Entropic MRT Lattice Boltzmann Model (KBC) & application on VPLBM

Mahmut Mustafa Tugtekin (B.Sc. Student) Advised by Dr.ir. MI Marc Gerritsma

Faculty of Aerospace Engineering, TU Delft, Netherlands

Honours Programme Delft

TU Delft

Abstract

The lattice Boltzmann method (LBM) is an alternative approach to computational fluid dynamics based on a fully discrete kinetic equation and fluid populations. The classical LBM scheme is 'weakly compressible'. It was also (LBGK) plagued by numerical instabilities in highly turbulent flows unless a more extensive domain or smaller time scale was used to increase resolution. Several improvements of LBM attempted to negate this issue. In particular, the multiple relaxation-times methods (MRT) take advantage of the additional degrees of freedom in the LBM kinetic system to stabilize the solution and improve accuracy. However, the MRT scheme introduced tuneable constants unique to each physical system, thus not a general solution for stability. With the introduction of ELBM (Entropic Lattice Boltzmann) that mimics Boltzmann's H theorem in discrete time, simulations of highly turbulent and thermal flows were possible. However, ELBM introduces varied viscosity over the domain, which can be negative. The smoke simulations and high turbulence flows require a stable scheme and preserved fine-grid details. As mentioned, for regular LBM to solve these systems, resolutions need to be increased further. Work by Wen[1] has tackled this problem by checking local flow properties at each point and artificially adding a decrease in these properties back to mesh. Although this solution works with three non-coupled meshes, it still does not tackle the stability problem but only solves the preservation problem. This report aims to solve the problem of creating a lattice method that, while preserving vorticity, tackles the stability issue with an ELBM and uses lower resolutions.

LB Method

The discrete Lattice Boltzmann equation is 1, which consists of a collision step and a streaming step. In1 left-hand side is streaming, and the right-hand side is the collision. Parameter β defines the rate of relaxation. here mirror state is $f_i^{mirr} = \alpha f_i^{eq} - f_i$ LB models are differentiated by their selection of parameter α, Lattice Bhatnar-Gross-Krook (LBGK) model [2] picks $\alpha = 2$.

$$f_i(\mathbf{x} + \Delta t \mathbf{v}_i, t + \Delta t) = (1 - \beta) f_i(\mathbf{x}, t) + \beta f_i^{mirr}(\mathbf{x}, t) \quad (1)$$

Here f^{eq} is the local equilibrium found from the discretization of local Maxwellian distribution depends only on locally conserved quantities, $f_i^{eq}(\mathbf{v}, t) = f_i^{eq}(\rho(\mathbf{x}, t), j_{alpha}(\mathbf{x}, t))$, the first and second order of the populations. Because Maxwellian distribution is the minima for the H function, collision steps take populations to a point closer to equilibrium at each step function.

$$f_i^{eq} = \omega \rho(\mathbf{x}, t) \left[1 + \frac{\mathbf{u}}{c_s^2} + \frac{(\mathbf{u} \cdot \mathbf{v}_i)^2 - c_s^2 (\mathbf{u} \cdot \mathbf{u})}{2 c_s^4} \right] \quad (2)$$

Taking Navier-Stokes equations as the target in hydrodynamic limit and using Chapman-Enskog expansion, the kinematic viscosity is related to the relaxation coefficient as:

$$\nu = c_s^2 \left(\frac{1}{\alpha \beta} - \frac{1}{2} \right) \Delta t \quad (3)$$

This also requires $c_s^2 = \frac{1}{3} c^2$ and $p = \frac{1}{3} \rho c^2$. Together these constitute a discrete velocity set as

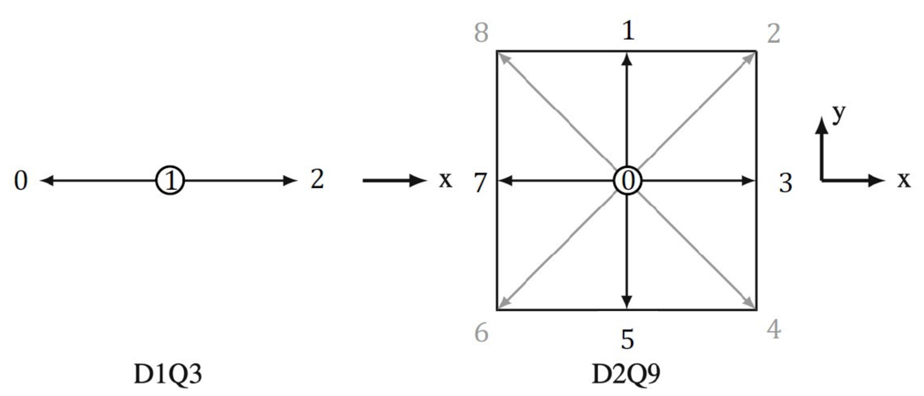

Figure 1. D1Q3 and D2Q9 velocity set

As stated, LBGK uses $\alpha = 2$ and over-relaxes populations toward equilibrium at a rate determined by relaxation coefficient β. While good for well-resolved grids, the BGK model has a narrow area of applicability and stability [3]. Especially for under-resolved high Reynolds flows, the LBGK model rapidly becomes unstable. To ensure stability under high vorticity smoke simulations KBC (Karlin, Bösch, and Chikatamarla) model will be used. In this model, the populations f_i are defined as a sum over kinematic (k_i), shear (s_i) and higher-order contributions (h_i):

$$f_i = k_i + s_i + h_i \quad (5)$$

Because moments of the populations are just linear transformations of the populations, inversely, populations can be constructed from moments. KBC is a two-relaxation-time model that relaxes all higher-order moment contributions h_i toward their equilibria with the same relaxation rate γ. In contrast, the shear moments s_i are over-relaxed according to the kinematic viscosity (α = 2). Therefore, in the KBC formulation, the mirror state can be defined as :

$$f_i^{mirr} = k_i + (\alpha s_i^{eq} - s_i) + [(1 - \gamma) h_i + \gamma h_i^{eq}] \quad (6)$$

The parameter γ is determined at each lattice node and time step so that the H function post-collision of a population is minimized given s moments over relax ($\alpha = 2$). This guarantees viscosity of shear moments cannot be negative, improving stability and giving improved control over the dissipation of vorticity. γ in a closed form can be found to be [5]:

$$\gamma_i = \frac{1}{\beta} - \left(2 - \frac{1}{\beta} \right) \frac{< \Delta s | \Delta h >}{< \Delta h | \Delta h >} \quad (7)$$

Where $< X|Y >$ designates the entropic dot product defined as $< X|Y >= \sum_{i=0}^{Q} \frac{X_i Y_i}{f_i^{eq}}$. Also, $\Delta s_i = s_i - s_i^{eq}$. The moment basis is:

$$k_i = k_i(\Pi_0, \Pi_x, Pi_y) = \rho, \rho u_x, \rho u_y; \quad s_i = s_i(\Pi_{xy}, \Pi_{xx}, \Pi_{yy}); \quad h_i = h_i(\Pi_{xxy}, \Pi_{xyy}, \Pi_{xxyy}) \quad (8)$$

This construction can be visualized with the figure 2

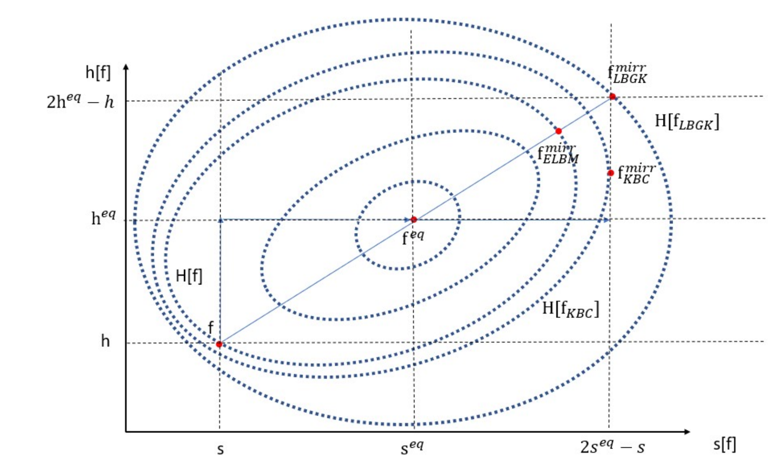

Figure 2. Entropy levelized map

In the future, a population that tracks vorticity will be added using D2Q5 scheme; since vorticity in the 2D domain is scalar, the governing equation for transportation of vorticity will be advection-diffusion

$$g_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - g_i(\mathbf{x}, t) = \frac{1}{\tau} (g_i^{eq}(\mathbf{x}, t) - g_i(\mathbf{x}, t)) + w_i \frac{\mathbf{c}_i \cdot \mathbf{F}_\omega}{c_s^2} \quad (9)$$

where F_ω is the extra force to be added on the grid as an external force to recover vorticity and is a function of the gradient of it.

$$g_i^{eq} = w_i \omega \left[1 + \frac{\mathbf{v}_i \mathbf{u}}{c_s^2} \right] \quad (10)$$

Where vorticity can be tracked from

$$\omega \sum_i g_i \quad (11)$$

Results

Validation is done by comparing the analytical solution to Taylor- Green vortex and the computational solution with L2 norm error. It can be observed the scheme does converge to an analytical solution, and it is faster with higher resolution.

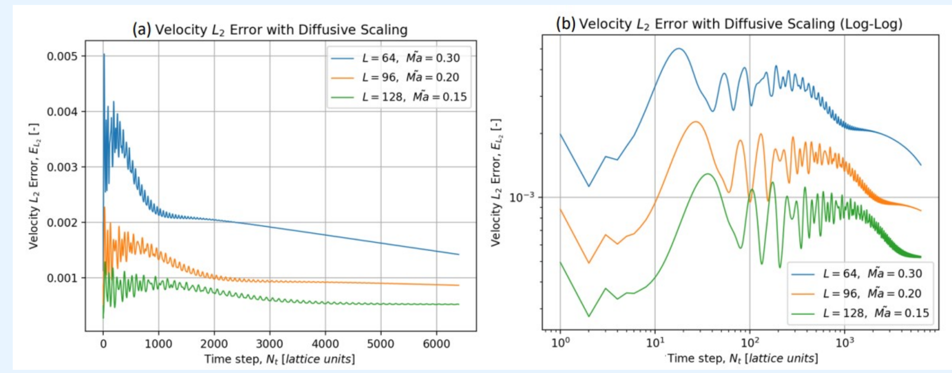

Figure 3. L2 Error with diffusive scaling

To inspect the vorticity field and the response of KBC to highly turbulent flow fields, the operator is tested with a doubly periodic shear layer. 4 Shows the established domain of stability as a function of U_0) and ν, found using L=128. It is evident that KBC extends the stability range of under-resolved simulations with sharp velocity gradients. It allows using lower values of ν for the same values of U_0), as well as higher values of U_0) for the same ν than the LBGK.

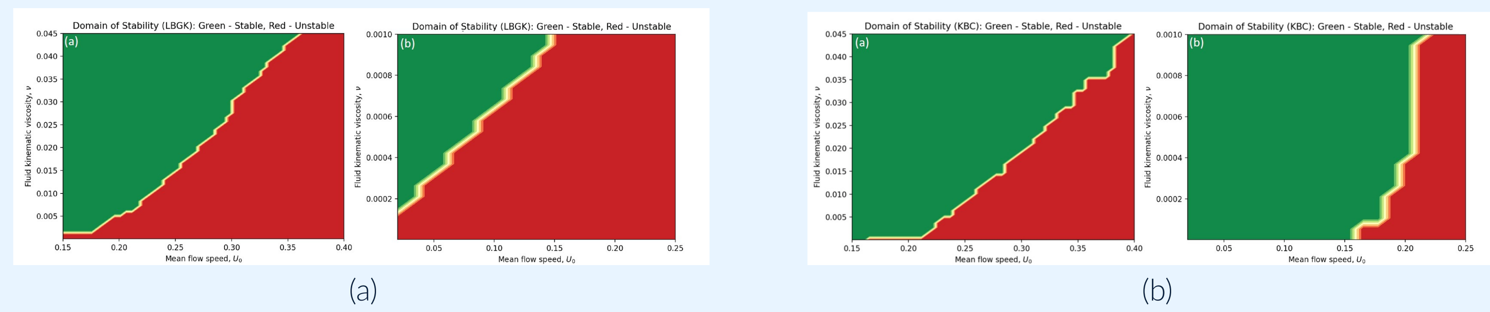

Figure 4. (a)-stability domain LBGK, (b)-stability domain KBC

5(a) shows a snapshot of the vorticity field on a fine grid $L = 512$ at a time $t = t_c$, and 5(b) spatial distribution of γ. Moreover, the values of γ are not necessarily confined to the [0,2] and can take both positive and negative values [4]. Due to the self-adaptation of γ to the flow domain, its spatial distribution resembles the vortex pattern. In locations with no large velocity gradients $\gamma \approx 2$, the KBC coincides with LBGK. Where $\gamma > 2$, it introduces additional dissipation, and where $\gamma < 2$, it reduces dissipation, and this adaptation of γ helps to represent low-order statistics and allows the numerical scheme to model physical dissipation correctly.

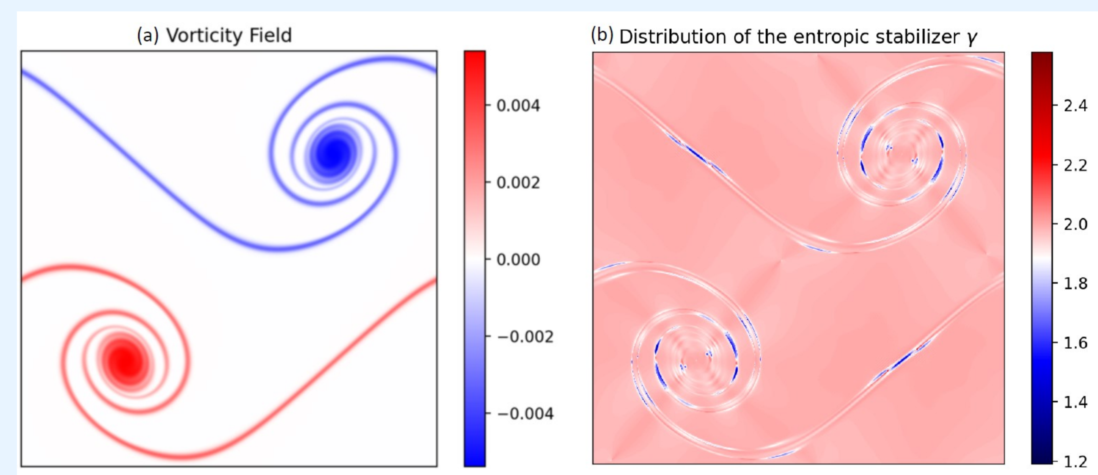

Figure 5. Entropic Stabilizer

[1] Wen, J., and Ma, H., "Real-time smoke simulation based on vorticity preserving lattice Boltzmann method," Visual Computer, Vol. 35, 2019. doi:10.1007/s00371-018-1514-x.19

[2] H. Chen, S. Chen, and W. H. Matthaeus, "Recovery of the Navier-Stokes equations using a lattice-gas Boltzmann method", Phys. Rev. A 45 (8 Apr. 1992), R5339–R5342.

[3]A. Krämer, D. Wilde, K. Küllmer, D. Reith, H. Foysi. Pseudoentropic derivation of the regularized lattice Boltzmann method. Phys. Rev. E, 100(2), 023302 1-16, 2019. American Physical Society. https://link.aps.org/doi/10.1103/PhysRevE.100.023302

M.M.Tugtekin@student.tudelft.nl