NTU

Lattice Boltzmann Method

A condensated Introduction

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May 23, 2012

NTU Outline

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NTU Introduction

What is the Lattice Boltzmann method?

In a nutshell:

"Is a way to simulate fluid flow and energy transfer on a discrete grid by using the Boltzmann transport equation at the messoscopic level rather using the macroscopic continuum level like the Navier-Stokes equations."

We do this by expressing the fluid in terms of the probabilistic motion of individual particles (effectivebly, in terms of motion of number densities) under the various macroscopic forces and microscopic interparticle interaction of the forces present in the system.

Introduction

Setting the perspective

Particles commonly are conceptualized as individual molecules which can have interaction with:

- Macroscopic Forces: Gravety, Big Electromagnetic sources.
- Microscopic Forces: Electromagnetic interactions between particles

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Setting the right perspective

we start by defining a function, $f(\vec{x}, \vec{p}, t)$ which would represents the number density of partciles with at position $\vec{x}$ at time t which has momentum $\vec{p} = m\vec{v}$, where m is the mass of each fluid particle and $\vec{v}$ is the particle velocity.

Example

definition of particle density

$$N(\vec{x}, \vec{p}, t) = f(\vec{x}, \vec{p}, t)dx^3dp^3 \tag{1}$$

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The Boltzmann Transport Equation, Part I

$$
\begin{aligned}
N(\vec{x} + \frac{\vec{p}}{m}dt, \vec{p}, t + dt) &= f(\vec{x} + \frac{\vec{p}}{m}dt, \vec{p}, t + dt)dx^3dp^3 \\
= N(\vec{x}, \vec{p}, t) &= f(\vec{x}, \vec{p}, t)dx^3dp^3
\end{aligned}
$$

NTU Introduction

The Boltzmann Transport Equation, Part II

$$
\begin{aligned}
N(\vec{x} + \frac{\vec{p}}{m}dt, \vec{p} + \vec{F}dt, t + dt) &= f(\vec{x} + \frac{\vec{p}}{m}dt, \vec{p} + \vec{F}dt, t + dt)dx^3 d \\
= N(\vec{x}, \vec{p}, t) &= f(\vec{x}, \vec{p}, t)dx^3 dp^3
\end{aligned}
$$

introduction

The Boltzmann Transport Equation, Part III

$$
\begin{aligned}
N(\vec{x} + \frac{\vec{p}}{m}dt, \vec{p} + \vec{F}dt, t + dt) &= f(\vec{x} + \frac{\vec{p}}{m}dt, \vec{p} + \vec{F}dt, t + dt)dx^3 d \\
= N(\vec{x}, \vec{p}, t) + \Omega dt dx^3 dp^3 &= f(\vec{x}, \vec{p}, t)dx^3 dp^3 + \Omega dt dx^3 dp^3
\end{aligned}
$$

The Transport Boltzmann Equation

$$
\frac{\vec{p}}{m} \cdot \nabla_{\vec{x}} f + \vec{F} \cdot \nabla_{\vec{p}} f + \frac{\partial f}{\partial t} = \Omega \qquad (2)
$$

NTU Prerequisites & Goals

Knowledge is a brick wall that you raise line by line forever

Boltzmann Transport Equation (without external forces)

$$\frac{\partial f}{\partial t} + c \cdot \nabla f = \Omega \tag{3}$$

where Ω is called the collision term.

The BGK Approximation

$$\Omega = \omega(f^{eq} - f) = \frac{1}{\tau}(f^{eq} - f) \tag{4}$$

Boltzmann BGK (without external forces)

$$\frac{\partial f}{\partial t} + c \cdot \nabla f = \frac{1}{\tau}(f^{eq} - f) \tag{5}$$

NTU The Lattice Boltzmann Method

How everything started

Basics of the method

In the lattice Boltzmann method, the above equation is discretized and assumed to be valid along specific directions -linkages- , this discrete equation can be written like:

$$\frac{\partial f_i}{\partial t} + c_i \cdot \nabla f_i = \frac{1}{\tau}(f_i^{eq} - f_i) \tag{6}$$

Using a forward difference in time and space, we found:

$$f_i(x + \Delta x, t + \Delta t) - f_i(x, t) = -\frac{\Delta t}{\tau}[f_i(x, t) - f_i^{eq}(x, t)] \tag{7}$$

which would is the working horse of LBM

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NTU LBM Lattice Arrangements

The name of Lattices

The lattice Arragements in LBM are designated by the terminology:

Terminology

DnQm

where:

- n is the dimension number of our lattice
- m is the number of linkages in our lattice

LBM Lattice Arrangements

The name of Lattices

As an example:

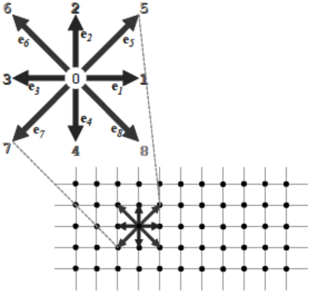

Figure: Example

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Lattice Arrangements

Lattices

The most used lattices are:

- For 1D problems:
  - D1Q2
  - D1Q3
  - D1Q5
- For 2D problems:
  - D2Q4
  - D2Q5
  - D2Q9
- For 3D problems:
  - D3Q15
  - D3Q19

NTU 1D Lattice Arrangements

D1Q2

Maybe the most basic of the lattices

Figure: D1Q2

For this lattice, the velocity vectors are: $\vec{c_1} = 1$ and $\vec{c_2} = -1$; the correspondent weighting factors are: $w_1 = 1/2$ and $w_2 = 1/2$; and the speed of sound in lattice $(\vec{C_s})$ is: $1/\sqrt{2}$.

NTU 1D Lattice Arrangements

D1Q3

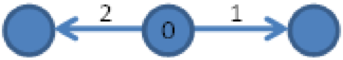


Figure: D1Q3

For this lattice, the velocity vectors are: $\vec{c_1} = 1$, $\vec{c_0} = 0$ and $\vec{c_2} = -1$; the correspondent weighting factors are: $w_1 = 1/6$, $w_0 = 4/6$ and $w_2 = 1/6$; and the speed of sound in lattice $(\vec{C_s})$ is: $1/\sqrt{3}$.

NTU 1D Lattice Arrangements

D1Q5

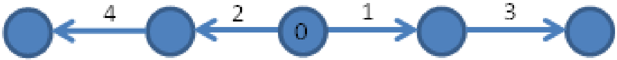


Figure: D1Q5

For this lattice, the velocity vectors are: $\vec{c_0} = 0$, $\vec{c_1} = 1$, $\vec{c_2} = -1$, $\vec{c_3} = 2$ and $\vec{c_4} = -2$; the correspondent weighting factors are: $w_0 = 6/12$, $w_1 = 1/12$, $w_2 = 1/12$, $w_3 = 2/12$ and $w_4 = 2/12$; and the speed of sound in lattice ($\vec{C_s}$) is: $1/\sqrt{3}$.

2D Lattice Arrangements

D2Q4

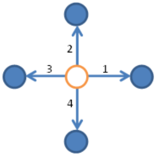


Figure: D2Q4

For this lattice, the velocity vectors are: $\vec{c_0} = (0, 1)$, $\vec{c_2} = (1, 0)$, $\vec{c_3} = (0, -1)$ and $\vec{c_4} = (-1, 0)$; the correspondent weighting factors are: $w_1 = w_2 = w_3 = w_4 = 1/4$.

2D Lattice Arrangements

D2Q5

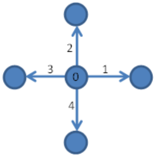


Figure: D2Q5

For this lattice, the velocity vectors are: $\vec{c_0} = (0,0)$, $\vec{c_0} = (0,1)$, $\vec{c_2} = (1,0)$, $\vec{c_3} = (0,-1)$ and $\vec{c_4} = (-1,0)$; the correspondent weighting factors are: $w_0 = 2/6$ and $w_1 = w_2 = w_3 = w_4 = 1/6$.

NTU 2D Lattice Arrangements

D2Q9

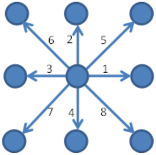


Figure: D2Q9

For this lattice, the velocity vectors are: $\vec{c_0} = (0,0)$, $\vec{c_1} = (0,1)$, $\vec{c_2} = (1,0)$, $\vec{c_3} = (0,-1)$, $\vec{c_4} = (-1,0)$, $\vec{c_5} = (1,1)$, $\vec{c_6} = (-1,1)$, $\vec{c_7} = (-1,-1)$ and $\vec{c_8} = (1,-1)$; the correspondent weighting factors are: $w_0 = 4/9$, $w_1 = w_2 = w_3 = w_4 = 1/9$ and $w_5 = w_6 = w_7 = w_8 = 1/36$.

NTU 3D Lattice Arrangements

D3Q15

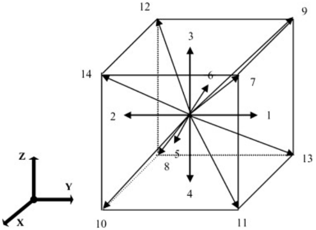


Figure: D3Q15

We can now figure out how the velocity vectors for any DnQm Lattice, therefore so the only information that we need to specify every time is the correspondent weighting factors: for $w_0 = 16/72$, for w_1 to w_6 is $8/72$ and for w_7 to w_14 is $1/72$.

NTU 3D Lattice Arrangements

D3Q19

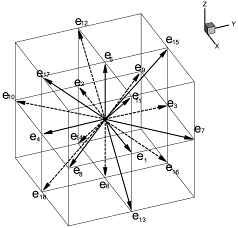


Figure: D3Q19

We can now figure out how the velocity vectors for any DnQm Lattice, therefore so the only information that we need to specify every time is the correspondent weighting factors: for $w_0 = 12/36$, for w_1 to w_6 is $2/36$ and for w_7 to w_18 is $1/36$.

NTU Equilibrium distribution Function

key to implemente LBM

The key element in appyling LBM for different problems is the equilibrium distribution function, f^{eq}.

We start from the normalized Maxwell's Distribution Function:

$$f = \frac{\rho}{2\pi/3} e^{-\frac{3}{2}(\vec{c}-\vec{u})^2} \tag{8}$$

which can be written as,

$$f = \frac{\rho}{2\pi/3} e^{-\frac{3}{2}(c^2)} e^{(2\vec{c}.\vec{u}-u^2/2)} \tag{9}$$

where $c^2 = \vec{c} \cdot \vec{c}$ and $u^2 = \vec{u} \cdot \vec{u}$. Recall that Taylor series expansion for e^{-x} is,

$$e^{-x} = 1 - x + \frac{x^2}{2!} - \frac{x^3}{3!} \dots \tag{10}$$

Equilibrium distribution Function

key to implemente LBM

Thefore the general equilibrium distribution can be writen as,

$$f = \frac{\rho}{2\pi/3} e^{-\frac{3}{2}(c^2)}[1 + 3(\vec{c} \cdot \vec{u}) - \frac{3}{2}u^2 + ...] \tag{11}$$

And the general from of the equilibrium distribution function can be written as,

$$f_i^{eq} = \phi\omega_i[A + B\vec{c}_i \cdot \vec{u} + C(\vec{c} \cdot \vec{u})^2 + Du^2] \tag{12}$$

NTU Outline

NTU The Lattice Boltzmann Method

by comparinson

First let's use a simple case: A 1-D Diffusion Equation:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{13}$$

and we are about to solve it by two methods:

- by Finite Difference Method (FDM)
- by Lattice Boltzmann Method (LBM)

NTU Finite Difference Approach

Using a uniform grid

Using a central difference in time and a second order central difference in space we get:

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2} \tag{14}$$

rearranging the above equation we get,

$$T_i^{n+1} - T_i^n = \frac{\alpha \Delta t}{\Delta x^2} T_{i+1}^n - 2T_i^n + T_{i-1}^n \tag{15}$$

and can be reformulated as,

$$T_i^{n+1} = T_i^n \left(1 - \frac{\alpha \Delta t}{\Delta x^2}\right) + \left(\frac{\alpha \Delta t}{\Delta x^2}\right) \frac{T_{i+1}^n + T_{i-1}^n}{2} \tag{16}$$

NTU Finite Difference Approach

Using a uniform grid

Now let

$$\omega = \frac{2\alpha\Delta t}{\Delta x^2} \tag{17}$$

Then our difference equation can be rewriten as;

Important equation

$$T_i^{n+1} = T_i^n (1-\omega) + \omega\frac{1}{2}\left(T_{i+1}^n + T_{i-1}^n\right) \tag{18}$$

NTU using the LBM approach

using a D1Q2 lattices

Start form the Boltzmann Equation

The kinetic equation for the distribution function (Temperature distribution, species distribution, etc), $f_k(x,t)$ can be written as:

$$\frac{\partial f_k(x,t))}{\partial t} + c_k \frac{\partial f_k(x,t))}{\partial x} = \Omega_k$$

for i=1,2 (for our one dimensional problem)

The left hand side term represents the streaming process, where the distribution function streams (advects along the lattice link with velocity $c_k = \frac{\Delta x}{\Delta t}$.

NTU using the LBM approach

using a D1Q2 lattices

using the BGK approximation for the collision operator:

$$\Omega_k = -\frac{1}{\tau}[f_k(x,t) - f_k^{eq}(x,t)]$$

The kinetic lattice boltzmann can be discretized as,

$$\frac{f_k(x, t+\Delta t)) - f_k(x,y)}{\Delta t} + c_k \cdot \frac{f_k(x+\Delta x, t+\Delta t) - f_k(x, t+\Delta t)}{\Delta x} = -\frac{1}{\tau}[f_k(x,t) - f_k^{eq}(x,t)] \tag{19}$$

Note that $\Delta x = c_k \Delta t$

NTU using the LBM approach

using a D1Q2 lattices

This would leads again to:

$$f_k(x+\Delta x, t+\Delta t) - f_k(x,t) = -\frac{\Delta t}{\tau}[f_k(x,t) - f_k^{eq}(x,t)]$$

if we do $\omega = \Delta t/\tau$ and re-arrange the variables as:

Do it looks familiar?

$$f_k(x+\Delta x, t+\Delta t) = f_k(x,t)\,(1-\omega) + \omega\frac{1}{2}\,(f_k^{eq})$$

This equation is the working horse of our diffusion problem and it represents a set of equations for each of the linkages of our lattice.

NTU using the LBM approach

using a D1Q2 lattices

for our case the dependent variable $T(x,t)$ can be related to the distribution function f_k as:

$$T(x,t) = \sum_{k=1}^{2} f_k(x,t) \tag{20}$$

and the equilibrium distribution can be choosen as $f_k^{eq} = w_k T(x,t)$ where w_k is the weighting factor in the direction of each linkage.

NTU using the LBM approach

using a D1Q2 lattices

We must remember that the weighting factor shoud sum 1, $\sum_{k=1}^{2} w_k = 1$ and the equilibrium distribution can be assumed valid along al k-directions,

$$T(x,t) = \sum_{k=1}^{2} f_k^{eq}(x,t) = \sum_{k=1}^{2} w_k T(x,t) \tag{21}$$

The relation between α and ω can be reduced from multi-scale expansion by using chapmann-Enskog expansion, which yield:

$$\alpha = \frac{\Delta x^2}{\Delta t D}(\tau - \frac{1}{2}) \tag{22}$$

where D is the dimension of the problem, 1, 2 or 3.

NTU using the LBM approach

using a D1Q2 lattices

Now we must define our Equilibrium function: Recall equation (12):

$$f_i^{eq} = T(x,t)w_i[A + B\vec{c}_i \cdot \vec{u} + C(\vec{c} \cdot \vec{u})^2 + Du^2]$$

it is appropiate that the equilibrium function be assumed constant, where no macroscopic velocity is involved, let:

$$f_i^{eq} = T(x,t)w_i A \tag{23}$$

and in this case A is assumed to be 1.

NTU using the LBM approach

using a D1Q2 lattices

and it must satisfy:

$$\sum_{i=1}^{2} f_k^{eq} = T(x,t) \tag{24}$$

$$\sum_{i=1}^{2} f_k^{eq} c_k = 0 \tag{25}$$

which leads to the equations:

$$A_1 + A_2 = T(x,t) \tag{26}$$

$$A_1 c_1 + A_2 c_2 = 0 \tag{27}$$

NTU using the LBM approach

using a D1Q2 lattices

but we know that $c_1 = 1$ and $c_2 = -1$, which leads us to

$$A_1 + A_2 = T(x,t) \tag{28}$$

$$A_1 - A_2 = 0 \mapsto A_1 = A_2 \tag{29}$$

thus $A_1 = A_2 = \mathrm{T(x,t)}/2$ or

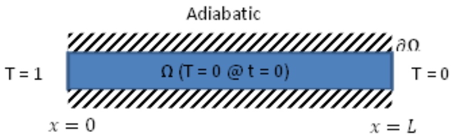
$$f_k^{eq} = 1/2\,T(x,t) \tag{30}$$

NTU Outline

1D Diffusion Case

Using LBM D1Q2

A slab initially at temperature equal to zero, $T = 0$. For time $t \geq 0$, the left surface of the slab is subjected to a high temperature and equal to unity, $T = 1$. The slab length is 30 units. Calculate the temperature distribution in the slab for t=200. Compare the of both methods, LBM and FDM, for $\alpha = 25$.



NTU 1D Diffusion Case

Using LBM D1Q2

Solution: Let us devide the domain of integration into $\Delta x = 1.0$ and $\Delta t = 1.0$ using $\alpha = 0.25$ we can compute $\omega : 0.25 = (1/\omega - 1/2)$ with gives $\omega = 4/3$.
we know from the equilibrium function analysis that for D1Q2, de equilibrium function is,

$$f_1^{eq}(x,t) = 0.5T(x,t) \tag{31}$$

$$f_2^{eq}(x,t) = 0.5T(x,t) \tag{32}$$

LBM consist of two steps, collision and streaming. The collision step is given by:

$$f_k^{eq}(x, t+\Delta t) = f_k(x,t)[1-\omega] + \omega f_k^{eq}(x,t)$$

And the Streaming step is:

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

1D Diffusion Case

Boundary Conditions

The boundary conditions for LBM are obtained by contrasting the macroscopic conditions with the streaming process near the boundaries. For our case we would use:

- Dirichlet Boundary Conditions.
- Neumann Boundary Conditions.

1D Diffusion Case

Boundary Conditions

- Dirichlet Boundary Condition

The detailed flux balance at the boundary, x=o for D1Q2 is as follows,

$$f_q^e q(0,t) - f_1(0,t) + f^{eq} - f_2(0,t) = 0$$

and,

$$\begin{aligned} f_1^{eq}(0,t) &= w_1 T_w = 0.5 T_w \\ f_2^{eq}(0,t) &= w_2 T_w = 0.5 T_w \end{aligned} \tag{33}$$

Therefore at $x = 0$, $f_1(0) + f_2(0) = T_w$, and from the streaming processes $f_1(0) = f_2(1)$, then $f_1(0)$ can be determined as $f_1(0) = T_w - f_2(0)$.

1D Diffusion Case

Boundary Conditions

- Neumann Boundary Condition

The temperature gradient is zero which implies that at x = n, $T(n) = T(n-1)$. Hence,

$$f_1(n) + f_2(n) = f_1(n-1) + f_2(n-1)$$

or

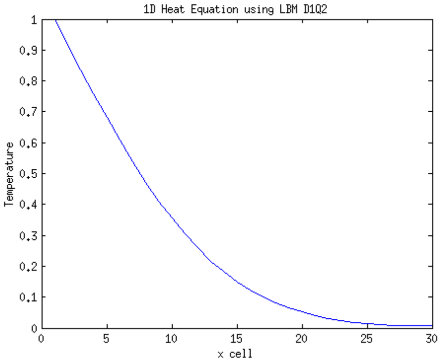
$$\begin{aligned} f_1(n) &= f_1(n-1) \\ f_2(n) &= f_2(n-1) \end{aligned}$$

where n denotes the lattice node.

NTU 1D Diffusion Case

Result using D1Q2

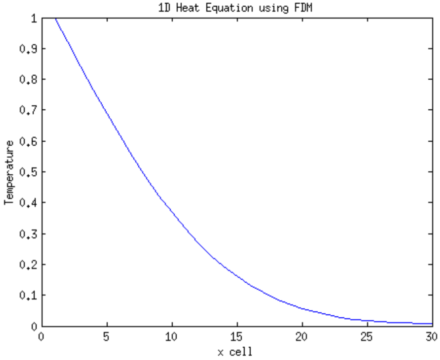
The result of our algorithm should be:



1D Diffusion Case

Result using FDM

The result of our algorithm should be:



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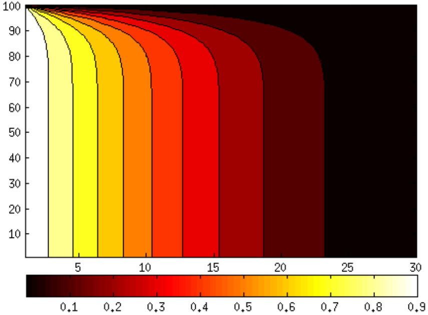
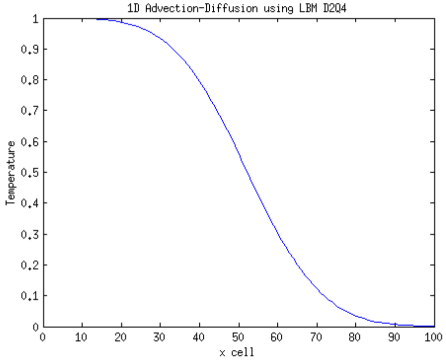
2D Diffusion Case

Result using D2Q4



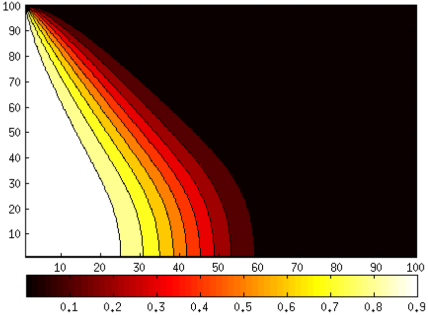
NTU 1D Advection-Diffusion Case

Result using D1Q2



2D Advection-Diffusion Case

Result using D2Q4



Resources

If you want to have more details on LBM

- Anne Hanna, "A short intro to LBM"
  http://icarusswims.blogspot.com/2011/04/
- A.A. Mohamad, "Lattice Boltzmann Method"
  http://www.springer.com/engineering/
- Sauro Succi, "The Lattice Boltzmann Equation"
  Oxford University Press

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Questions ?

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