Lattice Boltzmann Method

Foundations of Multiscale Modelling: Kinetics

Fedor Loginov

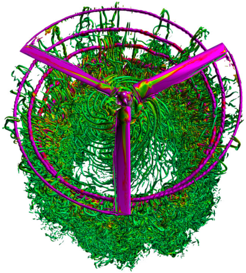
Mocsow, 2019

Plan

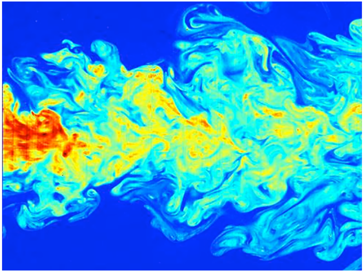
- Application of LBM
- Introduction to the theory
- Lattice Boltzmann
- Results
- Conclusion

Application of Lattice Boltzmann method

- Simulating a complex fluid dynamics
- Computing Quantum systems
- Modeling a Navier-Stokes



https://www.nas.nasa.gov



https://www.quantamagazine.org/

Introduction: Boltzmann equation

We consider a homogeneous system, where $f(\overrightarrow{r}, \overrightarrow{V}, t)$ (velocity distribution function) is independent of the spatial variable $\overrightarrow{r}$.

Boltzmann equation:

$$\frac{\partial}{\partial t} f(\overrightarrow{r}, \overrightarrow{V}, t) + \overrightarrow{V} \frac{\partial}{\partial \overrightarrow{r}} f(\overrightarrow{r}, \overrightarrow{V}, t) + \frac{\overrightarrow{F}}{m} \frac{\partial}{\partial \overrightarrow{V}} f(\overrightarrow{r}, \overrightarrow{V}, t) = I(f, f)$$

Normalization:

$$\int d\overrightarrow{V} \int d\overrightarrow{r} f(\overrightarrow{r}, \overrightarrow{V}, t) = N,$$

where N is a number of particles.

Introduction: equilibrium VDK

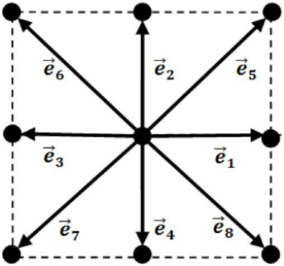
The Velocity distribution function(VDK) that satisfy $\frac{\partial f(\overrightarrow{V},t)}{\partial t} = I(f,f) = 0$ called equilibrium VDK.

$$f_{eq}(\overrightarrow{V},t) = f_M(\overrightarrow{V},t) = n\Big(\frac{m}{2\pi k_B T}\Big)^{3/2} \exp\Big(\frac{m(\overrightarrow{V} - \overrightarrow{u})^2}{2k_B T}\Big)$$

For considered case, where equilibrium VDK that independent of time is Maxwellian velocity distribution.

Lattice Boltzmann method(LBM) is a method solving sampled Boltzmann equation.

D2Q9



- All particles are confined in the nodes of lattice.
- The particle can move with velocity e_i or stay at rest.

Lattice Boltzmann

Two main steps:

- Computing of particles streaming
- Computing of particles collisions

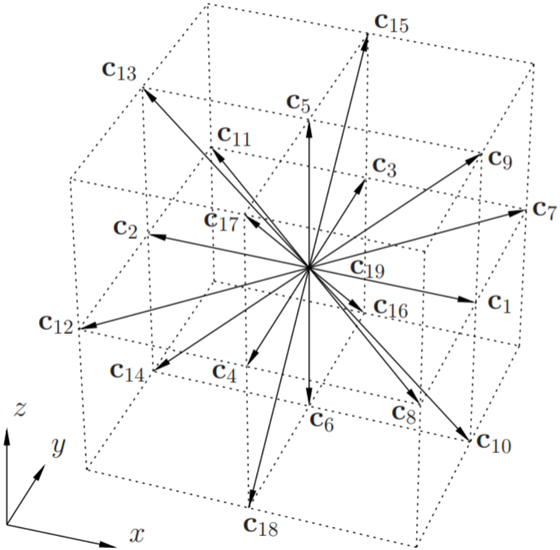
$f_i(\overrightarrow{V}, t)$ - is a probability of streaming in a particular direction.

$$\rho(\overrightarrow{r}, t) = \sum_{i=1}^{k} f_i(\overrightarrow{r}, t)$$

$$\overrightarrow{v}(\overrightarrow{r}, t) = \frac{1}{\rho(\overrightarrow{r})} \sum_{i=1}^{k} f_i(\overrightarrow{r}, t)\overrightarrow{c_i},$$

where k is the number of directions.

Lattice Boltzmann: D3Q19



Lattice Boltzmann: Bhatnagar-Gross-Krook model

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

with the lattice speed of sound $c_s = \frac{1}{\sqrt{3}}$ for the D3Q19 lattice and the lattice weights

$$w_i = \begin{cases} \frac{2}{36}, & i = 1 \ldots 6 \\ \frac{1}{36}, & i = 7 \ldots 18 \\ \frac{12}{36}, & i = 19 \end{cases}$$

Boundary conditions: bottom plane (z = 0)

$$v_z = 1 - \frac{1}{\rho}(f_1 + f_2 + f_3 + f_4 + f_7 + f_8 + f_{11} + f_{12} + f_{19} +$$

$$+2 * (f_6 + f_{10} + f_{14} + f_{16} + f_{18})$$

Consider nonequilibrium part of f_i: $f_i^* = f_i - f_i^{(eq)}$ The bounce-back condition in +z-direction (in normal direction to the boundary) would read as:

$$f_5^* = f_5 - f_5^{(eq)} = f_6^* = f_6 - f_6^{(eq)}$$

Boundary conditions: bottom plane (z = 0)

We have a system:

$$\begin{cases} \rho = \sum_{i=1}^{19} f_i \\ \overrightarrow{V} = \frac{1}{\rho} \sum_{i=1}^{k} f_i \overrightarrow{c_i} \\ f_5 - f_5^{(eq)} = f_6 - f_6^{(eq)} \end{cases}$$

Unknown variables: $f_9, f_{13}, f_{15}, f_{17}, \rho$

Boundary conditions: bottom plane ($z = 0$)

Solution:

$$\rho = \sum_{i=1}^{19} f_i$$

$$f_9 = f_{14} + \frac{2w_9}{c_s^2}\rho(v_z + v_x)$$

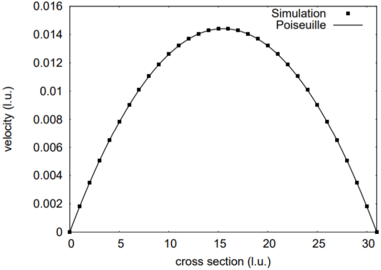
$$f_{13} = f_{10} + \frac{2w_{13}}{c_s^2}\rho(v_z - v_x)$$

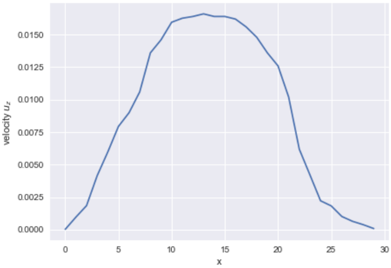
$$f_{15} = f_{18} + \frac{2w_{15}}{c_s^2}\rho(v_z + v_y)$$

$$f_{17} = f_{16} + \frac{2w_{17}}{c_s^2}\rho(v_z - v_y)$$

Results

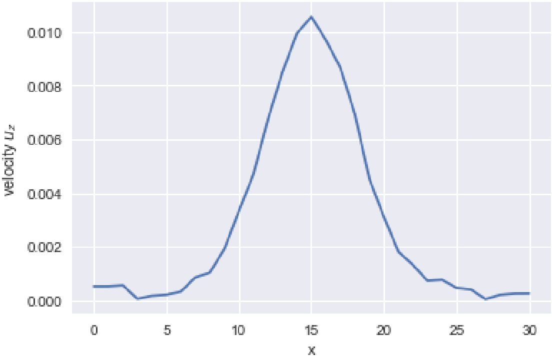
Box size: 30x30x30, $\tau = 4$





from Article (5000 iterations) my result (30 iterations,y=15)

Results



my result (30 iterations,y=10)

Results

Lattice Boltzmann method (D3Q19) with uniform boundaries has been realized on Python Notebook.
You can find the realisation and the presentation on the Github: https://github.com/FlyingArrogantCat/Kinetic

Literature and articles

- Implementation of on-site velocity boundary conditions for D3Q19 lattice Boltzmann *by Martin Hecht, Jens Harting*
- The Lattice Boltzmann Method:Principles and Practice *by Timm Kruger, Halim Kusumaatmaja,Alexandr Kuzmin*
- An immersed boundary-lattice Boltzmann model *by M. Navidbakhsh, M. Rezazadeh*

Thank you for your attention!