computationally effective and especially useful for solving thermal and aerodynamical solutions. This is due to the method's ability to deal with complex boundary conditions. Coupled with the ability to attach physical terms to the system, such as heat or viscosity, the LBM is widely useful. Due to computer efficiency, high speed aerodynamical fluid flows fail in the LBM due to the complexity in the calculations of just one iteration of the simplest LB Methods.

1 Background

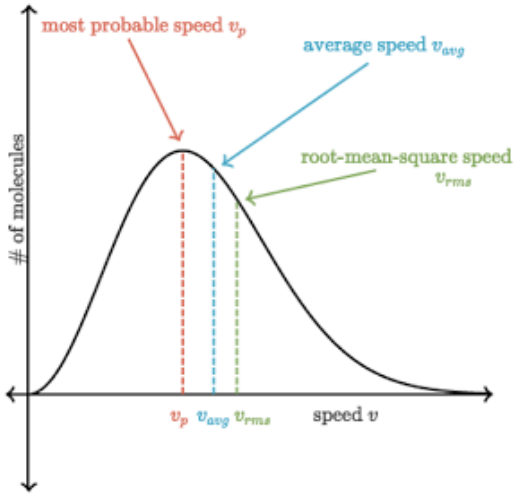
The LBM was developed by Guy R. McNamara and Gianluigi Zanetti in 1988 to help minimize the error involved in previous computational methods for simulating fluid flow. The LBM was also developed such that it's relation to the Boltzmann transport equation allows for physical characteristics such as heat and viscosity to be incorporated into the method by collision transfer. The LBM, similarly to other fluid-flow models, consists of a streaming step and a collision step. In the streaming step, particles move from one cell in the lattice to another, which takes a time step. In the collision step, energy is transferred between particles based on predetermined rules determined by the lattice shape, so long as the collisions obey conservation of mass and momentum. Theses collisions are instantaneous. In this paper, we will develop a 1D calculation for the Thermal LBM.

2 Introduction

CFD is useful for fluid-flows of gases and can be solved discretely for many previously unsolvable boundary conditions. That is, they can be solved algorithmically using a computer, leaving a numerical approximation with a certain amount of error. The LBM is a finite difference method for solving fluid systems

that follow the conditions of a newtonian-based collision model. That is, there are perfectly elastic collisions and that the distance between collisions is large enough to negate the effects of the volume of the particles such that we assume point-mass particles. This is the basis for what is known as Boltzmann's Kinetic Theory.

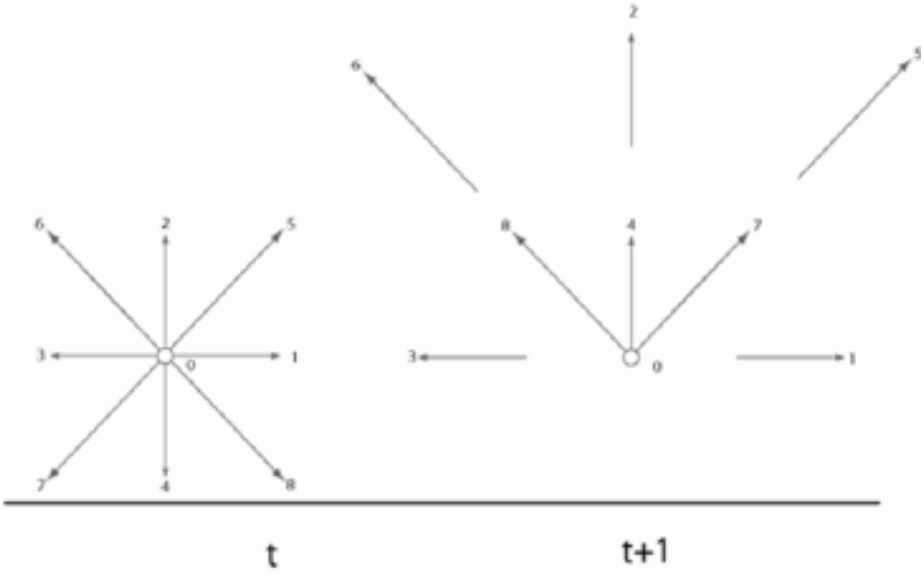
Along with these conditions comes the coupling of the method with the Maxwell-Boltzmann Distribution function.



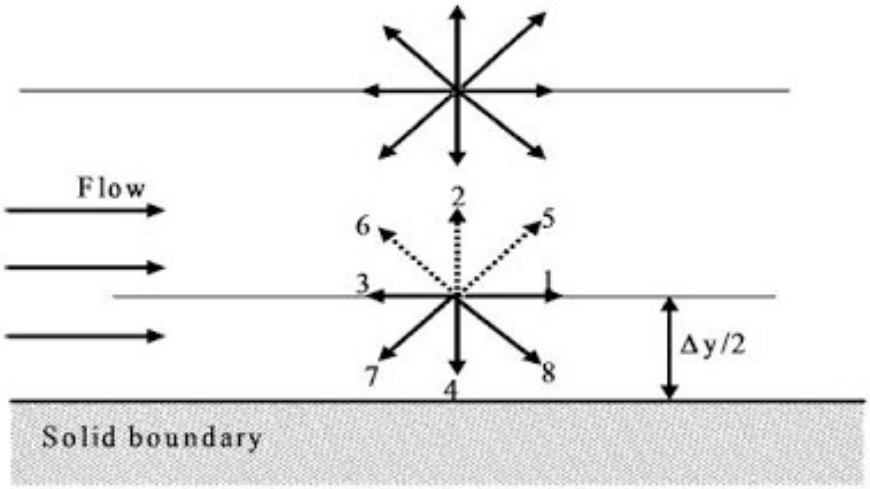
The Maxwell-Boltzmann Distribution function is a Guassian distribution that calculates the percentage of particles moving a particular speed at equilibrium in a system. Each particle or molecule has a unique distribution function. That is, smaller particles move faster, which stretches the function to the left and up; whereas heavier particles move slower, which stretches the function to the right and down. The usefulness of this function is that there an equation for it, and that it tells you about a system of particles at equilibrium.

3 Boundary Conditions

No-slip boundary conditions assume no slip upon contact with the boundary. For example, if in figure 1 the bottom of the lattice is a horizontal boundary condition, then for no-slip contact, $\vec{v_4} = \vec{v_2}$, $\vec{v_7} = \vec{v_5}$, and $\vec{v_8} = \vec{v_6}$. Periodic boundary conditions are also possible. This involves placing multiple boundary conditions in between lattices.



For simplicity consider our example for no-slip boundary conditions. Our unknown velocities are $\vec{v_2}$, $\vec{v_5}$, and $\vec{v_6}$ for our singular boundary condition, a. If we impose another horizontal boundary condition at a distance Δy and parallel from the first, then we know something about $\vec{v_2}$, $\vec{v_5}$, and $\vec{v_6}$ for a different lattice across the other boundary condition, b. We can then relate $\vec{v_{2,a}} = \vec{v_{2,b}}$, $\vec{v_{5,a}} = \vec{v_{5,b}}$, and $\vec{v_{6,a}} = \vec{v_{6,b}}$.



4 Origins of the LBM

The origins of the LBM start with the advent of the Navier-Stokes equations (NSE). The NSE is a set of continuous partial differential equations that describe the flow of viscous incompressable fluids. The continuity of the NSE allows it to take integral and differentiable form, which causes complications when solving for exact solutions given certain initial condition and boundary conditions. Similarly, the NSE is invariant of coordinate systems while later computational techniques,such as the LBM, rely on a lattice structure to solve. Before the LBM, the Lattice Gas Automaton (LGA) was developed to form a discrete model for describing fluid flow that would allow for non-integrable and non-differentiable solutions to be numerically approximated. The method of the LGA, like the LBM, is to reduce the degrees of freedom of movement of the particles, allowing one to describe particles through a probability distribution function $f_k(x, v, t)$ where x is position, v is velocity, and t is time. If some force is applied on a particles, positions and velocities change such that $x(t+\Delta t) = x(t)+v(t)dt$ and $v(t+\Delta t) = v(t)+a(t)dt$, where $a(t)$ is acceleration. f describes the probability that a particle will move in any particular direction and k describes which particle you're worried about.

If no collisions occur, then our probability distribution function is the same before and after our time step.

$$f_k(x + v_k dt, v + a_k dt, t + dt)dxdv = f_k(x, v, t)dxdv$$

If collisions do occur, then our probability distribution function before and after our time step varies by our collision operator Ω, which is dependent on time due to the time it takes for particles to relax after colliding.

$$f_k(x + v_k dt, v + a_k dt, t + dt)dxdv - f_k(x, v, t)dxdv = \Omega(f)dxdvdt$$

Our collision operator, $\Omega(f)$ acts on the distribution function to modify it with each time step.

Note that Ω can then be described as a difference quotient:

$$\Omega(f) = \frac{f_k(x + v_k dt, v + \vec{a_k} dt, t + dt)dxdv - f_k(x, v, t)dxdv}{dxdvdt} = \frac{Df}{dt}$$

This states that the rate of change of our distribution function is equal to the collision operator. Then, by the chain rule,

$$\frac{Df}{dt} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial t} + \frac{\partial f}{\partial t}$$

Note that $v = \frac{dx}{dt}$ and $a = \frac{dv}{dt}$.

If we assume that there are no external forces, then $F = 0$, $a = 0$, and

$$\Omega(f) = \frac{Df}{dt} = \frac{\partial f}{\partial x}(v) + \frac{\partial f}{\partial v}(0) + \frac{\partial f}{\partial t} = \vec{v} * \nabla f + \frac{\partial f}{\partial t}$$

for a multi-dimensional solution.

The collision operator can be solved for in many ways, but for the LBM we base the collision operator on the Bhatnagar, Gross, and Krook (BGK) solution to the collision operator:

$$\Omega(f_k) = \Omega_k = \frac{1}{\tau}(f_k^{eq} - f_k) = \vec{v} * \nabla f + \frac{\partial f}{\partial t}$$

where τ is the relaxation time towards equilibrium and f_k^{eq} is the equilibrium distribution function that can be determined from the Maxwell-Boltzmann Distribution function. This gives us our LBM equation:

$$\vec{v} * \nabla f + \frac{\partial f}{\partial t} = \frac{1}{\tau}(f_k^{eq} - f_k)$$

The BGK collision operator replaces the non-linear collision term, Ω, with the

$$\frac{1}{\tau}(f_k^{eq} - f_k)$$

term, which allows for easier descretization of the Lattice Boltzmann Equation. The BGK operator takes the difference in the distribution function with the equilibrium distribution function, derived from the Maxwell-Boltzmann Distribution, and multiplies it by the relaxation rate, $\frac{1}{\tau}$. The relaxation time, τ, is the time is takes for particles to relax after colliding, which must happen before they collide again. This time is related to the viscosity of the substance but takes on a numerical value depending on the physical attribute one is worried about. For example, for a thermal calculation, the relaxation time is related to the thermal diffusivity, α, of the substance, which is found in the heat equation. The thermal diffusivity of a substance is related to the relaxation time by

$$\alpha = \tau - \frac{\Delta t}{2}$$

, which is also derived from the Maxwell-Boltzmann distribution.

5 Discretizing the LBM

The LBM is a result of Boltzmann's kinetic theory which states that physical properties such as heat, viscosity, thermal, and electrical conductivity are maintained and transferred by the collisions of particles. These properties can thus be modelled by the Boltzmann transport equation which relates the rate of change of a probability distribution function to a collisions operator. This allows us to use our Lattice Boltzmann Method:

$$\vec{v} * \nabla f + \frac{\partial f}{\partial t} = \frac{1}{\tau}(f_k^{eq} - f_k)$$

Recall that,

$$\frac{f_k(x+v_k dt, v+a_k dt, t+dt)dxdv - f_k(x,v,t)dxdv}{dxdvdt} = \frac{1}{\tau}(f_k^{eq}(x,v,t) - f_k(x,v,t))$$

Then, we want to descretize our equation so as to develop an algorithm for numerically approximating the dynamics of our system. Thus,

$$\frac{f_k(x+v_k\Delta t, v+a_k\Delta t, t+\Delta t) - f_k(x,v,t)}{\Delta t} = \frac{1}{\tau}(f_k^{eq}(x,v,t) - f_k(x,v,t))$$

and

$$f_k(x+v_k\Delta t, v+a_k\Delta t, t+\Delta t) - f_k(x,v,t) = \frac{\Delta t}{\tau}(f_k^{eq}(x,v,t) - f_k(x,v,t))$$

and

$$f_k(x+v_k\Delta t, v+a_k\Delta t, t+\Delta t) = f_k(x,v,t) + \frac{\Delta t}{\tau}(f_k^{eq}(x,v,t) - f_k(x,v,t))$$

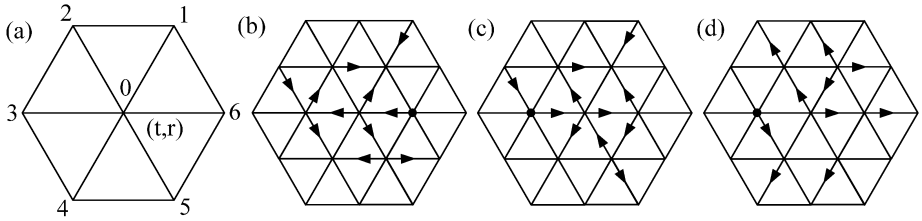
For a constant external force on the system, our equation is modified such that

$$f_k(x+v_k\Delta t, t+\Delta t) = f_k(\vec{x},t) + \frac{\Delta t}{\tau}(f_k^{eq} - f_k) + w_k\frac{\Delta t}{c_s^2}v_k F$$

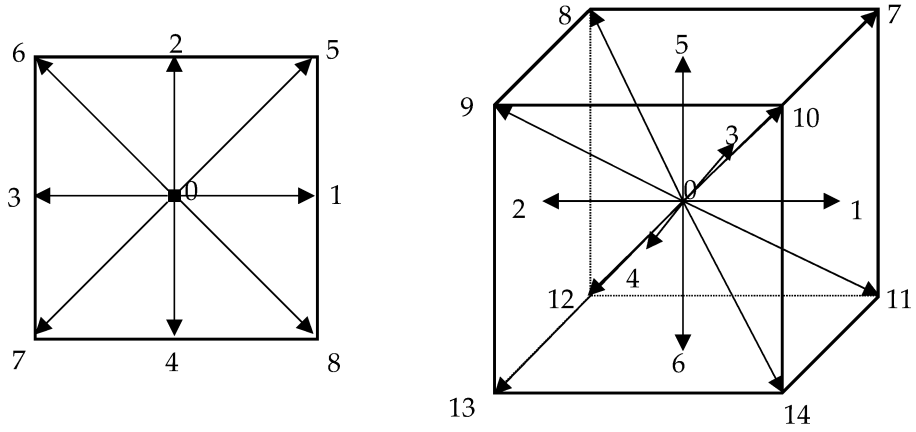
where w_k are the weighting factors for each node on the lattice and c_s is the speed of sound in the lattice. Both are parameters derived from the geometry of the lattice using the Maxwell-Boltzmann Distribution function.

6 Lattice Arrangements

Now that we have our discrete Lattice Boltzmann Equation, we can choose how we want to restrict the movement of particles for various systems. For the LGA, a hexagonal lattice was chosen so as to simulate gas kinetics and dynamics.



For the LBM, a Cartesian lattice is chosen and we assign the lattice the D_xQ_y notation, where x is the number of dimensions in the lattice and y is the number of directions that particles in a lattice can move. Two examples of lattice types are shown below.



Note for the lattice on the left, or the D_2Q_9 LBM, we restrict particles to moving in 9 direction in our 2 dimensional lattice.

$$\vec{v}_i = \begin{cases} (0,0) & \text{for } i = 0 \\ (1,0),(0,1),(-1,0),(0,-1) & \text{for } i = 1,2,3,4 \\ (1,1),(-1,1),(-1,-1),(1,-1) & \text{for } i = 5,6,7,8 \end{cases}$$

A similar derivation for possible velocity vectors is possible for the lattice on the right, which is also known as the D_3Q_{15} Lattice Boltzmann Method.
We can now perform calculations using the Lattice Boltzmann Method.

7 1D Thermal Lattice Boltzmann Method

Consider a 1D tube of gas with an initial temperature $T = 0$. When $t > 0$, the left boundary of the tube has a temperature $t = 1$. We will use a D_1Q_3 lattice arrangement with 3 total cells. Our possible velocity vectors are then

$$\vec{v}_i = \begin{cases} v_0 = 0 & \text{for } i = 0 \\ v_1 = 1 & \text{for } i = 1 \\ v_2 = -1 & \text{for } i = 2 \end{cases}$$

for each cell placed in the tube.
For the sake of calculation, we will assign our weighting factors for each velocity by

$$\vec{w}_i = \begin{cases} w_0 = \frac{4}{6} & \text{for } i = 0 \\ w_1 = \frac{1}{6} & \text{for } i = 1 \\ w_2 = \frac{1}{6} & \text{for } i = 2 \end{cases}$$

We will also assign our spacing between adjacent lattice centers as $\Delta x = 1$, our spacing between time steps $\Delta t = 1$, and our thermal diffusivity $\alpha = \frac{1}{4}$.

We can then determine the temperature at each node by setting our left most node to the addition of each weighting factor and all other nodes to the addition of the possible velocity vectors.

$$T(x,0) = \begin{cases} T(1,0) = f_0(1,0) + f_1(1,0) + f_2(1,0) = \frac{4}{6} + \frac{1}{6} + \frac{1}{6} = 1 \\ T(2,0) = f_0(2,0) + f_1(2,0) + f_2(2,0) = 0 + 1 + (-1) = 0 \\ T(3,0) = f_0(3,0) + f_1(3,0) + f_2(3,0) = 0 + 1 + (-1) = 0 \end{cases}$$

We can now calculate our equilibrium distribution functions, which for a thermal calculation is given by the weighting factors in each direction and the current temperature of the node:

$$f_k^{eq}(x,t) = w_k T(x,t) = \begin{cases} f_0^{eq}(1,0) = \frac{4}{6} \\ f_1^{eq}(1,0) = \frac{1}{6} \\ f_2^{eq}(1,0) = \frac{1}{6} \\ f_k^{eq}(2,0) = f_k^{eq}(3,0) = 0 \end{cases}$$

Using our value for thermal diffusivity, we can determine the relaxation time

$$\alpha = \tau - \frac{\Delta t}{2} \rightarrow \tau = \alpha + \frac{1}{2} \rightarrow \tau = \frac{1}{4} + \frac{1}{2} = \frac{3}{4}$$

Using the BGK Approximation for the Collision Operator, our collision step is given by:

$$f_k^*(\vec{x},t) = (1 - \frac{\Delta t}{\tau}) f_k(\vec{x},t) + \frac{\Delta t}{\tau} f_k^{eq}(\vec{x},t)$$

$$f_k^*(1,0) = \begin{cases} f_0^*(1,0) = (1 - \frac{4}{3})(\frac{4}{6}) + (\frac{4}{3})(\frac{4}{6}) = \frac{4}{6} \\ f_1^*(1,0) = (1 - \frac{4}{3})(\frac{1}{6}) + (\frac{4}{3})(\frac{1}{6}) = \frac{1}{6} \\ f_2^*(1,0) = (1 - \frac{4}{3})(\frac{1}{6}) + (\frac{4}{3})(\frac{1}{6}) = \frac{1}{6} \end{cases}$$

$$f_k(2,0) = \begin{cases} f_0^*(2,0) = (1 - \frac{4}{3})(0) + (\frac{4}{3})(0) = 0 \\ f_1^*(2,0) = (1 - \frac{4}{3})(1) + (\frac{4}{3})(0) = -\frac{1}{3} \\ f_2^*(2,0) = (1 - \frac{4}{3})(-1) + (\frac{4}{3})(0) = \frac{1}{3} \end{cases}$$

$$f_k(3,0) = \begin{cases} f_0^*(3,0) = (1 - \frac{4}{3})(0) + (\frac{4}{3})(0) = 0 \\ f_1^*(3,0) = (1 - \frac{4}{3})(1) + (\frac{4}{3})(0) = -\frac{1}{3} \\ f_2^*(3,0) = (1 - \frac{4}{3})(-1) + (\frac{4}{3})(0) = \frac{1}{3} \end{cases}$$

Now we want to move to the next time step. So we calculate our streaming step:

$$f_k(x,t) = f_k(x + v_k \Delta t, t + \Delta t)$$

$$f_0(x,1) = \begin{cases} f_0(1,1) = f_0^*(1,0) = \frac{4}{6} \\ f_0(2,1) = f_0^*(2,0) = 0 \\ f_0(3,1) = f_0^*(3,0) = 0 \end{cases}$$

$$f_1(x,1) = \begin{cases} f_1(1,1) = f_1^*(1,0) = \frac{1}{6} \\ f_1(2,1) = f_1^*(1,0) = \frac{1}{6} \\ f_1(3,1) = f_1^*(2,0) = -\frac{1}{3} \end{cases}$$

$$f_2(x,1) = \begin{cases} f_2(1,1) = f_2^*(1,0) = \frac{1}{6} \\ f_2(2,1) = f_2^*(3,0) = \frac{1}{3} \\ f_2(3,1) = f_2^*(3,0) = \frac{1}{3} \end{cases}$$

Now we can calculate the temperature at each node for $t = 1$ by adding the probabilities in each direction for each node.

$$T(x,1) = \sum_{n=1}^{3} f_i(x,1) = \begin{cases} T(1,1) = f_0(1,1) + f_1(1,1) + f_2(1,1) = \frac{4}{6} + \frac{1}{6} + \frac{1}{6} = 1 \\ T(2,1) = f_0(1,1) + f_1(1,1) + f_2(1,1) = 0 + \frac{1}{6} + \frac{1}{3} = \frac{1}{2} \\ T(3,1) = f_0(3,1) + f_1(3,1) + f_2(3,1) = 0 + \frac{-1}{3} + \frac{1}{3} = 0 \end{cases}$$

We can then recalculate our $f_k^{eq}(x,t) = w_k T(x,t)$ for $t = 1$ and run the simulation for as many time steps as desired.

8 Conclusion

In this paper the Lattice Boltzmann Method was introduced and the origins of it was discussed by it's relationship to Boltzmann's Kinetic Theory and Boltzmann's transport equation by a Newtonian based collision model. The Maxwell-Boltzmann distribution was also shown to illustrate particles velocities at equilibrium. Boundary conditions were hence explored and various lattice shapes were discussed starting with the Lattice Gas Automata and ending with the various Cartesian grids used in the LBM. We then introduced our simplest collision operator and the relation between relaxation time and thermal diffusivity for thermal dynamics was discussed. The LBM was then discretized and a hand calculation was performs for a 3 lattice, 1 dimensional form of the thermal Lattice Boltzmann Method.

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