Application of thermal Cascaded Lattice Boltzmann Method to 3D simulations in a high Prandtl number regime

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Introduction

In this contribution, a 3D thermal Cascaded Lattice Boltzmann Method is presented. Improvements to the LB collision kernel for both thermal and hydrodynamics field is introduced, by transforming the operations into the central moment space. The relaxation of central moments is defined in a reference frame moving with the fluid. Moreover, the moments of equilibria are calculated from continuous Maxwell-Boltzmann distribution, thus do not suffer from truncation error. As a consequence, CLBM enhances Galilean invariance, accuracy and stability of the method.
The Prandtl number (Pr), is defined as a ratio of molecular diffusivity of momentum to the molecular diffusivity of heat. For common fluids (e.g. oil), the Pr is usually high, which means that heat diffuses much slower than the momentum and the thermal boundary layer is contained within the velocity boundary layer. To reduce the computational overhead, a D3Q7 lattice is commonly used as it is enough to handle first-order moments of the discrete Boltzmann equation to recover the macroscopic advection-diffusion equation, which describes the temperature field. Unfortunately, in a high Pr regime, the low value of numerical conductivity leads to numerical artefacts known as a 'wiggles'. A natural remedy is to apply a lattice with a larger number of discrete velocities like D3Q27. It has been found, that to benefit from the usage of such a lattice, the commonly used cascaded relaxation scheme for advection-diffusion like equations needs to be modified to account for the higher-order moments of the thermal field. To demonstrate the accuracy of the proposed collision kernel, a mesh dependence study of steady forced convection from a confined cylinder is performed for different values of Pr number and compared against high-quality FEM solution.

Heat Transfer in LBM

Fixed Prandl Number problem
Macroscopic variables can be recovered from the moments of DF:

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

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

Such an approach together with the SRT collision operator would lead to the *fixed Prandtl Number problem* because thermal conductivity can not be tuned independently of kinematic viscosity.
There are three approaches to solve the issue:

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

(De)Coupling of N-S and Energy equations

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.

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,

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

Governing Equations

Simulate an incompressible flow coupled with heat transfer problem.

Hydrodynamics
The continuity and momentum equations are,

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

Energy-field
The Enthalpy balance equation is:

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

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

Lattice Boltzmann Method - Algorithm

The raw moments and central moments are defined as,

$$\Upsilon_{mn} = \sum_\alpha (e_{\alpha x})^m (e_{\alpha y})^n f_\alpha$$
$$\tilde{\Upsilon}_{mn} = \sum_\alpha (e_{\alpha x} - u_x)^m (e_{\alpha y} - u_y)^n f_\alpha$$

Density and velocity are interpreted as zeroth and first moment respectively,

$$\rho = \Upsilon_{00} = \sum_\alpha f_\alpha,$$
$$\rho\mathbf{u} = [u_x, u_y]^\top = [\Upsilon_{10}, \Upsilon_{01}]^\top = \sum_\alpha f_\alpha \mathbf{e}_\alpha + \frac{\mathbf{F}}{2}\delta t.$$

Hydrodynamics
1 Initialize $\boldsymbol{f}(\mathbf{x}, t)$,

2 Compute $\rho\mathbf{u} = [u_x, u_y]^\top = [k_{10}, k_{01}]^\top = \sum_\alpha f_\alpha \mathbf{e}_\alpha + \frac{\mathbf{F}}{2}\delta t$,

3 Compute
$\tilde{\boldsymbol{\Upsilon}}(\boldsymbol{x}, t) = \mathbb{N}\mathbb{M}\mathbf{f}(\boldsymbol{x}, t)$, $\tilde{\boldsymbol{\Upsilon}}^{eq}(\boldsymbol{x}, t) = \ldots$, $\tilde{\mathbf{F}}(\boldsymbol{x}, t) = \ldots$,

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

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

Energy-field
1 Initialize $\boldsymbol{h}(\mathbf{x}, t)$,

2 Compute $H = \sum_\alpha h_\alpha(\boldsymbol{x}, t)$

3 Compute
$\tilde{\boldsymbol{\Upsilon}}^H(\boldsymbol{x}, t) = \mathbb{N}\mathbb{M}\mathbf{h}(\boldsymbol{x}, t)$, $\tilde{\boldsymbol{\Upsilon}}^{H,eq}(\boldsymbol{x}, t) = \ldots$

4 Collision
$\tilde{\boldsymbol{\Upsilon}}^{H,*}(\mathbf{x}, t) = (\mathbb{1} - \mathbb{S}^H)\tilde{\boldsymbol{\Upsilon}}^H + \mathbb{S}^H\tilde{\boldsymbol{\Upsilon}}^{H,eq}$

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

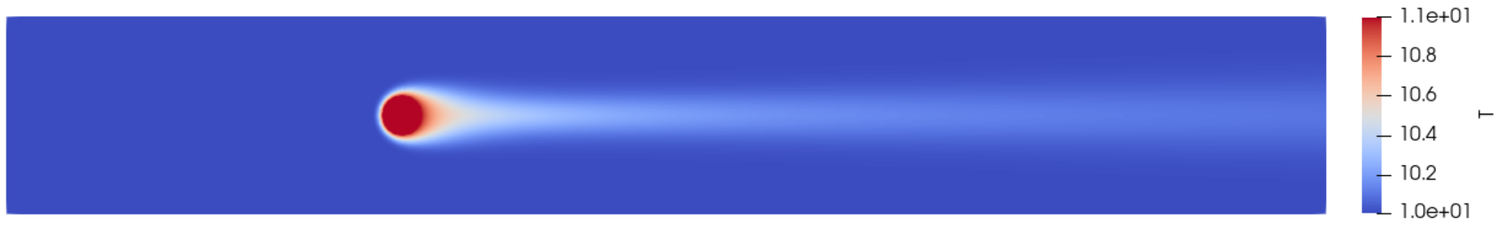

Figure 1: Flow over a hot cylinder: Re=10 Pr=10 D=120

Benchmark

To validate the properties of the proposed LBM model, a flow around a hot cylinder (see **??**) has been simulated with different collision kernels and compared against FEM reference result.

Case-ID	$Nu^{1st\ order\ bc}_{CM}$	$Nu^{2nd\ order\ bc}_{CM}$	$Nu^{1st\ order\ bc}_{CM\ SRT}$	$Nu^{2nd\ order\ bc}_{CM\ SRT}$	$Nu^{1st\ order\ bc}_{CM\ TRT}$	$Nu^{2nd\ order\ bc}_{CM\ TRT}$	Nu_{FEM}
$Pr10_{small}$	5.26	4.91	4.94	4.81	4.91	4.81	4.82
$Pr10_{medium}$	5.03	4.84	4.87	4.81	4.86	4.81	4.82
$Pr10_{large}$	4.92	4.83	4.84	4.81	4.83	4.81	4.82
$Pr100_{small}$	20.68	14.75	10.64	10.20	10.66	10.27	10.10
$Pr100_{medium}$	15.87	11.84	10.33	10.11	10.32	10.13	10.10
$Pr100_{large}$	12.96	10.64	10.20	10.09	10.19	10.08	10.10
$Pr1000_{small}$	166.42	102.27	-135.45	-138.08	27.09	24.58	21.43
$Pr1000_{medium}$	111.76	62.52	22.75	21.78	22.73	21.84	21.43
$Pr1000_{large}$	74.00	40.47	21.87	21.38	21.84	21.37	21.43

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

Case-ID	Lattice Size	Velocity set	Blockage Ratio	D	U	Pr	Re	ν	k
$Pr10_{small}$	1000x150x3	D3Q27Q27	1/5	30	0.01	10	10	3E-02	3E-03
$Pr10_{medium}$	2000x300x3	D3Q27Q27	1/5	60	0.005	10	10	3E-02	3E-03
$Pr10_{large}$	4000x600x3	D3Q27Q27	1/5	120	0.0025	10	10	3E-02	3E-03
$Pr100_{small}$	1000x150x3	D3Q27Q27	1/5	30	0.01	100	10	3E-02	3E-04
$Pr100_{medium}$	2000x300x3	D3Q27Q27	1/5	60	0.005	100	10	3E-02	3E-04
$Pr100_{large}$	4000x600x3	D3Q27Q27	1/5	120	0.0025	100	10	3E-02	3E-04
$Pr1000_{small}$	1000x150x3	D3Q27Q27	1/5	30	0.01	1000	10	3E-02	3E-05
$Pr1000_{medium}$	2000x300x3	D3Q27Q27	1/5	60	0.005	1000	10	3E-02	3E-05
$Pr1000_{large}$	4000x600x3	D3Q27Q27	1/5	120	0.0025	1000	10	3E-02	3E-05

Table 2: Case-ID: lookup table

Influence of relaxation matrix

The general relaxation matrix for the advection diffusion equation can presented as:

$$\mathbb{S}^H = diag\left([s_{000}, s_{100}, s_{010}, s_{001}, \ldots s_{ijk}\ldots, s_{122}, s_{212}, s_{221}, s_{222}]\right) \quad \text{and} \quad s^H = \frac{1}{\frac{k}{c_s^2\delta t} + 1/2}$$

- CM: The common approach for (central) moment based scheme for advection diffusion equation is to relax the first order moments only ($s_{i+j+k=1} = s^H$), while the higher order moments are set to equilibrium ($s_{i+j+k>1} = 1$). However, it turned out that such technique results in unacceptable 'wiggles' for numerically low conductivities.
- CM-TRT: The two-relaxation time approach requires the odd-moments to be relaxed with a common rate ($s_{odd} = s^H$), while the even moments are set to equilibrium ($s_{even} = 1$).
- CM-SRT: The a single relaxation time can be obtained by setting $s_{ijk} = s^H$.

Conclusions
To analyse flow of fluid having high Pr number, a lattice with large number of discrete velocities, like D3Q27, is necessary. Simulations on the D3Q7 lattice were unstable in the investigated regime. Proper treatment of collision kernel seems to have a more important role than the application of a second-order BC to represent the cylinder. The CM-TRT and CM-SRT kernels are superior to the kernels which relax first-order moments only.

The simulations were completed using the open-source TCLB solver available at:
`https://github.com/CFD-GO/TCLB`

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