CASCADED LATTICE BOLTZMANN METHODS BASED ON CENTRAL MOMENTS FOR THERMAL CONVECTION, MULTIPHASE FLOWS AND COMPLEX FLUIDS

by

FARZANEH HAJABDOLLAHI OUDERJI

BS, Bahonar University of Kerman (BUK), 2009
MS, Ferdowsi University of Mashhad, 2011

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Farzaneh Hajabdollahi Ouderji

has been approved for the

Engineering and Applied Science Program

by

Samuel Welch, Chair
Kannan Premnath, Advisor
Peter Jenkins
Sedat Biringen
Taeun Lee

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Lattice Boltzmann (LB) methods are kinetic schemes based on stream-and-collide procedures for the evolution of particle distribution functions, and are of much interest to the computational fluid dynamics community due to the locality of their algorithmic steps and other numerical features. Among the more recent developments in this area is the cascaded LB formulation, which is based on central moments and multiple relaxation times that was originally constructed for athermal, single-phase or single-fluid flows, and is promising due to its natural ability to impose Galilean invariance and its enhanced numerical properties such as improved numerical stability when compared to the other collision models. In this dissertation, we advance its state-of-the-art by proposing several new schemes based on cascaded LB approach with improved convergence and/or accuracy or numerical stability, with a common theme involving the use of double (or more) distribution functions that evolve under the relaxation of various central moments during the collision steps for the computation of various multi-physics fluid dynamics applications, including heat transfer and multiphase systems. Specifically, we present and analyze the following: (i) convergence acceleration by preconditioning of the cascaded LB method with additional Galilean invariant (GI) corrections to improve accuracy by reducing aliasing errors due to the discreteness and symmetries of the lattice for steady state flow simulations, (ii) implementation strategies for body forces and source terms in the simulations of fluid motion and scalar transport using cascaded LB schemes via operator splitting, (iii) cascaded LB methods for thermal convective flows in three-dimensions and cylindrical coordinates with axial symmetry, (iv) a kinetic approach for computing the vorticity fields locally in a double
distribution functions based LB formulation without relying on finite differences for spatial derivatives, and (v) cascaded LB schemes for incompressible, two-phase flows and interface capturing at high density ratios based on phase-field models, including extensions for representing surfactant effects. Numerical validation against a variety of complex flow benchmark problems demonstrate the accuracy and effectiveness of the approach for each of the new developments. We show significant improvements in convergence acceleration by preconditioning and accuracy by GI corrections, and improvements in stability with the use of cascaded LB formulations when compared to other collision models for simulations of thermal convective flows and multiphase systems. Overall, the cascaded LB schemes are found to be versatile and numerically robust for a variety of complex flows with attendant multi-physics effects.

The form and content of this abstract are approved. I recommend its publication.

Approved: Kannan Premnath
DEDICATION

This dissertation is dedicated to my family, and especially my sister, for their understanding, motivation and patience during the challenges of graduate school and life. I am truly thankful for having all of you in my life. I would to also dedicate this dissertation to my major Professor Prof. Kannan Premnath for his vital contributions to my professional development and for his numerous help during my graduate study. This work would not have been possible without his immense expertise that he shared and his ablest guidance.
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CHAPTER I

INTRODUCTION

1.1 Background and Motivation

Complex fluid motion arises widely in a number of engineering applications, geophysical contexts and biochemical systems. Of particular interests are those that involve thermal convective flows in configurations involving heat transfer and/or interfacial flows in multiphase or multi-fluid systems. Often the presence of nonlinearity and multiple scales inherent in such multiphysics situations make it quite challenging to investigate such systems. Simulations based on computational methods enable fundamental studies of the fluid mechanics and as predictive tools for engineering design of configurations that handle fluid flows. Thus, the development of accurate, efficient and robust numerical methods plays a pivotal role in computational fluid dynamics (CFD). Classical numerical techniques such as the finite difference, finite volume and finite element methods have traditionally been used to perform discretization of the partial differential equations such as the Navier-Stokes (NS) equations that represent the fluid motion including any attendant multiphysics effects. From a different perspective, more recently, the lattice Boltzmann (LB) method has demonstrated to be a very effective alternate numerical technique to simulate a variety of complex fluid flow systems [6, 7, 8].

The lattice Boltzmann method is a mesoscopic method based on local conservation and discrete symmetry principles, and may be derived as a special discretization of the Boltzmann equation [9]. Hence, it can be regarded as a kinetic scheme. Algorithmically, it involves the streaming of the particle distribution functions as a perfect shift advection step along the lattice directions and followed by a local collision step as a relaxation process towards an equilibria, and accompanied by special strategies for the implementation of impressed forces. The hydrodynamic fields char-
acterizing the fluid motion are then obtained via the various kinetic moments of the evolving distribution functions and its consistency to the NS equations may be established by a Chapman-Enskog expansion or Taylor series expansions under appropriate scaling between the discrete space step and time step. As such, the LB method has been applied for the computation of a wide range of complex flows including turbulence, multiphase and multicomponent flows, particulate flows and microflows (see e.g., [10, 11, 12]).

The LB method has the following advantages. Its streaming step is linear and exact and all nonlinearity is modeled locally in the collision step; by contrast, the convective term in the NS equation is nonlinear and nonlocal. The pressure field is obtained locally LB methods, circumventing the need for the solution of the time consuming elliptic Poisson equation as in traditional methods. The exact-advection in the streaming step combined with the collision step based on a relaxation model leads to a second order accurate method with relatively low numerical dissipation. The kinetic model for the collision step can be tailored to introduce additional physics as necessary and its additional degree of freedom can be tuned to improve numerical stability. Various boundary conditions for complex geometries can be represented using relatively simple rules for the particle populations. Finally, the locality of the method makes it amenable for almost ideal implementation on parallel computers for large scale flow simulations.

During the last decade or so, the LB method has undergone a number of refinements, especially with the development of more sophisticated collision models as well as in adopting advanced strategies from CFD to further improve its numerical stability, accuracy and efficiency. As such, the collision step, which represents various physics associated with the fluid motion including the momentum diffusion as a relaxation process, plays a main role in the numerical stability of the method. Among the earliest collision models is the single relaxation time (SRT) model [13], which, while being popular due to its simplicity, is susceptible to numerical instability at relatively high Reynolds numbers. A significant improvement is achieved by the multiple relaxation time model (MRT) [14] in which different raw moments relax at different rates. More re-
recently, further enhancement in stability was made possible by the introduction of a cascaded LB method, which is a multi-parametric scheme that is based on considering relaxation in terms of central moments, which are formulated by shifting the particle velocity by the local fluid velocity [15]. The significant advantages of such more advanced collision models were numerically demonstrated more recently (see e.g., [16, 17]).

Central moments based cascaded LB method has so far mainly been developed and applied for athermal flows (i.e., without heat transfer effects) and single-phase flows. In particular, development of new cascaded LB schemes for thermal convective flows in different spatial dimensions and two-phase flows with interfacial dynamics would significantly improve the state-of-the-art in the LB formulations and expand their scope for various complex fluid dynamics applications. In addition, strategies for convergence acceleration and for improvements in the accuracy of the cascaded LB method, and the construction of novel simpler and efficient approaches to handle body forces/sources for such methods would make further contributions of significant interest to the field. These are among the various topics of our research endeavors presented in this dissertation. Before we outline the specific original research goals and contributions of this dissertation later in this chapter, in what follows, we will first present some details of the LB method, including the cascaded formulation, which would serve as a basis for further improvements.

1.2 Single-Relaxation-Time (SRT) Lattice Boltzmann Method

First, we will briefly discuss the simplest version of the LB method, i.e., the single-relaxation time (SRT) approach, which will be used as a basis for comparison. A typical lattice in two-dimensions (2D) is the two-dimensional, nine velocity (D2Q9) lattice, which is illustrated in Fig. 1.1,
and components of the particle velocities are given by The particle velocity $e_\alpha$ may be written as

$$e_\alpha = \begin{cases} (0,0) & \alpha = 0 \\ (\pm 1,0), (0, \pm 1) & \alpha = 1, \cdots, 4 \\ (\pm 1, \pm 1) & \alpha = 5, \cdots, 8 \end{cases} \quad (1.1)$$

The lattice represents the discrete characteristic particle directions $e_\alpha$, where $\alpha = 0, 1, 2, \cdots, 8$ along which the discrete particle distribution function $f_\alpha$ advects (i.e., streams) and then undergo a scattering process (i.e., collision). According to the SRT LB method, the distribution function relaxes to its corresponding equilibrium distribution function $f^{eq}_\alpha$ at a single relaxation time $\tau$. Thus, the SRT LB method can be written as

$$f_\alpha(x + e_\alpha, t + 1) = f_\alpha(x, t) - \frac{1}{\tau} [f_\alpha(x, t) - f^{eq}_\alpha(x, t)], \quad (1.2)$$

where the equilibrium distribution function $f^{eq}_\alpha$ is related to the local fluid density $\rho$ and $u$ velocity fields, and is given by

$$f^{eq}_\alpha = w_\alpha \rho \left[ 1 + \frac{e_\alpha \cdot u}{c_s^2} + \frac{(e_\alpha \cdot u)^2}{2c_s^4} - \frac{u \cdot u}{2c_s^2} \right]. \quad (1.3)$$

Here, $w_\alpha$ are the weighting factors for different particle directions and given by $w_\alpha$ are given by $w_0 = 4/9$, $w_\alpha = 1/9$, where $\alpha = 1, 2, 3, 4$ and $w_\alpha = 1/36$, where $\alpha = 5, 6, 7, 8$ and $c_s^2 = 1/3$. Then, the hydrodynamic fields, i.e., the density and velocity are updated by taking zeroth and first moments, respectively, of $f_\alpha$, and the pressure field $p$ is obtained from density via an equation of state:

$$\rho = \sum_\alpha f_\alpha, \quad \rho u = \sum_\alpha f_\alpha e_\alpha, \quad p = c_s^2 \rho. \quad (1.4)$$

This method simulates the fluid motion, with the kinematic viscosity $\nu$ given by $\nu = c_s^2 (\tau - 1/2)$. It may be noted that the SRT LB method is prone to numerical instabilities when it is required to simulate fluid flows with relatively low viscosities, i.e., when $\tau \to 1/2$ and it does not possess any additional degrees of freedom to enhance its numerical properties to address such issues. It may be noted that various boundary formulations to represent the no-slip, free slip, open flow
FIGURE 1.1: Two-dimensional, nine-velocity (D2Q9) lattice.
boundary conditions, among others, in terms of their effect on the kinetic variables, i.e., the distribution function have been devised. For example, the no-slip condition can be represented by means of the so-called half-way bounce back scheme and its more sophisticated versions based on interpolations for curved walls. See Ref. [18] for details.

1.3 Cascaded Lattice Boltzmann Method based on Central Moments

We will now discuss a significantly improved version of the LB scheme based on central moments, which is referred to as the cascaded LB method [15], including the forcing terms [19]. It provides a context to this dissertation research, where we will further improve its efficiency and numerical accuracy, extend its capabilities, and broaden its scope of applications, in particular, to those related to thermo-fluid dynamics and complex fluids with interfaces. Generally, the cascaded LB method represents collision process via the relaxation of various central moments to their corresponding equilibria. Here, the central moments are defined as the sum over all particle directions of the products of the distribution function weighted with the monomials of the components of the particle velocity shifted by the fluid velocity (see below). The use of central moments naturally imposes Galilean invariance of those moment components independently supported by a given lattice (but not for those unsupported higher order moments that alias with the lower order ones due to the discreteness and symmetries of the lattice). In this regard, for the purpose of illustration, again the standard D2Q9 lattice is employed. As the cascaded LBM is a moment based approach, we start with a set of the following nine nonorthogonal basis vectors obtained
using the monomials $e_\alpha^m e_{\alpha y}^n$ in a ascending order:

\[
\Phi_0 = (1,1,1,1,1,1,1,1,1)^\dagger, \\
\Phi_1 = e_x = (0,1,0,-1,0,1,-1,-1,1)^\dagger, \\
\Phi_2 = e_y = (0,0,1,0,-1,1,1,-1,-1)^\dagger, \\
\Phi_3 = e_x \circ e_x + e_y \circ e_y, \\
\Phi_4 = e_x \circ e_x - e_y \circ e_y, \\
\Phi_5 = e_x \circ e_y, \\
\Phi_6 = e_x \circ e_x \circ e_y, \\
\Phi_7 = e_x \circ e_y \circ e_y, \\
\Phi_8 = e_x \circ e_x \circ e_y \circ e_y, \\
\tag{1.5}
\]

where $\dagger$ is the transpose operator. In the above, for any two $q$-dimensional vectors ($q = 9$ here) $a$ and $b$, we define the elementwise vector multiplication by $a \circ b$. That is, $(a \circ b)_\alpha = a_\alpha b_\alpha$, where $\alpha$ represents a component of the vector and the implicit summation convention is not assumed here. To facilitate the presentation in the following, we also define a standard scalar inner product of any two such vectors as $\langle a, b \rangle$. That is, $\langle a, b \rangle = \sum_{\alpha=0}^{q} a_\alpha b_\alpha$. By applying the Gram-Schmidt orthogonalization method they result into the following equivalent set of orthogonal basis vectors:

\[
K_0 = \Phi_0, \quad K_1 = \Phi_1, \quad K_2 = \Phi_2, \\
K_3 = 3\Phi_3 - 4\Phi_0, \quad K_4 = \Phi_4, \quad K_5 = \Phi_5, \\
K_6 = -3\Phi_6 + 2\Phi_2, \quad K_7 = -3\Phi_7 + 2\Phi_1, \quad K_8 = 9\Phi_8 - 6\Phi_3 + 4\Phi_0.
\tag{1.6}
\]

Collecting them as an orthogonal matrix $K$, we get

\[
K = [K_0, K_1, K_2, K_3, K_4, K_5, K_6, K_7, K_8],
\tag{1.6}
\]

See [15, 20, 19], which enumerates the details of the matrix $K$. Now we define the continuous equilibrium central moments as [15]:

\[
\hat{\Pi}^M_{x^m y^n} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f^M(\xi_x - u_x)^m(\xi_y - u_y)^n d\xi_x d\xi_y. 
\tag{1.7}
\]

where $f^M$ is the local Maxwell-Boltzmann distribution in the continuous particle velocity space $\xi = (\xi_x, \xi_y)$ and is given by: $f^M \equiv f^M(\rho, u, \xi) = \frac{\rho}{2\pi c_s^2} \exp\left[-\frac{(\xi-u)^2}{2c_s^2}\right]$. Here, $\rho$ is the density.
and $\mathbf{u} = (u_x, u_y)$ is the macroscopic fluid velocity. By evaluating $\hat{\Pi}_{m,n}^M$ in the increasing order of moments for the D2Q9 lattice we obtain

$$\hat{\Pi}_0^M = \rho, \quad \hat{\Pi}_x^M = 0, \quad \hat{\Pi}_y^M = 0, \quad \hat{\Pi}_{xx}^M = c_s^2 \rho, \quad \hat{\Pi}_{yy}^M = c_s^2 \rho, \quad \hat{\Pi}_{xy}^M = 0,$$

$$\hat{\Pi}_{xx}^M = 0, \quad \hat{\Pi}_{xy}^M = 0, \quad \hat{\Pi}_{xxy}^M = c_s^4 \rho.$$

Similarly, we define the central moments of the sources of order $(m + n)$ due to a force field $\mathbf{F} = (F_x, F_y)$ as

$$\hat{\Gamma}_{x^m y^n}^F = \frac{\Delta f^F}{\Delta s} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (\xi_x - u_x)^m (\xi_y - u_y)^n d\xi_x d\xi_y,$$  \hspace{1cm} (1.8)

where $\Delta f^F$ is the change in the distribution function due to force fields. Again we can evaluate Eq. (1.8) as

$$\hat{\Gamma}_0^F = 0, \quad \hat{\Gamma}_x^F = F_x, \quad \hat{\Gamma}_y^F = F_y, \quad \hat{\Gamma}_{xx}^F = 0, \quad \hat{\Gamma}_{yy}^F = 0, \quad \hat{\Gamma}_{xy}^F = 0,$$

$$\hat{\Gamma}_{xxy}^F = c_s^2 F_y, \quad \hat{\Gamma}_{xyy}^F = c_s^2 F_x, \quad \hat{\Gamma}_{xxyy}^F = 0.$$

Based on the above continuous central moments and using the trapezoidal rule for evaluating the source term to retain second order accuracy, the elements of the cascaded LBE can be formulated as follows [15, 19]:

$$f_\alpha(x + e_\alpha, t + 1) = f_\alpha(x, t) + \Omega_\alpha^c (f, t) + \frac{1}{2} [S_\alpha(x, t) + S_\alpha(x + e_\alpha, t + 1)]$$  \hspace{1cm} (1.9)

In the above equation, the collision term can be modeled by

$$\Omega_\alpha^c \equiv \Omega_\alpha^c (f, g) = (K \cdot \Delta g)_\alpha,$$  \hspace{1cm} (1.10)

where $f = (f_0, f_1, f_2, \ldots, f_8)^\dagger$ is the vector of distribution functions and $\Delta g = (\Delta g_0, \Delta g_1, \Delta g_2, \ldots, \Delta g_8)^\dagger$ is the vector of the unknown change in different moments supported by the lattice under collision that is given later. The discrete form of the source term $S_\alpha$ in the cascaded LBE represents the influence of the force field $(F_x, F_y)$ in the velocity space that is given as: $S = (S_0, S_1, S_2, \ldots, S_8)^\dagger$.

As Eq. (1.9) is semi-implicit, by using the standard variable transformation by He et al. [21, 22],
and, in particular, by He et al. [23] \( \overline{f}_\alpha = f_\alpha - \frac{1}{2}S_\alpha \), so that the implicitness is removed and a second-order accuracy is maintained, we get

\[
\overline{f}_\alpha(x + e_\alpha, t + 1) = \overline{f}_\alpha(x, t) + \Omega^c_\alpha(x, t) + S_\alpha(x, t).
\] (1.11)

In order to determine the structure of the cascaded collision operator and the source terms in the presence of general spatially and/or temporally variable body forces, we define the following set of central moments of order \((m + n)\), respectively, as

\[
\begin{pmatrix}
\hat{\kappa}_{x^m y^n} \\
\hat{\kappa}^{eq}_{x^m y^n} \\
\bar{\sigma}_{x^m y^n} \\
\overline{\kappa}_{x^m y^n}
\end{pmatrix}
= \sum_{\alpha}
\begin{pmatrix}
f_\alpha \\
f^{eq}_\alpha \\
S_\alpha \\
\overline{f}_\alpha
\end{pmatrix}
(e_{\alpha x} - u_x)^m(e_{\alpha y} - u_y)^n.
\] (1.12)

By equating the discrete central moments for both the distribution functions and source terms with the corresponding continuous central moments

\[
\hat{\kappa}^{eq}_{x^m y^n} = \hat{\Pi}^M_{x^m y^n}, \quad \bar{\sigma}_{x^m y^n} = \hat{\Gamma}^F_{x^m y^n},
\]

we get

\[
\begin{align*}
\hat{\kappa}_0 &= \rho, \quad \hat{\kappa}^{eq}_x = 0, \quad \hat{\kappa}^{eq}_y = 0, \quad \hat{\kappa}^{eq}_{xx} = c_s^2 \rho, \quad \hat{\kappa}^{eq}_{yy} = c_s^2 \rho, \quad \hat{\kappa}^{eq}_{xy} = 0, \\
\hat{\sigma}_0 &= 0, \quad \hat{\sigma}_x = F_x, \quad \hat{\sigma}_y = F_y, \quad \hat{\sigma}_{xx} = 0, \quad \hat{\sigma}_{yy} = 0, \quad \hat{\sigma}_{xy} = 0.
\end{align*}
\] (1.13)

Here, we apply the effect of the variable body forces only on the first order central moments of the sources to obtain consistent macroscopic equations [19]. Similarly, for the transformed central moments we have

\[
\begin{align*}
\hat{\kappa}_0 &= \rho, \quad \hat{\kappa}^{eq}_x = -\frac{1}{2}F_x, \quad \hat{\kappa}^{eq}_y = -\frac{1}{2}F_y, \quad \hat{\kappa}^{eq}_{xx} = c_s^2 \rho, \quad \hat{\kappa}^{eq}_{yy} = c_s^2 \rho, \quad \hat{\kappa}^{eq}_{xy} = 0, \\
\hat{\sigma}_0 &= 0, \quad \hat{\sigma}_x = -\frac{\epsilon}{2} F_y, \quad \hat{\sigma}_y = -\frac{\epsilon}{2} F_x, \quad \hat{\sigma}_{xx} = 0, \quad \hat{\sigma}_{yy} = 0, \quad \hat{\sigma}_{xy} = 0.
\end{align*}
\] (1.14)

On the other hand, the actual calculations in the cascaded formulation are carried out in the terms of the raw moments. Hence, we define the following set of raw moments (designated here
with the prime (‘) symbol), which will be used later:

\[
\begin{bmatrix}
\hat{\kappa}'_{x^m y^n} \\
\hat{\kappa}'_{x^m y^n} \\
\hat{\sigma}'_{x^m y^n} \\
\hat{\kappa}'_{x^m y^n}
\end{bmatrix} = \sum_{\alpha} \begin{bmatrix}
f^\alpha \\
f^\alpha \\
S_\alpha \\
\bar{f}^\alpha
\end{bmatrix} e^m_{\alpha x} e^n_{\alpha y}
\] (1.16)

We can readily convert the central moments into a combination of the raw moments by using the binomial theorem.

Thus, we first summarize the following set of raw moments for the source terms for the D2Q9 lattice:

\[
\hat{\sigma}'_0 = 0, \quad \hat{\sigma}'_x = \frac{F_x}{\gamma}, \quad \hat{\sigma}'_y = \frac{F_y}{\gamma},
\]

\[
\hat{\sigma}'_{xx} = \frac{2 F_x u_x}{\gamma^2}, \quad \hat{\sigma}'_{yy} = \frac{2 F_y u_y}{\gamma^2}, \quad \hat{\sigma}'_{xy} = \frac{F_x u_y + F_y u_x}{\gamma^2},
\]

\[
\hat{\sigma}'_{xxy} = F_y u_x^2 + 2 F_x u_x u_y, \quad \hat{\sigma}'_{xyy} = F_x u_y^2 + 2 F_y u_y u_x,
\]

\[
\hat{\sigma}'_{xxyy} = 2 F_x u_x u_y + 2 F_y u_y u_x^2.
\]

Next, as an intermediate step, the source moments projected to the orthogonal moment space \(\hat{m}^s_\beta = \langle \mathbf{K}_\beta, \mathbf{S} \rangle\) are obtained as

\[
\hat{m}^s_0 = 0, \quad \hat{m}^s_1 = F_x, \quad \hat{m}^s_2 = F_y,
\]

\[
\hat{m}^s_3 = 6 \mathbf{F} \cdot \mathbf{u}, \quad \hat{m}^s_4 = 2 (F_x u_x - F_y u_y), \quad \hat{m}^s_5 = (F_x u_y + F_y u_x),
\]

\[
\hat{m}^s_6 = (1 - 3 u_x^2) F_y - 6 F_x u_x u_y, \quad \hat{m}^s_7 = (1 - 3 u_y^2) F_x - 6 F_y u_y u_x,
\]

\[
\hat{m}^s_8 = 3 \left[ (6 u_y^2 - 2) F_x u_x + (6 u_x^2 - 2) F_y u_y \right].
\]

Equivalently, the above equations can be written in a matrix form as \(\mathbf{K} \cdot \mathbf{S} = (\hat{m}^s_0, \hat{m}^s_1, \hat{m}^s_2, \ldots, \hat{m}^s_8)^\dagger\). Now, inverting the above equation, we can obtain explicit expressions for \(S_\alpha\) in terms of the gen-
eral variable body force $F$ and fluid velocity $u$ in the particle velocity space as

$$S_0 = \frac{1}{9} [-\hat{m}_3 + \hat{m}_8],$$ \hspace{1cm} (1.17a)

$$S_1 = \frac{1}{36} [6\hat{m}_1 - \hat{m}_3 + 9\hat{m}_4 + 6\hat{m}_7 - 2\hat{m}_8],$$ \hspace{1cm} (1.17b)

$$S_2 = \frac{1}{36} [6\hat{m}_2 - \hat{m}_3 - 9\hat{m}_4 + 6\hat{m}_6 - 2\hat{m}_8],$$ \hspace{1cm} (1.17c)

$$S_3 = \frac{1}{36} [-6\hat{m}_1 - \hat{m}_3 + 9\hat{m}_4 - 6\hat{m}_7 - 2\hat{m}_8],$$ \hspace{1cm} (1.17d)

$$S_4 = \frac{1}{36} [-6\hat{m}_2 - \hat{m}_3 - 9\hat{m}_4 - 6\hat{m}_6 - 2\hat{m}_8],$$ \hspace{1cm} (1.17e)

$$S_5 = \frac{1}{36} [6\hat{m}_1 + 6\hat{m}_2 + 2\hat{m}_3 + 9\hat{m}_5 - 3\hat{m}_6 - 3\hat{m}_7 + \hat{m}_8],$$ \hspace{1cm} (1.17f)

$$S_6 = \frac{1}{36} [-6\hat{m}_1 + 6\hat{m}_2 + 2\hat{m}_3 - 9\hat{m}_5 - 3\hat{m}_6 + 3\hat{m}_7 + \hat{m}_8],$$ \hspace{1cm} (1.17g)

$$S_7 = \frac{1}{36} [-6\hat{m}_1 - 6\hat{m}_2 + 2\hat{m}_3 + 9\hat{m}_5 + 3\hat{m}_6 + 3\hat{m}_7 + \hat{m}_8],$$ \hspace{1cm} (1.17h)

$$S_8 = \frac{1}{36} [6\hat{m}_1 - 6\hat{m}_2 + 2\hat{m}_3 - 9\hat{m}_5 + 3\hat{m}_6 - 3\hat{m}_7 + \hat{m}_8].$$ \hspace{1cm} (1.17i)

Then, to determine the structure of the cascaded collision operator in the presence of forcing terms we start from the lowest-order nonconservative (i.e., second order) moments, and perform relaxation of various central moments to their corresponding equilibria, each carried out at different relaxation times. See Refs. [15, 19] for details. Thus, the change of different moments under
The cascaded collision can be summarized as

\begin{align}
\hat{g}_0 &= \hat{g}_1 = \hat{g}_2 = 0, \\
\hat{g}_3 &= \frac{\omega_3}{12} \left\{ \frac{2}{3} \rho + \frac{\rho (u_x^2 + u_y^2)}{\gamma} - (\hat{\kappa}'_{xx} + \hat{\kappa}'_{yy}) - \frac{1}{2} (\hat{\sigma}'_{xx} + \hat{\sigma}'_{yy}) \right\}, \\
\hat{g}_4 &= \frac{\omega_4}{4} \left\{ \frac{\rho (u_x^2 - u_y^2)}{\gamma} - (\hat{\kappa}'_{xx} - \hat{\kappa}'_{yy}) - \frac{1}{2} (\hat{\sigma}'_{xx} - \hat{\sigma}'_{yy}) \right\}, \\
\hat{g}_5 &= \frac{\omega_5}{4} \left\{ \frac{\rho u_x u_y}{\gamma} - \hat{\kappa}'_{xy} - \frac{1}{2} \hat{\sigma}'_{xy} \right\}, \\
\hat{g}_6 &= \frac{\omega_6}{4} \left\{ 2 \rho u_x^2 u_y + \hat{\kappa}'_{xxy} - 2 u_x \hat{\kappa}'_{xy} - u_y \hat{\kappa}'_{xx} - \frac{1}{2} \hat{\sigma}'_{xxy} \right\} - \frac{1}{2} u_y (3 \hat{g}_3 + \hat{g}_4) - 2 u_x \hat{g}_5, \\
\hat{g}_7 &= \frac{\omega_7}{4} \left\{ 2 \rho u_x^2 u_y + \hat{\kappa}'_{xxy} - 2 u_y \hat{\kappa}'_{xy} - u_x \hat{\kappa}'_{yy} - \frac{1}{2} \hat{\sigma}'_{xxy} \right\} - \frac{1}{2} u_x (3 \hat{g}_3 - \hat{g}_4) - 2 u_y \hat{g}_5, \\
\hat{g}_8 &= \frac{\omega_8}{4} \left\{ \frac{1}{9} \rho + 3 \rho u_x^2 u_y^2 - \left[ \hat{\kappa}'_{xxyy} - 2 u_x \hat{\kappa}'_{xxy} - 2 u_y \hat{\kappa}'_{xyy} + u_x^2 \hat{\kappa}'_{xyy} + u_y^2 \hat{\kappa}'_{xyy} ight. \\
&\quad \left. + 4 u_x u_y \hat{\kappa}'_{xy} - \frac{1}{2} \hat{\sigma}'_{xxyy} \right\} - 2 \hat{g}_3 - \frac{1}{2} \hat{g}_3 (3 \hat{g}_3 + \hat{g}_4) - \frac{1}{2} \hat{g}_3 (3 \hat{g}_3 - \hat{g}_4) \\
&\quad - 4 u_x u_y \hat{g}_5 - 2 u_y \hat{g}_6 - 2 u_x \hat{g}_7.
\end{align}

For ease of implementation, the cascaded lattice Boltzmann equation with forcing term can then be presented in terms of following collision and streaming steps, respectively:

\begin{align}
\tilde{f}_\alpha(x,t) &= \tilde{f}_\alpha(x,t) + \Omega^C_\alpha + S_\alpha(x,t) \\
\tilde{f}_\alpha(x + e_\alpha, t + 1) &= \tilde{f}_\alpha(x, t).
\end{align}

where, \( \Omega^C_\alpha \) is obtained using Eq. (7.41) and Eqs. (1.18a)–(1.18g). Finally, the explicit form of the
The hydrodynamic variables are then obtained as

\[ \begin{align*}
\tilde{f}_0 &= \tilde{f}_0 + [\tilde{g}_0 - 4(\tilde{g}_3 - \tilde{g}_8)] + S_0, \\
\tilde{f}_1 &= \tilde{f}_1 + [\tilde{g}_0 + \tilde{g}_1 - \tilde{g}_3 + \tilde{g}_4 + 2(\tilde{g}_7 - \tilde{g}_8)] + S_1, \\
\tilde{f}_2 &= \tilde{f}_2 + [\tilde{g}_0 + \tilde{g}_2 - \tilde{g}_3 - \tilde{g}_4 + 2(\tilde{g}_6 - \tilde{g}_8)] + S_2, \\
\tilde{f}_3 &= \tilde{f}_3 + [\tilde{g}_0 - \tilde{g}_1 - \tilde{g}_3 + \tilde{g}_4 - 2(\tilde{g}_7 + \tilde{g}_8)] + S_3, \\
\tilde{f}_4 &= \tilde{f}_4 + [\tilde{g}_0 - \tilde{g}_2 - \tilde{g}_3 - \tilde{g}_4 - 2(\tilde{g}_6 + \tilde{g}_8)] + S_4, \\
\tilde{f}_5 &= \tilde{f}_5 + [\tilde{g}_0 + \tilde{g}_1 + \tilde{g}_2 + 2\tilde{g}_3 + \tilde{g}_5 - \tilde{g}_6 - \tilde{g}_7 + \tilde{g}_8] + S_5, \\
\tilde{f}_6 &= \tilde{f}_6 + [\tilde{g}_0 - \tilde{g}_1 + \tilde{g}_2 + 2\tilde{g}_3 - \tilde{g}_5 - \tilde{g}_6 + \tilde{g}_7 + \tilde{g}_8] + S_6, \\
\tilde{f}_7 &= \tilde{f}_7 + [\tilde{g}_0 - \tilde{g}_1 - \tilde{g}_2 + 2\tilde{g}_3 + \tilde{g}_5 + \tilde{g}_6 + \tilde{g}_7 + \tilde{g}_8] + S_7, \\
\tilde{f}_8 &= \tilde{f}_8 + [\tilde{g}_0 + \tilde{g}_1 - \tilde{g}_2 + 2\tilde{g}_3 - \tilde{g}_5 + \tilde{g}_6 - \tilde{g}_7 + \tilde{g}_8] + S_8.
\end{align*} \]

The hydrodynamic variables are then obtained as

\[ \rho = \sum_{\alpha} f_{\alpha}, \quad \rho u = \sum_{\alpha} f_{\alpha} e_{\alpha} + \frac{1}{2} F, \quad p = c_s^2 \rho. \] (1.21)

It can be shown via the standard multiscale Chapman-Enskog expansion that the solution of the above cascaded LB method represents the weakly compressible Navier-Stokes equations (NSE) (see e.g., [19])

\[ \begin{align*}
\partial_t \rho + \nabla \cdot (\rho u) &= 0, \quad (1.22a) \\
\partial_t (\rho u) + \nabla \cdot (\rho uu) &= -\nabla p + \nabla \cdot [\rho \nu (2S - I) \nabla \cdot u] + \rho \zeta \nabla \cdot u + F, \quad (1.22b)
\end{align*} \]

where \( S = \frac{1}{2} (\nabla u + (\nabla u)^\dagger) \) and \( I \) are the strain rate tensor and identity tensor, respectively, and \( F = (F_x, F_y) \). The transport coefficients of the fluid motion, such as the kinematic bulk viscosity \( \zeta \) and kinematic shear viscosity \( \nu \) are related to the relaxation times of the second order moments via

\[ \zeta = (1/3) (1/\omega_3 - 1/2), \quad \nu = (1/3) (1/\omega_\beta - 1/2), \quad \beta = 4, 5 \]

and the relaxation times for higher order moments \( \omega_\beta \), where \( \beta = 6, 7, 8 \) can be independently adjusted to improve numerical stability. See Ref. [17] for a comparison of the cascaded LB method.
against LB methods based on other collision models for standard benchmark problems involving the solution of the 2D NSE.

1.4 Research Goals and Original Contributions of This Dissertation

The research detailed in this dissertation presents several new innovations that advances the state-of-the-art in the lattice Boltzmann method based on central moments and multiple relaxation times for flow simulations with attendant additional multiphysics effects. The overall thrust is to improve the efficiency, i.e., the convergence acceleration, and accuracy of the cascaded LB method for computation of steady state flows, to expand its ability to handle force/source terms via a time-splitting approach, and to develop new cascaded LB schemes for simulation of thermal convective flows in multiple dimensions as well as for two-phase flows in conjunction with the capturing of interfaces. In addition, for the first time, we propose a new strategy in the LB method that enable local vorticity computation without requiring the finite differencing for the spatial derivatives in simulations of flows with a passive scalar transport. A central theme in our research is the use of two (or more) distribution functions that evolve using unified advanced LB formulations based on multiple relaxation times and central moments for various applications that involve the computation of fluid motion in conjunction with the transport of a scalar or capturing of interfaces, such as in heat transfer and multiphase flow problems, respectively. The specific goals of this dissertation are to develop, analyze, and perform numerical studies of the following:

- Preconditioned cascaded LB scheme for convergence acceleration with improved Galilean invariance

- Symmetrized operator splitting formulations force/source implementations in cascaded LB methods for flow and scalar transport
• Three-dimensional cascaded LB method for thermal convective flows

• Axisymmetric central moment LB schemes for flows with heat transfer including swirling effects

• Local vorticity computation approach using double distribution functions based LB techniques for flow and scalar transport

• Cascaded LB methods for two-phase flows with interface capturing based on a phase-field model including surfactant effects

In the following, we will briefly expand on the details of the above research goals and expected outcomes.

1.4.1 Preconditioned cascaded LB scheme for convergence acceleration with improved Galilean invariance

Lattice Boltzmann models used for the computation of fluid flows represented by the Navier-Stokes (NS) equations on standard lattices can lead to non Galilean invariant (GI) viscous stress involving cubic velocity errors. This arises from the dependence of their third order diagonal moments on the first order moments for standard lattices, i.e., the aliasing effects due to the discreteness and symmetry of the lattice. Strategies have recently been introduced to restore GI without such errors using a modified collision operator involving either corrections to the relaxation times or to the moment equilibria. Convergence acceleration in the simulation of steady flows can be achieved by solving the preconditioned NS equations, which contain a preconditioning parameter that can be used to tune the effective sound speed, and thereby alleviating the numerical stiffness.

In this research contribution, we will present a GI formulation of the preconditioned cascaded
central moment LB method used to solve the preconditioned NS equations, which is free of cubic velocity errors on a standard lattice, for steady flows. A Chapman-Enskog analysis is used to reveal the structure of the spurious non-GI defect terms and it is demonstrated that the anisotropy of the resulting viscous stress is dependent on the preconditioning parameter, in addition to the fluid velocity. It is shown that partial correction to eliminate the cubic velocity defects is achieved by scaling the cubic velocity terms in the off-diagonal third-order moment equilibria with the square of the preconditioning parameter. Furthermore, we develop additional corrections based on the extended moment equilibria involving gradient terms with coefficients dependent locally on the fluid velocity and the preconditioning parameter. Such parameter dependent corrections eliminate the remaining truncation errors arising from the degeneracy of the diagonal third-order moments and fully restores GI without cubic defects for the preconditioned LB scheme on a standard lattice.

Several conclusions will be drawn from the analysis of the structure of the non-GI errors and the associated corrections, with particular emphasis on their dependence on the preconditioning parameter. The new GI preconditioned central moment LB method will be validated for a number of complex flow benchmark problems and its effectiveness to achieve convergence acceleration and improvement in accuracy will be demonstrated.

1.4.2 Symmetrized operator splitting formulations force/source implementations in cascaded LB methods for flow and scalar transport

Fluid motion are generally driven/influenced by local body forces, and similarly the transport of a scalar field, such as temperature, by the local (heat) sources. We will present operator split forcing schemes exploiting a symmetrization principle, i.e. Strang splitting, for cascaded LB methods in two- and three-dimensions for fluid flows with impressed local forces. We will also derive analogous scheme for the passive scalar transport represented by a convection-diffusion equa-
tion with a source term in a novel cascaded LB formulation. They are based on symmetric applications of the split solutions of the changes on the scalar field/fluid momentum due to the sources/forces over half time steps before and after the collision step. The latter step is effectively represented in terms of the post-collision change of moments at zeroth and first orders, respectively, to represent the effect of the sources on the scalar transport and forces on the fluid flow.

Such symmetrized operator split cascaded LB schemes are consistent with the second-order Strang splitting and naturally avoid any discrete effects due to forces/sources by appropriately projecting their effects for higher order moments. All the force/source implementation steps are performed only in the moment space and they do not require formulations as extra terms and their additional transformations to the velocity space. These result in particularly simpler and efficient schemes to incorporate forces/sources in the cascaded LB methods unlike those considered previously. We will demonstrate the validity and accuracy, as well as the second-order convergence rate of the symmetrized operator split forcing/source schemes for the cascaded LB methods based on a numerical study of various benchmark problems in 2D and 3D for fluid flow problems with body forces and scalar transport with sources.

1.4.3 Three-dimensional cascaded LB method for thermal convective flows

Fluid motion driven by thermal effects, such as that due to buoyancy in differentially heated three-dimensional (3D) enclosures, arise in several natural settings and engineering applications. It is represented by the solutions of the Navier-Stokes equations (NSE) in conjunction with the thermal energy transport equation represented as a convection-diffusion equation (CDE) for the temperature field. In this research, we will develop new 3D lattice Boltzmann (LB) methods based on central moments and using multiple relaxation times for the three-dimensional, fifteen velocity (D3Q15) lattice, as well as its subset, i.e., the three-dimensional, seven velocity (D3Q7)
lattice to solve the 3D CDE for the temperature field in a double distribution function framework. Their collision operators lead to a cascaded structure involving higher order terms. In this approach, the fluid motion is solved by another 3D cascaded LB model from prior work. Owing to the differences in the number of collision invariants to represent the dynamics of flow and the transport of the temperature field, the structure of the collision operator for the 3D cascaded LB formulation for the CDE will be shown to be markedly different from that for the NSE. We will validate the new 3D cascaded LB schemes for thermal convective flows for natural convection of air driven thermally on two vertically opposite faces in a cubic cavity enclosure at different Rayleigh numbers against prior numerical benchmark solutions.

1.4.4 Axisymmetric central moment LB schemes for flows with heat transfer including swirling effects

Fluid motion in cylindrical coordinates with axial symmetry that is driven by rotational effects and/or thermal buoyancy effects arise widely in a number of technological applications and geophysical contexts. Computational effort for such problems can be significantly reduced if axial symmetry can be exploited; in such cases the system of equations can be reduced to a set of quasi-two-dimensional (2D) problems in the meridian plane, where the simulations can be performed for broader ranges of the parameter spaces more efficiently. We will present a cascaded LB approach to simulate thermal convective flows, which are driven by buoyancy forces and/or swirling effects, in a cylindrical coordinate system with axial symmetry. In this regard, the dynamics of the axial and radial momentum components along with the pressure are represented by means of the 2D Navier-Stokes equations with geometric mass and momentum source terms in the pseudo Cartesian form, while the evolutions of the azimuthal momentum and the temperature field are each modeled by an advection-diffusion type equation with appropriate local source terms.

Based on these, cascaded LB schemes involving three distribution functions will be formulated
to solve for the fluid motion in the meridian plane using a D2Q9 lattice, and to solve for the azimuthal momentum and the temperature field each using a D2Q5 lattice. The geometric mass and momentum source terms for the flow fields and the energy source term for the temperature field are included using a new symmetric operator splitting technique, via pre-collision and post-collision source steps around the cascaded collision step for each distribution function. These will result in a particularly simple and compact formulation to directly represent the effect of various geometric source terms consistently in terms of changes in the appropriate zeroth and first order moments. We will validate this new axisymmetric cascaded LB approach by means of simulations of several complex buoyancy-driven thermal flows and including rotational effects in cylindrical geometries and comparisons of the computed results against prior benchmark numerical results. In addition, we will demonstrate significant improvements in numerical stability with the use of the cascaded LB formulation when compared to other collision models for axisymmetric flow simulations.

1.4.5 Local vorticity computation approach using double distribution functions based LB techniques for flow and scalar transport

Computation of vorticity, or the skew-symmetric velocity gradient tensor, in conjunction with the strain rate tensor plays an important role in fluid mechanics in the classification of flows, in identifying vortical structures and in the modeling of various complex flows. For the simulation of flows accompanied by the advection-diffusion transport of a scalar field, double distribution functions (DDF) based LB methods, involving a pair of lattice Boltzmann equations (LBEs) are commonly used. We will present a new local vorticity computation approach, i.e., without involving finite differences, by introducing an intensional anisotropy of the scalar flux in the third order, off-diagonal moment equilibria of the LBE for the scalar field, and then combining the second order non-equilibrium components of both the LBEs. As such, any pair of lattice sets in the DDF formulation that can independently support the third order off-diagonal moments would en-
able local determination of the complete flow kinematics, with the LBEs for the fluid motion and
the transport of the passive scalar providing the necessary moment relationships to respectively
determine the symmetric and skew-symmetric components of the velocity gradient tensor.

As an illustration of our approach, we will formulate a DDF-LB model for local vorticity compu-
tation using a pair of multiple relaxation times (MRT) based collision approaches on D2Q9 lat-
tices, where the necessary moment relationships to determine the velocity gradient tensor and the
vorticity will be established via a Chapman-Enskog analysis. We will present a numerical study
that validates the predicted vorticity fields against the analytical solutions with good accuracy
and second order convergence.

1.4.6 Cascaded LB methods for two-phase flows with interface capturing based on a phase-
field model including surfactant effects

Simulation of multiphase flows, which are ubiquitous in nature and engineering applications, re-
quire coupled capturing or tracking of the interfaces in conjunction with the fluid motion often
occurring at multiple scales. In this contribution, we will present unified cascaded LB methods
for the solution of the incompressible two-phase flows at high density ratios and for the captur-
ing of the interfacial dynamics. Based on a modified continuous Boltzmann equation (MCBE) for
two-phase flows, where a kinetic transformation to the distribution function involving the pres-
sure field is introduced to reduce the associated numerical stiffness at high density gradients, a
central moment cascaded LB formulation for fluid motion will be constructed. In this LB scheme,
the collision step is prescribed by the relaxation of various central moments to their equilibria
that are reformulated in terms of the pressure field obtained via matching to the continuous equi-
libria based on the transformed Maxwell distribution. Furthermore, the differential treatments
for the effects of the source term representing the change due to the pressure field and of the
source term due to the interfacial tension force and body forces appearing in the MCBE on dif-
ferent moments are consistently accounted for in this cascaded LB solver that computes the pressure and velocity fields. In addition, another cascaded LB scheme will be developed to solve for the interfacial dynamics represented by a phase field model based on the conservative Allen-Cahn equation that evolves interfaces by advection and under the competing effects due to a diffusion term and an interfacial sharpening or phase segregation flux term. The latter is introduced into the cascaded LB scheme via a modification to the moment equilibria.

The use of central moments natural maintains the Galilean invariance of the all moments independently supported by the chosen lattice and improves the numerical stability of the resulting unified cascaded LB formulation for two-phase flows. Based on numerical simulations of a variety of two-phase flow benchmark problems, we will validate the new approach and demonstrate improvements in numerical stability. Furthermore, for surfactant-laden interfacial flows, where the presence of surfactant can be used to tune the interfacial dynamics, another cascaded LB scheme that solves its concentration field based on a phase-field model will be constructed. The resulting approach will be validated for self-propulsion of a drop under an imposed linear gradient of surfactant distribution and equilibrium profile of surfactant concentration under adsorption effects.

1.5 Organization of This Dissertation

Based on the above introduction and research goals, this dissertation is organized into a number of chapters, each addressing a particular area of investigation. Thus, each chapter will include a literature review, mathematical formulations and numerical scheme associated with the specific topic being addressed, which will then be followed by results and discussion, and a summary of the main findings. As required, additional details supporting the discussion are given in various appendices. In Chapter 2, we present a new preconditioned formulation of the cascaded LB method for efficient simulations, which is further improved for accuracy by a modification to preserve its Galilean invariance without cubic velocity errors. A simpler strategy based
on symmetrized operator splitting for including local body forces in fluid motion and sources in passive scalar transport using the cascaded LB method is elaborated in Chapter 3. Central moments based cascaded LB schemes for thermal convective flows in three-dimensions and axisymmetric coordinates are discussed in Chapters 4 and 5, respectively. Chapter 6 discusses a new LB method for local vorticity computation via double distribution functions based approach for flow and scalar transport. Then, new cascaded LB schemes for two-phase flows, based on a phase field model are presented in Chapter 7. The modeling of attendant surfactant effects in two-phase flows using a cascaded LB approach is discussed in Appendix F. Finally, Chapter 8 summarizes this dissertation research, its main conclusions and outlook for future research investigations in this area.
CHAPTER II

GALILEAN INVARIANT PRECONDITIONED CENTRAL MOMENT LATTICE BOLTZMANN METHOD WITHOUT CUBIC VELOCITY ERRORS FOR EFFICIENT STEADY FLOW SIMULATIONS

2.1 Introduction

The lattice Boltzmann (LB) method has now been established as a powerful kinetic scheme based computational fluid dynamics approach ([24], [7], [18]). It is a mesoscopic method based on local conservation and discrete symmetry principles, and may be derived as a special discretization of the Boltzmann equation. During the last decade, many efforts were made to further improve its numerical stability, accuracy and efficiency. In particular, sophisticated collision models based on multiple relaxation times and involving raw moments, central moments or cumulants, and entropic formulations have significantly expanded the capabilities of the LB method. The significant achievements of these developments and their applications to a variety of complex flow problems have been discussed, for example, in [11, 12, 25, 26, 27, 28, 29, 17, 30, 31, 32, 33].

There exist various additional aspects in the LB approach that require further attention and present scope for improvements. In particular, the finiteness of the lattice can introduce certain truncation errors that manifest as non-Galilean invariant viscous stress, i.e. fluid velocity dependent viscosity. This lack of Galilean invariance (GI) arises due to the fact that the diagonal terms in the third-order moments are not independently supported by the standard tensor-product lattices (i.e. D2Q9 and D3Q27). More specifically, for example,

\[ \hat{\kappa}^{'}_{xxx} = \sum_{\alpha} e_{\alpha x}^{3} f_{\alpha} = \sum_{\alpha} e_{\alpha x} f_{\alpha} = \hat{\kappa}^{'}_{x}. \]

Here, and in the following, the primed quantities denote raw moments. In other words, there is a degeneracy of the third-order diagonal (longitudinal) moments that results in a deviation
between the emergent macroscopic equations derived by the Chapman-Enskog expansion and the Navier-Stokes (NS) equations. Such cubic-velocity truncation errors are grid independent and persist in finer grids especially under high shear and flow velocity. Moreover, such emergent anisotropic viscous stress may have a negative impact on numerical stability as a result of a negative dependence of the emergent viscosity on the fluid velocity. In order to overcome this shortcoming, various attempts have been made.

One possibility is to consider a lattice with a larger particle velocity set, such as the D2Q17 lattice in two-dimensions [34], which was pursued after [35] pointed out nonlinear, cubic-velocity deviations of the emergent equations of the LB models with standard lattice sets from the NS equations. This involved the use of higher order velocity terms in the equilibrium distribution. However, [36] showed that the specific equilibria adopted in [34] does not fully eliminate the cubic-velocity errors. Moreover, the use of non-standard lattice stencils with larger number of particle velocities increases the computational cost and propensity of the numerical instability at grid scales. On the other hand, it was shown more recently by various others ([37], [36], [38]) that partial corrections to the GI errors on the standard lattice (i.e. D2Q9 lattice) may be achieved by adopting special forms of the off-diagonal, third-order moments in the equilibria. That is,

\[
\hat{\kappa}_{eq}^{\prime} \kappa_{xxy} = c_s^2 \rho u_y + \rho u_x u_y, \quad \hat{\kappa}_{eq}^{\prime} \kappa_{xyy} = c_s^2 \rho u_x + \rho u_x u^2_y.
\]

Here, \(c_s\) is the speed of sound and the particular choices of the cubic-velocity terms that are underlined are crucial to partially restore GI for the above identified moments. Here, we also point out that the above forms of the off-diagonal, third-order raw moment equilibria that allow such partial GI corrections naturally arise in the central moment LB formulations, when the equilibrium central moment components are set to zero and then rewritten in terms of their corresponding raw moments. However, since \(\hat{\kappa}_{eq}^{\prime} \kappa_{xxx} = \hat{\kappa}_{x}^{eq}\) and \(\hat{\kappa}_{eq}^{\prime} \kappa_{yyy} = \hat{\kappa}_{y}^{eq}\) due to the degeneracy of the third-order longitudinal moments, which is inherent to the standard tensor-product lattices, additional corrections are required to restore GI completely free of cubic-velocity errors. In this regard, in order to compensate the terms which violate GI on standard lattices, LB schemes with
single relaxation time models were augmented with finite difference expressions [39, 40, 41]. On the other hand, more recently, [42] introduced small intentional anisotropies into a matrix collision operator that corrects the anisotropy in the resulting viscous stress tensor thereby addressing the above mentioned issue. In addition, independently, [43] introduced additional corrections involving velocity gradients to the equilibria that achieved equivalent results. These two studies provided strategies to represent the Navier-Stokes equations in LB models on standard lattices completely free of cubic-velocity errors. In addition, [44] presented finite difference based corrections to the method proposed in [45] to reduce the resulting spurious velocity dependent viscosity effects on standard lattices.

While the LB schemes have found applications to a wide range of fluid flow problems, there has also been considerable interest to an important class of problems related to low Reynolds number steady state flows. They include analysis and design optimization of a variety of Stokes flows through capillaries, porous media flows, heat transfer problems under stationary conditions, and since the LB methods are explicit marching in nature, efficient solution techniques need to be devised to accelerate their convergence (see e.g. [46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]). A recent review of the literature in the LB approach for such problems can be found in [58, 59]. Generally, multigrid and preconditioning techniques can be devised to improve the steady state convergence of the LB scheme. A comparison of a multigrid LB formulation with the conventional solvers showed significant improvement in efficiency [55]. At low Mach numbers, the convergence can be further accelerated by means of preconditioning for both the traditional single grid LB methods [49, 52, 53, 58, 59] and multigrid LB scheme [60]. The present chapter addresses a further refinement to the LB techniques for steady state flows, viz., improving the accuracy of the acceleration strategy based on the preconditioned LB formulation without GI cubic velocity and parameter dependent errors.

Thus, it is clear that another aspect of the LB method, similar to certain schemes based on the classical CFD, is its slow convergence to steady state at low Mach numbers. In such conditions,
there is a relatively large disparity between the sound speed and the convection speed of the fluid motion resulting in higher eigenvalue stiffness and larger number of iterations for convergence. This stiffness can be alleviated and convergence can be significantly improved by preconditioning. Reference [49] presented a preconditioned LB method based on a single relaxation time model by modifying the equilibrium distribution function by using a preconditioning parameter. Then, [52] and [53] presented preconditioned LB formulations based on multiple relaxation times. More recently, [58] presented a preconditioned scheme for the central moment based cascaded LB method [15] in the presence of forcing terms [19] and demonstrated significant convergence acceleration.

In general, such preconditioned LB schemes are intended to solve the preconditioned NS equations, which can be written as ([61], [62])

\[
\frac{\partial p}{\partial t} + \nabla \cdot (\rho u) = 0, \tag{2.1a}
\]

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot \left( \frac{\rho uu}{\gamma} \right) = -\frac{1}{\gamma} \nabla p^* + \frac{1}{\gamma} \nabla \cdot (\rho \nu S) + \frac{F}{\gamma}, \tag{2.1b}
\]

where \( p^* \), \( S \) and \( F \) are the pressure, strain rate tensor and the impressed force, respectively. Here, \( \gamma \) is the preconditioning parameter, which can be used to tune the pseudo-sound speed, thereby alleviating the eigenvalue stiffness and improving convergence acceleration (e.g. [58]). However, the existing LB models for the preconditioned NS equations are not Galilean invariant and are expected to involve both velocity- and parameter-dependent anisotropic form of the viscous stress tensor. Development of the Galilean invariant preconditioned central moment based LB method without cubic-velocity defects and parameter free truncation errors for steady flow simulations is the main focus of this study. It may be noted that the preconditioned NS equations may be considered as a specific example of what may be called as the generalized NS equations containing a free parameter. In the present case, such a parameter is imposed by numerics due to preconditioning. On the other hand, such generalized NS equations arise in other contexts such as in the simulation of the fluid saturated variable porous media flows represented by the Brinkman-Forchheimer-Darcy equation. In such cases, the free parameter appearing in the generalized NS
equations is imposed by physics, viz., the porosity. Thus, our present investigation on the development of the Galilean invariant LB models for the preconditioned NS equations on standard lattices without cubic-velocity and parameter dependent errors also has wider implications in other contexts.

In order to first identify such truncation errors, in this chapter we first perform a Chapman-Enskog analysis of the preconditioned central moment LB formulation and isolate various cubic-velocity and parameter dependent errors at various moment orders. It will be seen that the anisotropy of the stress tensor depends not just on the cubic-velocity terms (like in the previous studies), but also on the preconditioning parameter $\gamma$. Furthermore, we will also demonstrate that even to achieve partial corrections for the GI defects on the standard lattice, the cubic velocity terms appearing in the off-diagonal components of the third-order moment equilibria need to be appropriately scaled by $\gamma$ (e.g. $\tilde{\kappa}_{xxy}^c = c_s^2 \rho u_y + \rho u_x^2 u_y / \gamma^2$). In general, the various truncation error terms that arise due to the degeneracy of the third-order diagonal elements will be seen to have complex dependence on both the velocities and the preconditioning parameter. Once such GI defect terms are identified, new corrections are derived for the preconditioned central moment LB formulation based on the extended moment equilibria. This results in a GI central moment LB method for the preconditioned NS equations without cubic-velocity and parameter based defects on standard lattices. The present scheme is targeted towards efficient and accurate low Reynolds number steady state laminar flows by a preconditioned LB formulation without the discrete cubic velocity and parameter dependent effects via corrections to the moment equilibria.

This chapter is organized as follows. In the next section (Sec. 2.2), our previous central moment based preconditioned LBM with forcing terms on the D2Q9 lattice is summarized first. Section 3 performs a more refined analysis based on the Chapman-Enskog expansion and identifies various cubic-velocity and parameter dependent GI defect errors. Then, Sec 2.4 derives new corrections based on the extended moment equilibria and Sec. 2.5 presents a GI preconditioned central moment LB method free of cubic-velocity and parameter dependent errors. Numerical results are
presented in Sec. 2.6, which compares our numerical results for a variety of benchmark problems, including the lid-driven cavity flow, flow over a square cylinder, backward facing step flow, the Hartmann flow and the four-roll mills flow problem for the purpose of validation. In addition, convergence acceleration due to preconditioning and improvement in accuracy due to the GI corrected LB scheme are also illustrated. Finally, the main findings of this chapter are summarized in Sec. 2.7.

2.2 Preconditioned Cascaded Central Moment Lattice Boltzmann Method: Non-Galilean Invariant Formulation

In our previous work, we presented a modified cascaded central moment lattice Boltzmann method (LBM) with forcing terms for the computation of preconditioned NS equations [58]. However, this preconditioned LBM formulation is not Galilean invariant on standard lattices. This is because it results in grid-independent cubic-velocity errors that are sensitive to the preconditioning parameter. In fact, the derivation of the precise expression for the non-GI truncation errors will be derived in the next section. It may be noted that all other prior preconditioned LB schemes are also not Galilean invariant. However, the choice of central moments here partially corrects parts of the cubic velocity defects in the off-diagonal third order moments naturally (Sec. 2.3) and simplifies derivation of the correction terms to completely restore GI free of cubic velocity errors on standard lattice (Sec. 2.4). Here, we summarize our previous preconditioned central moment LB model setting the stage for further development in the following.

The preconditioned cascaded central moment LBM with forcing terms may be written as [58]

$$\tilde{f}_\alpha(x,t) = \bar{f}_\alpha(x,t) + (K \cdot \hat{g})_\alpha + S_\alpha(x,t), \quad (2.2a)$$

$$\bar{f}_\alpha(x + e_\alpha, t + 1) = \tilde{f}_\alpha(x, t), \quad (2.2b)$$

where a variable transformation $\tilde{f}_\alpha = f_\alpha - \frac{1}{2} S_\alpha$ is introduced to maintain second order accuracy in the presence of forcing terms. In the above, $K$ is the orthogonal transformation matrix and
\( \hat{g} \) is the collision operator. In order to list the expressions for the collision kernel for the standard two-dimensional, nine particle velocity (D2Q9) lattice, we first define various sets of raw moments as follows on which it is based:

\[
\begin{pmatrix}
\hat{\sigma}_{x'y'}^m
\hat{\sigma}_{x'y'}^{eq}
\hat{\sigma}_{x'y'}^{m}
\end{pmatrix} = \sum_{\alpha} \begin{pmatrix}
f_{\alpha}^m
f_{\alpha}^{eq}
S_{\alpha}
\end{pmatrix} \epsilon_{x'y'}^{m}
\tag{2.3}
\]

The preconditioned collision kernel set for the orthogonal moment basis using the preconditioning parameter \( \gamma \) can be written as [58]

\[
\tilde{g}_0 = \tilde{g}_1 = \tilde{g}_2 = 0,
\]

\[
\tilde{g}_3 = \frac{\omega_3}{12} \left\{ \frac{2}{3} \rho + \frac{\rho u_x^2 + u_y^2}{\gamma} - \tilde{K}_{xx} - \tilde{K}_{yy} - \frac{1}{2} (\tilde{\sigma}_{xx} + \tilde{\sigma}_{yy}) \right\},
\]

\[
\tilde{g}_4 = \frac{\omega_4}{4} \left\{ \frac{\rho u_x u_y}{\gamma} - \tilde{K}_{xy} - \frac{1}{2} \tilde{\sigma}_{xy} \right\},
\]

\[
\tilde{g}_5 = \frac{\omega_5}{4} \left\{ \frac{\rho u_x u_y}{\gamma} - \tilde{K}_{xy} - \frac{1}{2} \tilde{\sigma}_{xy} \right\},
\]

\[
\tilde{g}_6 = \frac{\omega_6}{4} \left\{ 2 \rho u_x^2 u_y + \tilde{K}_{xxy} - 2 u_x \tilde{K}_{xy} - u_y \tilde{K}_{xx} - \frac{1}{2} \tilde{\sigma}_{xx} \right\} - \frac{1}{2} u_y (\tilde{g}_3 + \tilde{g}_4) - 2 u_x \tilde{g}_5,
\]

\[
\tilde{g}_7 = \frac{\omega_7}{4} \left\{ 2 \rho u_x^2 u_y + \tilde{K}_{xxy} - 2 u_y \tilde{K}_{xy} - u_x \tilde{K}_{yy} - \frac{1}{2} \tilde{\sigma}_{xy} \right\} - \frac{1}{2} u_x (\tilde{g}_3 + \tilde{g}_4) - 2 u_y \tilde{g}_5,
\]

\[
\tilde{g}_8 = \frac{\omega_8}{4} \left\{ \frac{1}{2} \rho - 3 \rho u_x^2 u_y - \tilde{K}_{xxyy} - 2 u_x \tilde{K}_{xxy} - 2 u_y \tilde{K}_{xxy} + u_x^2 \tilde{K}_{yy} + u_y^2 \tilde{K}_{xx} + 4 u_x u_y \tilde{K}_{xy} \right\} - \frac{1}{2} \tilde{\sigma}_{xxyy} - 2 \tilde{g}_3 - \frac{1}{2} u_y (3 \tilde{g}_3 + \tilde{g}_4) - \frac{1}{2} u_x^2 (3 \tilde{g}_3 + \tilde{g}_4) - 4 u_x u_y \tilde{g}_5 - 2 u_y \tilde{g}_6 - 2 u_x \tilde{g}_7.
\]

For further details, and including the choice of the collision matrix \( K \) and source raw moments \( \hat{\sigma}_{x'y'}^{m} \), see [58]. This scheme results in a tunable pseudo-sound speed \( c_s^* = \gamma c_s \), where \( c_s = \frac{1}{\sqrt{3}} \delta_x / \delta_t \), and the emergent viscosity \( \nu \) is given by \( \nu = \frac{1}{3} (\omega_\beta - \frac{1}{2}) \), \( \beta = 4, 5 \). While this scheme is intended to simulate the preconditioned NS equations given in Eq. (1), as will be shown via a consistency analysis based on the Chapman-Enskog expansion in the next section that it leads to velocity-and preconditioning parameter-dependent non-GI truncation errors. In particular, it will be seen that the components of the non-equilibrium parts of the second order moments, which
contribute to the viscous stress tensor, depends on cubic velocity truncation errors and modulated by the preconditioning parameter $\gamma$.

2.3 Derivation of Non-Galilean Invariant Spurious Terms in the Preconditioned Cascaded Central Moment LB Method: Chapman-Enskog Analysis

In order to facilitate the Chapman-Enskog analysis, the central moment LB formulation can be equivalently rewritten in terms of a collision process involving relaxation to a generalized equilibria in the lattice or rest frame of reference [58]. This strategy is considered in this chapter to further investigate the structure of the cubic velocity non-GI truncation errors for our preconditioned LB method. In this regard, it is convenient to define the non-orthogonal transformation matrix $T$ which is the basis to obtain the orthogonal collision matrix $K$ used in the previous section and on which the subsequent analysis follows:

$$T = \begin{bmatrix} e_{a}^0, e_{ax}, e_{ay}, e_{ax}^2, e_{ay}^2, e_{ax}^2 - e_{ay}^2, e_{ax}e_{ay}, e_{ax}^2e_{ay}, e_{ax}e_{ay}^2, e_{ax}e_{ay}^2 \end{bmatrix},$$  

(2.5)

where the usual bra-ket notation is used to represent the raw and column vectors in the $q$-dimensional space ($q = 9$) for the D2Q9 lattice. Then, the relation between the various sets of the raw moments and their corresponding states in the velocity space can be defined via this nominal, non-orthogonal transformation matrix $T$ as

$$\tilde{m} = T\bar{f}, \quad \hat{m} = Tf, \quad \hat{m}^{eq} = T\bar{f}^{eq}, \quad \hat{S} = TS,$$  

(2.6)

where

$$\bar{f} = (f_0, f_1, f_2, \ldots, f_8)^\dagger, \quad f = (f_0, f_1, f_2, \ldots, f_8)^\dagger,$$

$$f^{eq} = (f_0^{eq}, f_1^{eq}, f_2^{eq}, \ldots, f_8^{eq})^\dagger, \quad S = (S_0, S_1, S_2, \ldots, S_8)^\dagger.$$
are the various quantities in the velocity space, and

\[
\hat{\mathbf{m}} = (\hat{m}_0, \hat{m}_1, \hat{m}_2, \ldots, \hat{m}_8)^\dagger = \left(\hat{\kappa}_0', \hat{\kappa}_x', \hat{\kappa}_y', \hat{\kappa}_{xx}', \hat{\kappa}_{xy}', \hat{\kappa}_{yy}', \hat{\kappa}_{xx}', \hat{\kappa}_{xy}', \hat{\kappa}_{yy}'\right)^\dagger, (2.7a)
\]

\[
\hat{\mathbf{m}} = (\hat{m}_0, \hat{m}_1, \hat{m}_2, \ldots, \hat{m}_8)^\dagger = \left(\hat{\kappa}_0', \hat{\kappa}_x', \hat{\kappa}_y', \hat{\kappa}_{xx}', \hat{\kappa}_{xy}', \hat{\kappa}_{yy}', \hat{\kappa}_{xx}', \hat{\kappa}_{xy}', \hat{\kappa}_{yy}'\right)^\dagger, (2.7b)
\]

\[
\hat{\mathbf{m}}^{eq} = (\hat{m}_0^{eq}, \hat{m}_1^{eq}, \hat{m}_2^{eq}, \ldots, \hat{m}_8^{eq})^\dagger = \left(\hat{\kappa}_0^{eq}, \hat{\kappa}_x^{eq}, \hat{\kappa}_y^{eq}, \hat{\kappa}_{xx}' + \hat{\kappa}_{xy}' + \hat{\kappa}_{yy}' - \hat{\kappa}_{xx}', \hat{\kappa}_{xy}', \hat{\kappa}_{yy}'\right)^\dagger, (2.7c)
\]

\[
\hat{S} = \left(\hat{S}_0, \hat{S}_1, \hat{S}_2, \ldots, \hat{S}_8\right)^\dagger = \left(\hat{\sigma}_0', \hat{\sigma}_x', \hat{\sigma}_y', \hat{\sigma}_{xx}', \hat{\sigma}_{xy}', \hat{\sigma}_{yy}'\right)^\dagger, (2.7d)
\]

are the corresponding states in the moment space.

To facilitate the Chapman-Enskog analysis, we can rewrite the preconditioned LB model presented in Eq. (2.2a) and Eq. (2.2b) in terms of the raw moment space given in Eq. (2.6) as ([19], [58])

\[
f(x + e_\alpha \delta_t, t + \delta_t) - f(x, t) = \mathbf{T}^{-1} \left[ -\hat{\Lambda} (\hat{\mathbf{m}} - \hat{\mathbf{m}}^{eq}) \right] + \mathbf{T}^{-1} \left[ \left( \mathbf{I} - \frac{1}{2} \hat{\Lambda} \right) \hat{\mathcal{S}} \right] \delta_t, (2.8)
\]

where the diagonal relaxation time matrix \(\hat{\Lambda}\) is defined as

\[
\hat{\Lambda} = \text{diag}(0, 0, 0, \omega_3, \omega_4, \omega_5, \omega_6, \omega_7, \omega_8). (2.9)
\]

The preconditioned raw moments of the equilibrium distribution and source terms can be represented as

\[
\hat{\kappa}_{xx}' = \rho + \frac{\rho u_x^2}{\gamma}, \quad \hat{\kappa}_{xy}' = \frac{\rho u_x u_y}{\gamma}, \quad \hat{\kappa}_{yy}' = \frac{\rho u_y^2}{\gamma},
\]

\[
\hat{\sigma}_0' = 0, \quad \hat{\sigma}_x' = \frac{F_x}{\gamma}, \quad \hat{\sigma}_y' = \frac{F_y}{\gamma}, \quad \hat{\sigma}_{xx}' = \frac{2F_x u_x}{\gamma^2}, \quad \hat{\sigma}_{xy}' = \frac{2F_x u_y + F_y u_x}{\gamma^2}, \quad \hat{\sigma}_{yy}' = \frac{F_y u_y^2 + 2F_x u_x u_y}{\gamma^2},
\]

\[
\hat{\sigma}_{xxy}' = 2(F_x u_x u_y^2 + F_y u_y u_x^2). (2.11)
\]
The following comments are in order here. Up to the second order moments, the above expressions coincide with those presented in our previous work [58]). In other words, \( u_i u_j \) terms in the moment equilibria are preconditioned by \( \gamma \), while the first and second order moment terms, i.e. \( F_i \) and \( F_i u_j \) are preconditioned by \( \gamma \) and \( \gamma^2 \), respectively. As a first new element towards a LB scheme with an improved GI, we precondition the third-order moment equilibria terms \( u_i u_j^2 \) terms by \( \gamma^2 \) (see the terms inside boxes in Eq. (2.10)). This partially restores GI without cubic velocity defects for the preconditioned LB model for the off-diagonal components of the third-order moments. In fact, as will be shown later in this section, in order to remove the spurious cross-velocity derivative terms appearing in the equivalent macroscopic equations of our preconditioned LB scheme (e.g. \( u_x u_y \partial_x u_y \) and \( u_y u_x \partial_y u_x \)), such a scaling of the cubic velocity terms in the third order moment equilibria is essential. Then, applying the standard Chapman-Enskog multiscale expansion to Eq. (2.8), i.e.

\[
\hat{m} = \sum_{n=0}^{\infty} \epsilon^n \hat{m}^{(n)},
\]

\[
\partial_t \hat{m} = \sum_{n=0}^{\infty} \epsilon^n \partial_{\tau_n}.
\]

where \( \epsilon \) is a small bookkeeping perturbation parameter, and also using a Taylor expansion to simplify the streaming operator in Eq. (2.8), i.e.

\[
f(x + e_\alpha \epsilon, t + \epsilon) = \sum_{n=0}^{\infty} \epsilon^n \left( \partial_t + e_\alpha \cdot \nabla \right)^n f(x, t).
\]

After converting all the resulting terms into the moment space using Eq. (2.6), we get the following moment equations at consecutive order in \( \epsilon \):

\[
O(\epsilon^0) : \quad \hat{m}^{(0)} = \hat{m}^{eq},
\]

\[
O(\epsilon^1) : \quad (\partial_{\tau_0} + \hat{E}_i \partial_i) \hat{m}^{(0)} = -\hat{\Lambda} \hat{m}^{(1)} + \hat{S},
\]

\[
O(\epsilon^2) : \quad \partial_i \hat{m}^{(0)} + (\partial_{\tau_0} + \hat{E}_i \partial_i) \left[ I - \frac{1}{2} \hat{\Lambda} \right] \hat{m}^{(1)} = -\hat{\Lambda} \hat{m}^{(2)},
\]

where \( \hat{E}_i = T(e_\epsilon, I)T^{-1}, i \in \{x, y\} \). The relevant components of the first-order \( O(\epsilon) \) equations Eq. (2.15b), i.e. up to the second order in moment space needed for deriving the preconditioned
macroscopic hydrodynamics equations are given as

\[ \partial_t \rho + \partial_x (\rho u_x) + \partial_y (\rho u_y) = 0, \]

(2.16a)

\[ \partial_t (\rho u_x) + \partial_x \left( \frac{1}{2} \rho + \frac{\rho u_x^2}{\gamma} \right) + \partial_y \left( \frac{\rho u_x u_y}{\gamma} \right) = \frac{F_x}{\gamma}, \]

(2.16b)

\[ \partial_t (\rho u_y) + \partial_x \left( \frac{\rho u_x u_y}{\gamma} \right) + \partial_y \left( \frac{1}{2} \rho + \frac{\rho u_y^2}{\gamma} \right) = \frac{F_y}{\gamma}, \]

(2.16c)

\[ \partial_t \left( \frac{2}{3} \rho + \frac{\rho(u_x^2 + u_y^2)}{\gamma} \right) + \partial_x \left( \frac{4}{3} \rho u_x + \frac{\rho u_x u_y}{\gamma} \right) + \partial_y \left( \frac{4}{3} \rho u_y + \frac{\rho u_x^2 u_y}{\gamma} \right) \]

\[ = -\omega_3 \hat{m}_3^{(1)} + \frac{2(F_x u_x + F_y u_y)}{\gamma}, \]

(2.16d)

\[ \partial_t \left( \frac{\rho(u_x^2 - u_y^2)}{\gamma} \right) + \partial_x \left( \frac{2}{3} \rho u_x - \frac{\rho u_x u_y^2}{\gamma} \right) + \partial_y \left( -\frac{2}{3} \rho u_y + \frac{\rho u_x^2 u_y}{\gamma} \right) \]

\[ = -\omega_4 \hat{m}_4^{(1)} + \frac{2(F_x u_x - F_y u_y)}{\gamma}, \]

(2.16e)

\[ \partial_t \left( \frac{\rho u_x u_y}{\gamma} \right) + \partial_x \left( \frac{1}{3} \rho u_x + \frac{\rho u_x u_y^2}{\gamma} \right) + \partial_y \left( \frac{1}{3} \rho u_y + \frac{\rho u_x^2 u_y}{\gamma} \right) \]

\[ = -\omega_5 \hat{m}_5^{(1)} + \frac{F_y u_y + F_y u_x}{\gamma}. \]

(2.16f)

Similarly, the leading order moment equations at \( O(\epsilon^2) \) can be obtained from Eq. (2.15c) as

\[ \partial_t \rho = 0, \]

(2.17a)

\[ \partial_t u_x + \partial_x \left[ \frac{1}{2} \left( 1 - \frac{1}{2} \omega_3 \right) \hat{m}_3^{(1)} + \frac{1}{4} \left( 1 - \frac{1}{2} \omega_4 \right) \hat{m}_4^{(1)} \right] + \partial_y \left[ \left( 1 - \frac{1}{2} \omega_5 \right) \hat{m}_5^{(1)} \right] = 0, \]

(2.17b)

\[ \partial_t u_y + \partial_x \left[ \frac{1}{4} \left( 1 - \frac{1}{2} \omega_5 \right) \hat{m}_5^{(1)} \right] + \partial_y \left[ \frac{1}{2} \left( 1 - \frac{1}{2} \omega_3 \right) \hat{m}_3^{(1)} - \frac{1}{2} \left( 1 - \frac{1}{2} \omega_4 \right) \hat{m}_4^{(1)} \right] = 0. \]

(2.17c)

In the above equations, the second-order, non-equilibrium moments \( \hat{m}_3^{(1)}, \hat{m}_4^{(1)} \) and \( \hat{m}_5^{(1)} \) (corresponding to, \( \hat{\kappa}_x^{(1)} + \hat{\kappa}_y^{(1)}, \hat{\kappa}_x^{(1)} - \hat{\kappa}_y^{(1)} \) and \( \hat{\kappa}_x^{(1)} \), respectively) are unknowns. Ideally, they should only be related to the strain rate tensor components to recover the correct physics related to the viscous stress. However, as will be shown below, on the standard D2Q9 lattice there will be non-GI contributions dependent on the preconditioning parameter \( \gamma \). In what follows, \( \hat{m}_3^{(1)}, \hat{m}_4^{(1)} \) and \( \hat{m}_5^{(1)} \) will be obtained from Eq. (2.16d), Eq. (2.16e) and Eq. (2.16f), respectively.
Now, from Eq. (2.16d), the non-equilibrium moment $\hat{m}_3^{(1)}$ can be written as

$$\hat{m}_3^{(1)} = \frac{1}{\omega_3} \left[ -\partial_t \left( \frac{2}{\gamma} \rho + \frac{\rho (u_x^2 + u_y^2)}{\gamma} \right) - \partial_x \left( \frac{4}{\gamma} \rho u_x + \frac{\rho u_x u_y}{\gamma} \right) - \partial_y \left( \frac{4}{\gamma} \rho u_y + \frac{\rho u_x^2}{\gamma} \right) + \frac{2 (F_x u_x + F_y u_y)}{\gamma^2} \right]. \tag{2.18}$$

In order to simplify Eq. (2.18) further, one needs to obtain expressions, in particular, for $\partial_t \left( \frac{\rho u_x^2}{\gamma} \right)$, $\partial_t \left( \frac{\rho u_y^2}{\gamma} \right)$, $\partial_x \left( \frac{\rho u_x u_y}{\gamma} \right)$ and $\partial_y \left( \frac{\rho u_x u_y}{\gamma} \right)$. It follows from Eq. (2.16b) that

$$\partial_t (\rho u_x) = -\frac{1}{3} \partial_x \rho - \partial_x \left( \frac{\rho u_x^2}{\gamma} \right) - \partial_y \left( \frac{\rho u_x u_y}{\gamma} \right) + \frac{F_x}{\gamma}. \tag{2.19}$$

Rearranging Eq. (2.19) as

$$\partial_t \left( \frac{\rho u_x^2}{\gamma} \right) = \frac{2 u_x}{\gamma} \partial_t (\rho u_x) + \frac{u_x^2}{\gamma} \partial_t \rho. \tag{2.20}$$

Using Eq. (2.19) and Eq. (2.16a) to replace the time derivative in the first and second terms respectively, on the right hand side of the above equation, we get.

$$\partial_t \left( \frac{\rho u_x^2}{\gamma} \right) = \frac{2 u_x}{\gamma} \left[ -\frac{1}{3} \partial_x \rho - \partial_x \left( \frac{\rho u_x^2}{\gamma} \right) - \partial_y \left( \frac{\rho u_x u_y}{\gamma} \right) + \frac{F_x}{\gamma} \right] + \frac{u_x^2}{\gamma} \left[ \partial_x (\rho u_x) + \partial_y (\rho u_y) \right]. \tag{2.21}$$

Similarly, we may write

$$\partial_t \left( \frac{\rho u_y^2}{\gamma} \right) = \frac{2 u_y}{\gamma} \left[ -\frac{1}{3} \partial_y \rho - \partial_y \left( \frac{\rho u_y^2}{\gamma} \right) - \partial_x \left( \frac{\rho u_x u_y}{\gamma} \right) + \frac{F_y}{\gamma} \right] + \frac{u_y^2}{\gamma} \left[ \partial_x (\rho u_x) + \partial_y (\rho u_y) \right]. \tag{2.22b}$$

Thus, the time derivative can be replaced with the spatial derivative. Also , it readily follows that

$$-\partial_x \left( \frac{\rho u_x u_y}{\gamma} \right) = -\frac{u_x^2}{\gamma} \partial_x (\rho u_x) - \frac{2 \rho u_x u_y}{\gamma^2} \partial_x u_y, \tag{2.22a}$$

$$-\partial_y \left( \frac{\rho u_x u_y}{\gamma} \right) = -\frac{u_y^2}{\gamma} \partial_y (\rho u_y) - \frac{2 \rho u_x u_y}{\gamma^2} \partial_y u_x. \tag{2.22b}$$

Rearranging Eq. (2.20) and simplifying it further by retaining all cubic velocity terms and neglecting all others higher order terms in velocity (e.g. fifth order and higher) we get

$$-\partial_t \left( \frac{\rho u_x^2}{\gamma} \right) = \frac{2 u_x}{\gamma} \partial_x \rho + \frac{2 u_x}{\gamma} \partial_x (\rho u_x^2) + \frac{2 u_y^2}{\gamma^2} \partial_x u_y + \frac{2 \rho u_x u_y}{\gamma^2} \partial_y u_x - \frac{F_x u_x}{\gamma^2} \partial_x (\rho u_x) - \frac{u_x^2}{\gamma} \partial_y (\rho u_y). \tag{2.23}$$
Similarly, it follows from Eq. (2.21) that

\[-\partial_0 \left( \frac{\rho u_x^2}{\gamma} \right) = \frac{2u_y}{\gamma^2} \partial_y \rho + \frac{2u_y}{\gamma^2} \partial_y (\rho u_y^2) + \frac{2\rho u_x^2}{\gamma^2} \partial_x u_x + \frac{2\rho u_x u_y}{\gamma^2} \partial_x u_y + \frac{2F_x u_y}{\gamma^2} - \frac{u_x^2}{\gamma} \partial_x (\rho u_x) - \frac{u_y^2}{\gamma} \partial_y (\rho u_y). \tag{2.24}\]

Now, to obtain an expression for \( \hat{m}_3^{(1)} \), we group all the higher order terms given in Eqs. (2.22a), (2.22b), (2.23) and (2.24). It follows that owing to the choice of the off-diagonal third-order equilibrium moments with the cubic velocity terms scaled by \( \gamma^2 \) (i.e. \( \hat{\kappa}^{eq}_{xy} = \frac{1}{3} \rho u_y + \frac{\rho u_x^2}{\gamma^2}, \hat{\kappa}^{eq}_{xy} = \frac{1}{3} \rho u_x + \frac{\rho u_y^2}{\gamma^2} \)) at the outset following Eq. (2.9) earlier, all the cross-derivative spurious terms, i.e. \(-2\rho u_x u_y \partial_x u_y\) and \(-2\rho u_x u_y \partial_y u_x\) cancel. Then, simplifying the grouping of all the remaining higher order terms in Eq. (2.22a), Eq. (2.22b), Eq. (2.23) and Eq. (2.24) and retaining all cubic velocity terms and neglecting terms of negligible higher orders and after considerable rearrangement, we get

\[-\partial_0 \left( \frac{\rho u_x^2}{\gamma} \right) - \partial_0 \left( \frac{\rho u_y^2}{\gamma} \right) - \partial_x \left( \frac{\rho u_x^2}{\gamma^2} \right) - \partial_y \left( \frac{\rho u_y^2}{\gamma^2} \right) \approx \frac{2}{3\gamma} (u_x \partial_x \rho + u_y \partial_y \rho) - \frac{2}{\gamma^2} (F_x u_x + F_y u_y) + \rho \left[ \left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) u_x^2 + \left( \frac{1}{\gamma^2} - \frac{1}{\gamma} \right) u_y^2 \right] \partial_x u_x + \rho \left[ \left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) u_y^2 + \left( \frac{1}{\gamma^2} - \frac{1}{\gamma} \right) u_x^2 \right] \partial_y u_y. \tag{2.25}\]

By substituting the above equation (Eq. (2.25)) in Eq. (2.18) and using \( \partial_0 \rho = -\partial_x (\rho u_x) - \partial_y (\rho u_y) \) from Eq. (2.16a) to further simplify the resulting expressions, we finally get the form of the non-equilibrium moment \( \hat{m}_3^{(1)} \) as

\[\hat{m}_3^{(1)} = -\frac{2\rho}{3\omega_3} (\partial_x u_x + \partial_y u_y) + \frac{2}{3\omega_3} \left( \frac{1}{\gamma} - 1 \right) (u_x \partial_x \rho + u_y \partial_y \rho) + \frac{\rho}{\omega_3} \left[ \left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) u_x^2 + \left( \frac{1}{\gamma^2} - \frac{1}{\gamma} \right) u_y^2 \right] \partial_x u_x + \rho \left[ \left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) u_y^2 + \left( \frac{1}{\gamma^2} - \frac{1}{\gamma} \right) u_x^2 \right] \partial_y u_y. \tag{2.26}\]

Similarly, using Eq. (2.16e) and following analogous procedure as above for \( \hat{m}_4^{(1)} \) and using Eq. (2.16f) for \( \hat{m}_5^{(1)} \) after considerable algebraic manipulations and simplifications we get the expressions for
the remaining non-equilibrium second-order moments as

\[ \hat{m}_4^{(1)} = \frac{-2\rho}{3\omega_4} (\partial_x u_x - \partial_y u_y) + \frac{2}{3\omega_4} \left( \frac{1}{\gamma} - 1 \right) (u_x \partial_x \rho - u_y \partial_y \rho) + \frac{\rho}{\omega_4} \left[ \left( \frac{4}{\gamma^2} - \frac{1}{2} \right) u_x^2 - \left( \frac{1}{\gamma^2} - \frac{1}{2} \right) u_y^2 \right] \partial_x u_x + \frac{\rho}{\omega_4} \left[ - \left( \frac{4}{\gamma^2} - \frac{1}{2} \right) u_y^2 + \left( \frac{1}{\gamma^2} - \frac{1}{2} \right) u_x^2 \right] \partial_y u_y, \]  

(2.27)

and

\[ \hat{m}_5^{(1)} = \frac{-\rho}{3\omega_5} (\partial_x u_y + \partial_y u_x) + \frac{1}{3\omega_5} \left( \frac{1}{\gamma} - 1 \right) (u_x \partial_y \rho + u_y \partial_x \rho) + \frac{1}{\omega_5} \left( \frac{1}{\gamma^2} - \frac{1}{4} \right) \rho u_x u_y (\partial_x u_x + \partial_y u_y). \]

(2.28)

The first terms, which are underlined, in the right hand sides of Eq. (2.26), Eq. (2.27) and Eq. (2.28) are associated with the required flow physics related to the components of the viscous stress tensor. All the remaining terms in these equations are non-Galilean invariant terms for the preconditioned LB scheme. These spurious terms arise because the diagonal third-order moments \( \hat{\kappa}_{xxx} \) and \( \hat{\kappa}_{yyy} \) are not supported by the standard D2Q9 lattice. However, such discrete effects are not observed in the C-E analysis of the continuous Boltzmann equation. In order to eliminate the non-GI error terms by other means in the next section on the standard lattice, we explicitly identify the various non-GI terms in the components of the second-order non-equilibrium moments as

\[ E_{3g\rho}^3 = 2 \frac{2}{3\omega_3} \left( \frac{1}{\gamma} - 1 \right) (u_x \partial_x \rho + u_y \partial_y \rho), \]

(2.29a)

\[ E_{3g\mu}^3 = \frac{\rho}{\omega_3} \left[ \left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) u_x^2 + \left( \frac{1}{\gamma^2} - \frac{1}{2} \right) u_y^2 \right] \partial_x u_x + \frac{\rho}{\omega_3} \left[ \left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) u_y^2 + \left( \frac{1}{\gamma^2} - \frac{1}{2} \right) u_x^2 \right] \partial_y u_y. \]

(2.29b)

\[ E_{4g\rho}^4 = 2 \frac{2}{3\omega_4} \left( \frac{1}{\gamma} - 1 \right) (u_x \partial_x \rho - u_y \partial_y \rho), \]

(2.30a)

\[ E_{4g\mu}^4 = \frac{\rho}{\omega_4} \left[ \left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) u_x^2 - \left( \frac{1}{\gamma^2} - \frac{1}{2} \right) u_y^2 \right] \partial_x u_x + \frac{\rho}{\omega_4} \left[ - \left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) u_y^2 + \left( \frac{1}{\gamma^2} - \frac{1}{2} \right) u_x^2 \right] \partial_y u_y. \]

(2.30b)
and
\[
E_{g\rho}^5 = \frac{1}{3\omega_5} \left( \frac{1}{\gamma} - 1 \right) (u_x \partial_y \rho + u_y \partial_x \rho), \quad (2.31a)
\]
\[
E_{gu}^5 = \frac{\rho}{\omega_5} \left( \frac{1}{\gamma^2} - \frac{1}{\gamma} \right) u_x u_y \partial_x u_x + \frac{\rho}{\omega_5} \left( \frac{1}{\gamma^2} - \frac{1}{\gamma} \right) u_x u_y \partial_y u_y. \quad (2.31b)
\]

Then, we can rewrite the non-equilibrium second-order moments
\[
\hat{m}_3^{(1)} = \tilde{\kappa}_{xx}^{(1)'} + \tilde{\kappa}_{yy}^{(1)'} = -\frac{2\rho}{3\omega_3} (\partial_x u_x + \partial_y u_y) + E_{g\rho}^3 + E_{gu}^3, \quad (2.32)
\]
\[
\hat{m}_4^{(1)} = \tilde{\kappa}_{xx}^{(1)'} - \tilde{\kappa}_{yy}^{(1)'} = -\frac{2\rho}{3\omega_4} (\partial_x u_x - \partial_y u_y) + E_{g\rho}^4 + E_{gu}^4, \quad (2.33)
\]
\[
\hat{m}_5^{(1)} = \tilde{\kappa}_{xy}^{(1)'} = -\frac{\rho}{3\omega_5} (\partial_x u_y + \partial_y u_x) + E_{g\rho}^5 + E_{gu}^5. \quad (2.34)
\]

Some interesting observations can be made from the above analysis: (i) when the LB scheme is preconditioned, i.e. \( \gamma \neq 1 \), non-GI terms persist in terms of velocity and density gradients for all the second-order non-equilibrium moments, including the off-diagonal moment (\( \hat{m}_5^{(1)} = \tilde{\kappa}_{xy}^{(1)'} \)), unlike that for the simulation of the standard NS equations (i.e. with \( \gamma = 1 \)). However, the non-GI cubic velocity contributions in \( \hat{m}_5^{(1)} \) vanish for incompressible flow (\( \nabla \cdot \mathbf{u} = 0 \)), i.e. \( E_{g\rho}^5 = 0 \). (ii). In general the prefactors appearing in the non-GI terms for the diagonal components, i.e. in \( \hat{m}_3^{(1)} \) and \( \hat{m}_4^{(1)} \) exhibit dramatically different behaviour for the asymptotic limit cases: No preconditioning case (\( \gamma \to 1 \)): \( \left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) \sim 3, \left( \frac{1}{\gamma^2} - \frac{1}{\gamma} \right) \sim 0 \); strong preconditioning case (\( \gamma \to 0 \)): \( \left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) \sim \frac{4}{\gamma^2}, \left( \frac{1}{\gamma^2} - \frac{1}{\gamma} \right) \sim \frac{1}{\gamma^2} \). Thus, due to the complicated structure of the truncation errors and their dependence on \( \gamma \), the non-GI terms in the diagonal moment components modify significantly as \( \gamma \) varies due to preconditioning. (iii) when \( \gamma = 1 \), i.e. when our preconditioned LB scheme reverts to the solution of the standard NS equations, \( E_{g\rho}^3 = E_{g\rho}^4 = E_{g\rho}^5 = 0, E_{gu}^3 = \frac{3\rho}{\omega_3} (u_x^2 \partial_x u_x + u_y^2 \partial_y u_y), E_{gu}^4 = \frac{3\rho}{\omega_4} (u_x^2 \partial_x u_x - u_y^2 \partial_y u_y), \) and \( E_{gu}^5 = 0 \). That is, the non-GI terms become identical to the results reported by [42] and [43].
2.4 Derivation of Corrections via Extended Moment Equilibria for Elimination of Cubic Velocity errors in Preconditioned Macroscopic Equations

In order to effectively eliminate the non-GI error terms given in Eq. (2.29a)-(2.31b) that appear in the non-equilibrium moments \( \hat{m}_3^{(1)}, \hat{m}_4^{(1)} \) and \( \hat{m}_5^{(1)} \) in the previous section (see Eqs. (2.32)-(2.34)) arising due to the third-order diagonal equilibrium moments \( \hat{\kappa}_{eq}^{xx}, \hat{\kappa}_{eq}^{yy} \) not being independently supported by the D2Q9 lattice, we consider an approach based on the extended moment equilibria. In other words, we extended the second-order moment equilibria by including extra gradient terms with unknown coefficients as follows:

\[
\hat{f}_{eq}^{(1)} = \begin{bmatrix}
\hat{m}_0^{eq(0)} \\
\hat{m}_1^{eq(0)} \\
\hat{m}_2^{eq(0)} \\
\hat{m}_3^{eq(0)} \\
\hat{m}_4^{eq(0)} \\
\hat{m}_5^{eq(0)} \\
\hat{m}_6^{eq(0)} \\
\hat{m}_7^{eq(0)} \\
\hat{m}_8^{eq(0)}
\end{bmatrix}
\begin{bmatrix}
0 \\
0 \\
0 \\
\hat{m}_3^{eq(1)} \\
\hat{m}_4^{eq(1)} \\
\hat{m}_5^{eq(1)} \\
0 \\
0 \\
0
\end{bmatrix}
= \begin{bmatrix}
\hat{\kappa}_0^{eq} \\
\hat{\kappa}_x^{eq} \\
\hat{\kappa}_y^{eq} \\
\hat{\kappa}_{xx}^{eq} + \hat{\kappa}_{yy}^{eq} \\
\hat{\kappa}_{xx}^{eq} - \hat{\kappa}_{yy}^{eq} \\
\hat{\kappa}_{xy}^{eq} \\
\hat{\kappa}_{xy}^{eq} \\
\hat{\kappa}_{xy}^{eq} \\
\hat{\kappa}_{xy}^{eq}
\end{bmatrix}
\begin{bmatrix}
0 \\
\theta_x^3 \partial_x u_x + \theta_y^3 \partial_y u_y + \lambda_x^3 \partial_x \rho + \lambda_y^3 \partial_y \rho \\
\theta_x^4 \partial_x u_x - \theta_y^4 \partial_y u_y + \lambda_x^4 \partial_x \rho - \lambda_y^4 \partial_y \rho \\
\theta_x^5 \partial_x u_x + \theta_y^5 \partial_y u_y + \lambda_x^5 \partial_x \rho + \lambda_y^5 \partial_y \rho \\
0 \\
0 \\
0
\end{bmatrix}
\]

(2.35)

In other words, the corrections to the second-order moments are given by

\[
\hat{m}_3^{eq(1)} = (\theta_x^3 \partial_x u_x + \theta_y^3 \partial_y u_y) + (\lambda_x^3 \partial_x \rho + \lambda_y^3 \partial_y \rho),
\]

(2.36a)

\[
\hat{m}_4^{eq(1)} = (\theta_x^4 \partial_x u_x - \theta_y^4 \partial_y u_y) + (\lambda_x^4 \partial_x \rho - \lambda_y^4 \partial_y \rho),
\]

(2.36b)

\[
\hat{m}_5^{eq(1)} = (\theta_x^5 \partial_x u_x + \theta_y^5 \partial_y u_y) + (\lambda_x^5 \partial_x \rho + \lambda_y^5 \partial_y \rho),
\]

(2.36c)

where the coefficients \( \theta_j^j, \theta_j^y, \lambda_j^x \) and \( \lambda_j^y \), where \( j = 3, 4, 5 \) are to be determined from a modified Chapman-Enskog analysis so that the non-GI cubic velocity terms are effectively removed from the emergent preconditioned macroscopic moment equations.
We now apply a Chapman-Enskog (C-E) expansion by taking into account the modified equilibria which is now given as \( \hat{m}^{eq} = \hat{m}^{eq(0)} + \delta_t \hat{m}^{eq(1)} \), where \( \hat{m}^{eq(0)} \) is the moment equilibria presented in the previous section and \( \hat{m}^{eq(1)} \) is the correction to this equilibria. As a result, the C-E expansion given as Eq. (2.12) and Eq. (2.13) are now replaced with

\[
\hat{m} = \hat{m}^{eq(0)} + \epsilon \hat{m}^{eq(1)} + \epsilon^2 \hat{m}^{(2)} + \cdots, \quad \delta_t = \partial_t + \epsilon \partial_{t_1} + \epsilon^2 \partial_{t_2} + \cdots. \tag{2.37}
\]

Then, by using a Taylor expansion given in Eq. (2.14) for the streaming operator in Eq. (2b) along with above modified C-E expansion Eq. (2.37), we get the following hierarchy of moment equations at different orders in \( \epsilon \):

\[
O(\epsilon^0) : \quad \hat{m}^{(0)} = \hat{m}^{eq}, \tag{2.38a}
\]

\[
O(\epsilon^1) : \quad (\partial_t + \hat{E}_i \partial_i) \hat{m}^{(0)} = -\hat{\Lambda} [\hat{m}^{(1)} - \hat{m}^{eq(1)}] + \hat{S}, \tag{2.38b}
\]

\[
O(\epsilon^2) : \quad \partial_t \hat{m}^{(0)} + (\partial_t + \hat{E}_i \partial_i) \left[ I - \frac{1}{2} \hat{\Lambda} \right] \hat{m}^{(1)} + (\partial_t + \hat{E}_i \partial_i) \left[ \frac{1}{2} \hat{\Lambda} \hat{m}^{eq(1)} \right] = -\hat{\Lambda} \hat{m}^{(2)}, \tag{2.38c}
\]

where \( \hat{E}_i = T(e_i)T^{-1} \) and \( i \in \{x, y\} \). The relevant \( O(\epsilon) \) equations for the first order moments are given in Eqs. (2.16a)-(2.16c). However, the equations of the second order moments are now modified due to the presence of the extended moment equilibria \( \hat{m}^{eq(1)} \) in Eq. (2.38b) which are now given by (instead of Eqs. (2.16d)-(2.16f))

\[
\partial_t \left( \frac{2}{3} \rho + \frac{\rho(u_x^2 + u_y^2)}{\gamma} \right) + \partial_x \left( \frac{4}{3} \rho u_x + \frac{\rho u_x u_y}{\gamma} \right) + \partial_y \left( \frac{4}{3} \rho u_y + \frac{\rho u_x u_y}{\gamma} \right) - \omega_3 \hat{m}_3^{(1)} + \omega_3 \hat{m}^{eq(1)} + \frac{2(u_x u_x + F_u u_y)}{\gamma^2}, \tag{2.39a}
\]

\[
\partial_t \left( \frac{\rho(u_x^2 - u_y^2)}{\gamma} \right) + \partial_x \left( \frac{2}{3} \rho u_x - \frac{\rho u_x u_y}{\gamma} \right) + \partial_y \left( -\frac{2}{3} \rho u_y + \frac{\rho u_x u_y}{\gamma} \right) - \omega_4 \hat{m}_4^{(1)} + \omega_4 \hat{m}^{eq(1)} + \frac{2(u_x u_x - F_u u_y)}{\gamma^2}, \tag{2.39b}
\]

\[
\partial_t \left( \frac{\rho u_x u_y}{\gamma} \right) + \partial_x \left( \frac{1}{3} \rho u_x + \frac{\rho u_x u_y}{\gamma} \right) + \partial_y \left( \frac{1}{3} \rho u_y + \frac{\rho u_x u_y}{\gamma} \right) - \omega_5 \hat{m}_5^{(1)} + \omega_5 \hat{m}^{eq(1)} + \frac{F_u u_y + F_y u_x}{\gamma^2}. \tag{2.39c}
\]

Similarly, the leading order moment equations of \( O(\epsilon^2) \) which are modified by \( \hat{m}^{eq(1)} \) as shown in
Eq. (2.38c) are obtained as (instead of Eqs. (2.17a)-(2.17c))

\[ \partial_t \rho = 0, \quad (2.40a) \]

\[
\partial_t (\rho u_x) + \partial_x \left[ \frac{1}{4} \left( 1 - \frac{1}{2} \omega_3 \right) \tilde{m}_3^{(1)} + \frac{1}{2} \left( 1 - \frac{1}{2} \omega_4 \right) \tilde{m}_4^{(1)} \right] + \partial_y \left[ (1 - \frac{1}{2} \omega_5) \tilde{m}_5^{(1)} \right] + \partial_x \left[ \frac{1}{4} \omega_3 \tilde{m}_3^{eq(1)} + \frac{1}{4} \omega_4 \tilde{m}_4^{eq(1)} \right] + \partial_y \left[ \frac{1}{4} \omega_5 \tilde{m}_5^{eq(1)} \right] = 0, \quad (2.40b) \]

\[
\partial_t (\rho u_y) + \partial_x \left[ (1 - \frac{1}{2} \omega_3) \tilde{m}_3^{(1)} \right] + \partial_y \left[ \frac{1}{4} \left( 1 - \frac{1}{2} \omega_3 \right) \tilde{m}_3^{(1)} - \frac{1}{2} (1 - \frac{1}{2} \omega_4) \tilde{m}_4^{(1)} \right] + \partial_x \left[ \frac{1}{4} \omega_3 \tilde{m}_3^{eq(1)} - \frac{1}{4} \omega_4 \tilde{m}_4^{eq(1)} \right] = 0. \quad (2.40c) \]

The non-equilibrium moment \( \tilde{m}_3^{(1)} \) is now obtained from Eq. (2.39a) as

\[
\tilde{m}_3^{(1)} \approx \left. \frac{1}{\omega_3} \left[ -\partial_u \left( \frac{2}{3} \rho + \frac{\rho (u_x^2 + u_y^2)}{\gamma} \right) - \partial_x \left( \frac{1}{3} \rho u_x + \frac{\rho u_x u_y}{\gamma} \right) - \partial_y \left( \frac{1}{3} \rho u_y + \frac{\rho u_x u_y}{\gamma} \right) + \frac{2 (F_x u_x + F_y u_y)}{\gamma^2} \right] \right| \tilde{m}_3^{eq(1)}. \quad (2.41) \]

All the terms within the square brackets in the above equation exactly corresponds to Eq. (2.32).

Hence, Eq. (2.41) reduces to

\[
\tilde{m}_3^{(1)} = -\frac{2 \rho}{3 \omega_3} (\partial_x u_x + \partial_y u_y) + E_{3y}^3 + E_{3x}^3 + \tilde{m}_3^{eq(1)}, \quad (2.42) \]

where the non-GI error terms \( E_{3y}^3 \) and \( E_{3x}^3 \) are given in Eqs. (2.29a) and (2.29b), respectively, and the extended moment equilibrium \( \tilde{m}_3^{eq(1)} \) in Eq. (2.36a). Similarly, the non-equilibrium moment \( \tilde{m}_4^{(1)} \) is obtained from Eq. (2.39b) and using Eq. (2.33) for simplification, and for \( \tilde{m}_5^{(1)} \) using Eqs. (2.39c) and (2.34), we finally get

\[
\tilde{m}_4^{(1)} = -\frac{2 \rho}{3 \omega_4} (\partial_x u_x - \partial_y u_y) + E_{4y}^4 + E_{4x}^4 + \tilde{m}_4^{eq(1)}, \quad (2.43) \]

\[
\tilde{m}_5^{(1)} = -\frac{\rho}{3 \omega_5} (\partial_x u_y + \partial_y u_x) + E_{5y}^5 + E_{5x}^5 + \tilde{m}_5^{eq(1)}. \quad (2.44) \]

Here, the non-GI error terms \( E_{4y}^4 \) and \( E_{4x}^4 \) are given in Eq. (2.30a) and Eq. (2.30b), respectively, and the correction equilibrium moment \( \tilde{m}_4^{eq(1)} \) in Eq. (2.36b). Likewise, \( E_{5y}^5 \) and \( E_{5x}^5 \) are obtained from Eqs. (2.31a) and (2.31b) respectively and \( \tilde{m}_5^{eq(1)} \) is presented in Eq. (2.36c).

Now, in order to obtain the preconditioned moment system for the conserved moments, we combine \( O(\epsilon) \) equations Eqs. (2.16a)-(2.16c) with \( \epsilon \times \) Eqs. (2.40a)-(2.40c) for the corresponding equa-
tions at $O(\epsilon^2)$, and using $\partial_t = \partial_{t_0} + \epsilon \partial_{t_1}$, we get
\begin{align}
\partial_t \rho + \partial_x (\rho u_x) + \partial_y (\rho u_y) &= 0, \\
\partial_t (\rho u_x) + \partial_x \left( \frac{1}{3} \rho + \frac{\rho u_x^2}{\gamma} \right) + \partial_y \left( \frac{\rho u_x u_y}{\gamma} \right) &= \frac{F_x}{\gamma} - \epsilon \partial_x \left[ \frac{1}{2} \left( 1 - \frac{\omega_3}{2} \right) \hat{m}_3^{(1)} + \frac{1}{2} \left( 1 - \frac{\omega_4}{2} \right) \hat{m}_4^{(1)} \right] - \epsilon \partial_y \left[ \frac{1}{2} \left( 1 - \frac{\omega_3}{2} \right) \hat{m}_5^{(1)} \right] \\
\partial_t (\rho u_y) + \partial_x \left( \frac{\rho u_x u_y}{\gamma} \right) + \partial_y \left( \frac{1}{3} \rho + \frac{\rho u_y^2}{\gamma} \right) &= \frac{F_y}{\gamma} - \epsilon \partial_x \left[ \frac{1}{2} \left( 1 - \frac{\omega_3}{2} \right) \hat{m}_3^{(1)} \right] - \epsilon \partial_y \left[ \frac{1}{2} \left( 1 - \frac{\omega_4}{2} \right) \hat{m}_4^{(1)} \right]
\end{align}
(2.45a)
(2.45b)
(2.45c)

Our goal is to show that the above equations (Eq. (2.45a)-(2.45c)) is consistent with the preconditioned NS equations (Eq. (1)) presented in Sec. 2.1 without the identified truncation errors, i.e. without involving the non-GI cubic velocity defects. Now, in order to relate the moment corrections $\hat{m}_3^{eq(1)}$, $\hat{m}_4^{eq(1)}$ and $\hat{m}_5^{eq(1)}$ appearing in the equilibria with the non-GI error terms, with a view to eliminate them, consider the right hand side of Eq. (2.45b) (i.e. the $x$-momentum equation) and substitute for $\hat{m}_3^{(1)}$, $\hat{m}_4^{(1)}$ and $\hat{m}_5^{(1)}$ from Eq. (2.42), Eq. (2.43) and Eq. (2.44), respectively, which becomes
\begin{align}
&= \frac{F_x}{\gamma} + \epsilon \partial_x \left[ \frac{1}{3} \left( \frac{1}{3} + \frac{1}{2} \right) \rho (\partial_x u_x + \partial_y u_y) + \frac{1}{3} \left( \frac{1}{3} - \frac{1}{2} \right) \rho (\partial_x u_x - \partial_y u_y) \right] \\
&\quad + \epsilon \partial_y \left[ \frac{1}{3} \left( \frac{1}{3} - \frac{1}{2} \right) \rho (\partial_x u_y + \partial_y u_x) \right]
\end{align}
\begin{align}
&- \epsilon \partial_x \left[ \frac{1}{2} \left( 1 - \frac{\omega_3}{2} \right) \left\{ E_{g3}^3 + E_{g3}^4 \right\} + \frac{1}{2} \left( 1 - \frac{\omega_4}{2} \right) \left\{ E_{g3}^4 + E_{g4}^4 \right\} \right] - \epsilon \partial_y \left[ \left( 1 - \frac{\omega_3}{2} \right) \left\{ E_{g3}^5 + E_{g4}^5 \right\} \right]
\end{align}
\begin{align}
&- \epsilon \partial_x \left[ \frac{1}{2} \hat{m}_3^{eq(1)} + \frac{1}{2} \hat{m}_4^{eq(1)} \right] - \epsilon \partial_y \left[ \hat{m}_5^{eq(1)} \right].
\end{align}
(2.46)

The first two lines in the above equations correspond to the physics, while the third line corresponds to the spurious non-GI terms arising from discrete lattice effects and the fourth line are related to equilibrium corrections.

In order to eliminate the cubic velocity truncation errors, it follows that the third and fourth
lines in the above equation (Eq. (2.46)) sum to zero. This yields

\[ \left(1 - \frac{\omega_3}{2}\right) \{ E_{g\rho}^3 + E_{gu}^3 \} + \hat{m}_3^{eq(1)} = 0, \]  
(2.47a)

\[ \left(1 - \frac{\omega_4}{2}\right) \{ E_{g\rho}^4 + E_{gu}^4 \} + \hat{m}_4^{eq(1)} = 0, \]  
(2.47b)

\[ \left(1 - \frac{\omega_5}{2}\right) \{ E_{g\rho}^5 + E_{gu}^5 \} + \hat{m}_5^{eq(1)} = 0. \]  
(2.47c)

The above equations Eqs. (2.47a)-(2.47c), represent the key constraint relations between the non-GI error terms and the moment equilibria correction terms to obtain a preconditioned cascaded central moment LB model without cubic velocity defects.

Further analysis shows that these constraints hold identically for the \( y \)-momentum as well (Eq. 2.45c)).

Now considering Eq. (2.47a) and using Eq. (2.29a) and (2.29b) for \( E_{g\rho}^3 \) and \( E_{gu}^3 \), respectively, the extend moment equilibrium \( \hat{m}_3^{eq(1)} \) is given as

\[ \hat{m}_3^{eq(1)} = (\theta_x^3 \partial_x u_x + \theta_y^3 \partial_y u_y) + (\lambda_x^3 \partial_x \rho + \lambda_y^3 \partial_y \rho), \]  

where the coefficients obtained after matching are given by

\[ \theta_x^3 = -\left(\frac{1}{\omega_3} - \frac{1}{2}\right) \rho \left[ \left(\frac{4}{\gamma^2} - \frac{1}{2}\right) u_x^2 + \left(\frac{1}{\gamma^2} - \frac{1}{\gamma}\right) u_y^2 \right], \]  
(2.48a)

\[ \theta_y^3 = -\left(\frac{1}{\omega_3} - \frac{1}{2}\right) \rho \left[ \left(\frac{4}{\gamma^2} - \frac{1}{2}\right) u_x^2 + \left(\frac{1}{\gamma^2} - \frac{1}{\gamma}\right) u_y^2 \right], \]  
(2.48b)

\[ \lambda_x^3 = -\frac{2}{3} \left(\frac{1}{\omega_3} - \frac{1}{2}\right) \left(\frac{1}{\gamma} - 1\right) u_x, \]  
(2.48c)

\[ \lambda_y^3 = -\frac{2}{3} \left(\frac{1}{\omega_3} - \frac{1}{2}\right) \left(\frac{1}{\gamma} - 1\right) u_y. \]  
(2.48d)

Similarly, from Eq. (2.30a),(2.30b), (2.36b) and (2.47b), we can obtain the coefficient of \( \hat{m}_4^{eq(1)} \), and from Eq. (2.31a), Eq. (2.31b), Eq. (2.36c) and Eq. (2.47c), those for \( \hat{m}_5^{eq(1)} \) can be determined. The results read as follows:

\[ \hat{m}_4^{eq(1)} = (\theta_x^4 \partial_x u_x - \theta_y^4 \partial_y u_y) + (\lambda_x^4 \partial_x \rho - \lambda_y^4 \partial_y \rho), \]  

\[ \hat{m}_5^{eq(1)} = (\theta_x^5 \partial_x u_x - \theta_y^5 \partial_y u_y) + (\lambda_x^5 \partial_x \rho - \lambda_y^5 \partial_y \rho). \]
where
\[ \theta_4^x = - \left( \frac{1}{\omega_4} - \frac{1}{2} \right) \rho \left[ \left( \frac{1}{\gamma} - \frac{1}{2} \right) u_x^2 - \left( \frac{1}{\gamma} - \frac{1}{7} \right) u_y^2 \right], \] (2.49a)
\[ \theta_4^y = \left( \frac{1}{\omega_4} - \frac{1}{2} \right) \rho \left[ - \left( \frac{1}{\gamma} - \frac{1}{2} \right) u_y^2 + \left( \frac{1}{\gamma} - \frac{1}{7} \right) u_x^2 \right], \] (2.49b)
\[ \lambda_4^x = - \frac{2}{3} \left( \frac{1}{\omega_4} - \frac{1}{2} \right) \left( \frac{1}{\gamma} - 1 \right) u_x, \] (2.49c)
\[ \lambda_4^y = - \frac{2}{3} \left( \frac{1}{\omega_4} - \frac{1}{2} \right) \left( \frac{1}{\gamma} - 1 \right) u_y, \] (2.49d)

and
\[ \tilde{m}_5^{eq(1)} = (\theta_5^5 \partial_x u_x + \theta_5^5 \partial_y u_y) + (\lambda_5^x \partial_x \rho + \lambda_5^y \partial_y \rho), \]

where
\[ \theta_5^5 = - \left( \frac{1}{\omega_5} - \frac{1}{2} \right) \rho \left( \frac{1}{\gamma} - \frac{1}{7} \right) u_x u_y, \] (2.50a)
\[ \theta_5^5 = - \left( \frac{1}{\omega_5} - \frac{1}{2} \right) \rho \left( \frac{1}{\gamma} - \frac{1}{7} \right) u_x u_y, \] (2.50b)
\[ \lambda_5^x = - \frac{1}{3} \left( \frac{1}{\omega_5} - \frac{1}{2} \right) \rho \left( \frac{1}{\gamma} - 1 \right) u_x, \] (2.50c)
\[ \lambda_5^y = - \frac{1}{3} \left( \frac{1}{\omega_5} - \frac{1}{2} \right) \rho \left( \frac{1}{\gamma} - 1 \right) u_y. \] (2.50d)

Note that, as a special case, when \( \gamma = 1 \), i.e. the LB model is used to solve the standard NS equations without preconditioning, then \( \theta_3^3 = -3\rho(\frac{1}{\omega_3} - \frac{1}{2})u_x^2, \theta_3^5 = -3\rho(\frac{1}{\omega_3} - \frac{1}{2})u_y^2, \theta_4^3 = -3\rho(\frac{1}{\omega_4} - \frac{1}{2})u_x^2, \theta_4^5 = -3\rho(\frac{1}{\omega_4} - \frac{1}{2})u_y^2, \) and all the remaining coefficient go to zero. In such a case, these moment corrections to the equilibria become identical to the GI corrections presented by [43] and equivalent to the alternative GI formulation without cubic velocity errors introduced by [42].

Finally, using the above extended moment equilibria (\( \tilde{m}_3^{eq(1)}, \tilde{m}_4^{eq(1)} \) and \( \tilde{m}_5^{eq(1)} \)) and the expression for the non-equilibrium moments (\( \tilde{m}_3^{(1)}, \tilde{m}_4^{(1)} \) and \( \tilde{m}_5^{(1)} \)) from Eq. (2.42)-Eq. (2.44) along with the constraint relations, i.e. Eqs. (2.47a)-(2.47c) in Eqs. (2.45a)-(2.45c), we get
\[ \partial_t \rho + \nabla \cdot j = 0, \] (2.51)
\[ \partial_t j_x + \nabla \cdot \left( \frac{j u_x}{\gamma} \right) = -\partial_x \frac{p^*}{\gamma} + \partial_x \left[ \frac{\varphi_4}{\gamma} (2 \partial_x j_x - \nabla \cdot j) + \frac{\varphi_3}{\gamma} \nabla \cdot j \right] \\
+ \partial_y \left[ \frac{\varphi_5}{\gamma} (\partial_x j_y + \partial_y j_x) \right] + \frac{F_x}{\gamma}, \] (2.52)
\[
\partial_t j_y + \nabla \cdot \left( \frac{j u_y}{\gamma} \right) = -\partial_y \frac{p^*}{\gamma} + \partial_x \left[ \frac{\vartheta_5}{\gamma} (\partial_x j_y + \partial_y j_x) \right] \\
+ \partial_y \left[ \frac{\vartheta_4}{\gamma} (2\partial_y j_y - \nabla \cdot j) + \frac{\vartheta_3}{\gamma} \nabla \cdot j \right] + \frac{F_y}{\gamma},
\]

(2.53)

where \( p^* = \frac{\gamma}{\gamma + 1} \rho \) is the pressure, \( j = \rho u \), and the bulk and shear viscosities are, respectively given by

\[
\vartheta_3 = \frac{\gamma}{3} \left( \frac{1}{\omega_3} - \frac{1}{2} \right), \quad \vartheta_4 = \frac{\gamma}{3} \left( \frac{1}{\omega_4} - \frac{1}{2} \right), \quad \vartheta_5 = \frac{\gamma}{3} \left( \frac{1}{\omega_5} - \frac{1}{2} \right).
\]

(2.54)

Thus, Eqs. (2.51)-(2.53) are consistent with the preconditioned NS equations given in Eqs. (2.1a)-(2.1b) without cubic velocity defects in GI due to the use of the extended moment equilibria presented earlier.

### 2.5 Galilean Invariant Preconditioned Cascaded Central Moment LBM without Cubic Velocity Errors on a Standard Lattice

The cascaded central moment LBM with forcing term presented in Eqs. (2.2a), (2.2b), (2.3) and (4) modify to enforce GI without cubic velocity errors as follows. Equations Eq. (2.2a), Eq. (2.2b) and Eq. (2.3) remains the same as before and the collision kernel given in Eq. (4) is modified to account for the extended moment equilibria in the second order moments as well as corrections to the third-order equilibrium moments. The change of moments \( \hat{g}_3, \hat{g}_4 \) and \( \hat{g}_5 \) for the second order components follow by augmenting the corresponding moment equilibria with the extended moment equilibria incorporating the GI corrections identified in the previous section. On the other hand, owing to the cascaded structure of the collision kernel, the GI corrections to the third order moment changes \( \hat{g}_6 \) and \( \hat{g}_7 \), which depend on the lower order moment changes, for the preconditioned central moment LB scheme need to be constructed carefully. They are obtained by prescribing the relaxation of the third order central moment components to their corresponding central moment equilibria. Following the derivation given in [19], they can then be represented as

\[
-6u_y \hat{g}_3 - 2u_y \hat{g}_4 - 8u_x \hat{g}_5 - 4\hat{g}_6 = \omega_6 [\hat{\kappa}^{eq}_{xxy} - \hat{\kappa}_{xxy}] \quad \text{and} \quad -6u_x \hat{g}_3 + 2u_x \hat{g}_4 - 8u_y \hat{g}_5 - 4\hat{g}_7 = \omega_7 [\hat{\kappa}^{eq}_{xyy} - \hat{\kappa}_{xyy}],
\]

where \( \hat{\kappa}_{xxy} \) and \( \hat{\kappa}_{xyy} \) are the third order central moment components, and \( \hat{\kappa}^{eq}_{xxy} \)
and $\tilde{\kappa}_{xy}^{eq}$, respectively, are their equilibria. Rewriting these central moment relaxations in terms of the relaxations of the raw moment components of the third and lower orders via the binomial theorem, it follows that

$$\tilde{g}_6 = \frac{\omega_6}{4} \left[ (\tilde{\kappa}'_{xxy} - \tilde{\kappa}_{xy}^{eq}) - 2u_x(\tilde{\kappa}'_{xy} - \tilde{\kappa}_{xy}^{eq}) - u_y(\tilde{\kappa}'_{xx} - \tilde{\kappa}_{xx}^{eq}) \right] - u_y \left( \frac{3}{2} \tilde{g}_3 + \frac{1}{2} \tilde{g}_4 \right) - 2u_x \tilde{g}_5,$$

$$\tilde{g}_7 = \frac{\omega_7}{4} \left[ (\tilde{\kappa}'_{xyy} - \tilde{\kappa}_{yy}^{eq}) - 2u_y(\tilde{\kappa}'_{xy} - \tilde{\kappa}_{xy}^{eq}) - u_x(\tilde{\kappa}'_{yy} - \tilde{\kappa}_{yy}^{eq}) \right] - u_x \left( \frac{3}{2} \tilde{g}_3 - \frac{1}{2} \tilde{g}_4 \right) - 2u_y \tilde{g}_5.$$

Now, using the components of the preconditioned raw moment equilibria, including those for the third order equilibrium moments with the GI corrections from Eq. (2.10), the final expressions for the change in moments for the collision kernel $\tilde{g}_6$ and $\tilde{g}_7$ can be derived. Thus, the modified preconditioned collision kernel with the GI corrections reads

$$\tilde{g}_0 = 0, \quad \tilde{g}_1 = 0, \quad \tilde{g}_2 = 0,$$

$$\tilde{g}_3 = \frac{\omega_3}{12} \left\{ \frac{2}{3} \rho + \rho(u_x^2 + u_y^2) / \gamma - (\tilde{\kappa}'_{xx} + \tilde{\kappa}'_{yy}) - \frac{1}{2} (\tilde{\sigma}'_{xx} + \tilde{\sigma}'_{yy}) + \left( \theta_x^3 \partial_x u_x + \theta_y^3 \partial_y u_y \right) \delta_t + \left( \lambda_x^3 \partial_x \rho + \lambda_y^3 \partial_y \rho \right) \delta_t \right\},$$

$$\tilde{g}_4 = \frac{\omega_4}{4} \left\{ \rho (u_x^2 - u_y^2) / \gamma - (\tilde{\kappa}'_{xx} - \tilde{\kappa}'_{yy}) - \frac{1}{2} (\tilde{\sigma}'_{xx} - \tilde{\sigma}'_{yy}) + \left( \theta_x^4 \partial_x u_x - \theta_y^4 \partial_y u_y \right) \delta_t + \left( \lambda_x^4 \partial_x \rho - \lambda_y^4 \partial_y \rho \right) \delta_t \right\},$$

$$\tilde{g}_5 = \frac{\omega_5}{4} \left\{ \rho u_x u_y / \gamma - \tilde{\kappa}'_{xy} - \frac{1}{2} \tilde{\sigma}'_{xy} + \left( \theta_x^5 \partial_x u_x + \theta_y^5 \partial_y u_y \right) \delta_t + \left( \lambda_x^5 \partial_x \rho + \lambda_y^5 \partial_y \rho \right) \delta_t \right\},$$

$$\tilde{g}_6 = \frac{\omega_6}{4} \left\{ \left( \frac{3}{7} - \frac{1}{10} \right) \rho u_x u_y + \tilde{\kappa}'_{xy} - 2u_x \tilde{\kappa}'_{xy} - u_y \tilde{\kappa}'_{xx} \right\} - \frac{1}{2} u_y (3 \tilde{g}_3 + \tilde{g}_4) - 2u_x \tilde{g}_5,$$

$$\tilde{g}_7 = \frac{\omega_7}{4} \left\{ \left( \frac{3}{7} - \frac{1}{10} \right) \rho u_x u_y + \tilde{\kappa}'_{xy} - 2u_y \tilde{\kappa}'_{xy} - u_x \tilde{\kappa}'_{yy} \right\} - \frac{1}{2} u_x (3 \tilde{g}_3 - \tilde{g}_4) - 2u_y \tilde{g}_5,$$

$$\tilde{g}_8 = \frac{\omega_8}{4} \left\{ \frac{1}{5} \rho + 3 \rho u_x^2 u_y^2 - \left[ \tilde{\kappa}'_{xyxy} - 2u_x \tilde{\kappa}'_{xyy} - 2u_y \tilde{\kappa}'_{xxy} + u_x^2 \tilde{\kappa}'_{yy} + u_y^2 \tilde{\kappa}'_{xx} + 4u_x u_y \tilde{\kappa}'_{xy} \right] \right\} - 2 \tilde{g}_3 - \frac{1}{2} u_y^2 (3 \tilde{g}_3 + \tilde{g}_4) - \frac{1}{2} u_x^2 (3 \tilde{g}_3 - \tilde{g}_4) - 4u_x u_y \tilde{g}_5 - 2u_y \tilde{g}_6 - 2u_x \tilde{g}_7.$$

where the various coefficients $\theta_x^j$, $\theta_y^j$, $\lambda_x^j$ and $\lambda_y^j$ where $j = 3, 4$ and 5 are given in Eqs. (2.48b)-(2.48d), and (2.49b)-(2.49d) and (2.50a)-(2.50d). The GI corrections are identified by means of the underlined terms in the cascaded collision kernel terms in the above equation.

It may be noted that other GI preconditioned LB schemes without cubic velocity errors can be
constructed from our results in the previous section. For example, a non-orthogonal moment
based multiple relaxation time LB method readily follows from the analysis presented before.
The spatial gradients for the velocity components and the density appearing in the extended
moment equilibria can be calculated using isotropic finite difference schemes. Alternatively, the
diagonal strain rate components \( \partial_x u_x \) and \( \partial_y u_y \) can be locally obtained from non-equilibrium
moments as follows, which is used in our simulation studies presented in the next section. From
Eqs. (2.42) and (2.47a) and rearranging, one may write the resulting expression as follows:

\[ -c_1 \partial_x u_x - c_2 \partial_y u_y = \hat{m}_3^{(1)} - e_\rho. \quad (2.55) \]

Similarly, from Eq. (2.43) and Eq. (2.47b), it follows that

\[ -\tilde{c}_1 \partial_x u_x + \tilde{c}_2 \partial_y u_y = \hat{m}_4^{(1)} - \tilde{e}_\rho, \quad (2.56) \]

where the coefficients \( c_1, c_2, \tilde{c}_1 \) and \( \tilde{c}_1 \) and the parameters \( e_\rho \) and \( \tilde{e}_\rho \) are defined as

\[
    c_1 = \left[ \frac{2}{3\omega_3} + P_\gamma \right] \rho, \quad \tilde{c}_1 = \left[ \frac{2}{3\omega_4} + \tilde{P}_\gamma \right] \rho, \\
    c_2 = \left[ \frac{2}{3\omega_3} + Q_\gamma \right] \rho, \quad \tilde{c}_2 = \left[ \frac{2}{3\omega_4} + \tilde{Q}_\gamma \right] \rho.
\]

(2.57) (2.58)

Here,

\[
    P_\gamma = -\frac{1}{2} (A_\gamma u_x^2 + B_\gamma u_y^2), \quad Q_\gamma = -\frac{1}{2} (A_\gamma u_y^2 + B_\gamma u_x^2), \\
    \tilde{P}_\gamma = -\frac{1}{2} (A_\gamma u_x^2 - B_\gamma u_y^2), \quad \tilde{Q}_\gamma = -\frac{1}{2} (A_\gamma u_y^2 - B_\gamma u_x^2)
\]

where \( A_\gamma = \left( \frac{4}{7^2} - \frac{1}{7} \right), B_\gamma = \left( \frac{1}{7^2} - \frac{1}{7} \right), C_\gamma = \left( \frac{1}{7} - 1 \right) \) and

\[
    e_\rho = \frac{1}{3} C_\gamma (u_x \partial_x \rho + u_y \partial_y \rho), \quad \tilde{e}_\rho = \frac{1}{3} C_\gamma (u_x \partial_x \rho - u_y \partial_y \rho).
\]

(2.59)

Solving Eqs. (2.55) and (2.56) for \( \partial_x u_x \) and \( \partial_y u_y \), we get

\[
    \partial_x u_x = \left[ \tilde{c}_2 (\hat{m}_3^{(1)} - e_\rho) + c_2 (\hat{m}_4^{(1)} - \tilde{e}_\rho) \right] / [-c_1 \tilde{c}_2 - \tilde{c}_1 c_2], \\
    \partial_y u_y = -\left[ c_1 (\hat{m}_4^{(1)} - \tilde{e}_\rho) + \tilde{c}_1 (\hat{m}_3^{(1)} - e_\rho) \right] / [-c_1 \tilde{c}_2 - \tilde{c}_1 c_2].
\]

(2.60a) (2.60b)
Here, the density gradients appearing in $e_\rho$ and $\tilde{\rho}$ Eqs. (2.59) may be computed using a isotropic finite difference scheme. In Eqs. (2.60a) and (2.60b), all the coefficients involving $\gamma$ need to be computed only once before the start of computations for efficient implementation; quantities such as $u_x^2$ and $u_y^2$ appearing in the factors $P$, $Q$, $\tilde{P}$ and $\tilde{Q}$ above need to be reused rather than perform the product calculations for every occurrence. A comparison of the computational costs for the uncorrected preconditioned LB scheme and the GI corrected preconditioned formulation is presented for a benchmark case study on the four-rolls mill flow problem at the end of the numerical results section (see Sec. 2.6.5), which also demonstrates a quantitative improvement in accuracy achieved with correction. The non-equilibrium moments $\hat{m}_3^{(1)}$ and $\hat{m}_4^{(1)}$ required in Eqs. (2.60a) and Eqs. (2.60b) are obtained as

\begin{align}
\hat{m}_3^{(1)} &= \sum_\alpha (e_{\alpha x}^2 + e_{\alpha y}^2) f_\alpha - \left[ \frac{2}{3} \rho + \frac{\rho (u_x^2 + u_y^2)}{\gamma} \right], \\
\hat{m}_4^{(1)} &= \sum_\alpha (e_{\alpha x}^2 - e_{\alpha y}^2) f_\alpha - \frac{\rho (u_x^2 - u_y^2)}{\gamma}.
\end{align}

### 2.6 Numerical Results

We will now present the validation of our new Galilean invariant preconditioned cascaded central moment LBM by making comparisons against prior numerical solutions for various complex flow benchmark problems. These include the lid-driven cavity flow, flow over a square cylinder, backward-facing step flow, the Hartmann flow and the four-roll mills flow problem. In addition, we will also demonstrate the convergence acceleration achieved using our preconditioning LB model for some of the benchmark flow problems.

#### 2.6.1 Lid-driven Cavity Flow

As the first test problem, the GI preconditioned central moment LB model is applied for the simulation of steady, two-dimensional flow within a square cavity driven by the motion of the
top lid. This is one of the classical internal flow benchmark problems with complex flow structures. The numerical simulations are computed at two different Reynolds numbers of 3200 and 5000, which are resolved by computational meshes with a resolution of $400 \times 400$. To implement the moving top wall at a velocity $U_p$, the standard momentum augmented half-way bounce back scheme is considered. In order to validate the numerical simulation results obtained with our GI preconditioned LB scheme, the computed dimensionless horizontal and vertical velocity profiles along the vertical and horizontal centerlines, respectively, for Reynolds number $Re = 3200$ and $5000$ and preconditioning parameter $\gamma = 0.1$, are presented with benchmark solutions of [2] in Fig. 2.1. The Mach number $Ma$ considered in the simulations is 0.05. It is clear that the velocity profiles for all the cases agree very well with the prior numerical data. Next, we investigate how the steady state convergence histories are influenced by the use of our new preconditioned formulation for this benchmark problem. Figure 2.2 presents the convergence histories for $Re = 3200$ obtained by varying the preconditioning parameter $\gamma$. Here $\gamma = 1$ corresponds to results without preconditioning. Obviously, the use of preconditioning accelerates the steady state convergence by at least one order of magnitude. For example, it can be seen that when compared to the case without preconditioning ($\gamma = 1$), the preconditioned GI cascaded LBM with $\gamma = 0.05$, is at least 15 times faster.

2.6.2 Laminar Flow over a Square Cylinder

Next, in order to validate our preconditioned LB formulation for an external complex flow example, a two dimensional laminar flow over a square cylinder in a channel is studied. The geometry details and the set up of the flow problem is provided in Fig. 2.3. A fully developed velocity profile is considered at the inlet, and at the outlet, a convective boundary condition is used which is given by

$$\partial_t u_i + U_{max} \partial_x u_i = 0$$  \hspace{1cm} (2.62)
FIGURE 2.1: Comparison of the computed horizontal velocity $u/U_p$ and vertical velocity $v/U_p$ profiles along the geometric centerlines of the cavity using the Galilean invariant preconditioned cascaded central moment LBM with the benchmark results of [2] (symbols) for $Re=3200$ and 5000 and $\gamma = 0.1$.

FIGURE 2.2: Convergence histories of the GI preconditioned cascaded central moment LBM and the standard cascaded LBM ($\gamma = 1$) for lid-driven cavity flow for $Re=3200$. 
where $U_{\text{max}}$ is the maximum velocity of the inflow profile. Computations were performed using $L = 50D$, $H = 8D$ and $L_1 = 12.5D$, where $D$ is side of square the cylinder, $L$ and $H$ are the total length and width of computation domain, respectively and the location of square cylinder from entrance is defined by $L_1$. In order to visualize the general complex features and patterns of the flow, the streamlines plots at four different Reynolds numbers $Re = 1$, $Re = 15$, $Re = 30$ and $Re = 200$ are presented in Fig. 2.4. In Fig. 2.4(a), as it may be expected, at a low Reynolds number, $Re = 1$, where the fluid velocity is relatively very slow and on the other hand, the viscosity is large, the fluid flow is creeping and symmetric without separation. However, with increasing Reynolds number an adverse pressure gradient is established which leads to the flow separation from the surface and a vortex pair regime is formed (Fig. 2.4(b)). As the Reynolds number is further increased further to $Re = 30$, the size of the recirculation zone increases; besides the flow is still steady and symmetric about the horizontal centerline (Fig. 2.4(c)). These general features and flow patterns are consistent with the prior benchmark results (e.g. [63], [3]).

Then, we present the velocity profiles along the centerline at different sections at $Re = 100$ with a mesh resolution of $1000 \times 320$. Figure. 2.5 illustrates the horizontal and vertical components of the velocity profiles of $u$ and $v$, respectively. By comparing the present results against the benchmark numerical results obtained using the Gas Kinetic scheme (GKS) [3], a good agreement between the computational results is observed. An important global feature of the flow over
FIGURE 2.4: Stream function contours for flow over a square cylinder for four different Reynolds numbers; Re=1, Re=15 and Re=30 using the GI preconditioned cascaded central moment LBM with $\gamma = 0.5$. 
a cylinder is the length of the recirculating flow pattern formed behind the cylinder. Quantitative characterization of this wake length $L_r$ and its dependence on the Reynolds number $Re$ is a key element in the validation of numerical scheme. A widely used empirical correlation for the wake length $L_r$ as a linear function of the Reynolds number is given by [63]

$$\frac{L_r}{D} \approx -0.065 + 0.0554Re, \text{ for } 5 < Re < 60.$$  (2.63)

As illustrated in Fig. 2.6a, the computed results for the wake length $L_r$ obtained using the GI preconditioned cascaded central moment LBM are in very good agreement with the empirical correlation presented in Eq. (2.63). As may be expected, for the steady 2D flow over a square cylinder which, at relatively low $Re$ is characterized by symmetry, the lift force is zero and, as a result, a main quantity of interest is the drag force or the drag coefficient $C_D$ in dimensionless form whose magnitude varies significantly with $Re$. We use the standard momentum exchange method to compute the drag force on the square cylinder in our preconditioned LB formulation.

A comparison of the computed drag coefficient $C_D$ obtained using our GI preconditioned LB scheme with the GKS scheme [3] based benchmark results is presented in Fig. 2.6b. It can be observed that the obtained results agree well with the benchmark solutions. Next, we analyze the influence of the precondition parameter $\gamma$ in our formulation on the steady state convergence of this complex flow problem. Figure 2.7 presents the convergence histories for $Re = 30$. It can be seen that when compared to the usual cascaded LBM without preconditioning ($\gamma = 1$), the preconditioned formulation (e.g. for $\gamma < 0.1$) is able converge to the steady state significantly faster, with the residual error being reduced to the machine round off error by a factor of least 15 times more rapidly. Thus, the GI preconditioned cascaded central moments LBM exhibits significant convergence acceleration for complex flows.
FIGURE 2.5: Comparison of the computed velocity profiles along and across the square cylinder along its centerline for both the horizontal $u$ and vertical $v$ velocity components obtained using the GI preconditioned cascaded central moment LBM with $\gamma = 0.5$ for $Re = 100$ with benchmark results obtained using the Gas Kinetic Scheme (GKS) [3].
FIGURE 2.6: Comparison of the computed Reynolds number dependence of the recirculating wake length $L_r$ on the left (a) and the Reynolds number dependence of the drag coefficient $C_D$ on the right with (b) benchmark correlation (Eq. (2.63)) and GKS-based numerical results [3] respectively.

FIGURE 2.7: Convergence histories of the GI preconditioned cascaded central moment LBM and the standard cascaded LBM ($\gamma = 1$) for flow over the square cylinder for $Re=30$. 

2.6.3 Backward-Facing Step Flow

As the third flow benchmark flow problem involving complex separation and reattachment effects, we consider a two-dimensional laminar flow over a backward facing step, which is computed using the GI preconditioned central moment LBM. The geometry and boundary conditions for the simulation are shown in Fig. 2.8. For a step of height $h$, the flow entry is placed at $L_1 = 10h$ behind the step and the exit is located $L_2 = 30h$ downstream of the step, and the channel height is defined as $H = 2h$. In this simulation, the number of nodes in resolving the step flow is defined by considering $h = 94$. At the entrance, a parabolic profile, and, at the outlet, a convective boundary condition are imposed, and, finally, the half-way bounce-back scheme is utilized for the no-slip boundary condition at the walls. The computational results are then presented for Reynolds numbers up to 800, where the Reynolds number is defined as $Re = \frac{2hU_{max}}{\nu}$. Here, $U_{max}$ is the maximum speed at the inlet channel. For the purpose of investigating the flow behavior in the vicinity of the step, the distributions of streamlines are plotted at four different Reynolds numbers in Fig. 2.9. Initially, a primary recirculation zone is created downstream of the step at $Re = 100$ (Fig. 2.9(a)). However, it can be seen from Fig. 2.9(a) to Fig. 2.9(d) that the Reynolds number has a remarkable effect on the structure recirculation regimes and the length of this zone is seen to increase by increasing the Reynolds number. Furthermore, a second recirculation zone occurs along the top wall at the higher Reynolds number of $Re = 500$ which becomes more vis-

\[ \text{FIGURE 2.8: Schematic representation of the flow over a backward-facing step in a 2D channel.} \]
ible at $Re = 800$. All these observed flow pattern are consistent with prior benchmark results. In order to more precisely determine the quantitative effect of the Reynolds number on the reattachment length in the primary recirculation zone, our computed results based on the GI preconditioned cascaded central moment LBM for different Reynolds numbers are computed with the numerical results of [4], which are presented in Fig. 2.10. It can be observed that the agreement between the predictions based on our GI preconditioned LB scheme and the benchmark results is excellent. Moreover, it can be clearly seen that by increasing the Reynolds number, the reattachment length increased, consistent with prior observations.

2.6.4 Hartmann Flow

In this section, in order to validate our preconditioned scheme for a problem involving a body force, the Hartmann flow of an incompressible fluid bounded by two parallel plates is studied. An external uniform magnetic field $B_z = B_0$ is applied perpendicular to the plates. Since the body force varies spatially arising due to the interaction of the flow velocity and the induced magnetic field, i.e. the Lorentz force, it represents appropriate test problem for the present study. In our preconditioned LB model, the moments of the source terms at different orders are preconditioned differently to correctly recover the macroscopic with variable body forces. The relationship between the external magnetic field $B_0$ and an induced magnetic field $B_x(z)$ across the channel is given by $B_x(z) = \frac{F_bL}{B_0} \left[ \frac{\sinh(Ha \frac{z}{L})}{\sinh(Ha)} - \frac{z}{L} \right]$, where $F_b$ and $L$ are driving force due to imposed pressure gradient and the half channel width, respectively, and $Ha$ is the Hartmann number, which measures the ratio of the Lorentz force to viscous force.

The Lorentz force component is then defined as $F_{mx} = B_0 \frac{dB_x}{dz}$. In consequence, the effective variable body force component is defined as $F_x = F_b + F_{mx}$. The analytical solution for the Hartmann flow has the following velocity profile $u_x(z) = \frac{F_bL}{B_0} \sqrt{\frac{2}{\nu}} \coth(Ha) \left[ 1 - \frac{\cosh(Ha \frac{z}{L})}{\cosh(Ha)} \right]$, where $\eta$ is the magnetic resistivity given by $\eta = B_0^2 L^2/(Ha^2 \nu)$. Figure 2.11 presents comparisons of the com-
FIGURE 2.9: Streamline contours for flow over a backward-facing step at (a) Re = 100, (b) Re = 300, (c) Re = 500, (d) Re = 800 computed using the GI preconditioned cascaded central moment LBM with $\gamma = 0.3$.

FIGURE 2.10: Comparison of the reattachment length as a function of the Reynolds number $Re$ computed using the GI preconditioned cascaded central moment LBM with $\gamma = 0.3$ (symbols) against the benchmark results of [4].
puted velocity profiles using the GI preconditioned cascaded LBM with $\gamma = 0.1$ and Mach number $Ma = 0.02$ against the exact solution for various values of $Ha$. It can be observed that the GI preconditioned cascaded central moment LBM is able to reproduce the benchmark solution very well. In particular, as $Ha$ is increased, the resulting higher magnitudes of the Lorentz force causes significant flattering of the velocity profiles and this effect of $Ha$ on the velocity profiles is represented by our preconditioned is model with very good accuracy.

FIGURE 2.11: Comparison of the computed velocity profile using the preconditioned GI cascaded central moment LBM ($\gamma = 0.1$) with the analytical solution for Hartmann flow for various $Ha$ at $Ma = 0.02$. The lines indicate analytical results, and the symbols are the solutions obtained by the GI preconditioned cascaded LBM.

2.6.5 Four-rolls Mill Flow Problem: Comparison between GI Corrected and Uncorrected Preconditioned Cascaded LBM

As seen in Sec. 2.3, the GI errors for the LBM on the standard, tensor product lattices, such as the D2Q9 lattice, are generally related to the strain rates in the principal directions ($\partial_x u_x$ and $\partial_y u_y$). Hence, in order to compare the GI corrected formulation (Sec. 2.5), which is constructed to eliminate such errors, with the uncorrected formulation (Sec. 2.2), we consider the four-rolls mill flow problem, which is characterized by local extensional/compression strain rates (i.e. $\partial_x u_x \neq 0, \partial_y u_y \neq 0$), and for which a well-defined analytical solution is available. It is a
modified form of the classical Taylor-Green vortex flow driven by a local body force, whose components are given by

\[ F_x(x, y) = 2\nu u_0 \sin x \sin y, \quad F_y(x, y) = 2\nu u_0 \cos x \cos y \]

in a periodic square domain of side length \(2\pi\) (\(0 \leq x, y \leq 2\pi\)), resulting in a steady vortical motion in the form of an array of counterrotating vortices. Here, \(\nu\) and \(u_0\) are the kinematic viscosity and the velocity scale, respectively, and a unit reference density is considered. The analytical solution of the velocity field, which follows from a simplification of the Navier-Stokes equations impressed by the above body force, reads

\[ u_x(x, y) = u_0 \sin x \sin y, \quad F_y(x, y) = u_0 \cos x \cos y. \]

Clearly, the local flow field is subjected to local diagonal strain rates, i.e. \(\partial_x u_x = -\partial_y u_y = u_0 \cos x \sin y\), and, as a result, the uncorrected LB scheme induces additional GI errors, which should be annihilated by the corrected LB method; and thus, the difference in the global flow fields against the analytical solution under a suitable norm in each case can be quantitatively studied and compared.

We performed computations on a square domain resolved by \(251 \times 251\) grid nodes with a velocity scale \(u_0 = 0.045\) for a Reynolds number \(Re = u_0 L/\nu\), where \(L = 2\pi\), of 20. Figure 2.12 shows the streamline patterns at the steady state computed using the GI corrected preconditioned LB scheme (\(\gamma = 0.3\)), which manifest as a set of counterrotating vortices. The computed velocity profile \(u_y(x, y = \pi)\) obtained using the GI corrected LB scheme along the horizontal centerline of the domain presented in Fig. 2.13 are compared against the analytical solution given above, which show good agreement.

Furthermore, Fig. 2.14 presents a surface plot of the diagonal strain rate component \(\partial_x u_x\), which is seen to have a significant local variation, due to which quantitative differences in the solutions between the GI corrected and uncorrected preconditioned LB schemes can be expected, which will now be demonstrated in the following.
FIGURE 2.12: Steady state streamline patterns for the four-rolls mill flow problem at $u_0 = 0.045$ and $\text{Re} = 20$ computed using the GI corrected preconditioned cascaded LB scheme with $251 \times 251$ grid nodes and $\gamma = 0.3$.

FIGURE 2.13: Comparison of the computed and analytical vertical velocity profiles $u_y(x)$ at $y = \pi$ for the four-rolls mill flow problem at $\text{Re} = 20$ obtained using the GI corrected preconditioned cascaded LB scheme with $251 \times 251$ grid nodes, $u_0 = 0.45$ and $\gamma = 0.3$. 
FIGURE 2.14: Distribution of the diagonal strain rate component $\partial_x u_x = -\partial_y u_y$ for the four-rolls mill flow problem with $u_0 = 0.045$. 
In order to make a quantitative comparison between the solutions obtained using the two different LB methods, we first define the global relative errors for the velocity field $||\text{GRE}_u^G||_2$ and $||\text{GRE}_v^G||_2$ between the components of the solution obtained using the GI corrected preconditioned LB scheme (i.e. $(u_c, v_c)$) and the analytical solution (i.e. $(u_a, v_a)$) under a discrete $\ell_2$ norm; and similarly $||\text{GRE}_u||_2$ and $||\text{GRE}_v||_2$ between the uncorrected preconditioned LB scheme (i.e. $(u_{uc}, v_{uc})$) and the analytical solution. These are written as follows:

$$||\text{GRE}_u^G||_2 = \sqrt{\sum (u_c - u_a)^2 / \sum u_a^2}, \quad ||\text{GRE}_v^G||_2 = \sqrt{\sum (v_c - v_a)^2 / \sum v_a^2},$$

$$||\text{GRE}_u||_2 = \sqrt{\sum (u_{uc} - u_a)^2 / \sum u_a^2}, \quad ||\text{GRE}_v||_2 = \sqrt{\sum (v_{uc} - v_a)^2 / \sum v_a^2},$$

where the summations in the above are carried out for the whole computational domain. Table 2.1 presents the above global relative errors for the velocity field components for both the preconditioned cascaded LB formulations for different values of the preconditioning parameter ($\gamma = 0.2, 0.3, 0.4$ and 0.5). It can be seen that significant improvements in accuracy is achieved by the GI corrected preconditioned LB scheme. In particular, the errors relative to the analytical solution are reduced by about a factor of two with the corrected preconditioned LB scheme for the conditions considered for the computation of this problem. Such improvements are consistent with the fact that the corrected LB scheme eliminates the additional GI errors arising in this flow subjected to the local variations of the diagonal (compression/extension) strain rates, which are present in the uncorrected LB scheme.

**TABLE 2.1:** Comparison between the global relative errors in the computed solutions for the velocity field using the GI corrected preconditioned cascaded LB scheme and the uncorrected preconditioned cascaded LB scheme for the four-rolls mill flow problem at Re = 20, $u_0 = 0.045$ and a grid resolution of $251 \times 251$.

| $\gamma$ | GI corrected u error $||\text{GRE}_u^G||_2$ | Uncorrected u error $||\text{GRE}_u||_2$ | GI corrected v error $||\text{GRE}_v^G||_2$ | Uncorrected v error $||\text{GRE}_v||_2$ |
|---------|-----------------|-----------------|-----------------|-----------------|
| 0.2     | $3.386 \times 10^{-3}$ | $6.662 \times 10^{-3}$ | $3.377 \times 10^{-3}$ | $6.665 \times 10^{-3}$ |
| 0.3     | $1.850 \times 10^{-3}$ | $4.104 \times 10^{-3}$ | $1.854 \times 10^{-3}$ | $4.126 \times 10^{-3}$ |
| 0.4     | $1.384 \times 10^{-3}$ | $2.851 \times 10^{-3}$ | $1.389 \times 10^{-3}$ | $2.865 \times 10^{-3}$ |
| 0.5     | $1.135 \times 10^{-3}$ | $2.113 \times 10^{-3}$ | $1.140 \times 10^{-3}$ | $2.123 \times 10^{-3}$ |
Finally, we now obtain an estimate for the additional computational cost associated with including the GI corrections. For the flow condition employed ($u_0 = 0.045$, $Re = 20$, and $251 \times 251$ grid nodes), with $\gamma = 0.3$, the uncorrected preconditioned LB scheme for 6000 iterations incurs a CPU time of 356.1 secs on a standard Dell workstation, while the GI corrected preconditioned LB scheme takes 390.9 secs. Thus, the additional computational overhead of applying the GI corrections is about 9.7%. These involved computations of the GI correction terms related to the velocity gradients using non-equilibrium moments and the finite-difference (FD) calculations of the density gradients in our present 2D simulations, with the latter taking 16.1 secs out of the total overhead of 34.8 secs. Also, it was found that there were negligible differences in the accuracy variations between using a isotropic FD scheme or a standard central difference FD scheme for the density gradients in the GI correction terms. Thus, especially in extensions to 3D, it may be more efficient to adopt the simpler standard FD schemes for density gradient calculations in the GI corrections terms. In summary, a significant improvement in accuracy was achieved with the use of the GI corrected preconditioned LB scheme when compared to the uncorrected preconditioning formulation with a relatively minor additional computational effort.

2.7 Summary and Conclusions

Lattice Boltzmann schemes on standard tensor product lattices can result in cubic-velocity errors in Galilean invariance (GI) as the third-order diagonal moments are not independently supported and degenerates to the first-order moments. Recent investigations have presented corrections to the collision operator to yield schemes free of these errors for the representation of the standard Navier-Stokes (NS) equations. Convergence acceleration of simulations of steady state flows can be achieved by solving the preconditioned NS equations involving a preconditioning parameter $\gamma$ to tune the pseudo-sound speed thereby alleviating the numerical stiffness. In our prior chapter, we devised a modified central moment based cascaded LBM to represent such preconditioned NS equations, which may be referred to as a specific example of an extended or generalized NS equa-
tions containing a free parameter, here the preconditioning parameter $\gamma$. In this chapter, we have presented a new preconditioned central moment based cascaded LB scheme that eliminates such non-GI cubic-velocity and parameter dependent errors for the simulation of steady state flows. A detailed analysis based on the Chapman-Enskog expansion reveals the structure of the non-GI truncation errors that appear in the second-order non-equilibrium moment components, which are related to the viscous stress. Subsequently, we prescribe an extended second-order moment equilibria that restores GI free of cubic-velocity errors for the preconditioned LB model on the standard D2Q9 lattice. The following are among the main findings arising from our analysis:

- In general, the use of central moments in a LB scheme provides a natural setting to partially restore GI for the third-order off-diagonal moments. In particular, by setting the third-order central moment equilibria of the off-diagonal components to zero (e.g. $\tilde{\kappa}_{xxxy}^eq = 0$), one naturally arrives at the precise forms of the corresponding raw moment equilibria (e.g. $\tilde{\kappa}_{xxxy}^{eq'} = c_s^2 \rho u_y + \rho u_y^2 u_y$) that restores GI of such components in the representation of the standard NS equations. On the other hand, in the preconditioned LB scheme, the cubic-velocity terms appearing in the third-order, off-diagonal moment equilibria needs to be scaled by $\gamma^2$ (e.g. $\tilde{\kappa}_{xxxy}^{eq'} = c_s^2 \rho u_y + \rho u_y^2 u_y / \gamma^2$) to fully eliminate the spurious cubic-velocity cross-derivative terms (e.g. $u_x u_y \partial_y u_x, u_y u_x \partial_x u_y$) appearing in the derivation of the preconditioned macroscopic equations.

- In order to effectively eliminate the non-GI, diagonal velocity gradient terms (e.g. $u_x^2 \partial_x u_x$), the second-order, diagonal moment equilibria needs additional corrections in both the velocity and density gradients when $\gamma \neq 1$, which are prescribed via extended moment equilibria. The velocity gradients can be locally and efficiently obtained using the non-equilibrium second order moment components; on the other hand, the density gradients can be computed using a finite-difference approximation.

- Unlike that for the standard NS equations, the representation of the preconditioned NS
equations using a LB scheme results in additional, non-GI, cross-coupling velocity terms (e.g. $u_y^2 \partial_x u_x$), which are also eliminated by our GI-corrected preconditioned LB scheme.

- For the second-order, off-diagonal moment equilibria, additional gradient velocity correction terms are needed to restore GI for these components when $\gamma \neq 1$. However, for incompressible flows ($\nabla \cdot \mathbf{u} = 0$), they vanish regardless of the value of $\gamma$. Such a situation is unique to the representation of the preconditioned NS equations using LB schemes, as the non-GI corrections are generally restricted only to the diagonal components of the second-order equilibria for the representation of the standard NS equations.

- In general, the prefactors in GI defect terms exhibit dramatically different behaviors for the asymptotic limit cases: For example, $\gamma \to 1$ (No preconditioning): $\left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) \sim 3$ and $\gamma \to 0$ (Strong preconditioning): $\left( \frac{4}{\gamma^2} - \frac{1}{\gamma} \right) \sim \frac{4}{\gamma^2}$.

- When $\gamma = 1$, i.e. when the present LB model is used to simulate flows represented by standard NS equations as a special case, all our results for the GI defect terms and corrections become identical with those derived by [42] and [43].

- Finally, the results of our present analysis can be extended to three-dimensions (e.g. D3Q27 lattice) and other collision models for the simulation of the preconditioned NS equations.

In addition, we have presented numerical validation of our new GI preconditioned LB scheme based on central moments against several complex flow benchmark problems including the lid-driven cavity flow, flow over a square cylinder, the backward facing step flow, the Hartmann flow and the four-roll mills flow problem. Comparison against prior numerical solutions show good agreement for the modified preconditioned scheme. In addition, it is demonstrated that our GI corrected preconditioned cascaded LB scheme results in significant convergence acceleration of complex flow simulations, and a quantitative improvement in accuracy when compared to the
uncorrected preconditioned LB scheme. Finally, it may be noted that our analysis of non-GI as-
pects for the preconditioned LB scheme has implications for LB schemes for other situations such
as the porous media flows. For example, there is a formal analogy between the preconditioned
NS equations and the Brinkman-Forchheimer-Darcy equations, where the porosity serves as a
free parameter (e.g. [64, 65]). LB models constructed for such flows (e.g. [66]) can be further im-
proved by the approach presented in this chapter.
3.1 Introduction

The lattice Boltzmann (LB) method is now a well established alternative numerical technique to computational fluid dynamics (CFD) problems. The collision step, which represents various physics associated with the fluid motion including the momentum diffusion as a relaxation process, plays a main role in the numerical stability of the method. Among the earliest collision models is the single relaxation time (SRT) model [67], which, while being popular due to its simplicity, is susceptible to numerical instability at relatively high Reynolds numbers. A significant improvement is achieved by the multiple relaxation time model (MRT) [14] in which different raw moments relax at different rates. More recently, further enhancement in stability was made possible by the introduction of a cascaded LB method, which is a multi-parametric scheme that is based on considering relaxation in terms of central moments, which are formulated by shifting the particle velocity by the local fluid velocity [15, 19]. The significant advantages of such more advanced collision models were numerically demonstrated more recently [43]. A strategy to accelerate the convergence of the cascaded LB method has also been devised and studied [58], which has been further extended with improved Galilean invariance properties [68].

Another aspect of the LB schemes, which is particularly important in applications, is the implementation strategy to represent the various impressed body forces, which can either arise within the fluids or imposed externally. Some examples include the local surface tension and phase segregation forces in multiphase fluid systems, Lorentz forces in magnetohydrodynamics, gravity and
Coriolis forces. In general, such body forces can be spatially varying and/or time dependent. Due to the kinetic nature of the LB method, special considerations are necessary and various forcing schemes have been introduced over the years ([69], [23], [70], [71], [72], [73]). In particular, the investigation by [71] highlighted the discrete effects arising in prior LB forcing schemes via the second order moments in the momentum flux tensor, and provided a consistent source term that avoids such spurious effects when used with the SRT collision model. This was further generalized to the MRT model by including source terms in the moment space in both two-dimensions (2D) and three-dimensions (3D) ([74], [75], [7]).

In the case of the cascaded LB method, the first consistent forcing scheme based on the central moments was presented by [19]. By taking the source term proposed by [76] as the starting point, they devised a forcing formulation without discrete effects, which was also shown to be a further generalization of that presented by [71] to the cascaded LB scheme under appropriate limits. Later, [77] constructed another type of forcing scheme for the cascaded LB method based on the exact difference method [73]. More recently, [78], [79] and [80] presented other variants of forcing schemes for LB methods based on central moments. While all these forcing schemes differ from one another due to the variations in the kinetic models for the source term, a common element among them is the presence of extra source terms or changes to the equilibria, which are usually taken together with the collision relaxation terms as part of the collision step. This generally involves computing source moments at different orders and transforming them back to the velocity space, which entails additional computational effort.

Based on the consideration that the LB schemes are generally fluid flow, i.e. Navier-Stokes (NS), solvers, and by avoiding the kinetic aspects for the implementation of the impressed forces, simpler and more efficient strategies can be constructed. The numerical framework for this is the operator splitting approach widely used to efficiently solve ordinary and partial differential equations arising in various applications including CFD ([81], [82]). The basis idea is to split the problem into a set of simpler subproblems and then devise a strategy that alternates between solv-
ing such simpler problems in certain sequence, which then approximate the solution to the full problem to a certain order of accuracy. Such operator splitting techniques are sometimes also referred to as the fractional step or time-splitting methods. Of particular importance is the Strang splitting [83], which achieves second-order accuracy by a symmetrized application of the solution method for one (or more) of the subproblems. The structure of the higher order splitting errors can be analyzed via the Taylor-Lie series [81] or using the Baker-Compbell-Hausdorff formulas [84]. From such a perspective, Dellar [85] presented a derivation of the lattice Boltzmann method based on Strang splitting with second order accuracy and interpreted both unsplit and time-split forcing schemes based on this approach. In particular, a uncoupled spin-step to implement body force in a SRT LB model introduced earlier by Salmon [86] was shown to be consistent with the Strang splitting. Furthermore, it was also extended to the MRT-LB models ([85], [87]).

In this chapter, our goal is to construct efficient body force implementation schemes based on the symmetrized operator (Strang) splitting for the cascaded LB methods. The lattice symmetry and the use of central moments naturally impose Galilean invariance for the chosen set of independent moments basis. The symmetric application of the separate body force steps in two half time steps in the cascaded LB formulation provides a second order accuracy. Unlike the unsplit forcing schemes presented earlier for the cascaded LB method [19], our approach does not require either the computation of various source moments at different orders or an extra transformation step to convert them back to velocity space. In essence, the operator-split forcing scheme involves one half application of the force before collision and the other half force step after collision. The latter step will be seen to lead to unique expressions for the post-collision change of first order moments in the cascaded collision operator. The precise structure of these expressions will be shown to depend on choice of the first order moment basis vectors associated with the type of lattice considered. In fact, we will present operator split forcing scheme for the cascaded LB method both in 2D and 3D for the computation of the fluid motion. In addition, in order to demonstrate the generality of our approach, we will extend it to represent the convective-diffusion equation
(CDE) with a source term, such as those arising in the convective thermal flows with internal heat generation. In this regard, a novel cascaded LB formulation for the solution of the CDE with source term using the Strang splitting will be constructed. Finally, we will present a numerical validation study of the symmetrized operator split forcing/source schemes for the cascaded LB method for fluid flow (i.e., the NS equations) and passive scalar transport (i.e., the CDE) and in different dimensions.

This chapter is organized as follows. In the next section (Sec. 2), we briefly review the various operator splitting approaches including the Strang splitting. Section 3 presents the general ideas behind the symmetrized operator splitting based forcing implementation in the LB method. Section 4 discusses the derivation and the algorithmic procedure of the symmetrized operator split forcing scheme for the 2D cascaded LB method for representing fluid flow subjected to local impressed forces. A corresponding 3D formulation is outlined in the Appendix A. Section 5 presents a symmetrized operator split approach source incorporation scheme for a 2D cascaded LB scheme for representing the convection-diffusion based transport of a passive scalar field with local sources. Numerical validation results of various symmetrized operator split forcing/source scheme are presented in Sec. 6. Finally, Sec. 7 summarizes our approach and presents the main conclusion arising from this work.

### 3.2 Operator Splitting Methods

We will now briefly review the various typical operator splitting methods, including the Strang splitting which will then be exploited to construct efficient second order accurate forcing schemes in the cascaded LB method. For the purpose of illustration, we will consider the numerical solutions of the following evolution problem:

\[
\frac{dy}{dt} = P y + Q y, \quad y(t) = y_0 \quad \text{on} \quad [t, t + \Delta t],
\]

(3.1)
where, for ease of presentation, \( P \) and \( Q \) are considered as linear operators. Nonlinear operators can be dealt with using Lie operator formalism \[84\]. Here, \( \Delta t \) is the time step. For reference, the unsplit solution \( y^U \) of the full problem can be represented as

\[
y^U = e^{\Delta t(P+Q)}y_0.
\] (3.2)

Now, a first order splitting scheme, which is sometimes known as the Lie-Trotter (LT) splitting or as the Godunov splitting scheme in the CFD literature, can be represented by means of the following steps, which compute solution to each subproblem involving \( P \) and \( Q \) separately:

**Step P**: Solve \( \frac{dy^*}{dt'} = Py^*, \quad y^*(t' = t) = y_0 \quad \text{on } [t, t + \Delta t], \) \hspace{1cm} (3.3a)

**Step Q**: Solve \( \frac{dy^{**}}{dt'} = Qy^{**}, \quad y^{**}(t' = t) = y^*(t + \Delta t) \quad \text{on } [t, t + \Delta t], \) \hspace{1cm} (3.3b)

**Solution**: \( y^{LT}(t + \Delta t) = y^{**}(t + \Delta t). \) \hspace{1cm} (3.3c)

This solution of the Lie-Trotter splitting or the \( P \cdot Q \) splitting scheme may be more compactly represented by means of the exponential operators as

\[
y^{LT}(t + \Delta t) = e^{\Delta tQ}e^{\Delta tP}y_0.
\] (3.4)

The local error \( (E_l) \) incurred over a small time step \( \Delta t \) due to splitting when compared to the unsplit solution (Eq. (3.2)) can be estimated by means of a Lie-Taylor series (factored product expansions) as \[81\]

\[
E_{l,LT} = y^{LT} - y^U = \frac{1}{2} [P, Q] y_0 \Delta t^2 + O(\Delta t^3),
\] (3.5)

where the symbol \([·, ·]\) represents the commutator, i.e., \([X, Y] = XY - YX\) for any two operators \( X \) and \( Y \). Then, the global error \( (E_g) \) over a time duration \( T \) or \( T/\Delta t \) number of steps is

\[
E_{g,LT} = (T/\Delta t) \cdot E_{l,LT} \sim O(\Delta t),
\]

which means that the Lie-Trotter scheme is first order accurate. This means that even if a higher order method is used to solve each subproblem (\( \text{Step P} \) and \( \text{Step Q} \)), the above splitting scheme is still overall first order accurate due to the decomposition error arising from the non-commuting operators, which is often the case in practice.
One possibility to improve the order of accuracy is to symmetrize the computation via taking the average of the two sequences of calculations, i.e. **Step P - Step Q** and **Step Q - Step P** results. Such an averaged scheme may be represented as \[ y^A = \frac{1}{2} (e^{\Delta t P} e^{\Delta t Q} + e^{\Delta t Q} e^{\Delta t P}) y_0. \] (3.6)

This approach introduces a local error relative to the unsplit solution (Eq. (3.2)), which can be written as \[ E_{l,A} = y^A - y^\prime = R' \Delta t^3 + O(\Delta t^4), \] where \[ R' = -\frac{1}{12} ([P, [P, Q]] + [Q, [Q, P]]) y_0. \]

Hence, the global error becomes \[ E_{g,A} = (T/\Delta t) \cdot E_{l,A} \sim O(\Delta t^2). \] While this is theoretically interesting to gain an order of accuracy, it is computationally expensive as, for each time step, double the effort is required when compared to the previous scheme (**P - Q** splitting).

A more efficient strategy to achieve a global second order accuracy is to devise the Strang (**S**) splitting \[83]. In this scheme, one of the operators (say **P**) is applied twice for a time step of length \(\Delta t/2\), before and after the solution of the other subproblem (say, involving **Step Q**), which is solved for full step length of \(\Delta t\). This may be represented as

**Step P^{1/2}**: Solve \[ \frac{dy^*}{dt'} = Py^*, \quad y^*(t' = t) = y_0 \text{ on } [t, t + \Delta t/2], \] (3.7a)

**Step Q**: Solve \[ \frac{dy^{**}}{dt'} = Qy^{**}, \quad y^{**}(t' = t) = y^*(t + \Delta t/2) \text{ on } [t, t + \Delta t], \] (3.7b)

**Step P^{1/2}**: Solve \[ \frac{dy^{***}}{dt'} = Py^{***}, \quad y^{***}(t' = t) = y^{**}(t + \Delta t) \text{ on } [t, t + \Delta t/2], \] (3.7c)

**Solution**: \[ y^S(t + \Delta t) = y^{***}(t + \Delta t/2). \] (3.7d)

This symmetric application of the operators in the \(P^{1/2} - Q - P^{1/2}\) scheme achieves second order accuracy, which may be deduced by first noting that the Strang splitting solution may be more compactly written in the exponential form as

\[ y^S(t + \Delta t) = e^{\Delta t/2 P} e^{\Delta t Q} e^{\Delta t/2 P} y_0. \] (3.8)
Its local error when compared to the unsplit solution (Eq. (3.2)) then follows via a Lie-Taylor series as [82]

\[ E_{l,S} = y^S - y^U = R\Delta t^3 + O(\Delta t^4), \]

(3.9)

where

\[ R = \frac{1}{24}([[P, Q], P] + 2 [[P, Q], Q])y_0. \]

(3.10)

Then, the global error \((E_g)\) over a time period \(T\) follows as \(E_{g,S} = (T/\Delta t) \cdot E_{l,S} \sim O(\Delta t^2)\) and hence this scheme is second order accurate. An equally valid possibility to achieve a similar second order accuracy is to consider the \(Q^{1/2} - P - Q^{1/2}\) splitting, which is useful when Step P is more expensive to compute than Step Q. It may be noted that a similar scheme was independently devised by [90], who further analyzed and elaborated on its variants (see also [91]), and hence it is sometimes referred to as the Strang-Marchuk splitting scheme.

### 3.3 Strang Splitting of Lattice Boltzmann Method Including Body Forces

Lattice Boltzmann (LB) schemes are generally constructed to represent the evolution of the dynamics of the fluid motion represented by

\[ \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \]

(3.11a)

\[ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \nabla \cdot \mathbf{\Pi}_V + \mathbf{F}, \]

(3.11b)

where \(\rho\) and \(\mathbf{u}\) are the fluid density and velocity, respectively, \(P\) is the pressure and \(\mathbf{\Pi}_V\) is the viscous stress tensor. Here, \(\mathbf{F}\) represents the effect of the local impressed body forces, which can vary spatially and may be time dependent, i.e. for e.g. in 2D, \(\mathbf{F} = (F_x, F_y)\) where \(F_x = F_x(\mathbf{x}, t)\) and \(F_y = F_y(\mathbf{x}, t)\). An efficient approach to solve the above fluid flow equation in the LB framework is to solve the Eqs. (3.11a) and (3.11b), but without the body force \(\mathbf{F}\) using the usual stream and collide procedure (subproblem A) and then separately solve \(\partial_t (\rho \mathbf{u}) = \mathbf{F}\) as a forcing step (subproblem B) and subsequently combined appropriately in a certain sequence to yield a second order accurate scheme. This can be achieved via symmetrization of the operator
splitting of the one of the subproblems over two half time steps. Dellar [85] performed a derivation and analysis of the LB method via Strang splitting, which will be used as formal starting point to construct efficient operator split forcing schemes for the cascaded LB method in the subsequent sections.

In the following, $S$, $C$ and $F$ are used to denote the operators used to perform the streaming step, collision step and the forcing step, respectively. For a lattice containing $\alpha = 0, 1, 2, \ldots b$ directions, the collision and streaming steps can be represented as

\begin{align}
\text{Step } C : & \quad f(x, t + \Delta t) = Cf(x, t) = f(x, t) + K \cdot \hat{g}, \\
\text{Step } S : & \quad f_\alpha(x, t + \Delta t) = S f_\alpha(x, t) \equiv f_\alpha(x - e_\alpha \Delta t, t).
\end{align}

(3.12a) (3.12b)

Here, $f = (f_0, f_1, f_2 \ldots f_b)^\dagger$ is a vector of size $(b+1)$ representing the distribution functions, where $\dagger$ is the transpose operator, $\hat{g} = (\hat{g}_0, \hat{g}_1, \hat{g}_2 \ldots \hat{g}_b)^\dagger$ is the vector representing the change of different moments under collision, and $K$ is the transformation matrix of the cascaded LB method that maps changes in moments back to changes in the distribution functions, which are specified later.

It may be noted that $C$ and $S$ operators represent the split solution operators of the discrete analog of $\partial_t f_\alpha = \Omega_\alpha$ and $\partial_t f_\alpha + e_\alpha \cdot \nabla f_\alpha = 0$, respectively, of the discrete velocity Boltzmann equation $\partial_t f_\alpha + e_\alpha \cdot \nabla f_\alpha = \Omega_\alpha$, whose emergent behavior represents the NS equations given in Eq. (3.11a) and Eq. (3.11b), but without $F$. Then, the forcing step separately solves the following:

$$\text{Step } F : \frac{\partial}{\partial t} (\rho u) = F.$$  

(3.13)

One possibility to combine the above split steps to effectively achieve second order accuracy is to perform a symmetric application of the forcing steps over two half time steps, before and after the collision step, which is akin to the spin steps for the force presented by Salmon ([86]):

$$f_\alpha(x, t + \Delta t) = SF^{1/2} CF^{1/2} f_\alpha(x, t),$$

(3.14)
where $F^{1/2}$ represents performing the solution of Eq. (3.13) over time step of length $\Delta t/2$. Ref. [85] showed that this achieves second order accuracy similar to the Strang splitting extended to three operators: $f_\alpha'(x, t + \Delta t) = C^{1/2} F^{1/2} S F^{1/2} C^{1/2} f_\alpha'(x, t)$, where the two are related by $f_\alpha = C^{1/2} F^{1/2} f_\alpha$. Since the momentum is conserved during collisions, a second order scheme with Eq. (3.14) can be obtained by $\rho u = \sum_\alpha f_\alpha f_\alpha' = F^{1/2}(\sum_\alpha f_\alpha e_\alpha)$. We will adopt the above strategy in our derivation of the symmetrized operator split forcing scheme for the cascaded LB method in the subsequent sections. Similar approach was recently adopted for the MRT LB models (e.g., [87]). In addition, Schiller [92] proposed a variant of the Strang splitting of forcing steps around streaming and collisions, where the half collision step is valid for the regime involving the relaxation time being much greater than the time step. Also, Dellar [42] showed that the Crank-Nicolson solution of the moment equations for combined collisions and time-independent forcing obtained by Strang splitting is equivalent to Kupershtokh’s exact difference method [73].

3.4 Body Force Scheme for 2D Cascaded LB Method for Fluid Flow via Strang Splitting

We will consider a 2D cascaded LB formulation for a two-dimensional, nine velocity (D2Q9) lattice. The components of the particle velocities are then represented by the following vectors using the standard Dirac’s bra-ket notation:

$$|e_x\rangle = (0, 1, 0, -1, 0, 1, -1, -1, 1)^\dagger, \quad (3.15a)$$

$$|e_y\rangle = (0, 0, 1, 0, -1, 1, 1, -1, -1)^\dagger. \quad (3.15b)$$

Their components for any particle velocity direction $\alpha$ (where $\alpha = 0, \ldots, 8$) are referred to as $e_{\alpha x}$ and $e_{\alpha y}$, respectively. Furthermore, we need the following 9-dimensional vector:

$$|1\rangle = (1, 1, 1, 1, 1, 1, 1, 1, 1)^\dagger. \quad (3.16)$$

The zeroth moment is the Euclidean inner product of this vector with the distribution function.

We then consider the following specific set of orthogonal basis vectors used in the collision term
of the cascaded LB method (e.g., [19]):

\[
\begin{align*}
|K_0\rangle &= |1\rangle, \quad |K_1\rangle = |e_x\rangle, \quad |K_2\rangle = |e_y\rangle, \quad |K_3\rangle = 3\left|e_x^2 + e_y^2\right| - 4|1\rangle, \\
|K_4\rangle &= |e_x^2 - e_y^2\rangle, \quad |K_5\rangle = |e_x e_y\rangle, \quad |K_6\rangle = -3\left|e_x e_y\right| + 2|e_y\rangle, \\
|K_7\rangle &= -3\left|e_x e_y\right| + 2|e_x\rangle, \quad |K_8\rangle = 9\left|e_x^2 e_y^2\right| - 6\left|e_x^2 + e_y^2\right| + 4|1\rangle.
\end{align*}
\] (3.17)

In the above, symbol such as \(|e_x^2 e_y\rangle = |e_x e_y e_x e_y\rangle\) represents a vector resulting from the element-wise vector multiplication (Hadamard product) of the sequence of vectors \(|e_x\rangle, |e_x\rangle\) and \(|e_y\rangle\). By combining the above 9 vectors, we then obtain the following orthogonal matrix

\[
K = [|K_0\rangle, |K_1\rangle, |K_2\rangle, |K_3\rangle, |K_4\rangle, |K_5\rangle, |K_6\rangle, |K_7\rangle, |K_8\rangle].
\] (3.18)

Here, \(K\) maps changes of moments under collisions back to changes in the distribution functions.

In order to determine the structure of the cascaded collision operator, we first define the following set of central moments of the distribution functions and its equilibria of order \((m+n)\), respectively, as

\[
\begin{pmatrix}
\hat{\kappa}_x^m y^n \\
\hat{\kappa}_x^\text{eq} y^n
\end{pmatrix} = \sum_{\alpha} \begin{pmatrix}
f_{\alpha} \\
f_{\alpha}^\text{eq}
\end{pmatrix} (e_{\alpha x} - u_x)^m (e_{\alpha y} - u_y)^n.
\] (3.19)

By equating the discrete central moments of the equilibrium distribution function with the corresponding continuous central moments based on the local Maxwellian ([15], [19], [20]), we get

\[
\begin{align*}
\hat{\kappa}_0^\text{eq} &= \rho, \quad \hat{\kappa}_x^\text{eq} = 0, \quad \hat{\kappa}_y^\text{eq} = 0, \quad \hat{\kappa}_{xx}^\text{eq} = c_s^2 \rho, \quad \hat{\kappa}_{yy}^\text{eq} = c_s^2 \rho, \\
\hat{\kappa}_{xy}^\text{eq} &= 0, \quad \hat{\kappa}_{xxy}^\text{eq} = 0, \quad \hat{\kappa}_{xyy}^\text{eq} = 0, \quad \hat{\kappa}_{xxyy}^\text{eq} = c_s^4 \rho.
\end{align*}
\] (3.20)

where \(c_s^2 = 1/3\) with \(c_s\) being the sound speed. This is set by applying the usual lattice units, i.e. \(\Delta x = \Delta t = 1\) or the particle speed \(c = \Delta x/\Delta t = 1\), and because \(c_s^2 = c^2/3\) for the athermal LB scheme used in this work (see e.g. [18]). On the other hand, the actual computations in the cascaded formulations are carried out in terms of raw moments, which are defined as (designated here with the \('\) symbol)

\[
\begin{pmatrix}
\hat{\kappa}'_x^m y^n \\
\hat{\kappa}'_x^\text{eq} y^n
\end{pmatrix} = \sum_{\alpha} \begin{pmatrix}
f_{\alpha} \\
f_{\alpha}^\text{eq}
\end{pmatrix} e_{\alpha x}^m e_{\alpha y}^n.
\] (3.21)
The collide and stream steps (C and S) of the 2D cascaded LB method can then be, respectively, written as [15, 19]

\begin{align*}
\text{Step C : } \quad f^p_\alpha &= f_\alpha + (K \cdot \mathbf{g})_\alpha \quad \text{(3.22a)} \\
\text{Step S : } \quad f_\alpha(x, t) &= f^p_\alpha(x - e_\alpha \Delta t, t), \quad \text{(3.22b)}
\end{align*}

where $f^p_\alpha$ represents the post-collision distribution function and $\mathbf{g} = (\tilde{g}_0, \tilde{g}_1, \tilde{g}_2 \ldots \tilde{g}_8)\uparrow$ is the change of different moments under collisions, which is determined based on the relaxation of various central moments to their corresponding equilibria in a cascaded fashion [15]. Since the mass and momentum are collision invariants, $\tilde{g}_0 = \tilde{g}_1 = \tilde{g}_2 = 0$. As a result, the cascaded structure starts from the non-conserved second order moments, and the corresponding components of the change of different moments under collisions are given by

\begin{align*}
\tilde{g}_3 &= \frac{\omega_3}{12} \left\{ \frac{2}{3} \rho + \rho(u_x^2 + u_y^2) - (\tilde{\kappa}_x' + \tilde{\kappa}_y') \right\}, \\
\tilde{g}_4 &= \frac{\omega_4}{4} \left\{ \rho(u_x^2 - u_y^2) - (\tilde{\kappa}_x' - \tilde{\kappa}_y') \right\}, \\
\tilde{g}_5 &= \frac{\omega_5}{4} \left\{ \rho u_x u_y - \tilde{\kappa}_{xy}' \right\}, \\
\tilde{g}_6 &= \frac{\omega_6}{4} \left\{ 2 \rho u_x^2 u_y + \tilde{\kappa}''_{xxy} - 2 u_x \tilde{\kappa}'_{xy} - u_y \tilde{\kappa}'_{xx} - \frac{1}{2} u_y (3 \tilde{g}_3 + \tilde{g}_4) - 2 u_x \tilde{g}_5, \\
\tilde{g}_7 &= \frac{\omega_7}{4} \left\{ 2 \rho u_x u_y^2 + \tilde{\kappa}''_{xxy} - 2 u_y \tilde{\kappa}'_{yy} - u_x \tilde{\kappa}'_{yy} - \frac{1}{2} u_x (3 \tilde{g}_3 - \tilde{g}_4) - 2 u_y \tilde{g}_5, \\
\tilde{g}_8 &= \frac{\omega_8}{4} \left\{ \frac{1}{9} \rho + 3 \rho u_x^2 u_y - \left[ \tilde{\kappa}''_{xxy} - 2 u_x \tilde{\kappa}'_{xyy} - 2 u_y \tilde{\kappa}'_{xxy} + u_x^2 \tilde{\kappa}'_{yy} + u_y^2 \tilde{\kappa}'_{xx} + 4 u_x u_y \tilde{\kappa}'_{xy} \right] - 2 \tilde{g}_3 - \frac{1}{2} u_y^2 (3 \tilde{g}_3 + \tilde{g}_4) - \frac{1}{2} u_x^2 (3 \tilde{g}_3 - \tilde{g}_4) \\
&\quad - 4 u_x u_y \tilde{g}_5 - 2 u_y \tilde{g}_6 - 2 u_x \tilde{g}_7 \right\}, \quad \text{(3.23)}
\end{align*}

where $\omega_3, \omega_4, \ldots, \omega_8$ are the relaxation parameters. These relaxation steps lead to the following expressions for the bulk and shear viscosities, respectively, as $\zeta = \frac{1}{3} \left( \frac{1}{\omega_3} - \frac{1}{2} \right) \Delta t$ and $\nu = \frac{1}{3} \left( \frac{1}{\omega_j} - \frac{1}{2} \right) \Delta t$ where $j = 4, 5$, and the pressure field $P$ is obtained via an equation of state as $P = \frac{1}{3} \rho$.

After the streaming step, i.e., Eq. (3.22b), we obtain the output velocity field components (desig-
nated with a superscript "o" as the first moment of \( f_\alpha \):

\[
\rho u^o_x = \sum_{\alpha=0}^{8} f_\alpha e_{ax}, \quad \rho u^o_y = \sum_{\alpha=0}^{8} f_\alpha e_{ay}.
\] (3.24)

We then introduce the effect of the body force \( \mathbf{F} = (F_x, F_y) \) as a solution of the subproblem in Eq. (3.13). This is accomplished by performing two symmetric steps of half time steps of length \( \Delta t/2 \), one before and the other after the collision step. Both these steps incorporate the effect of forces directly into the moment space. Solving Eq. (3.13) for the first part of the symmetric sequence of step yields

\[
\rho u_x - \rho u^o_x = F_x \frac{\Delta t}{2} \quad \text{and} \quad \rho u_y - \rho u^o_y = F_y \frac{\Delta t}{2}.
\]

Thus,

**Pre-collision Forcing Step \( F^{1/2} \):**

\[
u_x = \frac{1}{\rho} \left( \rho u^o_x + \frac{F_x}{2} \Delta t \right), \quad \nu_y = \frac{1}{\rho} \left( \rho u^o_y + \frac{F_y}{2} \Delta t \right).
\] (3.25)

Then, we use this updated velocity field \((\nu_x, \nu_y)\) in Eq. (3.23) to perform the cascaded relaxation collision step to determine the change of different moments under collisions, i.e. \( g_\beta, \beta = 3, 4, \ldots, 8 \). As a result of correctly projecting the effect of the forces in the various higher order moments, it naturally eliminates the discrete effects identified earlier [71] (see the discussion at the end of this section). Then, to implement the other part of the symmetrized force step with half step to solve Eq. (3.13) post collision, we set

\[
\rho u_x^p - \nu_x = F_x \frac{\Delta t}{2} \quad \text{and} \quad \rho u_y^p - \nu_y = F_y \frac{\Delta t}{2},
\]

where \((u_x^p, u_y^p)\) is the result of the target velocity field due to the forcing step after collision. Thus,

**Post-collision Forcing Step \( F^{1/2} \):**

\[
\nu_x = \nu_x^o + \frac{F_x}{2} \Delta t, \quad \nu_y = \nu_y^o + \frac{F_y}{2} \Delta t.
\] (3.26)

Note that this can also be rewritten in terms of the output velocity field \( u^o = (u^o_x, u^o_y) \) given in Eq. (3.24) by using Eq. (3.25) as

\[
\rho u_x^p = \rho u_x^o + F_x \Delta t, \quad \rho u_y^p = \rho u_y^o + F_y \Delta t.
\] (3.27)

A main issue here is how to effectively design the post-collision distribution function \( f^p_\alpha \) in the cascaded LB method so that Eq. (3.27) is precisely satisfied. Now, using

\[
f^p_\alpha = f_\alpha + (\mathbf{K} \cdot \mathbf{g})_\alpha
\]

and taking its first moments, we get

\[
\rho u_x^p = \Sigma_\alpha f^p_\alpha e_{ax} = \Sigma_\alpha f_\alpha e_{ax} + \Sigma_\beta \langle K_\beta e_x \rangle \tilde{g}_\beta, \quad (3.28a)
\]

\[
\rho u_y^p = \Sigma_\alpha f^p_\alpha e_{ay} = \Sigma_\alpha f_\alpha e_{ay} + \Sigma_\beta \langle K_\beta e_y \rangle \tilde{g}_\beta. \quad (3.28b)
\]
Based on the orthogonal basis vectors $|K_\beta\rangle$ given in Eq. (3.17), it follows that

$$
\Sigma_\beta \langle K_\beta|e_x \rangle g_\beta = 6 \tilde{g}_1, \quad \Sigma_\beta \langle K_\beta|e_y \rangle g_\beta = 6 \tilde{g}_2.
$$

(3.29)

Using Eqs. (3.24) and (3.29) in Eqs. (3.28a) and (3.28b) we get the desired velocity field as

$$
\rho u^p_x = \rho u^o_x + 6 \tilde{g}_1, \quad \rho u^p_y = \rho u^o_y + 6 \tilde{g}_2.
$$

(3.30)

Comparing the result of the target velocity field following the second half of the symmetrized forcing steps given in Eq. (3.27) with the change of moments based expressions in Eq. (3.30), we obtain

$$
\tilde{g}_1 = \frac{F_x}{6} \Delta t, \quad \tilde{g}_2 = \frac{F_y}{6} \Delta t.
$$

(3.31)

Equation (3.31) represents an algorithmic result that effectively implements the effect of the post-collision forcing step over a duration of half time step following collision. This is a consequence of the momentum needing to change by $F \Delta t$ over a time step, and the normalization is implied by our choice of basis for the moments. Then, the above relation (Eq. (3.31)) for the post-collision change of first moments due to the force field ($\tilde{g}_1$ and $\tilde{g}_2$) along with the change of different higher moments under collisions $\hat{g}_\beta$, where $\beta = 3, 4, \ldots, 8$, given in Eq. (3.23) effectively provide the desired post-collision states of the distribution function $f^p_\alpha$. Expanding Eq. (3.22a),
we get the expressions for the post-collision distribution functions as

\[ f_0^p = f_0 + \left[ g_0 - 4(g_3 - \hat{g}_8) \right], \]
\[ f_1^p = f_1 + \left[ g_0 + \hat{g}_1 - \hat{g}_3 + \hat{g}_4 + 2(\hat{g}_7 - \hat{g}_8) \right], \]
\[ f_2^p = f_2 + \left[ g_0 + \hat{g}_2 - \hat{g}_3 - \hat{g}_4 + 2(\hat{g}_6 - \hat{g}_8) \right], \]
\[ f_3^p = f_3 + \left[ g_0 - \hat{g}_1 - \hat{g}_3 + \hat{g}_4 - 2(\hat{g}_7 + \hat{g}_8) \right], \]
\[ f_4^p = f_4 + \left[ g_0 - \hat{g}_2 - \hat{g}_3 - \hat{g}_4 - 2(\hat{g}_6 + \hat{g}_8) \right], \]
\[ f_5^p = f_5 + \left[ g_0 + \hat{g}_1 + \hat{g}_2 + 2\hat{g}_3 + \hat{g}_5 - \hat{g}_6 - \hat{g}_7 + \hat{g}_8 \right], \]
\[ f_6^p = f_6 + \left[ g_0 - \hat{g}_1 + \hat{g}_2 + 2\hat{g}_3 - \hat{g}_5 - \hat{g}_6 + \hat{g}_7 + \hat{g}_8 \right], \]
\[ f_7^p = f_7 + \left[ g_0 - \hat{g}_1 - \hat{g}_2 + 2\hat{g}_3 + \hat{g}_5 + \hat{g}_6 + \hat{g}_7 + \hat{g}_8 \right], \]
\[ f_8^p = f_8 + \left[ g_0 + \hat{g}_1 - \hat{g}_2 + 2\hat{g}_3 - \hat{g}_5 + \hat{g}_6 - \hat{g}_7 + \hat{g}_8 \right]. \]  

(3.32)

Then, the algorithmic procedure of our symmetrized operator split forcing scheme for the 2D cascaded method can be summarized in terms of the following sequence of steps to evolve for a time duration \([t, t + \Delta t] \):

((i)) Obtain the updated the velocity \( \mathbf{u} = (u_x, u_y) \) based on the pre-collision forcing with half step using Eq. (3.25).

((ii)) Compute the change of moments under collisions, \( \hat{g}_\beta, \; \beta = 3, 4, \ldots, 8 \) using Eq. (3.23) based on the updated velocity \( (u_x, u_y) \) obtained in Step (i).

((iii)) Perform post-collision forcing with a half step effectively via the calculation of change of first order moments, i.e. \( \hat{g}_1 \) and \( \hat{g}_2 \) using Eq. (3.31).

((iv)) Compute the post-collision distribution functions \( f_\alpha^p, \; \alpha = 0, 1, \ldots, 8 \) using Eq. (3.32).

((v)) Perform the streaming step using Eq. (3.22b) to obtain the updated distribution functions \( f_\alpha, \; \alpha = 0, 1, \ldots, 8 \).
Finally, obtain the output velocity field \( \mathbf{u}^o = (u^o_x, u^o_y) \) via Eq. (3.24) and the density \( \rho \) using \( \rho = \sum_{\alpha=0}^{8} f_\alpha \).

Some of the main advantages of this symmetrized operator split forcing scheme of the cascaded LB method are:

(a) Using symmetrization principle with half-time step application of the body force before and after collision is consistent with Strang splitting and the scheme is formally second order accurate in time.

(b) The approach correctly projects the effects of the body force on the higher order moments via step (ii) above and hence naturally eliminates the discrete effects identified in prior works [71] (see below for details).

(c) The procedure is simple and efficient by involving the body force implementation directly only in the moment space and does not require additional terms due to forcing in the velocity space, which is usually obtained via cumbersome transformation from the moment space as in prior forcing schemes for the cascaded LB method. This aspect is especially advantageous in 3D. Appendix A outlines the implementation of this approach for a 3D central moment based LB scheme.

We will now present an analysis on how the spurious term \( F_i u_j + F_j u_i \) that can appear in the viscous stress is eliminated in our present central moments-based cascaded LB formulation using a split force implementation. This can be achieved by a continuous time equation for the second central moment whose evolution is independent of the body force. As a result, it can introduce a canceling second moment of the body force term at the leading order in the emergent PDE of the second raw moment of the distribution functions recovering correct flow physics. We will start with this latter aspect first and identify this compensating second raw moment of the body force by considering the discrete velocity Boltzmann equation \( \partial_t f_\alpha + \mathbf{e}_\alpha \cdot \nabla f_\alpha = \Omega_\alpha + S_\alpha \), where \( \Omega_\alpha \) and
\( S_\alpha \) are the collision operator and the source term due to the body force, respectively. Taking its zeroth and first moments lead to

\[
\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \quad \partial_t (\rho \mathbf{u}) + \nabla \cdot \mathbf{\Gamma} = \mathbf{F},
\]

(3.33)

and then taking its second moment, we obtain the following evolution equation

\[
\partial_t \mathbf{\Gamma} + \nabla \cdot \mathbf{\Lambda} = -\frac{1}{\tau} \mathbf{\Gamma}^{(\text{neq})} + \mathbf{T},
\]

(3.34)

where \( \mathbf{\Gamma} \) and \( \mathbf{\Lambda} \) are the second and third moments of the distribution functions, i.e., \( \sum_\alpha f_\alpha e_{\alpha i} e_{\alpha j} \) and \( \sum_\alpha f_\alpha e_{\alpha i} e_{\alpha j} e_{\alpha k} \), respectively, and \( \mathbf{T} \) is the required canceling second moment of the body force term, i.e., \( \sum_\alpha S_\alpha e_{\alpha i} e_{\alpha j} \), which should arise via a condition on the second central moment given in the following. In Eq. (3.34), \( \mathbf{\Gamma}^{(\text{neq})} \) is the non-equilibrium part of the second raw moment and \( \tau = 1/\omega_j \), where \( j = 4, 5 \), is the corresponding relaxation time, which are related to the viscous stress.

In order to determine the evolution equation for hydrodynamics at the leading order, we now apply the Chapman-Enskog (C-E) expansions of the distribution functions about its equilibria (local Maxwellian) and the time derivative, i.e., \( f_\alpha = f_\alpha^{(0)} + \epsilon f_\alpha^{(1)} + \epsilon^2 f_\alpha^{(2)} + \cdots \) and \( \partial_t = \partial_{t_0} + \epsilon \partial_{t_1} + \epsilon^2 \partial_{t_2} + \cdots \), respectively, where \( \epsilon \) is a small perturbation parameter. This is equivalent to the following expansions on the higher, non-conserved, raw moments

\[
\mathbf{\Gamma} = \mathbf{\Gamma}^{(0)} + \epsilon \mathbf{\Gamma}^{(1)} + \epsilon^2 \mathbf{\Gamma}^{(2)} + \cdots, \quad \mathbf{\Lambda} = \mathbf{\Lambda}^{(0)} + \epsilon \mathbf{\Lambda}^{(1)} + \epsilon^2 \mathbf{\Lambda}^{(2)} + \cdots,
\]

(3.35)

in the above moment system. To the leading order, the mass and momentum equations in Eq. (3.33) become

\[
\partial_{t_0} \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \quad \partial_{t_0} (\rho \mathbf{u}) + \nabla \cdot \mathbf{\Gamma}^{(0)} = \mathbf{F},
\]

(3.36)

where \( \mathbf{\Gamma}^{(0)} = c_s^2 \rho \mathbf{l} + \rho \mathbf{uu} \) is the equilibrium part of the second raw moment. On the other hand, the leading order second raw moment equation, via Eq. (3.34), reads as

\[
\partial_{t_0} \mathbf{\Gamma}^{(0)} + \nabla \cdot \mathbf{\Lambda}^{(0)} = -\frac{1}{\tau} \mathbf{\Gamma}^{(1)} + \mathbf{T}.
\]

(3.37)
In order to recover the physically correct viscous stress, the non-equilibrium part of the second moment $\Gamma^{(1)}$ in the above equation, Eq. (3.37), should only be related to $\nabla \cdot \Lambda^{(0)}$, which depends on the velocity gradients. However, the presence of the time derivative term in Eq. (3.37), i.e.,

$$\partial_t \Gamma^{(0)} = c_s^2 \partial_t \rho I + \partial_t (\rho uu),$$

in which the time derivatives of the velocity $\partial_t (\rho uu)$ via the leading momentum equation (Eq. (3.36)) give rise to an additional term of the form $Fu + uF$. This can be eliminated only if the corresponding moment of the body force $T$ becomes equal to

$$T = Fu + uF. \quad (3.38)$$

This necessary condition for the second raw moment of the body force $\sum_\alpha S_\alpha e_\alpha e_\beta = Fu + uF$, which is a classic result of the acceleration term in the Boltzmann equation, was given in [93]. This implies a vanishing second central moment of the body force, i.e., $\sum_\alpha S_\alpha (e_{\alpha x} - u_x)^m (e_{\alpha y} - u_y)^n = 0$ for $m + n = 2$, which appears explicitly in [94] and was considered in the previous unsplit forcing approach for the cascaded LB scheme [19].

In view of the above, in our present operator-split forcing based cascaded LB formulation, the PDE needed for the solving the split force step given in Eq. (3.13) is a central moment representation of the split kinetic equation $\partial_t f_\alpha = S_\alpha$. That is, taking the central moments of this equation of order $(m + n)$, we get an evolution equation as follows:

$$\text{Step } F : \frac{\partial}{\partial t} \hat{\kappa}_{xy}^{mn} = \sigma_{xy}^{mn}, \quad (3.39)$$

where $\hat{\kappa}_{xy}^{mn} = \sum_\alpha f_\alpha (e_{\alpha x} - u_x)^m (e_{\alpha y} - u_y)^n$ and $\sigma_{xy}^{mn} = \sum_\alpha S_\alpha (e_{\alpha x} - u_x)^m (e_{\alpha y} - u_y)^n$ are the central moments of the distribution functions and the source term due to the body force, respectively. It thus follows that, in particular, the continuous time equations for the change in the second central moment components for the split body force step are given as

$$\text{Step } F : \frac{\partial}{\partial t} \hat{\kappa}_{xx} = 0, \quad \frac{\partial}{\partial t} \hat{\kappa}_{yy} = 0, \quad \frac{\partial}{\partial t} \hat{\kappa}_{xy} = 0, \quad (3.40)$$

which implies the necessary condition for introducing the canceling second raw moment components of the body force, i.e., $2F_x u_x, 2F_y u_y$ and $F_x u_y + F_y u_x$ to eliminate the spurious effects in the viscous stress and thereby correctly recover the Navier-Stokes equations as mentioned above.
3.5 Extension of the Symmetrized Operator Split Implementation for Cascaded LB Method for Passive Scalar Transport Including Sources

In many applications, the transport of a passive scalar (e.g., temperature or species concentration) occurs, which is generally represented by means of the following convection-diffusion equation (CDE) with a source term

\[ \partial_t \phi + \nabla \cdot (u \phi) = \nabla \cdot (D_{\phi} \nabla \phi) + S_{\phi}. \] (3.41)

Here, \( \phi \) is the passive scalar variable, \( D_{\phi} \) is the diffusion coefficient, and \( S_{\phi} \) is the local source term (e.g. due to viscous dissipation, internal heat generation or chemical reaction). Various LB schemes have been investigated for modeling the CDE during the last two decades (e.g., [95, 21, 96, 97, 98, 99, 100, 101, 102, 87]). A novel numerical approach considered in this study for the solution of Eq. (3.41) is as follows. The velocity \( u \) in the above equation can be obtained from the cascaded LB scheme for the D2Q9 lattice presented in the previous section. Our goal is to solve for the passive scalar field \( \phi \) whose evolution is represented by the above CDE, but without the source term using a separate 2D cascaded scheme with collide and stream steps involving another distribution function; then implement the effect of the source term \( S_{\phi} \) via additional source steps using an operator split scheme based on a symmetrization principle. To meet this objective, we consider a new cascaded LB scheme for coupled fluid flow and scalar transport that we developed recently in different dimensions [33] and further accelerated by using multigrid [60].

Here, a two-dimensional, five velocity (D2Q5) lattice based cascaded LB method is introduced to represent the evolution of the passive scalar field via the CDE, which is adopted in this work for further extension using an operator split source implementation.

The D2Q5 lattice is represented by means of the following components of the particle velocity vectors \( |e_{x}\rangle \) and \( |e_{y}\rangle \):

\[ |e_{x}\rangle = (0, 1, 0, -1, 0)^\dagger, \] \( (3.42a) \)

\[ |e_{y}\rangle = (0, 0, 1, 0, -1)^\dagger. \] \( (3.42b) \)
In addition, we introduce the following $|1\rangle$ vector:

$$|1\rangle = (1, 1, 1, 1)^\dagger.$$  

(3.43)

The zeroth moment is the Euclidean inner product of this vector with the distribution functions.

The corresponding five orthogonal basis vectors are given by [60]

$$|L_0\rangle = |1\rangle, \quad |L_1\rangle = |e_x\rangle, \quad |L_2\rangle = |e_y\rangle,$$

$$|L_3\rangle = 5 |e_x^2 + e_y^2 - 4 |1\rangle, \quad |L_4\rangle = |e_x^2 - e_y^2\rangle,$$

(3.44)

which can be grouped together as the following transformation matrix $L$ for mapping changes in the moment space to those in the velocity space

$$L = [\begin{array}{cccc} |L_0\rangle & |L_1\rangle & |L_2\rangle & |L_3\rangle & |L_4\rangle \end{array}].$$

(3.45)

In order to represent the structure of the cascaded collision operator for the passive scalar field, we define the following central moments and raw moments, respectively, of the distribution function $g_\alpha$ and its equilibrium $g_{\alpha}^{eq}$ as

$$\left(\begin{array}{c} \hat{\kappa}^{\phi}_{x^m y^n} \\ \hat{\kappa}^{eq, \phi}_{x^m y^n} \end{array} \right) = \sum_\alpha \left(\begin{array}{c} g_\alpha \\ g_{\alpha}^{eq} \end{array} \right) (e_{\alpha x} - u_x)^m (e_{\alpha y} - u_y)^n,$$

(3.46)

and

$$\left(\begin{array}{c} \hat{\kappa}^{\phi'}_{x^m y^n} \\ \hat{\kappa}^{eq, \phi'}_{x^m y^n} \end{array} \right) = \sum_\alpha \left(\begin{array}{c} g_\alpha \\ g_{\alpha}^{eq} \end{array} \right) e_{\alpha x}^m e_{\alpha y}^n.$$

(3.47)

By equating the discrete central moments of the equilibrium distribution function with the corresponding continuous central moments based on the local Maxwellian (wherein the density is replaced by $\phi$), we get

$$\tilde{\kappa}^{eq, \phi}_0 = \phi, \quad \tilde{\kappa}^{eq, \phi}_x = 0, \quad \tilde{\kappa}^{eq, \phi}_y = 0, \quad \tilde{\kappa}^{eq, \phi}_{xx} = c_{s\phi}^2 \phi, \quad \tilde{\kappa}^{eq, \phi}_{yy} = c_{s\phi}^2 \phi,$$

(3.48)

which will be used in the construction of the collision operator later. In this work, we set $c_{s\phi}^2 = 1/3$. Then, the 2D cascaded LB scheme for the passive scalar transport without the source term
can be represented by means of the following collision and streaming steps:

\[ g_\alpha^p = g_\alpha + (\mathbf{L} \cdot \mathbf{h})_\alpha, \quad (3.49a) \]
\[ g_\alpha(x, t) = g_\alpha^p(x - e_\alpha \Delta t, t). \quad (3.49b) \]

The procedure to obtain the change of different moments under cascaded collision, i.e. \( \hat{\mathbf{h}} \) based on the central moment equilibria Eq. (3.48) is analogous to that used in the previous section for fluid flow, with the main difference being that in the present case, there is only one collisional invariant, i.e. \( \phi \), and hence \( \hat{\mathbf{h}}_0 = 0 \). Then, it follows that [60] (see also [33] that elaborates such a formulation for a 3D cascaded LBM for CDE)

\[ \begin{align*}
\hat{h}_1 &= \frac{\omega_1^\phi}{2} \left[ \phi u_x - \hat{\kappa}_x' \right], \\
\hat{h}_2 &= \frac{\omega_2^\phi}{2} \left[ \phi u_y - \hat{\kappa}_y' \right], \\
\hat{h}_3 &= \frac{\omega_3^\phi}{4} \left[ 2c_{s_0}^2 \phi - (\hat{\kappa}_{xx}' + \hat{\kappa}_{yy}') + 2(u_x \hat{\kappa}_x' + u_y \hat{\kappa}_y') + (u_x^2 + u_y^2) \phi \right] + u_x \hat{h}_1 + u_y \hat{h}_2, \\
\hat{h}_4 &= \frac{\omega_4^\phi}{4} \left[ -(\hat{\kappa}_{xx}' - \hat{\kappa}_{yy}') + 2(u_x \hat{\kappa}_x' - u_y \hat{\kappa}_y') + (u_x^2 - u_y^2) \phi \right] + u_x \hat{h}_1 - u_y \hat{h}_2. \quad (3.50)
\end{align*} \]

where \( \omega_1^\phi, \omega_2^\phi, \omega_3^\phi \) and \( \omega_4^\phi \) are the relaxation parameters. Notice that the cascaded structure of the expressions for the change of moments \( \hat{\mathbf{h}} \) starts from the first order moments for the CDE, unlike those for the NSE given the previous section. The relaxation parameters for the first order moments in the above determine the molecular diffusivity \( D_\phi \):

\[ D_\phi = c_{s_0}^2 \left( \frac{1}{\omega_j} - \frac{1}{2} \right) \Delta t, \ j = 1, 2. \]

After the streaming step in Eq. (3.49b), the output passive scalar field \( \phi^o \) is obtained as the zeroth moment of \( g_\alpha \) as

\[ \phi^o = \sum_{\alpha=0}^4 g_\alpha. \quad (3.51) \]

The effect of the source term \( S_\phi \) can then be introduced as the solution of the source subproblem split from Eq. (3.41): \( \partial_t \phi = S_\phi \). As before, this can be implemented by means of two symmetrized sequence of steps before and after collision, each using a time step \( \Delta t/2 \) and such a source operator will be denoted by \( \mathbf{R}^{1/2} \). Thus, the extension of the Strang splitting approach for the cascaded LBM to represent the source term in the CDE can be formulated as

\[ g_\alpha(x, t + \Delta t) = S \mathbf{R}^{1/2} \mathbf{C} \mathbf{R}^{1/2} g_\alpha(x, t). \quad (3.52) \]
Solving the above subproblem representing the evolution of the scalar field $\phi$ due to the source term $S_\phi$ yields the following step before collision

$$\text{Pre-collision Source Step } R^{1/2} : \phi = \phi^o + \frac{S_\phi}{2} \Delta t. \quad (3.53)$$

This updated $\phi$ is then used to perform the cascaded collision relaxation step and determine the change of different moments under collision $\hat{h}_\beta$, where $\beta = 1, 2, 3, 4$, given in Eq. (3.50). Analogously, the other source half step following collision can be represented as

$$\text{Post-collision Source Step } R^{1/2} : \phi^p = \phi + \frac{S_\phi}{2} \Delta t = \phi^o + S_\phi \Delta t. \quad (3.54)$$

In order to effectively implement this in the cascaded formulation, we take the zeroth moment of the post-collision distribution $g^p_\alpha$ given by $g^p_\alpha = g_\alpha + (L \cdot \hat{h})_\alpha$, which yields

$$\phi^p = \sum_\alpha g^p_\alpha = \sum_\alpha g_\alpha + \sum_\beta \langle K_\beta | 1 \rangle \hat{h}_\beta. \quad (3.55)$$

Based on the orthogonal basis vectors given in Eq. (3.44), it follows that $\sum_\beta \langle K_\beta | 1 \rangle \hat{h}_\beta = 5\hat{h}_0$, which when substituted in Eq. (3.55), and along with Eq. (3.51), we obtain

$$\phi^p = \phi^o + 5\hat{h}_0. \quad (3.56)$$

Comparing the target result Eq. (3.54) with the above constructed field (Eq. (3.56)), we get the following result for the zeroth order moment change due to the source $S_\phi$

$$\hat{h}_0 = \frac{S_\phi}{5} \Delta t. \quad (3.57)$$

This effectively implements the effect of the post-collision source step over a step length of $\Delta t/2$. Using this result (Eq. (3.57)) along with Eq. (3.50) for the change of moments under collision in Eq. (3.49a) and expanding $(K \cdot \hat{h})_\alpha$, we obtain the post-collision distribution functions, which read
\[
g'_0 = g_0 + \left[ \hat{h}_0 - \hat{h}_3 \right],
g'_1 = g_1 + \left[ \hat{h}_0 + \hat{h}_1 + \hat{h}_3 + \hat{h}_4 \right],
g'_2 = g_2 + \left[ \hat{h}_0 + \hat{h}_2 + \hat{h}_3 - \hat{h}_4 \right],
g'_3 = g_3 + \left[ \hat{h}_0 - \hat{h}_1 + \hat{h}_3 + \hat{h}_4 \right],
g'_4 = g_4 + \left[ \hat{h}_0 - \hat{h}_2 + \hat{h}_3 - \hat{h}_4 \right].
\] (3.58)

The overall sequence of computational steps for the 2D cascaded LB scheme for passive scalar transport with a source implementation based on the Strang splitting is similar to that for the fluid flow presented in the previous section. Moreover, such a symmetrized operator splitting formulation can also be used to represent forces/sources in the 3D central moment based LBM for thermal convective flows developed recently [33].

3.6 Results and Discussion

We will now present a numerical validation study of the various symmetrized operator split schemes to incorporate forces/sources in the cascaded LB method presented earlier by comparison of their computed results against a set of benchmark problems with analytical solutions. In the following, all the numerical results will be generally reported in the lattice units typical for LB simulations [18]. That is, unless otherwise specified, we consider \( \Delta x = \Delta t = 1 \) and hence the particle speed \( c = \Delta x/\Delta t \) is taken to be unity. The fluid velocity will be scaled by the particle speed \( c \), and the reference scale for the density \( \rho_0 \) is 1.0. For the cascaded LB method for fluid flow presented in Sec. 3.4, the considerations for the relaxation parameters are as follows: \( \omega_4 \) and \( \omega_5 \) determine the shear kinematic viscosity (via \( \omega_4 = \omega_5 = 1/\tau \) and \( \nu = \frac{1}{3}(\tau - \frac{1}{2})\Delta t \)), which can be specified from the problem statement. The parameter \( \omega_3 \) is related to the bulk viscosity (see e.g. [19]), while the remaining parameters for the higher order moments \( \omega_6, \omega_7 \) and \( \omega_8 \), along with
\( \omega_3 \) can be tuned to improve numerical stability. A detailed study of the influence of such parameters in the cascaded LB scheme was performed in [17]. For turbulent flow computations, care needs to be exercised in choosing the relaxation parameters for the higher order moments in order to avoid being over-dissipative. In this work, for the incompressible, laminar flow benchmark flow problems considered in the following, we use \( \omega_3 = \omega_6 = \omega_7 = \omega_8 = 1.0 \). On the other hand, for the cascaded LB method for the solution of the passive scalar transport presented in Sec. 3.5, the parameters \( \omega_1^\phi \) and \( \omega_2^\phi \), which are related to the coefficient of diffusivity (i.e. \( \omega_1^\phi = \omega_2^\phi = 1/\tau^\phi \) and \( D^\phi = \frac{1}{3}(\tau^\phi - \frac{1}{2})\Delta t \)), are assigned from the problem statement based on the characteristic dimensionless group; relaxation parameters \( \omega_j^\phi \), where \( j = 3, 4, 5 \), which influence the numerical stability, are set to unity in this work.

3.6.1 Poiseuille Flow

In these sections, we validate our 2D operator split forcing approach by considering various test problems involving different types of body force fields. For the first problem, a two-dimensional Poiseuille flow in a channel discretized with \( 3 \times 100 \) lattice nodes is considered. In our computations, at the top and bottom walls, a no-slip boundary condition, and at the inlet and outlet, periodic boundary conditions are applied. The no-slip boundary condition is implemented by using the classical half-way bounce back scheme in this work [103, 18]. The analytical solution of the velocity profile flow for this laminar flow problem can be written as follows:

\[
U(y) = U_{max}[1 - (\frac{y}{L})^2],
\]

where \( U_{max} = F_x L^2 / (2\rho \nu) \) is the maximum velocity along the central line. Here, \( L, \rho \) and \( \nu \) are the channel half-width, fluid density and kinematic viscosity respectively. \( F_x \) is a constant body force acting in the \( x \)-direction which drives the flow. Comparison of the simulation results of the velocity profile against the analytical solution is shown in Fig. 3.1, where the body forces for two cases with maximum velocities of 0.02 and 0.08 are set to the values of \( 10^{-8} \) and \( 10^{-7} \), respectively. For the former case, the relaxation time \( \tau \) is chosen to be 0.5019, which for the latter it is 0.5047. The corresponding Mach numbers \( Ma \) are 0.034 and 0.138, respectively.
It can be clearly seen that there is an excellent agreement between the numerical simulation carried out using the 2D symmetrized operator split cascaded LB forcing scheme and the analytical solution for the both cases.

**Grid Convergence Study**

In order to determine the order of accuracy of our symmetrized operator split forcing scheme, we perform a grid convergence test by applying a diffusive scaling. According to this scaling, Mach number $\text{Ma} = U/c_s$ reduces proportionally with the increase in the grid resolution at a fixed viscosity or fixed relaxation time $\tau = 1/\omega_j, \ j = 4, 5$, where $\omega_4$ and $\omega_5$ represent the relaxation parameters for the second order moments in the 2D cascaded LB scheme (see Sec. 4), so that the scheme has asymptotic convergence to the incompressible flow limit. For our simulation, we consider a Poiseuille flow with the same set up as considered earlier. We consider a sequence of $3 \times 15, 3 \times 31, \ldots, 3 \times 121$ lattice nodes to study grid convergence under diffusive scaling when the
relaxation time and Reynolds number are set to $\tau = 0.55$ and 100, respectively. Next, to quantify the grid convergence, we consider the global relative error ($E_{g,u}$) of the flow field under a discrete $\ell_2$-norm as follows:

$$\|E_{g,u}\|_2 = \sqrt{\frac{\sum (u_c - u_a)^2}{\sum (u_a)^2}},$$

(3.59)

where $u_c$ and $u_a$ is the computed and analytical solutions, respectively, and the summation is carried out for the flow domain. The relative error between the computed results and the analytical solution against different grid resolutions is illustrated in Fig. 3.2. The relative errors have a slope of 2.00 which indicates that our new approach based on the symmetrized operator split forcing scheme for the cascaded LB method is spatially second-order accurate.

FIGURE 3.2: Grid convergence for 2D Poiseuille flow with a constant Reynolds number $Re = 100$ and relaxation time $\tau = 0.55$ computed using the 2D symmetrized operator cascaded LB forcing scheme.

3.6.2 Hartmann Flow

As the next benchmark case study, a numerical comparison of the results with our 2D operator split forcing approach is made for a specific type of magnetohydrodynamic (MHD) flow, i.e., the flow between two unbounded plates subjected to a transverse magnetic field known as the Hartmann flow. This type of flow arises in a variety of engineering devices including MHD pumps,
fusion devices, generators and microfluidic devices. Furthermore, an inherent spatially-varying body force makes this benchmark a particularly suitable test problem for the present study. The fluid is driven by a constant body force $F_b$ and retarded by a local variable force (i.e. Lorentz force) arising by an interaction between a uniform steady magnetic field $B_y = B_0$, acting perpendicular to the channel walls and the fluid motion. By choosing the $x$ axis for the flow direction and the $y$ axis to be co-directional with the external magnetic field $B_y = B_0$, the induced magnetic field resulting from such an interaction can be represented as $B_x(y) = \frac{F_b L}{B_0} \left[ \frac{\sinh(Ha\frac{y}{L})}{\sinh(Ha)} - \frac{y}{L} \right]$. Here, the Hartmann number, $Ha$ is the square root of the ratio of the electromagnetic force to the viscous force and $L$ and $F_b$ are the channel half-width and the uniform driving force, respectively. Consequently, the effectively spatially varying body force which act on the flow is $F_x = F_b + F_{mx}$. This is a combination of the Lorentz force $F_{mx} = B_0 \frac{dB_x}{dy}$, and the uniform driving force $F_b$. The analytical solution for such a problem is $u_x(y) = \frac{F_b L}{B_0} \sqrt{\frac{\eta}{\nu}} \coth(Ha) \left[ 1 - \frac{\cosh(Ha\frac{y}{L})}{\cosh(Ha)} \right]$. Here, $\nu$ is the kinematic viscosity and $\eta$ is the magnetic resistivity, which can be represented by $\eta = B_0^2 L^2 / Ha^2 \nu$. We consider the same set up as considered for the Poiseuille flow simulation for the boundary conditions but now with spatially varying body forces. For two different values of $Ha$, 3 and 10, corresponding to Mach numbers of 0.013 and 0.004, respectively, the computed velocity profiles against the analytical solution are illustrated in Fig. 3.3. It can be observed that the present simulation is able to reproduce the analytical solution very well. In particular, the significant flattening of the velocity profile at higher $Ha$ is well reproduced by our forcing scheme.

3.6.3 Womersley Flow

We now turn to study the Womersley flow, which is a flow between two infinite parallel plates driven by a temporally oscillatory external force. This benchmark problem is used to assess the ability of our symmetrized operator split forcing scheme for representing time-dependent body forces. The external force $F_m \cos(\omega t)$ oscillates with an amplitude $F_m$ and with an angular fre-
FIGURE 3.3: Comparison of the computed velocity profiles using the 2D symmetrized operator split cascaded LB forcing scheme with the analytical solution for Hartmann flow for Hartmann numbers $Ha$ of 3 and 10. The lines indicate the analytical results, and the symbols are the solutions obtained by our present numerical scheme.
frequency \( \omega = 2\pi/T \), where \( T \) is the time period. Supposing that the flow is laminar and incompressible, the analytical solution for the velocity field is given as

\[
 u(y, t) = \text{Re} \left\{ i \frac{F_m}{\omega} \left[ 1 - \frac{\cos(\gamma y/L)}{\cos \gamma} \right] e^{(i\omega t)} \right\}, \tag{3.60}
\]

where \( \gamma = \sqrt{i \text{Wo}^2} \), \( \text{Wo} = L \sqrt{\omega/\nu} \) being the Womersley number, which is a non-dimensional parameter representing the ratio of the channel half width \( L \) to the diffusion length over an oscillation period (i.e., the Stokes layer thickness). \( \text{Re} \{ \cdot \} \) represents taking the real part of the expression within the brackets. The simulation parameters are set as follows. The computational domain is resolved by a \( 3 \times 100 \) mesh, the time period \( T = 10000 \) and the maximum force amplitude is set to \( F_m = 1 \times 10^{-5} \). The boundary condition at the inlet and the outlet is periodic and the half-way bounce-back scheme to represent the no-slip condition is used at the walls. The body force for this case is implemented as a solution of Eq. (3.13) to update the velocity field. Since the explicit form of the time-dependent force is known here, it can be either analytically integrated to perform the velocity update in the force step or solved numerically by representing the body force \( F_x \) via the trapezoidal rule as \( \frac{1}{2} F_m (\cos(\omega t) + \cos(\omega t + \Delta t/2)) \). The latter approach is used in the present study. In general cases, if the body force \( \mathbf{F} \) depends on \( \mathbf{u} \), then Eq. (3.13) needs to be numerically integrated and used as an implicit equation to solve for \( \mathbf{u} \). Simulations are carried out to obtain the velocity profiles across the channel at different time instants with the time period \( T \). Figure 6.5 shows a comparison for the velocity profiles for two values of the Womersley number, i.e. 4 and 10.7 at different time instants. It can be clearly seen that the numerical results agree well with the analytical solution represented by Eq. (3.60). Thus, the symmetrized operator split forcing scheme is able to represent flow profiles driven by time varying body forces with excellent accuracy.
FIGURE 3.4: Comparison of computed and analytical velocity profiles at different instants within a time period of pulsatile flow at two different Womersley numbers of $Wo = 4$ $Wo = 10.7$. Here, lines represent the analytical solution and symbols refer to the numerical results obtained using the 2D symmetrized operator split cascaded LB forcing scheme.
3.6.4 Flow through a Square Duct

In order to validate our 3D symmetrized operator split forcing scheme for a multidimensional flow subjected to a body force, we consider flow through a square duct driven by a constant body force $F_x$. In our computations, we apply periodic boundary conditions at the inlet and outlet and a no-slip boundary condition at the four wall surfaces. For a channel with width $2a$, this test problem has an analytical solution based on a Fourier series for the velocity field, which reads as

$$u(y, z) = \frac{16 a^2 F_x}{\rho \nu \pi^3} \sum_{n=1}^{\infty} (-1)^{(n-1)} \left[ 1 - \frac{\cosh\left(\frac{(2n-1)\pi y}{2a}\right)}{\cosh\left(\frac{(2n-1)\pi}{2}\right)} \right] \cos\left(\frac{(2n-1)\pi z}{2a}\right) \cos\left(\frac{(2n-1)\pi y}{2a}\right),$$

(3.61)

where $\rho$ and $\nu$ are the fluid density and kinematic viscosity, respectively and $x$ is the direction of the flow, and $-a < y < a$, $-a < z < a$ is the cross section of the duct. We chose a grid resolution of $3 \times 45 \times 45$, with a relaxation parameter $\tau$ equal to 0.76, and a body force magnitude of $F_x = 1 \times 10^{-7}$ is applied. Figure 3.5 illustrates the velocity profiles $u(y, z)$ computed using our 3D symmetrized operator split scheme to incorporate forcing terms in the 3D cascaded LB method for different values of $y$. In this figure, a comparison with the analytical solution given above is also made. It is evident that there is a very good agreement between our computed results and the analytical solution for this body force driven multidimensional flow problem.

3.6.5 Four-rolls Mill Flow Problem

Let us now consider a problem involving two-dimensional (2D), steady, fluid motion consisting of an array of counter-rotating vortices in a square domain of side $2\pi$ that is periodic in both $x$ and $y$ directions, driven by a spatially varying body force, i.e. $F_x = F_x(x, y)$ and $F_y = F_y(x, y)$. It is a modified form of the classical Taylor-Green vortex flow and has been used as a benchmark problem to test body force implementations in prior LBM studies (e.g., [104, 78]). The four-rolls
FIGURE 3.5: Comparison of the computed velocity profiles using the 3D symmetrized operator split cascaded LB forcing scheme and the analytical solution, for flow through a square duct in presence of a body force magnitude of $F_x = 10^{-7}$ for different values of $y$. Here, lines represent the analytical solution and symbols refer to the results obtained using the present numerical scheme.
fluid motion is established by imposing the following local body force components:

\[
F_x(x, y) = 2 \rho_0 \nu u_0 \sin x \sin y, \quad F_y(x, y) = 2 \rho_0 \nu u_0 \cos x \cos y,
\]

where \(0 \leq x, y \leq 2\pi\), \(\rho_0\) is the reference density, \(\nu\) is the kinematic viscosity, and \(u_0\) is the velocity scale. A simplification of the Navier-Stokes equations with the above local body force leads to the following analytical solution for the velocity field:

\[
u_x(x, y) = u_0 \sin x \sin y, \quad \nu_y(x, y) = u_0 \cos x \cos y.
\]

First, in order to validate the Strang splitting-based forcing scheme for the cascaded LBM, we consider \(u_0 = 0.01, \rho_0 = 1.0\) and \(\nu = 0.0011\), and the square domain of side \(2\pi\) is resolved by \(N \times N\) mesh grids, where \(N = 24, 48, 96, 192\). The mesh spacing \(\Delta x\) then is given by \(\Delta x = 2\pi/N\). Considering the convective scaling \(\Delta x/\Delta t = c = 1\), the kinematic viscosity may be written as \(\nu = \frac{1}{3}(\tau - \frac{1}{2})\Delta x\), where \(\tau = 1/\omega_4 = 1/\omega_5\). Figure 3.6 shows the velocity field \(\nu_y(x, y = \pi)\) computed using \(N = 96\) along the horizontal centerline of the domain and compared against the analytical solution given above. Excellent agreement is seen. Furthermore, Fig. 3.7 presents the 2D computed and analytical results for the streamlines, which are in very good agreement with each other. Evidently, counter-rotating pairs of vortices are well reproduced by the present forcing scheme for the cascaded LBM based on Strang splitting.

Grid Convergence Study

In order to verify the higher order accuracy provided by the Strang splitting, i.e., \(O(\Delta x^2) \sim O(\Delta t^2)\), we use the **convective** or **acoustic** scaling to study the convergence rate of the present operator-split forcing formulation for different grid resolutions, rather than the **diffusive** scaling considered earlier. Thus, we again use \(u_0 = 0.01, \nu = 0.0011\) and \(N = 24, 48, 96\) and 192. By maintaining \(\Delta x/\Delta t = c = 1\), for any pair of grid resolutions, \(N_i \times N_i\) and \(N_j \times N_j\), the corresponding relaxation parameters \(\tau_i\) and \(\tau_j\), respectively, under the convective scaling are related by \(\tau_j = \frac{1}{2} + (\tau_i - \frac{1}{2}) \frac{N_j}{N_i}\). Figure 3.8 illustrates rate of convergence using the relative error...
FIGURE 3.6: Comparison of the computed and analytical vertical velocity profiles $u_y(x)$ at $y = \pi$ for the four-rolls mill flow problem at $u_0 = 0.01$, $\nu = 0.0011$ and $N = 96$. Here, line represents the analytical solution and the symbol refers to the numerical results obtained using the 2D symmetrized operator split cascaded LB forcing scheme.

FIGURE 3.7: Streamlines (a) computed using the 2D symmetrized operator split cascaded LB forcing scheme and (b) obtained using the analytical solution for the four-rolls mill flow problem at $u_0 = 0.01$, $\nu = 0.0011$ and $N = 96$. 
between the computed and analytical solution for the $x$-component of the velocity field summed for the entire domain under the discrete $\ell_2$ norm (see Eq. (3.59)) for the above four different grid resolutions. It can be seen that the relative error varies with the grid resolution in the log-log scale with a slope of $-2.0$. Hence, the present forcing scheme based on the Strang splitting for the cascaded LBM is second order accurate under the convective scaling. In other words, this test demonstrates second order accuracy in time, while the earlier test for Poiseuille flow under diffusive scaling in Fig. 3.2 is not.

![Grid convergence for the four-rolls mill flow problem at $u_0 = 0.01$, $\nu = 0.0011$ computed using the 2D symmetrized operator split cascaded LB forcing scheme under the convective scaling.](image)

**FIGURE 3.8:** Grid convergence for the four-rolls mill flow problem at $u_0 = 0.01$, $\nu = 0.0011$ computed using the 2D symmetrized operator split cascaded LB forcing scheme under the convective scaling.

3.6.6 Thermal Couette Flow with Viscous Heat Dissipation

For the purpose of validating the symmetrized operator split cascaded source scheme for the solution of a scalar passive field represented by the CDE with a source term in Sec. 5, we perform the simulation of a thermal Couette flow with viscous heat dissipation. Here, the passive scalar field $\phi$ is the temperature $T$, which is evolved under a thermal diffusivity $D$, and modified by a
source term $S_r$ due to viscous dissipation arising from the shear flow. For such a one-dimensional Couette flow, the top wall moves with a constant velocity $U_0$ in a horizontal direction, which is maintained at a higher temperature $T_H$ and the bottom wall is at a lower temperature $T_L$ and remains stationary. The scalar source term $S_r$ resulting from the viscous heat dissipation is given by

$$S_r = \frac{2\nu}{C_v}(\mathbf{S} : \mathbf{S}),$$

(3.62)

where $\mathbf{S} = [\nabla u + (\nabla u)^T]/2$ is the strain rate tensor and $C_v$ is specific heat at constant volume. The source term due to the viscous heating $S_r$ in Eq. (3.62) is obtained in simulations from the cascaded LB solution for the flow field presented in Sec. 3.3. In particular, the strain rate tensor $\mathbf{S}$ in the cascaded LB formulation can be readily related to the second-order non-equilibrium moment components (see e.g., [19, 17]). For example, $S_{xy} = \frac{1}{2}(\partial_x u_y + \partial_y u_x) = -\frac{3\omega}{2\rho_0}(\sum_\alpha f_\alpha e_\alpha e_{\alpha y} - \rho u_x u_y)$. This problem has the following analytical solution for the temperature profile [105]

$$\frac{T - T_L}{T_H - T_L} = \frac{y}{H} + \frac{PrEc}{2} \frac{y}{H} \left(1 - \frac{y}{H}\right),$$

(3.63)

where $Pr = \nu/D$ is the Prandtl number and $Ec = U_0^2/[C_v(T_H - T_L)]$ is the Eckert number. In Fig. 3.9, the $Pr$ is fixed at 0.71 while the $Ec$ varies from 10 to 100 and the domain is discretized with $3 \times 64$ lattice nodes. The velocity of the top wall $U_0$ is taken as 0.05, the boundary temperature $T_L$ and $T_H$ are specified as 0.0 and 1.0, respectively, and the relaxation parameters $\tau$ and $\tau^\phi$ are chosen as 0.70 and 0.782, respectively. Computed results obtained using the symmetrized operator split cascaded source scheme are compared with the analytical solution given in Eq. (3.63). It is found that the numerical results are in excellent agreement with the analytical solution for various values of $Ec$, representing the source strength for this problem. In addition, the relative error between the computed results obtained using the Strang splitting-based source scheme and the analytical solution measured under the discrete $\ell_2$-norm (Eq. (3.59)) for the simulation of the thermal Couette flow are reported in Table 3.1.
TABLE 3.1: Relative error between the numerical results obtained using the 2D symmetrized operator split cascaded LB source scheme for a passive scalar transport and the analytical solution for the simulation of the thermal Couette flow at various Eckert numbers Ec.

<table>
<thead>
<tr>
<th>Eckert number Ec</th>
<th>Relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>$2.840 \times 10^{-5}$</td>
</tr>
<tr>
<td>20</td>
<td>$3.695 \times 10^{-5}$</td>
</tr>
<tr>
<td>40</td>
<td>$4.317 \times 10^{-5}$</td>
</tr>
<tr>
<td>60</td>
<td>$4.561 \times 10^{-5}$</td>
</tr>
<tr>
<td>80</td>
<td>$4.691 \times 10^{-5}$</td>
</tr>
<tr>
<td>100</td>
<td>$4.778 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

FIGURE 3.9: Comparison between numerical results of the temperature profile computed using the 2D symmetrized operator split cascaded LB source scheme for a passive scalar transport and the analytical solution for the thermal Couette flow for various values of the Eckert number Ec. Here, lines represent the analytical solution and symbols refer to the results obtained using the present numerical scheme.
3.7 Summary and Conclusions

Symmetrized operator split forcing schemes for flow simulations in 2D and 3D and a method for incorporating sources in a convection-diffusion transport of a scalar field using the cascaded lattice Boltzmann formulations are developed in this chapter. They involve force/source implementation steps before and following the collision step each taking a half time step, and are consistent with the Strang splitting, which has second order rate of convergence by construction. The post-collision half source/forcing step is effectively implemented in terms of the change of moments at the zeroth/first order that is a function of the source/body force and the time step, and a normalization factor arising from the choice of the basis for moments for the lattice set considered. The implementation of the pre-collision half source/forcing step properly projects the effects of the force/source to the higher order moments that undergo relaxation by collision and naturally eliminates the discrete effects. In contrast to the prior forcing schemes for the cascaded LB method that required using extra terms at different orders in the moment space and cumbersome lattice-dependent transformations to map them to the velocity space, the present symmetrized operator split forcing/source schemes result in a simpler formulation, with all the force/source related computations performed only in the moment space, which facilitates implementation. However, it may be noted that for efficient implementations of the LB algorithms, their performance on current hardware is limited entirely by memory bandwidth rather than by floating point operations, and the complexity of the aggregate collision operator (including forcing) does not affect performance. Comparisons of the numerical solutions obtained using the Strang splitting based forcing/source implementation methods for cascaded LB schemes against various benchmark solutions validate them for flow computations in both 2D and 3D as well as for the passive scalar transport with a local source. Furthermore, the numerical results demonstrate the second order accuracy for the convergence rate in time under the acoustic scaling of the symmetrized operator split forcing scheme.
CHAPTER IV

CENTRAL MOMENTS-BASED CASCADED LATTICE BOLTZMANN METHOD FOR THERMAL CONVECTIVE FLOWS IN THREE-DIMENSIONS

4.1 Introduction

The thermal energy transport equation for convective flows, represented by means of a convection-diffusion equation (CDE) for the temperature field, can be classified as a parabolic partial differential equation (PDE). Solution of an such equation has received considerable attention for its key role in the study of many transport phenomena arising in various thermal science and engineering applications. In addition, CDE-type models represent several important associated physical phenomena in fluid dynamics, such as the transport of the concentration of a chemical species as a passive scalar, and in the implicit capturing of interfaces in multiphase flows represented by phase field models. Whereas only for relatively simple geometries and boundary conditions, and under idealized physical situations exact analytical solutions of such equations are available, the development and applications of numerical methods play an essential role in investigations related to thermal convective flows, especially in three-dimensions (3D). Numerical techniques such as the finite difference, finite volume and finite element methods based on the direct discretization of the continuum PDEs such as the CDE have been investigated. From a different perspective, the lattice Boltzmann (LB) method has recently been demonstrated to be a very effective numerical approach for the representation of many complex fluid systems.

During their early stages of development, the LB models focused on applications to isothermal fluid flows. However, owing to numerous applications of thermal convection in fluids in natural settings and engineering, LB models for flows with heat transfer effects have also received con-
siderable attention more recently. Generally, the following types of approaches have been considered in the LB framework for simulation of thermal convective flows: (a) Multiphase (MS) LB schemes [106, 107, 108, 109], (b) hybrid approach (e.g. [110]), and (c) double distribution function (DDF) based LBM [21, 111, 112]. MS-Thermal LB models are obtained by including additional discrete velocities to the distribution function and using a higher order velocity expansion of the Maxwellian for modeling the equilibrium; here a single distribution function is used to represent the evolution of both velocity and temperature fields. Such approaches have severe restrictions in numerical stability and hence results in a narrow range of temperature variation. The hybrid approach considers using a LB model for the flow field and solvers the thermal energy equation by means of another numerical scheme such as the finite difference method. The DDF-LB schemes considers the evolution of two different distribution functions, which have overcome many of the limitation of other formulations, and are now more widely used.

Most of the prior studies related to the development of applications of DDF-based LB models consider SRT models and generally limited to two-dimensions (2D) [113, 114, 102]. The corresponding MRT based DDF-LB formulations were investigated by [115, 116, 117, 115, 112]. For practical applications, it is important to expand the capabilities of the LBM for thermal convective flows in 3D. However, only limited studies have so far been conducted in literature in this regard. One of the earliest 3D LB models for heat transfer based on a passive scalar approach was presented by [118], who performed simulations of Rayleigh-Benard convection using a SRT model. Subsequently, [119] developed a 3D SRT LB based on DDF approach and studied natural convection in a cubic cavity. More recently, [116] presented a MRT-LBE in 3D for CDE. Furthermore, [120, 121] and [122] employed DDF-based LB in 3D using MRT formulation for heat transfer problems.

In this chapter, we present new 3D formulations, based on cascaded approach using central moments within a DDF approach to represent flows with thermal convection. Such a collision model is constructed using a moving frame of reference and involving central moment relaxation based
on MRT. Due to the locality of the computational steps, these models maintain intrinsic parallelization properties enabling solution of large problems involving flows with heat transfer. Furthermore, the use of cascaded central moment formulation results in greater numerical stability to simulate 3D thermal convective flows. In this DDF approach, the cascaded LB scheme for the 3D fluid motion representing the solution of the Navier-Stokes equations (NSE) is based on a previous chapter. On the other hand, new cascaded LB formulation for the solution of the 3D thermal transport equation represented by the CDE will be derived and investigated. Here, it may be pointed out that structure of the 3D cascaded collision operators to represent the CDE will be seen to be very different from that corresponding to the solution of the NSE using the same lattice. Such difference in the expression for the collision kernels arise due to the number of collision invariants being different between solving the NSE (mass and momentum components, i.e. $1+3$) and the CDE (scalar field, i.e. $1$). In addition, in order to maintain generality of our 3D cascaded LB scheme, we consider representation of local heat source in the CDE via a source term in the velocity space using a variable transformation. We will discuss derivations of the 3D cascaded LBE for CDE representing the 3D thermal transport equations using both three-dimensional, fifteen velocity (D3Q15) lattice and its subset, viz., the three-dimensional, seven velocity (D3Q7) lattice. Finally, we present a quantitative validation of our 3D cascaded LB model for thermal convective flow by considering the simulation of 3D natural convection in a cubic cavity, which is a classical benchmark problem in this regard [1, 123, 124]. In particular, we will compare the structure of the velocity and temperature fields, as well as the heat transfer coefficient given in terms of the Nusselt number for different Rayleigh numbers, against a 3D benchmark solution.

This chapter is organized as follows. In the next section (Sec.2), we present the derivation of the 3D cascaded LBM for CDE representing the transport of the temperature field using the D3Q15 lattice following a brief presentation of the corresponding model for fluid flow, Section 3 presents the results and discussion of the numerical validation study involving the natural convection in a cubic enclosure containing air at different Rayleigh numbers. Finally, Sec.4 provides a summary
and conclusions arising from this work. In addition, Appendix B presents the derivation of the 3D cascaded LBM for CDE using a D3Q7 lattice.

### 4.2 Three-dimensional Cascaded LBE for Thermal Convective Flows Using D3Q15 Lattice

A DDF-based cascaded LBM for computation of coupled fluid motion and a scalar temperature field will now be constructed. Here, a distribution function \( f_\alpha \), whose evolution is represented by a cascaded LB formation for the solution of the Navier-Stokes equations (NSE), will be considered along with a separate distribution function \( g_\alpha \), whose dynamics is represented by another cascaded LB scheme for the convection-diffusion equation (CDE) of the scalar field. To maintain generality, the fluid motion, i.e. velocity \( u \), is considered to be influenced by a spatially/temporally varying body force \( F \) and the scalar \( \phi \) (such as the temperature \( T \)) by a local heat source \( R \). We derive the cascaded LB formulations for the typical lattice in 3D, i.e. the three-dimensional, fifteen velocity (D3Q15) lattice.

#### 4.2.1 3D Cascaded LB Model for Fluid Flow

Our goal is to first solve for the flow field represented by the NSE given by

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0, \tag{4.1a}
\]

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) = -\nabla P + \nabla \cdot \Pi + F, \tag{4.1b}
\]

where \( \rho = \rho(x, t) \) and \( u(x, t) \) are the local fluid density and velocity, respectively, at a location \( x = (x, y, z) \) and time \( t \). Here, \( P, \Pi \) and \( F \) represent the pressure, viscous stress tensor, and a local body force, respectively. It is assumed that \( F = F(x, t) \). The 3D central moment LBM for the solution of Eqs. (4.1a) and (4.1b), including a local source term \( S_\alpha \) in the velocity space for the D3Q15 lattice is presented in [125] as an extension of the model presented by [15]. A trapezoidal rule is considered in the characteristic integration of the source term to maintain second
order accuracy, and then a variable transformation \( \bar{f}_\alpha = f_\alpha - \frac{1}{2}S_\alpha \) is introduced to remove implicitness. Briefly, the 3D cascaded LBM for fluid flow with a body force may then be written as [125]

\[
\tilde{f}_\alpha(x, t) = \bar{f}_\alpha(x, t) + (K\hat{g})_\alpha + S_\alpha(x, t),
\]

\[(4.2a)\]

\[
\tilde{f}_\alpha(x + e_\alpha, t + 1) = \tilde{f}_\alpha(x, t).
\]

\[(4.2b)\]

Here, Eqs. (4.2a) and (4.2b) represent the collision and streaming steps, respectively. \( \tilde{f}_\alpha \) represents the post-collision distribution function, \( K \) is the orthogonal collision matrix, and \( \hat{g} \) is the collision kernel, which is obtained from central moment relaxation at different orders to their corresponding local equilibria. While the force here is on the derivation of a new cascaded LBE for 3D CDE as discussed in what follows, for \( K, \hat{g}, S_\alpha, \) and \( \tilde{f}_\alpha \) for the solution of the NSE in Appendix B. Once the distribution function is updated, the hydrodynamic variables are obtained from the various kinetic moments as

\[
\rho = \Sigma_\alpha \tilde{f}_\alpha, \quad \rho u = \Sigma_\alpha \tilde{f}_\alpha e_\alpha + \frac{1}{2} F.
\]

\[(4.3)\]

### 4.2.2 3D Cascaded LB Model for Transport of Temperature Field

We now present a derivation of a 3D cascaded LBM on a D3Q15 lattice for the transport of any generic scalar field \( \phi \) (such as temperature, where \( \phi = T \)), that satisfies the following

\[
CDE : \partial_t \phi + \nabla \cdot (u\phi) = \nabla \cdot (D_\phi \nabla \phi) + R.
\]

\[(4.4)\]

where \( \phi = \phi(x, t), \nabla = (\partial_x, \partial_y, \partial_z), D_\phi \) is the coefficient of diffusivity, \( R = R(x, t) \) is the local source term, and the velocity field \( u \) can be obtained from the LB model discussed earlier. The approach that can be taken in this regard consists of the following overall steps: (1) Construct an orthogonal moment basis starting from an initial set of linearly independent nonorthogonal basis vectors for the D3Q15 lattice. (2) Prescribe expressions for the continuous central moments
of equilibria and the source term at different orders and set them equal to their discrete central
moments used in the cascaded LB formulation; obtain corresponding raw moments at different
orders. (3) Determine the structure of the cascaded collision kernel via considering a central mo-
ment relaxation at different orders, and obtain the source terms in the velocity space. The com-
ponents of the particle velocity for the D3Q15 lattice can be written as

\[
|e_{\alpha x}| = (0, 1, -1, 0, 0, 0, 1, -1, 1, -1, 1, -1)\dagger,
|e_{\alpha y}| = (0, 0, 0, 1, -1, 0, 1, -1, 1, -1, 1, -1)\dagger,
|e_{\alpha z}| = (0, 0, 0, 0, 1, -1, 1, 1, 1, -1, -1, -1)\dagger,
\]

(4.5)

and a corresponding unit vector may be represented by

\[
|\phi| = (1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)\dagger.
\]

(4.6)

Here, we have used the notations \langle·| and |·⟩ to represent the row and the column vectors re-
spectively, and \dagger is the transpose operator. \langle a|b⟩ represent the dot product of any two vectors \textbf{a} and \textbf{b}. Using successively higher order orders of the monomials \(e_{\alpha x}^m e_{\alpha y}^n e_{\alpha z}^p\), we can write the following
nonorthogonal basis vectors

\[
|T_0⟩ = |\phi⟩,
|T_1⟩ = |e_{\alpha x}⟩, \quad |T_2⟩ = |e_{\alpha y}⟩, \quad |T_3⟩ = |e_{\alpha z}⟩,
|T_4⟩ = |e_{\alpha x} e_{\alpha y}⟩, \quad |T_5⟩ = |e_{\alpha x} e_{\alpha z}⟩, \quad |T_6⟩ = |e_{\alpha y} e_{\alpha z}⟩,
|T_7⟩ = |e_{\alpha x}^2 - e_{\alpha y}^2⟩, \quad |T_8⟩ = |e_{\alpha x}^2 - e_{\alpha z}^2⟩, \quad |T_9⟩ = |e_{\alpha x}^2 + e_{\alpha y}^2 + e_{\alpha z}^2⟩,
|T_{10}⟩ = |e_{\alpha x} (e_{\alpha x}^2 + e_{\alpha y}^2 + e_{\alpha z}^2)⟩, \quad |T_{11}⟩ = |e_{\alpha y} (e_{\alpha x}^2 + e_{\alpha y}^2 + e_{\alpha z}^2)⟩,
|T_{12}⟩ = |e_{\alpha z} (e_{\alpha x}^2 + e_{\alpha y}^2 + e_{\alpha z}^2)⟩, \quad |T_{13}⟩ = |e_{\alpha x} e_{\alpha y} e_{\alpha z}⟩,
|T_{14}⟩ = |e_{\alpha x}^2 e_{\alpha y}^2 + e_{\alpha x}^2 e_{\alpha z}^2 + e_{\alpha y}^2 e_{\alpha z}^2⟩.
\]

(4.7)

By applying the Gram-Schmidt orthogonalization method on the above set, we can obtain the
corresponding set of orthogonal basis vectors, which are grouped together into the following collision matrix $K$ as

$$K = [K_0, K_1, K_2, K_3, K_4, K_5, K_6, K_7, K_8, K_9, K_{10}, K_{11}, K_{12}, K_{13}, K_{14}]$$

where

$$K_0 = |\phi\rangle,$$

$$K_1 = |e_{ax}\rangle, \quad K_2 = |e_{ay}\rangle, \quad K_3 = |e_{az}\rangle,$$

$$K_4 = |e_{ax} e_{ay}\rangle, \quad K_5 = |e_{ax} e_{az}\rangle, \quad K_6 = |e_{ay} e_{az}\rangle,$$

$$K_7 = |e_{ax}^2 - e_{ay}^2\rangle, \quad K_8 = |e_{ax}^2 + e_{ay}^2 + e_{az}^2 - 3 |e_{az}^2\rangle, \quad K_9 = |e_{ax}^2 + e_{ay}^2 + e_{az}^2 - 2 |\phi\rangle,$$

$$K_{10} = 5 |e_{ax}(e_{ax}^2 + e_{ay}^2 + e_{az}^2)) - 13 |e_{ax}\rangle, \quad K_{11} = 5 |e_{ay}(e_{ax}^2 + e_{ay}^2 + e_{az}^2)) - 13 |e_{ay}\rangle,$$

$$K_{12} = 5 |e_{az}(e_{ax}^2 + e_{ay}^2 + e_{az}^2)) - 13 |e_{az}\rangle,$$

$$K_{13} = |e_{ax} e_{ay} e_{az}\rangle,$$

$$K_{14} = 30 |e_{ax}^2 e_{ay}^2 + e_{ax}^2 e_{az}^2 + e_{ay}^2 e_{az}^2\rangle - 40 |e_{ax}^2 + e_{ay}^2 + e_{az}^2\rangle + 32 |\phi\rangle. \quad (4.8)$$

Then, we define the continuous central moments of equilibria needed in the construction of the cascaded collision kernel for the 3D CDE as follows:

$$\hat{\Pi}_{x,y,z}^{\phi} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g^e(\xi - u)^m(\xi' - u)^n(\xi'' - u)^p d\xi dx dy dz, \quad (4.9)$$

where $g^e$ is the equilibrium distribution function in the continuous velocity space $(\xi, \xi', \xi'')$ for the scalar field $\phi$, which is given by $g^e = g^e(\phi, u, \xi) = \frac{\phi}{2\pi c_s^2} \exp\left[-\frac{(\xi - u)^2}{2c_s^2}\right]$. Here $c_s$ is a free parameter, which will be related to the desired coefficient of diffusivity $D_{\phi}$ later. Typically, we set $c_s^2 = \frac{1}{3}$, though it can be chosen to be at other values different from that for the cascaded LB model for the flow field. Moreover, $u$ in the above is the fluid velocity as defined in the previous section. It may be noted that the above equilibrium is obtained from the local Maxwellian by replacing the density with the scalar field $\phi$ used in our DDF scheme. Then, rewriting the com-
ponent of Eq. (4.9) in the increasing order of moments as

\[
\begin{align*}
\hat{\Pi}^{eq,\phi}_0 &= \phi, \\
\hat{\Pi}^{eq,\phi}_x &= \hat{\Pi}^{eq,\phi}_y = \hat{\Pi}^{eq,\phi}_z = 0, \\
\hat{\Pi}^{eq,\phi}_{xx} &= \hat{\Pi}^{eq,\phi}_{yy} = \hat{\Pi}^{eq,\phi}_{zz} = c_s^2 \phi, \\
\hat{\Pi}^{eq,\phi}_{xy} &= \hat{\Pi}^{eq,\phi}_{xz} = \hat{\Pi}^{eq,\phi}_{yz} = \hat{\Pi}^{eq,\phi}_{xyy} = \hat{\Pi}^{eq,\phi}_{xxy} = \hat{\Pi}^{eq,\phi}_{xxz} = \hat{\Pi}^{eq,\phi}_{xyz} = 0, \\
\hat{\Pi}^{eq,\phi}_{xxyy} &= c_s^4 \phi.
\end{align*}
\]

Here, and henceforth, the use of hat over a symbol represents any quantity in the moment space.

Similarly, for the continuous central moments due to source term \( R \) may be defined as

\[
\hat{\Gamma}^R_{x^m y^n z^p} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Delta g^R(\xi_x - u_x)^m(\xi_y - u_y)^n(\xi_z - u_z)^p d\xi_x d\xi_y d\xi_z.
\]

(4.10)

where \( \Delta g^R \) is the change in the distribution for the scalar field due to the source term. As the source term \( R \) can only effect the lowest, i.e. zeroth moment, the component of Eq. (4.10) maybe written as

\[
\begin{align*}
\hat{\Gamma}^R_0 &= R, \\
\hat{\Gamma}^R_x &= \hat{\Gamma}^R_y = \hat{\Gamma}^R_z = \hat{\Gamma}^R_{xx} = \hat{\Gamma}^R_{yy} = \hat{\Gamma}^R_{zz} = \hat{\Gamma}^R_{xy} = \hat{\Gamma}^R_{xz} = \hat{\Gamma}^R_{yz} = \hat{\Gamma}^R_{xyy} = \hat{\Gamma}^R_{xxy} = \hat{\Gamma}^R_{xxz} = \hat{\Gamma}^R_{xyz} = 0.
\end{align*}
\]

(4.11)

The cascaded LBE representing the transport of the 3D CDE can be obtained by applying a trapezoidal rule for the treatment of the source term in the characteristic integration to maintain second order accuracy. Thus, we havae

\[
g_\alpha(x + e_\alpha, t + 1) = g_\alpha(x, t) + \Omega^g_\alpha(x, t) + \frac{1}{2} \left[ S^\phi_\alpha(x, t) + S^\phi_\alpha(x + e_\alpha, t + 1) \right],
\]

(4.12)

where \( S^\phi_\alpha \) is the source term in the velocity space that effectively accounts for the term \( R(x, t) \) in the macroscopic CDE. In the above equation, the collision term \( \Omega^g_\alpha(x, t) \) can be modeled by

\[
\Omega^g_\alpha = \Omega^g_\alpha(g, \hat{h}) = (K \cdot \hat{h})_\alpha,
\]

(4.13)
where \( g = (g_0, g_1, \cdots, g_{14})^{\dagger} \) is the vector of the distribution function, and \( \hat{h} = (\hat{h}_0, \hat{h}_1, \cdots, \hat{h}_{14})^{\dagger} \) is the vector of the unknown collision kernel which will be determined later. For removing the implicitness, while maintaining a second-order accuracy, by applying a variable transformation [126],

\[
\bar{g}_\alpha = g_\alpha - \frac{1}{2} S_{\phi}^\alpha \quad \text{in Eq. (4.12)},
\]

we obtain

\[
\bar{g}_\alpha(x + e_\alpha, t + 1) = \bar{g}_\alpha(x, t) + \Omega_{\phi}^\alpha(x, t) + S_{\phi}^\alpha(x, t). \tag{4.14}
\]

This 3D central moment LBE may be rewritten in terms of the following collision and streaming steps for the purpose of implementation as

\[
\tilde{g}_\alpha(x, t) = \bar{g}_\alpha(x, t) + (K, \hat{h})_\alpha + S_{\phi}^\alpha(x, t), \tag{4.15a}
\]

\[
\tilde{g}_\alpha(x + e_\alpha, t + 1) = \tilde{g}_\alpha(x, t), \tag{4.15b}
\]

where the symbol \( \sim \) in the above represents the post collision distribution function. In order to build the structure of the cascaded collision and the source terms for representing the 3D CDE, we first define the following set of discrete central moments as

\[
\begin{pmatrix}
\hat{\kappa}_{x^m y^n z^p}
\hat{\kappa}_{eq x^m y^n z^p}
\hat{\sigma}_{x^m y^n z^p}
\hat{\tilde{\kappa}}_{x^m y^n z^p}
\end{pmatrix}
= \sum_{\alpha}
\begin{pmatrix}
g_\alpha
g_{eq}
g_{\phi}
S_{\phi}^\alpha
\end{pmatrix}
(e_{\alpha x} - u_x)^m (e_{\alpha y} - u_y)^n (e_{\alpha z} - u_z)^p, \tag{4.16}
\]

where \( \hat{\kappa}_{x^m y^n z^p} = \hat{\kappa}_{x^m y^n z^p} - \frac{1}{2} \hat{\sigma}_{x^m y^n z^p} \). Then, by equating the discrete central moments of the equilibrium distribution function and source term with their corresponding continuous central
moments at different orders, i.e. \( \hat{\kappa}_{x}^{eq, \phi} = \hat{\Gamma}_{x}^{eq, \phi} \) and \( \hat{\sigma}_{x}^{eq, \phi} = \hat{\Gamma}_{x}^{eq, \phi} \), respectively, we get

\[
\hat{\kappa}_{0}^{eq, \phi} = \hat{\phi},
\]

\[
\hat{\kappa}_{x}^{eq, \phi} = \hat{\kappa}_{x}^{eq, \phi} = \hat{\kappa}_{x}^{eq, \phi} = 0,
\]

\[
\hat{\kappa}_{xx}^{eq, \phi} = \hat{\kappa}_{yy}^{eq, \phi} = \hat{\kappa}_{zz}^{eq, \phi} = c_s^2 \hat{\phi},
\]

\[
\hat{\kappa}_{xy}^{eq, \phi} = \hat{\kappa}_{xz}^{eq, \phi} = \hat{\kappa}_{yz}^{eq, \phi} = \hat{\kappa}_{xyy}^{eq, \phi} = \hat{\kappa}_{xxy}^{eq, \phi} = \hat{\kappa}_{xxz}^{eq, \phi} = \hat{\kappa}_{xyz}^{eq, \phi} = 0,
\]

\[
\hat{\kappa}_{xxyy}^{eq, \phi} = c_s^4 \hat{\phi},
\]

\[
\text{(4.17)}
\]

and

\[
\hat{\sigma}_{0}^{\phi} = R,
\]

\[
\hat{\sigma}_{x}^{\phi} = \hat{\sigma}_{y}^{\phi} = \hat{\sigma}_{z}^{\phi} = 0,
\]

\[
\hat{\sigma}_{xx}^{\phi} = \hat{\sigma}_{yy}^{\phi} = \hat{\sigma}_{zz}^{\phi} = \hat{\sigma}_{xy}^{\phi} = \hat{\sigma}_{xz}^{\phi} = \hat{\sigma}_{yz}^{\phi} = 0,
\]

\[
\hat{\sigma}_{xyy}^{\phi} = \hat{\sigma}_{xxy}^{\phi} = \hat{\sigma}_{xxz}^{\phi} = \hat{\sigma}_{xyz}^{\phi} = 0,
\]

\[
\text{(4.18)}
\]

Since the actual calculations are carried out in term of various raw moments, we define the following set of the raw moment at different orders as

\[
\begin{pmatrix}
\hat{\kappa}_{x}^{eq, \phi} \\
\hat{\kappa}_{x}^{eq, \phi} \\
\hat{\sigma}_{x}^{eq, \phi} \\
\hat{\kappa}_{x}^{eq, \phi} \\
\hat{\sigma}_{x}^{eq, \phi} \\
\end{pmatrix} = \sum_{\alpha} \begin{pmatrix}
g_{\alpha} \\
g_{\alpha} \\
\tilde{g}_{\alpha} \\
\tilde{g}_{\alpha} \\
\tilde{g}_{\alpha} \\
\end{pmatrix} \begin{pmatrix}
g_{\alpha}^{eq} \\
g_{\alpha}^{eq} \\
S_{\alpha}^{\phi} \\
S_{\alpha}^{\phi} \\
S_{\alpha}^{\phi} \\
\end{pmatrix}
\]

\[
\text{(4.19)}
\]

where \( \hat{\kappa}_{x}^{eq, \phi} = \hat{\kappa}_{x}^{eq, \phi} = \hat{\kappa}_{x}^{eq, \phi} - \frac{1}{2} \hat{\sigma}_{x}^{eq, \phi} \), and the use of primes over the symbol here and henceforth refer to raw moments. From the above, we first determine the expressions for the source terms in the velocity space in Eq. (4.14). In this regard, as an intermediate step, by applying the binomial theorem on Eq. (4.18), we obtain the discrete raw moments of the source terms at different
Next, from this, we obtain the source terms projected to the orthogonal basis vector $\mathbf{K}$, i.e. $\hat{m}^{s,\phi} = (\mathbf{K} \cdot \mathbf{S}^\phi)$, where $\mathbf{S}^\phi = (S_0^\phi, S_1^\phi, S_2^\phi, \ldots, S_{14}^\phi)$. That is,

\[
\begin{align*}
\hat{m}_0^{s,\phi} &= R, \quad \hat{m}_1^{s,\phi} = \langle K_1 | S_\alpha \rangle = u_x R, \quad \hat{m}_2^{s,\phi} = \langle K_2 | S_\alpha \rangle = u_y R, \\
\hat{m}_3^{s,\phi} &= \langle K_3 | S_\alpha \rangle = u_z R, \quad \hat{m}_4^{s,\phi} = \langle K_4 | S_\alpha \rangle = u_x u_y R, \quad \hat{m}_5^{s,\phi} = \langle K_5 | S_\alpha \rangle = u_x u_z R, \\
\hat{m}_6^{s,\phi} &= \langle K_6 | S_\alpha \rangle = u_y u_z R, \quad \hat{m}_7^{s,\phi} = \langle K_7 | S_\alpha \rangle = (u_x^2 - u_y^2) R, \\
\hat{m}_8^{s,\phi} &= \langle K_8 | S_\alpha \rangle = (u_x^2 + u_y^2 - 2u_z^2 - 2) R, \quad \hat{m}_9^{s,\phi} = \langle K_9 | S_\alpha \rangle = (u_x^2 + u_y^2 + u_z^2) R, \\
\hat{m}_{10}^{s,\phi} &= \langle K_{10} | S_\alpha \rangle = 5 \left[ (u_x^2 + u_x u_y + u_x u_z^2) R \right] - 13u_x R, \\
\hat{m}_{11}^{s,\phi} &= \langle K_{11} | S_\alpha \rangle = 5 \left[ (u_x^2 u_y + u_y^3 + u_y u_z^2) R \right] - 13u_y R, \\
\hat{m}_{12}^{s,\phi} &= \langle K_{12} | S_\alpha \rangle = 5 \left[ (u_x^2 u_z + u_y^2 u_z + u_z^3) R \right] - 13u_z R, \\
\hat{m}_{13}^{s,\phi} &= \langle K_{13} | S_\alpha \rangle = u_x u_y u_z R, \\
\hat{m}_{14}^{s,\phi} &= \langle K_{14} | S_\alpha \rangle = 30 \left[ (u_x^2 u_y^2 + u_x^2 u_z^2 + u_y^2 u_z^2) R \right] - 40 \left[ (u_x^2 + u_y^2 + u_z^2) R \right] + 32 R. \tag{4.20}
\end{align*}
\]

Finally, by inverting the above, i.e. $S^\phi = \mathbf{K}^{-1} \cdot \hat{m}^{s,\phi}$, and exploiting the orthogonality of $\mathbf{K}$, we can determine the explicit expressions for the source terms in the velocity space $S_\alpha^\phi$, which are listed...
in Appendix C. In order to construct the collision kernel \( \hat{h} \) for the 3D cascaded collision operator for the scalar field \( \phi \), we need the raw moments of the collision kernel of different orders, i.e. \( \sum_{\alpha}(K \cdot \hat{h})_{\alpha}x^{m}y^{n}z^{p} \). Using the orthogonality property of \( \mathbf{K} \), and considering that the only conserved invariant of this 3D cascaded LBE is the scalar field \( \phi \) corresponding to the zeroth moment (i.e. \( \hat{h}_{0} = 0 \)), we get

\[
\sum_{\alpha}(K \cdot \hat{h})_{\alpha} = 0, \quad \sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ax} = 10\hat{h}_{1}, \quad \sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ay} = 10\hat{h}_{2}, \\
\sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{az} = 10\hat{h}_{3}, \quad \sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ay}e_{az} = 8\hat{h}_{4}, \quad \sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ax}e_{az} = 8\hat{h}_{5}, \\
\sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ax}^{2} = 2\hat{h}_{7} + 2\hat{h}_{8} + 6\hat{h}_{9}, \quad \sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ay}e_{az} = -4\hat{h}_{8} + 6\hat{h}_{9}, \\
\sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ax}e_{ay}e_{az} = 16\hat{h}_{10} + 8\hat{h}_{1}, \quad \sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ax}e_{ay}^{2} = 16\hat{h}_{10} + 8\hat{h}_{1}, \\
\sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ax}^{2}e_{ay} = 16\hat{h}_{11} + 8\hat{h}_{2}, \quad \sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ax}^{2}e_{az} = 16\hat{h}_{11} + 8\hat{h}_{2}, \\
\sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ax}e_{az}^{2} = 16\hat{h}_{12} + 8\hat{h}_{3}, \quad \sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ay}e_{az}^{2} = 16\hat{h}_{12} + 8\hat{h}_{3}, \\
\sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ax}e_{ay}e_{az} = 8\hat{h}_{13}, \quad \sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ax}^{2}e_{ay} = 8\hat{h}_{9} + 16\hat{h}_{14}, \\
\sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ax}^{2}e_{az} = 8\hat{h}_{9} + 16\hat{h}_{14}, \quad \sum_{\alpha}(K \cdot \hat{h})_{\alpha}e_{ay}^{2}e_{az} = 8\hat{h}_{9} + 16\hat{h}_{14}.
\]

At this point, it is important to highlight the significant difference in the derivation of the cascaded LBE for the fluid velocity \( \mathbf{u} \) (given in Appendix B) and that for the scalar field \( \phi \) considered here. In the case of the fluid flow, the mass and momentum are the conserved invariants for collision, and, hence its corresponding collision invariants kernel components will be zeroth, i.e. \( \hat{g}_{0} = \hat{g}_{1} = \hat{g}_{2} = \hat{g}_{3} \). However, in the present case, only the zeroth moment, i.e. the passive scalar field is the conserved moment during collision. Hence, \( \hat{h}_{0} \), but \( \hat{h}_{1} \neq \hat{h}_{2} \neq \hat{h}_{3} \). Due to these differences, it will be evident in the following that the expressions for the cascaded collision operator for the scalar field \( \phi \) is quite different from that for the fluid velocity \( \mathbf{u} \) given in Appendix B.

Finally based on the above, we determine the structure of the 3D cascaded collision operator for the scalar field \( \phi \) satisfying the CDE as follows: Beginning first at the lowest order non-conserved post-collision central moments, i.e. those for the first order moment component here, we set them
equal to their corresponding equilibrium states as an intermediate step. When the expression for a particular collision kernel component \( \hat{h}_\alpha (\alpha \geq 1) \) is obtained in this manner, we discard the equilibrium assumption and multiply it by a corresponding relaxation parameter \( \omega_\phi \). This step allows for a relaxation process in terms of the central moments to represent the effect of collision [15, 125]. After considerable algebraic manipulations and simplifications, and using the notation

\[
\tilde{\eta}_{x'y'z'} = \tilde{\eta}_{x'm'y'n'z'p} + \tilde{\kappa}_{x'm'y'n'z'p}
\]  

(4.21)

For, we summarize the final expressions for the collision kernel components \( \hat{h}_\alpha \) as

\[
\begin{align*}
\hat{h}_1 & = \frac{\omega_\phi}{10} \left[ \phi u_x - \tilde{\kappa}_x - \frac{1}{2} u_x R \right], \\
\hat{h}_2 & = \frac{\omega_\phi}{10} \left[ \phi u_y - \tilde{\kappa}_y - \frac{1}{2} u_y R \right], \\
\hat{h}_3 & = \frac{\omega_\phi}{10} \left[ \phi u_z - \tilde{\kappa}_z - \frac{1}{2} u_z R \right], \\
\hat{h}_4 & = \frac{\epsilon_\phi}{8} \left[ -\tilde{\eta}_{xy} + u_y \tilde{\eta}_x + u_x \tilde{\eta}_y - (\phi + \frac{1}{2} R) u_x u_y \right] + \frac{5}{4} u_y \hat{h}_1 + \frac{5}{4} u_x \hat{h}_2, \\
\hat{h}_5 & = \frac{\epsilon_\phi}{8} \left[ -\tilde{\eta}_{xz} + u_z \tilde{\eta}_x + u_x \tilde{\eta}_z - (\phi + \frac{1}{2} R) u_x u_z \right] + \frac{5}{4} u_z \hat{h}_1 + \frac{5}{4} u_x \hat{h}_3, \\
\hat{h}_6 & = \frac{\epsilon_\phi}{8} \left[ -\tilde{\eta}_{yz} + u_z \tilde{\eta}_y + u_y \tilde{\eta}_z - (\phi + \frac{1}{2} R) u_y u_z \right] + \frac{5}{4} u_z \hat{h}_2 + \frac{5}{4} u_y \hat{h}_3,
\end{align*}
\]  

(4.22-4.27)
\[
\begin{align*}
\hat{h}_7 & = \frac{\omega^\phi}{4} \left[ -\tilde{\eta}_{11}^\phi + 2(u_x \tilde{\eta}^\phi_y - u_y \tilde{\eta}^\phi_x) - (\phi + \frac{1}{2} R) (u_x^2 - u_y^2) \right] + \\
& \quad 5u_x \hat{h}_1 - 5u_y \hat{h}_2, \\
\hat{h}_8 & = \frac{\omega^\phi}{12} \left[ -\tilde{\eta}_{12}^\phi + 2(u_x \tilde{\eta}^\phi_y - u_y \tilde{\eta}^\phi_x) + 2(u_x \tilde{\eta}^\phi_x - u_y \tilde{\eta}^\phi_y - u_z \tilde{\eta}^\phi_z) - (\phi + \frac{1}{2} R) (u_x^2 + u_y^2 - 2u_z^2) \right] + \\
& \quad \frac{5}{3} u_x \hat{h}_1 + \frac{5}{3} u_y \hat{h}_2 - \frac{10}{3} u_z \hat{h}_3, \\
\hat{h}_9 & = \frac{\omega^\phi}{18} \left[ -\tilde{\eta}_{13}^\phi + 2(u_x \tilde{\eta}^\phi_y + u_y \tilde{\eta}^\phi_x + u_z \tilde{\eta}^\phi_z) - (\phi + \frac{1}{2} R) (u_x^2 + u_y^2 + u_z^2) \right] + \\
& \quad \frac{10}{9} (u_x \hat{h}_1 + u_y \hat{h}_2 + u_z \hat{h}_3), \\
\hat{h}_{10} & = \frac{\omega^\phi}{16} \left[ -\tilde{\eta}_{14}^\phi + 2u_y \tilde{\eta}^\phi_{xy} - u_y^2 \tilde{\eta}^\phi_x + u_x \tilde{\eta}^\phi_y - 2u_x u_y \tilde{\eta}^\phi_y + (\phi + \frac{1}{2} R) u_x u_y \right] \\
& \quad - \frac{5}{8} u_x^2 + \frac{1}{2} \hat{h}_1 - \frac{5}{8} u_x u_y \hat{h}_2 + u_y \hat{h}_4 + \frac{1}{8} u_x (-\hat{h}_7 + \hat{h}_8 + 3\hat{h}_9), \\
\hat{h}_{11} & = \frac{\omega^\phi}{16} \left[ -\tilde{\eta}_{15}^\phi + 2u_x \tilde{\eta}^\phi_y + u_y \tilde{\eta}^\phi_x - u^2 \tilde{\eta}^\phi_y - 2u_x u_y \tilde{\eta}^\phi_y + (\phi + \frac{1}{2} R) u_x u_y \right] \\
& \quad - \frac{5}{4} u_x u_y \hat{h}_1 - \frac{5}{4} u_x^2 + \frac{1}{2} \hat{h}_2 + u_x \hat{h}_4 + \frac{1}{4} u_y (-\hat{h}_7 + \hat{h}_8 + \hat{h}_9), \\
\hat{h}_{12} & = \frac{\omega^\phi}{16} \left[ -\tilde{\eta}_{16}^\phi + 2u_x \tilde{\eta}^\phi_y + u_y \tilde{\eta}^\phi_x + 2u_x \tilde{\eta}^\phi_y - u^2 \tilde{\eta}^\phi_y + (\phi + \frac{1}{2} R) u_x^2 u_y \right] \\
& \quad - \frac{5}{4} u_x u_y \hat{h}_1 + \frac{5}{4} u_x^2 + \frac{1}{2} \hat{h}_2, \\
\hat{h}_{13} & = \frac{\omega^\phi}{8} \left[ -\tilde{\eta}_{17}^\phi + u_x \tilde{\eta}^\phi_y + u_y \tilde{\eta}^\phi_x - u^2 \tilde{\eta}^\phi_y - u_x \tilde{\eta}^\phi_y - u_x u_y \tilde{\eta}^\phi_x + (\phi + \frac{1}{2} R) u_x u_y u_z \right] \\
& \quad - \frac{5}{4} u_y u_z \hat{h}_1 - \frac{5}{4} u_x u_z \hat{h}_2 - \frac{5}{4} u_x u_y \hat{h}_3 + u_z \hat{h}_4 + u_y \hat{h}_5 + u_x \hat{h}_6, \\
\hat{h}_{14} & = \frac{\omega^\phi}{16} \left[ -\tilde{\eta}_{18}^\phi + 2u_y \tilde{\eta}^\phi_{xy} + 2u_x \tilde{\eta}^\phi_{xy} - u_y^2 \tilde{\eta}^\phi_x + 4u_x u_y \tilde{\eta}^\phi_y + 2u_x^2 u_y \tilde{\eta}^\phi_y + c_s^4 \phi \\
& \quad - (\phi + \frac{1}{2} R) u_x^2 u_y^2 \right] \\
& \quad + \frac{5}{4} u_x u_y \hat{h}_1 + \frac{5}{4} u_x^2 \hat{h}_2 - 2u_x \tilde{\eta}^\phi_x + \frac{1}{8} (u_x^2 - u_y^2) \hat{h}_7 + \frac{1}{8} (u_x^2 + u_y^2) \hat{h}_8 \\
& \quad + \left(-\frac{3}{8} (u_x^2 + u_y^2) - \frac{1}{2}\right) \hat{h}_9 + 2u_x \hat{h}_{10} + 2u_y \hat{h}_{11} + u_y \hat{h}_2 + u_x \hat{h}_1. \\
\end{align*}
\]}

Here, the relaxation parameters \(\omega_\alpha^\phi\), where \(\alpha = 1, 2, \cdots 14\) satisfy the bounds \(0 < \omega_\alpha^\phi < 2\). The above cascaded collision kernel represents the 3D convection-diffusion equation for any scalar field \(\phi\) (such as temperature) with a source term, where the coefficient of diffusivity \(D_\phi\) is related to the relaxation times of the first order moments by

\[
D_\phi = c_s^2 \left( \frac{1}{\omega_j} - \frac{1}{2} \right), \quad j = 1, 2, 3
\]
The remaining relaxation parameters at higher orders influence numerical stability and can be tuned independently. In this chapter, we set them to unity. Notice that the structure of the collision kernel of the 3D cascaded LBE for the scalar field $\phi$ is markedly different from that for the fluid flow (see Appendix B). In particular, the "cascaded" structure starts for the scalar field from the second order moment components on, which that for the fluid flow begins from the third order moments owing to the differences in the number of collision invariants as mentioned earlier. Finally, by expanding the elements of the product $K \hat{h}$ in Eq. (4.13) and using it in Eq. (4.15a), the post-collision distribution function $\tilde{g}_\alpha$ is given by

$$
\tilde{g}_0 = \bar{g}_0 + \left[ \hat{h}_0 - 2\hat{h}_9 + 32\hat{h}_{14} \right] + S^\phi_0,
$$

$$
\tilde{g}_1 = \bar{g}_1 + \left[ \hat{h}_0 + \hat{h}_1 + \hat{h}_7 + \hat{h}_8 - \hat{h}_9 - 8\hat{h}_{10} - 8\hat{h}_{14} \right] + S^\phi_1,
$$

$$
\tilde{g}_2 = \bar{g}_2 + \left[ \hat{h}_0 - \hat{h}_1 + \hat{h}_7 + \hat{h}_8 - \hat{h}_9 + 8\hat{h}_{10} - 8\hat{h}_{14} \right] + S^\phi_2,
$$

$$
\tilde{g}_3 = \bar{g}_3 + \left[ \hat{h}_0 + \hat{h}_2 - \hat{h}_7 + \hat{h}_8 - \hat{h}_9 - 8\hat{h}_{11} - 8\hat{h}_{14} \right] + S^\phi_3,
$$

$$
\tilde{g}_4 = \bar{g}_4 + \left[ \hat{h}_0 - \hat{h}_2 - \hat{h}_7 + \hat{h}_8 - \hat{h}_9 + 8\hat{h}_{11} - 8\hat{h}_{14} \right] + S^\phi_4,
$$

$$
\tilde{g}_5 = \bar{g}_5 + \left[ \hat{h}_0 + \hat{h}_3 - 2\hat{h}_8 - \hat{h}_9 - 8\hat{h}_{12} - 8\hat{h}_{14} \right] + S^\phi_5,
$$

$$
\tilde{g}_6 = \bar{g}_6 + \left[ \hat{h}_0 - \hat{h}_3 - 2\hat{h}_8 - \hat{h}_9 + 8\hat{h}_{12} - 8\hat{h}_{14} \right] + S^\phi_6,
$$

$$
\tilde{g}_7 = \bar{g}_7 + \left[ \hat{h}_0 + \hat{h}_1 + \hat{h}_2 + \hat{h}_3 + \hat{h}_4 + \hat{h}_5 + \hat{h}_6 + \hat{h}_9 + 2\hat{h}_{10} + 2\hat{h}_{11} + 2\hat{h}_{12} + \hat{h}_{13} + 2\hat{h}_{14} \right] + S^\phi_7,
$$

$$
\tilde{g}_8 = \bar{g}_8 + \left[ \hat{h}_0 - \hat{h}_1 + \hat{h}_2 + \hat{h}_3 - \hat{h}_4 + \hat{h}_5 + \hat{h}_6 + \hat{h}_9 - 2\hat{h}_{10} + 2\hat{h}_{11} + 2\hat{h}_{12} - \hat{h}_{13} + 2\hat{h}_{14} \right] + S^\phi_8,
$$

$$
\tilde{g}_9 = \bar{g}_9 + \left[ \hat{h}_0 + \hat{h}_1 - \hat{h}_2 + \hat{h}_3 - \hat{h}_4 + \hat{h}_5 - \hat{h}_6 + \hat{h}_9 + 2\hat{h}_{10} - 2\hat{h}_{11} + 2\hat{h}_{12} - \hat{h}_{13} + 2\hat{h}_{14} \right] + S^\phi_9,
$$
\[ \tilde{g}_{10} = \bar{g}_{10} + \left[ \hat{h}_0 - \hat{h}_1 - \hat{h}_2 + \hat{h}_3 + \hat{h}_4 - \hat{h}_5 - \hat{h}_6 + \hat{h}_9 - 2\hat{h}_{10} - 2\hat{h}_{11} + 2\hat{h}_{12} + \hat{h}_{13} + 2\hat{h}_{14} \right] + S_{10}, \]
\[ \tilde{g}_{11} = \bar{g}_{11} + \left[ \hat{h}_0 - \hat{h}_1 + \hat{h}_2 + \hat{h}_3 + \hat{h}_4 + \hat{h}_5 - \hat{h}_6 + \hat{h}_9 + 2\hat{h}_{10} + 2\hat{h}_{11} - 2\hat{h}_{12} - \hat{h}_{13} + 2\hat{h}_{14} \right] + S_{11}, \]
\[ \tilde{g}_{12} = \bar{g}_{12} + \left[ \hat{h}_0 + \hat{h}_1 - \hat{h}_2 - \hat{h}_3 + \hat{h}_4 + \hat{h}_5 - \hat{h}_6 + \hat{h}_9 - 2\hat{h}_{10} - 2\hat{h}_{11} + 2\hat{h}_{12} + \hat{h}_{13} + 2\hat{h}_{14} \right] + S_{12}, \]
\[ \tilde{g}_{13} = \bar{g}_{13} + \left[ \hat{h}_0 - \hat{h}_1 + \hat{h}_2 - \hat{h}_3 - \hat{h}_4 + \hat{h}_5 + \hat{h}_6 + \hat{h}_9 + 2\hat{h}_{10} - 2\hat{h}_{11} - 2\hat{h}_{12} + \hat{h}_{13} + 2\hat{h}_{14} \right] + S_{13}, \]
\[ \tilde{g}_{14} = \bar{g}_{14} + \left[ \hat{h}_0 + \hat{h}_1 - \hat{h}_2 - \hat{h}_3 + \hat{h}_4 + \hat{h}_5 + \hat{h}_6 + \hat{h}_9 - 2\hat{h}_{10} - 2\hat{h}_{11} - 2\hat{h}_{12} - \hat{h}_{13} + 2\hat{h}_{14} \right] + S_{14}. \]

(4.37)

Upon performing the streaming step as given in Eq. (4.15b), using the updated distribution function, the scalar field \( \phi \) can be finally computed as

\[ \phi = \sum_{\alpha=0}^{14} g_{14} + \frac{1}{2} R \]

(4.38)

A simplified 3D cascaded LB formulation for the D3Q7 lattice is presented in Appendix D for completeness.

4.3 Results and Discussion

A main objective of this section is to validate the new 3D cascaded LB method discussed earlier for simulation of convective thermal flows. In this regard, we consider simulation of natural convection in a cubic cavity and a comparison of the computed flow and thermal characteristic against 3D benchmark numerical solutions. Natural convection of fluids in differentially heated enclosures has numerous engineering applications and arise in various natural settings. These include solar energy collectors, thermal energy storage systems, cooling of electronic devices, venti-
lation of buildings and crystal growth processes. It is chiefly characterized by the Rayleigh number representing the strength of the buoyancy effects relative to the counteracting thermal and momentum diffusion effects, and the Prandtl number. Some of the classic 2D benchmark solutions for this problem include the results reported by [127]. Given that the natural convective fluid motion in various cases of practical interest are three dimensional in nature, there have been considerable progress in obtaining benchmark numerical results for the 3D natural convection in a cubic enclosure [1] and our present study uses such data as part of the validation in the following.

A schematic of the geometric configuration for the physical model of the 3D cubic cavity considered and the coordinate system is shown in Fig.1. It consists of a cubic enclosure of side length $L$ and the left wall and the right wall surface are maintained at temperatures of $T_L$ and $T_H$, where $T_H > T_C$; all the other four wall surface are maintained to be adiabatic. The convective fluid motion then arises naturally from the buoyancy force due to a local temperature difference with respect to a reference temperature in the presence of a gravity field. This thermally driven flow may be represented by means of the following body force $F$ in the NSE in Eq. (4.1b) under Boussinesq approximation as

$$F = g \beta (T - T_0) \hat{k}$$

(4.39)

where $\beta$ is the coefficient of thermal expansion, $T = T(x, y, z, t)$ is the local temperature field, $T_0 = (T_L + T_H)/2$ is the reference temperature, $g$ is the acceleration due to gravity, and $\hat{k}$ is the unit vector in the positive $z$-direction in Fig.1. This body force is used in the 3D cascaded LBE for fluid flow is discusses in Sec.2.1, which the local temperature field needed in Eq. (4.38) is obtained from the other 3D cascaded LBE for the thermal energy equation presented in Sec.2.2.

The velocity and the temperature boundary conditions may be summarized as

$$u_x = u_y = u_z = 0 \quad \text{for all walls}$$

(4.40)

$$T(x, y = 0, z) = T_L, \quad T(x, y = L, z) = T_H,$$

(4.41)

$$\frac{\partial T}{\partial n} = 0 \quad \text{for all other walls}$$

(4.42)
where $\hat{n}$ is the wall normal direction. Half bounce back scheme is employed to implement the velocity boundary condition, and an anti-bounce back scheme is used to represent the Dirichlet boundary conditions for the scalar temperature field [116] and the Neumann boundary condition is implemented using the scheme given in [128]. The characteristic dimensionless Rayleigh number $Ra$ and the Prandtl number $Pr$ for this problem are given by

$$Ra = g\beta \Delta T L^3 / (\alpha \nu) \quad Pr = \nu / \alpha$$

(4.43)

where $\Delta T = T_H - T_L$ is the temperature difference between the hot and cold surface, $\alpha$ and $\nu$ are the thermal diffusivity and kinematic viscosity of the fluid, respectively. In the following, we will non-dimensionalize the coordinate lengths by the scale $L$, components of the velocity by $[g\beta L(T_H - T_L)]^{1/2}$ and the temperature by $T_0$. The corresponding dimensionless coordinates are
then denoted by \((x,y,z)\), the velocity field by \((u_x, u_y, u_z)\) and the temperature field by \(T\). A key parameter characterizing the thermal transport during natural convection is the Nusselt number. The mean Nusselt number at either the hot or cold wall maybe represented as

\[
Nu_{\text{mean}}(z) = \int_{x=0}^{1} \frac{\partial T(x,y)}{\partial y} \bigg|_{y=0 \text{ or } y=1} \, dx.
\] (4.44)

In the following, we will consider simulations of natural convection of air \((Pr = 0.71)\) at different values of the Rayleigh numbers \(Ra\). We will use the 3D cascaded LBM based on the D3Q15 lattice in this regard, and using a grid resolution of \(91 \times 91 \times 91\). Figure 4.2 presents the temperature and velocity profiles between the adiabatic bottom and top walls in the \(z\)-direction ((a) and (c), respectively) and between the cold and hot surfaces in the \(y\)--direction ((b) and (d)), respectively, along the symmetry plane \((x=0.5)\) at \(Ra = 10^5\) computed using our present 3D cascaded LBM. Also, plotted in these configurations in symbols are the prior reference benchmark solution based on the NSE [1]. It can be seen that the computed structure of both the temperature and velocity fields along different directions are in very good agreement with the benchmark numerical results. The slopes of the temperature fields near both the adiabatic and isothermal walls are found to be wall captured by our 3D cascaded LBM based on DDF formulation. Furthermore, from the velocity profiles shown in Figs.2(c) and 2(d), it is evident, in particular, that both the peak magnitudes and their locations of the fluid convection velocity are well reproduced by our 3D cascaded LB model.

Figure 3 presents the distribution of streamlines arising due to natural convective fluid currents from differentially heated enclosures at two different Rayleigh numbers of \(Ra = 10^4\) and \(Ra = 10^5\) along center planes in different coordinate directions. In the vertical \(y - z\) midplane \((x = 0.5)\), it can be seen that at lower \(Ra\) of \(10^4\), a central vortex appear as a dominant characteristic of the fluid motion. However, with increasing the Rayleigh number to \(10^5\), when the natural convection effects become more pronounced, the central vortex break up into a set of two vortices. In addition, it is evident that there is a clustering of streamlines near the wall surfaces. Scale anal-
FIGURE 4.2: Comparison of the temperature (top) and velocity profiles (bottom) for Rayleigh number $Ra = 10^5$ on the symmetry center plane $x - z$; symbols ” ◦” denote the reference benchmark solutions [1], and line ” − ” by present work.

ysis predicts the boundary layer thickness $\delta$ near an isothermal wall set up by natural convection scales as $Ra^{-1/4}$. Hence, there is a thinner layer of fluid near that drives a more vigorous natural convection at higher $Ra$. On the $x - z$ midplane ($y=0.5$), in which side walls are adiabatic, it is seen that the heated fluid rises up, with the colder fluid moving down and being replaced by the heated one. The flow pattern is found to be three-dimensional in nature. On the $x - y$ midplane ($z=0.5$), near the hot wall the fluid, which rises from the bottom of the cavity, moves towards the cold wall and after some distance changes the direction. For both the midplane as we increase the Rayleigh number, the thermal convective effects are found to be more dominate. These flow patterns are consistent with prior numerical solutions [1, 124].

The temperature distributions, represented by isotherms, in midplanes along different directions
FIGURE 4.3: Projections of streamlines in natural convection in a 3D cavity computed using 3D cascaded LBM on different center planes at Rayleigh number $Ra = 10^4$ (left) and $Ra = 10^5$ (right). Top row: $y - z$ plane, Middle row $x - z$ plane Bottom row: $y - x$ plane.
FIGURE 4.4: Temperature distribution in natural convection in a 3D cavity computed using 3D cascaded LBM on different center planes at Rayleigh numbers $Ra = 10^4$ (left) and $Ra = 10^5$ (right). Top row: $y-z$ plane, Middle row $x-z$ plane Bottom row: $y-x$ plane.
for $Ra$ of $10^4$ and $10^5$ are shown in Fig. 4. It can be seen that as the natural convection effect become more significant, at higher $Ra = 10^5$, the isotherms become more horizontal in the region around the centra of the cavity, and becomes nearly vertical in the thin boundary layers closer to the hot and cold walls. In general, as expected, significant temperature variations appear in the thin regions in the vicinity of the isothermal wall surfaces and more uniform distributions near the adiabatic wall surfaces.

In addition, in order to provide a quantitatively study of the numerical results we compare the following main flow and thermal characteristics of natural convection in a cubic cavity in the symmetry plane $(x = 0.5)$ at $Ra = 10^3$, $10^4$ and $10^5$ computed using our 3D cascaded LBM with the reference benchmark numerical solution [1]. The maximum horizontal velocity $u_{max}$ and its coordinate location $(y, x)$, the maximum vertical velocity $w_{max}$ and its coordinate location $(y, x)$; the maximum and minimum Nusselt numbers ($Nu_{mean}$ and $Nu_{min}$) and their location, and, finally, the average Nusselt number $Nu_{mean}$. The computed result, benchmark solutions of these quantities are presented in Table 1. It can be seen that the agreement between the DDF-based 3D cascaded LBM results and the benchmark solutions are in very good agreement.

<table>
<thead>
<tr>
<th>$Ra$</th>
<th>$10^3$</th>
<th>$10^4$</th>
<th>$10^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gridsize</td>
<td>$91 \times 91 \times 91$</td>
<td>$31 \times 31 \times 31$</td>
<td>$91 \times 91 \times 91$</td>
</tr>
<tr>
<td>$u_{max}$</td>
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<td>0.1314</td>
<td>0.1965</td>
</tr>
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<td>(0.5, 0.2000)</td>
<td>(0.5, 0.1910)</td>
</tr>
<tr>
<td>$w_{max}$</td>
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<td>0.1320</td>
<td>0.2232</td>
</tr>
<tr>
<td>Position $(y, x)$</td>
<td>(0.8426, 0.5)</td>
<td>(0.8333, 0.5)</td>
<td>(0.8876, 0.5)</td>
</tr>
<tr>
<td>$Nu_{max}$</td>
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<td>1.420</td>
<td>3.5815</td>
</tr>
<tr>
<td>Position $(y, x)$</td>
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<td>(0, 0.0833)</td>
<td>(0, 0.1685)</td>
</tr>
<tr>
<td>$Nu_{min}$</td>
<td>0.730</td>
<td>0.7639</td>
<td>0.5925</td>
</tr>
<tr>
<td>Position $(y, x)$</td>
<td>(0, 1.0)</td>
<td>(0, 1.0)</td>
<td>(0, 1.0)</td>
</tr>
<tr>
<td>$Nu_{mean}$</td>
<td>1.0977</td>
<td>1.105</td>
<td>2.2647</td>
</tr>
</tbody>
</table>

TABLE 4.1: Qualitative comparison of key flow and thermal characteristics in natural convection in a cubic cavity in the symmetry plane $(z=0.5)$ between the 3D cascaded LBM and the reference benchmark results obtained using a NSE solver [1]
4.4 Summary and Conclusions

Fluid flows with heat transfer effects via convective transport process and, in particular in three dimensions (3D), play a key role in a wide variety of problems of both fundamental and practical interests. Lattice Boltzmann methods are efficient computational kinetic model based approaches that can handle such multiphase fluid flow problem using double distribution function (DDF) formulations. In this chapter, we have constructed new 3D cascaded LB models for D3Q15 and D3Q7 lattices to solve the 3D convection-diffusion based thermal energy transport equation in the DDF framework, where the fluid motion is computed from another 3D cascaded LB model from a prior study. The collision step in this approach for the transport of the temperature field is obtained by the relaxation of central moments of different orders in a multiple relaxation time formulation. This involves considering the temperature field as the only collision invariant, while, by contrast, the LB model for the fluid flow is based on mass and the components of the momentum as the conserved variables. As a result, the cascaded structure of the 3D collision operator for the solution of the temperature field is quite different from that of the flow field. In particular, the cascaded structure emerges from the second moment onwards in the former case, while for the latter case, it begins from the third order. In addition, the transport coefficient, i.e. the thermal diffusivity for the temperature field is related to its relaxation times for the first order moments in the 3D cascaded collision model, while the kinematic viscosity of the fluid motion is dependent on the relaxation times of the second order moments of its corresponding 3D cascaded formulation. The new 3D cascaded LB models are then numerically investigated for the simulation of the 3D natural convection of air in differentially heated cubic enclosures at various Rayleigh numbers. Comparison of the computed structure of the velocity profiles and the temperature distribution against prior numerical results show good agreement. In addition, peak convection velocities and the heat transfer rates given in terms of the Nusselt number are in good quantitative agreement with the benchmark solutions at different Rayleigh numbers.
CHAPTER V

CASCADED LATTICE BOLTZMANN METHOD BASED ON CENTRAL MOMENTS FOR AXISYMMETRIC THERMAL FLOWS INCLUDING SWIRLING EFFECTS

5.1 Introduction

Fluid motion in cylindrical coordinates with axial symmetry that is driven by rotational effects and/or thermal buoyancy effects arise widely in a number of engineering applications and geophysical contexts (e.g., [129, 130, 131, 132, 133]). Some examples of technological applications encountering heat and mass transfer effects in axisymmetric flows include pipeline systems, heat exchangers, solar energy conversion devices, crystal growth and material processing systems, electronic cooling equipment and turbomachinery. Computational methods play an important role for both fundamental studies of the fluid mechanics and heat transfer aspects and as predictive tools for engineering design of such systems. In general, fluid motion in cylindrical coordinates due to swirling effects and buoyancy forces, and accompanied by thermal and mass transport is three-dimensional (3D) in nature. Computational effort for such problems can be significantly reduced if axial symmetry, which arise in various contexts, can be exploited; in such cases the system of equations can be reduced to set of quasi-two-dimensional (2D) problems in the meridian plane. Traditionally, numerical schemes based on finite difference, finite volume or finite elements were constructed to solve the axisymmetric Navier-Stokes (NS) equations for the fluid flow along with the advection-diffusion equation for the energy transport (e.g., [134, 135]).

On the other hand, lattice Boltzmann (LB) methods, which arise as minimal kinetic models of the Boltzmann equation, has attracted much attention and application to a wide range of fluid flows and heat and mass transfer problems [126, 6, 11, 8].
Following an approach for the solution of the Boltzmann equation in cylindrical coordinates [136], during the last two decades, various LB schemes for athermal flows (i.e., without heat transfer effects) have been introduced [137, 138, 139, 140, 141, 142, 143, 144, 145]. These approaches can be categorized according to the following: (i) Coordinate transformation method [137, 138, 139, 140, 141], in which the axisymmetric mass and momentum equations are reformulated as quasi-2D flow equations in the Cartesian forms with additional geometric source terms and then solved using a LB scheme. (ii) Vorticity-stream function approach [142], where LB models are introduced to simulate flows in cylindrical coordinates written in terms of the vorticity and stream function equations. (iii) Radius-weighted formulation [143], in which a simplified LB method is derived from a discretization of the continuous Boltzmann equation in cylindrical coordinates re-cast in a radius-weighted form. An analysis of these axisymmetric LB models were performed by [144]. Generally, these approaches solve for the axial and radial velocity components in the meridian plane using a popular single relaxation time (SRT) model for the representation of the collision step in the LB scheme. The azimuthal velocity field to represent axisymmetric swirling or rotational flows is computed using an additional LB scheme based on a separate distribution function in a double distribution function (DDF) framework [143, 145].

Further progress in the LB methods for the simulation of axisymmetric thermal flows have been reported in various studies [146, 147, 148, 149, 150, 151, 152, 153, 154, 155]. Earlier LB models in this regard [146, 147] used an hybrid approach, in which the energy equation was solved via a finite difference scheme. Later, [148, 149] solved the axisymmetric equation for the temperature field written in terms of a pseudo-2D advection-diffusion equation with a source term using a LB scheme based on a separation distribution function from that for the flow field. On the other hand, [150, 151] extended the radius-weighted formulation approach for axisymmetric fluid flow [143] for the simulation of thermal energy transport. A fractional-step based LB flux solver for axisymmetric thermal flow was presented in [153]. All these approaches were based on the common SRT model [13], in which, during the collision step, the distribution functions relax to
their local equilibria using a single relaxation parameter. This was further extended by the introduction of two tunable parameters as coefficients to the additional gradient terms in the equilibrium distribution functions [155]. Generally, SRT based LB schemes are known to be susceptible to numerical instabilities for convection-dominated flows or fluids with relatively low values of transport coefficients. In order to address this issue, the collision step based on a multiple relaxation time (MRT) model [156] has been constructed, in which raw moments of different orders relax at different rates. Few MRT LB schemes for axisymmetric thermal convective flows have recently been developed [149, 152, 153].

On the other hand, further improvements to the collision step enhancing the flow and thermal transport modeling capabilities can be achieved via the introduction of the cascaded collision model [15]. In this approach, the effects of collisions are represented in terms of relaxation of different orders of central moments, which are obtained by shifting the particle velocity, by the local fluid velocity at different rates. As the collision model is prescribed based on a local moving frame of reference, the relaxation steps for successive higher order moments exhibit a cascaded structure. The cascaded collision formulation was shown to be equivalent to considering relaxation to a generalized equilibrium in the rest or lattice frame of reference [157], and was augmented with forcing terms in 2D and 3D in [19]. Improvements in the numerical properties achieved using such advanced cascaded collision models based on central moments were recently demonstrated [16]. A modified formulation based on central moments involving relaxation to discrete equilibria rather than continuous Maxwellian equilibria was also proposed [158]. In order to accelerate convergence of steady flows, a preconditioned cascaded LB method was constructed and studied in [58], and whose Galilean invariance properties were significantly improved via corrections to equilibria in [68]. The cascaded LB scheme has recently been extended for simulating flows with heat transfer in 2D [159, 160] and in 3D in our recent work [33]. Some related recent papers that discuss about the forcing schemes as well as thermal sources are [80, 161, 162, 163]. However, for axisymmetric thermal convective flows including rotational effects, no such
advanced LB schemes are available in the literature.

In this chapter, we present a new cascaded LB formulation for thermal flows in cylindrical coordinate with axial symmetry, and including rotational effects. The mass, momentum (i.e., axial, radial and azimuthal components) and energy equations rewritten in pseudo-2D Cartesian forms in the meridian plane contain additional geometric source terms, which are included in the respective cascaded LB schemes via a novel symmetric time-split formulation [163]. In this approach, three separate distribution functions are considered: one for the density, axial and radial momentum components, another one for the azimuthal momentum component and finally third one for the temperature field. Each of the three distribution functions evolves according to a cascaded LB scheme. For this triple distribution functions framework, a two-dimensional, nine velocity (D2Q9) model is used to solve for the axisymmetric NS equations for the axial and radial momentum components, while a two-dimensional five velocity (D2Q5) model is employed to compute the azimuthal momentum and the temperature field, both of whose evolution are represented by advection-diffusion equations with source terms. The use of symmetric operation split formulations based on pre-collision and post-collision source steps for incorporating the geometric source terms for axisymmetric thermal flows including swirl effects leads to a particularly simplified formulation, which is consistent with the classical Strang splitting. The application of central moments based cascaded LB schemes using MRT can enhanced numerical stability of the LB simulations, and the use of symmetric operator splitting yields a scheme that is second order in time, as demonstrated numerically [163]. Such an axisymmetric cascaded LB approach for the simulation of thermally stratified and/or rotating flows in cylindrical geometries can lead to reduced computational and memory costs when compared to a 3D cascaded LB formulation. Several numerical axisymmetric benchmark problems focusing on buoyancy-driven flows and rotational effects are considered to validate our operator-split axisymmetric cascaded LB schemes for thermal flows. These include the Taylor-Couette flow, natural convection in an annulus between two co-axial vertical cylinders, Rayleigh-Benard convection in a vertical cylinder, cylindrical lid-
driven cavity flow, mixed convection in a tall vertical annulus and melt flow during Czochralski crystal growth in a vertical rotating cylinder.

This chapter is organized as follows. In the next section (Sec. 2), cascaded LB methods for axisymmetric thermal flows with swirl effects using a symmetric operator split formulation for the various geometric sources and forces are presented. Numerical results for various benchmark problems are presented and discussed in Sec.3. Finally, the paper concludes with a summary in Sec.4.

5.2 Cascaded LBM for Axisymmetric Thermal Convective Flows: Swirling Effects

We will now present cascaded LB methods based on central moments and MRT for the computation of thermal convective flows in the cylindrical coordinates with axial symmetry, by also taking into account azimuthal rotational/swirling effects. A triple distribution functions based LB approach is considered, where the geometric source terms arising in the pseudo-2D macroscopic equations are represented using symmetric operator splitting around the cascaded collision steps [163]. The solution of the resulting cascaded LB models then yields the local fluid flow variables such as the radial axial and azimuthal velocity fields, pressure (or density) field, and the temperature field in the meridian plane. First, we summarize the macroscopic governing equations for axisymmetric thermal flows subjected to rotation/swirl.

5.2.1 Governing equations for thermal flows in cylindrical coordinates with axial symmetry

For incompressible, axisymmetric thermal flows subjected to rotational/swirling effects, the macroscopic governing equations in the cylindrical coordinate system \((r, \theta, z)\) can be written as [143,
\[
\partial_t \rho + \partial_r (\rho u_r) + \partial_z (\rho u_z) = -\frac{u_r}{r}, \tag{5.1a}
\]
\[
\partial_t (\rho u_r) + \partial_r (\rho u_r^2) + \partial_z (\rho u_r u_z) = -\partial_r p + \partial_r (2\mu \partial_r u_r) + \partial_z [\mu (\partial_z u_r + \partial_z u_z)] \tag{5.1b}
\]
\[
+ \rho \frac{u_r^2}{r} - \rho \frac{u_z^2}{r} + 2\mu \frac{u_r}{r} - 2\mu \frac{u_r}{r^2} + F^b_r,
\]
\[
\partial_t (\rho u_z) + \partial_r (\rho u_r u_z) + \partial_z (\rho u_z^2) = -\partial_z p + \partial_r [\mu (\partial_r u_z + \partial_z u_r)] + \partial_z (2\mu \partial_z u_z) \tag{5.1c}
\]
\[
- \rho \frac{u_r u_z}{r} + \mu \frac{(\partial_z u_r + \partial_r u_z)}{r} + F^b_z,
\]
\[
\partial_t (\rho u_\theta) + \partial_r (\rho u_r u_\theta) + \partial_z (\rho u_z u_\theta) = \nu \left[ \frac{\partial^2}{\partial r^2} (\rho u_\theta) + \frac{\partial^2}{\partial z^2} (\rho u_\theta) \right] - 2\rho \frac{u_r u_\theta}{r}, \tag{5.1d}
\]
\[
+ \rho \nu \frac{u_r u_\theta}{r} - \rho \nu u_\theta - \frac{u_r u_\theta}{r^2},
\]
\[
\partial_t \phi + \partial_r (u_r \phi) + \partial_z (u_z \phi) = \partial_r (D_\phi \partial_r \phi) + \partial_z (D_\phi \partial_z \phi) - \frac{u_r \phi}{r} + \frac{D_\phi}{r} \partial_r \phi. \tag{5.1e}
\]

Here, \( r, z \) and \( \theta \) represent the coordinates in the radial, axial and azimuthal directions, respectively; accordingly, \( u_r, u_z \) and \( u_\theta \) denote the fluid velocity components in the respective directions, and \( F^b_r \) and \( F^b_z \) are radial and axial components of the external body forces, respectively. \( \rho \) and \( p \) represent the density and pressure, respectively, while \( \nu \) and \( \mu = \rho \nu \) correspond to the kinematic and dynamic viscosities of the fluid, respectively. \( \phi \) is the passive scalar variable, which is the temperature field \( T \) in the present study (i.e. \( \phi = T \)) and \( D_\phi \) is the coefficient of diffusivity. Equations (5.1a)-(5.1c) represent the axisymmetric NS equations for the axial and radial components of the velocity field in the meridian plane. The structure of the evolution equations for the azimuthal momentum (\( \rho u_\theta \)) and the scalar field (\( \phi \)) given in Eqs. (5.1d) and (5.1e) respectively, is similar in form, viz., advection-diffusion equation with a source, and hence they can be solved using the same numerical procedures.

In order to represent the above macroscopic equations in cylindrical coordinates in a set of pseudo-2D Cartesian forms, we apply the following coordinate/variable transformations:

\[
(r, z) \mapsto (y, x), \quad (u_r, u_z) \mapsto (u_y, u_x), \quad \rho u_\theta \mapsto \psi. \tag{5.2}
\]

Then, the resulting equations in pseudo-Cartesian forms involve additional terms when compared
to the standard flow and thermal transport equations in 2D, which can be regarded as geometric source terms. The latter will be introduced via a symmetric operator splitting technique in the respective cascaded LB formulation in the following. Thus, the mass and momentum equations for the fluid motion in the meridian plane (Eqs.(5.1a)-(5.1c)) can be written in pseudo-2D Cartesian forms as

\[ \partial_t \rho + \partial_y (\rho u_y) + \partial_x (\rho u_x) = M^A, \]  
\[ \partial_t (\rho u_x) + \partial_r (\rho u_x^2) + \partial_y (\rho u_x u_y) = - \partial_x p + \partial_x [2 \mu \partial_x u_x] + \partial_y [\mu (\partial_y u_x + \partial_x u_y)] + F^A_x + F^b_x, \]  
\[ \partial_t (\rho u_y) + \partial_x (\rho u_x u_y) + \partial_y (\rho u_y^2) = - \partial_y p + \partial_x [\mu (\partial_x u_y + \partial_y u_x)] + \partial_y [2 \mu \partial_y u_y] + F^A_y + F^b_y, \]  

where the geometric mass source \( M^A \) and the momentum source vector \( F^A = (F^A_x, F^A_y) \) can be represented as

\[ M^A = - \rho \frac{u_y}{y}, \]  
\[ F^A_x = - \rho \frac{u_x u_y}{y} + \mu \frac{\partial_x u_y + \partial_y u_x}{y}, \]  
\[ F^A_y = \frac{\psi^2}{\rho y} - \rho \frac{u_y^2}{y} + 2 \mu \frac{\partial_y u_y}{y} - 2 \mu \frac{u_y}{y^2}. \]  

Then, the total force \( F = (F_x, F_y) \) in this approach becomes

\[ F_x = F^A_x + F^b_x, \quad F_y = F^A_y + F^b_y. \]  

Here, the body force \( F^b = (F^b_x, F^b_y) \) could be a volumetric force such as the buoyancy force or the Lorentz force. Similarly, the azimuthal momentum equation for \( \psi = \rho u_\theta \) can be written as

\[ \partial_t \psi + \partial_x (u_x \psi) + \partial_y (u_y \psi) = D_\psi (\partial_x^2 \psi + \partial_y^2 \psi) + S_\psi, \]  

where the corresponding geometric source term \( S_\psi \) can be expressed as

\[ S_\psi = - \frac{2 u_y \psi}{y} + \frac{\mu}{y} \partial_y \left( \frac{\psi}{\rho} \right) - \frac{\nu \psi}{y^2}. \]
and $D_\psi$ is the coefficient of diffusivity, which is equal to the kinematic viscosity of the fluid $\nu$, i.e. $D_\psi = \nu$. Finally, the axisymmetric advection-diffusion equation for the scalar, i.e., temperature field ($\phi = T$) in the pseudo-2D cartesian coordinate system reads as

$$\partial_t \phi + \partial_x (u_x \phi) + \partial_y (u_y \phi) = \partial_x (D_\phi \partial_x \phi) + \partial_y (D_\phi \partial_y \phi) + S_\phi,$$

(5.8)

where the source term $S_\phi$ is given as

$$S_\phi = -\frac{u_y \phi}{y} + \frac{D_\phi}{y} \partial_y \phi.$$  

(5.9)

Our goal, then, is to represent the evolution of the axial and radial momentum components along with density (Eqs.(5.3)-(5.5)) using a distribution function $f_\alpha$, azimuthal momentum (Eqs.(5.6)-(5.7)) using another distribution function $g_\alpha$, and the scalar temperature field (Eqs.(5.8)-(5.9)) using a third distribution function $h_\alpha$. We use a D2Q9 lattice for $f_\alpha$, while for both $g_\alpha$ and $h_\alpha$, a D2Q5 lattice would suffice since to represent advection-diffusion type equations, the lattice is required to satisfy only a lower degree of symmetry than the lattice used for the Navier-Stokes equations. In each case, a cascaded LB scheme based on a symmetric operator splitting will be constructed in the following.

5.2.2 Cascaded LB scheme for axial and radial velocity fields: operator splitting for mass and momentum source terms

In order to consistently include the geometric mass and momentum sources along with any external body force given in Eqs.(5.4) and (5.5) in a cascaded LB scheme, we will employ a symmetric operator splitting strategy around its collision term [163]. First, we define the following components of the particle velocities for the D2Q9 lattice:

$$|e_x\rangle = (0, 1, 0, -1, 0, 1, -1, -1, 1)^\dagger,$$

(5.10a)

$$|e_y\rangle = (0, 0, 1, 0, -1, 1, -1, -1)^\dagger,$$

(5.10b)
where $\dagger$ is the transpose operator and their components for any particle direction $\alpha$ are denoted by $e_{\alpha x}$ and $e_{\alpha y}$, where $\alpha = 0, 1, \cdots 8$. We also need the following 9-dimensional vector
\[
|1\rangle = (1, 1, 1, 1, 1, 1, 1, 1)\dagger
\] (5.11)
whose inner product with the distribution function $f_\alpha$ defines its zeroth moment. Here, and in the following, we have used the standard Dirac’s bra-ket notation to represent the vectors. The corresponding nine orthogonal basis vectors may be represented by (e.g. [19]):
\[
K_0 = |1\rangle, \quad K_1 = |e_x\rangle, \quad K_2 = |e_y\rangle, \quad K_3 = 3|e_x^2 + e_y^2\rangle - 4|1\rangle,
\]
\[
K_4 = |e_x^2 - e_y^2\rangle, \quad K_5 = |e_x e_y\rangle, \quad K_6 = -3|e_x^2 e_y\rangle + 2|e_y\rangle,
\]
\[
K_7 = -3|e_x e_y^2\rangle + 2|e_x\rangle, \quad K_8 = 9|e_x^2 e_y^2\rangle - 6|e_x^2 + e_y^2\rangle + 4|1\rangle.
\] (5.12)

Here and henceforth, symbols such as $|e_x^2 e_y\rangle = |e_x e_x e_y\rangle$ denote a vector that result from the element wise vector multiplication of vectors $|e_x\rangle$, $|e_x\rangle$ and $|e_y\rangle$. The above set of vectors can be organized by the following orthogonal matrix
\[
\mathbf{K} = [K_0, K_1, K_2, K_3, K_4, K_5, K_6, K_7, K_8],
\] (5.13)
which maps changes of moments under collisions due to a cascaded central moment relaxation back to changes in the distribution function (see below). As the cascaded collision operator is built on the moment space, we first define the central moments and raw moments of order $(m + n)$ of the distribution function $f_\alpha$ and its equilibrium $f_{\alpha}^{eq}$ as
\[
\begin{pmatrix}
\hat{\kappa}_{x^m y^n} \\
\hat{\kappa}_{x^m y^n}^{eq}
\end{pmatrix}
= \sum_\alpha \begin{pmatrix}
f_\alpha \\
f_{\alpha}^{eq}
\end{pmatrix}
\begin{pmatrix}
e_{\alpha x} - u_x \\
e_{\alpha y} - u_y
\end{pmatrix}^m \begin{pmatrix}
e_{\alpha y} - u_y \\
e_{\alpha x} - u_x
\end{pmatrix}^n,
\] (5.14)
and
\[
\begin{pmatrix}
\hat{\kappa}'_{x^m y^n} \\
\hat{\kappa}'_{x^m y^n}^{eq}
\end{pmatrix}
= \sum_\alpha \begin{pmatrix}
f_\alpha \\
f_{\alpha}^{eq}
\end{pmatrix}
\begin{pmatrix}
e_{\alpha x}^m e_{\alpha y}^n \\
e_{\alpha y}^m e_{\alpha x}^n
\end{pmatrix},
\] (5.15)
respectively. Here and in what follows, the prime (') symbols denote various raw moments. The central moments of the equilibrium are constructed to be equal to those for the Maxwellian, which
then serve as attractors during the cascaded collision represented as a relaxation process [15].

In the following, an operator splitting based cascaded LB scheme will be constructed to solve Eqs.(5.3)-(5.5). First, we represent the solution of the mass and momentum equations in the meridian plane (Eq.(5.3)) without the respective source terms (i.e. \( M_A, F_x^A, F_y^A, F_x^b, F_y^b \)) by means of the evolution of the distribution function \( f_\alpha \) using the usual collision and streaming steps (\( C \) and \( S \), respectively) as

\[
\text{Step } C: \quad f_\alpha^C = f_\alpha + (\mathbf{K} \cdot \mathbf{p})_\alpha, \quad (5.16a)
\]

\[
\text{Step } S: \quad f_\alpha(x, t) = f_\alpha^C(x - e_\alpha \Delta t, t), \quad (5.16b)
\]

where \( e_\alpha = (e_{\alpha x}, e_{\alpha y}) \), \( \Delta t \) is the time step, \( f_\alpha^C \) is the post-collision distribution function at a location \( x \) and time \( t \). \( \mathbf{p} = (\hat{p}_0, \hat{p}_1, \hat{p}_2 \ldots \hat{p}_8) \) denotes the changes of different moments under collision based on the relaxation of central moments to their equilibria in a cascaded fashion [15]. With the mass and momentum being conserved during collision \( \hat{p}_0 = \hat{p}_1 = \hat{p}_2 = 0 \), and the changes in the higher order non-conserved moments are given by ([15, 157, 19])

\[
\hat{p}_3 = \frac{\omega_3}{12} \left\{ 2c_s^2 \rho + \rho (u_x^2 + u_y^2) - (\bar{\kappa}_{xx} + \bar{\kappa}_{yy}) \right\},
\]

\[
\hat{p}_4 = \frac{\omega_4}{4} \left\{ \rho (u_x^2 - u_y^2) - (\bar{\kappa}_{xx} - \bar{\kappa}_{yy}) \right\},
\]

\[
\hat{p}_5 = \frac{\omega_5}{4} \left\{ \rho u_x u_y - \bar{\kappa}_{xy} \right\},
\]

\[
\hat{p}_6 = \frac{\omega_6}{4} \left\{ 2 \rho u_x^2 u_y + \bar{\kappa}_{xxy} - 2 u_x \bar{\kappa}_{xy} - u_x \bar{\kappa}_{xx} - \frac{1}{2} u_y (3\hat{p}_3 + \hat{p}_4) - 2 u_x \hat{p}_5, \right\}
\]

\[
\hat{p}_7 = \frac{\omega_7}{4} \left\{ 2 \rho u_x^2 u_y + \bar{\kappa}_{xxy} - 2 u_y \bar{\kappa}_{xy} - u_x \bar{\kappa}_{yy} - \frac{1}{2} u_x (3\hat{p}_3 - \hat{p}_4) - 2 u_y \hat{p}_5, \right\}
\]

\[
\hat{p}_8 = \frac{\omega_8}{4} \left\{ c_s^4 \rho + 3 \rho u_x^2 u_y - \left[ \bar{\kappa}_{xxy} - 2 u_x \bar{\kappa}_{xy} - 2 u_y \bar{\kappa}_{yy} - u_x^2 \bar{\kappa}_{xx} + u_y^2 \bar{\kappa}_{yy} + u_x^2 \bar{\kappa}_{xy} \right. \right.
\]

\[
\left. + 4 u_x u_y \bar{\kappa}_{xy} \right\} - 2 \hat{p}_3 - \frac{1}{2} u_y^2 (3\hat{p}_3 + \hat{p}_4) - \frac{1}{2} u_x^2 (3\hat{p}_3 - \hat{p}_4) - 4 u_x u_y \hat{p}_5 - 2 u_y \hat{p}_6 - 2 u_x \hat{p}_7.
\]

(5.17)

Here, \( \omega_3, \omega_4 \cdots \omega_8 \) are relaxation parameters, where \( \omega_3, \omega_4 \) and \( \omega_5 \) are related to the bulk and shear viscosities and the other \( \omega_i \) influence the numerical stability of the method. In particular, the bulk viscosity is given by \( \xi = c_s^2 (\frac{1}{\omega_3} - \frac{1}{2}) \Delta t \) and the shear viscosity by \( \nu = c_s^2 (\frac{1}{\omega_4} - \frac{1}{2}) \Delta t \),
where \( j = 4, 5 \), and \( c_s^2 = c^2/3 \), where \( c = \Delta x/\Delta t \). In this work, we consider the lattice units, where \( \Delta x = \Delta t = 1 \) and hence the speed of sound \( c_s = 1/\sqrt{3} \), and the higher order relaxation parameters \( \omega_6, \omega_7 \) and \( \omega_8 \) are set to unity for simplicity. After the streaming step (see Eq.(5.16b)), the output density field and the velocity field components (designated with a superscript "0") as the zeroth and first moments of \( f_\alpha \), respectively:

\[
\rho^0 = \sum_{\alpha=0}^{8} f_\alpha, \quad \rho^0 u_x^0 = \sum_{\alpha=0}^{8} f_\alpha e_{\alpha x}, \quad \rho^0 u_y^0 = \sum_{\alpha=0}^{8} f_\alpha e_{\alpha y}
\]  

(5.18)

We then introduce the influence of the mass source \( M_A \) in Eq. (5.3a) and the momentum sources \( F_x^A = F_x^A + F_y^b \) and \( F_y = F_y^A + F_y^b \) in Eqs. (5.3b) and (5.3c), respectively, as the solution of the following two sub problems, referred to as the mass source step \( M \) and momentum source step \( F \), respectively:

\[
\text{Step } M : \partial_t \rho = M^A, \quad (5.19a)
\]

\[
\text{Step } F : \partial_t (\rho u) = F = F^A + F^b, \quad (5.19b)
\]

where \( u = (u_x, u_y) \) and \( F_A = (F_x^A, F_y^A) \) etc. In our previous work [163], we constructed a symmetric operator splitting based approach to incorporate a single momentum source in a cascaded LB method. In the present work, we further extend this approach to symmetric splitting of multiple operators related to mass and momentum sources. In other words, we perform two symmetric steps of half time steps of length \( \Delta t/2 \) of \( M \) and \( F \), one before and the other after the collision step. The overall symmetrized operator splitting based cascaded LB algorithm implementing all the four operators (\( C, S, M \) and \( F \)) during the time interval \([t, t + \Delta t]\) may be written as

\[
f_\alpha(x, t + \Delta t) = M_1^{1/2} F_1^{1/2} C F_1^{1/2} M_1^{1/2} S f_\alpha(x, t), \quad (5.20)
\]

where \( M_1^{1/2} \) and \( F_1^{1/2} \) represent solving Eqs. (5.19a) and (5.19b), respectively, over time step \( \Delta t/2 \). Both of these steps introduce the effect of geometric mass and momentum source and the body forces directly in the momentum space.
Solving Eqs. (5.19a) and (5.19b) for the first part of symmetric sequence needed in Eq. (5.20) yields \( \rho - \rho^o = M^A \frac{\Delta t}{2} \), \( \rho u_x - \rho u^o_x = F_x \frac{\Delta t}{2} \) and \( \rho u_y - \rho u^o_y = F_y \frac{\Delta t}{2} \). Thus, we have

Pre-collision Mass Source Step \( \mathbf{M}^{1/2} \):

\[
\rho = \rho^o + M^A \frac{\Delta t}{2} \tag{5.21a}
\]

Pre-collision Momentum Source Step \( \mathbf{F}^{1/2} \):

\[
\begin{align*}
\rho u_x &= \rho u^o_x + F_x \frac{\Delta t}{2} \tag{5.21b} \\
\rho u_y &= \rho u^o_y + F_y \frac{\Delta t}{2} \tag{5.21c}
\end{align*}
\]

where \( M^A, F_x \) and \( F_y \) are given in Eqs. (5.4a)-(5.4c) and (5.5). Based on Eq. (5.20), the next step is the collision step, which is performed using the updated density and velocity fields \( (\rho, u_x, u_y) \) given in Eqs. (5.21a)-(5.21c) and then determining the change of moments under collision \( \hat{p}_\beta (\beta = 3, 4, \ldots, 8) \) using Eq. (5.17). Then, implementing the other part of the symmetrized mass and momentum steps with using a half time step to solve Eqs. (5.19a) and (5.19b), we obtain the target density and velocity field after collision represented as \( (\rho^p, u^p_x, u^p_y) \) via \( \rho^p - \rho = M^A \frac{\Delta t}{2} \), \( \rho u^p_x - \rho u_x = F_x \frac{\Delta t}{2} \) and \( \rho u^p_y - \rho u_y = F_y \frac{\Delta t}{2} \). Thus, we have

Post-collision Momentum Source Step \( \mathbf{F}^{1/2} \):

\[
\begin{align*}
\rho u^p_x &= \rho u^o_x + F_x \frac{\Delta t}{2} \\
u^p_y &= \rho u^o_y + F_y \frac{\Delta t}{2},
\end{align*}
\]

(5.22a)

Post-collision Mass Source Step \( \mathbf{M}^{1/2} \):

\[
\rho^p = \rho + M^A \frac{\Delta t}{2},
\]

(5.22b)

By rewriting the above results for the post-collision source steps in terms of the output density \( \rho^o \) and velocity field \( \mathbf{u}^o = (u^o_x, u^o_y) \) via Eqs. (5.21a)-(5.21c), we get

\[
\begin{align*}
\rho^p &= \rho^o + M^A \Delta t, & \rho u^p_x &= \rho u^o_x + F_x \Delta t, & \rho u^p_y &= \rho u^o_y + F_y \Delta t.
\end{align*}
\]

(5.23)

To effectively design the post-collision distribution function \( f^p_\alpha \) in the cascaded LB scheme so that Eq. (5.23) is precisely satisfied, we consider \( f^p_\alpha = f_\alpha + (\mathbf{K} \cdot \hat{\mathbf{p}})_\alpha \) and taking its zeroth and first moments, we obtain

\[
\begin{align*}
\rho^p &= \sum_\alpha f^p_\alpha = \sum_\alpha f_\alpha + \sum_\beta \langle K_\beta | 1 \rangle \hat{p}_\beta, \tag{5.24a} \\
\rho u^p_x &= \sum_\alpha f^p_\alpha e_{ax} = \sum_\alpha f_\alpha e_{ax} + \sum_\beta \langle K_\beta | e_x \rangle \hat{p}_\beta, \tag{5.24b} \\
\rho u^p_y &= \sum_\alpha f^p_\alpha e_{ay} = \sum_\alpha f_\alpha e_{ay} + \sum_\beta \langle K_\beta | e_y \rangle \hat{p}_\beta. \tag{5.24c}
\end{align*}
\]
Since the orthogonal basis vectors $|K_\beta\rangle$ given in Eq. (5.12) satisfy $\Sigma_\beta\langle K_\beta|1 \rangle = 9\hat{p}_0$, $\Sigma_\beta\langle K_\beta|e_x \rangle = 6\hat{p}_1$, $\Sigma_\beta\langle K_\beta|e_y \rangle = 6\hat{p}_2$, Eqs. (5.24a)-(5.24c) become

$$\rho^o = \rho^o + 9\hat{p}_0, \quad \rho u_x^o = \rho u_x^o + 6\hat{p}_1, \quad \rho u_y^o = \rho u_y^o + 6\hat{p}_2. \quad (5.25)$$

Comparing Eqs. (5.23) and (5.25), it follows that the change of the zeroth moment ($\hat{p}_0$) and the first moments ($\hat{p}_1$ and $\hat{p}_2$) due to mass and momentum source can be written as

$$\hat{p}_0 = \frac{M_A}{9} \Delta t, \quad \hat{p}_1 = \frac{F_x}{6} \Delta t, \quad \hat{p}_2 = \frac{F_y}{6} \Delta t. \quad (5.26)$$

where $M_A$ follows from Eq. (5.4a), $F_x$ and $F_y$ are given in Eq. (5.5) and (5.4b)-(5.4c). These expressions effectively provide the desired post-collision states of the distribution function, i.e. $f^o_\alpha$ due to mass and momentum sources. The overall scheme presented above based on operator splitting provides a consistent approach to represent mass and momentum sources in the fluid motion. In particular, the pre-collision steps each over a half time step length shown in Eqs. (5.21a)-(5.21c) introduce the effect of mass source and the forces into the moment equilibria of all orders before they undergo central moment relaxation (Eq. (5.17)). As a result, in particular, they eliminate the spurious terms such as $F_i u_j + F_j u_i$ arising in the second order non-equilibrium moments related to the viscous stress in the Chapman-Enskog analysis and correctly recover the Navier-Stokes equations [85, 163]. In addition, the use of two half mass source/force steps around the collision step is consistent with the classical Strang splitting of multiple operators and is second order accurate (see [85, 163] for details and also [87] for its application to a multiple relaxation formulation). An alternative approach to introduce forcing terms based on an unsplit formulation for the cascaded LB method has been presented recently in [80, 161]. Thus, finally expanding $(K \cdot \hat{p})_\alpha$ in Eq. (5.16a), the components of the post-collision distribution func-
tions read as

\[
\begin{align*}
    f_0^p &= f_0 + [\hat{p}_0 - 4(\hat{p}_3 - \hat{p}_8)], \\
    f_1^p &= f_1 + [\hat{p}_0 + \hat{p}_1 - \hat{p}_3 + \hat{p}_4 + 2(\hat{p}_7 - \hat{p}_8)], \\
    f_2^p &= f_2 + [\hat{p}_0 + \hat{p}_2 - \hat{p}_3 - \hat{p}_4 + 2(\hat{p}_6 - \hat{p}_8)], \\
    f_3^p &= f_3 + [\hat{p}_0 - \hat{p}_1 - \hat{p}_3 + \hat{p}_4 - 2(\hat{p}_7 + \hat{p}_8)], \\
    f_4^p &= f_4 + [\hat{p}_0 - \hat{p}_2 - \hat{p}_3 - \hat{p}_4 - 2(\hat{p}_6 + \hat{p}_8)], \\
    f_5^p &= f_5 + [\hat{p}_0 + \hat{p}_1 + \hat{p}_2 + 2\hat{p}_3 + \hat{p}_5 - \hat{p}_6 - \hat{p}_7 + \hat{p}_8], \\
    f_6^p &= f_6 + [\hat{p}_0 - \hat{p}_1 + \hat{p}_2 + 2\hat{p}_3 - \hat{p}_5 - \hat{p}_7 + \hat{p}_8], \\
    f_7^p &= f_7 + [\hat{p}_0 - \hat{p}_1 - \hat{p}_2 + 2\hat{p}_3 + \hat{p}_5 + \hat{p}_6 + \hat{p}_7 + \hat{p}_8], \\
    f_8^p &= f_8 + [\hat{p}_0 + \hat{p}_1 - \hat{p}_2 + 2\hat{p}_3 - \hat{p}_5 + \hat{p}_7 + \hat{p}_8].
\end{align*}
\]

(5.27)

where \(\hat{p}_0, \hat{p}_1, \text{ and } \hat{p}_2\) are obtained from Eq. (26) and \(\hat{p}_3, \hat{p}_4, \ldots, \hat{p}_8\) from Eq. (5.17) *

5.2.3 Cascaded LB scheme for azimuthal velocity field: operator splitting for source term

* We now construct a novel cascaded LB scheme for the solution of the equation of the azimuthal momentum component \((\psi = \rho u_\theta)\) given in Eqs. (5.6) and (5.7) using a D2Q5 lattice [163]. First, defining the vectors corresponding to particle velocity components and a 5-dimensional vector \(|1\rangle\) as

\[
\begin{align*}
|e_x\rangle &= (0, 1, 0, -1, 0)^\dagger, \\
|e_y\rangle &= (0, 0, 1, 0, -1)^\dagger, \\
|1\rangle &= (1, 1, 1, 1, 1)^\dagger,
\end{align*}
\]

(5.28a)

(5.28b)

(5.28c)
where taking the inner product of the distribution function \( g_\alpha \) with \( |1\rangle \) defines its zeroth moment. Using these, the five orthogonal basis vectors can be written as

\[
L_0 = |1\rangle, \quad L_1 = |e_x\rangle, \quad L_2 = |e_y\rangle, \\
L_3 = 5 |e_x^2 + e_y^2\rangle - 4 |1\rangle, \quad L_4 = |e_x^2 - e_y^2\rangle,
\]

which can be grouped together as the following transformation matrix that converts the changes in moments to those in the distribution functions:

\[
L = [L_0, L_1, L_2, L_3, L_4].
\]

In order to design a cascaded collision operator to solve for the azimuthal momentum, which acts as a passive scalar field \( \psi = \rho u_\theta \) described by an advection-diffusion equation under the action of a local source term (Eqs. (5.6) and (5.7)), we define the following central moments and raw moments of the distribution function \( g_\alpha \) and its equilibrium \( g_{eq\alpha} \) as

\[
\begin{pmatrix}
\hat{\kappa}_{\psi x}^{m,n} \\
\hat{\kappa}_{eq\psi x}^{m,n}
\end{pmatrix} = \sum_\alpha \begin{pmatrix}
g_\alpha \\
g_{eq\alpha}
\end{pmatrix} (e_{\alpha x} - u_x)^m (e_{\alpha y} - u_y)^n,
\]

and

\[
\begin{pmatrix}
\hat{\kappa}_{\psi' x}^{m,n} \\
\hat{\kappa}_{eq\psi' x}^{m,n}
\end{pmatrix} = \sum_\alpha \begin{pmatrix}
g_\alpha \\
g_{eq\alpha}
\end{pmatrix} e_{\alpha x}^m e_{\alpha y}^n,
\]

respectively. The central moments of the equilibrium \( \hat{\kappa}_{\psi x}^{m,n} \) are devised be equal to those for the Maxwellian after replacing the density with the scalar field in its expression. Then the cascaded collision step is written in terms of relaxation of different central moments to their equilibria.

Similar to the previous section, a symmetrized operator split scheme will now be developed to solve Eqs. (5.6) and (5.7) in the cascaded LB formulation. First, we represent the solution of Eq. (5.6) without the source term (Eq. (5.7)) through the collision and streaming steps of the distribution function \( g_\alpha \) as

\[
\text{Step C:} \quad g_\alpha^p = g_\alpha + (L \cdot \hat{q})_\alpha, \quad (5.33a)
\]

\[
\text{Step S:} \quad g_\alpha(x, t) = g_\alpha^p(x - e_{\alpha} \Delta t, t). \quad (5.33b)
\]
where $g^p_\alpha$ is the post-collision distribution function and $\hat{q} = (\hat{q}_0, \hat{q}_1, \cdots \hat{q}_4)$ represents the changes of different moments under a cascaded collision prescribed as a relaxation process in terms of central moments, which reads as \[163\]

\begin{align*}
\hat{q}_1 &= \frac{\omega_1^\psi}{2} \left[ \psi u_x - \hat{r}^{\psi'}_{xx} \right], \\
\hat{q}_2 &= \frac{\omega_2^\psi}{2} \left[ \psi u_y - \hat{r}^{\psi'}_{yy} \right], \\
\hat{q}_3 &= \frac{\omega_3^\psi}{4} \left[ 2c_{s\psi}^2 \left( \hat{r}^{\psi'}_{xx} + \hat{r}^{\psi'}_{yy} \right) + 2(u_x \hat{r}^{\psi'}_x + u_y \hat{r}^{\psi'}_y) + (u_x^2 + u_y^2)\psi \right] + u_x \hat{q}_1 + u_y \hat{q}_2, \\
\hat{q}_4 &= \frac{\omega_4^\psi}{4} \left[ -\left( \hat{r}^{\psi'}_{xx} - \hat{r}^{\psi'}_{yy} \right) + 2(u_x \hat{r}^{\psi'}_x - u_y \hat{r}^{\psi'}_y) + (u_x^2 - u_y^2)\psi \right] + u_x \hat{q}_1 - u_y \hat{q}_2, 
\end{align*}

(5.34)

where $\omega_1^\psi$, $\omega_2^\psi$, $\omega_3^\psi$, and $\omega_4^\psi$ are the relaxation parameters. Since $\psi$ is conserved during collision, \( \hat{q}_0 = 0 \). The relaxation parameters for the first order moments ($\omega_1^\psi$ and $\omega_2^\psi$) are related to diffusivity $D_\psi = \nu = c_{s\psi}^2 \left( \frac{1}{\omega_j} - \frac{1}{2} \right) \Delta t$, $j=1,2$ where $c_{s\psi}^2$ is a free parameter, which is set to $1/3$. The relaxation parameters for the higher order moments, which influence numerical stability, are taken to be unity in this study. After the streaming step in Eq.(5.33b), the output passive azimuthal momentum field $\psi^o$ is computed as the zeroth moment of $g_\alpha$ as

$$
\psi^o = \sum_{\alpha} g_\alpha. 
$$

(5.35)

The source term $S_\psi$, which was eliminated in the above, will now be introduced by appropriately combining its effect after solution of the following such problem:

**Step $\mathbf{R}$:** \[\quad \partial_t \psi = S_\psi \]

(5.36)

Its solution will now be combined with the split solution obtained in the absence of the source term in Eqs.(5.33a) and (5.33b) via a symmetric operator splitting technique over a time interval $[t, t + \Delta t]$, analogous to that considered in the previous subsection. This can be represented as

$$
g_\alpha(x, t + \Delta t) = S \mathbf{R}^{1/2} \mathbf{C} \mathbf{R}^{1/2} g_\alpha(x, t), 
$$

(5.37)

The pre-collision source step $\mathbf{R}^{1/2}$ is executed via a solution of Eq.(5.36) over a duration $\Delta t/2$, which yields $\psi - \psi^o = S_\phi \frac{\Delta t}{2}$, and hence

**Pre-collision Source Step $\mathbf{R}^{1/2}$:** \[\quad \psi = \psi^o + S_\psi \frac{\Delta t}{2} \]

(5.38)
Based on this updated scalar field, the changes of different moments under collision \( \hat{q}_\beta, \beta = 1, 2, 3, 4 \), given in Eq.(5.34) can be computed. Similarly, the other part of the source step \( \mathbf{R}^{1/2} \) with half time step following collision can be performed by solving Eq.(5.36), which can be expressed as

\[
\text{Post-collision Source Step } \mathbf{R}^{1/2} : \psi^p = \psi + S_\psi \frac{\Delta t}{2}
\]  

(5.39)

where \( \psi^p \) is the target scalar field after collision. By rewriting it in terms of the output scalar field \( \psi^o \) using Eq. (5.38), we have

\[
\psi^p = \psi^o + S_\psi \Delta t. 
\]  

(5.40)

In order for the post-collision distribution function \( g^p_\alpha = g_\alpha + (\mathbf{L} \cdot \hat{q})_\alpha \) to satisfy Eq. (5.40), we write its zeroth moment as

\[
\psi^p = \Sigma_\alpha g^p_\alpha = \Sigma_\alpha g_\alpha + \Sigma_\beta \langle L_\beta | 1 \rangle \hat{q}_\beta. 
\]  

(5.41)

Since \( \Sigma_\beta \langle L_\beta | 1 \rangle q_\beta = 5\hat{q}_0 \) via orthogonal of basis vectors (see Eq.(5.29)), it follows from Eqs.(5.35) and (5.41) that \( \psi^p = \psi^o + 5\hat{q}_0 \). Comparing this with Eq.(5.40), we get the change of the zeroth moment \( \hat{q}_0 \) due to the presence of the source term \( S_\psi \) as

\[
\hat{q}_0 = \frac{S_\psi}{5} \Delta t. 
\]  

(5.42)

The modeling of the source term for the transport of a scalar field via the above operator splitting approach provides a consistent representation of their effect in the convection-diffusion equation. This is due to the fact that the use of the pre-collision source step over a half time step (Eq. (5.38)) introduces the effect of the scalar source term into the moment equilibria of all orders before they participate in the collision step via the relaxation of various central moments (Eq. (5.34)). Moreover, the symmetric application of pre- and post-collision source steps over a half time step length in each case makes it consistent with the Strang splitting [163]. Similar considerations hold for the strategy for including the local heat sources presented in the next section. Another equivalent approach based on an unsplit formulation to incorporate the source term for the scalar field is discussed in [162]. Finally, the components of the post-collision distribution
function in Eq.(5.33a) can be expressed after expanding \((L \hat{q})_\alpha\) as
\[
\begin{align*}
g^p_0 & = g_0 + [\hat{q}_0 - 4\hat{q}_3], \\
g^p_1 & = g_1 + [\hat{q}_0 + \hat{q}_1 + \hat{q}_3 + \hat{q}_4], \\
g^p_2 & = g_2 + [\hat{q}_0 + \hat{q}_2 + \hat{q}_3 - \hat{q}_4], \\
g^p_3 & = g_3 + [\hat{q}_0 - \hat{q}_1 + \hat{q}_3 + \hat{q}_4], \\
g^p_4 & = g_4 + [\hat{q}_0 - \hat{q}_2 + \hat{q}_3 - \hat{q}_4], \\
\end{align*}
\] (5.43)
where \(\hat{q}_0\) (i.e., the change of the zeroth moment due to source) is given in Eq. (5.42) and \(\hat{q}_\beta, \beta = 1, 2, 3, 4\) (i.e., the changes of the higher, non-conserved, moments under collision) is obtained from Eq. (5.34).

5.2.4 Cascaded LB scheme for temperature field: operator splitting for source term

As in the previous section, we consider a D2Q5 lattice, and use the orthogonal basis vectors \(L_\beta\) and the transformation matrix \(L\) given in Eqs. (5.29) and (5.30), respectively, to design a cascaded LB scheme for the solution of the temperature field \(\phi = T\). Its evolution is presented by the advection-diffusion equation with a source term given in Eqs. (5.8) and (5.9). The various central moments and raw moments of the corresponding distribution function \(h_\alpha\) and its equilibrium \(h^\text{eq}_\alpha\) are defined as
\[
\begin{pmatrix}
\hat{k}^\phi_{x^m y^n} \\
\hat{k}^\text{eq,}\phi_{x^m y^n}
\end{pmatrix} = \sum_\alpha \begin{pmatrix}
h_\alpha \\
h^\text{eq}_\alpha
\end{pmatrix} (e^{m}_{\alpha x} - u_{x})^m(e^{n}_{\alpha y} - u_{y})^n, \\
(5.44)
\]
and
\[
\begin{pmatrix}
\hat{k}'^\phi_{x^m y^n} \\
\hat{k}'^\text{eq,}\phi_{x^m y^n}
\end{pmatrix} = \sum_\alpha \begin{pmatrix}
h_\alpha \\
h^\text{eq}_\alpha
\end{pmatrix} e^{m}_{\alpha x} e^{n}_{\alpha y}. \\
(5.45)
\]
As before, we use the symmetrized operator splitting to include the source term \(S_\phi\) in the cascaded LB scheme, which can be presented as:
\[
h_\alpha(x, t + \Delta t) = S R^{1/2} C R^{1/2} h_\alpha(x, t), \\
(5.46)
\]
where $C$ and $S$ denote the collision and streaming steps, respectively, of $g_{\alpha}$ used to solve Eq. (5.8) (without $S_{\phi}$)

**Step C:** $h_{\alpha}^{p} = h_{\alpha} + (\mathbf{L} \cdot \mathbf{\hat{r}})_{\alpha}$,  \hspace{1cm} (5.47a)

**Step S:** $h_{\alpha}(x, t) = h_{\alpha}^{p}(x - e_{\alpha} \Delta t, t)$.  \hspace{1cm} (5.47b)

Here, $h_{\alpha}^{p}$ is the post-collision distribution function and $\mathbf{\hat{r}} = (\mathbf{\hat{r}}_{o}, \mathbf{\hat{r}}_{1}, \mathbf{\hat{r}}_{2}, \mathbf{\hat{r}}_{3}, \mathbf{\hat{r}}_{4})$ is the change of different moments under collision, with $\mathbf{\hat{r}}_{o} = 0$ due to $\phi$ being a collision invariant. In the above, after the streaming step, the solution of the output scalar field $\phi^{o}$ is computed via the zeroth moment of $h_{\alpha}$ as

$$\phi^{o} = \sum_{\alpha=0}^{4} h_{\alpha}. \hspace{1cm} (5.48)$$

The operator $R^{1/2}$ applied twice in Eq.(5.46) represents the split solution of the scalar field due to the source term of the evolution equation $\partial_{t} \phi = S_{\phi}$ before and after collision over a half time step $\Delta t/2$. Thus, the pre-collision source step can be expressed as

**Pre-collision Source Step $R^{1/2}$:** $\phi = \phi^{o} + \frac{S_{\phi}}{2} \Delta t. \hspace{1cm} (5.49)$

This updated scalar field $\phi$ is then used to compute the changes of different moments under collision $\mathbf{\hat{r}}_{\beta}, \beta = 1, 2, 3, 4$, which can be written as

$$\mathbf{\hat{r}}_{1} = \frac{\omega_{1}^{\phi}}{2} \left[ \phi u_{x} - \mathbf{\hat{r}}_{x}^{\phi'} \right],$$

$$\mathbf{\hat{r}}_{2} = \frac{\omega_{2}^{\phi}}{2} \left[ \phi u_{y} - \mathbf{\hat{r}}_{y}^{\phi'} \right],$$

$$\mathbf{\hat{r}}_{3} = \frac{\omega_{3}^{\phi}}{4} \left[ 2c_{s_{\phi}}^{2} \phi - (\mathbf{\hat{r}}_{x}^{\phi'} + \mathbf{\hat{r}}_{y}^{\phi'}) + 2(u_{x} \mathbf{\hat{r}}_{x}^{\phi'} + u_{y} \mathbf{\hat{r}}_{y}^{\phi'}) + (u_{x}^{2} + u_{y}^{2}) \phi \right] + u_{x} \mathbf{\hat{r}}_{1} + u_{y} \mathbf{\hat{r}}_{2},$$

$$\mathbf{\hat{r}}_{4} = \frac{\omega_{4}^{\phi}}{4} \left[ -(\mathbf{\hat{r}}_{x}^{\phi'} - \mathbf{\hat{r}}_{y}^{\phi'}) + 2(u_{x} \mathbf{\hat{r}}_{x}^{\phi'} - u_{y} \mathbf{\hat{r}}_{y}^{\phi'}) + (u_{x}^{2} - u_{y}^{2}) \phi \right] + u_{x} \mathbf{\hat{r}}_{1} - u_{y} \mathbf{\hat{r}}_{2}, \hspace{1cm} (5.50)$$

where the relaxation parameters $\omega_{1}^{\phi}$ and $\omega_{2}^{\phi}$ are related to the thermal diffusivity $D_{\phi}$ via $D_{\phi} = c_{s_{\phi}}^{2} (\frac{1}{\omega_{j}^{\phi}} - \frac{j}{2}) \Delta t, j = 1, 2$, where $c_{s_{\phi}}^{2} = \frac{1}{3}$ and $\omega_{3}^{\phi} = \omega_{4}^{\phi} = 1$ in this work. Following this, the post-collision source step $R^{1/2}$ can be represented as

**Post-collision Source Step $R^{1/2}$:** $\phi^{p} = \phi + \frac{S_{\phi}}{2} \Delta t \hspace{1cm} (5.51)$
where \( \phi^p \) is the target scalar field following collision, which via Eq.(5.49) reads as \( \phi^p = \phi^o + S_\phi \Delta t \).

The post-collision distribution function \( h^p_\alpha = h_\alpha + (L \cdot \hat{r})_\alpha \) can be made to satisfy this condition using Eq. (5.48) and using \( \Sigma_{\beta} (L_{\beta}|1) \hat{r}_\beta = 5\hat{r}_0 \) after taking its zeroth moment, i.e. \( \phi^p = \sum_\alpha h^p_\alpha \).

This provides the following zeroth moment change due to \( S_\phi \) after collision

\[
\hat{r}_0 = \frac{S_\phi}{5} \Delta t.
\] (5.52)

Finally, the post-collision distribution function \( h^p_\alpha \) can be explicitly written after expanding \( (L \cdot \hat{r})_\alpha \) in Eq.(5.47a) as follows:

\[
\begin{align*}
h^p_0 &= h_0 + \left[ \hat{r}_0 - 4\hat{r}_3 \right], \\
h^p_1 &= h_1 + \left[ \hat{r}_0 + \hat{r}_1 + \hat{r}_3 + \hat{r}_4 \right], \\
h^p_2 &= h_2 + \left[ \hat{r}_0 + \hat{r}_2 + \hat{r}_3 - \hat{r}_4 \right], \\
h^p_3 &= h_3 + \left[ \hat{r}_0 - \hat{r}_1 + \hat{r}_3 + \hat{r}_4 \right], \\
h^p_4 &= h_4 + \left[ \hat{r}_0 - \hat{r}_2 + \hat{r}_3 - \hat{r}_4 \right],
\end{align*}
\] (5.53)

where \( \hat{r}_\beta \) is obtained form Eq. (5.52) and \( \hat{r}_\beta, \beta = 1, 2, 3 \) and 4, follows from Eq. (5.50) due to various non-conserved moment changes under collision.

### 5.3 Results and Discussion

In this section, the cascaded LB schemes described above will be applied to and studied for different complex flow benchmark problems to validate them for simulations of axisymmetric flows with heat transfer and including rotational/swirling effects. These include the following: (a) Taylor-Couette flow between two rotating circular cylinders, (b) natural convection in an annulus between two stationary coaxial vertical cylinders, (c) Rayleigh-Benard convection inside vertical cylinder heated at the bottom and cooled at the top, (d) cylindrical cavity flow driven by the motion of the top lid, (e) mixed convection in a slender vertical annulus subjected to the inner cylinder rotation, and (f) melt flow in a cylinder during Czochralski crystal growth process.
5.3.1 Taylor-Couette flow

As the first test problem, the classical shear-driven circular Couette flow between two circular cylinders is considered [164]. This problem is used to assess the cascaded LB scheme for the azimuthal velocity component $u_\theta$ given in Sec. 2.3, whose evolution is represented by Eqs. (5.6) and (7). The radii of the inner and outer cylinders are defined as $R_i$ and $R_o$, respectively. Let the angular velocities of the inner and outer cylinders be $\Omega_i$ and $\Omega_o$, respectively, which induce an azimuthal flow within their annulus gap. The analytical solution for such a cylindrical Couette flow is given in terms of the radial variation of the azimuthal velocity as follows:

$$u_\theta(r) = Ar + \frac{B}{r},$$

where $A = \frac{\Omega_o R_o^2 - \Omega_i R_i^2}{R_o^2 - R_i^2}$, $B = \frac{(\Omega_i - \Omega_o) R_i^2 R_o^2}{R_o^2 - R_i^2}$. Here, $r$ is the radial distance from the cylindrical axis. For ease of representation, this can be written in a non-dimensional form as

$$\frac{u_\theta(r)}{u_o} = \frac{1}{1 - \beta^2} \left( (\kappa - \beta^2) \frac{r}{R_i} + \frac{R_i}{r} (1 - \kappa) \right),$$

where $u_o = \Omega_i R_i$, $\beta$ is the radius ratio given by $\beta = R_i/R_o$ and $\kappa$ denotes the angular velocity ratio, i.e., $\kappa = \Omega_o/\Omega_i$.

In our simulation, periodic boundary conditions are applied in the axial direction and the values of the azimuthal velocities at the inner and outer cylinder are prescribed as $u_\theta(r = R_i) = \Omega_i R_i = u_o$ and $u_\theta(r = R_o) = \Omega_o R_o = \frac{\kappa}{\beta} u_o$, respectively using the Dirichlet boundary condition implementation scheme associated with the advection-diffusion equation representing the dynamics of $u_\theta$ [100]. The outer cylinder radius is resolved by 200 lattice nodes and the lattice location for the inner cylinder fixed using $R_i = \beta R_o$ for different choices of $\beta$. The periodic axial direction is discretized using 3 lattice nodes. The relaxation times in the cascaded LB scheme representing the kinematic shear viscosity are set as $\omega_j = 1/\tau, j = 4, 5$, where $\tau = 0.6$, and $u_o$ is chosen such that the rotational Reynolds number $Re = u_o R_i/\nu$ becomes 5. Figure 1 presents a comparison of the velocity profiles computed using the cascaded LB scheme against the analytical solution at
the angular velocity ratio $\kappa = 0.1$ for various values of the radius ratio $\beta$ ($\beta = 0.103, 0.203, 0.303$ and 0.503). It is clear that the agreement between the numerical and analytical solution is very good.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5_1.png}
\caption{Comparison between the analytical velocity profile (solid lines) and the cascaded LB solution (symbols) for the Taylor-Couette flow between two circular cylinders at an angular velocity ratio $\kappa = 0.1$ and for various values of the radius ratio $\beta$.}
\end{figure}

**Order of accuracy**

We will now examine our new axisymmetric cascaded LB scheme for this benchmark problem to establish its order of accuracy. In this regard, we consider the diffusive scaling, i.e., an increase in the grid resolution is accompanied by a proportional decrease in the Mach number at a fixed viscosity or a fixed relaxation time, which corresponds to an asymptotic convergence to the incompressible flow limit. For this purpose, the global relative error ($E_{g,u}$) is defined as follows:

$$E_{g,u} = \sqrt{\frac{\sum(u_e - u_a)^2}{\sum(u_a^2)}},$$

(5.54)
where $u_c$ is the numerical velocity field computed using the axisymmetric cascaded LB scheme and $u_a$ is the analytical solution given above, and the summation is carried out for the whole domain. We consider fixed values of the Reynolds number $Re = 5$, radius ratio $\beta = 1/3$, relaxation time that determines the momentum diffusivity, i.e., the viscosity as $\tau = 0.6$. Four different grid resolutions of $24 \times 3$, $48 \times 3$, $96 \times 3$, and $192 \times 3$ are considered and the corresponding relative errors are computed. As displayed in Fig. 5.2, the global relative errors have a slope of $-2.0$ in the log-log scale, and thus evidently our axisymmetric cascaded LB scheme is second order accurate.

![Graph showing relative errors vs grid resolution](image)

**FIGURE 5.2**: Evaluation of order of accuracy for Taylor-Couette flow with a constant Reynolds number $Re = 5$, radius ratio $\beta = 1/3$ and relaxation time $\tau = 0.6$ at different grid resolutions computed using the axisymmetric cascaded LB scheme.

5.3.2 Natural convection in an annulus between two coaxial vertical cylinders

In order to validate our cascaded LB schemes for axisymmetric flows with heat transfer, we simulate a buoyancy-driven flow between two coaxial stationary cylinders, which is a prototype problem of both fundamental and practical interest. Since the flow field is coupled to the temperature...
field via the buoyancy force in view of Eqs. (5.3a)-(5.3c), (5.4a)-(5.4c), (5.5), (5.8) and (5.9), this problem facilitates a thorough examination of the efficacy of the coupling between the cascaded LB schemes presented in Sec. 2.2 and 2.4. The schematic of this problem is depicted in Fig. 5.3, where \( R_i, R_o, H \) and \( g \) are the radii of the inner cylinder and outer cylinder, the height of the cylinder and the gravitation acceleration, respectively.

![FIGURE 5.3: Schematic illustration of the geometry and boundary conditions for natural convection in a vertical annulus.](image)

For the velocity field, no-slip boundary conditions are considered on all four walls involving the inner and outer cylindrical surfaces, and top and bottom walls. The inner and outer walls of the lateral cylindrical side walls are maintained at temperatures of \( T_H \) and \( T_L \), respectively, where \( T_H > T_L \), while the top and bottom walls are considered to be thermally insulated (adiabatic). As a result, this generates a body force due to buoyancy in the axial direction, which under the Boussinesq approximation, can be written as \( g\beta(T - T_o) \), where \( \beta \) is the thermal expansion coefficient, and \( T_o = (T_H + T_L)/2 \). This body force component is added to the geometric source terms in Eq. (5.5) for \( F_b^x \), which then sets up natural convection within the annulus of the axisymmetric geometry. This thermally driven flow problem is characterized by two dimensionless numbers, viz., the Rayleigh number \( Ra \) and Prandtl number \( Pr \) defined as

\[
Ra = \frac{g\beta(T_H - T_L)L^3}{\alpha \nu}, \quad Pr = \frac{\nu}{\alpha},
\]

where \( L = R_o - R_i \) is the annual gap serving as the characteristic length, and \( \nu \) and \( \alpha \) are the
kinematic viscosity and thermal diffusivity, respectively. In addition, the geometric parameters influencing this problem are the aspect ratio $H/L$ and the radius ratio $R_o/R_i$, both of which are set to 2 in the present study. The no-slip conditions for the velocity field are implemented using the standard half-way bounce back scheme in the cascaded LB method, while the imposed temperature and no heat flux conditions on the boundaries are represented using the approach presented in [100]. All the spatial derivatives needed in the source terms in Eqs.(5.4b), (5.4c) and (5.9) are computed using a central difference scheme. The characteristic velocity due to natural convection $\sqrt{g\beta(T_H - T_L)}R_i$ is kept small so that the flow can be regarded as incompressible. We performed simulations at $Pr = 0.7$ and $Ra = 10^3$, $10^4$ and $10^5$ corresponding to the parameter spaces considered in prior studies [165, 166, 152]. In addition, we have also performed additional simulations at higher Rayleigh numbers of $Ra = 10^6$ and $Ra = 10^7$ that could serve as possible reference results for future research work in this area. The computational domain is resolved using a grid resolution of $200 \times 200$ in the axial and radial directions, respectively, for the lower Rayleigh number cases (i.e., $Ra = 10^3$, $10^4$ and $10^5$) and using $300 \times 300$ for higher Rayleigh number considered (i.e., $Ra = 10^6$ and $Ra = 10^7$).

Figure 5.4 presents the computed streamlines and isotherms for three different $Ra = 10^3$, $10^4$ and $10^5$. It is clear that as $Ra$ increases, the vortical patterns turn to be progressively more complex, with the $Ra = 10^5$ case generating additional pairs of vortices around the middle of the annulus. Furthermore, as $Ra$ increase, the isotherms are greatly distorted, and the velocity and thermal boundary layers become thinner near the hot and cold lateral walls signifying the strengthened convection mode of heat transfer. It may be noted that all these observations are consistent with prior studies based on other numerical methods (e.g., [165, 166, 152]). Furthermore, the results for the computed streamlines and the isotherms at the higher $Ra = 10^6$ and $Ra = 10^7$ are presented in Fig. 5.5. It can be seen that the streamline patterns become more complex, with the resulting buoyancy-driven convection becoming more intense. Also, as can be expected from scaling arguments, the thermal boundary layers near the cylinder walls become thinner thereby mono-
FIGURE 5.4: Streamlines and isotherms for the natural convection between two co-axial vertical cylinders at $Pr = 0.7$ and (a,d) $Ra = 10^3$, (b,e) $Ra = 10^4$ and (c,f) $Ra = 10^5$ computed using cascaded LB schemes. Top row presents streamlines and the bottom row the isotherms.
tonically increasing the heat transfer rate for these higher $Ra$ cases.

Then in order to quantify the rates of heat transfer on the lateral walls, the overall Nusselt numbers $Nu_i$ and $Nu_o$ on the inner and outer cylinders can be defined as

$$Nu_i = \frac{-R_i}{H(T_H - T_L)} \int_o^H (\partial_y T)_i dx, \quad Nu_o = \frac{-R_o}{H(T_H - T_L)} \int_o^H (\partial_y T)_o dx,$$

and hence the average Nusselt number $\overline{Nu} = (Nu_i + Nu_o)/2$.

First, we have conducted grid sensitivity analysis to identify the minimum grid resolution necessary to provide converged heat transfer rate results for each Rayleigh number. For example, Table 5.1 reports the results of a grid convergence test in terms of the average Nusselt number $\overline{Nu}$ for a typical $Ra = 10^4$ by repeating the simulations for three different mesh resolutions of $100 \times 100, 200 \times 200, 250 \times 250$. From this table, it can be seen that for this benchmark problem, while the $\overline{Nu}$ results between the grid resolution cases $100 \times 100$ and $200 \times 200$ cases vary appreciably, that between $200 \times 200$ and $250 \times 250$ show relatively negligible variations. Hence, the results with using $200 \times 200$ can be deemed to have shown grid convergence for $Ra = 10^4$. In a similar manner, we have performed a sensitivity study and established the grid convergence for various $Ra$ for different benchmark problems.

**TABLE 5.1:** Grid convergence study given in terms of the average Nusselt number $\overline{Nu}$ for $Ra = 10^4$ for natural convection in a cylindrical annulus computed using axisymmetric cascaded LB schemes.

<table>
<thead>
<tr>
<th>Grid Resolution</th>
<th>$\overline{Nu}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$100 \times 100$</td>
<td>3.172</td>
</tr>
<tr>
<td>$200 \times 200$</td>
<td>3.199</td>
</tr>
<tr>
<td>$250 \times 250$</td>
<td>3.202</td>
</tr>
</tbody>
</table>

Table 5.2 shows a comparison of the average Nusselt number computed using the cascaded LB scheme for $Ra = 10^3, 10^4, 10^5$ against prior numerical benchmark results [165, 166, 152]. It can be seen that our predictions for the average Nusselt numbers agree well with those obtained by other methods. In addition, this table also includes new results for the higher $Ra$ of $10^6$ and
FIGURE 5.5: Streamlines and isotherms for the natural convection between two co-axial vertical cylinders at $Pr = 0.7$ and (a,c) $Ra = 10^6$, (b,d) $Ra = 10^7$ computed using cascaded LB schemes. Top row presents streamlines and the bottom row the isotherms. Grid resolution used is $300 \times 300$. 
It is evident that increasing the Rayleigh number increases the average Nusselt number. For example, the heat transfer rate increases by about six times when $Ra$ increases from $10^4$ to $10^7$. The new quantitative data for $\bar{Nu}$ for $Ra = 10^6$ and $10^7$, in particular, could serve as possible benchmark results for future research work.

**TABLE 5.2**: Comparison of the average Nusselt number $\bar{Nu}$ for different $Ra$ for natural convection in a cylindrical annulus computed using axisymmetric cascaded LB schemes with other reference numerical solutions and new results for $Ra = 10^6$ and $10^7$.

<table>
<thead>
<tr>
<th>$Ra$</th>
<th>Cascaded LB schemes</th>
<th>Ref. [165]</th>
<th>Ref. [166]</th>
<th>Ref. [152]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$</td>
<td>1.688</td>
<td>-</td>
<td>-</td>
<td>1.692</td>
</tr>
<tr>
<td>$10^4$</td>
<td>3.199</td>
<td>3.037</td>
<td>3.163</td>
<td>3.215</td>
</tr>
<tr>
<td>$10^5$</td>
<td>5.781</td>
<td>5.760</td>
<td>5.882</td>
<td>5.798</td>
</tr>
<tr>
<td>$10^6$</td>
<td>10.421</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$10^7$</td>
<td>18.411</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

### 5.3.3 Swirling flow in a lid-driven cylindrical container

In this section, we investigate the ability of the axisymmetric cascaded LB schemes to accurately simulate the dominant role played by the swirling motion and its coupling with the complex radial and axial flow induced in the meridian plane. In this regard, we consider the symmetry breaking flow in a cylindrical container of radius $R$ and height $H$ driven by a rotating top end wall at angular velocity $\Omega$ (see Fig. 6).

The dynamics of this flow is presented by Eqs. (5.3a)-(5.3c), (5.4a)-(5.4c), (5.6) and (5.7), whose solution scheme via our cascaded LB formulation is presented in Sec.2.2 and 2.3. Briefly, as the fluid in the vicinity of the top lid gains azimuthal motion, it is ejected radially outward, and then downward due to the constraining effect of the side wall. Subsequently as the fluid reaches the bottom it is pushed radially inward, and when it is closer to the axis, it travels upward, thereby completing flow circulation in the meridian plane. The details of the physics and the flow pattern depend on the aspect ratio $R_A = H/R$ and the rotational Reynolds number $Re = R^2\Omega/\nu$. Various experiments (e.g., [167, 168]) and numerical simulations (e.g., [169, 170, 171]) have revealed
FIGURE 5.6: Schematic of swirling flow in a confined cylinder driven by a rotating top lid.
that for certain combinations of the characteristic parameters $R_A$ and $Re$, distinct recirculation regain around the cylinder axis, designated as the vortex breakdown bubble, may occur. For example, Refs. [168, 5] show that for cases $(R_A, Re)$ equal to (1.5, 990) and (2.5, 1010), no vortex breakdown bubbles occur whereas for (1.5, 1290), they do occur.

In order to asses and validate our cascaded LB schemes presented earlier to simulate such complex swirling flow, we consider the following four test cases: $Re = 990$ and $Re = 1290$ with $R_A = 1.5$ and $Re = 1010$ and $Re = 2020$ with $R_A = 2.5$. The computational domain is resolved using a mesh resolution of $100 \times 150$ for $R_A = 1.5$ and $100 \times 250$ for $R_A = 2.5$. No-slip boundary conditions are used at bottom, lateral and top walls: $u_\theta = u_r = u_z = 0$ at $z = 0$ and $r = R$, and $u_\theta = r\Omega$, $u_r = u_z = 0$ at $z = H$. The streamlines computed using the cascaded LB schemes for the above four cases are in Fig. 7. It can be seen that no vortex break-down bubbles appear for $(R_A, Re)$ equal to (1.5, 990) and (1.5, 1010). On the other hand, one vortex break down bubble is seen at (1.5, 1290) and two break down bubbles occur in the vicinity of the cylinder axis. These distinct regimes in swirling flows and the complex flow structure for different $(R_A, Re)$ cases are strikingly consistent with prior numerical solution (e.g., [5, 143, 145, 172]). Quantitative comparison of the computed structure of the axial velocities along the axis of symmetry obtained using the axisymmetric cascaded LB schemes for the above four sets of the aspect ratios $R_A$ and Reynolds number $Re$ against the results from a NS-based solver (given in [5]) are shown in Fig. 8. Here, the axial velocity is scaled by the maximum imposed azimuthal velocity $u_o = \Omega R$ on the rotating lid and the axial distance $z$ by the cylinder height $H$. The numerical results of our central moments based cascaded LB method for the axial velocity profiles are in very good agreement with the NS-based solution approach [5]. Also, in particular, notice local negative values for the axial velocities for the cases $Re = 1290$ and $R_A = 1.5$ and $Re = 2200$ and $R_A = 2.5$, which is an indication of the presence of one or more vortex breakdown bubbles. As such, both the magnitudes and the shapes of the axial velocity distributions are well reproduced by our cascaded LB approach using operator splitting to represent complex flows in cylindrical coordinates.
FIGURE 5.7: Computed streamline patterns in the meridian plane due to swirling flow in a confined cylinder driven by a rotating lid at various aspect ratios and Reynolds numbers using the axisymmetric cascaded LB schemes: (a) $R_A = 1.5$ and $Re = 990$, (b) $R_A = 1.5$ and $Re = 1290$, (c) $R_A = 2.5$ and $Re = 1010$ and (d) $R_A = 2.5$ and $Re = 2200$. 
FIGURE 5.8: Dimensionless axial velocity profile $u_z/u_o$ as a function of the dimensional axial distance $z/H$ for (a) $R_A = 1.5$ and $Re = 990$, (b) $R_A = 1.5$ and $Re = 1290$ (c) $R_A = 2.5$ and $Re = 1010$ and (d) $R_A = 2.5$ and $Re = 2200$: Comparison between axisymmetric cascaded LB scheme predictions and NS-based solver results ([5])
5.3.4 Mixed convection in a slender vertical annulus between two coaxial cylinders

We will now assess our new axisymmetric LB computational approach based on central moments to simulate the combined effects of rotation and buoyancy forces on the flow and heat transfer in confined cylindrical spaces. In this regard, we investigate mixed convection in a slender vertical annulus between two coaxial cylinders arising due to inner side wall rotation, which has numerous applications related to rotating machinery and various other heat transfer systems. This problem involving both natural convection and forced convection due to rotation can test all the three axisymmetric cascaded LB formulations (Secs. 2.2-2.4) in a unified manner.

A schematic arrangement of this axisymmetric thermal flow problem is shown in Fig. 9. It consists of two coaxial cylinders of height $H$, with an annular gap $D = R_o - R_i$, where $R_i$ and $R_o$ are the radii of the inner and outer cylinders, respectively. The lateral walls of the inner and outer cylinders are maintained at temperatures $T_H$ and $T_L$, respectively, where $T_H > T_L$, and their bottom and top ends are thermally insulated. The inner cylinder is subjected to rotation at an angular velocity $\Omega_i$, while the outer cylinder and the end walls are considered to be rigidly fixed.
As noted in a recent study [154], this problem is governed by the following characteristic dimensionless parameters: Prandtl number $Pr = \nu/\alpha$, radius ratio $R_{io} = R_o/R_i$, slenderness ratio $\eta = H/(R_o - R_i)$, Reynolds number $Re = \Omega_i R_i D/\nu$, Grashof number $Gr = g\beta(T_H - T_L)D^3/\nu^2$, and $\sigma = Gr/Re^2$, where the parameter $\sigma$ is used to measure the strength of the buoyancy force relative to the centrifugal force. Hence, $\sigma$ characterizes the degree of mixed convection.

In the present study, we set $Pr = 0.7$, $R_{io} = 2$, $\eta = 10$, $Re = 100$, and three cases of $\sigma$ are considered: $\sigma = 0$, 0.01 and 0.05. The grid resolution used for all the three cases is $40 \times 400$, in which the location of the inner cylinder from the axis $R_i$ is at 40. Figure 10 shows the computed contours of the azimuthal velocity, temperature field, vorticity and streamlines for the above three values of $\sigma$. When $\sigma = 0$, there is no buoyancy force and the flow and the temperature fields are influenced by the centrifugal force and the forced convection effects, which manifest in the form of five pairs of counter-rotating cells, viz., the classical Taylor vortex cells arising from centrifugal flow instability between curved walls [130]. As $\sigma$ is increased, the presence of buoyancy forces and the associated natural convective fluid currents alter the overall flow structure and the temperature field by their complicated interactions with primary vortex cells induced by the swirling effects from inner wall rotation. For example, when $\sigma = 0.05$, a four-pairs based Taylor vortex structure, rather than five-pair of vortex cells observed for $\sigma = 0$, arises from the relative weakening effects of the centrifugal forces in the presence of heating. The strength of the Taylor vortex in the positive azimuthal direction $\theta$ is seen to be enhanced, while that negative $\theta$ direction appear to be diminished and these observations are consistent with the benchmarks results [173, 174] and recent numerical simulations [153]. In order to quantify the heat transfer rate in the presence of mixed convection, a mean equivalent thermal conductivity at the inner cylinder can be defined as

$$\bar{k}_{eq}|_i = \frac{lnR_{io}}{\mu} \int_0^H \left(-r\frac{\partial T}{\partial r}|_{r=R_i}\right) dr.$$  

Table 3 presents a comparison of the equivalent thermal conductively computed using the axisymmetric cascaded LB formulations against the benchmark results [173, 174] for different values
FIGURE 5.10: Contours of (a) azimuthal velocity, (b) temperature, (c) vorticity, and (d) streamlines for mixed convection in a slender cylindrical annulus for three different values of $\sigma$ computed using the axisymmetric cascaded LB schemes.
of \( \sigma \). Very good quantitative agreement is seen and this validates the ability of the cascaded LB schemes in the cylindrical coordinate system to represent complex flows with heat transfer.

**TABLE 5.3:** Comparison of the mean equivalent thermal conductivity at the inner cylinder in a slender vertical cylindrical annulus during mixed convection for \( Re = 100, Pr = 0.7, R_{io} = 2, \eta = 10 \) at different values of \( \sigma \).

<table>
<thead>
<tr>
<th>( \sigma )</th>
<th>Ref. [174]</th>
<th>Ref. [173]</th>
<th>Present Work</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.473</td>
<td>1.393</td>
<td>1.395</td>
</tr>
<tr>
<td>0.01</td>
<td>1.370</td>
<td>1.383</td>
<td>1.378</td>
</tr>
<tr>
<td>0.05</td>
<td>1.324</td>
<td>1.323</td>
<td>1.321</td>
</tr>
</tbody>
</table>

5.3.5 Melt flow and convection during Czochralski crystal growth in a rotating cylindrical crucible

As the last test problem, we simulate melt flow and convection during Czochalski crystal growth, based on a configuration reported by Wheeler [175], using our axisymmetric cascaded LB schemes. This Wheeler’s benchmark problem involved both forced convection due to the rotation of the crucible and the crystal and natural convection arising from heating effects in the presence of gravity. It has been studied by a variety of numerical schemes (e.g., [176, 177, 146, 154]). The geometric arrangement of this problem is shown in Fig. 11.

Liquid melt in a cylindrical rotating crucible of radius \( R_c \) and height \( H \) at an angular rotation rate of \( \Omega_c \) undergoes stirred vortical motion in the meridian plane, which is aided by the angular rotation of the solid crystal of radius \( R_x \) at rate \( \Omega_x \). In addition, natural convection is set up due to the buoyancy force generated from a differential heating, where the bottom is insulated and its crucible side is maintained at a temperature \( T_H \), while the crystal is at a lower temperature \( T_L \) (i.e., \( T_L < T_H \)). These can be prescribed in terms of the following boundary conditions,
FIGURE 5.11: Geometric arrangement of melt flow and convection during Czochralski crustal growth in a rotating crucible—Wheeler’s benchmark problem.
where the \((x, z)\) coordinates are scaled by \(R_c\):

\[
\begin{align*}
\frac{\partial u_r}{\partial r} &= \frac{\partial u_z}{\partial r} = \frac{\partial T}{\partial r} = 0 & \text{for } r = 0 \quad 0 \leq z \leq \alpha\\
u_r &= u_z = 0, \quad u_\theta = \Omega_c R_c, \quad T = T_H & \text{for } r = 1 \quad 0 \leq z \leq \alpha\\
u_r &= u_z = 0, \quad u_\theta = r \Omega_c, \quad \frac{\partial T}{\partial z} = 0 & \text{for } z = 0 \quad 0 \leq r \leq 1\\
u_r &= u_z = 0, \quad u_\theta = r \Omega_x, \quad T = T_L & \text{for } z = \alpha \quad 0 \leq r \leq \beta\\rac{\partial u_r}{\partial r} &= \frac{\partial u_\theta}{\partial z} = 0, \quad u_z = 0, \quad T = T_L + \frac{r - \beta}{1 - \beta} (T_H - T_L) & \text{for } z = \alpha \quad \beta \leq r \leq 1
\end{align*}
\]

where \(\alpha = H/R_c, \beta = R_x/R_c\). This flow problem is characterized by the following dimensionless parameters: Reynolds numbers due to crucible and crystal rotations \(Re_c = R_c^2 \Omega_c/\nu\) and \(Re_x = R_x^2 \Omega_x/\nu\), and Prandtl number \(Pr = \nu/\alpha\). We investigate the ability of the axisymmetric cascaded LB schemes for the simulation of mixed convection associated with the Wheeler’s benchmark problem for the following two cases: (a) \(Re_x = 100, \ Re_c = -25\) and (b) \(Re_x = 1000, \ Re_c = -250\), where the negative sign denotes that the sense of rotation of the crystal is apposite to that of the crucible. We take \(Pr = 0.05\), \(\alpha = 1\), and \(\beta = 1\) and use a grid resolution of \(100 \times 200\) for the simulation of both the cases.

Figure 12 shows the streamlines and isotherm contours in the meridian plane of the liquid melt motion for the two cases. It can be seen that a recirculating vortex appears around the upper left region below the crystal in both cases in addition to the primary vortex. The center of this secondary vortex is found to move to the right at higher Reynolds numbers as a result of higher associated centrifugal forces. On the other hand, the forced convection has modest effect on the temperature distribution, as they are largely alike for both the cases due to the relatively low Reynolds numbers considered.

Table 4 shows the computed absolute maximum values of the streamfunction \(\psi_{max}\) for the above two cases and compared with prior numerical results presented in [146, 176]. In the pseudo-2D
FIGURE 5.12: Streamlines (upper row) and isotherms (bottom row) corresponding to two cases of the Wheeler’s benchmark problem of melt flow and convection during Czochralski crystal growth: $Re_x = 100, Re_c = -25$ (left) and $Re_x = 1000, Re_c = -250$ (right).
Cartesian coordinates, this is obtained by solving for $\psi$ using $\partial \psi / \partial y = -y u_x$ and $\partial \psi / \partial x = y u_y$.

The good agreement confirms that the new axisymmetric cascaded LB schemas presented in this study can effectively simulate complex flow and heat transfer problems in cylindrical geometries.

**TABLE 5.4:** Comparison of the maximum value of the stream function $\psi_{\text{max}}$ computed using the axisymmetric cascaded LB schemes with reference numerical solutions for the Wheeler’s benchmark problem.

<table>
<thead>
<tr>
<th>Reference</th>
<th>$Re_x = 10^2, Re_c = -25$</th>
<th>$Re_x = 10^4, Re_c = -250$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present Work</td>
<td>0.1183</td>
<td>1.123</td>
</tr>
<tr>
<td>Ref. [119]</td>
<td>0.1140</td>
<td>1.114</td>
</tr>
<tr>
<td>Ref. [176]</td>
<td>0.1177</td>
<td>1.148</td>
</tr>
</tbody>
</table>

5.3.6 Comparison of single relaxation time and cascaded LB models for axisymmetric flow simulations

We will now make a direct comparison between the performance of the single relaxation time (SRT) LB scheme and the proposed cascaded LB formulation based on central moments for axisymmetric flow simulations. In particular, a study of the numerical stability characteristics of these schemes for flow simulations in the cylindrical coordinates represents a key aspect with important practical implications. In this regard, we consider the computation of lid-driven swirling flow in a cylindrical container discussed in Sec. 5.3.3, as the flow is set up by a shear in the presence of a geometric singularity between the stationary cylindrical walls and the rotating lid.

For a fixed angular rotation rate $\Omega$ of the lid of the cylindrical container of radius $R$ and height $H$ (see Sec. 5.3.3 for the nomenclature) at different aspect ratios $R_A = H/A$, we will now make a comparison between the maximum attainable Reynolds number $Re = R^2 \Omega / \nu$ with the axisymmetric SRT [145] and cascaded LB schemes. In this regard, we gradually reduce the viscosity, or equivalently, the relaxation time $\tau$ for a specific grid resolution until the computation becomes numerically unstable. In the case of the cascaded LB formulation, this is equivalent varying the relaxation times for the second order moments $\omega_j = 1/\tau$, where $j = 4, 5$, and the remaining relax-
ation times for the higher order moments are set to unity for simplicity.

In particular, for two different grid resolutions of $101 \times 101$ and $101 \times 151$ corresponding to the aspect ratios $R_A$ of 1.0 and 1.5, respectively, at a fixed angular velocity $\Omega = 0.0014$, simulations are carried out using both these LB models by reducing the relaxation time $\tau$ until the computation becomes, which then determines the maximum attainable $Re$ in each case. Since the radius $R = 100$ for both these grid resolution cases, the maximum imposed linear velocity of the cylindrical lid $R\Omega$ is 0.14. The onset of instability is determined when the relative global error increases rapidly as the simulation progress. Such a computational investigation is an extension of those considered for the LB models in the Cartesian coordinates recently [17]. The results are displayed in Fig. 5.13, which show significant improvements in numerical stability with the use of the axisymmetric cascaded LB approach. It can be seen that the cascaded LB computations can reach Reynolds numbers that are about 7 times higher than those with using the SRT LB scheme for the $R_A = 1.0$, i.e., when the grid resolution used is $100 \times 100$. As the cylindrical confined space for the fluid motion undergoing shearing motion becomes narrower and slender ($R_A = 1.5$) that is resolved using $101 \times 150$ grid nodes, the maximum attainable $Re$ with the central moments based cascaded LB formulation becomes even higher, by as much as 10 times when compared to the SRT model.

It may be noted that when the cascaded LB scheme is used to solve the governing equations for axisymmetric flows, it incurs about 20% additional computational effort, in terms of the CPU time, when compared to the SRT-LB scheme similar to that observed in the respective 2D Cartesian formulations [17]. On the other hand, the cascaded LB formulation is seen to be much more stable than the SRT scheme. As a result, for practical simulations of axisymmetric flows including swirl effects, the central moments based formulation holds important advantages over other collision models. These significant improvements in numerical stability with cascaded LB schemes, which allow efficient simulation of axisymmetric flows with broader ranges of parameter spaces, for a given resolution is consistent with the recent results obtained for simulations of flows in the
FIGURE 5.13: Comparison of the maximum Reynolds number for numerical stability of single relaxation time (SRT) and cascaded LB methods for simulation of the shear driven swirling flow in a confined cylinder at different grid resolutions.
5.4 Summary and Conclusions

Thermally stratified fluid convection including rotational effects within cylindrical confined spaces represents an important class of flows with numerous engineering applications. Exploiting axial symmetry in such problems leads to their representation in terms of a quasi-2D system of equations with geometric source terms in the meridian plane, which can significantly reduce computational and memory costs when compared to their 3D modeling.

In this work, we have presented axisymmetric cascaded LB schemes for convective flows with combined rotation and thermal stratification effects in cylindrical geometries. A triple distribution function based approach is employed in this regard, in which the axial and radial momentum as well as the pressure field are solved using a D2Q9 lattice based cascaded LB scheme, while the azimuthal momentum and the temperature field are solved using the two other cascaded LB schemes, each based on a D2Q5 lattice. The collision step in these three schemes is based on the relaxation of different central moments at different rates to represent the dynamics of the fluid motion as well as the advection-diffusion transport of the passive scalar fields in a consistent framework. The geometric mass, momentum and energy source terms arising in the quasi-2D formulation are incorporated using a simpler operator splitting based approach involving a symmetric application of their effects given in terms of appropriate change of moments for two half time steps around the collision step. This new computational approach is then used to simulate a variety of complex axisymmetric benchmark thermal flow problems including natural convection between two coaxial cylinders, Rayleigh-Benard convection in a vertical cylinder, mixed convection in a slender vertical annulus between two cylinders under combined rotation and buoyancy forces, and convective flow of a melt during Czochralski crystal growth in a rotating cylindrical crucible. Comparison of the computed results obtained using the axisymmetric
cascaded LB schemes for such thermal convective flows for the structures of the flow and thermal fields, as well as the heat transfer rates given in terms of the Nusselt number against prior benchmark numerical solutions demonstrate their good accuracy and validity.
CHAPTER VI

LOCAL VORTICITY COMPUTATION IN DOUBLE DISTRIBUTION
FUNCTIONS BASED LATTICE BOLTZMANN MODELS FOR FLOW AND
SCALAR TRANSPORT

6.1 Introduction

Qualitative distribution and quantitative measures of vorticity are of fundamental interest in fluid mechanics. Indeed, fluid motions are often associated with vortical structures, which can be characterized by vorticity, and, more generally, by certain invariants of the velocity gradient tensor [178, 179]. The significance of the rigid-body like rotational component of the fluid element was first identified in a pioneering work by Helmholtz [180] and the subject has a long and rich history [181, 182]. This local rotational property of the flow, given by the curl of the velocity field, was termed vorticity by Lamb [183]. While there is no consensus on a rigorous definition of a vortex, various quantitative measures have been devised to identify regions associated with more rigid-body rotations than stretching or shearing motions that aid in flow classification [184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196]. Such approaches are based on a complete knowledge of the velocity gradient tensor, and the local, Eulerian based methods for coherent structure identification are popular. In more detail, the velocity gradient tensor $A_{ij} \equiv \partial_j u_i$ of the velocity field $u_i$ can be decomposed into symmetric $S_{ij}$ and anti- or skew-symmetric parts $\Omega_{ij}$ as

$$\partial_j u_i = \frac{1}{2}(\partial_j u_i + \partial_i u_j) + \frac{1}{2}(\partial_j u_i - \partial_i u_j) = S_{ij} + \Omega_{ij},$$

where $S_{ij}$ is the strain rate tensor and $\Omega_{ij}$ is the intrinsic rotation rate (spin) tensor, with $\Omega_{ij} = -\frac{1}{2}\epsilon_{ijk}\omega_k$. Here, $\omega_k$ is the Cartesian component of the vorticity and $\epsilon_{ijk}$ is the Levi-Civita (permutation) tensor, and the vorticity can be defined as $\omega_i = \epsilon_{ijk}\partial_j u_k$ or $\omega = \nabla \times u$. Both $\omega_i$ and
$S_{ij}$, or, in general, $\partial_j u_i$ play an important role in eduction techniques for vortex structure identification. In particular, many of these methods [197] are based on the second and third invariants of the velocity gradient tensor $\partial_j u_i$, i.e., $Q = -\frac{1}{2} S_{ij} S_{ij} + \frac{1}{4} \omega_k \omega_k$ and $R = \frac{1}{3} (S_{ij} S_{jk} S_{ki} + \frac{2}{3} \omega_i \omega_j S_{ij})$.

Similarly, sometimes the Lamb vector $L_i = \epsilon_{ijk} \omega_j u_k$ plays a prominent role in the analysis of vortex dynamics [198]. Thus, a complete knowledge of the local velocity gradient tensor $\partial_j u_i$, or equivalently, $S_{ij}$ and $\Omega_{ij}$ or $\omega_k$ is of basic interest in structure identification and classification of flows. This also allows a local determination of the components of the convective acceleration of the fluid elements. In addition, the distribution of vorticity is related to the sound generation and propagation in flow generated acoustics [199]. Furthermore, many models for the representation of turbulence, rheological fluid flows such as those involving viscoelasticity, and complex fluid systems such as liquid crystals and polar fluids depend on the local measures of the complete velocity gradient tensor $\partial_j u_i$ [200]. It is thus highly desirable for computational methods for fluid dynamics that allow especially local determination of all components of the velocity gradient tensor, including the skew symmetric part (i.e., the vorticity).

The lattice Boltzmann (LB) method is a kinetic computational approach for a variety of fluid mechanics and transport problems [201, 14, 24, 11, 12, 7, 43, 18]. Generally, the standard versions of the LB models can only represent the symmetric part of $\partial_j u_i$, i.e., the strain rate tensor $S_{ij}$ via the second order non-equilibrium moments of the distribution function, which are, in turn, related to the spatial derivatives of the first and third order moment equilibria. The latter are constructed based on symmetry and isotropy considerations that respect the underlying isotropy of the viscous stress tensor of the fluid motion represented by the Navier-Stokes equations. It is known that such LB approaches can recover the strain rate tensor components locally with second order accuracy (see e.g., Refs. [202, 203, 17]). However, most of the existing LB models are not constructed to recover the antisymmetric velocity gradient tensor $\Omega_{ij}$ locally without relying on the use of finite difference approximation for the spatial derivatives of the velocity field components. One notable exception is the recent and interesting work [204], which
introduced an approach based on modifying the fifth order moment equilibria of the LB solver for fluid flow that enables vorticity computation. This approach is restricted to only lattices that can support fifth order independent moments and thus is applicable only to the three-dimensional, twenty seven velocity (D3Q27) lattice, and not for other standard lattice sets, including the common two-dimensional, nine velocity (D2Q9) lattice. Furthermore, since it is based on a certain prescribed form of the higher order moment equilibria, it may be challenging to extend it for thermal flows as well as those with significant compressibility effects that involve constraints on the higher moments of the single distribution function, and may also impact its Galilean invariance of solving the fluid motion.

Our approach is based on different considerations than the above mentioned work for vorticity computation. The goal is to simulate the fluid motion along with an advection-diffusion transport of a scalar field, represented by the following Navier-Stokes equations (NSE) and the convection-diffusion equation (CDE), respectively:

\[
\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (6.2)
\]

\[
\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{T} + \mathbf{F}, \quad (6.3)
\]

\[
\partial_t \phi + \nabla \cdot (\phi \mathbf{u}) = \nabla \cdot (D_\phi \nabla \phi), \quad (6.4)
\]

where \( \rho, \mathbf{u} \) and \( p \) are the fluid density, velocity, and pressure, respectively, \( T_{ij} = 2\nu S_{ij} - \frac{2}{d} \rho \nu \partial_k u_k \delta_{ij} + \rho \zeta \partial_k u_k \delta_{ij} \) is the deviatoric stress tensor (with \( \nu \) and \( \zeta \) being the kinematic shear and bulk viscosities, respectively, and \( d \) being the number of spatial dimensions), \( \mathbf{F} \) is the local body force, and \( \phi \) is the scalar field (with \( D_\phi \) being its diffusivity). These equations can be solved by means of a double distribution functions (DDF) based approach using two lattice Boltzmann equations (LBEs) – one for the flow field and the other for the scalar field. Such situations related to solving the additional passive scalar field dynamics arise widely, including those related to the transport of energy or temperature field in thermal convection, and of the concentration field of a chemical species in reacting systems, and in the interface capturing using phase field models in
multiphase flows. Indeed, the modeling of flow and scalar transport using DDF based LBEs is quite common and is a subject of a number of investigations (e.g., Refs. [95, 21, 96, 97, 98, 99, 100, 101, 102, 87, 33, 205, 206]). In such cases, our essential philosophy is to use the additional degrees of freedom (DOF) available in the LBE for the solution of the CDE to construct a procedure for local vorticity computation. This is possible because as the evolution of the scalar field \( \phi \) is influenced by the local fluid velocity \( u \), its solution procedure can, in principle, contain the complete kinematics of the flow field, which can be obtained from the corresponding LBE with careful construction of its equilibria.

The basic idea behind our approach is as follows. Local vorticity computation in the DDF-LBEs can be achieved by prescribing an intensional anisotropy of the scalar flux in the third order, off-diagonal moment equilibria of the LBE for the scalar field and then combining the second order, off-diagonal non-equilibrium moment components of both the LBEs. In essence, the LBE for the fluid flow provides local expressions for the strain rate tensor \( S_{ij} \) and the LBE for the scalar field yields local relations for the skew-symmetric velocity gradient tensor \( \Omega_{ij} \), and hence the vorticity \( \omega_k \). This formulation leads to various advantages. The numerical characteristics of the LBE for the fluid motion are preserved as no additional constraints on its equilibria are imposed (but only on those for the scalar field) and the resulting eduction approach is non-invasive in representing the fluid flow. The freedom from the need to prescribing extra constraints for higher moments for the LBE flow solver allows ready extension to construct LBE model for complex flow physics. In addition, any pair of lattice sets, each supporting only lower (i.e., third) order independent moments, in this DDF-LBE approach can enable local vorticity computation. Thus, this method is applicable for all standard lattices (e.g., D2Q9, D3Q15, D3Q19 and D3Q27) and in different dimensions. Furthermore, the since method is based on two distribution functions which by themselves are generally solved with second order accuracy, the numerically predicted vorticity magnitudes are second order by construction, just like the computed strain rate tensor. Finally, the local expressions for the vorticity field naturally lend themselves to parallel computation.
For the purpose of illustration without losing generality, in this work, we will specialize our DDF approach by formulating two LBEs using natural (non-orthogonal) moment basis and multiple relaxation times (MRT) for the solution of flow and scalar transport using the standard D2Q9 lattice to locally compute the complete information about the flow kinematics, i.e., all the 1291 components of the velocity gradient tensor, including the skew-symmetric components. However, our method can be readily extended to LBE based on other collision models, such as the single relaxation time LBE, MRT-LBE with other moment basis, cascaded LBE and cumulant LBE, and various other lattice sets in different dimensions. This chapter is organized as follows. The next section (Sec. 6.2 will present a MRT-LBE for computing the fluid motion, and its Chapman-Enskog (C-E) analysis to determine the symmetric components of the velocity gradient tensor. Section 6.3.1 will then discuss another MRT-LBE for representing the advection-diffusion transport of a scalar field, and its C-E analysis to obtain the necessary relations for the skew-symmetric components of the velocity gradient tensor. The expression for the local computation of the vorticity field is derived in Sec. 6.4. Then, results and discussion of the comparisons of the computed vorticity fields against the analytical solutions for various representative fluid flow problems are given in Sec. 6.5. Finally, Sec. 7.8 presents a summary and conclusions of this chapter.

6.2 MRT-LBE for Fluid Motion

In order to solve the fluid motion in two-dimensions (2D) represented by the mass and momentum conservation equations given in Eqs. (6.2) and (6.3), respectively, we will now present a MRT-LBE using a natural, non-orthogonal moment basis [19]. In this regard, a D2Q9 lattice is used, and whose particle velocities are given by the following:

\[ |e_x\rangle = (0, 1, 0, -1, 0, 1, -1, -1, 1)^\dagger, \]  
\[ |e_y\rangle = (0, 0, 1, 0, -1, 1, 1, -1, -1)^\dagger, \]
where $\dagger$ is the transpose operator and the standard Dirac’s bra-ket notation is used to represent the vectors. The Cartesian components for any particle direction $\alpha$ are represented by $e_{\alpha x}$ and $e_{\alpha y}$, where $\alpha = 0, 1, \ldots, 8$. In addition, we need the following 9-dimensional vector whose inner product with the particle distribution function $f_\alpha$ yields its zeroth moment:

$$
|1\rangle = (1, 1, 1, 1, 1, 1, 1, 1, 1)^\dagger.
$$

(6.6)

The non-orthogonal basis vectors can then be written as

$$
T_0 = |1\rangle, \quad T_1 = |e_x\rangle, \quad T_2 = |e_y\rangle, \quad T_3 = |e_x^2 + e_y^2\rangle, \quad T_4 = |e_x^2 - e_y^2\rangle,
\quad T_5 = |e_x e_y\rangle, \quad T_6 = |e_x^2 e_y\rangle, \quad T_7 = |e_x e_y^2\rangle, \quad T_8 = |e_x^2 e_y^2\rangle.
$$

(6.7)

In the above, symbols such as $|e_x^2 e_y\rangle = |e_x e_x e_y\rangle$ denote a vector that arise from the elementwise vector multiplication of vectors $|e_x\rangle$, $|e_x\rangle$ and $|e_y\rangle$. In order to map changes of moments back to changes in the distribution function, we group the above set of vectors as a transformation matrix $T$, which reads as

$$
T = [T_0, T_1, T_2, T_3, T_4, T_5, T_6, T_7, T_8].
$$

(6.8)

We then define the raw moments of order $(m + n)$ of the distribution function $f_\alpha$, its equilibrium $f_{\alpha}^{eq}$, and the source terms $S_\alpha$ to represent the body force, respectively, as

$$
\begin{pmatrix}
\hat{m}_x^m y^n \\
\hat{m}_{x,y}^{eq} \\
\hat{\sigma}_{x,m,y}^{eq}
\end{pmatrix} = \sum_{\alpha=0}^{8} \begin{pmatrix}
f_\alpha \\
f_{\alpha}^{eq} \\
S_\alpha
\end{pmatrix} e_{\alpha x}^m e_{\alpha y}^n.
$$

(6.9)

Here, and in what follows, the prime (‘) symbols denote various raw moments. In terms of the nominal, nonorthogonal transformation matrix $T$ the relation between the various moments and their corresponding states in the velocity space can be written as

$$
\hat{m} = Tf, \quad \hat{m}^{eq} = Tf^{eq}, \quad \hat{S} = TS,
$$

(6.10)
where

\[ f = (f_0, f_1, f_2, \ldots, f_8)^\dagger, \quad f_{eq} = (f_{eq}^0, f_{eq}^1, f_{eq}^2, \ldots, f_{eq}^8)^\dagger, \]

\[ S = (S_0, S_1, S_2, \ldots, S_8)^\dagger \]

are the various quantities in the velocity space, and

\[ \hat{m} = (\hat{m}_0, \hat{m}_1, \hat{m}_2, \ldots, \hat{m}_8)^\dagger \]
\[ \hat{m}^{eq} = (\hat{m}_0^{eq}, \hat{m}_1^{eq}, \hat{m}_2^{eq}, \ldots, \hat{m}_8^{eq})^\dagger \]
\[ \hat{S} = (\hat{S}_0, \hat{S}_1, \hat{S}_2, \ldots, \hat{S}_8)^\dagger \]

are the corresponding states in the moment space.

The MRT-LBE with trapezoidal rule to represent the source term with second order accuracy can be written as

\[
\begin{align*}
    f (x + e_\alpha \delta t, t + \delta t) - f (x, t) &= T^{-1} \left[ -\hat{A} (\hat{m} - \hat{m}^{eq}) \right] \\
    &+ \frac{1}{2} T^{-1} \left[ \hat{S} (x + e_\alpha \delta t, t + \delta t) + \hat{S} (x, t) \right] \delta t.
\end{align*}
\]

where the diagonal relaxation time matrix \( \hat{A} \) can be represented as

\[
\hat{A} = \text{diag}(0, 0, 0, \omega_3, \omega_4, \omega_5, \omega_6, \omega_7, \omega_8).
\]

In order to obtain an effectively explicit scheme, we apply the transformation \([69, 23]\) \( \bar{f}_\alpha = f_\alpha - \frac{1}{2} S_\alpha \delta t \), or equivalently \( \hat{m} = \hat{m} + \frac{1}{2} \hat{S} \delta t \) and \( \hat{k}'_{x'y^n} = \hat{k}'_{x'y^n} - \frac{1}{2} \sigma'_{x'y^n} \delta t \), and the MRT-LBE can be written as

\[
\begin{align*}
    \bar{f} (x + e_\alpha \delta t, t + \delta t) - \bar{f} (x, t) &= T^{-1} \left[ -\hat{A} (\hat{m} - \hat{m}^{eq}) \right] + T^{-1} \left[ \left( 1 - \frac{1}{2} \hat{A} \right) \hat{S} \right] \delta t.
\end{align*}
\]
The moment equilibria $\kappa_{x\alpha y\beta}^{eq}$ at different orders can be written as [19]

\[
\begin{align*}
\tilde{\kappa}_0^{eq} &= \rho, \\
\tilde{\kappa}_x^{eq} &= u_x, \\
\tilde{\kappa}_y^{eq} &= u_y, \\
\tilde{\kappa}_{xx}^{eq} &= c_s^2 \rho + p u_x^2, \\
\tilde{\kappa}_{yy}^{eq} &= c_s^2 \rho + p u_y^2, \\
\tilde{\kappa}_{xy}^{eq} &= c_s^2 \rho u_x u_y, \\
\tilde{\kappa}_{xxy}^{eq} &= c_s^4 \rho + c_s^2 \rho (u_x^2 + u_y^2) + p u_x^2 u_y^2, \\
\tilde{\kappa}_{xyy}^{eq} &= c_s^4 \rho + c_s^2 \rho (u_x^2 + u_y^2) + p u_x^2 u_y^2, \\
\tilde{\kappa}_{xxyy}^{eq} &= 2(c_s^4 \rho + c_s^2 \rho (u_x^2 + u_y^2) + p u_x^2 u_y^2),
\end{align*}
\]

which are obtained from the discrete representation of the local Maxwellian by transforming back their central moments at a given order to their corresponding raw moments. Here, $c_s$ is the speed of sound, and in the present work, we typically set $c_s^2 = 1/3$. Also, moments of the source terms $\tilde{\sigma}_{x\alpha y\beta}^{eq}$ follow as [19]

\[
\begin{align*}
\tilde{\sigma}_0' &= 0, \\
\tilde{\sigma}_x' &= F_u x, \\
\tilde{\sigma}_y' &= F_u y, \\
\tilde{\sigma}_{xx}' &= 2 F_u u_x, \\
\tilde{\sigma}_{yy}' &= 2 F_u u_y, \\
\tilde{\sigma}_{xy}' &= F_u u_x + F_u u_y, \\
\tilde{\sigma}_{xxy}' &= 2(F_u u_x u_y + F_u u_y u_x),
\end{align*}
\]

where $F = (F_x, F_y)$. The hydrodynamic fields are given by

\[
\begin{align*}
\rho &= \sum_{\alpha=0}^{8} \bar{f}_\alpha, \\
\rho u &= \sum_{\alpha=0}^{8} \bar{f}_\alpha e_\alpha + \frac{1}{2} F \delta_t, \\
p &= c_s^2 \rho.
\end{align*}
\]

The above represents the solution of the NSE (Eqs. (6.2) and (6.3)), with the kinematic bulk and shear viscosities related to the relaxation times via $\zeta = c_s^2 \left( \frac{1}{\omega_3} - \frac{1}{2} \right) \delta_t$ and $\nu = c_s^2 \left( \frac{1}{\omega_j} - \frac{1}{2} \right) \delta_t$, where $j = 4, 5$ respectively. The remaining relaxation times for the higher order moments, which influence the numerical stability, are set to unity in this work.

6.2.1 Moment relationships for the symmetric velocity gradient tensor: Chapman-Enskog Analysis

We will now perform a Chapman-Enskog analysis [207] to determine the expressions that relate the symmetric velocity gradient tensor to certain components of the local (non-equilibrium) mo-
ponents up to the second order are necessary, which read as (see Appendix E for details)

\[ \hat{\mathbf{m}} = \sum_{j=0}^{\infty} \epsilon^j \hat{\mathbf{m}}^{(j)}, \quad \partial_t = \sum_{j=0}^{\infty} \epsilon^j \partial_j, \]  

(6.18)

where \( \epsilon \) is a small bookkeeping perturbation parameter, and also performing a Taylor series expansion of the streaming operator in Eq. (6.14), i.e.,

\[ \hat{f}(\mathbf{x} + \epsilon \mathbf{c} \mathbf{e}_i, t + \epsilon) = \sum_{j=0}^{\infty} \epsilon^j (\partial_t + \epsilon \mathbf{c} \mathbf{e}_i \cdot \nabla)^j \hat{f}(\mathbf{x}, t). \]  

(6.19)

and converting all quantities in the velocity space to the moment space (via Eq. (6.10)) and using \( \hat{\mathbf{m}} = \hat{\mathbf{m}} - \frac{1}{2} \hat{\mathbf{S}} \partial_t \), we obtain the following system of moment equations at consecutive order in \( \epsilon \):

\[ O(\epsilon^0) : \quad \hat{\mathbf{m}}^{(0)} = \hat{\mathbf{m}}^{eq}, \]  

(6.20a)

\[ O(\epsilon^1) : \quad (\partial_{t_0} + \hat{\mathbf{E}} \partial_{\mathbf{c}}) \hat{\mathbf{m}}^{(0)} = -\hat{\mathbf{A}} \hat{\mathbf{m}}^{(1)} + \hat{\mathbf{S}}, \]  

(6.20b)

\[ O(\epsilon^2) : \quad \partial_{t_1} \hat{\mathbf{m}}^{(0)} + (\partial_{t_0} + \hat{\mathbf{E}} \partial_{\mathbf{c}}) \left[ \mathbf{I} - \frac{1}{2} \hat{\mathbf{A}} \right] \hat{\mathbf{m}}^{(1)} = -\hat{\mathbf{A}} \hat{\mathbf{m}}^{(2)}, \]  

(6.20c)

where \( \hat{\mathbf{E}}_i = \mathbf{T}(\mathbf{e}_i) \mathbf{T}^{-1}, i \in \{x, y\} \). In order to obtain the hydrodynamic macroscopic equations, in the \( O(\epsilon) \) system (see Eq. (6.20b)), the equations representing the evolution of the moment components up to the second order are necessary, which read as (see Appendix E for details)

\[ \partial_{t_0} \rho + \partial_x (\rho u_x) + \partial_y (\rho u_y) = 0, \]  

(6.21a)

\[ \partial_{t_0} (\rho u_x) + \partial_x (c_s^2 \rho + \rho u_x^2) + \partial_y (\rho u_x u_y) = F_x, \]  

(6.21b)

\[ \partial_{t_0} (\rho u_y) + \partial_x (\rho u_x u_y) + \partial_y (c_s^2 \rho + \rho u_y^2) = F_y, \]  

(6.21c)

\[ \partial_{t_0} (2c_s^2 \rho + \rho (u_x^2 + u_y^2)) + \partial_x [(1 + c_s^2) \rho u_x + \rho u_x u_y^2] + \partial_y [(1 + c_s^2) \rho u_y + \rho u_x^2 u_y] \]
\[ = -\omega_3 \hat{m}_3^{(1)} + 2(F_x u_x + F_y u_y), \]  

(6.21d)

\[ \partial_{t_0} (\rho (u_x^2 - u_y^2)) + \partial_x [(1 - c_s^2) \rho u_x - \rho u_x u_y^2] + \partial_y [(-1 + c_s^2) \rho u_y + \rho u_x^2 u_y] \]
\[ = -\omega_4 \hat{m}_4^{(1)} + 2(F_x u_x - F_y u_y), \]  

(6.21e)

\[ \partial_{t_0} (\rho u_x u_y) + \partial_x (c_s^2 \rho u_y + \rho u_x^2 u_y) + \partial_y (c_s^2 \rho u_x + \rho u_x^2 u_y) \]
\[ = -\omega_5 \hat{m}_5^{(1)} + F_x u_y + F_y u_x. \]  

(6.21f)
Analogously, at the $O(\epsilon)^2$ level (see Eq. (6.20c)), the relevant moment equations to recover the equations of the fluid motion written up to the first order as

\begin{align}
\partial_t \rho &= 0, \\
\partial_t (\rho u_x) + \partial_x \left[ \frac{1}{2} (1 - \frac{1}{2} \omega_3) \tilde{m}_3^{(1)} + \frac{1}{2} (1 - \frac{1}{2} \omega_4) \tilde{m}_4^{(1)} \right] + \partial_y \left[ (1 - \frac{1}{2} \omega_5) \tilde{m}_5^{(1)} \right] &= 0, \\
\partial_t (\rho u_y) + \partial_x \left[ (1 - \frac{1}{2} \omega_5) \tilde{m}_5^{(1)} \right] + \partial_y \left[ \frac{1}{2} (1 - \frac{1}{2} \omega_3) \tilde{m}_3^{(1)} - \frac{1}{2} (1 - \frac{1}{2} \omega_4) \tilde{m}_4^{(1)} \right] &= 0.
\end{align}

Here, the components of the second-order non-equilibrium moments $\tilde{m}_3^{(1)}$, $\tilde{m}_4^{(1)}$ and $\tilde{m}_5^{(1)}$ (which represent $\tilde{\kappa}_xx^{(1)} + \tilde{\kappa}_yy^{(1)}$, $\tilde{\kappa}_xx^{(1)} - \tilde{\kappa}_yy^{(1)}$ and $\tilde{\kappa}_xy^{(1)}$, respectively) are unknowns. They can be obtained from Eqs. (6.21d), (6.21e) and (6.21f), respectively, where the time derivatives $\partial_0 \left( 2c_s^2 \rho + \rho(u_x^2 + u_y^2) \right)$, $\partial_0 \left( \rho(u_x^2 - u_y^2) \right)$ and $\partial_0 (\rho u_x u_y)$ are eliminated in favor of the spatial derivatives using the leading order mass and momentum equations (i.e., Eqs. (6.21a)–(6.21c), respectively). For details, see e.g., Refs. [19, 68]. Neglecting all terms of $O(u^3)$ and higher, we can obtain the expressions for the various components of the non-equilibrium second order moments related to the symmetric part of the velocity gradient tensor $S_{ij} = \frac{1}{2} (\partial_j u_i + \partial_i u_j)$ (i.e., $\partial_x u_x$, $\partial_y u_y$ and $\partial_y u_x + \partial_x u_y$), which read as [19, 68]

\begin{align}
\tilde{m}_3^{(1)} &= \tilde{\kappa}_xx^{(1)} + \tilde{\kappa}_yy^{(1)} = - \frac{2c_s^2 \rho}{\omega_3} (\partial_x u_x + \partial_y u_y), \\
\tilde{m}_4^{(1)} &= \tilde{\kappa}_xx^{(1)} - \tilde{\kappa}_yy^{(1)} = - \frac{2c_s^2 \rho}{\omega_4} (\partial_x u_x - \partial_y u_y), \\
\tilde{m}_5^{(1)} &= \tilde{\kappa}_xy^{(1)} = - \frac{2c_s^2 \rho}{\omega_5} (\partial_x u_y + \partial_y u_x).
\end{align}

When these expressions are substituted in Eqs. (6.22b) and (6.22c), and then combining the $O(\epsilon)$ and $O(\epsilon^2)$ moment equations up to the first order, the NSE given Eqs. (6.2) and (6.3) follows. The non-equilibrium moment relations given in Eqs. (6.23a)–(6.23c) will be combined further with the developments given in the next section to develop a local computing approach for the vorticity field later in Sec. 6.4.
6.3 MRT-LBE for Transport of a Passive Scalar

The solution of the advection-diffusion of the passive scalar field \( \phi \) given by the CDE in Eq. (6.4) will now be represented by using another MRT-LBE. Considering the D2Q9 lattice again, which, as required, supports the off-diagonal third order moment equilibria independently as noted in the Introduction, we use the same natural moment basis given in Eq. (6.7) as well as the resulting transformation matrix \( \mathbf{T} \) (see Eq. (6.8)). First, we define the relation between the various raw moments and the corresponding distribution function \( g_\alpha \) and their equilibria \( g_{\alpha}^{eq} \) for this MRT-LBE as

\[
\hat{\mathbf{n}} = \mathbf{T} g, \quad \hat{\mathbf{n}}^{eq} = \mathbf{T} g^{eq},
\]

(6.24)

where

\[
g = (g_0, g_1, g_2 \ldots g_8)^\dagger, \quad g^{eq} = (g_0^{eq}, g_1^{eq}, g_2^{eq} \ldots g_8^{eq})^\dagger
\]

(6.25)

are given in the velocity space, and

\[
\hat{\mathbf{n}} = (\hat{n}_0, \hat{n}_1, \hat{n}_2 \ldots \hat{n}_8)^\dagger
\]

\[
= (\hat{\eta}_0, \hat{\eta}_1, \hat{\eta}_2 \ldots \hat{\eta}_8)^\dagger
\]

(6.26)

\[
\hat{\mathbf{n}}^{eq} = (\hat{n}_0^{eq}, \hat{n}_1^{eq}, \hat{n}_2^{eq} \ldots \hat{n}_8^{eq})^\dagger
\]

\[
= (\hat{\eta}_0^{eq}, \hat{\eta}_1^{eq}, \hat{\eta}_2^{eq} \ldots \hat{\eta}_8^{eq})^\dagger
\]

(6.27)

represent the equivalent states in the moment space. Here, the various sets of raw moments are defined as follows:

\[
\begin{pmatrix}
\hat{\eta}_{x^m y^n}^l \\
\hat{\eta}_{x^m y^n}^{eq}
\end{pmatrix}
= \sum_{\alpha=0}^{8} \begin{pmatrix}
g_\alpha \\
g_{\alpha}^{eq}
\end{pmatrix} e_{m}^{x} e_{n}^{y},
\]

(6.28)

Then the MRT-LBE using a non-orthogonal moment basis for the solution of the CDE can be written as

\[
g(x + e_\alpha \delta_t, t + \delta_t) - g(x, t) = -\mathbf{T}^{-1} [\hat{\mathbf{A}}(\hat{\mathbf{n}} - \hat{\mathbf{n}}^{eq})],
\]

(6.29)
where $\hat{\Lambda}^\phi$ is the diagonal relaxation time matrix given by

$$\hat{\Lambda}^\phi = \text{diag}(0, \omega_1^\phi, \omega_2^\phi, \omega_3^\phi, \omega_4^\phi, \omega_5^\phi, \omega_6^\phi, \omega_7^\phi, \omega_8^\phi, \omega_9^\phi, \omega_{10}^\phi, \omega_{11}^\phi, \omega_{12}^\phi)$$

A key element in this work is the prescription of the moment equilibria $\hat{n}^eq$ (Eq. (6.27)) used in Eq. (6.29) to enable a local computation of the antisymmetric velocity gradient tensor or the vorticity field. The passive scalar $\phi$ is advected by the local velocity field $u$, and hence its solution procedure, in principle, has a complete information on the kinematics of the fluid elements undergoing a variety of motion when it is carefully designed. As such, most of the components of the moment equilibria $\hat{n}^eq$ can be constructed in analogy with $\hat{m}^eq$ given in Eq. (6.15), where the density $\rho$ is replaced by the scalar field $\phi$. On the other hand, in view of the above consideration, in order to extract the local intrinsic rotation rate of the fluid element related to the antisymmetric velocity gradient tensor, we prescribe anisotropy in the scalar flux ($\phi u$) components used in the third order moment equilibria, which, as we shall see in the following, does not affect recovering of the macroscopic CDE. Thus, we set

$$\tilde{\eta}^eq_0 = \phi, \quad \tilde{\eta}^eq_x' = \phi u_x, \quad \tilde{\eta}^eq_y = \phi u_y,$$

$$\tilde{\eta}^eq_x' = c_{s\phi}^2 \phi + \phi u_x^2, \quad \tilde{\eta}^eq_y' = c_{s\phi}^2 \phi + \phi u_y^2, \quad \tilde{\eta}^eq_{xy} = \phi u_x u_y,$$

$$\tilde{\eta}^eq_{xx}' = \beta_1 c_{s\phi}^2 \phi u_y + \phi u_x^2 u_y, \quad \tilde{\eta}^eq_{yy}' = \beta_2 c_{s\phi}^2 \phi u_x + \phi u_y^2 u_x,$$

$$\tilde{\eta}^eq_{xxyy} = c_{s\phi}^4 \phi + c_{s\phi}^2 \phi(u_x^2 + u_y^2) + \phi u_x^2 u_y^2,$$

(6.31)

where $c_{s\phi}$ is an independent parameter related to the diffusivity $D_\phi$ (see below), and we typically set $c_{s\phi}^2 = 1/3$ in this work. Here, $\beta_1$ and $\beta_2$ are free parameters that prescribe anisotropy on the scalar flux appearing in the third order moment equilibria. Typically, $\beta_1 \approx 1$ and $\beta_2 \approx 1$, but $\beta_1 - \beta_2 \neq 0$, i.e., a small intentional anisotropy is introduced to locally recover the magnitude of the intrinsic rotation rate of the fluid motion (see the following section). The scalar field $\phi$ is then obtained as the zeroth moment of the distribution function $g_\alpha$, which evolves according to
Eq. (6.29) in the form of the standard collide-and-steam steps:

\[ \phi = \sum_{\alpha=0}^{8} g_{\alpha}. \]  

(6.32)

Then, the above represents the solution of the CDE (Eq. (6.4)), with the diffusivity related to the relaxation times via \( D_{\phi} = \frac{c_{s\phi}^2}{2} \left( \frac{1}{\omega_j} - \frac{1}{2} \right) \delta t \) where \( j = 1, 2 \).

6.3.1 Moment relationships for the scalar gradient vector and skew-symmetric velocity gradient tensor: Chapman-Enskog Analysis

We will now perform a C-E analysis of the MRT-LBE for the passive scalar field. Applying the moment expansion about its equilibria and a multiscale expansion of the time derivative to Eq. (6.29)

\[ \hat{n} = \sum_{j=0}^{\infty} \epsilon^j \hat{n}^{(j)}, \quad \partial_t = \sum_{j=0}^{\infty} \epsilon^j \partial_{tj}, \]  

(6.33)

where \( \epsilon = \delta t \) and also using a Taylor expansion of the streaming operator \( g_{\alpha}(x + e_{\alpha}\epsilon, t + \epsilon) = \sum_{j=0}^{\infty} \frac{\epsilon^j}{j!} (\partial_t + e_{\alpha} \cdot \nabla) g(x, t) \), the following moment equations at consecutive order in \( \epsilon \) can be obtained:

\[ O(\epsilon^0) : \quad \hat{n}^{(0)} = \hat{n}^{eq}, \]  

(6.34a)

\[ O(\epsilon^1) : \quad (\partial_{t0} + \hat{E}_i \partial_i) \hat{n}^{(0)} = -\hat{\Lambda} \phi \hat{n}^{(1)}, \]  

(6.34b)

\[ O(\epsilon^2) : \quad \partial_{t1} \hat{n}^{(0)} + (\partial_{t0} + \hat{E}_i \partial_i) \left[ I - \frac{1}{2} \hat{\Lambda} \phi \right] \hat{n}^{(1)} = -\hat{\Lambda} \phi \hat{n}^{(2)}, \]  

(6.34c)
where $\hat{\mathbf{E}}_i$ is the same as that given earlier. Some of the relevant components at the leading order (i.e., $O(\epsilon)$) of the moment system (see Eq. (6.34b)) are given as

$$\partial_t \phi + \partial_x (\phi u_x) + \partial_y (\phi u_y) = 0, \quad (6.35a)$$

$$\partial_t (\phi u_x) + \partial_x (c_{s\phi}^2 + \phi u_x^2) + \partial_y (\phi u_x u_y) = -\omega_1 \hat{n}_1^{(1)}, \quad (6.35b)$$

$$\partial_t (\phi u_y) + \partial_x (\phi u_x u_y) + \partial_y (c_{s\phi}^2 + \phi u_y^2) = -\omega_2 \hat{n}_2^{(1)}, \quad (6.35c)$$

$$\partial_t (2c_{s\phi}^2 + \phi (u_x^2 + u_y^2)) + \partial_x \left[(1 + \beta_2 c_{s\phi}^2) \phi u_x + \phi u_x u_y^2\right] + \partial_y \left[(1 + \beta_1 c_{s\phi}^2) \phi u_y + \phi u_x^2 u_y\right] = -\omega_3 \hat{n}_3^{(1)}, \quad (6.35d)$$

$$\partial_t (\phi (u_x^2 - u_y^2)) + \partial_x \left[(1 - \beta_2 c_{s\phi}^2) \phi u_x + \phi u_x u_y^2\right] + \partial_y \left[-(1 + \beta_1 c_{s\phi}^2) \phi u_y + \phi u_x^2 u_y\right] = -\omega_4 \hat{n}_4^{(1)}, \quad (6.35e)$$

$$\partial_t (\phi u_x u_y) + \partial_x \left[\beta_1 c_{s\phi}^2 \phi u_y + \phi u_x^2 u_y\right] + \partial_y \left[\beta_2 c_{s\phi}^2 \phi u_x + \phi u_x u_y^2\right] = -\omega_5 \hat{n}_5^{(1)}, \quad (6.35f)$$

where the above can be obtained by replacing $\hat{\kappa}_{x_m y_n}^{eq'}$ in the corresponding C-E analysis for the fluid motion with $\hat{\eta}_{x_m y_n}^{eq'}$ (see the previous section and for details) and allowing for the relaxation of the first order moments, since only the scalar field $\phi$ is conserved in the present case. Similarly, the leading component (i.e., the zeroth order) of the moment system at the $O(\epsilon^2)$ level to recover the CDE is obtained from Eqs. (6.34c) can be written as

$$\partial_t \phi + \partial_x \left[\left(1 - \frac{\omega_1^{\phi}}{2}\right) \hat{n}_1^{(1)}\right] + \partial_y \left[\left(1 - \frac{\omega_2^{\phi}}{2}\right) \hat{n}_2^{(1)}\right] = 0. \quad (6.36)$$

Now, in order to derive the CDE, we need to combine Eq. (6.35a) and $\epsilon$ times Eq. (6.36) by using $\partial_t = \partial_{t_0} + \epsilon \partial_{t_1}$, which requires $\hat{n}_1^{(1)}$ and $\hat{n}_2^{(1)}$. These first order non-equilibrium moments ($\hat{n}_1^{(1)}$ and $\hat{n}_2^{(1)}$) can be obtained from Eqs. (6.35b) and (6.35c), respectively, where the time derivatives are eliminated in favor of the spatial derivatives by using the leading order mass, momentum and scalar conservation equations (i.e., Eqs. (6.21a), (6.21b), (6.21c) and (6.35a)). Hence after some simplification, and neglecting terms of $O(u^2)$ and higher, we get the components of the first or-
der non-equilibrium moments in terms of the components of the scalar gradient vector \( \partial_i \phi \) as

\[
\begin{align*}
\hat{n}_1^{(1)} &= \hat{n}_x^{(1)}' = -\frac{1}{\omega_1^\phi} c_{s\phi}^2 \partial_x \phi, \\
\hat{n}_2^{(1)} &= \hat{n}_y^{(1)}' = -\frac{1}{\omega_2^\phi} c_{s\phi}^2 \partial_y \phi,
\end{align*}
\]

(6.37a) (6.37b)

It may be noted that in the derivation of these non-equilibrium moment components, only the spatial derivatives of the second order moment equilibria (i.e., \( \hat{\eta}_{eq}^{\prime \prime \prime} \), \( \hat{\eta}_{eq}^{\prime \prime} \) and \( \hat{\eta}_{eq}^{\prime} \)) are involved and do not involve the introduced anisotropy, which appears at a higher order level, i.e., for the third order moments of the equilibrium distribution via the factors \( \beta_1 \) and \( \beta_2 \) and hence the advection-diffusion of the passive scalar transport is correctly recovered.

As shown in the previous section, the symmetric components of the velocity gradient tensor \( \partial_x u_x, \partial_y u_y \) and \( \partial_x u_y + \partial_y u_x \) can be obtained from the MRT-LBE for fluid flow. In order to obtain the skew-symmetric component, i.e., \( \partial_x u_y - \partial_y u_x \), which would then provide a complete information about the velocity gradient tensor \( \partial_j u_i \) and hence the vorticity field, we now exploit the additional degree of freedom available in the off-diagonal, second-order non-equilibrium moment equation resulting from the MRT-LBE for CDE, i.e., Eq. (6.35f). Simplifying this equation by eliminating the time derivative in favor of spatial derivatives and eliminating higher order terms (i.e., \( O(u^2) \)) and above), we get

\[
\begin{align*}
\beta_1 c_{s\phi}^2 \partial_x (\phi u_y) + \beta_2 c_{s\phi}^2 \partial_y (\phi u_x) &= -\omega_5^\phi \hat{n}_5^{(1)},
\end{align*}
\]

(6.38)

which can be rewritten as

\[
\hat{n}_5^{(1)} = -\frac{c_{s\phi}^2}{\omega_5^\phi} \left[ \phi (\beta_1 \partial_x u_y + \beta_2 \partial_y u_x) + (\beta_1 u_y \partial_x \phi + \beta_2 u_x \partial_y \phi) \right].
\]

(6.39)

Clearly, the anisotropy introduced into the scalar flux components in the third order moment equilibria results in an additional flexibility via an independent equation given above (Eq. (6.39)). In this equation, the gradients of the scalar field in the Cartesian coordinate directions \( \partial_x \phi \) and \( \partial_y \phi \) can be obtained locally from Eq. (6.37a) and Eq. (6.37b); and with the knowledge of the off-diagonal second-order non-equilibrium moment component \( \hat{n}_5^{(1)} \), then Eq. (6.39) represents an ad-
ditional independent equation to compute the antisymmetric velocity gradient tensor component, which will be exploited further in the next section.

6.4 Derivation of local expressions for the complete velocity gradient tensor and vorticity field

In order to separately determine the cross-derivative components of the velocity gradient tensor, i.e., \( \partial_y u_x \) and \( \partial_x u_y \), we combine the analysis presented in the two earlier sections. In particular, the Eq. (6.23c) resulting from the solution of the MRT-LBE for fluid flow and Eq. (6.39) from the MRT-LBE for CDE, can be rewritten as

\[
\begin{align*}
\partial_x u_y + \partial_y u_x &= N_{xy}, \\
\beta_1 \partial_x u_y + \beta_2 \partial_y u_x &= N_{xy}^\phi,
\end{align*}
\]

where, when \( \phi \neq 0 \),

\[
\begin{align*}
N_{xy} &= -\frac{\omega_5}{\rho c_s^2} \hat{m}_3^{(1)} , \\
N_{xy}^\phi &= -\frac{\omega_5}{\rho c_s^2} \hat{n}_5^{(1)} - \frac{1}{\phi} (\beta_1 u_y \partial_x \phi + \beta_2 u_x \partial_y \phi).
\end{align*}
\]

Solving Eqs. (6.40a) and (6.40b), we get following independent and local expressions for the off-diagonal components or the cross derivatives of the velocity field, which is one of the main results of this work:

\[
\begin{align*}
\partial_x u_y &= \frac{N_{xy} - \beta_2 N_{xy}}{\beta_1 - \beta_2}, \\
\partial_y u_x &= \frac{\beta_1 N_{xy} - N_{xy}^\phi}{\beta_1 - \beta_2}.
\end{align*}
\]

The diagonal components of the velocity gradient tensor, i.e., \( \partial_x u_x \) and \( \partial_y u_y \) follow from solving the Eqs. (6.23a) and (6.23b) resulting from the MRT-LBE for the fluid motion, which reads as

\[
\begin{align*}
\partial_x u_x &= -\frac{1}{4c_s^2 \rho} \left[ \omega_3 \hat{m}_3^{(1)} + \omega_4 \hat{m}_4^{(1)} \right], \\
\partial_y u_y &= -\frac{1}{4c_s^2 \rho} \left[ \omega_3 \hat{m}_3^{(1)} - \omega_4 \hat{m}_4^{(1)} \right].
\end{align*}
\]
and this completes the determination of all the components of the velocity gradient tensor. Finally, a local expression for the pseudo-vector, viz., the vorticity field \( \omega = \nabla \times u = (0, 0, \omega_z) \) can be obtained by combining Eqs. (6.42a) and (6.42b) as

\[
\omega_z = \partial_x u_y - \partial_y u_x = \frac{2N_{xy}^\phi - (\beta_1 + \beta_2)N_{xy}}{(\beta_1 - \beta_2)},
\]

(6.44)

which is another key result arising from our analysis.

The terms \( N_{xy} \) and \( N_{xy}^\phi \) given in Eqs. (6.41a) and (6.41b), respectively, which are needed in Eqs. (6.42a), (6.42b) and (6.44) can be evaluated locally using

\[
\hat{m}_{5}^{(1)} = \hat{\kappa}_{xy}' - \hat{\kappa}_{xy}^{eq} = \hat{\kappa}_{xy} - \rho u_x u_y,
\]

(6.45a)

\[
\hat{n}_{5}^{(1)} = \hat{\eta}_{xy}' - \hat{\eta}_{xy}^{eq} = \hat{\eta}_{xy} - \phi u_x u_y,
\]

(6.45b)

and also since \( \hat{n}_1^{(1)} = \hat{\eta}_x - \hat{\eta}_x^{eq} = \hat{\eta}_x - \phi u_x \) and \( \hat{n}_2^{(1)} = \hat{\eta}_y - \hat{\eta}_y^{eq} = \hat{\eta}_y - \phi u_y \), and from Eqs. (6.37a) and (6.37b), we have the required local expressions for the derivatives of the scalar field, which read as

\[
\partial_x \phi = -\frac{\omega_1^\phi}{c_s^2} [\hat{\eta}_x - \phi u_x], \quad \partial_y \phi = -\frac{\omega_2^\phi}{c_s^2} [\hat{\eta}_y - \phi u_y]
\]

(6.46)

Note that \( \beta_1 \approx 1 \) and \( \beta_2 \approx 1 \), but \( \beta_1 \neq \beta_2 \) and are otherwise free parameters. We typically set \( \beta_1 = 1, \beta_2 = 0.9 \) in this work. In addition, the expressions for \( \hat{m}_3^{(1)} \) and \( \hat{m}_4^{(1)} \) needed in the diagonal components of the velocity gradient tensor, i.e., Eqs. (6.43a) and (6.43b) can be written as

\[
\hat{m}_3^{(1)} = (\hat{\kappa}_{xx}' + \hat{\kappa}_{yy}') - (2c_s^2 \rho + \rho (u_x^2 + u_y^2)), \quad (6.47a)
\]

\[
\hat{m}_4^{(1)} = (\hat{\kappa}_{xx}' - \hat{\kappa}_{yy}') - \rho (u_x^2 - u_y^2). \quad (6.47b)
\]

In the above, \( \hat{\kappa}_{xx}', \hat{\kappa}_{yy}', \hat{\kappa}_{xy}', \hat{\eta}_x', \hat{\eta}_y', \hat{\eta}_{xy}' \) are the raw moment components of different orders of the respective distribution functions. The formulation presented above thus allows local computation of the complete velocity gradient tensor and the vorticity field.
6.5 Results and discussion

In this section, we will perform a numerical validation study of the new DDF MRT-LB scheme for vorticity computation. In this regard, we will consider a set of well-defined benchmark flow problems for which the analytical solutions for the vorticity field are available or can be derived. In the simulations results presented in the following, the relaxation times for the second order moments of the MRT-LBE for the flow field \( \omega_4 = \omega_5 = 1/\tau \) are chosen to specify the desired fluid viscosity, while those for the first order moments of the MRT-LBE for the scalar field \( \omega_1^\phi = \omega_2^\phi = 1/\tau^\phi \) are prescribed to select the diffusivity. The relaxation times of all the higher order moments for both the LBEs are set to unity for simplicity. Unless otherwise specified, we consider the use of lattice units, i.e., \( \delta_x = \delta_t = 1.0 \) typical for LB simulations and a reference density of unity is considered in this work. For all the benchmark problems reported in what follows, we set the coefficients for the scalar flux terms in the third order moment equilibria of the MRT-LBE for the scalar field to \( \beta_1 = 1.0 \) and \( \beta_2 = 0.9 \).

6.5.1 Poiseuille flow

As the first benchmark problem, a steady flow between two parallel plates with a width \( 2L \) driven by a constant body force \( F_x \), i.e., the Poiseuille flow, is simulated. This flow problem has an analytical solution for the vorticity field as the linear profile \( \omega_z(y) = 2U_{max}y/L^2 \), which can be derived from the parabolic velocity profile \( u_x(y) = U_{max}[1 - \frac{y^2}{L^2}] \), where \( U_{max} = \frac{F_x L^2}{2 \nu \rho} \) is the maximum centerline velocity, \( \nu \) and \( \rho \) are fluid kinematic viscosity and density, respectively. Periodic boundary conditions are employed in the streamwise direction and no-slip condition for the velocity field are imposed using the half-way bounce back scheme. The computational domain is resolved using \( 3 \times 151 \) lattice nodes. For the scalar field, we consider fixed values at the bottom and top walls as \( \phi_L = 1.0 \) and \( \phi_H = 2.0 \), respectively, and its diffusivity is specified by choosing \( \tau^\phi = 0.57 \). At a fixed body force \( F_x = 3 \times 10^{-6} \), computations are carried by adjusting the fluid
kinematic viscosity such that the following five sets of maximum centerline velocities are considered: $U_{\text{max}} = 0.01, 0.03, 0.05,$ and $0.08$. Figure 6.1 shows a comparison between numerical results for the vorticity profiles obtained using the DDF MRT-LB scheme and the analytical solutions for the above set of values for $U_{\text{max}}$. Excellent agreement is seen.

FIGURE 6.1: Comparison of the computed profiles of the vorticity field and the analytical solution in a Poiseuille flow for different values of the centerline velocity $U_{\text{max}} = 0.01, 0.03, 0.05,$ and $0.08$ obtained by varying the fluid viscosity at a fixed body force $F_x = 3 \times 10^{-6}$. Here, the lines represent the analytical solution and symbols refer to the numerical results obtained by the present DDF MRT-LB scheme.

6.5.2 Four-rolls mill flow

In order to examine the validity of our approach for a flow problem with fully two-dimensional (2D) spatially varying distribution of the vorticity field, we consider next the four-rolls mill flow. It is a steady, rotational flow consisting of an array of counter-rotating vortices generated by the stirring action of a suitably specified local body force $F_x = F_x(x,y)$ and $F_y = F_y(x,y)$ in a periodic square domain of size $2\pi \times 2\pi$. It is a modified form of the Taylor-Green vortex flow. The spatially varying driving body force can be written as $F_x(x,y) = 2\rho_0 \nu u_0 \sin x \sin y$ and
\[ F_y(x, y) = 2\rho_0 \nu u_0 \cos x \cos y, \] where \( \rho_0 \) is the reference density, \( \nu \) is kinematic viscosity and \( u_0 \) is the velocity scale and \( 0 \leq x, y \leq 2\pi \). A solution of the simplified form of the Navier-Stokes equations with the above described body force yields the explicit form of the local velocity field, which reads as \( u_x(x, y) = u_0 \sin x \sin y \) and \( u_y(x, y) = u_0 \cos x \cos y \). Then, the analytical solution for the local vorticity field \( \omega_z(x, y) \) can be derived by taking the curl of the above velocity field, which can be written as

\[
\omega_z(x, y) = -2u_0 \sin x \cos y. \tag{6.48}
\]

For the purpose of setting up simulations, the Reynolds number for this flow problem can be defined as \( \text{Re} = u_0 2\pi/\nu \) and the viscosity can be written as \( \nu = \frac{1}{3}(\tau - \frac{1}{2})\Delta x \), where \( \Delta x = \Delta t = 2\pi/N \), where \( N \) is the number of grid nodes in each direction. We consider a grid resolution of \( 84 \times 84 \) and a velocity scale \( u_0 = 0.035 \) to simulate four-rolls mill flow at \( \text{Re} = 40 \). The scalar field is initialized to a uniform value of 2.0 in this periodic domain with the relaxation time \( \tau^{\phi} = 0.57 \).

Figure 6.2 presents a comparison between the spatial distribution of the computed vorticity field obtained using the DDF MRT-LB scheme and the analytical solution. Due to the presence of a system of counter-rotating vortices, the vorticity field, represented by harmonic functions analytically, dramatically varies both in its magnitude and sign. Good agreement between the two results are evident. Furthermore, in order to make a more head-on comparison, Fig. 6.3 shows the computed vorticity profiles \( \omega_z(x, y) \) computed using our LB scheme along various horizontal sections at \( y = 0, \pi/4, \pi/2, \pi, 5\pi/4 \) along with results based on the analytical solution. It is evident that there is a very good agreement between our numerical results and the analytical solution.

Grid convergence study

We will now assess the order of accuracy of the convergence of the vorticity computation via our DDF MRT-LB scheme. In this regard, at a fixed viscosity of \( \nu = 0.00218 \) with a velocity scale \( u_0 = 0.045 \), we consider the following sequence of four different resolutions: \( 24 \times 24, 48 \times 48, \ldots \).
FIGURE 6.2: Comparison of the spatial distribution of the computed vorticity field with the analytical solution in a four-rolls mill flow within a square domain of size $2\pi \times 2\pi$ for $Re = 40$. The surface plot on the left corresponds to the numerical results obtained by the present DDF MRT-LB scheme and that on the right is based on the analytical solution.

FIGURE 6.3: Comparison of computed profiles of the vorticity field and the analytical solution in a four-rolls mill flow along various horizontal sections at $y = 0, \pi/4, \pi/2, \pi, 5\pi/4$. Here, the lines represent the analytical solution and symbols refer to the numerical results obtained by the present DDF MRT-LB scheme.
96x96 and 192x192. For each case, we measure the following global relative error \(E_{g,\omega}\) between the vorticity field computed using the DDF MRT-LB scheme given by \(\omega_c\) and the corresponding analytical solution denoted by \(\omega_a\):

\[
E_{g,\omega} = \sqrt{\frac{\Sigma (\omega_c - \omega_a)^2}{\Sigma (\omega_a)^2}},
\]

where the summations in the above are for the whole computational domain. The rate of convergence of the global relative error is depicted using a log-log scale in Fig. 6.4. From this figure, it can be seen that the relative error exhibits a slope of -2.0, which demonstrates that the vorticity computation using our approach is second order accurate.

6.5.3 Womersley flow

In order to validate our approach for the calculation of the vorticity field in unsteady flows, a 2D pulsatile flow between two parallel plates separated by a width \(2L\) driven by a sinusoidally time-dependent body force \(F_x(t)\) is considered. This classical Womersley flow problem is subjected to a periodic body force given by \(F_x = F_m \cos(\Omega t)\), where \(F_m\) is the maximum amplitude of the force and \(\Omega = 2\pi/T\) is the angular frequency and \(T\) being the time period. Considering that this pulsatile flow is laminar and incompressible, the analytical solution for velocity field is given as [208]

\[
u(y,t) = R\{i\frac{F_m}{\Omega} \left[ 1 - \frac{\cos(\gamma y/L)}{\cos \gamma} \right] e^{i\Omega t}\},
\]

where \(\gamma = \sqrt{iWo^2}\) and \(Wo = L\sqrt{(\Omega/\nu)}\) is the Womersley number. Here, and in the following \(R\{\cdot\}\) refers to the real part of the expression. Then, the analytical solution for the local time-dependent vorticity field \(\omega_z(y,t)\) can be readily obtained by taking the curl of the velocity field as

\[
\omega_z(y,t) = R\left\{ i\frac{F_m}{\mu L} \left[ \frac{\sin(\gamma y/L)}{\cos \gamma} \right] e^{i\mu t} \right\}.
\]

We consider a grid resolution of \(3 \times 101\), maximum force amplitude \(F_m = 1.0 \times 10^{-5}\) with a time period \(T = 10,000\) and two different values of the Womersley number, i.e., \(Wo = 4.0\) and
FIGURE 6.4: Evaluation of the order of accuracy of the present DDF MRT-LB scheme for vorticity computation in the four-rolls mill flow problem with a constant kinematic viscosity $\nu = 0.00218$ at different grid resolutions.
Wo = 7.0, which are specified by setting the relaxation times for the MRT-LBE for the flow field to be $\tau = 0.781$ and $\tau = 0.596$, respectively. Periodic boundary conditions and the no-slip boundary conditions are considered for the inlet/outlet in the streamwise direction and along the two parallel walls, respectively. The parameters and the boundary conditions for the scalar field are the same as those considered for the Poiseuille flow simulations discussed earlier. Figure 6.5 presents a comparison between the computed vorticity profiles obtained using the DDF MRT-LB scheme and the corresponding analytical solution at different time instants within a time period $T$. It is evident that the vorticity field is subjected to strong temporal and spatial variations, which are very well reproduced quantitatively by our local computational approach.

FIGURE 6.5: Comparison of computed profiles of the vorticity field and the analytical solution in a pulsatile flow in a channel (i.e., Womersley flow) at different instants within a time period for two different Womersley numbers of Wo = 4.0 and Wo = 7.0. Here, lines represent the analytical solution and the symbols refer to the numerical results obtained using the present DDF MRT-LB scheme.

6.6 Summary and Conclusions

A quantitative knowledge of the local skew-symmetric velocity gradient tensor, or equivalently the vorticity field, in conjunction with the symmetric velocity gradient tensor, in flow simulation methods is crucial for various applications, including those related to techniques for the identification of flow structures and in the modeling of complex fluids. In many situations, it is required to compute the fluid motion coupled to the transport by advection and diffusion of a
scalar field. In the mesoscopic LB methods, the hydrodynamics (i.e., the NSE) and the scalar transport (i.e., the CDE) are commonly computed via the evolution of a pair of distribution functions represented by means of two LBEs. In such double distribution functions (DDF) based LB approaches, we present a new strategy for computing the vorticity field locally via exploiting the additional degrees of freedom available in the construction of the higher order moment equilibria in the collision model for the representation of the scalar transport to obtain the necessary additional independent relations. In particular, we have shown that this can be achieved by introducing an intensional anisotropy in the scalar flux components in the third order, off-diagonal moment equilibria, and then combining the second-order, off-diagonal non-equilibrium moment components of both the LBEs. This approach for local vorticity computation has several advantages, which include the following. Any pair of lattice sets in the DDF-LBEs that support the third order off diagonal moments independently, which includes the various standard lattice velocity models in different dimensions, can allow a local determination of the complete flow kinematics, including the skew-symmetric velocity gradient tensor. It imposes no additional constraints on the higher order equilibrium moments of the LBE for the flow field, which can be solved by using any standard formulation without modification thereby maintaining its numerical characteristics intact. Since the vorticity computation are based on distribution functions, which are generally solved to be second order accurate, the resulting mesoscopic and local computation of vorticity and the strain rate tensor are second order accurate as well. The presented strategy is general and is applicable for a variety of collision models.

In the present work, for the purpose of illustration, we specialize our approach by constructing a DDF formulation using a MRT-LBE for the solution of the fluid motion and another MRT-LBE involving an anisotropy in the scalar flux components in the third order equilibria for the transport of a scalar field, each on a D2Q9 lattice. By means of a Chapman-Enskog analysis, we have shown that the former provides the necessary second order non-equilibrium moment equations to determine the symmetric velocity gradient tensor, while the latter yields additional correspond-
ing moment relations to obtain the skew-symmetric velocity gradient tensor. For simplicity, the MRT-LBEs are constructed using natural, non-orthogonal moment bases. In order to validate our new approach, we have presented comparisons of the computed vorticity fields against the analytical solutions for various benchmark problems such as the steady flow in a channel, four-rolls mill flow and the pulsatile (Womersley) flow in a channel, which demonstrate its good accuracy. In addition, an analysis of the method for various grid resolutions establishes its second order convergence for computing vorticity. The DDF-LB approach for local vorticity computation, while specialized here for the D2Q9 model, can be extended in 3D for various lattice sets (i.e., D3Q15, D3Q19 and D3Q27).
CHAPTER VII

CASCADED LATTICE BOLTZMANN METHOD FOR PHASE-FIELD MODELING OF INCOMPRESSIBLE MULTIPHASE FLOWS

7.1 Introduction

Multiphase flows arise in a number of technological and scientific applications, including in chemical and petroleum processing and power generation systems as well as microfluidic devices, and are common in nature. Such flows, whose prototypical configuration involves a continuous fluid phase and a dispersed phase, such as bubbles or droplets, are characterized by surface tension along interfaces and phase segregation effects [209]. Simulation of multiphase flows are challenging due to the simultaneous capturing or tracking of interfacial motion and the computation of fluid motion, which are generally nonlinear and can occur at multiple scales. There are various interface capturing approaches that are used in conjunction with the direct discretization of the Navier-Stokes equations (NSE), which include the volume-of-fluid method [210], front tracking method [211] and the level set method [212].

During the last two decades, the lattice Boltzmann (LB) methods based on kinetic formulations that represent the evolution of particle distribution functions have emerged as a promising addition to the techniques available for computational fluid dynamics [126, 10, 24, 11, 18]. Significant interest in such methods are largely due to the locality of their the stream-and-collide algorithm and ease of implementation of boundary conditions based on kinetic approaches on Cartesian grids. For simulation of multiphase flows, the LB methods have been further extended to incorporate various models and techniques to represent interfacial dynamics and fluid motion. Among them, some of the early approaches represented the phase segregation and the effect of surface tension via either a color model [213, 214], a pseudopotential formulation [215] or a free-energy
based formulation [216] and their thermodynamic consistency were analyzed in [70, 217, 94]. A significantly improved LB method using a kinetic theory based mean field model was presented in [22], which allowed accurate simulation of multiphase flows at moderate density ratios. This approach used one LB scheme for the fluid motion and captured the interfacial motion via an index function, whose evolution was represented by another LB scheme where the phase segregation was achieved using a Carnahan-Starling nonideal equation of state. This was further improved for simulation of two-phase flows at high density ratios by means of a stable discretization scheme [218]. The latter work motivated developments of consistent LB techniques for interfacial capturing techniques based on phase field models.

Phase field models represent interfaces to be diffuse, which comprise thin transitional regions of nonzero thickness across which various fluid properties vary continuously from one phase to the other [219, 220, 221, 222]. Such diffuse interface methods capture interfacial motion implicitly via the evolution of an order parameter, which serves as a phase field to distinguish between different fluid phases. The dynamics of the order parameter is often based on a thermodynamic free energy functional formulation, of which the Cahn-Hilliard equation (CHE) [223] is a common choice. A LB scheme to represent the convective CHE was presented in [224], which was shown to be applicable only for density-matched two-fluid systems in [225], who then proposed a modification to handle multiphase flows at moderate density ratios. The latter work was further improved in the investigations presented in [226, 227] to represent incompressible multiphase flows based on modified CHE for capturing of interfaces.

The challenges associated with the use of CHE, such as the need to calculate fourth order derivatives, motivated other phase field type approaches. The Allen-Cahn equation (ACE) is another type of diffuse interface model used that was originally developed for material science applications [228]. More recently, the ACE was reformulated based on a counter term approach [229] to eliminate curvature driven interfacial motion in order to make it applicable for two-phase flows [230], in which the geometric information such as the interface normal and curvature are computed
readily by expressing them in terms of a hyperbolic tangent variation of the order parameter across the interface. Then, Ref. [231] further modified the ACE to make it mass conservative, which was shown to be equivalent to a conservative level set approach [232]. Such a conservative ACE results in a simpler formulation with less numerical dispersion than the modified CHE, as the former requires the computation of only lower, i.e., second, order derivatives of the phase field variable when compared to the latter as noted above. Based on such conservative ACE, LB schemes for interface capturing were developed in [233, 234].

The collision step plays an important role in the LB method especially for the solution of the fluid motion. The single relaxation time (SRT) model to represent the change in the distribution functions due to collision is a common approach [67]. However, it is known to be susceptible to numerical instability issues at relatively low values of the transport coefficients or at higher Reynolds number. This can be overcome to a significant extent by considering the relaxation of various raw moments to their equilibria using multiple relaxation times (MRT) to represent the effect of collisions [14]. A further improvement can be achieved by considering the relaxation in terms of central moments [15]. It naturally maintains the Galilean invariance of all independent moments supported by a chosen lattice and the resulting method was termed as the cascaded LB method. The method was interpreted by considering relaxation in terms of a generalized equilibrium in a rest frame of reference [20]. A scheme based on central moments to incorporate local forces and its consistency to the Navier-Stokes equations (NSE) via a Chapman-Enskog analysis was presented in [19]. Significant improvements in the numerical stability of the cascaded LB method were shown in [43, 17]. More recently, various refinements and extensions of the central moments based LB formulation were considered (see e.g., [158, 162, 205, 160, 33, 206]).

In this contribution, we present new unified cascaded LB methods for incompressible two-phase flows at high density ratios. In our formulation, one cascaded LB scheme for the solution of the multiphase fluid motion and another cascaded LB scheme for the representation of interface capturing will be developed. For the former case, the starting point is the modified continuous Boltz-
mann equation (MCBE) for incompressible two-phase flows [22], where a transformation to the
distribution function is introduced to reduce the numerical stiffness associated with high density
gradients and the resulting hydrodynamic variables are given in terms of the pressure and velocity
fields via their zeroth and first moments, respectively. Based on this MCBE, a new discrete
cascaded LB method based on central moments and multiple relaxation times for two-phase fluid
flow will be constructed. In this regard, we will formulate its collision step in terms of relaxation
to various central moment equilibria which will be expressed by matching the central moments of
the modified continuous Maxwell distribution and given in terms of the pressure field arising via
the transformation mentioned above. The MCBE [22] also contains source terms related to the
pressure changes and those due to the interfacial (surface tension) force and a body force, whose
respective effects on the changes in various moments are different. In order to account for the dif-
fferential effects of the source term due to pressure and that due to the interfacial and body forces
for handling the simulation of two-phase flows, we will present a consistent source/force treat-
ment scheme, which is an extension of and modification to the central moment based approach
that was given in a previous work for single phase flows [19]. The interfacial dynamics will be
captured using the conservative ACE phase field formulation that evolves interfaces via advection
and under the competing effects of a diffusion term and an interface sharpening term. In this
regard, by extending the work of Ref. [233], another MRT based modified cascaded LB scheme
developed for the solution of the convection diffusion equation [205, 33], where the sharpening
term due to the phase separation flux is introduced as a modification to the moment equilib-
ria, will be constructed to represent the evolution of the phase field variable. All fluid properties
such as the density and viscosities across the phase interfaces are then expressed as smooth affine
functions of the phase field variable. Since the resulting cascaded LB solvers are based on pre-
scribing collision and sources via matching their continuous values in a moving of reference based
on local fluid velocity, it naturally maintains their Galilean invariance for the independent mo-
mements supported by the chosen lattice. They can improve numerical stability for the simulation
of two-phase flows at high density ratios and at relatively low fluid viscosities, thereby widening
the parametric ranges for simulations. In this work, the cascaded central moment LB formulation for the coupled solution of the two-phase flow and interfacial motion will be presented on two-dimensional, nine velocity (D2Q9) lattice sets, which will then be validated for a set of numerical benchmark problems to demonstrate its accuracy and improvements in stability.

This chapter is organized as follows. In Sec. 7.2, we will present the governing equations for the incompressible two-phase flow and the phase field model based on the conservative ACE for the capturing of interfaces. Section 7.3 discusses the discrete velocity Boltzmann equation for two-phase flows that represents the starting point for the construction of the central moments based kinetic formulation for its solution procedure. Then, the cascaded LB method for the solution of the two-phase flow in terms of the pressure and velocity fields is derived in Sec. 7.4. Subsequently, Sec. 7.5 presents another cascaded LB method for interfacial dynamics based on the conservative ACE. Section 7.6 discusses the numerical validation study of the new cascaded LB formulation for a variety of two-phase flow benchmark problems. A comparison of numerical stability different collision models is presented in Sec. 7.7. Finally, the conclusions of this work are summarized in Sec. 7.8. An extension for phase-field modeling of surfactant-Laden multiphase flows using a cascaded LB approach is presented in Appendix F.

7.2 Governing Macroscopic Equations: Interface Capturing and Two-Phase Fluid Motion

In order to capture the interfacial dynamics, we consider a phase field method based on the conservative Allen-Cahn equation (ACE). This was originally formulated for two-phase flows by removing the curvature-driven motion [230] via a counter term approach [229] and then re-expressed in a conservative form [231]. Let \( \phi \) be an order parameter or the phase field variable, with \( \phi = \phi_A \) representing the fluid in phase \( A \) and \( \phi = \phi_B \) denoting that in phase \( B \). Then, the interface propagation given in terms of the phase field variable based on the conservative ACE can be
written as
\[ \frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = \nabla \cdot [M_\phi (\nabla \phi - \theta \mathbf{n})], \] (7.1)
where \( \mathbf{u} \) is the fluid velocity, \( \mathbf{n} \) is the unit normal vector, which can be computed via the order parameter \( \phi \) as \( \mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|} \), and \( M_\phi \) is the mobility. In the above, the variable \( \theta \) can be expressed as
\[ \theta = \frac{-4(\phi - \phi_A)(\phi - \phi_B)}{W(\phi_A - \phi_B)}, \] (7.2)
where the parameter \( W \) is related to the width of the interface. The right hand side of Eq. (7.1) is obtained by removing the curvature-driven interface motion \( u_\kappa \mathbf{n} = -M_\kappa \kappa \mathbf{n} \) by canceling it out by adding a counteracting term based on computing the curvature \( \kappa_m \), where \( \kappa_m = \nabla \cdot \mathbf{n} \) with \( \mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|} \), directly in terms of a kernel function given by the following hyperbolic tangent profile of the order parameter
\[ \phi(\zeta) = \frac{1}{2}(\phi_A + \phi_B) + \frac{1}{2}(\phi_A - \phi_B) \tanh \left( \frac{2\zeta}{W} \right), \] (7.3)
which represents the equilibrium profile of the phase field variable, where \( \zeta \) is a spatial coordinate along the normal with the origin at the interface. Thus, Eq. (7.1) effectively represents the relaxation of any arbitrary initial distribution of the order parameter to a hyperbolic tangent profile across the interface, which is then sustained during interfacial advection. Equivalently, this equation can be interpreted as the interface propagating via advection (given by its LHS) under the competing effects of a diffusion term and an interface sharpening term or a separation flux term (given by the first and second terms on the RHS, respectively). In the above, \( W \) and \( M_\phi \) are numerical parameters, with \( W \) representing the interface thickness, while \( M_\phi \) controlling the relaxation rate of any initial \( \phi \) to its equilibrium profile across the interfaces (Eq. (7.3)) as well as the dissipation of any interface singularities via diffusion.

On the other hand, the two-phase fluid flow is represented by the following incompressible Navier-
Stokes equations (NSE):

\[ \nabla \cdot \mathbf{u} = 0, \quad (7.4) \]

\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) \right) = -\nabla p + \nabla \cdot \left[ \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^\intercal) \right] + \mathbf{F}_s + \mathbf{F}_{\text{ext}}, \quad (7.5) \]

where \( p \) is the hydrodynamic pressure, \( \rho \) is the fluid density, \( \mu \) is its viscosity, \( \mathbf{F}_s \) is the smoothed formulation of the surface tension force and \( \mathbf{F}_{\text{ext}} \) is an external body force (e.g., gravity).

In the above, there are several ways to express the surface tension force \( \mathbf{F}_s \) as a smoothed representation based on the order parameter. One approach is based on a thermodynamic (Gibbs-Duhem) formulation in which the surface tension force is calculated from the negative product of the gradient of the chemical potential \( \tilde{\mu}_\phi \) and the phase field variable \( \phi \) as follows (see e.g., [220]):

\[ \mathbf{F}_s = -\phi \nabla \tilde{\mu}_\phi, \quad \tilde{\mu}_\phi = 4\beta (\phi - \phi_A)(\phi - \phi_B) (\phi - (\phi_A + \phi_B)/2) - \kappa \nabla^2 \phi. \quad (7.6) \]

Here, the parameters \( \beta \) and \( \kappa \) are used to control the surface tension \( \sigma \) and the interface thickness \( W \) via the following relations

\[ \kappa = \frac{3}{2} \sigma W, \quad \beta = \frac{12 \sigma}{W}. \quad (7.7) \]

Additionally, geometric approaches such as the continuous surface force formulation can be considered [235]. In particular, a geometric approach for the surface tension force developed originally for level set methods and adapted for phase field methods [236] can be written as

\[ \mathbf{F}_s = -\tilde{\kappa} |\nabla \phi|^2 (\nabla \cdot \mathbf{n}) \mathbf{n}. \quad (7.8) \]

Here, the parameter \( \tilde{\kappa} \) is related to the surface tension \( \sigma \) via \( \tilde{\kappa} = \gamma \sigma W \), where the coefficient \( \gamma \) satisfies \( \gamma \int_{-\infty}^{\infty} (d\phi/d\zeta)^2 d\zeta = 1 \), which arises from interpreting the surface tension in terms of interfacial energy per unit surface area by considering the equilibrium phase field variable profile given in Eq. (7.3) and matching it with the sharp interface limit for a flat interface [236]. In this work, this latter (geometric) approach is adopted for representing the surface tension force \( \mathbf{F}_s \) for performing two-phase flow simulations using cascaded LB formulations discussed in what follows. Finally, the jumps in fluid properties such as the density and viscosity across the interface
are smoothed as well and can be written as a continuous function of the phase field variable $\phi$ and then used in Eq. (7.5) in different ways. In this study, we employ a linear interpolation for representing the interfacial variations of the fluid properties (see e.g., [221]). Thus,

$$\rho = \rho_B + \frac{\phi - \phi_A}{\phi_A - \phi_B} (\rho_A - \rho_B), \quad \mu = \mu_B + \frac{\phi - \phi_A}{\phi_A - \phi_B} (\mu_A - \mu_B),$$

(7.9)

where $\rho_A$ and $\rho_B$ are the densities and $\mu_A$ and $\mu_B$ are the dynamic viscosities in the fluid phases denoted by $\phi_A$ and $\phi_B$, respectively. In this work, we consider $\phi_B = 0$ and $\phi_A = 1$.

### 7.3 Modified Continuous Boltzmann Equation for Two-Phase Flows and Central Moments of Equilibria and Sources

To solve the incompressible Navier-Stokes equations (NSE) for two-phase flows (Eqs. (7.4) and (7.5)) in a kinetic formulation, the starting point is the two-dimensional (2D) continuous Boltzmann equation given by [22]

$$\frac{Df}{Dt} \equiv \frac{\partial f}{\partial t} + \xi \cdot \nabla f = -\frac{1}{\tau} (f - f^M) + \frac{(\xi - u)}{\rho c_s^2} \cdot (F_t - \nabla \psi) f^M,$$

(7.10)

where $f = f(x,t;\xi)$ is the density distribution function at a location $x$ and at time $t$, corresponding to the particle velocity $\xi = (\xi_x, \xi_y)$. Here, $f^M$ is the local Maxwell distribution function defined as

$$f^M \equiv f^M(\rho, u) = \frac{\rho}{2\pi c_s^2} \exp \left[ -\frac{(\xi - u)^2}{2c_s^2} \right],$$

(7.11)

where $c_s$ is the speed of sound and fluid velocity $u = (u_x, u_y)$. The effect of collisions is typically represented as a relaxation of $f$ to its equilibrium, i.e., $f^M$ with a characteristic time scale $\tau$. The continuous formulation of the interfacial tension force $F_s$, which is discussed in the previous section, along with any local body force $F_{ext}$ are grouped as the total force $F_t = F_s + F_{ext}$.

This total force along with the gradient contribution of the net effect of the hydrodynamic pressure $p$ relative to that from the ideal equation of state $\rho c_s^2$, i.e., $\psi(\rho) = p - \rho c_s^2$ are accounted for via a source term in Eq. (7.10). In general, multiphase flows can be associated with relatively
large jumps in fluid properties across the interfaces. In particular, as the density gradients $\nabla \rho$ or $\nabla \psi$ become relatively large, Eq. (7.10) becomes numerically stiff.

To alleviate such numerical stiffness, the following kinetic transformation to the distribution can be introduced [22]

$$g = f c_s^2 + (p - \rho c_s^2) \frac{f^M(\rho, \mathbf{0})}{\rho},$$  \hspace{1cm} (7.12)

where $g$ can be regarded as the pressure distribution function. Here, $f^M(\rho, \mathbf{0})$ is the local Maxwellian with null macroscopic fluid velocity, which follows from Eq. (7.11) as

$$f^M(\rho, \mathbf{0}) = \frac{\rho}{2 \pi c_s^2} \exp \left[ - \frac{\xi^2}{2 c_s^2} \right].$$  \hspace{1cm} (7.13)

Then, by applying the above transformation (Eq. (7.12)) to the continuous Boltzmann equation (Eq. (7.10)) and assuming two-phase flows in the incompressible limit, i.e., $|\mathbf{u}| \ll 1$, the following kinetic equation for the distribution function $g$ can be obtained [22]

$$\frac{Dg}{Dt} = -\frac{1}{\tau} (g - g^{eq}) + (\xi - \mathbf{u}) \cdot \mathbf{F}_t \frac{f^M(\rho, \mathbf{u})}{\rho} + (\xi - \mathbf{u}) \cdot \mathbf{F}_p \left\{ \frac{f^M(\rho, \mathbf{u})}{\rho} - \frac{f^M(\rho, \mathbf{0})}{\rho} \right\} \text{O}(\mathbf{u}),$$  \hspace{1cm} (7.14)

which is referred to as the modified continuous Boltzmann equation (MCBE) in this work. In Eq. (7.14), $g^{eq}$ is the transformed local Maxwellian or the modified equilibrium distribution function, which reads as

$$g^{eq} = c_s^2 f^M(\rho, \mathbf{u}) + (p - \rho c_s^2) \frac{f^M(\rho, \mathbf{0})}{\rho}$$  \hspace{1cm} (7.15)

and $\mathbf{F}_p$ is the net effect of the hydrodynamic pressure $p$ relative to the contribution from the ideal equation of state dependent on density, which is referred as the net gradient pressure force, and can be expressed as

$$\mathbf{F}_p = -\nabla (p - \rho c_s^2) \equiv -\nabla \psi.$$  \hspace{1cm} (7.16)

In the MCBE (Eq. (7.14)), even though $\mathbf{F}_p$ can be large at high density ratios, since it is multiplied by $\left\{ \frac{f^M(\rho, \mathbf{u})}{\rho} - \frac{f^M(\rho, \mathbf{0})}{\rho} \right\}$, which is $O(\mathbf{u})$ and small, the associated numerical stiffness issues
on the evolution of the distribution function $g$ is reduced significantly. Hence, the MCBE serves as the starting point in the construction of a discrete kinetic scheme for the solution of the incompressible two-phase flows with high phase density contrasts. The hydrodynamic pressure and velocity fields are then obtained as the zeroth and first kinetic moments of the distribution function $g$, respectively. That is,

$$p = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g \xi_d d\xi_y, \quad \rho c_s^2 u = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g \xi_d d\xi_y.$$  \tag{7.17}

### 7.3.1 Continuous Central Moments of Equilibria and Sources of MCBE

As a prelude to constructing a cascaded LB scheme from the discretization of the MCBE, which is discussed in the next section, we will first need the continuous central moments of its equilibria and various sources. They are based on the contributions from the corresponding continuous Maxwell distribution function evaluated with and without the macroscopic fluid velocity in view of the kinetic transformation introduced above.

First, defining the continuous central moments of the local Maxwellian for a moving fluid, i.e., with the macroscopic fluid velocity, of order $(m + n)$ as

$$\hat{\Pi}^M_{mn} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f^M(\rho, u)(\xi_x - u_x)^m(\xi_y - u_y)^n d\xi_x d\xi_y,$$  \tag{7.18}

and then defining the continuous central moments of the local Maxwellian with the null macroscopic fluid velocity of order $(m + n)$ as

$$\hat{\Pi}^M(0)_{mn} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f^M(\rho, 0)(\xi_x - u_x)^m(\xi_y - u_y)^n d\xi_x d\xi_y.$$  \tag{7.19}

The definite integrals given in Eqs. (7.18) and (7.19) can be evaluated exactly via standard quadrature rules. The D2Q9 lattice used in the construction of the cascaded LB scheme based on a matching principle in the next section supports nine independent moment components. In this regard, we will need the corresponding components of $\hat{\Pi}^M_{mn}$ and $\hat{\Pi}^M(0)_{mn}$ as intermediate results.
Thus, calculating the components of the continuous central moments of the Maxwellian \( \hat{\Pi}_{mn}^M \) (Eq. (7.18)) at various orders, which reads as

\[
\hat{\Pi}_{00}^M = \rho, \quad \hat{\Pi}_{10}^M = 0, \quad \hat{\Pi}_{01}^M = 0, \quad \hat{\Pi}_{20}^M = \rho c_s^2, \quad \hat{\Pi}_{02}^M = \rho c_s^2, \quad \hat{\Pi}_{11}^M = 0, \quad \hat{\Pi}_{21}^M = 0, \quad \hat{\Pi}_{12}^M = 0, \quad \hat{\Pi}_{22}^M = \rho c_s^4. \tag{7.20}
\]

and those of \( \hat{\Pi}_{mn}^{M(0)} \) (Eq. (7.19)) may be written as

\[
\hat{\Pi}_{00}^{M(0)} = 1, \quad \hat{\Pi}_{10}^{M(0)} = -u_x, \quad \hat{\Pi}_{01}^{M(0)} = -u_y, \quad \hat{\Pi}_{20}^{M(0)} = (u_x^2 + c_s^2), \quad \hat{\Pi}_{02}^{M(0)} = (u_y^2 + c_s^2), \quad \hat{\Pi}_{11}^{M(0)} = u_x u_y, \quad \hat{\Pi}_{21}^{M(0)} = -(u_x^2 + c_s^2)u_y, \quad \hat{\Pi}_{12}^{M(0)} = -(u_y^2 + c_s^2)u_x, \quad \hat{\Pi}_{22}^{M(0)} = (u_x^2 + c_s^2)(u_y^2 + c_s^2).
\]

Then, in order to discretize Eq. (7.14) in a cascaded LB formulation, we need the continuous central moments of the equilibrium pressure distribution function or the transformed Maxwellian \( g_{eq} \) (Eq. (7.15)) of order \((m + n)\). By defining it as

\[
\hat{\Pi}_{mn}^{eq,g} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g_{eq}(\xi_x - u_x)^m(\xi_y - u_y)^n d\xi_x d\xi_y, \tag{7.21}
\]

it readily follows that Eq. (7.21) satisfies the following relation

\[
\hat{\Pi}_{mn}^{eq,g} = c_s^2 \hat{\Pi}_{mn}^M + \psi(\rho)\hat{\Pi}_{mn}^{M(0)}. \]

Evaluating its nine components, we get

\[
\hat{\Pi}_{00}^{eq,g} = p, \quad \hat{\Pi}_{10}^{eq,g} = -\psi(\rho)u_x, \quad \hat{\Pi}_{01}^{eq,g} = -\psi(\rho)u_y, \quad \hat{\Pi}_{20}^{eq,g} = pc_s^2 + \psi(\rho)u_x^2, \quad \hat{\Pi}_{02}^{eq,g} = pc_s^2 + \psi(\rho)u_y^2, \quad \hat{\Pi}_{11}^{eq,g} = \psi(\rho)u_x u_y, \quad \hat{\Pi}_{21}^{eq,g} = -\psi(\rho)(c_s^2 + u_x^2)u_y, \quad \hat{\Pi}_{12}^{eq,g} = -\psi(\rho)(c_s^2 + u_y^2)u_x, \quad \hat{\Pi}_{22}^{eq,g} = c_s^6 + \psi(\rho)(u_x^2 + c_s^2)(u_y^2 + c_s^2). \tag{7.22}
\]

Next, we need the continuous central moments of the source term due to the total (interfacial and local body) force \( F_t = (F_{tx}, F_{ty}) \) of order \((m + n)\) in MCBE (Eq. (7.14)), which can be defined as

\[
\hat{\Gamma}_{mn}^t = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} S^t(\xi_x - u_x)^m(\xi_y - u_y)^n d\xi_x d\xi_y, \tag{7.23}
\]
where
\[
S_t = (\xi - \mathbf{u}) \cdot \mathbf{F}_t \frac{f_M(\rho, \mathbf{u})}{\rho}.
\] (7.24)

It can be shown that this continuous central moment satisfies the following identity that depends on the those of the Maxwellian
\[
\hat{\Gamma}^t_{mn} = F_{tx} \frac{\hat{\Pi}^M_{m+1,n}}{\rho} + F_{ty} \frac{\hat{\Pi}^M_{m,n+1}}{\rho}.
\]

By evaluating its components and dealiasing the resulting central moment components higher than the second order by setting them to zero, as they do not influence the recovery of the hydrodynamics via the Chapman-Enskog expansion [19], the results can be summarized as
\[
\hat{\Gamma}^t_{00} = 0, \quad \hat{\Gamma}^t_{10} = c_s^2 F_{tx}, \quad \hat{\Gamma}^t_{01} = c_s^2 F_{ty}, \quad \hat{\Gamma}^t_{20} = 0, \quad \hat{\Gamma}^t_{02} = 0, \quad \hat{\Gamma}^t_{11} = 0,
\]
\[
\hat{\Gamma}^t_{21} = 0, \quad \hat{\Gamma}^t_{12} = 0, \quad \hat{\Gamma}^t_{22} = 0.
\] (7.25)

Finally, we define the continuous central moments of the source term due to the net gradient pressure force \( \mathbf{F}_p = (F_{px}, F_{py}) \) in Eq. (7.14) of order \((m + n)\) as
\[
\hat{\Gamma}^p_{mn} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} S^p(\xi - \mathbf{u})^m(\xi' - \mathbf{u}'')^n d\xi d\xi',
\] (7.26)

where
\[
S^p = (\xi - \mathbf{u}) \cdot \mathbf{F}_p \left\{ \frac{f_M(\rho, \mathbf{u})}{\rho} - \frac{f_M(\rho, \mathbf{0})}{\rho} \right\}.
\] (7.27)

Based on its definition, this central moment \( \hat{\Gamma}^p_{mn} \) can be demonstrated to satisfy the following identity
\[
\hat{\Gamma}^p_{mn} = F_{px} \left( \frac{\hat{\Pi}^M_{m+1,n}}{\rho} - \frac{\hat{\Pi}^M_{m+1,n}}{\rho} \right) + F_{py} \left( \frac{\hat{\Pi}^M_{m,n+1}}{\rho} - \frac{\hat{\Pi}^M_{m,n+1}}{\rho} \right).
\]

By using this and deriving the expressions for the nine components, where, as before, we retain the results only up to the second order moments that determine the two-phase fluid motion and set the higher order ones to zero, they can be summarized as
\[
\hat{\Gamma}^p_{00} = (F_{px} u_x + F_{py} u_y), \quad \hat{\Gamma}^p_{10} = -u_x \hat{\Gamma}^p_{00}, \quad \hat{\Gamma}^p_{01} = -u_y \hat{\Gamma}^p_{00}, \quad \hat{\Gamma}^p_{20} = 2c_s^2 F_{px} u_x + (u_x^2 + c_s^2) \hat{\Gamma}^p_{00},
\]
\[
\hat{\Gamma}^p_{02} = 2c_s^2 F_{py} u_y + (u_y^2 + c_s^2) \hat{\Gamma}^p_{00}, \quad \hat{\Gamma}^p_{11} = c_s^2 (F_{px} u_y + F_{py} u_x) + u_x u_y \hat{\Gamma}^p_{00},
\]
\[
\hat{\Gamma}^p_{21} = 0, \quad \hat{\Gamma}^p_{12} = 0, \quad \hat{\Gamma}^p_{22} = 0.
\] (7.28)
7.4 Cascaded LB Method for Solution of Two-Phase Fluid Motion

We will now present a cascaded central moment LB method based on the discretization of the MCBE discussed in the previous section for the solution of incompressible two-phase flow. In this regard, we consider the D2Q9 lattice, whose components of the particle velocities are represented by the following vectors using the standard Dirac’s bra-ket notation:

\[
|e_x\rangle = (0, 1, 0, -1, 0, 1, -1, 1)^\dagger, \tag{7.29a}
\]
\[
|e_y\rangle = (0, 0, 1, 0, -1, 1, -1, -1)^\dagger. \tag{7.29b}
\]

In addition, we need to define the following nine-dimensional vector

\[
|1\rangle = (1, 1, 1, 1, 1, 1, 1, 1, 1)^\dagger, \tag{7.30}
\]

whose inner product with a discrete distribution function \(g_\alpha\) (see below), where \(\alpha = 0, 1, 2, \cdots, 8\) represents the particle velocity direction, i.e., its zeroth moment yields the pressure field. Using the above, the following set of orthogonal moment basis vectors can be used to constructed the cascaded LB formulation:

\[
|K_0\rangle = |1\rangle, \quad |K_1\rangle = |e_x\rangle, \quad |K_2\rangle = |e_y\rangle, \quad |K_3\rangle = 3|e_x^2 + e_y^2\rangle - 4|1\rangle, \quad
|K_4\rangle = |e_x^2 - e_y^2\rangle, \quad |K_5\rangle = |e_x e_y\rangle, \quad |K_6\rangle = -3|e_x^2 e_y\rangle + 2|e_y\rangle, \quad
|K_7\rangle = -3|e_x e_y^2\rangle + 2|e_x\rangle, \quad |K_8\rangle = 9|e_x^2 e_y^2\rangle - 6|e_x^2 + e_y^2\rangle + 4|1\rangle. \tag{7.31}
\]

In the above, a symbol such as \(|e^2_y\rangle = |e_x e_y\rangle\) represents a vector resulting from the element-wise vector multiplication of the sequence of vectors \(|e_x\rangle, |e_x\rangle\) and \(|e_y\rangle\). By combining the above nine independent vectors, we then obtain the following orthogonal moment basis matrix

\[
\mathbf{K} = [|K_0\rangle, |K_1\rangle, |K_2\rangle, |K_3\rangle, |K_4\rangle, |K_5\rangle, |K_6\rangle, |K_7\rangle, |K_8\rangle]. \tag{7.32}
\]

Then, we perform the standard spatial and temporal discretization of the MCBE (Eq. (7.14)) along the characteristic directions of the particle velocities over a time step \(\delta_t\) (typically \(\delta_t = 1\) in...
lattice units), where we apply a trapezoidal rule for the treatment of the source term to maintain a second order accuracy [22], which yields

\[ g_\alpha(x + e_\alpha \delta t, t + \delta t) = g_\alpha(x, t) + \left( K \cdot \hat{h} \right)_\alpha + \frac{1}{2} \left[ S_\alpha(x, t) + S_\alpha(x + e_\alpha \delta t, t + \delta t) \right] \delta t. \]  

(7.33)

Here, \((K \cdot \hat{h})_\alpha\) is the cascaded collision operator, where \(\hat{h} = (\hat{h}_0, \hat{h}_1, \hat{h}_2, \ldots, \hat{h}_8)^\dagger\) is a vector representing the changes in all the nine moments supported by the lattice under collision which will be determined in what follows. \(S_\alpha\) is the total source term representing the cumulative effect of the discrete version of the source due to the interfacial and local body force \(S^d_\alpha\) (via Eq. (7.24)) and that due to the net gradient pressure force \(S^p_\alpha\) (via Eq. (7.27)):

\[ S_\alpha = S^d_\alpha + S^p_\alpha. \]  

(7.34)

In order to remove implicitness in Eq. (7.33), we apply a variable transformation \(\overline{g}_\alpha = g_\alpha - \frac{1}{2} S_\alpha \delta t\), which then results in the following effectively explicit cascaded LB scheme

\[ \overline{g}_\alpha(x + e_\alpha \delta t, t + \delta t) = \overline{g}_\alpha(x, t) + (K \cdot \hat{h})_\alpha + \delta g^\delta_\alpha, \]  

(7.35)

where \(\delta g^\delta_\alpha\) is a modified cumulative source term under the variable transformation, which we prescribe to be the following:

\[ \delta g^\delta_\alpha = K^{-1} \left( I - \frac{1}{2} \hat{\Lambda} \right) KS. \]  

(7.36)

Here, \(S = (S_0, S_1, S_2, \ldots, S_8)^\dagger\) represents a vector of all the nine components of the discrete source term and \(\hat{\Lambda} = \text{diag}(\omega_0, \omega_1, \omega_2, \ldots, \omega_8)\) is a relaxation time matrix used in the development of the cascaded collision operator under relaxation of different central moments later. Since the effects of the two sources \(S^d_\alpha\) and \(S^p_\alpha\) appearing in the cumulative source term \(S_\alpha\) on the changes of various moments are different, we consider a modification to the earlier central moments based strategy [19] in this regard. The expression given in Eq. (7.36) is motivated to remove any spurious effects due to the source term in the second order non-equilibrium moments, which are related to the viscous stress tensor, in order to consistently recover the incompressible NSE for two-phase flows. Similar approach has been considered in the MRT-LBE with forcing term pre-
viously (see e.g., [75]), but the form of $\delta g^s_{\alpha}$ in Eq. (7.36) will be still determined by a central moments based strategy in what follows.

In order of derive the expressions for $\hat{h}$ and $\delta g^s_{\alpha}$ to complete the formulation of the cascaded LB scheme for two-phase fluid motion, we first define the discrete central moments of the distribution function, its equilibrium and the source term as

$$
\begin{pmatrix}
\hat{\eta}_{mn} \\
\hat{\eta}'_{mn} \\
\hat{\sigma}_{mn} \\
\hat{\eta}'_{mn}
\end{pmatrix} = \sum_{\alpha} \begin{pmatrix}
g_{\alpha} \\
g_{\alpha}^e \\
S_{\alpha} \\
g_{\alpha}
\end{pmatrix} \left( e_{ax} - u_x \right)^m \left( e_{ay} - u_y \right)^n,
$$

(7.37)

where $\hat{\eta}_{mn} = \hat{\eta}_{mn} - \frac{1}{2} \hat{\sigma}_{mn} \delta_t$ and the corresponding raw moments as

$$
\begin{pmatrix}
\eta'_{mn} \\
\eta'_{mn} \\
\sigma'_{mn} \\
\eta'_{mn}
\end{pmatrix} = \sum_{\alpha} \begin{pmatrix}
g_{\alpha} \\
g_{\alpha}^e \\
S_{\alpha} \\
g_{\alpha}
\end{pmatrix} e_{ax}^m e_{ay}^n,
$$

(7.38)

where $\hat{\eta}'_{mn} = \hat{\eta}'_{mn} - \frac{1}{2} \hat{\sigma}'_{mn} \delta_t$. Then, we need to determine the expressions for the discrete central moments of the equilibrium distribution function and the source term. In this regard, we apply a matching principle [15, 19], where they are respectively set equal to their continuous values for all orders supported by the lattice. That is,

$$
\hat{\eta}^{eq}_{mn} = \hat{\Pi}^{eq,g}_{mn}, \quad \hat{\sigma}_{mn} = \hat{\Gamma}_{mn} \equiv \hat{\Gamma}^t_{mn} + \hat{\Gamma}^p_{mn},
$$

(7.39)

where the continuous central moment components of the equilibrium $\hat{\Pi}^{eq,g}_{mn}$ is given in Eq. (7.22), while those for the source terms $\hat{\Gamma}^t_{mn}$ and $\hat{\Gamma}^p_{mn}$ can be found in Eqs. (7.25) and (7.28), respectively. This step effectively preserve the Galilean invariance of all the moments independently supported by the lattice.

Based on Eq. (7.39), the first step in deriving the modified cumulative source term in the velocity space due to various sources/forces $\delta g^s_{\alpha}$ is to convert the central moments $\hat{\sigma}_{mn}$ to the correspond-
ing raw moments $\hat{\sigma}_{mn}$ at various orders via the binomial transform. Performing this and setting all the cumulative source moments of second and higher order to zero as they do not affect recovering the hydrodynamics of the two-phase fluids in the Chapman-Enskog analysis [19, 205], we get

\[
\hat{\sigma}_{00} = \hat{\Gamma}_{00}^p \equiv (F_{px}u_x + F_{py}u_y), \quad \hat{\sigma}_{10} = c_s^2F_{tx}, \quad \hat{\sigma}_{01} = c_s^2F_{ty},
\]

\[
\hat{\sigma}_{20} = 2c_s^2(F_{tx}u_x + F_{px}u_x) = 2c_s^2(\hat{\sigma}_{00} + \hat{\sigma}_{02}) + 2c_s^2\hat{\Gamma}_{00}^p, \quad \hat{\sigma}_{02} = 2c_s^2(F_{ty}u_y + F_{py}u_y) + c_s^2\hat{\Gamma}_{00}^p,
\]

\[
\hat{\sigma}_{11} = c_s^2(F_{tx}u_y + F_{ty}u_x) = c_s^2(F_{px}u_y + F_{py}u_x), \quad \hat{\sigma}_{21} = 0, \quad \hat{\sigma}_{12} = 0, \quad \hat{\sigma}_{22} = 0.
\]

Using this, we then evaluate the various source moments projected to the orthogonal basis vectors and with a scaling based on the relaxation time for avoiding any spurious effects in the second order non-equilibrium moments as mentioned earlier, i.e., $\hat{m}^s_j = (1 - \frac{1}{2}\omega_j) \langle K_j | S_\alpha \rangle$, which yields

\[
\hat{m}^s_0 = \left(1 - \frac{1}{2}\omega_0\right) \hat{\sigma}_{00}, \quad \hat{m}^s_1 = \left(1 - \frac{1}{2}\omega_1\right) \hat{\sigma}_{10}, \quad \hat{m}^s_2 = \left(1 - \frac{1}{2}\omega_2\right) \hat{\sigma}_{01},
\]

\[
\hat{m}^s_3 = \left(1 - \frac{1}{2}\omega_3\right) \left[3(\hat{\sigma}_{20} + \hat{\sigma}_{02}) - 4\hat{\sigma}_{00}\right], \quad \hat{m}^s_4 = \left(1 - \frac{1}{2}\omega_4\right) \left[\hat{\sigma}_{20} - \hat{\sigma}_{02}\right],
\]

\[
\hat{m}^s_5 = \left(1 - \frac{1}{2}\omega_5\right) \hat{\sigma}_{11}, \quad \hat{m}^s_6 = \left(1 - \frac{1}{2}\omega_6\right) \left[-3\hat{\sigma}_{21} + 2\hat{\sigma}_{01}\right], \quad \hat{m}^s_7 = \left(1 - \frac{1}{2}\omega_7\right) \left[-3\hat{\sigma}_{12} + 2\hat{\sigma}_{10}\right],
\]

\[
\hat{m}^s_8 = \left(1 - \frac{1}{2}\omega_8\right) \left[9\hat{\sigma}_{22} - 6(\hat{\sigma}_{20} + \hat{\sigma}_{02}) - 8\hat{\sigma}_{00}\right].
\]

Finally, by exploiting the orthogonal property of $K$ in $\delta g^s_\alpha = K^{-1} \hat{m}^s$, where $\hat{m}^s = (1 - \frac{1}{2}\hat{\Lambda}) KS$, with $\hat{m}^s = (\hat{m}^s_0, \hat{m}^s_1, \hat{m}^s_2, \cdots, \hat{m}^s_8)^\dagger$, we get the modified cumulative source term due to various
Next, the structure of the cascaded collision operator \( (\mathbf{K} \cdot \hat{\mathbf{h}})_\alpha \) based on the discrete equilibrium central moments \( \hat{\eta}_{m0}^{\text{eq}} \) given in Eq. (7.39) is determined as follows. For all non-conserved moments, i.e., for \( (m + n) \geq 2 \), we prescribe the relaxation of the discrete central moments \( \hat{\eta}_{mn} \) to their corresponding central moment equilibria \( \hat{\eta}_{mn}^{\text{eq}} \) at a relaxation time \( \omega_\beta [15, 19] \). That is, \[
\sum_\alpha (\mathbf{K} \cdot \hat{\mathbf{h}})_\alpha (e_{ax} - u_x)^m (e_{ay} - u_y)^n = \omega_\beta (\hat{\eta}_{m0}^{\text{eq}} - \hat{\eta}_{mn}).
\]
For the transformed distribution function \( \bar{g}_\alpha \) employed in the cascaded LB scheme (Eq. (7.35)), during a time step \( \delta t \), its zeroth moment change needs to be \( \delta \sigma'_{00} \), while its first order moments are required to change by \( \delta \sigma'_{10} \) and \( \delta \sigma'_{01} \) in order to consistently update the pressure field and the fluid momentum via the interfacial and body forces. On the other hand, the respective moment changes due to the sources given earlier are \( \hat{m}_0' = (1 - \frac{1}{2}\omega_0) \hat{\sigma}'_{00}, \hat{m}_1' = (1 - \frac{1}{2}\omega_1) \hat{\sigma}'_{10}, \) and \( \hat{m}_2' = (1 - \frac{1}{2}\omega_2) \hat{\sigma}'_{01}. \) Hence, to meet the above physical constraints, we effectively need to satisfy the following constraints: \[
\sum_\alpha (\mathbf{K} \cdot \hat{\mathbf{h}})_\alpha = \frac{\omega_0}{2} \delta \hat{\sigma}'_{00},
\sum_\alpha (\mathbf{K} \cdot \hat{\mathbf{h}})_\alpha e_{ax} = \frac{\omega_1}{2} \delta \hat{\sigma}'_{10} \text{ and } \sum_\alpha (\mathbf{K} \cdot \hat{\mathbf{h}})_\alpha e_{ay} = \frac{\omega_2}{2} \delta \hat{\sigma}'_{01}. \]
Based on these considerations for the lower order moment changes and the central moment relaxation for the higher order moments under collision mentioned above, the expressions for the components of the moment change vec-
tor \( \hat{h} = (\hat{h}_0, \hat{h}_1, \hat{h}_2, \ldots, \hat{h}_8)^\dagger \) can be determined, which are summarized as follows:

\[
\begin{align*}
\hat{h}_0 &= \frac{\omega_0}{2} \frac{\hat{F}_p^{\rho}}{9}, \quad \hat{h}_1 = \frac{\omega_1}{2} \frac{c_s^2 F_{tx}}{6}, \quad \hat{h}_2 = \frac{\omega_2}{2} \frac{c_s^2 F_{ty}}{6}, \\
\hat{h}_3 &= \frac{\omega_3}{12} \left[ 2 \rho c_s^2 + \rho c_s^2 (u_x^2 + u_y^2) - (\eta_{20} + \eta_{02}) \right], \\
\hat{h}_4 &= \frac{\omega_4}{4} \left[ \rho c_s^2 (u_x^2 - u_y^2) - (\eta_{20} - \eta_{02}) \right], \\
\hat{h}_5 &= \frac{\omega_5}{4} \left[ \rho c_s^2 u_x u_y - \eta_{11} \right], \\
\hat{h}_6 &= \frac{\omega_6}{4} \left[ \psi(\rho) (\dot{c}_s^2 + u_x^2) u_y + \eta_{21} - u_y \eta_{12} - 2 u_x \eta_{11} + 3 \rho u_x^2 u_y - u_x^2 u_y p \right] \\
&\quad \quad \quad - u_y \left( \frac{3}{2} h_3 + \frac{1}{2} h_4 \right) - 2 u_x \hat{h}_5, \\
\hat{h}_7 &= \frac{\omega_7}{4} \left[ \psi(\rho) (\dot{c}_s^2 + u_y^2) u_x + \eta_{12} - 2 u_y \eta_{11} - u_x \eta_{02} + 3 \rho u_x u_y^2 - u_x u_y^2 p \right] \\
&\quad \quad \quad - u_x \left( \frac{3}{2} h_3 - \frac{1}{2} h_4 \right) - 2 u_y \hat{h}_5, \\
\hat{h}_8 &= \frac{\omega_8}{4} \left[ \dot{c}_s^2 \rho + \psi(\rho) (\dot{c}_s^2 + u_x^2) (\dot{c}_s^2 + u_y^2) - \eta_{22} + 2 (u_y \eta_{21} + u_x \eta_{12}) \\
&\quad \quad \quad - (u_x^2 \eta_{20} + u_x^2 \eta_{02}) - 4 u_x u_y \eta_{11} + 4 \rho u_x^2 u_y^2 - u_x^2 u_y^2 p \right] - \frac{3}{2} \frac{u_y^2}{2} (3 \hat{h}_3 + \hat{h}_4) \\
&\quad \quad \quad - \frac{1}{2} u_x^2 (3 \hat{h}_3 - \hat{h}_4) - 4 u_x u_y \hat{h}_5 - 2 u_y \hat{h}_6 - 2 u_x \hat{h}_7. \quad (7.41)
\end{align*}
\]

Finally, the post-collision distribution function represented by \( \bar{g}_\beta \) can be obtained by expanding \((K \cdot \hat{h})_\alpha\) in Eq. (7.35), which read as

\[
\begin{align*}
\bar{g}_0 &= \bar{g}_0 + \left[ \hat{h}_0 - 4(\hat{h}_3 - \hat{h}_8) \right] + \delta g_0^s, \\
\bar{g}_1 &= \bar{g}_1 + \left[ \hat{h}_0 + \hat{h}_1 - \hat{h}_3 + \hat{h}_4 + 2(\hat{h}_7 - \hat{h}_8) \right] + \delta g_1^s, \\
\bar{g}_2 &= \bar{g}_2 + \left[ \hat{h}_0 + \hat{h}_2 - \hat{h}_3 - \hat{h}_4 + 2(\hat{h}_6 - \hat{h}_8) \right] + \delta g_2^s, \\
\bar{g}_3 &= \bar{g}_3 + \left[ \hat{h}_0 - \hat{h}_1 - \hat{h}_3 + \hat{h}_4 - 2(\hat{h}_7 + \hat{h}_8) \right] + \delta g_3^s, \\
\bar{g}_4 &= \bar{g}_4 + \left[ \hat{h}_0 - \hat{h}_2 - \hat{h}_3 - \hat{h}_4 - 2(\hat{h}_6 + \hat{h}_8) \right] + \delta g_4^s, \\
\bar{g}_5 &= \bar{g}_5 + \left[ \hat{h}_0 + \hat{h}_1 + \hat{h}_2 + 2 \hat{h}_3 + \hat{h}_5 - \hat{h}_6 - \hat{h}_7 + \hat{h}_8 \right] + \delta g_5^s, \\
\bar{g}_6 &= \bar{g}_6 + \left[ \hat{h}_0 - \hat{h}_1 + \hat{h}_2 + 2 \hat{h}_3 - \hat{h}_5 - \hat{h}_6 + \hat{h}_7 + \hat{h}_8 \right] + \delta g_6^s, \\
\bar{g}_7 &= \bar{g}_7 + \left[ \hat{h}_0 - \hat{h}_1 - \hat{h}_2 + 2 \hat{h}_3 + \hat{h}_5 + \hat{h}_6 + \hat{h}_7 + \hat{h}_8 \right] + \delta g_7^s, \\
\bar{g}_8 &= \bar{g}_8 + \left[ \hat{h}_0 + \hat{h}_1 - \hat{h}_2 + 2 \hat{h}_3 - \hat{h}_5 + \hat{h}_6 - \hat{h}_7 + \hat{h}_8 \right] + \delta g_8^s. \quad (7.42)
\end{align*}
\]
This represents the collision step, and the streaming step then follows from rearranging Eq. (7.35) as \( \tilde{g}_\alpha(x, t + \delta t) = \widetilde{g}_\alpha(x - e_\alpha \delta t, t) \), where \( \alpha = 0, 1, 2, \cdots, 8 \). Once the cascaded collision and streaming steps are performed, the two-phase flow fields, i.e., the hydrodynamic pressure and the velocity can be obtained via the zeroth and first moments of the transformed distribution function as

\[
p = \sum_\alpha g_\alpha + \frac{1}{2} F_p \cdot u \delta t, \quad \rho \epsilon_s^2 u = \sum_\alpha g_\alpha e_\alpha + \frac{1}{2} c_s^2 F_t \delta t.
\]

(7.43)

Based on the Chapman-Enskog multiscale expansion (see e.g., [19]), it can be shown that the above cascaded LB scheme represents the incompressible two-phase fluid motion, where the fluid viscosity \( \mu \) is related to the relaxation times of the second order moments as

\[
\mu = \rho \nu = \rho \epsilon_s^2 \left( \frac{1}{\omega_j} - \frac{1}{2} \right) \delta t, \quad j = 4, 5,
\]

(7.44)

and the rest of the relaxation times, which can influence numerical stability, are set to unity in this work. It may be noted that in the implementation of our cascaded LB formulation, all the spatial gradients of the phase field variable \( \phi \) required in the computation of the interfacial normal \( \mathbf{n} = (n_x, n_y) \) and the surface tension force \( F_s \) are obtained using a second order isotropic finite difference scheme. In addition, in view of Eq. (7.9), the spatial gradients of the density \( \rho \) are directly expressed in terms of those of \( \phi \). The solution procedure for the evolution of the phase field will be discussed next.

### 7.5 Cascaded LB Method for Solution of Phase-Field based Interfacial Dynamics

We will now construct another cascaded LB scheme for the solution of the conservative Allen-Cahn equation (ACE) given in Eq. (7.1). Since the ACE is a convection-diffusion equation (CDE) with an additional interface sharpening flux term, our solution approach is based on modifying the central moment cascaded approach that we developed recently for CDE in a MRT formulation [205, 33, 206], where this additional term is included in the first order moment equilibria. This strategy is an extension of the approach proposed in [233]. In this regard, we con-
sider a D2Q9 lattice using the same orthogonal moment basis vectors and the matrix given in Eqs. (7.31) and (7.32), respectively.

Then, the collision and streaming steps of such a cascaded LB scheme for the evolution of the discrete distribution function \( f_\alpha \) can be respectively represented as

\[
\tilde{f}_\alpha(x, t) = f_\alpha(x, t) + (K \cdot \hat{g})_{\alpha}, \quad (7.45a)
\]

\[
f_\alpha(x, t + \delta t) = \tilde{f}_\alpha(x - e_\alpha \delta t, t). \quad (7.45b)
\]

In order to design a cascaded collision operator to solve for the phase field variable \( \phi \) described by an conservative Allen-Cahn equation (ACE), we first define the following central moments and raw moments of the distribution function \( f_\alpha \) and its equilibrium \( f^\text{eq}_\alpha \), respectively, as

\[
\left( \hat{\kappa}_{mn} \right) = \sum_\alpha \left( \begin{array}{c} f_\alpha \\ f^\text{eq}_\alpha \end{array} \right) (e_{ax} - u_x)^m (e_{ay} - u_y)^n, \quad (7.46)
\]

\[
\left( \hat{\kappa}'_{mn} \right) = \sum_\alpha \left( \begin{array}{c} f_\alpha \\ f^\text{eq}_\alpha \end{array} \right) e_{ax}^m e_{ay}^n. \quad (7.47)
\]

Then, we consider the continuous central moments of the equilibria

\[
\hat{\Pi}_{mn}^{\text{eq}, \phi} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f^\text{eq}(\xi_x - u_x)^m (\xi_y - u_y)^n d\xi_x d\xi_y \quad (7.48)
\]

by defining the equilibrium distribution function \( f^\text{eq} \) in analogy with the local Maxwell distribution function by replacing the density with the phase field variable \( \phi \): 

\[
f^\text{eq} \equiv f^\text{eq}(\phi, u, \xi) = \frac{\phi}{2\pi c_s^2 \phi} \exp \left[ -\frac{(\xi - u)^2}{2c_s^2 \phi} \right].
\]

Here \( c_s \phi \) is a free parameter, which will be related to the coefficient of diffusivity \( M_\phi \) later. Typically, we set \( c_s^2 \phi = \frac{1}{3} \). The relaxation of the central moments to the corresponding equilibria given above only models a diffusion process. In order to account for the counteracting phase separation flux components \( -\theta n_x \) and \( -\theta n_y \) appearing in the conservative ACE (Eq. (7.1)), where \( n = (n_x, n_y) \) is the interface normal, we modify the first order continuous central moments from being null to \( \hat{\Pi}_{10}^{\text{eq}, \phi} = M_\phi \theta n_x \) and \( \hat{\Pi}_{01}^{\text{eq}, \phi} = M_\phi \theta n_y \). Then, by matching of the
discrete and continuous central moments of the equilibria, i.e., \( \hat{\kappa}_{mn}^{eq} = \hat{\Pi}_{mn}^{eq}\phi \) for all the nine independent moments supported by the lattice, we obtain the components of \( \kappa_{mn}^{eq} \) as

\[
\hat{\kappa}_{00}^{eq} = \phi, \quad \hat{\kappa}_{10}^{eq} = M_\phi \theta n_x, \quad \hat{\kappa}_{01}^{eq} = M_\phi \theta n_y, \quad \hat{\kappa}_{20}^{eq} = c_{s\phi}^2 \phi, \quad \hat{\kappa}_{02}^{eq} = c_{s\phi}^2 \phi, \quad \hat{\kappa}_{11}^{eq} = 0, \\
\hat{\kappa}_{21}^{eq} = 0, \quad \hat{\kappa}_{12}^{eq} = 0, \quad \hat{\kappa}_{22}^{eq} = c_{s\phi}^4 \phi.
\]

The cascaded collision operator can then be constructed by prescribing the relaxation of central moments of different orders to their equilibria, i.e., \( \sum_{\alpha} (K \cdot \hat{g})_{\alpha} (e_{ax} - u_x)^m (e_{ay} - u_y)^n = \omega_3^\phi (\kappa_{mn}^{eq} - \hat{\kappa}_{mn}) \), where only the zeroth moment being conserved \( (\hat{\kappa}_{00}^{eq} = \hat{\kappa}_{00} = \phi) \), and \( \omega_3^\phi \) are the various relaxation times. The resulting changes in all the nine components of moments under collision, i.e., \( \hat{g} = (\hat{g}_0, \hat{g}_1, \hat{g}_2, \ldots, \hat{g}_8) \) can be summarized as follows:

\[
\begin{align*}
\hat{g}_0 &= 0, \quad \hat{g}_1 = \frac{\omega_1^\phi}{6} \left[ \phi u_x + \left[ M_\phi \theta n_x - \kappa_{10}' \right] \right], \quad \hat{g}_2 = \frac{\omega_2^\phi}{6} \left[ \phi u_y + \left[ M_\phi \theta n_y - \kappa_{01}' \right] \right], \\
\hat{g}_3 &= \frac{\omega_3^\phi}{12} \left[ 2c_{s\phi}^2 \phi - (u_x^2 + u_y^2) \phi - (\kappa_{20}' + \kappa_{02}') + 2(u_x \kappa_{10}' + u_y \kappa_{01}') \right] + u_x \hat{g}_1 + u_y \hat{g}_2, \\
\hat{g}_4 &= \frac{\omega_4^\phi}{4} \left[ -(u_x^2 - u_y^2) \phi - (\kappa_{20}' - \kappa_{02}') + 2(u_x \kappa_{10}' - u_y \kappa_{01}') \right] + 3(u_x \hat{g}_1 - u_y \hat{g}_2), \\
\hat{g}_5 &= \frac{\omega_5^\phi}{4} \left[ -u_x u_y \phi - \kappa_{11}' + (u_x \kappa_{01}' + u_y \kappa_{10}') \right] + \frac{3}{2} (u_x \hat{g}_2 + u_y \hat{g}_1), \\
\hat{g}_6 &= \frac{\omega_6^\phi}{4} \left[ -u_x u_y \phi - \kappa_{12}' - u_y \kappa_{02}' - 2u_x \kappa_{11}' + 2u_x u_y \kappa_{10}' + u_x^2 \kappa_{01}' \right] + 3u_x u_y \hat{g}_1 \\
&\quad + \left( \frac{3}{2} u_x^2 + 1 \right) \hat{g}_2 - \frac{3}{2} u_y \hat{g}_3 - \frac{1}{2} u_y \hat{g}_4 - 2u_x \hat{g}_5, \\
\hat{g}_7 &= \frac{\omega_7^\phi}{4} \left[ -u_x u_y^2 \phi - \kappa_{11}' - u_x \kappa_{02}' - 2u_x \kappa_{11}' + 2u_x u_y \kappa_{01}' + u_y^2 \kappa_{10}' \right] + \left( \frac{3}{2} u_y^2 + 1 \right) \hat{g}_1 \\
&\quad + 3u_x u_y \hat{g}_2 - \frac{3}{2} u_y \hat{g}_3 + \frac{3}{2} u_x \hat{g}_4 - 2u_y \hat{g}_5, \\
\hat{g}_8 &= \frac{\omega_8^\phi}{4} \left[ c_{s\phi}^4 \phi - \kappa_{22}' + 2(u_x \kappa_{12}' + u_y \kappa_{21}') - (u_y^2 \kappa_{20}' + u_x^2 \kappa_{02}') - 4u_x u_y \kappa_{11}' - 2(u_x u_y \kappa_{01}' + u_x^2 \kappa_{01}') \right] \\
&\quad - u_x^2 u_y^2 \phi + (2u_x + 3u_x^2 u_y) \hat{g}_1 + (2u_y + 3u_x u_y^2) \hat{g}_2 - (2 + \frac{3}{2} (u_x^2 + u_y^2)) \hat{g}_3 + \frac{1}{2} (u_x^2 - u_y^2) \hat{g}_4 \\
&\quad - 4u_x u_y \hat{g}_5 - 2u_y \hat{g}_6 - 2u_x \hat{g}_7, \quad (7.49)
\end{align*}
\]

where the relaxation times of the first order moments \( \omega_1^\phi \) and \( \omega_2^\phi \) are related to the mobility parameter \( M_\phi \) in Eq. (7.1) via \( M_\phi = c_{s\phi}^2 \left( \frac{1}{\omega_j^\phi} - \frac{1}{2} \right) \delta_{t,j} \), \( j = 1, 2 \), and therest of the relaxation times are set to unity. Finally, the post-collision distribution function \( f_\alpha \) can be explicitly written after
expanding \((\mathbf{K} \cdot \dot{\mathbf{g}})_{\alpha}\) in Eq. (7.45a) as

\[
\begin{align*}
\tilde{f}_0 &= f_0 + [\dot{\gamma}_0 - 4(\dot{\gamma}_3 - \dot{\gamma}_8)], \\
\tilde{f}_1 &= f_1 + [\dot{\gamma}_0 + \dot{\gamma}_1 - \dot{\gamma}_3 + \dot{\gamma}_4 + 2(\dot{\gamma}_7 - \dot{\gamma}_8)], \\
\tilde{f}_2 &= f_2 + [\dot{\gamma}_0 + \dot{\gamma}_2 - \dot{\gamma}_3 - \dot{\gamma}_4 + 2(\dot{\gamma}_6 - \dot{\gamma}_8)], \\
\tilde{f}_3 &= f_3 + [\dot{\gamma}_0 - \dot{\gamma}_1 - \dot{\gamma}_3 + \dot{\gamma}_4 - 2(\dot{\gamma}_7 + \dot{\gamma}_8)], \\
\tilde{f}_4 &= f_4 + [\dot{\gamma}_0 - \dot{\gamma}_2 - \dot{\gamma}_3 - \dot{\gamma}_4 - 2(\dot{\gamma}_6 + \dot{\gamma}_8)], \\
\tilde{f}_5 &= f_5 + [\dot{\gamma}_0 + \dot{\gamma}_1 + \dot{\gamma}_2 + 2\dot{\gamma}_3 + \dot{\gamma}_5 - \dot{\gamma}_6 - \dot{\gamma}_7 + \dot{\gamma}_8], \\
\tilde{f}_6 &= f_6 + [\dot{\gamma}_0 - \dot{\gamma}_1 + \dot{\gamma}_2 + 2\dot{\gamma}_3 - \dot{\gamma}_5 - \dot{\gamma}_6 + \dot{\gamma}_7 + \dot{\gamma}_8], \\
\tilde{f}_7 &= f_7 + [\dot{\gamma}_0 - \dot{\gamma}_1 - \dot{\gamma}_2 + 2\dot{\gamma}_3 + \dot{\gamma}_5 + \dot{\gamma}_6 + \dot{\gamma}_7 + \dot{\gamma}_8], \\
\tilde{f}_8 &= f_8 + [\dot{\gamma}_0 + \dot{\gamma}_1 - \dot{\gamma}_2 + 2\dot{\gamma}_3 - \dot{\gamma}_5 + \dot{\gamma}_6 - \dot{\gamma}_7 + \dot{\gamma}_8].
\end{align*}
\]

(7.50)

This is followed by performing the streaming step shown in Eq. (7.45b), which then updates the phase field variable \(\phi\) via taking the zeroth moment of \(f_{\alpha}\) as

\[
\phi = \sum_{\alpha} f_{\alpha}.
\]

(7.51)

### 7.6 Results and Discussion

We will now present a validation study of our new cascaded LB approach developed for incompressible two-phase flows for a variety of benchmark problems. Since the LB formulation for the interface capturing based on the conservative ACE has been analyzed in Ref. [233], we will limit the validation of our implementation in this regard for one benchmark problem below (Sec. 7.6.1). Instead, most of our focus in what follows will be on investigating the cascaded LB methods presented in the previous two sections for the coupled solution of the two-phase fluid motion with interfacial dynamics, especially at high density ratios and under different interfacial flow configurations.
7.6.1 Evolution of a circular interface in imposed shear flow

We will first assess the ability of the cascaded LB scheme for conservative ACE (see Sec. 7.5) to capture the kinematical effects of the interfacial motion under deformation and rotational effects with good fidelity. In this regard, we consider a circular interface subjected to an imposed shear flow given by the following velocity field in a periodic square domain of size $L_0$ [237]

$$
\begin{align*}
    u_x(x, y) &= -U_0 \pi \cos \left( \pi \left( \frac{x}{L_0} - \frac{1}{2} \right) \right) \sin \left( \pi \left( \frac{y}{L_0} - \frac{1}{2} \right) \right) \\
    u_y(x, y) &= U_0 \pi \sin \left( \pi \left( \frac{x}{L_0} - \frac{1}{2} \right) \right) \cos \left( \pi \left( \frac{y}{L_0} - \frac{1}{2} \right) \right),
\end{align*}
$$

where $U_0$ is the velocity scale. In our simulations, we take the radius of the circular interface to be $R = L_0/5$, whose center is initially located at $(x_c, y_c) = (L_0/2, 3L_0/10)$ in a square computational domain resolved with $L_0 = 200$. Moreover, the numerical parameters of the conservative ACE, i.e., the width $W$ and the mobility $M_\phi$ are set as follows: $W = 3$ and latter is obtained by considering a Peclet number $Pe = U_0 W / M_\phi = 60$. To guide interface undergoing deformation and rotation to return to its original position at $T = 2T_f$, where $T_f = L_0 / U_0$, the velocity field given above is reversed at $T = T_f$. Figure 7.1 presents snapshots of the interface, identified by the contours of $(\phi_A + \phi_B) / 2$ at the instants $T = 0, 0.5T_f, T_f, 1.5T_f, 2T_f$. It can be seen that the interface undergoes advection with complex shape changes under shear, and the cascaded LB method faithfully recovers the original circular shape with good accuracy after completing a cycle.

7.6.2 Laplace-Young relation of a static drop

We will now make a quantitative verification of the ability of the coupled cascaded LB formulations in the computation of the various forces and their balances in a static drop immersed in a fluid medium by considering high density ratios. In this regard, according the analytical predictions of the Laplace-Young’s relation, for a 2D drop at rest, the pressure difference between the it and the ambient fluid ($\Delta P$) is related to the surface tension $\sigma$ and its radius of curvature
FIGURE 7.1: Snapshots of the interface under an imposed shear flow with an initially circular shape computed by the cascaded LB method.
(1/R) via \( \Delta P = \sigma/R \), which we will use for comparison. In the simulations, we consider a drop of density \( \rho_A \) surrounded by an ambient fluid of density \( \rho_B \) and placed in the center of a periodic square domain resolved by 200 \( \times \) 200 grid nodes. We first performed simulations with a drop of radius \( R = 30 \) by considering a surface tension \( \sigma = 1 \times 10^{-3} \) at various density ratios of \( \rho_A/\rho_B = 10, 100, 1000 \) till they reached equilibrium. Figure 7.2 shows the surface contours of the pressure differences between the drop and the ambient fluid. It is evident that the pressure distribution within the drop is smooth and uniform and the jump across the interface is sharp and independent of the density ratio as expected. The cascaded LB method is seen to be robust even at relatively high density contrasts. Then, Fig. 7.3 shows a comparison between the computed pressure differences between the drop and the ambient fluid as a function of its curvature for three different values of the surface tension \( \sigma = 1 \times 10^{-3}, 5 \times 10^{-3}, 1 \times 10^{-4} \) at a density ratio of 1000 against the predictions given by the Laplace-Young relation. It verifies the expected linear dependence between \( \Delta P \) and \( 1/R \) and the computed results are found to be in good quantitative agreement with the analytical solution.
FIGURE 7.3: Comparison of the computed pressure differences (symbols) obtained using the cascaded LB method against the analytical predictions using the Laplace-Young relation for various values of the drop curvature $1/R$ with surface tension $\sigma = 5 \times 10^{-3}, 1 \times 10^{-3}, 1 \times 10^{-4}$. 
7.6.3 Rayleigh-Taylor instability

Next, we will investigate the cascaded LB methods for simulation of the classical Rayleigh-Taylor (R-T) instability. Such a gravitational acceleration-driven instability arises when a heavier fluid of density $\rho_A$ is placed on top of a lighter fluid of density $\rho_B$ in the presence of gravity, and the interface between the two fluids undergoes complex unsteady motion. A mesh size of $L \times 4L$, where $L = 201$, is employed, and periodic boundary conditions along the lateral vertical sides and no-slip boundary conditions at the top and bottom boundaries are imposed. The initial perturbation at the interface between the two fluids to initiate instability is described by a cosinusoidal function given by $y_0 = 2L + 0.1L \cos(2\pi x/L)$, where the origin of the coordinate system is fixed at the left bottom corner of the computational domain. The interfacial instability is characterized by the Reynolds number $\text{Re} = \rho_A \sqrt{gL}/\mu$ based on a velocity scale $U_c = \sqrt{gL}$, and the Atwood number $\text{At} = (\rho_A - \rho_B)/(\rho_A + \rho_B)$. Here, $\mu$ is the dynamic viscosity and $g$ is the acceleration due to gravity. The dimensionless timescale $T$ is then defined based on $U_c$ and $L$ as $T = U_c/(L\sqrt{\text{At}})$. In addition, for interface capturing, we consider $W = 5$, and the Peclet number $\text{Pe} = U_c L/M_\phi = 3000$.

By fixing $\text{At} = 0.5$, we performed simulations for two cases of the Reynolds number, i.e., $\text{Re} = 256$ and 3000. Figure 7.4 presents the evolution of the interface under flow instability at these two Reynolds numbers. In general, the spike formation by the heavier fluid moving downward is accompanied by a bubble of the lighter fluid rising upwards. The interface between the fluids undergoes complex shape changes leading to a roll-up of its tails under the dynamical effects of the two moving fluids. Moreover, at higher $\text{Re}$, when the inertial effects predominate over the viscous effects, small scale flow structures emerge. The snapshots of the simulated results of the R-T instability at various time instants are in overall agreement with the prior numerical results at $\text{Re} = 256$ (e.g., [22, 238]) and $\text{Re} = 3000$ (e.g., [221, 239]). Moreover, Fig. 7.5 shows quantitative comparisons of the computed values of the non-dimensional locations of the spike and
FIGURE 7.4: Snapshots of simulation of Rayleigh-Taylor instability at At = 0.5 and (a) Re = 256 and (b) Re = 3000.
bubble fronts scaled by \( L \) at both \( \text{Re} \) against prior numerical reference data. It can be that the numerical results obtained using the cascaded LB formulations for time evolution of the interface locations evaluated at the center (spike) and at the edges (bubble) are in good quantitative agreement with the respective reference results at both \( \text{Re} = 256 \) and \( \text{Re} = 3000 \).

![Graphs showing time evolution of bubble front and spike tip positions](image)

**FIGURE 7.5:** Time evolution of the positions of the bubble front and the spike tip for Rayleigh-Taylor instability at \( At = 0.5 \) and (a) \( \text{Re} = 256 \) and (b) \( \text{Re} = 3000 \).

### 7.6.4 Falling drop under gravity

We will now consider another unsteady two-phase flow problem involving a drop falling under a gravitational field. In such a case, during the descent of the drop, it undergoes significant shape changes due to deformation, which arises from a complex interplay between the gravity force, surface tension force and the viscous force. A drop of diameter \( D = 30 \) with a density \( \rho_A \) is placed initially at a location of \( (75, 300) \) in a rectangular domain that is divided into \( 151 \times 451 \) lattice nodes (with the origin of the coordinate system being located at the left bottom corner), and filled with a lighter ambient fluid of density \( \rho_B \). Free-slip boundary conditions are imposed on the top and bottom boundaries and lateral vertical sides are taken to be periodic. For this
computational set up, the gravitational force is applied everywhere by setting $F_{ext} = -(\rho - \rho_B)gj$.

The drop dynamics is characterized by the following non-dimensional numbers: Eotvos number $Eo = g(\rho_A - \rho_B)D^2/\sigma$ representing the gravity force relative to the surface tension and the Ohnesorge number $Oh = \mu_A/\sqrt{\rho_A D\sigma}$ representing the viscous effects. Following Ref. [240], we fix $\rho_A/\rho_B = 5$, $Eo = 43$ and study the influence of $Oh$ by considering $Oh = 0.3, 0.7$ and $1.0$, with $\nu_A = \nu_B = \nu$. These three values of $Oh$ are obtained by setting $\nu = 0.1, 0.2333$ and $0.3333$, respectively. For reporting results, the instantaneous time $t$ is non-dimensionalized as $T = t/\sqrt{D/g}$.

Figure 7.6 presents the snapshots of the evolution of the interface of the falling drop for the above three cases of $Oh$. In general, it can be seen that as $Oh$ increases, the viscous force increases relative to the surface tension force and hence the drop deformation is reduced. Thus, at a large value of $Oh = 1.0$, the drop undergoes relative small deformation attaining a steady state, while at $Oh = 0.7$, it is stretched more along the horizontal direction by the surface tension force after initially taking an ellipsoidal shape. On the other hand, at a still lower $Oh = 0.3$, the drop becomes considerably slender along the sides, while exhibiting bag-like shape due to shear under gravity in the presence of the prevailing surface tension force with smaller viscous force effects at later stages. These computed drop shape variations at different times with $Oh$ are consistent with the findings reported in Ref. [240].

7.6.5 Buoyancy-driven rising bubble

Next, we examine the ability of our cascaded LB formulations to simulate a well-defined two-phase flow problem involving a moving dispersed phase in a continuous phase with high density contrasts than those considered in the previous two cases. In this regard, we consider a bubble of diameter $D$ and density $\rho_B$ rising in an ambient fluid of density $\rho_A$, with $\rho_A/\rho_B$ being 1000, by buoyancy forces under various parametric conditions. This represents the buoyant motion of an
FIGURE 7.6: Evolution of a deforming drop falling under gravity for various values of the Ohnesorge number Oh of 0.3, 0.7 and 1.0 at a fixed Eotvos number Eo = 43 shown at time instants $T = 0, 2.04, 3.05, 4.07, 5.09, 6.11, 7.13, 8.14, \text{ and } 9.16$ (from top to bottom).
air bubble in water and is of practical interest. Our goal is to test the robustness of the cascaded LB approach to capture the various shape changes the bubble undergoes due to the balance between the different competing forces as well as simulate the time history of the bubble path with quantitative accuracy.

The computational configuration consists of a rectangular domain with a grid resolution of 161 × 481 in which a bubble of diameter resolved with 64 grid nodes is initially centered at a location (40, 120) (with the coordinate system’s origin being situated at the bottom left corner of the domain). Free slip boundary conditions are imposed on the two vertical sides and the no-slip conditions are considered on the top and bottom boundaries. This set up corresponds to that discussed in Refs. [241, 242]. The bubble is set in motion by applying a body force given by \( F_{ext} = -(\rho - \rho_A)gj \). The characteristic scales of this two-phase flow problem are: the length scale \( L = D \), the velocity scale \( U_g = \sqrt{gD} \), which represents the gravitational velocity, and the time scale \( T = L/U_g \). Based on these and the various competing forces (i.e., buoyancy, viscous and surface tension), the non-dimensional parameters of this two-phase flow problem are the Reynolds number \( Re = \rho_AU_gD/\mu_A \) and the Eotvos number \( Eo = \rho_AU_g^2D/\sigma \), along with the ratios of the fluid properties \( \rho_A/\rho_B \) and \( \mu_A/\mu_B \). The non-dimensional time for reporting time histories is represented by \( t^* = t/T \). Depending on the magnitudes of these dimensionless groups, the bubble undergoes complex interfacial shape changes, attaining either spherical-cap, dimpled ellipsoidal-cap or skirted configurations, among various possibilities [243].

By setting \( \rho_A/\rho_B = 1000 \) and \( \mu_A/\mu_B = 100 \) at a fixed Reynolds number \( Re = 35 \), we performed buoyancy-driven bubble rise simulations at various values of the Eotvos numbers \( Eo = 10, 50 \) and 125 (as in Refs. [242, 238]) using the cascaded LB methods. Figure 7.7 presents the computed evolution of the interface of the rising bubble at these three values of \( Eo \). When the role of the surface tension force is relatively significant in comparison with the other forces, as when the Eotvos number is low (\( Eo = 10 \)), the bubble undergoes smaller deformation that is initiated at its rear end, which then results in a flattening of that side as the bubble rises For the intermediate
case \((Eo = 35)\), the driving buoyancy force predominates the surface tension under the prevailing viscous force, resulting in a much larger deformation by stretching that leads to the formation of tails that elongates at later times. At even higher \(Eo = 125\), this process is more pronounced and the skirted shape accompanied by the pair of tails is further elongated and straightened. These computed shape variations with different \(Eo\) at various time are very similar with the results based on other methods \([242, 238]\). Furthermore, in order to make a quantitative comparison, we then compute the vertical coordinate of the center of mass of the rising bubble as it undergoes shape changes using 
\[
y_c = \frac{\int_{\Omega_b} y \, dx}{\int_{\Omega_b} 1 \, dx},
\]
where \(\Omega_b\) represents the region occupied by the bubble, for the case \(Re = 35\) and \(Eo = 125\). Figure 7.8 shows the non-dimensional center of mass as a function of the non-dimensional time computed using the cascaded LB schemes against the reference numerical results from Ref. \([238]\). It is evident that our approach is in good quantitative agreement with the available numerical data for the temporal evolution of the bubble paths, thereby verifying its accuracy and robustness for this high density ratio two-phase flow problem.

7.6.6 Impact of a drop on a thin liquid layer

As a final benchmark problem, we consider an inertia-driven two-phase flow problem at a high density ratio, i.e., the impact of a circular drop on a thin layer of fluid and the study of its subsequent outcomes. Such impact dynamics of drops leads to a rich variety of outcomes depending on the characteristic parameters representing the ratios of various attendant forces \([244]\). The computational set up considered for this example is described in Ref. \([245]\). Both the drop and the thin layer are considered to be the of the same liquid of density \(\rho_A\) and the ambient fluid is of density \(\rho_B\). We consider a high density ratio \(\rho_A/\rho_B = 1000\) to represent the impact of a water drop surrounded by air. The computational domain is resolved with 501 × 1501 grid nodes, in which the liquid layer is discretized by 150 grid nodes, while the drop radius \(R\) is represented by 100 mesh nodes. The interface thickness \(W\) is set to be 5. We impose periodic conditions on the two vertical boundaries, no-slip boundary condition on the bottom wall, and free-slip con-
FIGURE 7.7: Evolution of the interface of a buoyancy-driven rising bubble at \( Re = 35 \) and (a) \( Eo = 10 \), (b) \( Eo = 50 \), (c) \( Eo = 125 \).
FIGURE 7.8: Time history of the non-dimensional center of mass of a buoyancy-driven rising bubble at Re = 35 and Eo = 125.
dition on the top boundary. The drop is set into downward motion by setting it with an initial impact velocity $U = 0.05$. The dynamics and the impact outcomes of this problem is determined by the following non-dimensional parameters: the Reynolds number $Re = 2\rho_A UR/\mu_A$ and the Weber number $We = 2\rho_A U^2 R/\sigma$, which represents the ratio of the inertial force to the surface tension force, in addition to the ratios of the fluid properties, and the timescale is given as $2R/U$. In our cascaded LB simulations, with the density ratio given above, we set $\mu_A/\mu_B = 10$, the Weber number is fixed at $We = 8000$, and consider two different values of the Reynolds numbers: $Re = 20$ and $Re = 100$.

Figure 7.9 presents the evolutions of interfaces at these two Reynolds numbers upon drop impact. At the lower $Re = 20$, since the kinetic energy of the drop impact is relatively low, it merges with the liquid film, which is accompanied by the interfacial wave moving outwards. This results in the deposition of the drop as the outcome. On the other hand, as the $Re$ is increased to 100, upon drop impact, the interface initially spreads outcomes, and then with the higher attendant kinetic energy, it leads an ejecta sheet formation. This, in turn, spreads outwards by evolving into a splashing lamella that curls at its edges due to the competing surface tension and viscous frictional effects, leading to the splashing as the final outcome. These computed behaviors are consistent with other recent numerical results (e.g., [245]), which demonstrate the ability of the cascaded LB schemes to handle inertia-driven two-phase flows at high density ratios.

7.7 Comparative study of numerical stability of different collision models

Generally, it is known that the LB methods can be susceptible to numerical instabilities as the kinematic viscosity of the fluid being simulated is significantly lowered, which is strongly influenced by the type of collision model used. We will now assess the robustness of our cascaded LB formulation in achieving relatively low fluid kinematic viscosities, when compared to a single relaxation time (SRT) formulation for a two-fluid case study involving capillary oscillations of a
FIGURE 7.9: Evolution of the splashing of a drop on a thin film at $\text{We} = 8000$ and $\rho_A/\rho_B = 1000$ for (a) $\text{Re} = 20$ (b) $\text{Re} = 100$. 
liquid cylinder in another ambient lighter fluid. The SRT formulation for two-phase flows used for comparison is based on one SRT LB solver obtained as a discretization of the MCBE for two-phase fluid motion and another SRT LB scheme for capturing interfacial dynamics represented by the conservative ACE. We consider a periodic domain of resolution $200 \times 200$ in which a liquid cylinder of density $\rho_A$ is placed in another lighter ambient fluid of density $\rho_B$, where $\nu_A = \nu_B$ for simplicity, undergoes free oscillations. The oscillations are initiated from an initially elliptic configuration of the cylinder (semi-major axis $a = 25$ and semi-minor axis $b = 15$) via the capillary effects on its interface. Figure 7.10 shows a typical example of the evolution of the interface of the liquid cylinder undergoing free oscillations. Now, employing each of the two collision models,

![Graph](image_url)

FIGURE 7.10: Evolution of the interface of an oscillating liquid cylinder starting from an initial elliptic shape configuration with semi-major axis $a = 25$ and semi-minor axis $b = 15$; surface tension parameter $\tilde{\kappa} = 0.1$, kinematic viscosity $\nu_A = \nu_B = 0.01$ and density ratio $\rho_A/\rho_B = 100$.

for the above initial geometric configuration of the liquid cylinder with surface tension parameter $\tilde{\kappa} = 0.01$, and for four sets of values of the density ratios $\rho_A/\rho_B = 500, 600, 800$ and $900$, the kinematic viscosity of the fluids $\nu_A = \nu_B$ are gradually reduced till the simulations becomes unstable. Figure 7.11 reports the ratios of the minimum achievable viscosities for SRT and cascaded
LB formulations that allow stable simulations for the above values of density ratios. It is evident that dramatic improvements in numerical stability, by over one or two orders of magnitude, is achieved by the cascaded LB schemes when compared to the SRT LB schemes for this two-fluid case study. For example, even at high density ratio of 900, the lowest viscosity achieved by the cascaded LB schemes is smaller by a factor of over 55, when compared to that attained using the SRT LB schemes, and such factors are significantly higher at more moderate density ratios. These numerical stability improvements associated with using the cascaded LB formulations for two-phase flow simulations are consistent with the findings of previous studies on single-phase flows (e.g., [17, 206]).
7.8 Summary and Conclusions

In this chapter, we discussed new cascaded LB formulations based on central moments and multiple relaxation times for computation of two-phase, incompressible flows at high density ratios. Using the modified continuous Boltzmann equation (MCBE) for two-phase flows, which involves a kinetic transformation to handle numerical stiffness at high density gradients, as a starting point, a cascaded LB scheme for the solution of the incompressible two-phase fluid motion directly in terms of the pressure and velocity fields is constructed. This involves the representation of the collision step via the relaxation of various central moments to their equilibria that are obtained by matching the corresponding continuous central moments of the modified Maxwell distribution expressed in terms of the pressure field. In addition, a consistent forcing scheme to handle the surface tension and body forces, as well as the net gradient pressure force, whose effects on the changes in various moments are different, is constructed. In order to capture the interfacial dynamics, another cascaded LB method that solves the phase field based conservative Allen-Cahn (ACE), which evolves interfaces by advection due to fluid motion under competing effects of diffusion and sharpening terms, is developed. This is achieved by a modification of first order central moments of the corresponding equilibrium distribution function via the addition of the interface sharpening term. Simulations of a variety of benchmark problems, including the equilibrium of a static drop, Rayleigh-Taylor instability, falling drop under gravity, buoyancy-driven rising bubble, drop impact on a thin liquid layer, validated the ability of the cascaded LB schemes to reproduce complex two-phase interfacial flows at high density ratios with good accuracy. In addition, dramatic improvements in numerical stability in reaching relatively low viscosities in two-phase systems with the use of cascaded LB approach when compared to a single relaxation time formulation is demonstrated. Thus, the cascaded LB methods for coupled solution of the fluid motion and interfacial dynamics, based on the MCBE and conservative ACE, are accurate and robust for two-phase flow simulations with high contrasts in fluid properties. In addition, in Appendix F the efficacy of a phase field modeling the surfactant effects on two-phase flows using
a central moments based formulation is demonstrated.
Lattice Boltzmann (LB) methods, based on their compact and efficient collide-and-stream algorithmic steps, are among the important classes of kinetic schemes for computational fluid dynamics. Among the various collision models available for the LB methods, the cascaded formulation based on central moments and multiple relaxation times, which was originally constructed for athermal, single phase flows, is promising due to its natural ability to impose Galilean invariance and its enhanced numerical features such as improved numerical stability when compared to other approaches. In this dissertation, we advanced the state-of-the-art in this area by proposing several new schemes based on cascaded LB formulations with improved convergence and/or accuracy or enhanced numerical stability for a variety of complex fluid dynamics problems. A central theme in our research is the use of double (or more number of) distribution functions that evolve under central moments relaxations during the collision steps for computation of various multi-physics fluid flow applications, including heat transfer and multiphase systems. In particular, we presented and analyzed the following new developments: (i) convergence acceleration by preconditioning of the cascaded LB method with additional Galilean invariant corrections to improve solution accuracy for steady state flow simulations, (ii) implementation strategies for body forces and source terms in the simulations of fluid motion and scalar transport using cascaded LB schemes via operator splitting, (iii) cascaded LB methods for thermal convective flows in three-dimensions and cylindrical coordinates with axial symmetry, (iv) a kinetic approach for computing the vorticity fields locally in a double distribution functions (DDF) based LB formulation without relying on finite differences for spatial derivatives, and (v) cascaded LB schemes for two-phase flows and interface capturing based on phase-field models, with extensions for representing surfactant effects. In what follows, we will briefly summarize our research contributions in the above areas along with the findings made in each chapter of this dissertation:
Following the introduction in Chapter 1 that highlighted our research goals, Chapter 2 presented a cascaded LB method for the solution of the preconditioned Navier-Stokes (NS) equations to achieve convergence acceleration of steady state flows. The preconditioned NS equations involves a preconditioning parameter $\gamma$, which can be tuned to adjust the pseudo-sound speed in order to alleviate the numerical stiffness arising at low Mach numbers and thereby improve convergence. The preconditioned cascaded LB scheme is constructed by modifying its moment equilibria and source terms with using the preconditioning parameter. Simulations for a variety of complex benchmark flows demonstrated significant convergence acceleration, by one or more orders of magnitude, with the use of preconditioning. Furthermore, it is known that the LB schemes on standard lattices such as the D2Q9 lattice can result additional cubic-velocity errors in Galilean invariance (GI) due to the aliasing effects arising from the finiteness and symmetries of the lattice, irrespective of the collision model. In particular, the third-order diagonal moments degenerates to the first moments that result in the additional truncation error contributions to the recovery of the NS equations. In Chapter 1, we showed that for the solution of the preconditioned NS equations in a LB formulation, such cubic-velocity errors depend also on the preconditioning parameter, in addition to the fluid velocity. The structure of such non-GI truncation errors that are related to the velocity and density gradient terms with coefficients related to $\gamma$ was obtained using a Chapman-Enskog analysis and then a strategy to eliminate them via corrections to the moment equilibria of the preconditioned cascaded LB method was presented. Simulations with GI-corrected preconditioned central moment formulation showed significant improvements in accuracy and thus it can be concluded that our approach allows higher fidelity and faster simulations of steady state flows.

Chapter 3 focuses on new implementation strategies for the body forces in the solution of the fluid motion and source terms in the computation of the advection-diffusion transport of a scalar field in the cascaded LB framework. We proposed symmetrized operator splitting based approaches for body force/sources, which involves performing a pair of force/source steps with half time
steps before and after the collision step. They are implemented in terms of the changes on the moments of appropriate orders due to the source term/body force. This formulation is consistent with the classical Strang splitting, and is considerably simpler than the previous body force implementations in cascaded LB method, which involved lattice-dependent constructions and cumbersome implementations. Simulations with using our new algorithm for a variety of benchmark problems demonstrated its accuracy in the solution of the fluid motion and passive scalar transport influenced by body forces and source terms, respectively. In addition, our symmetrical time-splitting approach was found to be second order accuracy in time.

Thermal convective flows in three-dimensions (3D) arise in many engineering systems, nature and biophysical contexts. Chapter 4 presents new 3D cascaded LB formulations for the solution of the fluid motion in conjunction with that for the energy equation represented via the convection-diffusion of the temperature field based on a DDF approach. In particular, the derivations of the new cascaded collision operators based on central moments and multiple relaxation times for the solution of the temperature field on the D3Q15 and D3Q7 lattices are discussed in detail in this chapter, and the solution of the fluid flow is performed using another cascaded LB method proposed in a prior work. It is demonstrated that the structure of the cascaded collision operator for the scalar field is markedly different from that for the hydrodynamic fields due to the differences number of conserved quantities under collision, involving one (scalar field) in the former case and four (density and components of the velocity field) in the latter case. We then performed numerical simulations of buoyancy-driven convection of air in differentially heated cubic cavity at various Rayleigh numbers Ra. The numerical results for the non-dimensional peak convection velocities and the heat transfer rates at different Ra were found to be in good agreement with prior benchmark data, thereby validating our new 3D cascaded LB scheme for flows with heat transfer.

Thermally-driven fluid motion under buoyancy forces and rotational effects in cylindrical configurations is an important class of problems, which can be more efficiently solved by exploiting any inherent axial symmetry, as it can significantly alleviate the computational overhead when
compared to the full 3D simulations. Chapter 5 proposes axisymmetric cascaded LB schemes for the solution of thermal convective flows including swirling effects in a quasi-2D representation with geometric source terms based on a triple distribution functions approach. One cascaded LB scheme solves for the fluid motion in the meridian plane, i.e., the radial and axial velocity components and the pressure field using a D2Q9 lattice, the second scheme solves for the temperature field using a D2Q5 lattice, and the third scheme computes the azimuthal velocity component representing the swirling effects also using a more compact D2Q5 lattice. The collision steps in all the three schemes are based on central moments and multiple relaxation times, and the geometric source terms are incorporated via the symmetrized operator splitting technique proposed in Chapter 3. This unified cascaded LB formulation is then used to compute a wide range of complex axisymmetric thermal convective benchmark problems, including natural convection between two coaxial cylinders, Rayleigh-Bénard convection in a vertical cylinder, mixed convection in a slender vertical annulus between two cylinders under combined rotation and buoyancy forces, and convective flow of a melt during Czochralski crystal growth in a rotating cylindrical crucible. The computed results for the structures of the flow and temperature fields and the Nusselt number for various characteristic parameters are found to be in very good agreement with prior numerical benchmark data for these problems. Moreover, this validated axisymmetric cascaded LB approach is found to be second order accurate under grid agreement and exhibits significantly improved numerical stability when compared to other existing LB schemes based on other collision models for these problems.

Chapter 6 reports an interesting outcome of our research investigations related to the DDF-based LB formulations. Quantitative estimates of the vorticity field, or equivalently the skew-symmetric velocity gradient tensor, plays a central role in fluid mechanics, ranging from identification of flow structures to modeling of complex fluids. As indicated above, in many instances, it is necessary to compute fluid motion in conjunction with the advection-diffusion transport of a scalar field (e.g., temperature or concentration fields), which can be accomplished using DDF-LB method.
using any applicable collision model. In this chapter, for the first time in the LB literature, we propose a new kinetic strategy to locally compute the vorticity field by exploiting the additional degrees of freedom available in the collision model used for the solution of the scalar field. By means of a Chapman-Enskog analysis, we construct such an approach via introducing an intensional anisotropy in the scalar flux components in the third order, off-diagonal moment equilibria, and then combining the second-order, off-diagonal non-equilibrium moment components of both the LB schemes. This vorticity computation approach is entirely local in nature and avoids the need to use finite-differences for the spatial derivatives and hence naturally lend themselves for efficient implementation on modern parallel computing systems. The method is general as it can be constructed for any pair of lattice sets in the DDF-LB schemes that can independently support third order off diagonal moments, which includes several standard available lattice sets in different spatial dimensions. For the purpose of demonstration, we implement this strategy using a DDF-LB formulation using multiple relaxation times involve one LB scheme for the fluid motion and another one for the scalar transport, each using a D2Q9 lattice. Simulations of a variety of benchmark flow problems with analytical solutions validate the accuracy of our local vorticity computation method. Furthermore, it is also shown that the method converges with second order spatial convergence for the solution of the vorticity field.

Finally, an advanced application of our research endeavor related to multiphase flow modeling and simulations is presented in Chapter 7. It discusses a new cascaded LB formulation for incompressible, two-phase flows at high density ratios. One cascaded LB scheme for the solution of the hydrodynamics, i.e., the pressure and velocity fields, is constructed from the discretization of the modified continuous Boltzmann equation for two-phase flows obtained via a kinetic transformation to handle stiffness issues at high density gradients. As before, the collision step is prescribed via relaxation of various central moments to their equilibria. The latter are obtained by matching the continuous central moments of the modified Maxwell distribution function given in terms of the pressure field. The surface tension and body forces, as well as the net gradient
pressure force, are incorporated into this schemes via additional terms to consistently account for their effects on the changes of different moments. On the other hand, the interfacial dynamics is captured using another cascaded LB scheme based a phase field model represented by the conservative Allen-Cahn equation. This equation prescribes the evolution of interfaces by advection due to fluid motion and diffusion that is counteracted by an interface sharpening term. The latter is incorporated into the cascaded LB scheme as an additional term to its moment equilibria. We performed simulations of various two-phase flow benchmark problems, including the Rayleigh-Taylor instability, falling drop under gravity, buoyancy-driven rising bubble and drop impact on a thin liquid layer, which validated the accuracy of our formulation to represent complex interfacial flows at high density ratios. Moreover, we demonstrated that our cascaded LB scheme results in major improvements in numerical stability in attaining relatively low fluid viscosities in two-phase systems when compared to a LB scheme based on a SRT collision model. Finally, in order to further extend the capabilities of our two-phase cascaded LB formulation, we also introduced the effect of surfactants via an additional tangential surface tension gradient term in the interfacial force (See Appendix F). The surface concentration equation, based on a phase field model, is solved using yet another cascaded LB scheme. This approach is validated by comparisons against the analytical solutions for the terminal velocity of the self-migration of a drop under imposed linear surfactant concentration gradient and in the representation of equilibrium surfactant concentration profile.

Overall, this dissertation demonstrated the versatility of our advanced cascaded LB formulations based on central moments and multiple relaxation times with very good numerical properties, in terms of convergence, accuracy, and stability, i.e., robustness, in their applications to a wide range of complex flows with attendant multiphysics effects that are of broader interest. There are a number of areas in which the new methods that have been presented in this dissertation can be further extended and applied. In the following, we will highlight some of the potential research topics for future investigations that follows from the various developments discussed above:
• Combine preconditioning techniques discussed in Chapter 2 with multigrid (MG) methods in the cascaded LB scheme to further improve convergence acceleration to solve steady state flows.

• Extend the Galilean-invariant (GI) corrections approach presented in Chapter 2 for other parameter-dependent models for fluid flows, such as the volume-averaged representation of porous media flows via the Brinkman-Forchheimer-Darcy equation to improve solution accuracy by eliminating porosity and velocity dependent truncation errors.

• Develop MG-LB schemes based on double distribution functions such as those discussed in Chapters 4 and 5 for efficient simulation for flows with heat transfer.

• Extend the new DDF LB schemes developed for local vorticity computation in the simulations of flows with scale transport in 2D (see Chapter 6) to 3D and with using other advanced collision models and validate for high Reynolds number turbulent flows.

• Develop three-dimensional cascaded LB schemes for incompressible two-phase flows at high density ratios based on phase field models as an extension of the formulation discussed in Chapter 7.

• Extend and validate the diffuse-interface model for surfactant dynamics presented in Chapter 7 Appendix F to 3D.

• Combine the last two items above, and study the physics of surfactant-laden bubble dynamics in turbulent flows.
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APPENDIX A

1.1 Strang Splitting Implementation of Body Forces in 3D Central Moment LB Method

For the propose of illustration, we will consider the 3D central moment LB method using the three-dimensional, fifteen velocity (D3Q15) \[125\] lattice, but can be readily extended for other lattices such as the D3Q27 lattice. The components of the particle velocity vectors along with the $|1\rangle$ vector (which is used to represent the zeroth moment with the distribution function) for this lattice are

$$
|e_x\rangle = (0, 1, -1, 0, 0, 0, 1, -1, 1, -1, 1, -1, 1, -1)^\dagger,
$$

$$
|e_y\rangle = (0, 0, 0, 1, -1, 0, 0, 1, -1, 1, -1, 1, -1)^\dagger,
$$

$$
|e_z\rangle = (0, 0, 0, 0, 1, -1, 1, 1, 1, -1, -1, -1)^\dagger,
$$

$$
|1\rangle = (1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)^\dagger.
$$

The corresponding linearly independent orthogonal basis vectors are given by \[125\]

$$
|K_0\rangle = |1\rangle, \quad |K_1\rangle = |e_x\rangle, \quad |K_2\rangle = |e_y\rangle, \quad |K_3\rangle = |e_z\rangle,
$$

$$
|K_4\rangle = |e_x e_y\rangle, \quad |K_5\rangle = |e_x e_z\rangle, \quad |K_6\rangle = |e_y e_z\rangle,
$$

$$
|K_7\rangle = |e_x^2 - e_y^2\rangle, \quad |K_8\rangle = |e_x^2 + e_y^2 + e_z^2\rangle - 3 |e_z^2\rangle, \quad |K_9\rangle = |e_x^2 + e_y^2 + e_z^2\rangle - 2 |1\rangle,
$$

$$
|K_{10}\rangle = 5 |e_x(e_x^2 + e_y^2 + e_z^2)\rangle - 13 |e_x\rangle,
$$

$$
|K_{11}\rangle = 5 |e_y(e_x^2 + e_y^2 + e_z^2)\rangle - 13 |e_y\rangle, \quad |K_{12}\rangle = 5 |e_z(e_x^2 + e_y^2 + e_z^2)\rangle - 13 |e_z\rangle,
$$

$$
|K_{13}\rangle = |e_x e_y e_z\rangle,
$$

$$
|K_{14}\rangle = 30 |e_x^2 e_y^2 + e_x^2 e_z^2 + e_y^2 e_z^2\rangle - 40 |e_x^2 + e_y^2 + e_z^2\rangle + 32 |1\rangle.
$$

(1.1)
Then, the orthogonal matrix $K$ follows as

$$K = |K_0⟩, |K_1⟩, |K_2⟩, |K_3⟩, |K_4⟩, |K_5⟩, |K_6⟩, |K_7⟩, |K_8⟩,$$

$$|K_9⟩, |K_{10}⟩, |K_{11}⟩, |K_{12}⟩, |K_{13}⟩, |K_{14}⟩⟩,$$  \hspace{1cm} (1.3)

which maps the change of moments under collisions back to the changes in the distribution functions. The central moments and raw moments of the distribution function and its equilibrium of order $(m + n + p)$ are defined, respectively, as

$$\begin{pmatrix} \dot{\hat{\kappa}}_{x^m y^n z^p} \\ \hat{\kappa}_{eq}^{x^m y^n z^p} \end{pmatrix} = \sum_{\alpha} \begin{pmatrix} f_{\alpha} \\ f_{eq}^{\alpha} \end{pmatrix} (e_{\alpha x} - u_x)^m (e_{\alpha y} - u_y)^n (e_{\alpha z} - u_z)^p,$$ \hspace{1cm} (1.4)

and

$$\begin{pmatrix} \dot{\hat{\kappa}}'_{x^m y^n z^p} \\ \hat{\kappa}'_{eq}^{x^m y^n z^p} \end{pmatrix} = \sum_{\alpha} \begin{pmatrix} f_{\alpha} \\ f_{eq}^{\alpha} \end{pmatrix} e_{\alpha x}^m e_{\alpha y}^n e_{\alpha z}^p.$$ \hspace{1cm} (1.5)

The central moment equilibria used for the construction of the 3D cascaded collision operator for the D3Q15 lattice is presented in [125]. The collide and stream steps of the 3D cascaded method are formally represented in Eqs. (3.22a) and (3.22b), respectively. Owing to the mass and momentum being collision invariants, it follows that $\hat{g}_0 = \hat{g}_1 = \hat{g}_2 = \hat{g}_3 = 0$. For the non-conserved
The output velocity field \( u^0 = (u_x^o, u_y^o, u_z^o) \) is obtained following the streaming step as

\[
\rho u_x^o = \sum_{\alpha=0}^{14} f_{\alpha} c_{\alpha x}, \quad \rho u_y^o = \sum_{\alpha=0}^{14} f_{\alpha} c_{\alpha y}, \quad \rho u_z^o = \sum_{\alpha=0}^{14} f_{\alpha} c_{\alpha z}. \tag{1.7}
\]

As in the 2D case, the pre-collision forcing step \( F^{1/2} \) involves the following update to the velocity field:

\[
u_x = \frac{1}{\rho} \left( \rho u_x^o + \frac{F_x}{2} \Delta t \right), \quad u_y = \frac{1}{\rho} \left( \rho u_y^o + \frac{F_y}{2} \Delta t \right), \quad u_z = \frac{1}{\rho} \left( \rho u_z^o + \frac{F_z}{2} \Delta t \right), \tag{1.8}
\]

which will be used in the determination of the cascaded collision based change of different moments, i.e. \( \tilde{g}_3 \), where \( \beta = 4, 5, \ldots, 14 \) as given in Eq. (1.6). Analogously, the other post-collision step \( F^{1/2} \) in the symmetrized operator splitting can be written as

\[
\rho u_x^o = \rho u_x + \frac{F_x}{2} \Delta t, \quad \rho u_y^o = \rho u_y + \frac{F_y}{2} \Delta t, \quad \rho u_z^o = \rho u_z + \frac{F_z}{2} \Delta t, \tag{1.9}
\]
which, via Eq. (1.8), reads as

\[\rho u_x^p = \rho u_x^o + F_x \Delta t, \quad \rho u_y^p = \rho u_y^o + F_y \Delta t, \quad \rho u_z^p = \rho u_z^o + F_z \Delta t.\]  

(1.10)

In order to effectively introduce this effect into the 3D cascaded formulation, we take the first order moments of the post-collision distribution function \(f_x^p = f_\alpha + (K \cdot \mathbf{g})_\alpha\), which yields

\[\rho u_x^p = \sum_\alpha f_x^p e_{\alpha x} = \Sigma_\alpha f_\alpha e_{\alpha x} + \Sigma_\beta (K_\beta|e_x) \tilde{g}_\beta, \]  

(1.11a)

\[\rho u_y^p = \sum_\alpha f_y^p e_{\alpha y} = \Sigma_\alpha f_\alpha e_{\alpha y} + \Sigma_\beta (K_\beta|e_y) \tilde{g}_\beta, \]  

(1.11b)

\[\rho u_z^p = \sum_\alpha f_z^p e_{\alpha z} = \Sigma_\alpha f_\alpha e_{\alpha z} + \Sigma_\beta (K_\beta|e_z) \tilde{g}_\beta. \]  

(1.11c)

Based on the orthogonal basis vectors \(K_\beta\) given in Eq. (1.2), it follows that

\[\Sigma_\beta (K_\beta|e_x) g_\beta = 10 \tilde{g}_1, \quad \Sigma_\beta (K_\beta|e_y) g_\beta = 10 \tilde{g}_2, \quad \Sigma_\beta (K_\beta|e_z) g_\beta = 10 \tilde{g}_3. \]  

(1.12)

Using Eqs. (1.11a)-(1.11c) along with Eqs. (1.7) and (1.12) and comparing with (1.10), we obtain the following result for the change of first order moments due to the force field:

\[\tilde{g}_1 = \frac{F_x}{10} \Delta t, \quad \tilde{g}_2 = \frac{F_y}{10} \Delta t, \quad \tilde{g}_3 = \frac{F_z}{10} \Delta t. \]  

(1.13)

Finally, using Eq. (1.13) and Eq. (1.6) for the change of moments under cascaded collision in \((K \cdot \mathbf{g})_\alpha\) and expanding it, we get the expressions for the post collision-distribution function, which
read as

\[
\begin{align*}
  f_0^p &= f_0 + [\tilde{g}_0 - 2\tilde{g}_9 + 32\tilde{g}_{14}], \\
  f_1^p &= f_1 + [\tilde{g}_0 + \tilde{g}_1 + \tilde{g}_7 + \tilde{g}_8 - \tilde{g}_9 - 8\tilde{g}_{10} - 8\tilde{g}_{14}], \\
  f_2^p &= f_2 + [\tilde{g}_0 - \tilde{g}_1 + \tilde{g}_7 + \tilde{g}_8 - \tilde{g}_9 + 8\tilde{g}_{10} - 8\tilde{g}_{14}], \\
  f_3 &= f_3 + [\tilde{g}_0 + \tilde{g}_2 - \tilde{g}_7 + \tilde{g}_8 - \tilde{g}_9 - 8\tilde{g}_{11} - 8\tilde{g}_{14}], \\
  f_4^p &= f_4 + [\tilde{g}_0 - \tilde{g}_2 - \tilde{g}_7 + \tilde{g}_8 - \tilde{g}_9 + 8\tilde{g}_{11} - 8\tilde{g}_{14}], \\
  f_5^p &= f_5 + [\tilde{g}_0 + \tilde{g}_3 - 2\tilde{g}_8 - \tilde{g}_9 - 8\tilde{g}_{12} - 8\tilde{g}_{14}], \\
  f_6^p &= f_6 + [\tilde{g}_0 - \tilde{g}_3 - 2\tilde{g}_8 - \tilde{g}_9 + 8\tilde{g}_{12} - 8\tilde{g}_{14}], \\
  f_7^p &= f_7 + [\tilde{g}_0 + \tilde{g}_1 + \tilde{g}_2 + \tilde{g}_3 + \tilde{g}_4 + \tilde{g}_5 + \tilde{g}_6 + \tilde{g}_9 + 2\tilde{g}_{10} + 2\tilde{g}_{11} + 2\tilde{g}_{12} \\
  &\quad + \tilde{g}_{13} + 2\tilde{g}_{14}], \\
  f_8^p &= f_8 + [\tilde{g}_0 - \tilde{g}_1 + \tilde{g}_2 + \tilde{g}_3 - \tilde{g}_4 + \tilde{g}_5 + \tilde{g}_6 + \tilde{g}_9 - 2\tilde{g}_{10} - 2\tilde{g}_{11} + 2\tilde{g}_{12} \\
  &\quad - \tilde{g}_{13} + 2\tilde{g}_{14}], \\
  f_9^p &= f_9 + [\tilde{g}_0 + \tilde{g}_1 - \tilde{g}_2 + \tilde{g}_3 - \tilde{g}_4 + \tilde{g}_5 - \tilde{g}_6 + \tilde{g}_9 + 2\tilde{g}_{10} - 2\tilde{g}_{11} + 2\tilde{g}_{12} \\
  &\quad - \tilde{g}_{13} + 2\tilde{g}_{14}], \\
  f_{10}^p &= f_{10} + [\tilde{g}_0 - \tilde{g}_1 - \tilde{g}_2 + \tilde{g}_3 + \tilde{g}_4 - \tilde{g}_5 - \tilde{g}_6 + \tilde{g}_9 - 2\tilde{g}_{10} - 2\tilde{g}_{11} + 2\tilde{g}_{12} \\
  &\quad + \tilde{g}_{13} + 2\tilde{g}_{14}], \\
  f_{11}^p &= f_{11} + [\tilde{g}_0 + \tilde{g}_1 + \tilde{g}_2 - \tilde{g}_3 + \tilde{g}_4 + \tilde{g}_5 - \tilde{g}_6 + \tilde{g}_9 + 2\tilde{g}_{10} + 2\tilde{g}_{11} - 2\tilde{g}_{12} \\
  &\quad - \tilde{g}_{13} + 2\tilde{g}_{14}], \\
  f_{12}^p &= f_{12} + [\tilde{g}_0 - \tilde{g}_1 + \tilde{g}_2 - \tilde{g}_3 - \tilde{g}_4 + \tilde{g}_5 - \tilde{g}_6 + \tilde{g}_9 - 2\tilde{g}_{10} + 2\tilde{g}_{11} - 2\tilde{g}_{12} \\
  &\quad - \tilde{g}_{13} + 2\tilde{g}_{14}], \\
  f_{13}^p &= f_{13} + [\tilde{g}_0 + \tilde{g}_1 - \tilde{g}_2 - \tilde{g}_3 - \tilde{g}_4 - \tilde{g}_5 + \tilde{g}_6 + \tilde{g}_9 + 2\tilde{g}_{10} - 2\tilde{g}_{11} - 2\tilde{g}_{12} \\
  &\quad + \tilde{g}_{13} + 2\tilde{g}_{14}], \\
  f_{14}^p &= f_{14} + [\tilde{g}_0 - \tilde{g}_1 - \tilde{g}_2 - \tilde{g}_3 + \tilde{g}_4 + \tilde{g}_5 + \tilde{g}_6 + \tilde{g}_9 - 2\tilde{g}_{10} - 2\tilde{g}_{11} - 2\tilde{g}_{12} \\
  &\quad - \tilde{g}_{13} + 2\tilde{g}_{14}].
\end{align*}
\]
The overall algorithmic sequence of steps for the 3D cascaded LB method with the operator split forcing implementation is similar to that presented in Sec. 4. Notice the significant simplification offered by the present 3D symmetrized operator split forcing scheme, when compared to that presented in [125].
APPENDIX B

2.1 Structure of the 3D Central Moment-based Collision Kernel for Fluid Flow using a D3Q15 Lattice

The details of the derivation of the 3D cascaded LBM for fluid motion with forcing terms using the D3Q15 lattice is presented in [125]. Here, we summarize the main results for completeness and for comparison with the corresponding 3D cascaded LB model for the solution of the transport of a scalar field represented by the CDE. The collision kernel $\hat{g} = (\hat{g}_0, \hat{g}_1, \ldots, \hat{g}_{14})$ in the 3D cascaded LBE for field flow given in Eq. (4.2a) depends on the following set of moments:

$$
\begin{pmatrix}
\hat{\kappa}'_{x \mid y \mid z \mid p} \\
\hat{\kappa}'_{x \mid y \mid z \mid p} \\
\hat{\sigma}'_{x \mid y \mid z \mid p} \\
\hat{\kappa}'_{x \mid y \mid z \mid p}
\end{pmatrix}
= 
\sum_{\alpha}
\begin{pmatrix}
\bar{f}_{\alpha} \\
\bar{f}_{\alpha} \\
S_{\alpha} \\
\bar{f}_{\alpha}
\end{pmatrix}
\begin{pmatrix}
f_{\alpha} \\
f_{\alpha} \\
\epsilon_{\alpha x} \epsilon_{\alpha y} \epsilon_{\alpha z}
\end{pmatrix},
$$

(2.1)

where $\hat{\kappa}'_{x \mid y \mid z \mid p} = \hat{\kappa}'_{x \mid y \mid z \mid p} - \frac{1}{2} \hat{\sigma}'_{x \mid y \mid z \mid p}$. The specific expressions for raw moments of the source term $\hat{\sigma}'_{x \mid y \mid z \mid p}$ as well as the corresponding source terms in the velocity space $S_{\alpha}$ representing the effect of a body force is presented in [125]. Using the notation $\hat{\eta}'_{x \mid y \mid z \mid p} = \hat{\kappa}'_{x \mid y \mid z \mid p} + \hat{\sigma}'_{x \mid y \mid z \mid p}$ and by prescribing a central moment relaxation at different orders for the D3Q15 lattice, the structure of the collision kernel components for $\hat{g}$ can be expressed as (see [125] for details)
\[ \hat{g}_0 = \hat{g}_1 = \hat{g}_2 = \hat{g}_3 = 0, \quad (2.2) \]
\[ \hat{g}_4 = \frac{\omega_4}{8} \left[ -\tilde{\eta}_{xy} + \rho u_x u_y + \frac{1}{2} (\tilde{\sigma}_x^\prime u_y + \tilde{\sigma}_y u_x) \right], \quad (2.3) \]
\[ \hat{g}_5 = \frac{\omega_5}{8} \left[ -\tilde{\eta}_{zz} + \rho u_x u_z + \frac{1}{2} (\tilde{\sigma}_x^\prime u_z + \tilde{\sigma}_z u_x) \right], \quad (2.4) \]
\[ \hat{g}_6 = \frac{\omega_6}{8} \left[ -\tilde{\eta}_{yz} + \rho u_y u_z + \frac{1}{2} (\tilde{\sigma}_y^\prime u_z + \tilde{\sigma}_z u_y) \right], \quad (2.5) \]
\[ \hat{g}_7 = \frac{\omega_7}{4} \left[ -\tilde{\eta}_{xx} - \tilde{\eta}_{yy} + \rho(u_x^2 - u_y^2) + (\tilde{\sigma}_x^\prime u_x - \tilde{\sigma}_y^\prime u_y) \right], \quad (2.6) \]
\[ \hat{g}_8 = \frac{\omega_8}{12} \left[ -\tilde{\eta}_{xx} + \tilde{\eta}_{yy} - 2\tilde{\eta}_{zz} + \rho(u_x^2 + u_y^2 + 2u_z^2) \right. \]
\[ \left. + (\tilde{\sigma}_x^\prime u_x + \tilde{\sigma}_y^\prime u_y - 2\tilde{\sigma}_z^\prime u_z) \right], \quad (2.7) \]
\[ \hat{g}_9 = \frac{\omega_9}{18} \left[ -\tilde{\eta}_{xx} + \tilde{\eta}_{yy} + \tilde{\eta}_{zz} + \rho(u_x^2 + u_y^2 + u_z^2) \right. \]
\[ \left. + (\tilde{\sigma}_x^\prime u_x + \tilde{\sigma}_y^\prime u_y + \tilde{\sigma}_z^\prime u_z) + \rho \right], \quad (2.8) \]
\[ \hat{g}_{10} = \frac{\omega_{10}}{16} \left[ -\tilde{\eta}_{xyy} + 2u_y \tilde{\eta}_{xy} + u_x \tilde{\eta}_{yy} - 2\rho u_x u_y^2 - \frac{1}{2} \tilde{\sigma}_y u_x^2 - \tilde{\sigma}_y^\prime u_y u_x \right] \]
\[ + u_y \hat{g}_4 + \frac{1}{8} u_x (-\hat{g}_7 - \hat{g}_8 + 3\hat{g}_9), \quad (2.9) \]
\[ \hat{g}_{11} = \frac{\omega_{11}}{16} \left[ -\tilde{\eta}_{xxy} + 2u_x \tilde{\eta}_{xx} + u_y \tilde{\eta}_{xy} - 2\rho u_x u_x^2 - \frac{1}{2} \tilde{\sigma}_x^\prime u_x^2 - \tilde{\sigma}_x^\prime u_x u_y \right] \]
\[ + u_x \hat{g}_4 + \frac{1}{8} u_y (\hat{g}_7 + \hat{g}_8 + 3\hat{g}_9), \quad (2.10) \]
\[ \hat{g}_{12} = \frac{\omega_{12}}{16} \left[ -\tilde{\eta}_{xxz} + 2u_x \tilde{\eta}_{xz} + u_z \tilde{\eta}_{zx} - 2\rho u_x u_z^2 - \frac{1}{2} \tilde{\sigma}_x^\prime u_x^2 - \tilde{\sigma}_x^\prime u_x u_z \right] \]
\[ + u_x \hat{g}_5 + \frac{1}{8} u_z (\hat{g}_7 + \hat{g}_8 + 3\hat{g}_9), \quad (2.11) \]
\[ \hat{g}_{13} = \frac{\omega_{13}}{8} \left[ -\tilde{\eta}_{xyz} + u_x \tilde{\eta}_{y} + u_y \tilde{\eta}_{xz} + u_z \tilde{\eta}_{xy} - 2\rho u_x u_y u_z - \frac{1}{2} (\tilde{\sigma}_x^\prime u_x u_z \right. \]
\[ \left. + \tilde{\sigma}_y^\prime u_x u_y + \tilde{\sigma}_z^\prime u_x u_y) \right] + u_z \hat{g}_4 + u_y \hat{g}_5 + u_x \hat{g}_6, \quad (2.12) \]
\[ \hat{g}_{14} = \frac{\omega_{14}}{16} \left[ -\tilde{\eta}_{xyxyy} + 2u_x \tilde{\eta}_{xyxy} + u_y \tilde{\eta}_{xxxy} - u_x \tilde{\eta}_{yyxy} - u_x^2 \tilde{\eta}_{xx} - 4u_x u_y \tilde{\eta}_{xy} \right. \]
\[ \left. + \tilde{\eta}_{xxy} + 3\rho u_x u_x^2 + \tilde{\sigma}_x^\prime u_x u_y^2 + \tilde{\sigma}_y^\prime u_y u_x^2 \right] - 2u_x u_y \hat{g}_4 + \frac{1}{8} (u_x^2 - u_y^2) \hat{g}_7 \]
\[ + \frac{1}{8} (-u_x^2 - u_y^2) \hat{g}_8 + \left( \frac{3}{8}(-u_x^2 - u_y^2) - \frac{1}{2} \right) \hat{g}_9 + 2u_x \hat{g}_{10} + 2u_y \hat{g}_{11}, \quad (2.13) \]

where \( \omega_4, \omega_5, \ldots, \omega_{14} \) are the relaxation parameters \((0 < \omega_\beta < 2 \text{ for } \beta = 4, 5, \ldots, 14) \). The relaxation times for the second order moments control the kinematic viscosity \( \nu \) of the fluid being
simulated through \( \nu = c_s^2 \left( \frac{1}{\omega_j} - \frac{1}{T} \right) \), where \( j = 5, \cdots, 9 \). The rest of the relaxation parameters, which influence numerical stability, are set to unity in the present work. Finally, by expanding the product \( \mathbf{K}\mathbf{g} \) in Eq. (4.2a), the post-collision values of the distribution function are given by

\[
\tilde{f}_0 = f_0 + [g_0 - 2\tilde{g}_9 + 32\tilde{g}_{14}] + S_0,
\]

\[
\tilde{f}_1 = f_1 + [g_0 + \tilde{g}_1 + \tilde{g}_7 + \tilde{g}_8 - \tilde{g}_9 - 8\tilde{g}_{10} - 8\tilde{g}_{14}] + S_1,
\]

\[
\tilde{f}_2 = f_2 + [g_0 - \tilde{g}_1 + \tilde{g}_7 + \tilde{g}_8 - \tilde{g}_9 + 8\tilde{g}_{10} - 8\tilde{g}_{14}] + S_2,
\]

\[
\tilde{f}_3 = f_3 + [g_0 + \tilde{g}_2 - \tilde{g}_7 + \tilde{g}_8 - \tilde{g}_9 - 8\tilde{g}_{11} - 8\tilde{g}_{14}] + S_3,
\]

\[
\tilde{f}_4 = f_4 + [g_0 - \tilde{g}_2 - \tilde{g}_7 + \tilde{g}_8 - \tilde{g}_9 + 8\tilde{g}_{11} - 8\tilde{g}_{14}] + S_4,
\]

\[
\tilde{f}_5 = f_5 + [g_0 + \tilde{g}_3 - 2\tilde{g}_8 - \tilde{g}_9 - 8\tilde{g}_{12} - 8\tilde{g}_{14}] + S_5,
\]

\[
\tilde{f}_6 = f_6 + [g_0 - \tilde{g}_3 - 2\tilde{g}_8 - \tilde{g}_9 + 8\tilde{g}_{12} - 8\tilde{g}_{14}] + S_6,
\]

\[
\tilde{f}_7 = f_7 + [g_0 + \tilde{g}_1 + \tilde{g}_2 + \tilde{g}_3 + \tilde{g}_4 + \tilde{g}_5 + \tilde{g}_6 + \tilde{g}_9 + 2\tilde{g}_{10} + 2\tilde{g}_{11} + 2\tilde{g}_{12}
+ \tilde{g}_{13} + 2\tilde{g}_{14}] + S_7,
\]

\[
\tilde{f}_8 = f_8 + [g_0 - \tilde{g}_1 + \tilde{g}_2 + \tilde{g}_3 - \tilde{g}_4 - \tilde{g}_5 - \tilde{g}_6 - \tilde{g}_9 - 2\tilde{g}_{10} + 2\tilde{g}_{11} + 2\tilde{g}_{12}
- \tilde{g}_{13} + 2\tilde{g}_{14}] + S_8,
\]

\[
\tilde{f}_9 = f_9 + [g_0 + \tilde{g}_1 - \tilde{g}_2 + \tilde{g}_3 + \tilde{g}_4 + \tilde{g}_5 - \tilde{g}_6 + \tilde{g}_9 + 2\tilde{g}_{10} - 2\tilde{g}_{11} + 2\tilde{g}_{12}
- \tilde{g}_{13} + 2\tilde{g}_{14}] + S_9,
\]

\[
\tilde{f}_{10} = f_{10} + [\tilde{g}_0 - \tilde{g}_1 - \tilde{g}_2 + \tilde{g}_3 + \tilde{g}_4 - \tilde{g}_5 - \tilde{g}_6 + \tilde{g}_9 - 2\tilde{g}_{10} - 2\tilde{g}_{11} + 2\tilde{g}_{12}
+ \tilde{g}_{13} + 2\tilde{g}_{14}] + S_{10},
\]

\[
\tilde{f}_{11} = f_{11} + [\tilde{g}_0 + \tilde{g}_1 + \tilde{g}_2 - \tilde{g}_3 - \tilde{g}_4 - \tilde{g}_5 - \tilde{g}_6 + \tilde{g}_9 + 2\tilde{g}_{10} + 2\tilde{g}_{11} - 2\tilde{g}_{12}
- \tilde{g}_{13} + 2\tilde{g}_{14}] + S_{11},
\]

\[
\tilde{f}_{12} = f_{12} + [\tilde{g}_0 - \tilde{g}_1 + \tilde{g}_2 - \tilde{g}_3 + \tilde{g}_4 - \tilde{g}_5 - \tilde{g}_6 + \tilde{g}_9 - 2\tilde{g}_{10} + 2\tilde{g}_{11} - 2\tilde{g}_{12}
- \tilde{g}_{13} + 2\tilde{g}_{14}] + S_{12},
\]

\[
\tilde{f}_{13} = f_{13} + [\tilde{g}_0 + \tilde{g}_1 - \tilde{g}_2 - \tilde{g}_3 + \tilde{g}_4 + \tilde{g}_5 + \tilde{g}_6 + \tilde{g}_9 + 2\tilde{g}_{10} - 2\tilde{g}_{11} - 2\tilde{g}_{12}
+ \tilde{g}_{13} + 2\tilde{g}_{14}] + S_{13},
\]
\[ \tilde{f}_{14} = \tilde{f}_{14} + [\hat{g}_0 - \hat{g}_1 - \hat{g}_2 - \hat{g}_3 + \hat{g}_4 + \hat{g}_5 + \hat{g}_6 + \hat{g}_9 - 2\hat{g}_{10} - 2\hat{g}_{11} - 2\hat{g}_{12} - \hat{g}_{13} + 2\hat{g}_{14}] + S_{14}. \] (2.14)

Then, after performing the streaming step as given in Eq. (4.2b), we get the updated distribution function from which the velocity field \( \mathbf{u} \) can be computed as shown in Eq. (4.3).
3.1 Source Terms for the 3D Cascaded LBE for Scalar Field using D3Q15 Lattice

Using the source moments projected to the orthogonal basis vectors $\hat{m}^{s,\phi}$ defined in Eq. (4.20) and inverting it by using $S^\phi = K^{-1} \cdot \hat{m}^{s,\phi}$, and exploiting the orthogonality of the collision matrix $K$, we get following expressions for the source terms in the velocity space for the D3Q15 lattice used in the solution of the 3D CDE as

\[
\begin{align*}
S_0^\phi &= \frac{1}{45} \left[ 3\hat{m}_{0}^{s,\phi} - 5\hat{m}_{9}^{s,\phi} + \hat{m}_{14}^{s,\phi} \right], \\
S_1^\phi &= \frac{1}{180} \left[ 12\hat{m}_{0}^{s,\phi} + 18\hat{m}_{1}^{s,\phi} + 45\hat{m}_{7}^{s,\phi} + 15\hat{m}_{8}^{s,\phi} - 10\hat{m}_{9}^{s,\phi} - 9\hat{m}_{10}^{s,\phi} - \hat{m}_{14}^{s,\phi} \right], \\
S_2^\phi &= \frac{1}{180} \left[ 12\hat{m}_{0}^{s,\phi} - 18\hat{m}_{1}^{s,\phi} + 45\hat{m}_{7}^{s,\phi} + 15\hat{m}_{8}^{s,\phi} - 10\hat{m}_{9}^{s,\phi} + 9\hat{m}_{10}^{s,\phi} - \hat{m}_{14}^{s,\phi} \right], \\
S_3^\phi &= \frac{1}{180} \left[ 12\hat{m}_{0}^{s,\phi} + 18\hat{m}_{2}^{s,\phi} - 45\hat{m}_{7}^{s,\phi} + 15\hat{m}_{8}^{s,\phi} - 10\hat{m}_{9}^{s,\phi} - 9\hat{m}_{11}^{s,\phi} - \hat{m}_{14}^{s,\phi} \right], \\
S_4^\phi &= \frac{1}{180} \left[ 12\hat{m}_{0}^{s,\phi} - 18\hat{m}_{2}^{s,\phi} - 45\hat{m}_{7}^{s,\phi} + 15\hat{m}_{8}^{s,\phi} - 10\hat{m}_{9}^{s,\phi} + 9\hat{m}_{11}^{s,\phi} - \hat{m}_{14}^{s,\phi} \right], \\
S_5^\phi &= \frac{1}{180} \left[ 12\hat{m}_{0}^{s,\phi} + 30\hat{m}_{8}^{s,\phi} - 10\hat{m}_{9}^{s,\phi} - 9\hat{m}_{12}^{s,\phi} - \hat{m}_{14}^{s,\phi} \right], \\
S_6^\phi &= \frac{1}{180} \left[ 12\hat{m}_{0}^{s,\phi} - 18\hat{m}_{3}^{s,\phi} - 30\hat{m}_{8}^{s,\phi} - 10\hat{m}_{9}^{s,\phi} + 9\hat{m}_{12}^{s,\phi} - \hat{m}_{14}^{s,\phi} \right], \\
S_7^\phi &= \frac{1}{720} \left[ 48\hat{m}_{0}^{s,\phi} + 72\hat{m}_{1}^{s,\phi} + 72\hat{m}_{2}^{s,\phi} + 72\hat{m}_{3}^{s,\phi} + 90\hat{m}_{4}^{s,\phi} + 90\hat{m}_{5}^{s,\phi} + 90\hat{m}_{6}^{s,\phi} + 40\hat{m}_{9}^{s,\phi} \right].
\end{align*}
\]
\[ \begin{align*}
S_8^\phi &= \frac{1}{720} \left[ 48\hat{m}_0^s,\phi + 72\hat{m}_1^s,\phi + 72\hat{m}_2^s,\phi + 72\hat{m}_3^s,\phi - 90\hat{m}_4^s,\phi + 90\hat{m}_5^s,\phi + 90\hat{m}_6^s,\phi + 40\hat{m}_9^s,\phi \\
&\quad - 9\hat{m}_{10}^s,\phi + 9\hat{m}_{11}^s,\phi + 9\hat{m}_{12}^s,\phi - 90\hat{m}_{13}^s,\phi + \hat{m}_{14}^s,\phi \right], \\
S_9^\phi &= \frac{1}{720} \left[ 48\hat{m}_0^s,\phi - 72\hat{m}_1^s,\phi - 72\hat{m}_2^s,\phi + 72\hat{m}_3^s,\phi - 90\hat{m}_4^s,\phi + 90\hat{m}_5^s,\phi - 90\hat{m}_6^s,\phi + 40\hat{m}_9^s,\phi \\
&\quad + 9\hat{m}_{10}^s,\phi - 9\hat{m}_{11}^s,\phi + 9\hat{m}_{12}^s,\phi - 90\hat{m}_{13}^s,\phi + \hat{m}_{14}^s,\phi \right], \\
S_{10}^\phi &= \frac{1}{720} \left[ 48\hat{m}_0^s,\phi - 72\hat{m}_1^s,\phi - 72\hat{m}_2^s,\phi + 72\hat{m}_3^s,\phi + 90\hat{m}_4^s,\phi - 90\hat{m}_5^s,\phi - 90\hat{m}_6^s,\phi + 40\hat{m}_9^s,\phi \\
&\quad - 9\hat{m}_{10}^s,\phi - 9\hat{m}_{11}^s,\phi + 9\hat{m}_{12}^s,\phi + 90\hat{m}_{13}^s,\phi + \hat{m}_{14}^s,\phi \right], \\
S_{11}^\phi &= \frac{1}{720} \left[ 48\hat{m}_0^s,\phi + 72\hat{m}_1^s,\phi + 72\hat{m}_2^s,\phi - 72\hat{m}_3^s,\phi + 90\hat{m}_4^s,\phi - 90\hat{m}_5^s,\phi - 90\hat{m}_6^s,\phi + 40\hat{m}_9^s,\phi \\
&\quad + 9\hat{m}_{10}^s,\phi + 9\hat{m}_{11}^s,\phi - 9\hat{m}_{12}^s,\phi - 90\hat{m}_{13}^s,\phi + \hat{m}_{14}^s,\phi \right], \\
S_{12}^\phi &= \frac{1}{720} \left[ 48\hat{m}_0^s,\phi - 72\hat{m}_1^s,\phi + 72\hat{m}_2^s,\phi - 72\hat{m}_3^s,\phi - 90\hat{m}_4^s,\phi + 90\hat{m}_5^s,\phi - 90\hat{m}_6^s,\phi + 40\hat{m}_9^s,\phi \\
&\quad - 9\hat{m}_{10}^s,\phi + 9\hat{m}_{11}^s,\phi - 9\hat{m}_{12}^s,\phi + 90\hat{m}_{13}^s,\phi + \hat{m}_{14}^s,\phi \right], \\
S_{13}^\phi &= \frac{1}{720} \left[ 48\hat{m}_0^s,\phi + 72\hat{m}_1^s,\phi - 72\hat{m}_2^s,\phi - 72\hat{m}_3^s,\phi - 90\hat{m}_4^s,\phi + 90\hat{m}_5^s,\phi + 90\hat{m}_6^s,\phi + 40\hat{m}_9^s,\phi \\
&\quad + 9\hat{m}_{10}^s,\phi - 9\hat{m}_{11}^s,\phi - 9\hat{m}_{12}^s,\phi + 90\hat{m}_{13}^s,\phi + \hat{m}_{14}^s,\phi \right], \\
S_{14}^\phi &= \frac{1}{720} \left[ 48\hat{m}_0^s,\phi - 72\hat{m}_1^s,\phi - 72\hat{m}_2^s,\phi - 72\hat{m}_3^s,\phi + 90\hat{m}_4^s,\phi + 90\hat{m}_5^s,\phi + 90\hat{m}_6^s,\phi + 40\hat{m}_9^s,\phi \\
&\quad - 9\hat{m}_{10}^s,\phi - 9\hat{m}_{11}^s,\phi - 9\hat{m}_{12}^s,\phi + 90\hat{m}_{13}^s,\phi + \hat{m}_{14}^s,\phi \right](3.1)
\end{align*} \]
4.1 3D Cascaded LB Model for Transport of Temperature Field using a D3Q7 Lattice

The CDE for the scalar field \( \phi \), such as the temperature, given in Eq. (4.4) has the diffusion term with lower degree of symmetry than that of the viscous stress tensor term in the NSE. As a result, the lattice set to represent the CDE can possibly satisfy lower degree of symmetry and isotropy requirements than that for the NSE. Hence, one can also construct a simplified 3D cascaded LBE for the CDE using a three-dimensional, seven velocity (D3Q7) lattice. In this regard, the components of the particle velocity along with the unit vector for this lattice are given by

\[
|e_{\alpha x}\rangle = (0, 1, -1, 0, 0, 0, 0)^\dagger, \\
|e_{\alpha y}\rangle = (0, 0, 0, 1, -1, 0, 0)^\dagger, \\
|e_{\alpha z}\rangle = (0, 0, 0, 0, 0, 1, -1)^\dagger, \\
|\phi\rangle = (1, 1, 1, 1, 1, 1, 1)^\dagger. \quad (4.1)
\]

Starting from the nominal basis vectors

\[
T_0 = |\phi\rangle, \\
T_1 = |e_{\alpha x}\rangle, \quad T_2 = |e_{\alpha y}\rangle, \quad T_3 = |e_{\alpha z}\rangle, \\
T_4 = |e_{\alpha x}^2 - e_{\alpha y}^2\rangle, \quad T_5 = |e_{\alpha x}^2 - e_{\alpha z}^2\rangle \\
T_6 = |e_{\alpha x}^2 + e_{\alpha y}^2 + e_{\alpha z}^2\rangle,
\]
and applying the Gram-Schmidt procedure, the corresponding linearly independent orthogonal basis vectors are given by

\[ K_0 = |\phi \rangle, \quad K_1 = |e_{ax} \rangle, \quad K_2 = |e_{ay} \rangle, \quad K_3 = |e_{az} \rangle, \quad K_4 = |e_{ax}^2 - e_{ay}^2 \rangle, \]
\[ K_5 = 2 |e_{ax}^2 - e_{ay}^2 \rangle - |e_{ax}^2 - e_{ay}^2 \rangle, \quad K_6 = 7 |(e_{ax}^2 + e_{ay}^2 + e_{az}^2) - 6 |\phi \rangle. \]

Next, the orthogonal collision matrix can be written as

\[ K = [K_0, K_1, K_2, K_3, K_4, K_5, K_6, K_7]. \quad (4.2) \]

The discrete central moments of various quantities and their corresponding raw moments are given in Eq. (4.16) and Eq. (4.19), respectively, where \( \alpha = 0, 1, \cdots, 6 \) is considered. Following the overall procedure discussed in Sec. 2 and adopting it for the D3Q7 lattice, various results can now be summarized. First, the raw moments of the source term at different orders are given by

\[ \hat{\sigma}_{0}^{\phi} = R, \]
\[ \hat{\sigma}_{x}^{\phi} = u_x R, \quad \hat{\sigma}_{y}^{\phi} = u_y R, \quad \hat{\sigma}_{z}^{\phi} = u_z R, \]
\[ \hat{\sigma}_{xx}^{\phi} = u_x^2 R, \quad \hat{\sigma}_{yy}^{\phi} = u_y^2 R, \quad \hat{\sigma}_{zz}^{\phi} = u_z^2 R. \quad (4.3) \]

Then, as in Sec. 2 transforming them to the velocity space, the source term in the particle velocity space are given as

\[ S_0^{\phi} = \frac{1}{7} \left[ \tilde{m}_0^{s,\phi} - \tilde{m}_6^{s,\phi} \right], \]
\[ S_1^{\phi} = \frac{1}{84} \left[ 12 \tilde{m}_0^{s,\phi} + 42 \tilde{m}_1^{s,\phi} + 21 \tilde{m}_4^{s,\phi} + 7 \tilde{m}_5^{s,\phi} + 2 \tilde{m}_6^{s,\phi} \right], \]
\[ S_2^{\phi} = \frac{1}{84} \left[ 12 \tilde{m}_0^{s,\phi} - 42 \tilde{m}_1^{s,\phi} + 21 \tilde{m}_4^{s,\phi} + 7 \tilde{m}_5^{s,\phi} + 2 \tilde{m}_6^{s,\phi} \right], \]
\[ S_3^{\phi} = \frac{1}{84} \left[ 12 \tilde{m}_0^{s,\phi} + 42 \tilde{m}_1^{s,\phi} - 21 \tilde{m}_4^{s,\phi} + 7 \tilde{m}_5^{s,\phi} + 2 \tilde{m}_6^{s,\phi} \right], \]
\[ S_4^{\phi} = \frac{1}{84} \left[ 12 \tilde{m}_0^{s,\phi} - 42 \tilde{m}_1^{s,\phi} - 21 \tilde{m}_4^{s,\phi} + 7 \tilde{m}_5^{s,\phi} + 2 \tilde{m}_6^{s,\phi} \right], \]
\[ S_5^{\phi} = \frac{1}{42} \left[ 6 \tilde{m}_0^{s,\phi} + 21 \tilde{m}_3^{s,\phi} - 7 \tilde{m}_5^{s,\phi} + \tilde{m}_6^{s,\phi} \right], \]
\[ S_6^{\phi} = \frac{1}{42} \left[ 6 \tilde{m}_0^{s,\phi} - 21 \tilde{m}_3^{s,\phi} - 7 \tilde{m}_5^{s,\phi} + \tilde{m}_6^{s,\phi} \right]. \quad (4.4) \]
where

\[ \hat{m}_0^{\rho,\phi} = R, \quad \hat{m}_1^{\rho,\phi} = \langle K_1 | S_{\alpha} \rangle = u_x R, \quad \hat{m}_2^{\rho,\phi} = \langle K_2 | S_{\alpha} \rangle = u_y R, \]

\[ \hat{m}_3^{\rho,\phi} = \langle K_3 | S_{\alpha} \rangle = u_z R, \quad \hat{m}_4^{\rho,\phi} = \langle K_4 | S_{\alpha} \rangle = (u_x^2 - u_y^2) R, \]

\[ \hat{m}_5^{\rho,\phi} = \langle K_5 | S_{\alpha} \rangle = (u_x^2 + u_y^2 - 2u_z^2) R, \]

\[ \hat{m}_6^{\rho,\phi} = \langle K_6 | S_{\alpha} \rangle = (7u_x^2 + u_y^2 + u_z^2) R - 6R. \]  \hspace{1cm} (4.5)

Then, by prescribing central moment relaxation to their corresponding equilibria for first and higher orders, and following the approach presented in Sec. 2, we get the collision kernel for the D3Q7 lattice as

\[ \hat{h}_1 = 0, \]

\[ \hat{h}_1 = \frac{\omega_1^{\phi}}{2} \left[ \phi u_x - \widehat{\eta}_{xx} - \frac{R}{2} u_x \right], \]

\[ \hat{h}_2 = \frac{\omega_2^{\phi}}{2} \left[ \phi u_y - \widehat{\eta}_{yy} - \frac{R}{2} u_y \right], \]

\[ \hat{h}_3 = \frac{\omega_3^{\phi}}{2} \left[ \phi u_z - \widehat{\eta}_{zz} - \frac{R}{2} u_z \right], \]

\[ \hat{h}_4 = \frac{\omega_4^{\phi}}{4} \left[ -(\widehat{\eta}_{xx} + \widehat{\eta}_{yy} + \widehat{\eta}_{zz}) + 2(u_x \widehat{\eta}_{xx} - u_y \widehat{\eta}_{yy}) - (\phi + \frac{R}{2})(u_x^2 - u_y^2) \right] + \]

\[ \frac{1}{3}(u_x \hat{h}_1 + u_y \hat{h}_2 - 2u_z \hat{h}_3), \]

\[ \hat{h}_5 = \frac{\omega_5^{\phi}}{12} \left[ -(\widehat{\eta}_{xx} + \widehat{\eta}_{yy} + \widehat{\eta}_{zz} + 2u_x \widehat{\eta}_{xx} + u_y \widehat{\eta}_{yy} - 2u_z \widehat{\eta}_{zz}) - (\phi + \frac{R}{2})(u_x^2 + u_y^2 - 2u_z^2) \right] + \]

\[ \frac{2}{3}(u_x \hat{h}_1 + u_y \hat{h}_2 + u_z \hat{h}_3), \]  \hspace{1cm} (4.6)

where \( \omega_1^{\phi}, \omega_2^{\phi}, \ldots, \omega_6^{\phi} \) are relaxation parameters. The coefficient of diffusivity of the scalar field in the CDE, i.e. \( D_\phi \) in Eq. (4.4) is related to the relaxation parameters for the first order moments through \( D_\phi = \frac{c_s^2}{\omega_0^{\phi}} \left( \frac{1}{\omega_j^{\phi}} - \frac{1}{2} \right) \), where \( j = 1, 2, 3 \). Finally, the post-collision values of the distribution
function are obtained from Eq. (4.15a) after expanding $(\mathbf{K}\hat{\mathbf{h}})_\alpha$ for the D3Q7 lattice as

$$
\tilde{g}_0 = g_0 + [\hat{h}_0 - 6\hat{h}_6] + S^\phi_0,
$$

$$
\tilde{g}_1 = g_1 + [\hat{h}_0 + \hat{h}_1 + \hat{h}_4 + \hat{h}_5 + \hat{h}_6] + S^\phi_1,
$$

$$
\tilde{g}_2 = g_2 + [\hat{h}_0 - \hat{h}_1 + \hat{h}_4 + \hat{h}_5 + \hat{h}_6] + S^\phi_2,
$$

$$
\tilde{g}_3 = g_3 + [\hat{h}_0 + \hat{h}_2 - \hat{h}_4 + \hat{h}_5 + \hat{h}_6] + S^\phi_3,
$$

$$
\tilde{g}_4 = g_4 + [\hat{h}_0 - \hat{h}_2 - \hat{h}_4 + \hat{h}_5 + \hat{h}_6] + S^\phi_4,
$$

$$
\tilde{g}_5 = g_5 + [\hat{h}_0 + \hat{h}_3 - 2\hat{h}_5 + \hat{h}_6] + S^\phi_5,
$$

$$
\tilde{g}_6 = g_6 + [\hat{h}_0 - \hat{h}_3 - 2\hat{h}_5 + \hat{h}_6] + S^\phi_6. \quad (4.7)
$$
APPENDIX E

5.1 Relation between non-equilibrium moments and spatial derivatives of components of moment equilibria for D2Q9 lattice

For better clarity, the $O(\epsilon)$ moment system using a non-orthogonal moment basis given in Eq. (6.20b) in Sec. 6.2, i.e., $(\partial_t + \hat{\mathbf{E}}_i \partial_i)\hat{\mathbf{m}}(0) = -\hat{\mathbf{H}}\hat{\mathbf{m}}(1) + \hat{\mathbf{S}}$, which forms a main element in the derivation, can be expanded explicitly in terms of their various components as follows:

\[
\begin{align*}
\partial_t \hat{\chi}^{eq} + \partial_x \hat{\chi}^{eq} + \partial_y \hat{\chi}^{eq} &= \hat{\sigma}_0', \\
\partial_t \hat{\chi}^{eq} + \partial_x \hat{\chi}^{eq} + \partial_y \hat{\chi}^{eq} &= \hat{\sigma}_x', \\
\partial_t \hat{\chi}^{eq} + \partial_x \hat{\chi}^{eq} + \partial_y \hat{\chi}^{eq} &= \hat{\sigma}_y', \\
\partial_t (\hat{\chi}^{eq}_{xx} + \hat{\chi}^{eq}_{yy}) + \partial_x (\hat{\chi}^{eq}_{xx} + \hat{\chi}^{eq}_{xy}) + \partial_y (\hat{\chi}^{eq}_{yy} + \hat{\chi}^{eq}_{xy}) &= -\omega_3 \hat{m}_3^{(1)} + \hat{\sigma}_{xx} + \hat{\sigma}_{yy}, \\
\partial_t (\hat{\chi}^{eq}_{xx} - \hat{\chi}^{eq}_{yy}) + \partial_x (\hat{\chi}^{eq}_{xx} - \hat{\chi}^{eq}_{xy}) + \partial_y (\hat{\chi}^{eq}_{yy} + \hat{\chi}^{eq}_{xy}) &= -\omega_4 \hat{m}_4^{(1)} + \hat{\sigma}_{xx} - \hat{\sigma}_{yy}, \\
\partial_t \hat{\chi}^{eq}_{xy} + \partial_x \hat{\chi}^{eq}_{xy} + \partial_y \hat{\chi}^{eq}_{xy} &= -\omega_5 \hat{m}_5^{(1)} + \hat{\sigma}_{xy}, \\
\partial_t \hat{\chi}^{eq}_{xx} + \partial_x \hat{\chi}^{eq}_{xx} + \partial_y \hat{\chi}^{eq}_{xy} &= -\omega_6 \hat{m}_6^{(1)} + \hat{\sigma}_{xx}, \\
\partial_t \hat{\chi}^{eq}_{yy} + \partial_x \hat{\chi}^{eq}_{xy} + \partial_y \hat{\chi}^{eq}_{xy} &= -\omega_7 \hat{m}_7^{(1)} + \hat{\sigma}_{xy}, \\
\partial_t \hat{\chi}^{eq}_{xyy} + \partial_x \hat{\chi}^{eq}_{xyy} + \partial_y \hat{\chi}^{eq}_{xyy} &= -\omega_8 \hat{m}_8^{(1)} + \hat{\sigma}_{xyy}.
\end{align*}
\]

In general, it can be seen that any non-equilibrium moment of order $n$ depends on the spatial derivatives of equilibrium moments of order $(n + 1)$ and $(n - 1)$. In particular, the diagonal components of the second order moment ($\hat{m}_3^{(1)}$ and $\hat{m}_4^{(1)}$) depend on the moment equilibria of first order ($\hat{\chi}^{eq}_x$ and $\hat{\chi}^{eq}_y$) and third order ($\hat{\chi}^{eq}_{xx}$ and $\hat{\chi}^{eq}_{xy}$), while the off-diagonal second order moment ($\hat{m}_5^{(1)}$) depends only on that of third order equilibrium moments ($\hat{\chi}^{eq}_{xy}$ and $\hat{\chi}^{eq}_{xyy}$). These considerations are important in establishing the relationship between the non-equilibrium second-order
moments and the velocity gradient tensor components. In the case of the LBE for computing fluid flow, the symmetry of their moment equilibria to respect the isotropy of the viscous stress tensor limits the dependence of the corresponding non-equilibrium second order moments to only on the symmetric part of the velocity gradient tensor (i.e., the strain rate tensor). However, the construction of the LBE for computing the transport of a passive scalar represented by the CDE does not need to satisfy these restrictive constraints, and the additional degrees of freedom available for the higher order moments can be suitably exploited. Indeed, since the diffusion term of the CDE need only to satisfy a lower degree of isotropy than that of the viscous term of the NSE, the third order moment equilibria for the former case can be specifically designed to locally represent the skew-symmetric part of the velocity gradient tensor via the respective off-diagonal non-equilibrium second-order moment (based on an equation analogous to the sixth equation in the above moment system with $\hat{\kappa}_{x,m,y,n}^{eq}$ replaced by $\hat{\eta}_{x,m,y,n}^{eq}$ and $\hat{m}_{j}^{(1)}$ by $\hat{n}_{j}^{(1)}$ — Sec. 6.3.1).
APPENDIX F

6.1 Phase-field modeling of effect of soluble surfactant dynamics on two-phase flows

6.1.1 Introduction

Surface-active materials or surfactants play an important role in numerous two-phase or two-fluid dispersed systems where they strongly modulate phenomena associated with droplets and bubbles, such as in oil recovery, atomization systems, manufacturing processes related to biochemical and cosmetic products, and microfluidic devices. For example, the coalescence or breakup of dispersed phases and their transport, as well as the generation of stable droplet emulsions are crucially dependent on the presence of surfactants in interfacial flows. Surfactants preferentially adsorb on interfaces with nonuniform distribution, which then lowers the local surface tension and can induce additional fluid motion around interfaces via the tangential surface tension gradients or Marangoni stresses. Due to the complex nature of the transport of the surfactant between the bulk fluids and interfaces, and its coupling with the interfacial dynamics and the two-fluid motion, it is challenging to model and simulate surfactant-laden two-phase flows. Various computational methods, which can be classified according to either sharp-interface or diffuse-interface methods (see e.g., [246] for a review). Within the latter approaches, of particular interest to the present investigation are the phase-field methods.

A phase-field model for soluble surfactant dynamics coupled to two-fluid hydrodynamics was presented in [247], which was further generalized in [248]. The work of [249] pointed out some issues associated with the well-posedness of these models and then presented some modifications to the free-energy functional that avoided them. Moreover, in order to circumvent the rendering of the
interface thickness artificially dependent on the surfactant concentration, [250] presented an ad hoc solution by neglecting the effect of surfactant concentration on the chemical potential that drives the interfacial dynamics based on the Cahn-Hilliard equation (CHE) and also simplified the modeling of surface tension forces on surfactant-laden interfaces, which was adopted recently in [251] for studying the surfactant effect on droplet coalescence.

Given the ad hoc manner in which the chemical potential appearing in the CHE needs to be modified to eliminate the spurious surfactant concentration effects on the interfacial profile in the previous investigations, we present an alternate approach to capture interfaces in surfactant-laden two-phase flows based on the conservative Allen-Cahn equation (ACE). As also discussed in more detail earlier, the conservative ACE is a simpler approach with some better numerical properties such as smaller dispersive errors than the CHE as the former requiring computation of only second-order derivatives when compared to the latter that depends on fourth-order derivatives in its formulation. In addition, the solution of the two-phase fluid motion in our approach will be based on a kinetic theory formulation that is derived from the modified continuous Boltzmann equation (MCBE) for two-phase flows given in an earlier section, in which we will introduce a simpler geometric approach to formulate the effect of surfactants on the surface tension force, i.e., the lower of the local magnitude of surface tension and the Marangoni effects. Moreover, the chemical potential appearing in the surfactant concentration equation will be based on a well-posed gradient-free delta function formulation to represent adsorption effects [249], which is consistent with other modifications mentioned above. Finally, the solution of the surfactant concentration equation will be based on an advanced formulation using the cascaded LB method. As a result, the solution of the two-phase fluid motion, capturing of interfaces and the surfactant concentration will all be performed in a unified central moments based approach.
6.1.2 Surfactant concentration evolution equation

We will now present a phase-field based evolution equation for the surfactant concentration field. For ease of presentation, the surfactant concentration will be non-dimensionalized by its maximum or saturation value for the surfactant monolayer on the interface given by $\psi_\infty$. Hence, the non-dimensional local surfactant concentration $\psi = \psi(x, t)$ is restricted $0 \leq \psi \leq 1$. The distribution of the surfactant concentration $\psi(x, t)$ is determined under the competing effects of adsorption and diffusive processes as well as solubility effects as it undergoes advection from the fluid motion. On the other hand, the interfacial dynamics is represented by the evolution of the phase-field variable $\phi(x, t)$ represented by the conservative ACE (Eq. (7.1)), with the bulk fluid in each phase is identified as either $\phi_A$ or $\phi_B$. Its solution procedure based on a cascaded LB method is presented in Sec. 7.5. The diffuse interfacial profile and its thickness are thus independent of the surfactant concentration, which is required to avoid spurious effects and maintain physically consistent interfacial dynamics [250, 251].

Then, the transport of the surfactant concentration is represented by the following evolution equation

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = \nabla \cdot (M\psi \nabla \mu\psi),$$

(6.1)

where $M\psi$ is the local surfactant mobility that can be expressed as $M\psi = m\psi (1 - \psi)$, with $m\psi$ being the scale for the mobility parameter, and $\mu\psi$ represents the chemical potential, whose gradients drive the diffusion-adsorption dynamics of the advecting surfactant concentration field. Defining the following based on the order parameter of the phase field variable $\phi$ used to capture the interfacial dynamics

$$\phi_m = (\phi_A + \phi_B)/2, \quad \phi_0 = (\phi_A - \phi_B)/2,$$

the chemical potential $\mu\psi$ in earlier phase-field formulations can be written as [247, 248]

$$\mu\psi = \lambda \ln \left( \frac{\psi}{1 - \psi} \right) - \frac{s}{2} |\nabla \phi|^2 + \frac{w}{2} (\phi - \phi_m)^2.$$ 

(6.2)
In particular, second term on the RHS of the above chemical potential represents the preferential effect of the surfactant adsorption on the interface in terms of a delta function via a square gradient of the order parameter. However, for well-posedness with better numerical properties for wider ranges of parameter choices, Ref. [249] (see also the recent study [251]) suggested replacing it by means of a gradient-free regularized delta function formulation obtained using the hyperbolic tangent profile across the interface in the normal direction for the phase field variable \( \phi \). By adopting this latter strategy, the chemical potential used in this work can be rewritten as

\[
\mu_\psi = \lambda \ln \left( \frac{\psi}{1 - \psi} \right) - \frac{s}{2} \frac{4}{\phi^2_0 W^2} \left[ \phi^2_0 - (\phi - \phi_m)^2 \right]^2 + \frac{w}{2} (\phi - \phi_m)^2. \tag{6.3}
\]

Here, \( \lambda, s \) and \( w \) are model parameters that characterize the strengths of various competing processes. Each term on the RHS of the chemical potential appearing in Eq. (6.3) can be interpreted as follows (see e.g., [251]): the first term is referred to as the entropy term that bounds the surfactant concentration between 0 and 1 and denotes decrease in the system entropy when the surfactant is uniformly distributed everywhere, with higher \( \lambda \) driving stronger diffusion that tends to redistribute \( \psi \) more uniformly throughout the domain; the second term, also known as the adsorption term, expresses the energetic preference of surfactant to get adsorbed on interfaces, whose strength can be tuned by the parameter \( s \); finally, the last term is a penalty term the penalizes the presence of surfactant in the bulk fluids and expresses solubility effects, whose magnitude is controlled by the parameter \( w \), and hence it can also be referred to as the bulk term.

These last two terms oppose the diffusive process (first term) and sharpen the surfactant concentration profile around interfaces. Substituting Eq. (6.3) in Eq. (6.1) and rearranging, the evolution equation for the surfactant concentration field \( \psi \) can be rewritten as

\[
\frac{\partial \psi}{\partial t} + u \cdot \nabla \psi = \nabla \cdot (\lambda m_\psi \nabla \psi) + \nabla \cdot (m_\psi \psi (1 - \psi) P), \tag{6.4}
\]

where the second term of the RHS of the above equation can be interpreted as a flux term related to the adsorption and solubility of the surfactant, and \( P \) is given by

\[
P = \nabla \left( - \frac{s}{2} \frac{4}{\phi^2_0 W^2} \left[ \phi^2_0 - (\phi - \phi_m)^2 \right]^2 + \frac{w}{2} (\phi - \phi_m)^2 \right). \tag{6.5}
\]
Following the notations given in [249], with $U$, $L$ and $W$ being the velocity scale, length scale and interface thickness, respectively, the non-dimensional forms of various model parameters can be expressed as follows: $\text{Pe}_\psi = UL/m_\psi$ is the Peclet number, $\text{Ex} = 4s/(wW^2)$ is a number that characterizes the relative strength of adsorption and solubility effects, and $\text{Pi} = \lambda W^2/(8\tilde{\kappa}_0)$ is a number denoting the relative role of surfactant diffusion.

6.1.3 Interfacial force in the presence of surfactants via a geometric approach for the two-fluid motion

The solution of the surfactant-laden two-phase fluid motion that computes the pressure $p$ and the velocity fields $\mathbf{u}$ will be obtained from the cascaded LB method described in Sec. 7.4, which, in turn, is based on the modified continuous Boltzmann equation (MCBE) (see Sec. 7.3). The surface tension force $\mathbf{F}_s$ appearing in Eq. (7.8) needs to be modified to account for surfactant effects. In this regard, we will adopt the geometric formulation presented in [250]. The smoothed surface tension formulation for surfactant-laden interfacial flows with a local surfactant concentration $\psi$ can be written as

$$
\mathbf{F}_s = -\tilde{\kappa}(\psi)|\nabla \phi|^2 (\nabla \cdot \mathbf{n}) \mathbf{n} + |\nabla \phi|^2 \nabla_s \tilde{\kappa}(\psi),
$$

where $\nabla_s$ is the surface gradient operator given by $\nabla_s \equiv \nabla - \mathbf{n}(\mathbf{n} \cdot \nabla)$ or in index notation

$$
\partial_{si} = (\delta_{ij} - n_i n_j) \partial_j,
$$

where $i,j \in (x,y)$. The first term on the RHS of Eq. (6.6) represents the capillary force, where the lowering of the local surface tension by the presence of surfactant is accounted through the dependence of the surface tension parameter $\tilde{\kappa}$ on $\psi$, i.e., $\tilde{\kappa}(\psi)$ (see below for details). The second term represents the effects of the tangential gradients of the surface tension, or the Marangoni force, arising from the non-uniform concentration of the surfactant on the interface. The Cartesian components of the surface tension force for surfactant-laden interfaces
can then be expressed as

\[ F_{sx} = -\tilde{\kappa}(\psi) |\nabla \phi|^2 (\nabla \cdot \mathbf{n}) n_x + |\nabla \phi|^2 \left[ (1 - n_x^2) \partial_x \tilde{\kappa}(\psi) - n_x n_y \partial_y \tilde{\kappa}(\psi) \right], \tag{6.7a} \]

\[ F_{sy} = -\tilde{\kappa}(\psi) |\nabla \phi|^2 (\nabla \cdot \mathbf{n}) n_y + |\nabla \phi|^2 \left[ (1 - n_y^2) \partial_y \tilde{\kappa}(\psi) - n_x n_y \partial_x \tilde{\kappa}(\psi) \right], \tag{6.7b} \]

where \( n_x \) and \( n_y \) are the components of the interfacial unit normal \( \mathbf{n} = (n_x, n_y) = \nabla \phi / |\nabla \phi| \).

Such a geometric strategy enhances flexibility as the effect of surfactant on the surface tension force is naturally tunable with an appropriate choice of the interfacial equation of the state, when compared to the earlier approaches [247, 248]. In this work, the interface equation of state to represent the influence of the surfactant on (lowering) the local surface tension is given by the following non-linear dependence based on the Langmuir isotherm, i.e., \( \sigma(\psi) = \sigma_0 [1 + \beta \ln(1 - \psi)] \), or, equivalently

\[ \tilde{\kappa}(\psi) = \tilde{\kappa}_0 [1 + \beta \ln(1 - \psi)], \tag{6.8} \]

where \( \beta \) is the Gibbs elasticity number that parametrizes the sensitivity of the surface tension to the local surfactant concentration, and \( \sigma_0 \) and \( \tilde{\kappa}_0 \) correspond to those for the clean interfaces, i.e., without the presence of surfactant.

6.1.4 Cascaded LB method for the solution of the surfactant concentration field

The order parameter \( \phi \) for the capturing of interfaces and the two-phase fluid motion represented by the pressure and velocity fields can be computed using the respective cascaded LB methods discussed in Secs. 7.5 and 7.4, respectively. Then, in order to solve for the surfactant concentration \( \psi \) represented by the evolution equation, Eq. (6.4), in what follows, we construct another cascaded LB scheme. The collision and streaming steps of such a scheme for the evolution of the discrete distribution function \( h_\alpha \) can be respectively represented as

\[ \tilde{h}_\alpha(x, t) = h_\alpha(x, t) + (K \cdot \tilde{q})_\alpha, \tag{6.9a} \]

\[ h_\alpha(x, t + \delta_t) = \tilde{h}_\alpha(x - e_\alpha \delta_t, t), \tag{6.9b} \]
on a D2Q9 lattice and by considering the same moment basis as used in the previous sections
(Secs. 7.4 and 7.5).

For the construction of the collision operator, we first define the following central moments and
raw moments of \( h_\alpha \) and its equilibrium \( h_\alpha^{\text{eq}} \), respectively, as

\[
\left( \begin{array}{c}
\hat{\chi}_{mn}
\hat{\chi}^{\text{eq}}_{mn}
\end{array} \right) = \sum_{\alpha} \left( \begin{array}{c}
h_\alpha
h_\alpha^{\text{eq}}
\end{array} \right) (e_\alpha x - u_x)^m (e_\alpha y - u_y)^n,
\]

\( (6.10) \)

\[
\left( \begin{array}{c}
h_\alpha
h_\alpha^{\text{eq}}
\end{array} \right) e_\alpha^{m} e_\alpha^{n},
\]

\( (6.11) \)

Next, we define the continuous central moments of the equilibria

\[
\hat{\Pi}_{mn}^{\text{eq},\psi} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} h^{\text{eq}}(\xi_x - u_x)^m (\xi_y - u_y)^n d\xi_x d\xi_y
\]

\( (6.12) \)

by expressing the equilibrium distribution function \( h^{\text{eq}} \) in analogy with the local Maxwell dis-
tribution function by replacing the density with the surfactant concentration field \( \psi \): \( h^{\text{eq}} \equiv h^{\text{eq}}(\psi, u, \xi) = \frac{\psi}{2\pi c_s\psi} \exp \left[ -\frac{(\xi - u)^2}{2c_s^2\psi} \right] \). Here \( c_s\psi \) is a free parameter, which will be related to the coefficient of mo-
bility \( m_\psi \) later. Typically, we use \( c_s^2\psi = \frac{1}{3} \). The relaxation of the central moments to the corre-
sponding equilibria given above only models a diffusion process. In order to account for the flux
components due to the surfactant adsorption on the interface and its solubility effects in the bulk
fluids, i.e., \( m_\psi \psi(1 - \psi)P_x \) and \( m_\psi \psi(1 - \psi)P_y \), where \( P = (P_x, P_y) \) is given in Eq. (6.5) that
appears in the surfactant concentration evolution equation (Eq. (6.4)), we modify the first order
continuous central moments from being null to

\[
\hat{\Pi}_{10}^{\text{eq},\psi} = m_\psi \psi(1 - \psi)P_x \quad \text{and} \quad \hat{\Pi}_{01}^{\text{eq},\psi} = m_\psi \psi(1 - \psi)P_y.
\]

Then, by matching of the discrete and continuous central moments of the equilibria, i.e., \( \hat{\chi}^{\text{eq}}_{mn} = \hat{\Pi}_{mn}^{\text{eq},\psi} \) for all the nine independent moments supported by the lattice, we can get the components
of \( \hat{\chi}^{\text{eq}}_{mn} \), which are summarized as

\[
\hat{\chi}^{\text{eq}}_{00} = \psi, \quad \hat{\chi}^{\text{eq}}_{10} = m_\psi \psi(1 - \psi)P_x, \quad \hat{\chi}^{\text{eq}}_{01} = m_\psi \psi(1 - \psi)P_y, \quad \hat{\chi}^{\text{eq}}_{20} = c_s^2\psi, \quad \hat{\chi}^{\text{eq}}_{02} = c_s^2\psi,
\]

\[
\hat{\chi}^{\text{eq}}_{11} = 0, \quad \hat{\chi}^{\text{eq}}_{21} = 0, \quad \hat{\chi}^{\text{eq}}_{12} = 0, \quad \hat{\chi}^{\text{eq}}_{22} = c_s^4\psi.
\]
The cascaded collision operator can then be derived by expressing the relaxation of central moments of different orders to their equilibria, i.e., \( \sum_\alpha (\mathbf{K} \cdot \hat{\mathbf{q}})_\alpha (e_{\alpha x} - u_x)^m (e_{\alpha y} - u_y)^n = \omega_\beta^\psi (\hat{e}_{\alpha m}^{eq} - \hat{e}_{\alpha m}) \), where only the zeroth moment being conserved \( (\hat{e}_{00}^{eq} = \hat{e}_{00}) = \psi \), and \( \omega_\beta^\psi \) are the various relaxation times. The resulting changes in all the nine components of moments under collision, i.e., \( \hat{\mathbf{q}} = (\hat{q}_0, \hat{q}_1, \hat{q}_2, \ldots, \hat{q}_8) \) can be written as follows:

\[
\begin{align*}
\hat{q}_0 &= 0, & \hat{q}_1 &= \frac{\omega_1^\psi}{6} \left[ \psi u_x - \hat{\chi}_{10}' \right], & \hat{q}_2 &= \frac{\omega_2^\psi}{6} \left[ \psi u_y - \hat{\chi}_{01}' \right], \\
\hat{q}_3 &= \frac{\omega_3^\psi}{12} \left[ 2 c^2_{s^\psi} \psi - (u_x^2 + u_y^2) \psi - (\hat{\chi}_{20} - \hat{\chi}_{02}') + 2(u_x \hat{\chi}_{10} + u_y \hat{\chi}_{01}') \right] + u_x \hat{q}_1 + u_y \hat{q}_2, \\
\hat{q}_4 &= \frac{\omega_4^\psi}{4} \left[ -(u_x^2 - u_y^2) \psi - (\hat{\chi}_{10} - \hat{\chi}_{01}') + 2(u_x \hat{\chi}_{10} - u_y \hat{\chi}_{01}') \right] + 3(u_x \hat{q}_1 - u_y \hat{q}_2), \\
\hat{q}_5 &= \frac{\omega_5^\psi}{4} \left[ -u_x u_y \psi - \hat{\chi}_{11}' + (u_x \hat{\chi}_{01} + u_y \hat{\chi}_{10}') \right] + \frac{3}{2} (u_x \hat{q}_2 + u_y \hat{q}_1), \\
\hat{q}_6 &= \frac{\omega_6^\psi}{4} \left[ -u_x^2 u_y \psi + \hat{\chi}_{21}' - u_y \hat{\chi}_{20} + 2u_x \hat{\chi}_{11} + 2u_x u_y \hat{\chi}_{10} + u_y \hat{\chi}_{01}' \right] + 3u_x u_y \hat{q}_1 \\
&\quad + \left( \frac{3}{2} u_x^2 + 1 \right) \hat{q}_2 - \frac{3}{2} u_y \hat{q}_3 - \frac{1}{2} u_y \hat{q}_4 - 2u_x \hat{q}_5, \\
\hat{q}_7 &= \frac{\omega_7^\psi}{4} \left[ -u_x u_y \hat{\chi}_{12}' - u_x \hat{\chi}_{02}' - 2u_y \hat{\chi}_{11} + 2u_x u_y \hat{\chi}_{01} + u_y \hat{\chi}_{02}' \right] + \left( \frac{3}{2} u_y^2 + 1 \right) \hat{q}_1 \\
&\quad + 3u_x u_y \hat{q}_2 - \frac{3}{2} u_y \hat{q}_3 + \frac{1}{2} u_x \hat{q}_4 - 2u_y \hat{q}_5, \\
\hat{q}_8 &= \frac{\omega_8^\psi}{4} \left[ \left( u_y \hat{\chi}_{22}' - 2(u_x \hat{\chi}_{12} + u_y \hat{\chi}_{21}') - (u_y \hat{\chi}_{20} + u_x \hat{\chi}_{02}) - 4u_x u_y \hat{\chi}_{11} + 2(u_x u_y \hat{\chi}_{10} + u_x^2 u_y \hat{\chi}_{01}) \right) \\
&\quad - u_x^2 u_y^2 \hat{\chi} \right] + (2u_x + 3u_x u_y') \hat{q}_1 + (2u_y + 3u_x^2 u_y) \hat{q}_2 - (2 + \frac{3}{2} (u_x^2 + u_y^2)) \hat{q}_3 + \frac{1}{2} (u_x^2 - u_y^2) \hat{q}_4 \\
&\quad - 4u_x u_y \hat{q}_5 - 2u_y \hat{q}_6 - 2u_x \hat{q}_7, 
\end{align*}
\]

and accounting for the adsorption and solubility effects, we prescribe the changes in the first order moment components as

\[
\hat{q}_1 = \hat{q}_1 + \frac{\omega_1^\psi}{6} m_\psi \psi (1 - \psi) P_x, \quad \hat{q}_2 = \hat{q}_2 + \frac{\omega_2^\psi}{6} m_\psi \psi (1 - \psi) P_y, 
\]

(6.14)

Here, the relaxation times of the first order moments \( \omega_1^\psi \) and \( \omega_2^\psi \) are related to the mobility parameter \( m_\psi \) and the diffusion parameter \( \lambda \) in Eq. (6.4) via \( \lambda m_\psi = \epsilon_{s^\psi} \left( \frac{1}{\omega_j^\psi} - \frac{1}{2} \right) \delta_{ij}, j = 1, 2 \), and the rest of the relaxation times are set to unity. Using the above, the post-collision distribution
function $\tilde{h}_\alpha$ can be written in the component form after expanding $(\mathbf{K} \cdot \mathbf{q})_\alpha$ in Eq. (6.9a) as

$$
\tilde{h}_0 = h_0 + [\hat{q}_0 - 4(\hat{q}_3 - \hat{q}_8)],
$$

$$
\tilde{h}_1 = h_1 + [\hat{q}_0 + \hat{q}_1 - \hat{q}_4 + 2(\hat{q}_7 - \hat{q}_8)],
$$

$$
\tilde{h}_2 = h_2 + [\hat{q}_0 + \hat{q}_2 - \hat{q}_3 - \hat{q}_4 + 2(\hat{q}_0 - \hat{q}_8)],
$$

$$
\tilde{h}_3 = h_3 + [\hat{q}_0 - \hat{q}_1 - \hat{q}_3 + \hat{q}_4 - 2(\hat{q}_7 + \hat{q}_8)],
$$

$$
\tilde{h}_4 = h_4 + [\hat{q}_0 - \hat{q}_2 - \hat{q}_3 - \hat{q}_4 - 2(\hat{q}_0 + \hat{q}_8)],
$$

$$
\tilde{h}_5 = h_5 + [\hat{q}_0 + \hat{q}_1 + \hat{q}_2 + 2\hat{q}_3 + \hat{q}_5 - \hat{q}_6 + \hat{q}_7 + \hat{q}_8],
$$

$$
\tilde{h}_6 = h_6 + [\hat{q}_0 - \hat{q}_1 + \hat{q}_2 + 2\hat{q}_3 - \hat{q}_5 - \hat{q}_6 + \hat{q}_7 + \hat{q}_8],
$$

$$
\tilde{h}_7 = h_7 + [\hat{q}_0 - \hat{q}_1 - \hat{q}_2 + 2\hat{q}_3 + \hat{q}_5 + \hat{q}_6 + \hat{q}_7 + \hat{q}_8],
$$

$$
\tilde{h}_8 = h_8 + [\hat{q}_0 + \hat{q}_1 - \hat{q}_2 + 2\hat{q}_3 - \hat{q}_5 + \hat{q}_6 - \hat{q}_7 + \hat{q}_8].
$$

(6.15)

This is followed by performing the streaming step shown in Eq. (6.9b), which then finally updates the surfactant concentration field $\psi$ via taking the zeroth moment of $h_\alpha$ as

$$
\psi = \sum h_\alpha.
$$

(6.16)

It may be noted that for the implementation of the above scheme, we need to initialize the distribution function, which can be expressed in terms of its equilibrium in the velocity space as

$$
h_{\alpha}^{eq} = w_{\alpha}\psi\left[1 + \frac{e_{\alpha} \cdot \mathbf{u}}{c_s^2 \psi} + \frac{(e_{\alpha} \cdot \mathbf{u})^2}{2c_s^4 \psi} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2 \psi}\right] + m_\psi\psi(1 - \psi)w_\alpha\frac{e_{\alpha} \cdot \mathbf{P}}{c_s^2 \psi},
$$

(6.17)

where the weighting factors $w_{\alpha}$ are given by $w_0 = 4/9, w_\alpha = 1/9$, where $\alpha = 1, 2, 3, 4$ and $w_\alpha = 1/36$, where $\alpha = 5, 6, 7, 8$.

6.1.5 Numerical results

Young’s problem: Drop migration under imposed constant surfactant concentration gradient

First, we will validate the correctness of the implementation of the surface tension force for the surfactant-laden interfacial motion, i.e., Eqs. (6.7a) and (6.7b), and in particular the Marangoni
force, in our formulation. In this regard, we consider the classical Young’s problem of thermo-
capillary migration of a drop [252, 253] and recast into the equivalent surfactant concentration
gradient driven problem. According to this problem, a neutrally-buoyant drop of fluid $A$ with di-
ameter $D$ solely under an imposed linear surfactant concentration profile $\psi(y) = a + G_\Gamma y$ (i.e., $G_\Gamma$
being the constant gradient of the surfactant concentration field and $y$ is the vertical coordinate)
will self-propel in the ambient fluid $B$ and its terminal migration velocity under the assumption
of creeping flow has the following analytical solution:

$$V_\Gamma = -\frac{\sigma_\Gamma G_\Gamma D}{6\mu_B + 9\mu_A},$$

where $\sigma_\Gamma$ is the sensitivity of the surface tension with the surfactant concentration, which, ac-
cording to the linearized form of the Langmuir’s isotherm for dilute surfactant concentration, can
be expressed as $\sigma_\Gamma \equiv \partial \sigma / \partial \psi = -\sigma_0 \beta$. $\mu_A$ and $\mu_B$ are the respective dynamic viscosities.

We consider a drop with diameter $D = 30$ initially located near the bottom of a rectangular
domain resolved with $51 \times 201$ grid nodes. Periodic boundary conditions along the two verti-
cal sides and no-slip boundary conditions along the two horizontal sides are imposed. By using
a density ratio of unity, we consider the same dynamic viscosities in both the fluids by setting
the kinematic viscosities as $\nu_A = \nu_B = 0.05$. Furthermore, we impose a linear variation of the
surfactant concentration along the vertical direction by setting $G_\Gamma = 9.95 \times 10^{-5}$. Figure 6.1
shows the computed the drop migration velocities for three different surface tension sensitivities
$\sigma_0 \beta = 0.0048, \sigma_0 \beta = 0.0146$ and $\sigma_0 \beta = 0.0244$ and their comparisons against the available analytical solution for the terminal velocity. It is evident that after the initial transients, the computed migration velocities in the long time limit are in good agreement with the analytical terminal velocity. In addition, some snapshots of the evolution of a migrating drop for all the above three cases are presented in Fig. 6.2. As it can be seen, the drop self-propels under non-uniform surface tension (i.e., Marangoni force) arising due to an imposed constant concentration gradient without any smearing effects to the shape of the drop. Thus, the above numerical simulation results val-

idate our implementation of the surface tension force in the presence of a spatial distribution of
FIGURE 6.1: Comparison of computed drop migration velocity under imposed constant surfactant concentration gradient in the simulation of Young's problem (solid lines) with the analytical solution for the terminal velocity (dashed lines) for surface tension sensitivities $\sigma_0\beta = 0.0048$, $\sigma_0\beta = 0.0146$ and $\sigma_0\beta = 0.0244$. 
surfactant concentration.

Simulation of equilibrium surfactant concentration profile for a planar interface

In addition, we will now test the implementation of the cascaded LB scheme for the solution of the surfactant concentration equation. In this regard, an analytical solution for the equilibrium surfactant concentration profile for a planar interface can be used to make comparison. Such an analytical solution can be obtained under the condition that the chemical potential $\mu_\psi$ is uniform throughout the domain. In other words, by setting $\mu_\psi = \mu_\psi, b$, where $\mu_\psi, b$ is the value in the bulk region given by $\mu_\psi, b = \lambda \ln \psi_b + w(\phi_A - \phi_B)^2 / 8$, we get the analytical solution of the equilibrium surfactant concentration profile as

$$\psi_c^e(\zeta) = \frac{\psi_b}{\psi_b + \psi_c(\zeta)}, \quad (6.18)$$

where $\psi_b$ is the prescribed bulk surfactant concentration loading, and $\psi_c(\zeta)$ in an auxiliary function given by

$$\psi_c(\zeta) = \exp \left\{ -\frac{s}{2\lambda} \left[ \frac{2}{W} \phi_m \text{sech}^2 \left( \frac{2\zeta}{W} \right) \right]^2 + \frac{w}{2\lambda} \left[ \phi(\zeta) - \phi_m \right]^2 - \frac{w}{8} (\phi_A - \phi_B)^2 \right\}. \quad (6.19)$$

Here, $\phi(\zeta) = \phi_m + \phi_0 \tanh(2\zeta/W)$ is the corresponding equilibrium hyperbolic profile of the phase field variable. In the above, $\zeta$ is a coordinate along the normal direction originating at the interface.

We consider a computational domain with grid resolution $3 \times 10^1$ and choose the interface width $W = 3$, and the non-dimensional numbers are taken as $\text{Ex} = 1$, $\Pi = 49100$, from which the values of the parameters $s$ and $w$ can be obtained. For three different values of the bulk surfactant concentration, i.e., $\psi_b = 0.0001, \psi_b = 0.0002$, and $\psi_b = 0.0003$, the equilibrium surfactant concentration profiles are obtained through numerical simulations, which are presented in Fig. 6.3 along with the analytical solution for comparison. It can be seen that the surfactant concentration peaks at the interface. This reflects the preferential adsorption of surfactant around the in-
FIGURE 6.2: Snapshots of the evolution of a migrating drop under imposed constant surfactant concentration gradient in the simulation of Young’s problem for surface tension sensitivities $\sigma_0 \beta = 0.0048$, $\sigma_0 \beta = 0.0146$ and $\sigma_0 \beta = 0.0244$. 
terface, which is counteracted by the diffusion. Moreover, the computed equilibrium profiles are in good agreement with the analytical solution, which validates our implementation of the cascaded LB scheme for the surfactant concentration equation.

FIGURE 6.3: Comparison of computed (symbols) and analytical (linear) equilibrium profiles for surfactant concentration $\psi$ for a planar interface. Simulations are performed for the imposed surfactant concentrations in the bulk fluids $\psi_b = 0.0001$, $\psi_b = 0.0002$ and $\psi_b = 0.0003$. 