Lattice Boltzmann Method - Overview

A top-down approach

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Simulation Frameworks
Dresden

February 8, 2024

Outline

1. Introduction
   - Mesoscopic Approach
   - 1D Heat Equation
2. Advantages and Disadvantages
3. Typical LBM applications
4. Lattice Boltzmann equation
5. Lattice Boltzmann method
6. Advanced collision operators
7. For Further Reading

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Introduction

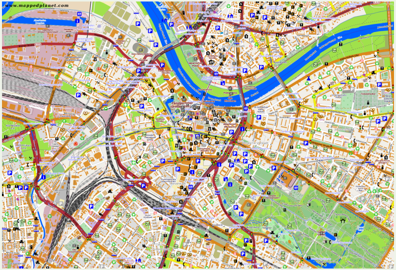
- Imagine to model the traffic in Dresden.
- There are 3 approaches.

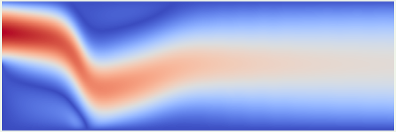
Traffic modeling - Macroscopic approach

Macroscopic

Each street is modeled as a pipe in which cars (fluid) flow. Divide streets in segments. → Local average behavior.

Comparison with fluid world





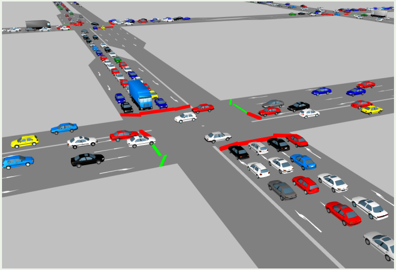
[1]

Traffic modeling - Microscopic approach

Microscopic

Each car (particle) is modeled. Too much data to process. → Particle behavior.

Comparison with fluid world



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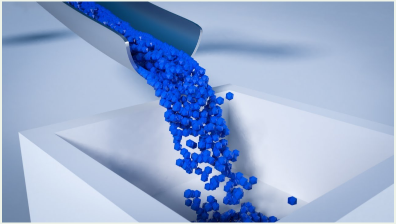

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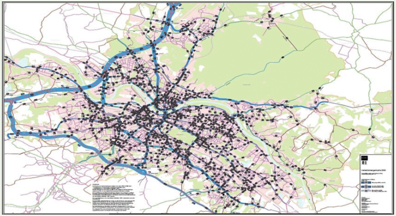
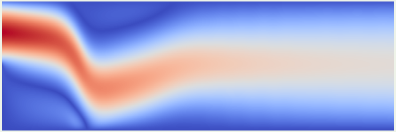
Traffic modeling - Mesoscopic approach

Mesoscopic

Vehicles are grouped together. A good quantity of data to process. → Particle average behavior.

Comparison with fluid world





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Conclusions

- LBM works in the mesoscopic world!
- Gas kinetic theory is the king of mesoscopic world.
- The properties of each group of particles are represented by distribution functions (derived from the Boltzmann equation).

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Example: heat equation

- We want to solve the heat equation on a 1D rod:

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

- On the right side we have adiabatic boundary condition:

$$\left.\frac{\partial T}{\partial x}\right|_{x=L} = 0.$$

- On the left side we have a fix temperature:

$$T(x = 0) = 1.$$

- As initial condition we set:

$$T(x, t = 0) = 0.$$

Example: heat equation

lattice BGK equation (LBGK)

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} \left[f_i^{\mathrm{eq}}(\mathbf{x}, t) - f_i(\mathbf{x}, t) \right]$$

Macroscopic variables

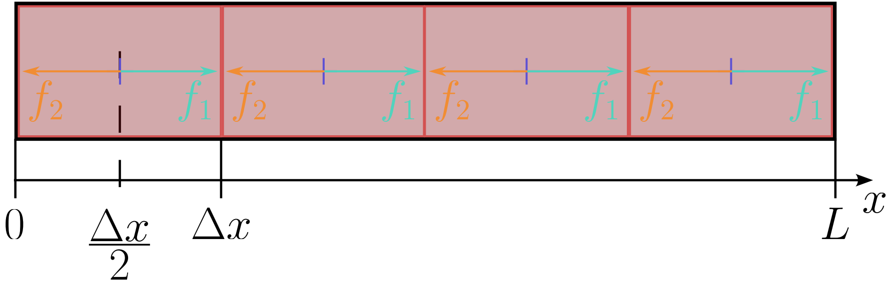
$$T(\mathbf{x}, t) = \sum_{i=0}^{q} f_i(\mathbf{x}, t)$$

$$f_i^{\mathrm{eq}} = T w_i$$

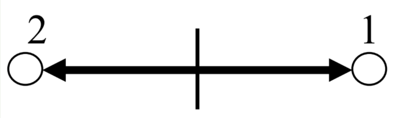
$$\alpha = \left(\tau - \frac{\Delta t}{2} \right) c_s^2$$

where, τ is a relaxation time.

Example: heat equation



$D1Q2$ velocity space discretization



$w_i = 0.5$

$c_s = 1$

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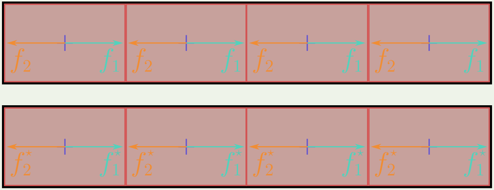
Example: heat equation

lattice BGK equation (LBGK)

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} \left[f_i^{\mathrm{eq}}(\mathbf{x}, t) - f_i(\mathbf{x}, t) \right]$$

Collision

$$f_i^{\star}(\mathbf{x}, t) = f_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} \left[f_i^{\mathrm{eq}}(\mathbf{x}, t) - f_i(\mathbf{x}, t) \right]$$



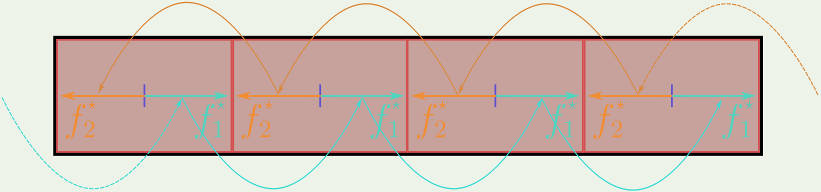
Example: heat equation

lattice BGK equation (LBGK)

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} \left[f_i^{\mathrm{eq}}(\mathbf{x}, t) - f_i(\mathbf{x}, t) \right]$$

Streaming

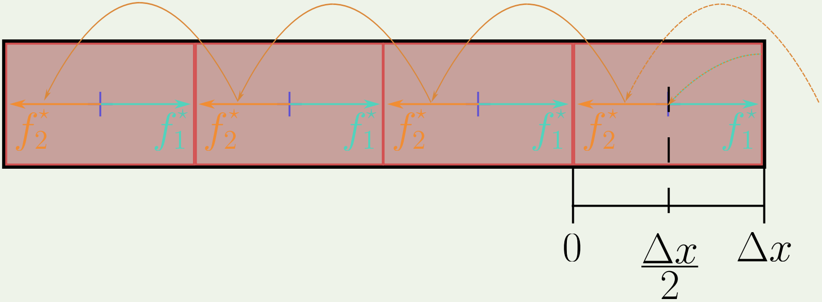
$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i^{\star}(\mathbf{x}, t)$$



Example: heat equation

Boundary Conditions - Adiabatic

$$f_2(x = L, t + \Delta t) = f_1^\star(x = L, t)$$

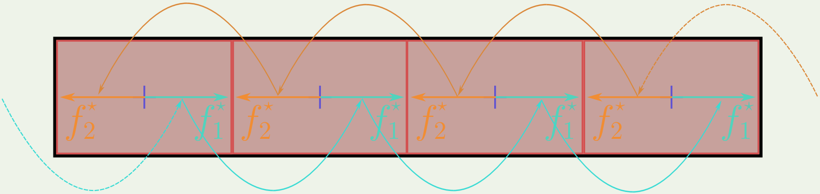


Example: heat equation

Boundary Conditions - Dirichlet

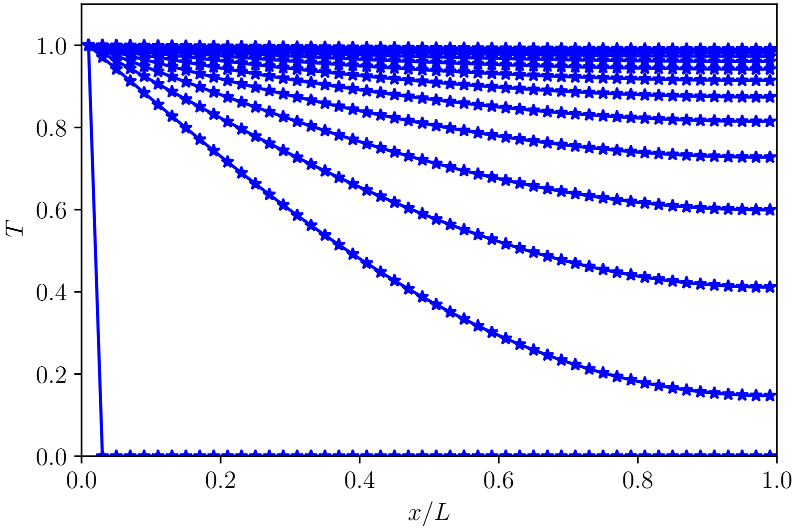
$$T_w = \sum_{i=1}^{2} f_i(\mathbf{x}, t + \Delta t)$$

$$f_1(x = 0, t + \Delta t) = T_w - f_2(x = 0, t + \Delta t)$$



Example: heat equation

Result with 50 elements on the rod



Conclusions

- LBM works in the mesoscopic world!
- Links between macroscopic and mesoscopic variables.
- Simple 1D temperature diffusion application.

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Advantages and Disadvantages

Pros

- Solves simple arithmetic equations.
- Only unknowns are the distribution functions.
- Current value of distribution functions depends solely on previous conditions. $\rightarrow$ Easy to implement in parallel.
- Boundary conditions are simple even for complex geometries.
- Well suited for aeroacoustic sound generation.
- Works on regular square grids.

Advantages and Disadvantages

Cons

- Works on regular square grids.
- Numerically not stable for small viscosity.
- Number of elements strongly depends on the Re number.
- Extra sensitive to Ma number $\rightarrow$ typically used for weakly compressible flows.
- Memory-intensive, especially during streaming.
- Time-dependent, not efficient for steady flows.

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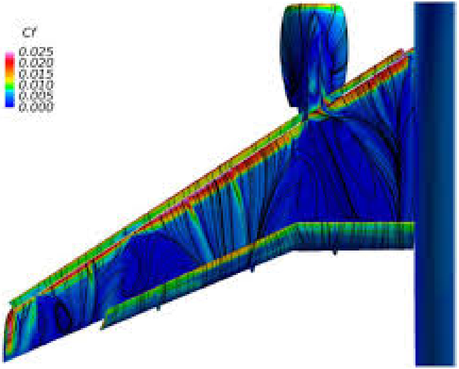
Typical LBM applications - Aerospace



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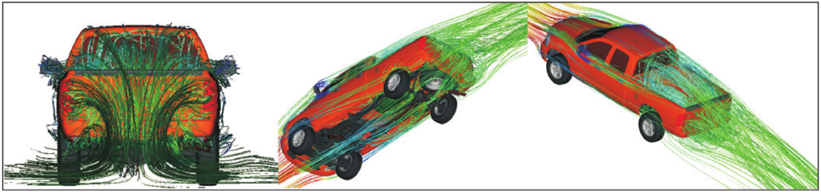
- Incompressible / Weakly compressible
- Easy to implement BCs on complex geometries
- Turbulence models available
- Collision models exist also for transonic/supersonic regime

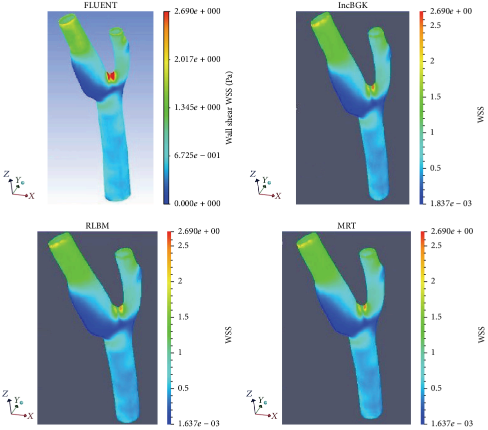
Typical LBM applications - Automotive



[11]

- Incompressible / Weakly compressible
- Easy to implement BCs on complex geometries
- Turbulence models available

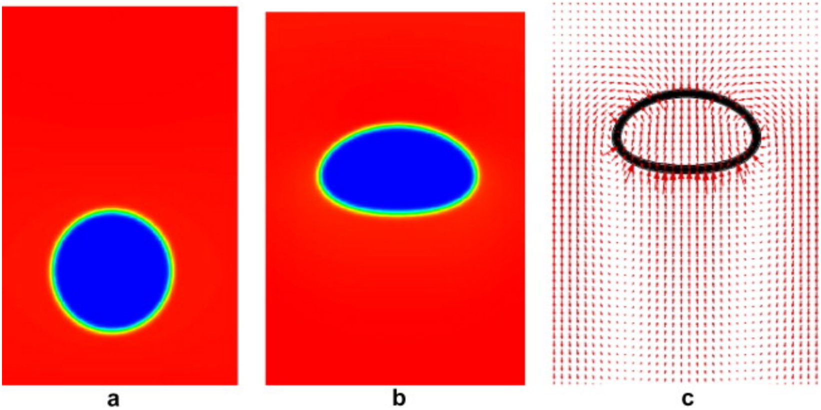
Typical LBM applications - Medicine



[12]

- Incompressible / Weakly compressible
- Easy to implement BCs on complex geometries
- Unsteady flows

Typical LBM applications - Multi-phase flow



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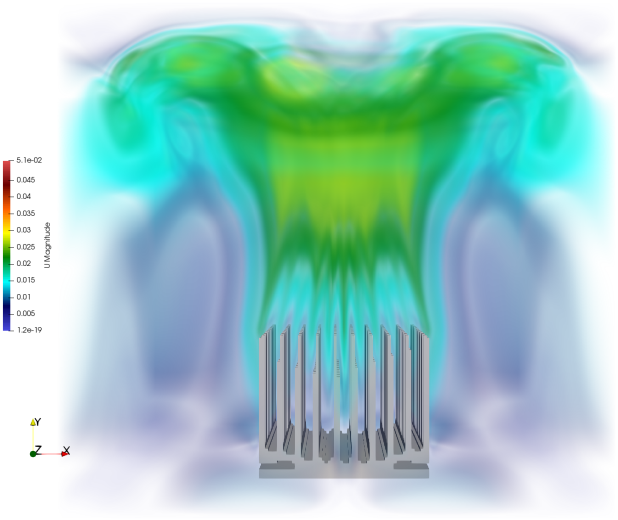
Typical LBM applications - Conjugate heat transfer



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Disclaimer

Most of the content from this section on, is based on the book of Krüger et al. 2017[1]. The author of these slides found it to be very well written and exhaustive to introduce any newcomer to the fantastic world of LBM.

[1]Timm Krüger et al. (2017). *The Lattice Boltzmann Method. Principles and Practice*. Springer Cham. DOI: 10.1007/978-3-319-44649-3

Lattice Boltzmann equation

Non-dimensional quantities (*)

$$\frac{\partial}{\partial t^\star} = \frac{\ell}{V}\frac{\partial}{\partial t}, \quad \frac{\partial}{\partial x^\star} = \ell\frac{\partial}{\partial x}, \quad \frac{\partial}{\partial \xi^\star} = V\frac{\partial}{\partial \xi}$$

where the reference variables are ρ_0, V, ℓ

Non-dimensional force-free Boltzmann equation

$$\boxed{\frac{\partial f^\star}{\partial t^\star} + \xi_\alpha^\star\frac{\partial f^\star}{\partial x_\alpha^\star} = \Omega^\star(f^\star)}$$

where

$f^\star = fV^d/\rho_0, \quad \rho^\star = \rho/\rho_0, \quad \Omega^\star = \Omega\ell V^2/\rho_0, \quad \theta^\star = RT/V^2$

Lattice Boltzmann equation

Let us drop the * notation

Non-dimensional force-free Boltzmann equation

$$\boxed{\frac{\partial f}{\partial t} + \xi_\alpha \frac{\partial f}{\partial x_\alpha} = \Omega(f)}$$

Conversation constraints are represented by the moments of the collision operator:

- mass conservation: $\int \Omega(\mathbf{x}, t)\,\mathrm{d}^3\xi = 0$
- momentum conservation: $\int \boldsymbol{\xi}\Omega(\mathbf{x}, t)\,\mathrm{d}^3\xi = \mathbf{0}$
- total energy conservation: $\int |\boldsymbol{\xi}|^2\Omega(\mathbf{x}, t)\,\mathrm{d}^3\xi = 0$

Lattice Boltzmann equation

Bhatnagar-Gross-Krook (BGK) collision operator

$$\Omega(f) = -\frac{1}{\tau}(f - f^{\mathrm{eq}})$$

where, τ - relaxation time and f^{eq} - equilibrium distribution.

Non-dimensional equilibrium distribution

$$f^{\mathrm{eq}}(\rho, \mathbf{V}, \theta, \boldsymbol{\xi}) = \frac{\rho}{(2\pi\theta)^{d/2}} \exp\left(-\frac{(\boldsymbol{\xi} - \mathbf{V})^2}{2\theta}\right)$$

- $\rho(\mathbf{x}, t) = \int f^{\mathrm{eq}}(\mathbf{x}, \boldsymbol{\xi}, t)\, \mathrm{d}^3\xi$
- $\rho(\mathbf{x}, t)\mathbf{V}(\mathbf{x}, t) = \int \boldsymbol{\xi}(\mathbf{x}, t) f^{\mathrm{eq}}(\mathbf{x}, \boldsymbol{\xi}, t)\, \mathrm{d}^3\xi$
- $\rho(\mathbf{x}, t)E(\mathbf{x}, t) = 0.5 \int |\boldsymbol{\xi}(\mathbf{x}, t)|^2 f^{\mathrm{eq}}(\mathbf{x}, \boldsymbol{\xi}, t)\, \mathrm{d}^3\xi$

Lattice Boltzmann equation

Expanding Non-dim equilibrium distribution function only upto the first 3 expansion coefficients of Hermit Polynomials (HP) expansion is sufficient to properly resolve the Navier-Stokes equations (NSe).

Non-dim. eq. distribution for NSe

$$f^{\mathrm{eq}}(\rho, \mathbf{V}, \theta, \boldsymbol{\xi}) = \rho\omega(\boldsymbol{\xi})\left\{1 + \xi_\alpha V_\alpha + \left[V_\alpha V_\beta + (\theta - 1)\delta_{\alpha\beta}\right](\xi_\alpha\xi_\beta - \delta_{\alpha\beta})\right\}$$

Lattice Boltzmann equation

Velocity discretization stencil - $DdQq$

- One dimension $\rightarrow D1Q3$
- Two dimensions $\rightarrow D2Q9$
- Three dimensions $\rightarrow D3Q27$

Low order stencils exist, such as $D3Q15$ and $D3Q19$ which still recover hydrodynamic moments up to second order (energy), but the truncation error is different. Some of these truncation terms are not rotational invariant causing problems with turbulent flows.

Lattice Boltzmann equation

We discretize the integrals with the Gauss-Hermite quadrature rule to attain a second order approximation and we obtain

Equilibrium distribution function for NSe

$$f_i^{\mathrm{eq}} = \rho w_i \left\{ 1 + \xi_{i\alpha} V_\alpha + 0.5 \left[V_\alpha V_\beta + (\theta - 1)\delta_{\alpha\beta} \right] (\xi_\alpha \xi_\beta - \delta_{\alpha\beta}) \right\}$$

We now assume that the flow is isothermal $\rightarrow \theta = 1$. Furthermore we introduce $c_i = \xi_i / \sqrt{3}$.

Equilibrium distribution function for NSe

$$\boxed{f_i^{\mathrm{eq}} = \rho \omega_i \left[1 + \frac{c_{i\alpha} V_\alpha}{c_s^2} + \frac{V_\alpha V_\beta (c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta})}{2 c_s^4} \right]}$$

Lattice Boltzmann equation

By following the same procedure for f, we obtain

Discrete-Velocity Boltzmann Equation (DVBE)

$$\boxed{\frac{\partial f_i}{\partial t} + c_{i\alpha}\frac{\partial f_i}{\partial x_\alpha} = \Omega(f_i)}$$

Macroscopic quantities

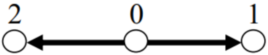
- $\rho(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t) = \sum_i f_i^{\mathrm{eq}}(\mathbf{x}, t)$
- $\rho(\mathbf{x}, t)\mathbf{V}(\mathbf{x}, t) = \sum_i \mathbf{c}_i f_i(\mathbf{x}, t) = \sum_i \mathbf{c}_i f_i^{\mathrm{eq}}(\mathbf{x}, t)$
- $\rho(\mathbf{x}, t)E(\mathbf{x}, t) = 0.5\sum_i |\mathbf{c}_i|^2 f_i(\mathbf{x}, t) = 0.5\sum_i |\mathbf{c}_i|^2 f_i^{\mathrm{eq}}(\mathbf{x}, t)$

Construction of velocity sets

In order to consistently solve NSe via LBM, the moments of the weights w_i and velocities $c_{i\alpha}$ need to be isotropic up to the fifth order. This leads to the following conditions

1. $w_i > 0$
2. $\sum_i w_i = 1$
3. $\sum_i w_i c_{i\alpha} = 0$
4. $\sum_i w_i c_{i\alpha} c_{i\beta} = c_s^2 \delta_{\alpha\beta}$
5. $\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} = 0$
6. $\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\mu} = c_s^4 (\delta_{\alpha\beta}\delta_{\gamma\mu} + \delta_{\alpha\gamma}\delta_{\beta\mu} + \delta_{\alpha\mu}\delta_{\beta\gamma})$
7. $\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\mu} c_{i\nu} = 0$

Construction of velocity sets - D1Q3



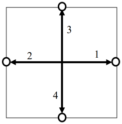
[5]

- $i = 0, 1, 2$
- $\alpha = 1 = x$
- $c_i = 0, \pm 1$

1. $w_0 > 0, w_1 > 0, w_2 > 0$
2. $w_0 + w_1 + w_2 = 1$
3. $w_1 - w_2 = 0$
4. $w_1 + w_2 = c_s^2$
5. $w_1 - w_2 = 0$
6. $w_1 + w_2 = 3c_s^4$

Solution: $w_0 = 2/3, w_1 = w_2 = 1/6, c_s^2 = 1/3$

Construction of velocity sets - D2Q4



[5]

- $i = 1, 2, 3, 4$
- $\alpha = 2 = x, y$
- $c_i = (1, 0); (-1, 0); (0, 1); (0, -1)$

1. $w_1 > 0, w_2 > 0,$
   $w_3 > 0, w_4 > 0$
2. $w_1 + w_2 + w_3 + w_4 = 1$
3. $(x)w_1 - w_2 = 0$
   $(y)w_3 - w_4 = 0$
4. $(x^2)w_1 + w_2 = c_s^2$
   $(y^2)w_3 + w_4 = c_s^2$
5. $(x^3)w_1 - w_2 = 0;$
   $(y^3)w_3 - w_4 = 0$
6. $(x^4)w_1 + w_2 = 3c_s^4;$
   $(y^4)w_3 + w_4 = 3c_s^4$

Solution: $w_1 = w_2 = w_3 = w_4 = 1/4, c_s^2 = 1/2$ but eq. 6 is not satisfied.

Lattice Boltzmann equation

Last step is the discretization in time and space of the DVBE via the method of Characteristics, to obtain the

lattice Boltzmann equation

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Delta t \Omega(f_i)$$

BGK collision operator

$$\Omega(f_i) = -\frac{1}{\tau}(f_i - f_i^{\mathrm{eq}})$$

$$0 = \sum_i \Omega_i(\mathbf{x}, t), \quad \mathbf{0} = \sum_i \mathbf{c}_i \Omega_i(\mathbf{x}, t), \quad 0 = \sum_i |\mathbf{c}_i|^2 \Omega_i(\mathbf{x}, t)$$

lattice BGK equation (LBGK)

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} \left[f_i^{\mathrm{eq}}(\mathbf{x}, t) - f_i(\mathbf{x}, t) \right]$$

Lattice Boltzmann equation

Second-order Chapman-Enskog expansion of f

$$f_i = f_i^{\mathrm{eq}} + \underbrace{\varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \ldots}_{f^{\mathrm{neq}}}$$

where ε is the Knudsen number, truncated to

$$\boxed{f_i \approx f_i^{\mathrm{eq}} + \varepsilon f_i^{(1)}}$$

The idea is to apply this form of expansion to the LBGK and to its derivatives. Let us define $f^{\mathrm{neq}} = f - f^{\mathrm{eq}}$, after some algebra we obtain two sets of equations belonging to first (ε) and second (ε^2) order in Knudsen number. Where the second order can be seen as a correction to the first order.

Lattice Boltzmann equation

Second-order Chapman-Enskog expansion of LBGK

$$\left(\varepsilon\partial_t^{(1)} + \varepsilon^2\partial_t^{(2)}\right)\rho + \varepsilon\partial_\gamma^{(1)}(\rho V_\gamma) = 0$$

$$\left(\varepsilon\partial_t^{(1)} + \varepsilon^2\partial_t^{(2)}\right)(\rho V_\alpha) + \varepsilon\partial_\beta^{(1)}\Pi_{\alpha\beta}^{\mathrm{eq}} = -\varepsilon^2\partial_\beta^{(1)}\left(1 - \frac{\Delta t}{2\tau}\right)\Pi_{\alpha\beta}^{(1)}$$

$$\Pi_{\alpha\beta}^{eq} = \rho V_\alpha V_\beta + \rho c_s^2\delta_{\alpha\beta}$$

$$\Pi_{\alpha\beta}^{(1)} = -\rho c_s^2\tau\left(\partial_\beta^{(1)} V_\alpha + \partial_\alpha^{(1)} V_\beta\right) + \tau\partial_\gamma^{(1)}(\rho V_\alpha V_\beta V_\gamma)$$

The last element of this equation is the leading error of the LBGK $\mathcal{O}(u^3)$. This becomes insignificant if $\mathrm{Ma}^2 << 1 \rightarrow \mathcal{O}(\mathrm{Ma}^2)$.

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Lattice Boltzmann equation

Combining all equations together and reverting the expansions of the derivatives we can recover the Navier-Stokes equations, neglecting $\mathcal{O}(\mathrm{Ma}^2)$ terms

Navier-Stokes equations

$$\partial_t \rho + \partial_\gamma (\rho V_\gamma) = 0$$

$$\partial_t (\rho V_\alpha) + \partial_\beta (\rho V_\alpha V_\beta) = -\partial_\beta \underbrace{(\rho c_s^2)}_{p} \quad (1)$$

$$+ \partial_\beta \underbrace{\left(1 - \frac{\Delta t}{2\tau}\right) \rho c_s^2 \tau}_{\mu} [\partial_\beta V_\alpha + \partial_\alpha V_\beta] \quad (2)$$

Conclusions

- Formulation of equilibrium distribution function.
- Only the first 3 expansions coefficients are required to resolve the NSe.
- Introduction and derivation of velocity discretization stencils - $DdQq$.
- Formulation of the DVBE.
- Formulation of the lattice Boltzmann equation.
- Formulation of the LBGK equation.
- Introduction to Chapman-Enskog expansion.
- Leading order of the LGBK as $\mathcal{O}(\mathrm{Ma}^2)$.
- Recovery of NS equations.

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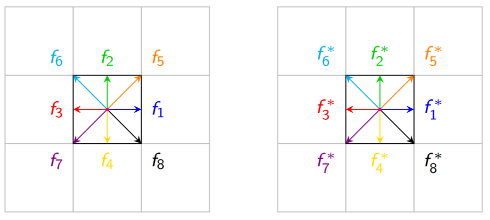
Lattice Boltzmann method

lattice BGK equation (LBGK)

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} \left[f_i^{\mathrm{eq}}(\mathbf{x}, t) - f_i(\mathbf{x}, t) \right]$$

Collision

$$f_i^{\star}(\mathbf{x}, t) = f_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} \left[f_i^{\mathrm{eq}}(\mathbf{x}, t) - f_i(\mathbf{x}, t) \right]$$

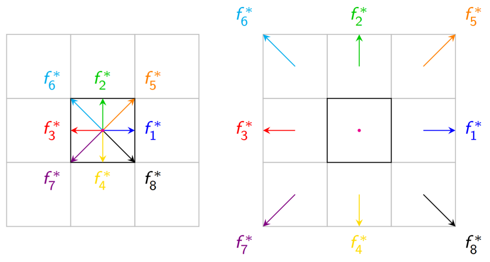


[6]

Lattice Boltzmann method

Streaming

$$f_i(\mathbf{x} + c_i \Delta t, t + \Delta t) = f_i^\star(\mathbf{x}, t)$$



[6]

Lattice Boltzmann method

Equilibrium distribution function for NSe

$$f_i^{\mathrm{eq}} = \rho w_i \left[1 + \frac{c_{i\alpha} V_\alpha}{c_s^2} + \frac{V_\alpha V_\beta (c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta})}{2 c_s^4} \right]$$

Macroscopic quantities

- $\rho(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t) = \sum_i f_i^{\mathrm{eq}}(\mathbf{x}, t)$
- $\rho(\mathbf{x}, t)\mathbf{V}(\mathbf{x}, t) = \sum_i \mathbf{c}_i f_i(\mathbf{x}, t) = \sum_i \mathbf{c}_i f_i^{\mathrm{eq}}(\mathbf{x}, t)$
- $p = c_s^2 \rho$
- $\sigma_{\alpha\beta} \approx -\left(1 - \frac{\Delta t}{2\tau}\right) \sum_i \mathbf{c}_{i\alpha} c_{i\beta} f_i^{\mathrm{neq}}(\mathbf{x}, t)$

where, ρ - density, $\rho\mathbf{V}$ - momentum, p - pressure and $\sigma_{\alpha\beta}$ - deviatoric stress tensor.

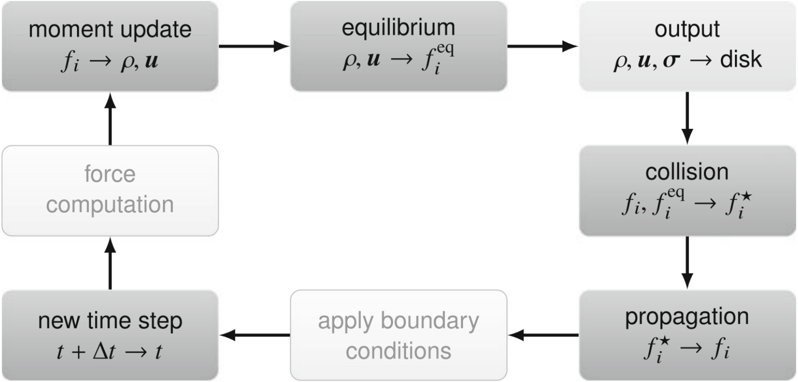
Lattice Boltzmann method

Relation between relaxation time τ and kinematic viscosity ν

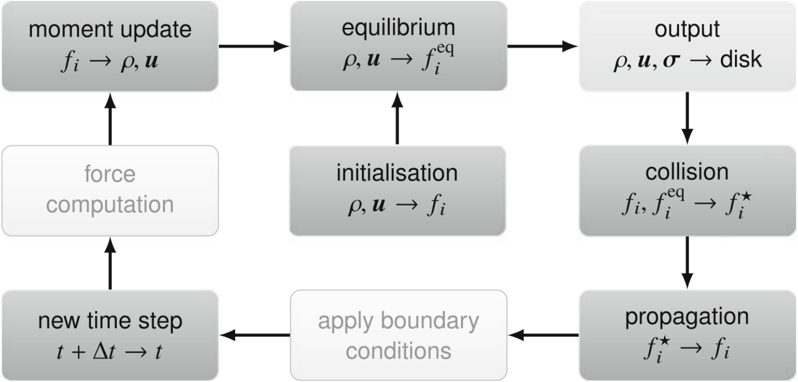
$$\nu = \left(\tau - \frac{\Delta t}{2}\right) c_s^2$$

The equation of ν should be always positive to hold its physical meaning. Stability region $\tau > \Delta t/2$. With this formulation the LBM is second order accurate in both time and space.

Lattice Boltzmann method



Lattice Boltzmann method



Lattice Boltzmann method - Initial Conditions

Assign

$$\rho_0 = \rho(\mathbf{x}, t = 0), \quad \mathbf{V}_0 = \mathbf{V}(\mathbf{x}, t = 0)$$

Calculate

$$f_i^{\mathrm{eq}} = f_i^{\mathrm{eq}}(\rho_0, \mathbf{V}_0)$$

$$f_i^{\mathrm{neq}} = f_i^{\mathrm{neq}}(\rho_0, \mathbf{V}_0)$$

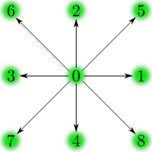
$$f_i^{\mathrm{neq}} \approx -w_i \frac{\tau \rho}{c_s^2} Q_{i\alpha\beta} \underbrace{\partial_\alpha V_{0_\beta}}_{\mathrm{FD}}$$

$$Q_{i\alpha\beta} = c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta} = \mathcal{H}^{(2)}_{i\alpha\beta}$$

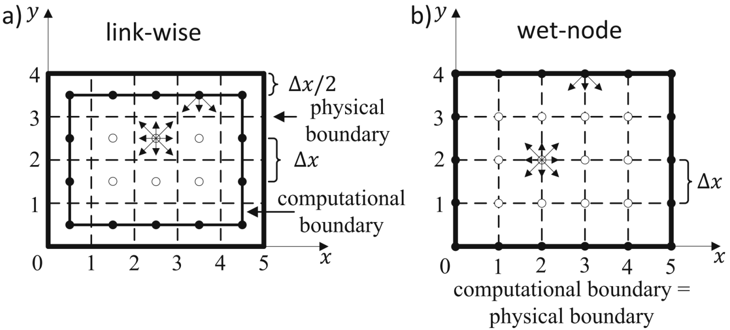
$$f_i = f_i^{\mathrm{eq}} + f_i^{\mathrm{neq}}$$

Now we can start with the *collision* step!

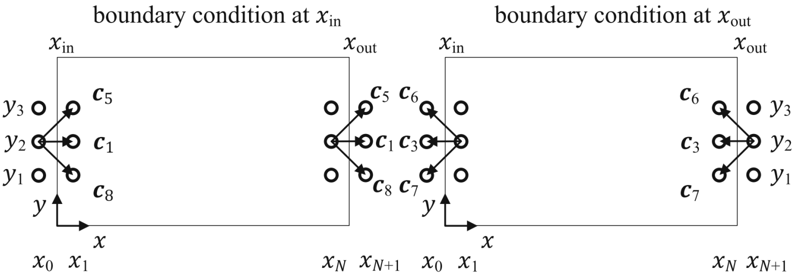
Lattice Boltzmann method - Boundary Conditions



[7]



Lattice Boltzmann method - Periodic BC

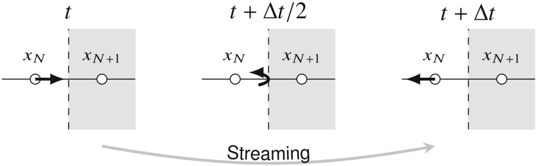


$$f^{\star}_{1,5,8}(\mathbf{x}_0) = f^{\star}_{1,5,8}(\mathbf{x}_N)$$

$$f^{\star}_{3,6,7}(\mathbf{x}_{N+1}) = f^{\star}_{3,6,7}(\mathbf{x}_1)$$

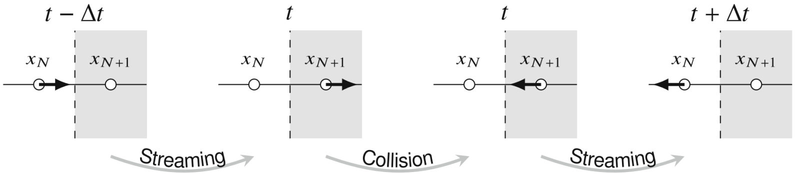
Lattice Boltzmann method - Wall BC

Case a: half-way bounce back



$$f_3(x_N, t + \Delta t) = f_1^\star(x_N, t)$$

Case b: full-way bounce back

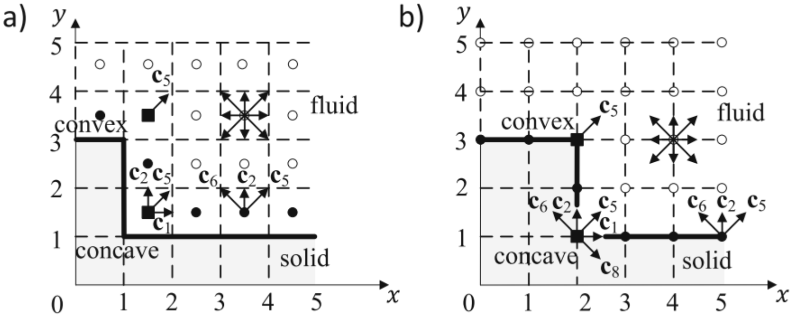


$$f_1(x_{N+1}, t) = f_1^\star(x_N, t - \Delta t)$$

$$f_3^\star(x_{N+1}, t) = f_1(x_{N+1}, t)$$

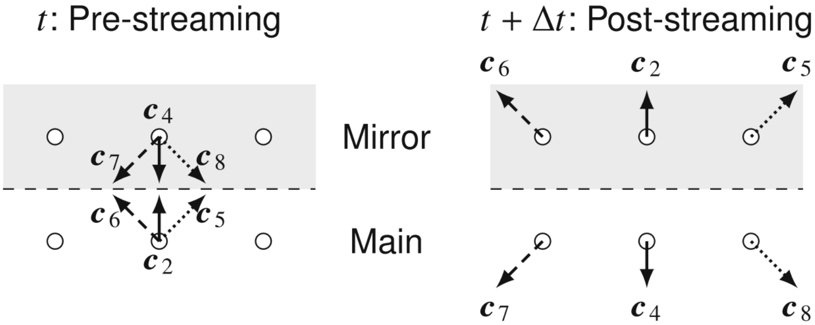
$$f_3(x_N, t + \Delta t) = f_3^\star(x_{N+1}, t)$$

Lattice Boltzmann method - Wall BC Corners



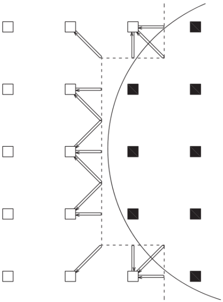
$$f_{6,2,5}(\mathbf{x}_b) = f^{\star}_{8,4,7}(\mathbf{x}_N)$$

Lattice Boltzmann method - Slip BC

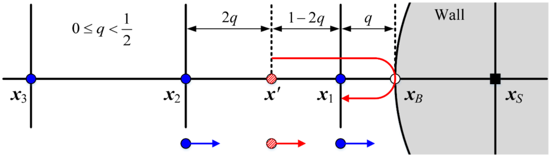


$$f_{6,2,5}(\mathbf{x}_b) = f^{\star}_{7,4,8}(\mathbf{x}_N)$$

Lattice Boltzmann method - Wall BC Curved

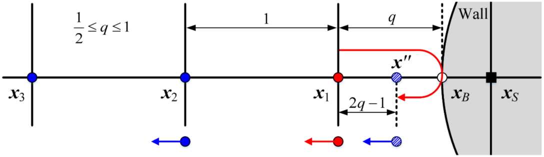


[8]



[9]

$$f_i(\mathbf{x}_1, t+\Delta t) = 2q f_i^\star(\mathbf{x}_1, t) + (1-2q) f_i^\star(\mathbf{x}_2, t)$$



[9]

1. Find the links.
2. Calculate q.
3. Interpolate.

$$f_i(\mathbf{x}_1, t+\Delta t) = \frac{1}{2q} f_i^\star(\mathbf{x}_1, t) + \left(1 - \frac{1}{2q}\right) f_i^\star(\mathbf{x}_1, t)$$

Lattice Boltzmann method - Force

Collision

$$f_i^{\star}(\mathbf{x}, t) = f_i(\mathbf{x}, t) + \frac{\Delta t}{\tau}\left[f_i^{\mathrm{eq}}(\mathbf{x}, t) - f_i(\mathbf{x}, t)\right] + \left(1 - \frac{\Delta t}{2\tau}\right) F_i \Delta t$$

Macroscopic quantities

$$\rho(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t) + 0.5\Delta t \sum_i F_i(\mathbf{x}, t)$$

$$\rho(\mathbf{x}, t)\mathbf{V}(\mathbf{x}, t) = \sum_i \mathbf{c}_i f_i(\mathbf{x}, t) + 0.5\Delta t \sum_i \mathbf{c}_i F_i(\mathbf{x}, t)$$

$$\sigma_{\alpha\beta} \approx -\left(1 - \frac{\Delta t}{2\tau}\right) \sum_i \mathbf{c}_{i\alpha} c_{i\beta} f_i^{\mathrm{neq}}(\mathbf{x}, t) - \frac{\Delta t}{2}\left(1 - \frac{\Delta t}{2\tau}\right)(F_\alpha V_\beta + V_\alpha F_\beta)$$

Lattice Boltzmann method - Unit Conversion

Conversion factor

$$C_l = \frac{l_{\mathrm{phy}}}{l_{\mathrm{lat}}}$$

where l is any unit we need to convert.

Lattice units

- $\Delta x_{\mathrm{lat}} = 1 \rightarrow C_\ell = \Delta x_{\mathrm{phy}}$
- $\Delta t_{\mathrm{lat}} = 1 \rightarrow C_t = \Delta t_{\mathrm{phy}}$
- $\rho_{\mathrm{lat}} = 1 \rightarrow C_\rho = \rho_{\mathrm{phy}}$

Relation between τ_{lat} and ν_{phy}

$[\nu] = m^2/s \rightarrow C_\nu = C_\ell^2/C_t = \Delta x_{\mathrm{phy}}^2/\Delta t_{\mathrm{phy}}$

$$\nu_{\mathrm{phy}} = \nu_{\mathrm{lat}} C_\nu = c_{s,\mathrm{lat}}^2(\tau_{\mathrm{lat}} - 0.5)\frac{\Delta x_{\mathrm{phy}}^2}{\Delta t_{\mathrm{phy}}}$$

Lattice Boltzmann method - Unit Conversion

Law of similarity

Flow systems are dynamically similar if they have the same Reynolds number, Mach number and geometry.

Definitions

- $\mathrm{Re} = \ell V / \nu$
- $\mathrm{Ma} = V / c_s$

Conversion factors

- $\mathrm{Ma}_{\mathrm{phy}} = \mathrm{Ma}_{\mathrm{lat}} \rightarrow V_{\mathrm{phy}} / V_{\mathrm{lat}} = c_{s,\mathrm{phy}} / c_{s,\mathrm{lat}} = C_V \rightarrow$ $\boxed{\Delta t_{\mathrm{phy}} = C_t = C_\ell / C_V = \Delta x_{\mathrm{phy}} c_{s,\mathrm{lat}} / c_{s,\mathrm{phy}}}$
- $\mathrm{Re}_{\mathrm{lat}} = \mathrm{Re}_{\mathrm{phy}} \rightarrow \ell_{\mathrm{lat}} / \ell_{\mathrm{phy}} V_{\mathrm{lat}} / V_{\mathrm{phy}} = \nu_{\mathrm{lat}} / \nu_{\mathrm{phy}} \rightarrow C_\ell C_V = C_\nu \rightarrow C_\nu = C_\ell^2 / C_t \rightarrow$ $\boxed{C_\nu = \Delta x_{\mathrm{phy}}^2 / \Delta t_{\mathrm{phy}}}$

Lattice Boltzmann method - Turbulence modeling

Eddy-viscosity model

$$\nu_{\mathrm{tot}} = \nu_{\mathrm{fluid}} + \nu_{\mathrm{turb}}$$

Smagorinsky model Smagorinsky 1963

$$\nu_{\mathrm{turb}} = (K\Delta x)^2 \sqrt{2 S_{\alpha\beta} S_{\alpha\beta}}$$

$$S_{\alpha\beta} = 0.5 \left(\frac{\partial V_\alpha}{\partial x_\beta} + \frac{\partial V_\beta}{\partial x_\alpha} \right)$$

In LBM, the strain rate tensor $S_{\alpha\beta}$ can be computed from non-equilibrium distribution:

$$S_{\alpha\beta} = -\frac{1}{2\rho\tau_{\mathrm{tot}} c_s^2} \sum_i \mathbf{c}_{i\alpha} c_{i\beta} f_i^{\mathrm{neq}}(\mathbf{x}, t)$$

DLR

Conclusions

- Flow chart of the Lattice Boltzmann Method.
- Stability region of τ.
- Proper initialization of f.
- Link-wise and Wet-node approach.
- Overview of BCs and corners' problem.
- Implementation of curved BCs.
- Introducing the force term into LBM.
- Unit conversion.
- Introduction to turbulence modeling.

Outline

1. Introduction
   - Mesoscopic Approach
   - 1D Heat Equation
2. Advantages and Disadvantages
3. Typical LBM applications
4. Lattice Boltzmann equation
5. Lattice Boltzmann method
6. Advanced collision operators
7. For Further Reading

Advanced collision operators - MRT

Multi Relaxation Time LBM (MRT-LBM)

$$\boxed{f_i^\star(\mathbf{x}, t) = f_i(\mathbf{x}, t) + \mathbf{MS}^{-1}\left[m_i^{\mathrm{eq}}(\mathbf{x}, t) - m_i(\mathbf{x}, t)\right]}$$

Collision

$$\Omega = \mathbf{M}^{-1}\mathbf{S}\left[\mathbf{m}^{\mathbf{eq}}(\mathbf{x}, t) - \mathbf{m}(\mathbf{x}, t)\right]$$

$$\mathbf{m} = \mathbf{Mf}$$

- $\mathbf{M}$ constructed via orthogonal basis d'Humières 2002.
- Other options available Coreixas, Chopard, and Latt 2019.
- Values of $\mathbf{M}, \mathbf{S}, \mathbf{m}^{\mathbf{eq}}$ available here d'Humières 2002; Suga et al. 2015; Tölke, Freudiger, and Krafczyk 2006.
- More stable than BGK.
- Infinite choices for the $\mathbf{S}$ values.

Advanced collision operators - HRR

Hybrid Recursive Regularized BGK (HRR-BGK)

$$\boxed{f_i^\star(\mathbf{x},t) = f_i^{\mathrm{eq}}(\mathbf{x},t) + (1-\omega) f_i^{\mathrm{neq}}(\mathbf{x},t)}$$

Hermite polynomials (HP) expansions

$$f_i^{\mathrm{eq}}(\mathbf{x},t) = w_i \sum_{n=0}^{N} \frac{1}{n!} \mathbf{a}_0^{(n)} : \boldsymbol{\mathcal{H}}_i^{(n)}$$

$$f_i^{\mathrm{neq}}(\mathbf{x},t) = w_i \sum_{n=2}^{N} \frac{1}{n!} \mathbf{a}_1^{(n)} : \boldsymbol{\mathcal{H}}_i^{(n)}$$

- The $\boldsymbol{\mathcal{H}}_i^{(n)}$ and the expression for $\mathbf{a}_0^{(n)}, \mathbf{a}_1^{(n)}$ are given in Feng et al. 2019.

Advanced collision operators - HRR

HP second order coefficients blending

$$\mathbf{a}_1^{(2,\mathrm{HRR})} = \sigma \mathbf{a}_1^{(2)} + (1-\sigma)\mathbf{a}_1^{(2,\mathrm{PRR})}$$

$$a_{1,\alpha\beta}^{(2)} = \sum_{i=0}^{q-1} c_{i,\alpha} c_{i,\beta} f_i^{\mathrm{neq}}$$

$$a_{1,\alpha\beta}^{(2),\mathrm{PRR}} = -\rho c_s^2 \tau \left(\frac{\partial V_\beta}{\partial x_\alpha} + \frac{\partial V_\alpha}{\partial x_\beta} \right)$$

- $\mathbf{a}_1^{(2),\mathrm{PRR}}$ evaluated via finite-difference $\rightarrow$ increases stability of the scheme.
- Higher order HP coefficients ($n > 2$) are computed recursively Malaspinas 2015 using the equilibrium coefficients $\mathbf{a}_0^{(n)}$.
- Regularization can be expressed as an MRT model with a Hermite vector product basis, where the non-hydrodynamic moments are relaxed to their equilibrium value.

Advanced collision operators - Cumulant

- Derived to overcome drawbacks of MRT Geier et al. 2015.
- Formulation based on statistically independent observable quantities of the distribution functions, the cumulants $c_{\alpha\beta\gamma}$.
- We work in the wave number space $\boldsymbol{\Xi}$, rather than velocity space $\boldsymbol{\xi}$.

Two-sided Laplace transformation of f

$$F(\boldsymbol{\Xi}) = \mathcal{L}[f(\boldsymbol{\xi})] = \int_{-\infty}^{\infty} f(\boldsymbol{\xi}) \exp(-\boldsymbol{\Xi} \cdot \boldsymbol{\xi}) \,\mathrm{d}\boldsymbol{\xi}$$

Cumulant expression

$$c_{\alpha\beta\gamma} = c^{-\alpha-\beta-\gamma} \frac{\partial^\alpha \partial^\beta \partial^\gamma}{\partial \Xi^\alpha \partial \Upsilon^\beta \partial Z^\gamma} \ln [F(\Xi, \Upsilon, Z)] \Big|_{\Xi=\Upsilon=Z=0}$$

Advanced collision operators - Cumulant

Collision

$$c^{\star}_{\alpha\beta\gamma} = \omega_{\alpha\beta\gamma} c^{\mathrm{eq}}_{\alpha\beta\gamma} + (1 - \omega_{\alpha\beta\gamma}) c_{\alpha\beta\gamma}$$

- 27 different cumulants $c_{\alpha\beta\gamma}$.
- Different collision frequency $\omega_{\alpha\beta\gamma}$ for each cumulant.
- By rotational invariance considerations, the number of independent collision frequencies is reduced to 10.

Conclusions

- Introduced the MRT scheme.
- Introduced the HRR-BGK scheme.
- Introduced the Cumulant scheme.

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7. For Further Reading

For Further Reading

- Coreixas, Christophe, Bastien Chopard, and Jonas Latt (2019). "Comprehensive comparison of collision models in the lattice Boltzmann framework: Theoretical investigations". In: *Physical Review E* 100.3.
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Vielen Dank für Ihre Aufmerksamkeit! Haben Sie Fragen?

[15]

URLs for pictures

1. http://www.mappedplanet.com/karten/214/1.png
2. https://i0.wp.com/www.tecnocarreteras.es/wp-content/uploads/sites/2/2015/04/1672-como-y-por-que-usar-simuladores-de-trafico-para-optimizar-la-gestion-del-mismo.jpg?w=660&ssl=1
3. https://i.ytimg.com/vi/JJfknCScENs/maxresdefault.jpg
4. https://www.researchgate.net/profile/Andrew-Tembo/publication/331330381_Hierarchical_analysis_of_the_influencing_factors_on_the_variation_of_PAHs_in_RDS/links/5c7442709285lc69504133b8/Hierarchical-analysis-of-the-influencing-factors-on-the-variation-of-PAHs-in-RDS.pdf?origin=publication_detail
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