

Appendix A The origin of Lattice Boltzmann Method

The Lattice Boltzmann Method originates from the continuous Boltzmann equation, Eqn. (A1).

$$\frac{Df(x, \boldsymbol{\xi}, t)}{Dt} = \left(\frac{\partial}{\partial t} + \xi_\alpha \frac{\partial}{\partial x_\alpha} \right) f(x, \xi, t) = \Omega(f) \quad (\text{A1})$$

The collision operator (Ω) is a highly complex term whose fundamental role is to restore the system to the Maxwellian state by directing f toward its Maxwell-Boltzmann equilibrium distribution (f^{eq}). The operator vanishes when the system reaches its equilibrium ($f = f^{eq}$) [1]. For ideal gas, this thermodynamic equilibrium state is formulated in Eqn. (A2).

$$f^{eq}(\mathbf{x}, |\boldsymbol{\xi} - \mathbf{u}|, t) = \rho \left(\frac{1}{(2\pi\bar{r}T)} \right)^{D/2} \exp \left(-\frac{|\boldsymbol{\xi} - \mathbf{u}|^2}{2\bar{r}T} \right) \quad (\text{A2})$$

where ρ and $\mathbf{u}$ are the mixture density and velocity, respectively. D is the spatial dimension, T is the temperature, and $\bar{r}$ is the gas constant of the mixture.

$$\bar{r} = \frac{R}{\bar{W}} \quad \bar{W} = \frac{1}{\sum_{k=1}^N Y_k / W_k} \quad (\text{A3})$$

The gas constant of the mixture is formed with the universal gas constant ($R = 8.3145$ kJ/kmol/K), and the mixture molecular weight ($\bar{W}$), Eqn. (A3).

The fluid physics derived from the BE at the macroscale is consistent with the Navier-Stokes equations. This indicates that the individual atoms are no longer distinguishable nor of primary interest. The Chapman-Enskog expansion connects the Boltzmann formulation to the macroscopic Navier-Stokes equations [2].

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_\alpha} (\rho u_\alpha) = 0 \quad (\text{A4})$$

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial}{\partial x_\beta} (\rho u_\alpha u_\beta) = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial \mathcal{T}_{\alpha\beta}}{\partial x_\beta} \quad (\text{A5})$$

where the pressure can be approximated by the ideal gas law ($p = \rho \bar{r} T$).

The zeroth and first order moments of the velocity distribution function f yields the local density (ρ), and momentum $\rho \mathbf{u}(\mathbf{x}, t)$, respectively.

$$\begin{aligned} \rho(\mathbf{x}, t) &= \int f(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} \\ \rho \mathbf{u}(\mathbf{x}, t) &= \int f(\mathbf{x}, \boldsymbol{\xi}, t) \boldsymbol{\xi} d\boldsymbol{\xi} \end{aligned} \quad (\text{A6})$$

Although the continuous Boltzmann equation can be applied to the mass and momentum conservation laws, the high-dimensional, integro-differential nature of the VDF

and the collision term makes direct solutions prohibitively challenging, if not impossible [3]. Thus, continuous kinetic theory is discretized by evaluating the VDF along specific discrete velocity directions. This discrete formulation decouples the fluid evolution into a collision step that relaxes f toward equilibrium and a streaming step that advects f . While discretization strategies vary (e.g., D1Q3, D2Q9, D3Q19), we select the two-dimensional, nine-directional D2Q9 scheme for this study due to its symmetric nature and low memory usage [4]. However, because the set of discrete velocities is finite, deviations between the continuous and discrete moments arise. To counterbalance these inconsistencies, an additional forcing term should be added to the evolution of the distribution function [5].

Eqn. (A7) defines the discrete distribution functions (f_i) traveling with the velocity of $\mathbf{c}_i$ in the discrete lattice directions. w_i are the Gaussian weights, and $\omega(\mathbf{c}_i)$ is the weighting function.

$$f_i(\mathbf{x}, t) = \frac{w_i}{\omega(\mathbf{c}_i)} f(\mathbf{x}, \mathbf{c}_i, t) \quad (\text{A7})$$

Another cornerstone of LBM is the construction of the collision operator. Over the years, various collision models have been developed to improve numerical performance. The most renowned approaches include the Single Relaxation Time (SRT) model, also called the Bhatnagar-Gross-Krook (BGK) operator [6], two-relaxation time (TRT) models [7, 8], multi-relaxation time (MRT) models [8, 9], and regularization models [10–12]. While the BGK operator is preferred for its simplicity, it suffers from numerical instability in high-shear flows [13]. TRT and MRT models enhance the stability margin by tuning the relaxation times of higher-order moments. Addressing the same stability limitation, the regularized collision kernels extend the stability boundaries by filtering the nonequilibrium parts of the distribution function.

Appendix B Initial Conditions and Flame Metrics

The initial thermodynamic states for the burnt and unburnt mixtures are obtained from Cantera’s chemical equilibrium solver [14]. As a representative case, Table B1 presents the initial conditions for an equivalence ratio of unity. For the chemical kinetics, we utilize the 9-species, 12-step reduced hydrogen mechanism developed by Boivin et al. [15].

We compute the flame speed (S_L) using the flame consumption speed approach (FCS). This strategy integrates the consumption rate of the limiting reactant (fuel, $\dot{w}_F$, or oxidizer, $\dot{w}_O$) along the flame-surface normal, and subsequently determines S_L through normalization with reactant’s consumed mass density [16]. Unlike multidimensional configurations, the one-dimensional flame front is perpendicular to the domain axis and propagates only along this direction. This simplification reduces the spatial integral to a simple line integral. Thus, the FCS approach is advantageous in the 1-D case, as it captures the global flame behavior without requiring explicit flame-front reconstruction.

Variables	Fresh Gases	Burnt Gases
T	300 K	2381 K
P	101325 Pa	101325 Pa
Y_{H_2}	$2.85 \cdot 10^{-2}$	$1.12 \cdot 10^{-3}$
Y_{O_2}	$2.26 \cdot 10^{-1}$	$8.49 \cdot 10^{-3}$
Y_{H_2O}	0	$2.39 \cdot 10^{-1}$
Y_H	0	$7.30 \cdot 10^{-5}$
Y_O	0	$4.29 \cdot 10^{-4}$
Y_{OH}	0	$5.72 \cdot 10^{-3}$
Y_{HO_2}	0	$1.86 \cdot 10^{-6}$
$Y_{H_2O_2}$	0	$2.06 \cdot 10^{-7}$
Y_{N_2}	$7.45 \cdot 10^{-1}$	$7.45 \cdot 10^{-1}$

Table B1: CANTERA computed initial conditions of Fresh and Burnt Gases

$$\begin{aligned}
S_L &= -\frac{1}{\rho_U(Y_{F_U} - Y_{F_B})} \cdot \int_{-\infty}^{\infty} \dot{w}_F dx \quad \text{when } \phi \leq 1 \\
S_L &= -\frac{1}{\rho_U(Y_{O_U} - Y_{O_B})} \cdot \int_{-\infty}^{\infty} \dot{w}_O dx \quad \text{when } \phi > 1
\end{aligned} \tag{B1}$$

The flame consumption speed (FCS) formulation is given in Eqn. (B1). The limiting reactant is the fuel (subscript F) under lean conditions ($\phi \leq 1$), and the oxidizer (subscript O) under rich conditions ($\phi > 1$). The subscripts U and B denote the unburnt and burnt states, respectively.

We also calculate the thermal flame thickness (δ) using the maximum temperature gradient approach. This is defined as the ratio of the temperature difference between the burnt and unburnt states to the maximum temperature gradient across the flame front ($\delta = (T_B - T_U)/(dT/dx)_{max}$).

References

- [1] Chen, S., Doolen, G.D.: Lattice boltzmann method for fluid flows. Annual Review of Fluid Mechanics **30**, 329–364 (1998) <https://doi.org/10.1146/annurev.fluid.30.1.329>
- [2] Chapman, S., Cowling, T.G.: The Mathematical Theory of Non-uniform Gases : an Account of the Kinetic Theory of Viscosity, Thermal Conduction and Diffusion in Gases. London: Cambridge U.P, Cambridge (1970)

- [3] He, X., Chen, S., Doolen, G.D.: A novel thermal model for the lattice boltzmann method in incompressible limit. *Journal of Computational Physics* **146**, 282–300 (1998) <https://doi.org/10.1006/jcph.1998.6057>
- [4] Krüger, T., Kusumaatmaja, H., Kuzmin, A., Shardt, O., Silva, G., Viggen, E.M.: *The Lattice Boltzmann Method*. Springer, Switzerland (2017)
- [5] Farag, G., Zhao, S., Chiavassa, G., Boivin, P.: Consistency study of lattice-boltzmann schemes macroscopic limit. *Physics of Fluids* **33**(3), 037101 (2021) <https://doi.org/10.1063/5.0039490>
- [6] Qian, Y.H., D’Humières, D., Lallemand, P.: Lattice bgk models for navier-stokes equation. *Europhysics Letters* **17**, 479–484 (1992) <https://doi.org/10.1209/0295-5075/17/6/001>
- [7] Ginzburg, I., Verhaeghe, F., d’Humières, D.: Two-relaxation-time lattice boltzmann scheme: about parametrization, velocity, pressure and mixed boundary conditions. *Communications in Computational Physics* **3**, 427–478 (2008) <https://doi.org/10.1006/jcph.1998.6057>
- [8] Khirevich, S., Ginzburg, I., Tallarek, U.: Coarse- and fine-grid numerical behavior of mrt/trt lattice-boltzmann schemes in regular and random sphere packings. *Journal of Computational Physics* **281**, 708–742 (2015) <https://doi.org/10.1016/j.jcp.2014.10.038>
- [9] d’Humières, D.: Multiple-relaxation-time lattice boltzmann models in three dimensions. *Computers & Mathematics with Applications* **360**, 437–451 (2002) <https://doi.org/10.1098/rsta.2001.0955>
- [10] Latt, J., Chopard, B.: Lattice boltzmann method with regularized pre-collision distribution functions. *Mathematics and Computers in Simulation* **72**, 165–168 (2006) <https://doi.org/10.1016/j.matcom.2006.05.017>
- [11] Malaspinas, O.: Increasing stability and accuracy of the lattice Boltzmann scheme: recursivity and regularization (2015). <https://arxiv.org/abs/1505.06900>
- [12] Coreixas, C., Wissocq, G., Puigt, G., Boussuge, J.-F., Sagaut, P.: Recursive regularization step for high-order lattice boltzmann methods. *Phys. Rev. E* **96**, 033306 (2017) <https://doi.org/10.1016/j.matcom.2006.05.017>
- [13] Hosseini, S.A., Darabiha, N., Thévenin, D.: Theoretical and numerical analysis of the lattice kinetic scheme for complex-flow simulations. *Phys. Rev. E* **99**, 023305 (2019) <https://doi.org/10.1103/PhysRevE.99.023305>
- [14] Goodwin, D.G., Moffat, H.K., Schoegl, I., Speth, R.L., Weber, B.W.: *Cantera: An Object-oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes*. <https://www.cantera.org>. Version 3.1.0 (2024). <https://www.cantera.org>

[//doi.org/10.5281/zenodo.14455267](https://doi.org/10.5281/zenodo.14455267)

- [15] Boivin, P., Jimenez, C., Sanchez, A.L., Williams, F.A.: An explicit reduced mechanism for h₂–air combustion. *Proceedings of the Combustion Institute* **33**, 517–523 (2011) <https://doi.org/10.1016/j.proci.2010.05.002>
- [16] Giannakopoulos, G.K., Frouzakis, C.E., Shikhar, M., Tomboulides, A.G., Mat-
alon, M.: Consumption and displacement speeds of stretched premixed flames
- theory and simulations. *Combustion and Flame* **208**, 164–181 (2019) <https://doi.org/10.1016/j.combustflame.2019.06.027>