Application of the Cascaded Lattice Boltzmann Method with interpolated boundary conditions to heat transfer problems

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Introduction

Goal

Simulate an incompressible flow coupled with heat transfer problem.

The continuity and momentum equations are:

$$\begin{cases} \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \\ \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \left(\mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^\top] \right) + \mathbf{F} \end{cases}$$

The Enthalpy balance equation is:

$$\frac{\partial}{\partial t}(\rho c_p T) + \nabla \cdot (\mathrm{u} \rho c_p T) = \nabla \cdot (k \nabla T) + \dot{q}$$

Lattice Boltzmann Method

Probability of finding a particle in the phase space:

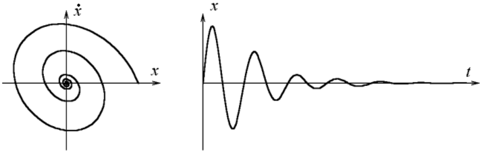

Figure 1: $\Psi = \Psi(t, \mathrm{x}, \dot{\mathrm{x}})$

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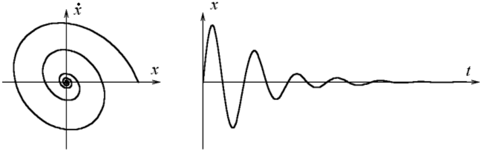

Figure 1: $\Psi = \Psi(t, \mathrm{x}, \dot{\mathrm{x}})$

In an infinitesimally small volume of the phase space $d\mathrm{x}d\mathrm{u}$:

$$\Psi_{no\ collisions}(t + dt, \mathrm{x} + d\mathrm{x}, \mathrm{u} + d\mathrm{u})d\mathrm{x}d\mathrm{u} = \Psi_{no\ collisions}(t, \mathrm{x}, \mathrm{u})d\mathrm{x}d\mathrm{u}$$

Probability of finding a particle in the phase space:

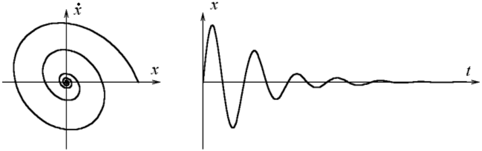

Figure 1: $\Psi = \Psi(t, \mathbf{x}, \dot{\mathbf{x}})$

In an infinitesimally small volume of the phase space $d\mathbf{x}d\mathbf{u}$:

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Now, include the collision term $\mathbb{C}(\Psi)$:

$$\Psi(t + dt, \mathbf{x} + d\mathbf{x}, \mathbf{u} + d\mathbf{u})d\mathbf{x}d\mathbf{u} = \Psi(t, \mathbf{x}, \mathbf{u})d\mathbf{x}d\mathbf{u} + \mathbb{C}(\Psi)d\mathbf{x}d\mathbf{u}dt$$

Taylor series expansion:

$$\Psi(t+dt, \mathsf{x}+d\mathsf{x}, \mathsf{u}+d\mathsf{u}) = \Psi(t, \mathsf{x}, \mathsf{u}) + \frac{\partial \Psi}{\partial t} dt + \nabla_{\mathsf{x}} \Psi d\mathsf{x} + \nabla_{\mathsf{u}} \Psi d\mathsf{u}$$

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Plug in:

$$\left[\Psi(t, \mathsf{x}, \mathsf{u}) + \frac{\partial \Psi}{\partial t} dt + \nabla_{\mathsf{x}} \Psi d\mathsf{x} + \nabla_{\mathsf{u}} \Psi d\mathsf{u}\right] d\mathsf{x} d\mathsf{u} = \left[\Psi(t, \mathsf{x}, \mathsf{u}) + \mathbb{C}(\Psi) dt\right] d\mathsf{x} d\mathsf{u}$$

Taylor series expansion:

$$\Psi(t+dt, \mathbf{x}+d\mathbf{x}, \mathbf{u}+d\mathbf{u}) = \Psi(t, \mathbf{x}, \mathbf{u}) + \frac{\partial \Psi}{\partial t}dt + \nabla_{\mathbf{x}}\Psi d\mathbf{x} + \nabla_{\mathbf{u}}\Psi d\mathbf{u}$$

Plug in:

$$\left[\Psi(t, \mathbf{x}, \mathbf{u}) + \frac{\partial \Psi}{\partial t}dt + \nabla_{\mathbf{x}}\Psi d\mathbf{x} + \nabla_{\mathbf{u}}\Psi d\mathbf{u}\right] d\mathbf{x}d\mathbf{u} = \left[\Psi(t, \mathbf{x}, \mathbf{u}) + \mathbb{C}(\Psi)dt\right]d\mathbf{x}d\mathbf{u}$$

Reformulate velocity $\mathbf{u} = \frac{d\mathbf{x}}{dt}$ and acceleration $\frac{d\mathbf{u}}{dt} = \frac{\mathbf{F}}{\rho}$:

$$\frac{\partial \Psi}{\partial t} + (\mathbf{u} \cdot \nabla_{\mathbf{x}})\Psi + (\frac{\mathbf{F}}{\rho} \cdot \nabla_{\mathbf{u}})\Psi = \mathbb{C}(\Psi)$$

Streaming and Collision:

$$\underbrace{\Psi(t+dt, \mathbf{x}+d\mathbf{x}, \mathbf{u}+d\mathbf{u})d\mathbf{x}d\mathbf{u}}_{\textit{Streaming}} = \underbrace{\Psi(t, \mathbf{x}, \mathbf{u})d\mathbf{x}d\mathbf{u} + \mathbb{C}(\Psi)d\mathbf{x}d\mathbf{u}dt}_{\textit{Collision}}$$

The Boltzmann equation can be viewed as a substantial derivative (of an intensive quantity Ψ) which is equal to the collision term $\mathbb{C}$ applied to the distribution function of Ψ:

$$\frac{\partial \Psi}{\partial t} + (\mathbf{u} \cdot \nabla_{\mathbf{x}})\Psi + (\frac{\mathbf{F}}{\rho} \cdot \nabla_{\mathbf{u}})\Psi = \mathbb{C}(\Psi)$$

$$\underbrace{f_i(\mathrm{x} + \mathrm{e_i}\Delta \mathrm{x}, t + \Delta t)}_{\textit{Streaming}} = \underbrace{f_i(\mathrm{x}, t) - \frac{1}{\tau}(f_i - f_i^{eq}) + F_i(\mathrm{x}, t)}_{\textit{Collision}}$$

- $\tau = \tau(\nu)$ relaxation parameter, ν is the kinematic viscosity
- f_i - discrete probability distribution function
- F_i - source term (ex. gravity force)

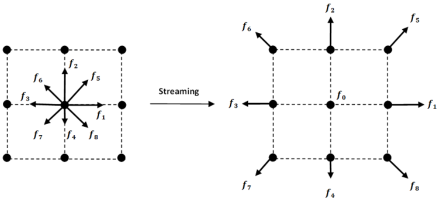

Figure 2: D2Q9: Streaming

Algorithm: Fluid

1 Initialize f_i^{in}

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2 Compute

$\rho = \sum_{i=0}^{8} f_i^{in}(\mathrm{x}, t)$ *and* $\mathrm{u}(\mathrm{x}, t) = \frac{1}{\rho}\sum_{i=0}^{8} f_i^{in}(\mathrm{x}, t)\mathrm{e}_i + \frac{\mathbf{F}}{2\rho}\delta t$

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3 Compute $f_i^{eq}(\mathrm{x}, t) = w_i \rho \left[1 + \frac{\mathrm{e}_i \mathrm{u}}{c_s^2 e^2} + \frac{(\mathrm{e}_i \mathrm{u})^2}{2 c_s^4 e^4} - \frac{\mathrm{u}^2}{2 c_s^2 e^2} \right]$ where $c_s^2 = \frac{1}{3}$

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4 Collision $f_i^{out}(\mathbf{x}, t) = f_i^{in}(\mathbf{x}, t) - \frac{1}{\tau_f}\left[f_i^{in}(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)\right] + F_i(\mathbf{x}, t)$

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5 Streaming $f_i^{in}(\mathrm{x} + \mathrm{e}_i, t + 1) = f_i^{out}(\mathrm{x}, t)$

Heat Transfer in LBM

Macroscopic variables can be recovered from the moments of DF:

$$\textit{mass density:} \quad \rho = \int f(\mathrm{x}, \boldsymbol{\xi}, t, T) d^3\xi$$

$$\textit{momentum density:} \quad \rho \mathrm{u} = \int \boldsymbol{\xi} f(\mathrm{x}, \boldsymbol{\xi}, t, T) d^3\xi$$

$$\textit{internal energy density:} \quad \rho i = \frac{1}{2} \int |\boldsymbol{\xi} - \mathrm{u}|^2 f(\mathrm{x}, \boldsymbol{\xi}, t, T) d^3\xi$$

Why not extract the temperature from the internal energy as $i = c_v T$?

Macroscopic variables

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Why <u>not</u> extract the temperature from the internal energy as $i = c_v T$?

Such approach together with the SRT collision operator would lead to the *fixed Prandl Number problem*, because thermal conductivity can not be tuned independently of kinematic viscosity.

Fixed Prandl Number problem

The are three approaches to solve the issue:

1. Multi Relaxation Time + Multispeed LBM (there are not enough moments on standard lattices).
2. Introduce new distribution function, which can evolve in its own way, responsible for the energy field.
3. Use LBM for hydrodynamic coupled with another solver (e.g. finite difference) for temperature field.

Algorithm: Energy Field

'Advection - Diffusion' of H is solved on a separate D2Q9 lattice

1 Initialize $h_i^{in}(\mathrm{x}, t)$

2 Compute $H = \sum_{i=0}^{9} h_i^{in}(\mathrm{x}, t)$

3 Compute $h_i^{eq}(\mathrm{x}, t) = Hw_i \left[1 + \frac{\mathrm{e}_i \mathrm{u}}{c_s^2 e^2} + \frac{(\mathrm{e}_i \mathrm{u})^2}{2c_s^2 e^4} - \frac{\mathrm{u}^2}{2c_s^2 e^2}\right]$

4 Collision $h_i^{out}(\mathrm{x}, t) = h_i^{in}(\mathrm{x}, t) - \frac{1}{\tau_T}\left[h_i^{in}(\mathrm{x}, t) - h_i^{eq}(\mathrm{x}, t)\right] + \frac{\dot{q}}{\rho c_p}$

5 Streaming $h_i^{in}(\mathrm{x} + \mathrm{e}_i, t + 1) = h_i^{out}(\mathrm{x}, t)$

Now, the temperature field can be solved in a fluid:

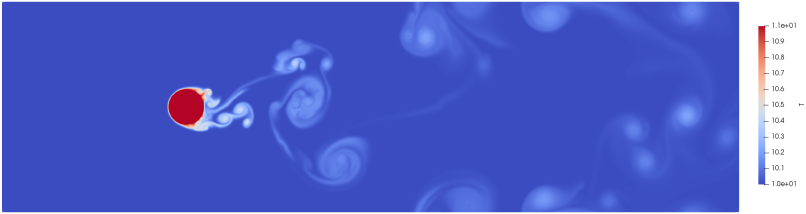

Figure 3: Re = 1000, Pr = 0.71, D = 128 [lu]

Physically, equations are coupled:

- Energy Eq. $\rightarrow$ NS: equation of state $f(p, \rho, T) = 0$.
  Usually, ideal gas $p(\rho, T) = \rho RT = \rho c_s^2$ is assumed for single phase LBM models.
- NS $\rightarrow$ Energy Eq.: kinetic energy + dissipation (viscous heating) and compression work.

(De)Coupling of N-S and Energy equations

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- NS $\rightarrow$ Energy Eq.: kinetic energy + dissipation (viscous heating) and compression work.

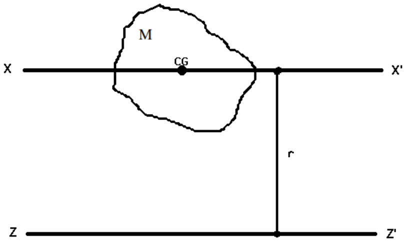
In simplified models, the NS equation is decoupled from energy eq.
The equation of state has a constant temperature
$p(\rho, T) = \rho c_s^2 = \rho RT_0$ and the sound speed is fixed as $c_s = \sqrt{RT_0}$.
As a result, these models are incompressible.
To account for thermal advection the Boussinesq approximation can be employed,

$$\rho(T) \approx \rho_0(1 - \alpha_V(T - T_0)),$$

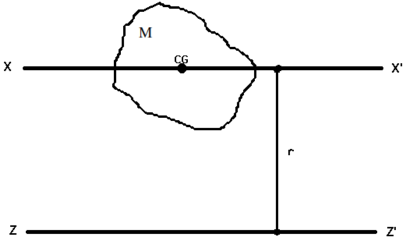
$$F_{bouyancy} = [\rho(T) - \rho_0]g = -g\rho_0\alpha_V(T - T_0).$$

Theory - deeper dive

(Central) Moments


M
CG
X
X'
r
Z
Z'

'Statistical' refreshment



$$
\begin{aligned}
m_0 &= M = \int r^0 \rho(r) d\Omega \\
m_1 &= \mu = \frac{1}{M} \int r^1 \rho(r) d\Omega \\
m_2 &= I_{zz'} = \int r^2 \rho(r) d\Omega \\
\sigma^2 &= I_{xx'} \int (r-\mu)^2 \rho(r) d\Omega
\end{aligned}
$$

Moments

The raw moments and central moments:

$$\kappa_{mn} = \sum_i (e_{i,x})^m (e_{i,y})^n f_i$$

$$\tilde{\kappa}_{mn} = \sum_i (e_{i,x} - u_x)^m (e_{i,y} - u_y)^n f_i$$

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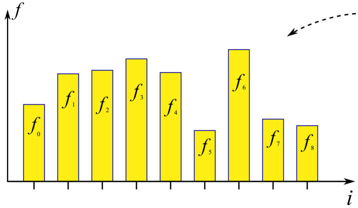
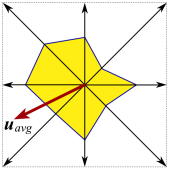
Physical interpretation:

$$\rho = \kappa_{00} = \sum_i f_i$$

$$\rho \mathbf{u} = [u_x, u_y]^\top = [\kappa_{10}, \kappa_{01}]^\top = \sum_i f_i \mathbf{e}_i + \frac{\mathbf{F}}{2}\delta t$$





Alternatively, moments can be expressed in terms of matrix transformations:

$$\boldsymbol{\Upsilon} = \mathbb{M}\mathsf{f}$$
$$\tilde{\boldsymbol{\Upsilon}} = \mathbb{N}\boldsymbol{\Upsilon}$$

The resulting order of central moments is:

$$\tilde{\boldsymbol{\Upsilon}} = [\tilde{\kappa}_{00}, \tilde{\kappa}_{10}, \tilde{\kappa}_{01}, \tilde{\kappa}_{20}, \tilde{\kappa}_{02}, \tilde{\kappa}_{11}, \tilde{\kappa}_{21}, \tilde{\kappa}_{12}, \tilde{\kappa}_{22}]^\top$$

The Maxwell-Boltzmann equilibrium distribution function in a continuous velocity space is known as:

$$\Psi^{M\text{-}B,\,eq} = \Psi^{M\text{-}B,\,eq}(\phi, \boldsymbol{\xi}, \mathrm{u}) = \frac{\phi}{(2\pi c_s^2)^{D/2}} exp\left[-\frac{(\boldsymbol{\xi} - \mathrm{u})^2}{2c_s^2}\right]$$

where:

ϕ	–	quantity of interest
$\boldsymbol{\xi}$	–	microscopic ‘particle‘ velocity
u	–	macroscopic ‘flow‘ velocity

The continuous definition of the central moments is:

$$\tilde{\kappa}_{mn} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(\xi_x - u_x)^m(\xi_y - u_y)^n\Psi(\phi, \boldsymbol{\xi}, \mathrm{u})d\xi_x d\xi_y$$

Algorithm fluid - revisited

1 Initialize f_i^{in}

2 Compute $\mathbf{u} = [u_x, u_y]^\top = [\kappa_{10}, \kappa_{01}]^\top = \frac{1}{\rho}\sum_i f_i \mathbf{e}_i + \frac{\mathbf{F}}{2\rho}\delta t$

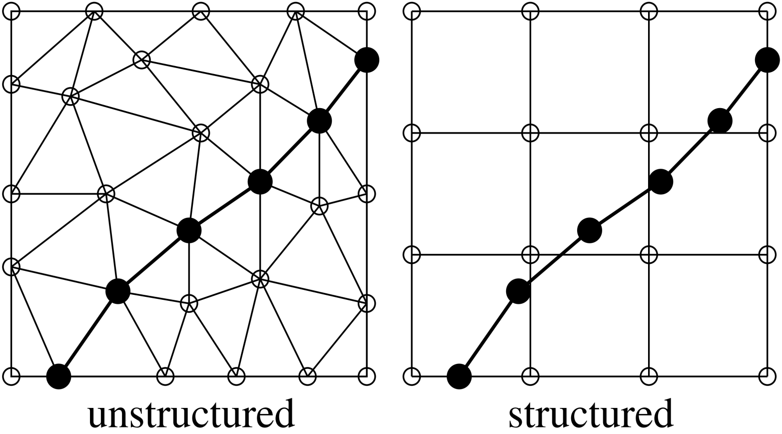
3 Compute
$\tilde{\boldsymbol{\Upsilon}}(\mathrm{x}, t) = \mathbb{N}\mathbb{M}\mathbf{f}(\mathrm{x}, t)$,
$\tilde{\boldsymbol{\Upsilon}}^{eq} = [\rho, 0, 0, c_s^2\rho, c_s^2\rho, 0, 0, 0, c_s^4\rho]^\top$
$\tilde{\mathrm{F}} = [0, F_x/\rho, F_y/\rho, 0, 0, 0, c_s^2 F_y/\rho, c_s^2 F_x/\rho, 0]^\top$

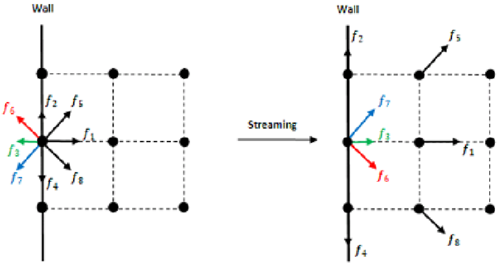
4 Collision $\tilde{\boldsymbol{\Upsilon}}(\mathbf{x}, t + \delta t) = \tilde{\boldsymbol{\Upsilon}} - \mathbb{S}(\tilde{\boldsymbol{\Upsilon}} - \tilde{\boldsymbol{\Upsilon}}^{eq}) + (\mathbb{1} - \mathbb{S}/2)\tilde{\mathbf{F}}$

5 Streaming $f_i(\mathbf{x} + \mathbf{e}\delta t, t + \delta t) = \mathbb{M}^{-1}\mathbb{N}^{-1}\tilde{\boldsymbol{\Upsilon}}_i(\mathbf{x}, t + \delta t)$

(Un)structured Mesh

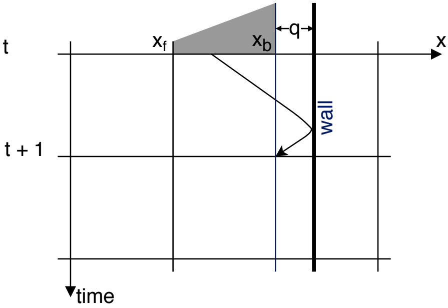
(Un)structured Mesh?





$$f_{\bar{i}}(x_b, t + \Delta t) = f_i(x_b, t)$$

It is assumed that during each streaming step, the population travels a distance $|e_i|\Delta t$.



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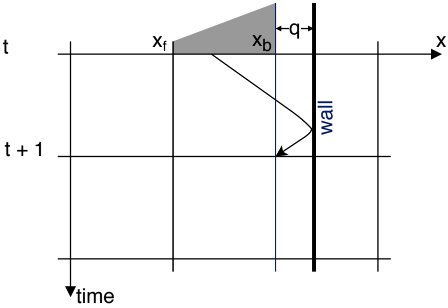
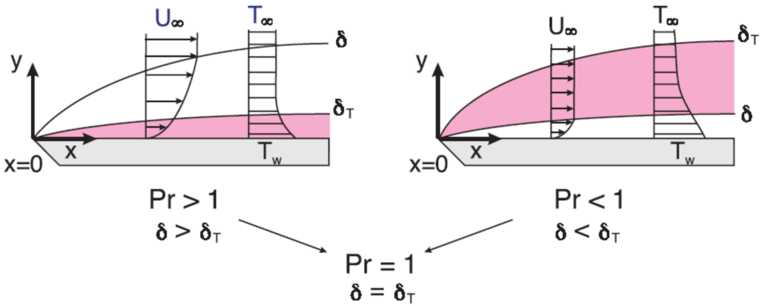


$$f_{\bar{i}}(x_b, t+\Delta t) = \begin{cases} 2q f_i^*(x_b, t) + (1-2q) f_i^*(x_f, t) & \text{for } q \in [0, 0.5] \\ \frac{1}{2q} f_i^*(x_b, t) + \frac{2q-1}{2q} f_{\bar{i}}^*(x_b, t) & \text{for } q \in (0.5, 1], \end{cases}$$

$$Nu = \frac{h\Delta T}{k(\Delta T/D)} = \frac{hD}{k} \sim \frac{\text{convective heat transfer}}{\text{conductive heat transfer}}$$

$$Pr = \frac{\nu}{\alpha} = \frac{\nu\rho c_p}{k} \sim \frac{\text{molecular diffusivity of momentum}}{\text{molecular diffusivity of heat}}$$



Scenarios

Case-ID	Lattice Size	Velocity set	Blockage Ratio	D	U	Pr	Re	ν	k
$\mathrm{Pr10}_{small}$	1000x150x3	D3Q27Q27	1/5	30	0.01	10	10	3E-02	3E-03
$\mathrm{Pr10}_{medium}$	2000x300x3	D3Q27Q27	1/5	60	0.005	10	10	3E-02	3E-03
$\mathrm{Pr10}_{large}$	4000x600x3	D3Q27Q27	1/5	120	0.0025	10	10	3E-02	3E-03
$\mathrm{Pr100}_{small}$	1000x150x3	D3Q27Q27	1/5	30	0.01	100	10	3E-02	3E-04
$\mathrm{Pr100}_{medium}$	2000x300x3	D3Q27Q27	1/5	60	0.005	100	10	3E-02	3E-04
$\mathrm{Pr100}_{large}$	4000x600x3	D3Q27Q27	1/5	120	0.0025	100	10	3E-02	3E-04
$\mathrm{Pr1000}_{small}$	1000x150x3	D3Q27Q27	1/5	30	0.01	1000	10	3E-02	3E-05
$\mathrm{Pr1000}_{medium}$	2000x300x3	D3Q27Q27	1/5	60	0.005	1000	10	3E-02	3E-05
$\mathrm{Pr1000}_{large}$	4000x600x3	D3Q27Q27	1/5	120	0.0025	1000	10	3E-02	3E-05

Table 1: Case-ID: lookup table

Case-ID	$Nu^{1st\ order\ bc}_{CM\ HIGHER}$	$Nu^{2nd\ order\ bc}_{CM\ HIGHER}$	$Nu^{1st\ order\ bc}_{Cumulants}$	$Nu^{2nd\ order\ bc}_{Cumulants}$	Nu_{FEM}
$Pr10_{small}$	4.91	4.81	5.04	4.83	4.82
$Pr10_{medium}$	4.86	4.81	4.92	4.82	4.82
$Pr10_{large}$	4.83	4.81	4.87	4.81	4.82
$Pr100_{small}$	10.66	10.27	14.50	11.52	10.1
$Pr100_{medium}$	10.32	10.13	11.82	10.36	10.1
$Pr100_{large}$	10.19	10.08	10.83	10.13	10.1
$Pr1000_{small}$	27.09	24.58	94.31	58.33	21.43
$Pr1000_{medium}$	22.73	21.84	53.97	34.19	21.43
$Pr1000_{large}$	21.84	21.37	34.04	24.56	21.43

Table 2: Influence of kernel and BC on Nu number.
1st order bc = BB (hydrodynamics) + EQ (thermodynamics)
2nd order bc = IBB (hydrodynamics) + IABB (thermodynamics)

Memory requirements

	No [-]	[double]	[Bytes]
DF	2x27	54	432
DF temp	2x27	54	432
q	2x27	13.5	108
flag	1	0.5	4
memory per node		122	976

Table 3: Theoretical memory requirements for:
3D, DDF model with interpolated BC

Memory requirements

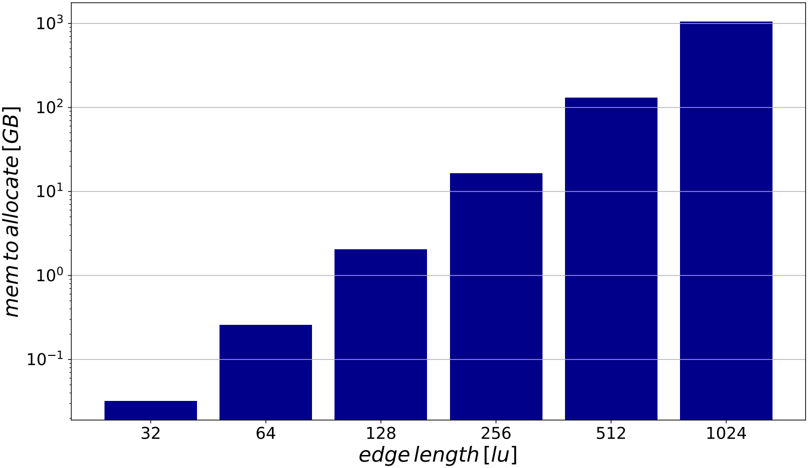


Figure 4: Theoretical memory requirements for:
3D, DDF model with interpolated BC

Q: Does the high memory requirement limits applicability of LBM?

Memory requirements

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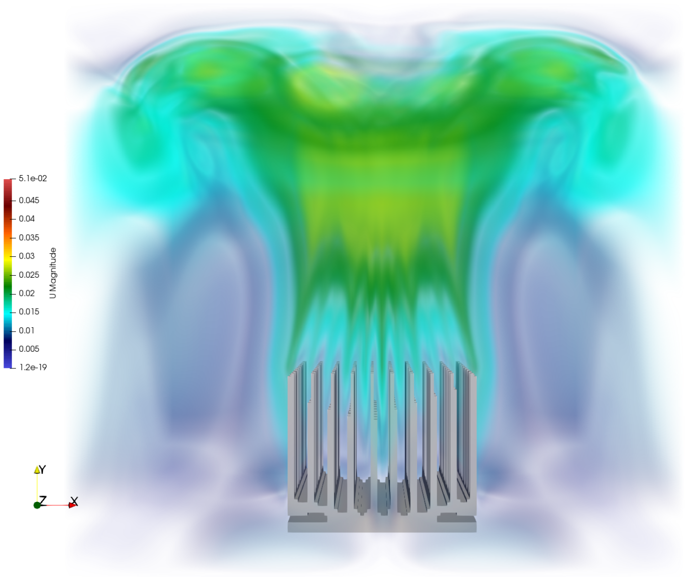
Not necassary. Similar problems occur in other CFD methods like VOF, FEM, FD. The common solutions are:

1. Mesh refinement.
2. Chimera (overlapping) mesh.

Questions?



5.1e-02
0.045
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
1.2e-19
U Magnitude
Y
Z
X