A new splitting scheme to the discrete Boltzmann equation for non-ideal gases on non-uniform meshes

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Abstract

We present a novel numerical procedure for solving the discrete Boltzmann equations (DBE) on non-uniform meshes. Our scheme is based on the Strang splitting method where we seek to investigate two-phase flow applications. In this note, we investigate the onset of parasitic currents which arise in many computational two-phase algorithms. To the best of our knowledge, the results presented in this work show, for the first time, a spectral element discontinuous Galerkin (SEDG) discretization of a discrete Boltzmann equation which successfully eliminates parasitic currents on non-uniform meshes. With the hope that this technique can be used for applications in complex geometries, calculations are performed on non-uniform mesh distributions by using high-order (spectral), body-fitting quadrilateral elements. Validation and verification of our work is carried out by comparing results against the classical 2D Young-Laplace law problem for a static drop.

Keywords: Multiphase, Spectral-element method, Discontinuous Galerkin method, Lattice Boltzmann method

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1. Introduction

Flows with interfaces between two phases are ubiquitous in nature and industry: rain drops falling on plant leaves, inkjet printing, and steam-water mixtures in a boiling water reactor (BWR). The interface represents a rapid but smooth transition of physical quantities between the bulk fluid values. Microscopic, long-range interactions among molecules along the interface place these fluids in tension. An accurate representation of the surface tension is critical when performing simulations of complex phenomena such as jet/droplet breakup or coalescence. Over the last few decades, one major challenge in modelling the surface tension has been the existence of parasitic or spurious currents. According to Lafaurie *et al.* [1], these currents are described as a “small amplitude velocity field due to a slight unbalance between stresses in the interfacial region.” Such currents may persist indefinitely thereby preventing the achievement of a true equilibrium state, and, possibly creating oscillations strong enough to entirely destroy the interface.

The lattice Boltzmann method (LBM) [2] does not directly solve the Navier-Stokes equations

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(NSE). Instead, lattice Boltzmann models solve simplified kinetic equations at the micro/meso-scopic level, so that macroscopic averaged properties obey the desired Navier-Stokes behavior. The LBM’s ability to incorporate intermolecular interactions at the microscopic level allow for appropriate recovery of interfacial dynamics at the macroscopic level. This has made the LBM a useful tool for simulating multiphase flows. We refer the reader to the following references for a more detailed review [2]-[8].

Similar to NSE solvers, LB-based schemes are also plagued by the onset of parasitic currents. Connington and Lee [9] provide a thorough review of multiphase LB models and their associated remedies to reduce or eliminate parasitic currents. One of the major contributions cited in their work is the model proposed by Lee and Fischer [10] where a free energy approach is adopted. Using a non-conservative formulation of the intermolecular force, known as the *potential* form, as well as an isotropic finite difference (FD) discretization of relevant gradients, they were able to successfully remove spurious currents for a static 2D droplet.

The goal of this work is to extend the approach of Lee and Fischer to non-uniform meshes. Most, if not all, of the previous LB models have been proposed for regular, isotropic lattice mesh which allows for the simple “perfect shift” implementation of the streaming procedure in LB schemes. Based upon our literature review, there is little analysis showing the reduction or elimination of spurious currents on non-uniform meshes. In the context of the LBM, there have been numerous models and algorithms proposed to tackle and study non-uniform meshes [11]-[17]. However, little work has been done on applying weighted residual schemes like the DG discretization or continuous finite element method (FEM) to multiphase flows. Wardle and Lee [18] utilized a standard Galerkin finite element method to discretize a non-homogeneous (i.e. with source term) streaming step in order to study free-surface flow in a concentric cylinder. Wang *et al.* [19] proposed a multiphase flow solver based on a finite volume discretization to a modified version of the Navier-Stokes equations which incorporated moment formulations of the macroscopic variables and momentum flux tensor. Yet, their work lacked any analysis on the reduction or elimination of parasitic currents. Since many multiphase engineering applications involve complex geometries (i.e. nuclear fuel assemblies or gas turbine engines), we believe that an LB-based analysis on how parasitic currents can be eliminated on non-uniform grids is required.

In this study, we apply the spectral element discontinuous Galerkin (SEDG) [14, 20] method to the Lee and Fischer [10] multiphase flow model. In particular, we seek to solve the discrete Boltzmann equation on non-uniform meshes using an SEDG discretization of the streaming step. Based upon our investigations, the common approach of calculating the effect of interfacial forces in the so called collision step does not eliminate parasitic currents. As a remedy, we propose a unique algorithm based on the Strang splitting [21, 22] procedure to solve DBE for non-ideal gases. Our procedure includes a source term within the streaming step. By coupling the SEDG method with a stable time-stepping technique, our scheme can easily handle the source term in a numerical sense. Such a procedure would be almost impossible if one sought to include a source term into the perfect shift implementation. We believe that this is the first time a SEDG method has been used in conjunction with a multiphase lattice Boltzmann model to successfully eliminate spurious currents.

This article is organized as follows. In section 2, we begin by presenting the relevant governing equations to our approach, namely the discrete Boltzmann equation (DBE) for non-ideal gases with a forcing term that was proposed by Guo *et al.* [23]. Also in this section, we derive two different procedures for solving the DBE from the perspective of Strang splitting. The first is the proposed, novel procedure which includes a portion of Guo's forcing term into the streaming step. The second is a well-known and popular technique that is based on the work of He, Shan and Doolen [3]. This section also includes a discussion on how to treat source terms explicitly. We illustrate this with the use of a common time-marching scheme. Finally, we conclude the section with a comparison between the two Strang splitting procedure and provide insight on how the latter Strang splitting procedure can lead to the onset of parasitic currents on non-uniform grids. Numericals tests are presented in section 4 where we investigate the spurious current phenomena for a static two-dimensional drop on unstructured and non-uniform meshes. In addition, we carry out a convergence test to validate the new scheme for the Young-Laplace law. We summarize our findings in section 5.

2. Governing Equations and Mathematical Model

The mathematical model that we choose for this study begins with the discrete Boltzmann equation (DBE) for isothermal non-ideal gases which undergo a collision process according to the BGK approximation [8]:

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla f_\alpha = -\frac{f_\alpha - f_\alpha^{eq}}{\lambda} + F_\alpha, \quad (1)$$

where f_α ($\alpha = 0, 1, \dots, N_\alpha$) is the single-particle density distribution function in the α -direction of the lattice model. Each function, f_α , is defined at a discrete set of spatial points, $\mathbf{x}$ and time levels t . Furthermore, the functions traverse the computational domain in the direction of their microscopic velocity $\mathbf{e}_\alpha$. The parameter λ is the relaxation time and controls the viscosity of the Navier-Stokes equations that are recovered from Eq. (1). N_α is the number of microscopic velocities. The equilibrium distribution function is given by

$$f_\alpha^{eq} = t_\alpha \rho \left[1 + \frac{(\mathbf{e}_\alpha \cdot \mathbf{u})}{c_s^2} + \frac{(\mathbf{e}_\alpha \mathbf{e}_\alpha - c_s^2 \mathbf{I}) : \mathbf{u} \mathbf{u}}{2c_s^4} \right], \quad (2)$$

where $\mathbf{u}$ is the macroscopic velocity; t_α are the weighting factors; ρ is the density of the fluid and c_s is the speed of sound and considered a constant. For this study, we choose a two-dimensional model commonly known as the D2Q9 model and values for $\mathbf{e}_\alpha$, t_α and c_s are given in [8, 14]. The second term on the right-hand side of Eq. (1) represents an external force applied to each particle and is based on the formulation provided by Guo *et al.* [23] who derived the following expression:

$$F_\alpha = t_\alpha \left(\frac{\mathbf{e}_\alpha}{c_s^2} + \frac{(\mathbf{e}_\alpha \cdot \mathbf{u}) \mathbf{e}_\alpha - \mathbf{u} c_s^2}{c_s^4} \right) \cdot \mathbf{F} \quad (3)$$

$\mathbf{F}$ is the intermolecular interaction force which can depend on both, space and time. We consider model proposed by Lee and Lin [8], called the *potential* form, where $\mathbf{F}$ is written as

$$\mathbf{F} = \nabla \rho c_s^2 - \rho \nabla (\mu_0 - \kappa \nabla^2 \rho). \quad (4)$$

μ_0 is the chemical potential of the bulk energy of the fluid and κ is a gradient parameter that is related to the interface thickness, D . The chemical potential, μ_0 , is a function of the bulk free energy, E_0 . Subsequent to [8], Lee and Fischer [10] incorporated this term into the model of He, Shan and Doolen [3].

2.1. Strang Splitting Method

The Strang splitting [21] technique is an alternative method to solving Eq. (1) while retaining second-order accuracy in time. We adopt this approach and propose the following method to compute f_α^{n+1} from f_α^n :

$$f_\alpha^{n+1} = C_\lambda^{A,I}(\delta t/2) \circ S_{\mathbf{e}_\alpha}^A(\delta t) \circ C_\lambda^{A,E}(\delta t/2) f_\alpha^n. \quad (5)$$

Here $C_\lambda^{A,I}(\delta t/2)$ and $C_\lambda^{A,E}(\delta t/2)$ represents the numerical solution operator for the following ordinary differential equation (ODE) system

$$\frac{df_\alpha}{dt} = -\frac{f_\alpha - f_\alpha^{eq}}{\lambda} + F_\alpha^* \quad (6)$$

over a half time-step, $\delta t/2$, and $S_{\mathbf{e}_\alpha}^A(\delta t)$ is the numerical solution operator for the following system:

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla f_\alpha = F_\alpha^* \quad (7)$$

over the full timestep, δt . With $F_\alpha^* = t_\alpha \left(\frac{\mathbf{e}_\alpha}{c_s^2} \right) \cdot \mathbf{F}$ and $F_\alpha^{**} = t_\alpha \left(\frac{(\mathbf{e}_\alpha \cdot \mathbf{u}) \mathbf{e}_\alpha - \mathbf{u} c_s^2}{c_s^4} \right) \cdot \mathbf{F}$. The superscripts E and I in Eq. (5) respectively indicate explicit and implicit Euler time-stepping schemes. Figure 1 shows a visual representation for the general Strang splitting scheme that is being proposed. The white circles in the figures represent intermediate values that have been determined by $C_\lambda^{A/B,E}(\delta t/2)$ and $S_{\mathbf{e}_\alpha}^{A/B}(\delta t)$ and are then evolved to f_α^{n+1} . The superscript B refers to an alternative Strang splitting technique described later in this section.

Figure 1: Time-stepping Table

Eq. (7) is a hyperbolic equation with a source term that can be fairly stiff. By coupling non-centered finite difference quotients for the spatial derivatives with a Runge-Kutta time integration method, Warming *et.al* [24] were one of the first to develop an explicit solution method to solve a hyperbolic equation with a source term. Later LeVeque and Yee [25], modified MacCormack's method to easily include a source term which was solved explicitly. Using a linearly implicit method and a careful treatment of the source term in the corrector step, their scheme achieved second-order accuracy overall. Upon further examination, we may re-write Eq. (7) in the following way:

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla (f_\alpha - t_\alpha \rho) + \vec{\pi}_\alpha \cdot \nabla \mu = 0 \quad (8)$$

where $\vec{\pi}_\alpha = \frac{\rho t_\alpha}{c_s^2} \mathbf{e}_\alpha$ and $\mu = \mu_0 - \kappa \nabla^2 \rho$. Eq. (8) now includes the $O(|\mathbf{e}_\alpha|)$ term of Eq. (3) and is represented using advection operators. One of the benefits to writing Eq. (8) is the opportunity to use a consistent spatial discretization, like upwinding, for the second and third term. Setting $\tau = \lambda/\delta t$, the proposed Strang splitting method takes the overall form given by:

$$C_\lambda^{A,E}(\delta t/2) : \quad f_\alpha^* = f_\alpha^n - \frac{(f_\alpha - f_\alpha^{eq})^n}{2\tau} + \frac{\delta t}{2} F_\alpha^{**,n} \quad (9)$$

$$S_{\mathbf{e}_\alpha}^A(\delta t) : \quad \frac{df_\alpha^*}{dt} = \mathbf{H}(f_\alpha^*, \rho, \mu) \quad (10)$$

$$C_\lambda^{A,I}(\delta t/2) : \quad f_\alpha^{n+1} = f_\alpha^{**} - \frac{(f_\alpha - f_\alpha^{eq})^{n+1}}{2\tau} + \frac{\delta t}{2} F_\alpha^{**,n+1}. \quad (11)$$

Hereinafter, we refer to this method as the Strang-splitting, Advection-with-Source, discrete Boltzmann method or **SAS-DBM** for short. The operation given by $S_{\mathbf{e}_\alpha}^A(\delta t)$ in Eq. (10) now represents a system of ODEs in time and forms a semi-discretized representation or a method-of-lines approach.

f_α^{**} represents the solution which is found from the streaming step, $S_{\mathbf{e}_\alpha}^A(\delta t)$. In this instance, the $\mathbf{H}$ represents the differential spatial operators in Eq. (8) and includes boundary information. From a computational perspective, we can make the Strang splitting procedure of Eqs.(9)–(11) more efficient by combining the implicit and explicit steps. This can be done by re-arranging the post-streaming step, $C_\lambda^{A,I}(\delta t/2)$, in the following manner:

$$f_\alpha^{n+1} = \frac{f_\alpha^{**} + \frac{1}{2\tau} f_\alpha^{eq,n+1} + \frac{\delta t}{2} F_\alpha^{**,n+1}}{1 + \frac{1}{2\tau}}, \quad (12)$$

and substituting into the pre-streaming step of $C_\lambda^{A,E}(\delta t/2)$.

The alternative to Eq. (5) is the splitting approach given by:

$$f_\alpha^{n+1} = C_\lambda^{B,I}(\delta t/2) \circ S_{\mathbf{e}_\alpha}^B(\delta t) \circ C_\lambda^{B,E}(\delta t/2) f_\alpha^n, \quad (13)$$

In a similar but slightly different formulation to the process above, $C_\lambda^{B,I}(\delta t/2)$ and $C_\lambda^{B,E}(\delta t/2)$ represents the numerical solution operator for the following ordinary differential equation (ODE) system

$$\frac{df_\alpha}{dt} = -\frac{f_\alpha - f_\alpha^{eq}}{\lambda} + F_\alpha \quad (14)$$

over a half time-step, $\delta t/2$, and $S_{\mathbf{e}_\alpha}^B(\delta t)$ is the numerical solution operator for the following system:

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla f_\alpha = 0 \quad (15)$$

Eq. (15) is the homogeneous linear advection equation written in the Eulerian form [15]. The overall form is now given by:

$$C_\lambda^{B,E}(\delta t/2) : f_\alpha^* = f_\alpha^n - \frac{(f_\alpha - f_\alpha^{eq})^n}{2\tau} + \frac{\delta t}{2} F_\alpha^n \quad (16)$$

$$S_{\mathbf{e}_\alpha}^B(\delta t) : \frac{df_\alpha^*}{dt} = \mathbf{L}(f_\alpha^*) \quad (17)$$

$$C_\lambda^{B,I}(\delta t/2) : f_\alpha^{n+1} = f_\alpha^{**} - \frac{(f_\alpha - f_\alpha^{eq})^{n+1}}{2\tau} + \frac{\delta t}{2} F_\alpha^{n+1}, \quad (18)$$

where $F_\alpha = F_\alpha^* + F_\alpha^{**}$ is defined by Eq. (3). Hereinafter, we refer to this method as the Strang-splitting, Advection-with-No Source, discrete Boltzmann method or **SANS-DBM** for short. The $\mathbf{L}$ represents the differential spatial operator in Eq. (15) and includes boundary information. Again, by combining the implicit (Eq. (18)) and explicit (Eq. (16)) steps via a re-arrangement to the implicit step (similar to Eq. (12)), the computations can be made more efficient. In fact, after appropriate variable substitutions are made, this procedure is easily recognized to be the popular scheme of He, Shan and Doolan [3] with the exception that the forcing term is now provided by Guo [23]. Furthermore, the solution to Eq. (15) is of little concern to most practitioners since this operation is carried out using the perfect shift implementation on regular grids where lattice points reside along characteristics.

2.2. Streaming on non-uniform meshes: An explicit treatment to the Source Term

A crucial component of the splitting methods written above are the streaming steps, described by Eqs. (7) and (15), as well as their respective numerical implementations $S_{\mathbf{e}_\alpha}^A(\delta t)$ and $S_{\mathbf{e}_\alpha}^B(\delta t)$. At the moment, it is difficult, if not impossible, to solve the streaming step with a source term when using the perfect shift implementation on a regular lattice grid. On the other hand, rigorous numerical techniques have been applied to Eqs. (7) and (15) which give accurate solutions on a variety of meshes including unstructured meshes where grid points may not necessarily reside along characteristics [13, 15, 14]. The semi-discretized forms in Eqs. (10) and (17), given by $S_{\mathbf{e}_\alpha}^A(\delta t)$ and $S_{\mathbf{e}_\alpha}^B(\delta t)$, are well-suited to be solved by a host of temporal integration methods like multi-step, predictor-corrector or Runge-Kutta methods.

In general, the conventional LBM adopts a combination of an explicit scheme for the streaming step and an implicit scheme for the collision step. This can be seen in the form of a trapezoidal rule [3, 14] which is used to integrate the right-hand side of Eq. (1) along characteristics. To benefit from a larger timestep (i.e. larger CFL number), implicit schemes for the streaming and collision operations have been proposed [15], however this procedure requires the inversion of the matrix which can become an expensive computational cost. In practice, many adopt a fully explicit numerical algorithm [3], which makes the LBM an attractive means to investigate interfacial flows. It is in this spirit where we seek to present a technique that can treat the source term in Eq. (7) explicitly. For example, the second-order Runge-Kutta (RK2) formula [26] for $S_{\mathbf{e}_\alpha}^A(\delta t)$ in Eq. (10) could be presented in the following (predictor-corrector) format:

• Predictor

$$f_\alpha^{*,n+1/2} = f_\alpha^{*,n} + \frac{\delta t}{2} \mathbf{H}^n, \quad (19)$$

• Corrector

$$f_\alpha^{*,n+1} = f_\alpha^{*,n} + \delta t \mathbf{H}^{n+1/2}, \quad (20)$$

where $\mathbf{H}^n \equiv F_\alpha^{*,n} - \mathbf{e}_\alpha \cdot \nabla f_\alpha^{*,n}$ and $\mathbf{H}^{n+1/2} = (\mathbf{H}^{n+1} + \mathbf{H}^n)/2$. This procedure can be written in the one-step form:

$$f_\alpha^{*,n+1} = f_\alpha^{*,n} + \delta t (F_\alpha^{*,n+1/2} - \mathbf{e}_\alpha \cdot \nabla f_\alpha^{*,n}) + \frac{\delta t^2}{2} \mathbf{e}_\alpha \cdot \nabla [\mathbf{e}_\alpha \cdot \nabla f_\alpha^{*,n} - F_\alpha^{*,n}]. \quad (21)$$

where $F_\alpha^{*,n+1/2} = (F_\alpha^{*,n+1} + F_\alpha^{*,n})/2$. A further approximation to terms at the $n + 1/2$ time level can be made by noting that $F_\alpha^{*,n+1} = F_\alpha^{*,n} + \delta t \frac{\partial F_\alpha^{*,n}}{\partial t} + O(\delta t^2)$ [27]. Hence, $F_\alpha^{*,n+1/2} = (2F_\alpha^{*,n} + \delta t \frac{\partial F_\alpha^{*,n}}{\partial t} + O(\delta t^2))/2 = F_\alpha^{*,n} + \frac{\delta t}{2} \frac{\partial F_\alpha^{*,n}}{\partial t} + O(\delta t^2/2)$. As a result, we arrive at the following explicit scheme

$$f_\alpha^{*,n+1} = f_\alpha^{*,n} + \delta t (F_\alpha^{*,n} - \mathbf{e}_\alpha \cdot \nabla f_\alpha^{*,n}) + \frac{\delta t^2}{2} \left[\mathbf{e}_\alpha \cdot \nabla [\mathbf{e}_\alpha \cdot \nabla f_\alpha^{*,n} - F_\alpha^{*,n}] + \frac{\partial F_\alpha^{*,n}}{\partial t} \right]. \quad (22)$$

A similar procedure for $S_{\mathbf{e}_\alpha}^B(\delta t)$ in Eq. (18) arrives at the following

$$f_\alpha^{*,n+1} = f_\alpha^{*,n} - \delta t (\mathbf{e}_\alpha \cdot \nabla f_\alpha^{*,n}) + \frac{\delta t^2}{2} \mathbf{e}_\alpha \cdot \nabla [\mathbf{e}_\alpha \cdot \nabla f_\alpha^{*,n}]. \quad (23)$$

It is worth noting that this procedure is identical to the one resulting from a Taylor-Galerkin or Lax-Wendroff (LW) procedure [15] and the additional, higher-order terms of Eqs. (22) and (23), help to stabilize the scheme by introducing diffusion in the characteristic or streamline direction, $\mathbf{e}_\alpha$ [27].

2.3. Comparing the two Strang-splitting schemes

Using the RK2/LW equations above, we may combine the collision and streaming steps of Eq. (11) into one complete equation that is given by

$$\begin{aligned} (f_\alpha^{n+1} - f_\alpha^n)|_{\text{SAS}} &= \delta t \left(-\frac{(f_\alpha - f_\alpha^{eq})^n}{2\lambda} - \frac{(f_\alpha - f_\alpha^{eq})^{n+1}}{2\lambda} + \frac{F_\alpha^{**,n+1} + F_\alpha^{**,n}}{2} + F_\alpha^{*,n} - \mathbf{e}_\alpha \cdot \nabla f_\alpha^n \right) \\ &+ \frac{\delta t^2}{2} [\mathbf{e}_\alpha \cdot \nabla] \left(\frac{(f_\alpha - f_\alpha^{eq})^n}{\lambda} - (F_\alpha^n - \mathbf{e}_\alpha \cdot \nabla f_\alpha^n) \right) \\ &+ \frac{\delta t^3}{4} [\mathbf{e}_\alpha \cdot \nabla]^2 \left(-\frac{(f_\alpha - f_\alpha^{eq})^n}{\lambda} + F_\alpha^{**,n} \right). \end{aligned} \quad (24)$$

Similarly, we may combine the collision and streaming steps of eq. (18) to give

$$\begin{aligned} (f_\alpha^{n+1} - f_\alpha^n)|_{\text{SANS}} &= \delta t \left(-\frac{(f_\alpha - f_\alpha^{eq})^n}{2\lambda} - \frac{(f_\alpha - f_\alpha^{eq})^{n+1}}{2\lambda} + \frac{F_\alpha^{n+1} + F_\alpha^n}{2} - \mathbf{e}_\alpha \cdot \nabla f_\alpha^n \right) \\ &+ \frac{\delta t^2}{2} [\mathbf{e}_\alpha \cdot \nabla] \left(\frac{(f_\alpha - f_\alpha^{eq})^n}{\lambda} - (F_\alpha^n - \mathbf{e}_\alpha \cdot \nabla f_\alpha^n) \right) \\ &+ \frac{\delta t^3}{4} [\mathbf{e}_\alpha \cdot \nabla]^2 \left(-\frac{(f_\alpha - f_\alpha^{eq})^n}{\lambda} + F_\alpha^n \right). \end{aligned} \quad (25)$$

It is important to mention that we have dropped the temporal derivative of F_α^n in Eq. (22) for the purpose of illustrating the difference between the two Strang splitting schemes. The main difference between these two equations occurs in the terms of $O(\delta t)$ and $O(\delta t^3)$. From one perspective, we may consider the behavior of these equations for the steady-state case. If the steady-state is reached, then we would expect the terms on the right-hand side of Eqs. (24) and (25) to vanish. In this instance we may perform Taylor expansions, up to order $O(\delta t^2)$, for terms on the right-hand side at the $n+1$ time level. The expansion introduces temporal derivatives which may be dropped since we assume

the steady-state is reached. Eqs. (24) and (25) then become

$$\begin{aligned}
(f_\alpha^{n+1} - f_\alpha^n)|_{\text{SAS}} &= \delta t \left(-\frac{(f_\alpha - f_\alpha^{eq})^n}{\lambda} + F_\alpha^n - \mathbf{e}_\alpha \cdot \nabla f_\alpha^n \right) \\
&+ \frac{\delta t^2}{2} [\mathbf{e}_\alpha \cdot \nabla] \left(\frac{(f_\alpha - f_\alpha^{eq})^n}{\lambda} - (F_\alpha^n - \mathbf{e}_\alpha \cdot \nabla f_\alpha^n) \right) \\
&+ \frac{\delta t^3}{4} [\mathbf{e}_\alpha \cdot \nabla]^2 \left(-\frac{(f_\alpha - f_\alpha^{eq})^n}{\lambda} + F_\alpha^{*,n} \right). \tag{26}
\end{aligned}$$

$$\begin{aligned}
(f_\alpha^{n+1} - f_\alpha^n)|_{\text{SANS}} &= \delta t \left(-\frac{(f_\alpha - f_\alpha^{eq})^n}{\lambda} + F_\alpha^n - \mathbf{e}_\alpha \cdot \nabla f_\alpha^n \right) \\
&+ \frac{\delta t^2}{2} [\mathbf{e}_\alpha \cdot \nabla] \left(\frac{(f_\alpha - f_\alpha^{eq})^n}{\lambda} - (F_\alpha^n - \mathbf{e}_\alpha \cdot \nabla f_\alpha^n) \right) \\
&+ \frac{\delta t^3}{4} [\mathbf{e}_\alpha \cdot \nabla]^2 \left(-\frac{(f_\alpha - f_\alpha^{eq})^n}{\lambda} + F_\alpha^n \right). \tag{27}
\end{aligned}$$

Furthermore, for the steady-state case, we note that Eq. (1) becomes a balance between the collision, force and advection terms. In other words, the temporal term vanishes to arrive at

$$\mathbf{e}_\alpha \cdot \nabla f_\alpha = -\frac{f_\alpha - f_\alpha^{eq}}{\lambda} + F_\alpha. \tag{28}$$

Incorporating Eq. (28) into Eqs. (26) and (27) shows that the terms of $O(\delta t)$ and $O(\delta t^2)$ vanish and what remains are

$$(f_\alpha^{n+1} - f_\alpha^n)|_{\text{SAS}} = \frac{\delta t^3}{4} [\mathbf{e}_\alpha \cdot \nabla]^2 (\mathbf{e}_\alpha \cdot \nabla f_\alpha - F_\alpha^{*,n}). \tag{29}$$

$$(f_\alpha^{n+1} - f_\alpha^n)|_{\text{SANS}} = \frac{\delta t^3}{4} [\mathbf{e}_\alpha \cdot \nabla]^2 (\mathbf{e}_\alpha \cdot \nabla f_\alpha). \tag{30}$$

In bulk phase regions, far from the interface, density gradients vanish and Eqs. (29) and (30) show that the steady-state is certainly achieved where $f_\alpha^{n+1} = f_\alpha^n$. On the other hand, in the vicinity of the interface, density gradients are not negligible. As a result, the advection term in Eq. (30) suggests a contribution to the solution that is not balanced by any term in the original discrete Boltzmann equation (i.e Eq. (1)). Including the source term via eq. (7) suggests that a proper balance is achieved at steady-state and no additional terms are introduced.

3. Numerical Tests

In this section, we investigate the parasitic current phenomena for a 2D stationary drop with stationary walls (i.e. $\mathbf{u}_b = \mathbf{0}$) using the **SAS-DBM** and **SANS-DBM** mentioned above. The spatial discretization to the streaming steps are based on the spectral-element discontinuous Galerkin (SEDG) method. Details on this discretization can be found in [20]. The results include calculations that have been performed on non-uniform meshes which are the result of using high-order, spectral elements. We also include the convergence of the Young-Laplace law.

3.1. Two-Dimensional (2D) Stationary Drop

In this section, we present computational results for a two-dimensional stationary droplet. The computational domain is a square box, defined via $\Omega := [-1, 1]^2$, and is filled with quadrilateral spectral elements. A droplet is placed in the center of the domain with radius, $R_o = 0.5$. Using the *D2Q9* microscopic model, we perform our analysis on uniform and non-uniform distributions of spectral elements. Fig. 2 shows the velocity fields for the three different numerical schemes. In each case, the density ratio is $\rho_l/\rho_v = 10$ where $\rho_l = 1.0$ and $\rho_v = 0.1$. The influence of the surface tension, σ , is manifest in the parameter, $\beta = \frac{12\sigma}{(\rho_l^{sat} - \rho_v^{sat})^4 D}$ [10]. The interface thickness is $D = 0.05$. We choose $\beta = 0.01$, and $\tau = 0.5$. In each image, the initial condition and static density profile is given by the hyperbolic tangent function: $\rho(s) = \frac{\rho_l^{sat} + \rho_v^{sat}}{2} + \frac{\rho_l^{sat} - \rho_v^{sat}}{2} \tanh\left(\frac{2s}{D}\right)$. s is the coordinate normal to the interface. The image on the left shows the velocity vectors, magnified by 10^{15} , for the **SAS-DBM** scheme. The right image shows velocity vectors, magnified by $\sim 10^2$, for the **SANS-DBM** scheme. The red line in the figure shows the $\rho = .55$ contour. In both cases, the velocity vectors are shown after $\sim 10^6$ timesteps, which is when a steady-state solution is assumed. The calculations were performed on a uniform mesh of size $E = 32 \times 32$ elements with the polynomial order of $N = 5$. The **SANS-DBM** show the presence of parasitic currents near in the vicinity of the interface while they disappear rapidly as you move further away. Using the proposed **SAS-DBM** scheme, the parasitic currents are nearly eliminated - confirmed in the image on the left. These results shed light on the differences between Eqs. (29) and (30) - suggesting that the advection term (without a source term to provide the necessary balance) can lead to spurious effects. To the best of our knowledge, the results from the **SAS-DBM** represent the first time a weighted residual method (like the SEDG method) has been applied to the lattice Boltzmann equations for non-ideal gases which can successfully eliminate parasitic currents.

Based upon the results from Fig. 2, we focus the remainder of our investigation on the elimination of parasitic currents by examining the **SAS-DBM** for a variety of parameters. To begin, we test the method on a non-uniform mesh distribution. Fig. 3 shows a non-uniform mesh using $E = 16 \times 16$ elements, where the elements are refined in the vicinity of the drop. We employ polynomial order of $N = 7$ for a stationary drop with interface thickness of $D = 0.05$. Fig. 4 shows the time evolution of the maximum kinetic energy for variable β (i.e. surface tension) and for variable relaxation times (τ). To physically characterize these investigations we introduce the non-dimensional Laplace (La) number, defined as

$$La = \frac{\sigma 2R_o}{\rho \nu^2}. \quad (31)$$

We may interpret the Laplace number as a way to understand the magnitude of the capillary wave generated by the interface relative to the momentum transport via viscous diffusion. In the plots, the time is non-dimensionalized to the viscous time of the vapor phase, $t_v = \rho_v \nu_v R / \sigma$. In both cases, the maximum kinetic energy diminishes exponentially to round-off with time. In the case of fixed τ and variable β , we see that the curves collapse almost entirely onto a single curve with the non-dimensionalization of time. For larger β , which indicates higher a surface-tension coefficient and smaller compressibility, we notice that the rate at which the max. kinetic energy achieves

Figure 2: Momentum field, $\rho\mathbf{u}$, after 10^6 timesteps for the **SAS-DBM** (left) magnified by 10^{15} and the **SANS-DBM** (right), magnified by 10^2 . Results are shown for $D = 0.05$ and $\beta = 0.01$. Momentum field is taken after 10^6 timesteps. The red line in the figure shows the $\rho = 0.55$ contour.

equilibrium is slightly faster than the smaller β values. It is worth noting how the variable relaxation times influence the evolution of the kinetic energy. In particular, for values of $\tau < 0.5$ (hence smaller viscosities), the kinetic energy lingers in time suggesting that the volumetric surface tension force dominates the momentum field over the diffusion of the field. While for larger relaxation time (i.e. $\tau > 0.5$), the diffusion of the momentum plays a larger role and equilibrium is achieved much earlier.

The influence of the polynomial order (N) is of importance as this defines the resolution of the problem. Fig. 5 shows the influence of the polynomials on a static drop with $\beta = 0.01$, $\tau = 0.5$, and $D = 0.05$. For the image on the left the timestep is fixed. For $N = 3$, we see that the max. kinetic energy is higher than for the other orders. This is most likely due to the lack of resolution to properly represent the interface. It is also worth noting that the lower polynomial orders ($N = 4$ and $N = 5$) show quicker relaxation to equilibrium than the higher orders.

To further verify our scheme, we investigate the convergence behavior of our scheme for the Young-Laplace law. For a stationary droplet, Laplace's law states $\Delta p = p_{liq} - p_{vap} = \sigma/R$, where p_{liq} and p_{vap} are the pressure within the liquid and vapor respectively. The pressure for this scheme is computed via the following [28]: $P = P_o - \frac{\kappa}{2}(\nabla\rho) \cdot (\nabla\rho)$. Where P_o is the thermodynamic pressure defined by the following equation of state (EOS): $P_o = \rho \frac{\partial H_o}{\partial \rho} - H_o$. For the Young-Laplace law, we let σ be an input parameter and allow β to vary. Fig. 6 shows the relative error of the computed pressure difference to the analytic pressure difference (given by Laplace's law) as a function of M which is a measure of interface thickness (left image). The relaxation parameter is set to $\tau = 0.5$. We choose the interface thickness based on the minimum spacing between nodal points, $\Delta\mathbf{x}_{min}$. M is a multiplier, where $D = M\Delta\mathbf{x}_{min}$. The interface profile is given by the hyperbolic tangent profile described above. $\Delta\mathbf{x}_{min}$ is based on the polynomial order and the mesh distribution, which, for this

Figure 3: Non-Uniform Mesh Distribution with for $E = 16 \times 16$ elements

Figure 4: Time evolution of the maximum kinetic energy for variable β (left) and variable relaxation time τ (right). Both computations are performed on the non-uniform mesh distribuiton

test we use $N = 7$ and the non-uniform mesh distribution given by Fig. 3. An interesting feature of this figure shows that the perfomance of the SEDG discretization is comparable and somewhat better than a second-order scheme. This might be due to the high-order polynomial interpolations that are utilized to discretize and approximate density gradients. Fig. 6 also shows the convergence of the Young-Laplace law for variable polynomial orders. By increasing the the polynomial order we are increasing the resolution of the interface and thus showing fairly good convergence.

Figure 5: Time evolution of the maximum kinetic energy for $La = 10^3$. Left image shows results for variable polynomial order N at fixed timestep.

Figure 6: Convergence of the Laplace law. Left image shows results for variable interface thickness D - measured in terms of a multiplier M , where $D = M\Delta x_{min}$. Right images shows results for variable polynomial order N .

3.2. 2D Stationary Droplet - Perturbed Mesh

In order to take further advantage of the body-fitting nature of the scheme, we conduct similar 2D droplet tests on a perturbed mesh. We consider a perturbation to the simple 2D box mesh. Fig. 7 portrays the mesh we consider. This perturbation is introduced via a simple “zig-zagged” distribution that is based on the angle, θ . The reason behind this perturbation is to observe the performance of the **SAS-DBM** on poorly designed meshes. We recognize that these types of skewed meshes are not ideal in resolving interfacial dynamics. Rather, we take this opportunity to test the performance of the **SAS-DBM** for worst-case scenario implementations. The image on the right shows the time evolution of the maximum kinetic energy at different angles, θ . The measure of the perturbation is given by the coefficient $\alpha = \tan \theta$. For each α that is considered, the plots collapse almost entirely on the same curve. The evolution of the kinetic energy shows a gradual elimination of parasitic currents - especially for elements which are highly skewed (i.e. larger α).

Figure 7: Left Image: A perturbed mesh - the zig-zagged distribution. The degree of perturbation is based on a skewness coefficient, $\alpha = \tan \theta$. θ is an angle measured from a straight vertical edge that would otherwise (i.e. without perturbation) exist. Right Image: Time evolution of the maximum kinetic energy on perturbed mesh for variable α . Results are shown for $D = 0.05$, $\beta = 0.01$, $\tau = 0.5$, and $La = 10^3$.

4. Conclusions

We have presented a novel algorithm for solving the discrete Boltzmann equations on non-uniform meshes. The proposed method, a Strang-splitting, Advection-with-Source, discrete Boltzmann method or **SAS-DBM** for short is shown to successfully eliminate parasitic currents. In our analysis, we compare the **SAS-DBM** with another counterpart known as the Strang-splitting, Advection-with-No Source, discrete Boltzmann method or **SANS-DBM**. Our investigation reveals that spurious currents prevail with the **SANS-DBM**. By utilizing a common time-stepping scheme (RK2), we show that an imbalance between source (collision and force) and advection ($\mathbf{e}_\alpha \cdot \nabla$) operators may contribute to non-vanishing parasitic currents. Numerical results for the **SAS-DBM** show that parasitic currents vanish for a range of Laplace (La) numbers and polynomial orders. The 2D Young-Laplace law for a static droplet has been verified for a range of interfacial thicknesses and polynomial orders. Finally, we test the scheme for poorly designed meshes by perturbing a uniform distribution of elements. Results indicate that the **SAS-DBM** performs well by eliminating the currents for a range of skewness coefficients. Future work includes the investigation of more complex two-phase applications such as rising bubble dynamics and wetting phenomena.

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