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An Absorbing Boundary Condition for the Lattice Boltzmann Method Based on the Perfectly Matched Layer

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Abstract

The Lattice Boltzmann Method (LBM) is a well established computational tool for fluid flow simulations. This method has been recently utilized for low Mach number computational aeroacoustics. Robust and nonreflective boundary conditions, similar to those used in Navier-Stokes solvers, are needed for LBM-based aeroacoustics simulations. The goal of the present study was to develop an absorbing boundary condition based on the perfectly matched layer (PML) concept for LBM. The derivation of formulations for both two and three dimensional problems are presented. The macroscopic behavior of the new formulation is discussed. The new formulation was tested using benchmark acoustic problems. The perfectly matched layer concept appears to be very well suited for LBM, and yielded very low acoustic reflection factor.

Keywords

non-reflective boundary conditions; lattice Boltzmann method; computational aeroacoustics

1. Introduction

In recent years, the Lattice Boltzmann Method (LBM) has emerged as a robust computational tool in fluid dynamics [1]. The LBM offers some intrinsic advantages over conventional Navier-Stokes schemes. For instance, Navier-Stokes equations are second-order partial differential equations, while the LBM is derived from a set of first-order PDE's. Navier-Stokes solvers need to treat nonlinear convection terms, while the LBM formulation does not include such nonlinearity. Navier-Stokes solvers for incompressible flows often need to solve a Poisson equation to obtain the pressure. This involves global data communication. In the LBM, pressure is determined directly from the equation of state avoiding such communication overhead. Furthermore, the lattice Boltzmann algorithms are simple to code. Complex boundary geometries can be handled without the need for the analytic description of the grid geometry.

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Recently, the LBM has been used computational aeroacoustics (CAA) studies. Course et al. [2] studied the accuracy of the LBM for some canonical acoustic problems. Their study of a planar wave and 2D Gaussian pulse propagation quantified the numerical dispersion and dissipation of the LBM, and the effect of grid resolution. A driven acoustic standing-wave in a tube was also studied to investigate the possibility of implementing sound-absorbing boundaries. Marié et al. [3] studied the behavior of the lattice Boltzmann equation (LBE) analytically. Their analysis led to a modal decomposition of the LBM which provides the dispersion and dissipation relation for the shear and propagating modes. Using Chapman-Enskog analysis, they successfully recovered the acoustic and shear modes at macroscopic scales. Li et al. [4, 5] studied the accuracy of a modified lattice Boltzmann scheme for some canonical wave problems. The LBM results were compared with those obtained from a direct numerical simulation (DNS). The LBM and the DNS yielded identical results for the studies cases, suggesting that the LBM can be used to correctly simulate aeroacoustic problems.

The LBM has also been used for more applied problems in CAA. Lew et al. [6] used this method to simulate the noise generated by a subsonic round jet and compared the LBM results with those obtained from a Navier-Stokes LES code. Their results showed that the LBM is computationally more efficient for low Mach number flows. LBM-CAA simulations of some complex problems such as landing gear noise [7], and jet noise suppression through the use of micro-jets [8] have also been reported.

Nonreflective boundary conditions are of crucial importance for accurate CAA simulations. Robust nonreflective boundary conditions are not yet available for LBM. With the exception of one study [9], no rigorous studies have been made on this subject, to the authors' best knowledge. Kam et al. [9] studied non-reflective boundary conditions for the lattice Boltzmann method. Most notably, they introduced a sponge-layer formulation by adding an additional damping term to the Lattice Boltzmann equations.

In general, the development of nonreflective boundary conditions for the LBM is challenging due to the fact that such boundary conditions should be formulated in terms of the particle distribution function rather than macroscopic quantities such as density, velocity, and pressure. The purpose of the present study was to develop and implement a robust absorbing layer boundary condition, based on the Perfectly Matched Layer (PML) concept, in the framework of the Lattice Boltzmann method. The PML technique was first introduced by Berenger for Maxwell's equations in electromagnetics [10]. This type of absorbing layers is in theory nonreflective for any angle and frequency of the incident waves.

Following Berenger's approach, Hu developed a PML formulation for linearized Euler equations in a series of papers [11, 12, 13]. More recently, Hu et al. [14] have developed absorbing boundary conditions for nonlinear Euler and Navier-Stokes equations based on the PML method. Despite significant progress over the past few years, a stable PML has not yet been developed for mean flows with arbitrary directions. No rigorous PML formulation exists for viscous flow simulations [15]. Consequently, there has been limited applications of PML in CAA.

In the present paper, an absorbing boundary condition is presented for Lattice Boltzmann equations (LBE) which is formulated based on the PML concept. A brief introduction to the LBM is presented in Sec. 1.1. The theoretical background on the PML formulation for general hyperbolic equations is presented in Sec. 2. Section 3 deals with the derivation of the PML method for the LBM. The PML formulation is derived for both two- and three-dimensional problems. Some verification studies are presented in Sec. 4. Conclusions are drawn in Sec. 5

1.1. The Lattice Boltzmann Method

1.1.1. The Boltzmann Equation—Consider the Cartesian coordinates, $\mathbf{x}$, of a point in physical space and molecular velocity $\mathbf{c}$. We can define a distribution function, f , such that

$$f(\mathbf{c}, \mathbf{x}, t) d\mathbf{x} d\mathbf{c} \quad (1)$$

denotes the probable number of molecules with velocities in the range $d\mathbf{c} = dc_1 dc_2 dc_3$ in the position range $d\mathbf{x} = dx_1 dx_2 dx_3$ about the position $\mathbf{x}$ at time t [16]. The distribution function can be scaled by the molecular mass and is usually referred to as mass density distribution or density weighted distribution function. The macroscopic properties such as the density $\rho(\mathbf{x}, t)$, momentum $\rho \mathbf{u}(\mathbf{x}, t)$, internal energy $\rho e(\mathbf{x}, t)$, stress tensor $\sigma_{ij}(\mathbf{x}, t)$ and the heat flux vector $\mathbf{q}(\mathbf{x}, t)$, are obtained by the moments of the mass distribution function ¹:

$$\rho(\mathbf{x}, t) = \int f(\mathbf{x}, \mathbf{c}, t) d\mathbf{c}, \quad (2)$$

$$\rho u_i(\mathbf{x}, t) = \int c_i f(\mathbf{x}, \mathbf{c}, t) d\mathbf{c} \quad (3)$$

$$\rho e(\mathbf{x}, t) = \frac{1}{2} \int \tilde{c}_i \tilde{c}_i f(\mathbf{x}, \mathbf{c}, t) d\mathbf{c}, \quad (4)$$

$$\sigma_{ij}(\mathbf{x}, t) = - \int \tilde{c}_i \tilde{c}_j f(\mathbf{x}, \mathbf{c}, t) d\mathbf{c}, \quad (5)$$

$$q_i(\mathbf{x}, t) = \frac{1}{2} \int \tilde{c}_i (\tilde{c}_j \tilde{c}_j) f(\mathbf{x}, \mathbf{c}, t) d\mathbf{c}, \quad (6)$$

where the peculiar velocity, $\tilde{\mathbf{c}} = \mathbf{c} - \mathbf{u}$, is the particle velocity with respect to the flow velocity.

The governing equation of kinetic theory, which is the evolution equation for the distribution function, is the Boltzmann equation,

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = \Omega(f), \quad (7)$$

where the collision operator $\Omega(f)$ models the rate of change of the distribution function due to molecular collisions. Considering binary collisions between spherical molecules in the dilute limit, the collision takes the form [16]

$$\Omega(f) = \frac{1}{m} \int |\mathbf{c}_1 - \mathbf{c}| (f'_1 f'_1 - f f_1) dS d\mathbf{c}, \quad (8)$$

where dS is the collision cross section. Primed variables denote the state of particles before the collision, while variables without prime correspond to the state of particles after the collision. The collision operator has the following important property:

¹Vector quantities are denoted by bold symbols. The italic symbols with indices denote components of the vectors and follow the index notation rules.

$$\int \Omega(f) \begin{bmatrix} 1 \\ c_i \\ c_i c_i \end{bmatrix} d\mathbf{c} = 0. \quad (9)$$

These equalities reflect the conservation of mass, momentum, and energy. For this reason, 1, c_i , and $c_i c_i$ are frequently called the elementary collision invariants.

1.1.2. The BGK approximation—The collision operator of the Boltzmann equation, eq. (8), yields a complex integro-differential equation. To simplify the equation, Bhatnagar, Gross, and Krook assumed that the effect of collision among particles is to cause the gas to approach its equilibrium state [17]. More precisely, the Bhatnagar, Gross, and Krook (BGK) approximation, also known as the collision interval theory [16], assumes that during the time interval dt a fraction, dt/τ' , of molecules in a differential volume undergo collisions, which alter their distribution from f to the Maxwell-Boltzmann distribution f^{eq} which is given by

$$f^{eq}(\mathbf{c}) = \frac{\rho}{(2\pi RT)^{3/2}} e^{-(c_i - u_i)^2 / (2RT)}. \quad (10)$$

This implies that the rate of change of distribution functions due to collision, which is by definition the collision operator $\Omega(f)$, is equal to $-(f - f^{eq})/\tau'$. Therefore, the Boltzmann equation becomes

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = -\frac{f - f^{eq}}{\tau'}. \quad (11)$$

The above form of the Boltzmann equation is usually referred to as the *Boltzmann-BGK* equation. The relaxation time, τ' , controls the transport properties of the gas [16].

1.1.3. The BGK-Lattice Boltzmann Equation—Discretization of the BGK Boltzmann equation, eq. (11), yields

$$f(\mathbf{c}, \mathbf{x} + \mathbf{c}\Delta t, t + \Delta t) - f(\mathbf{c}, \mathbf{x}, t) = \frac{-1}{\tau} [f(\mathbf{c}, \mathbf{x}, t) - f^{eq}(\mathbf{c}, \mathbf{x}, t)], \quad (12)$$

where $\tau = \Delta t/\tau'$. Further discretization of the phase space on a set of velocity directions which form a Hermite base [18, 19, 20] lead to the BGK-Lattice Boltzmann equation:

$$f_\alpha(\mathbf{x} + \mathbf{c}_\alpha \Delta t, t + \Delta t) - f_\alpha(\mathbf{x}, t) = \frac{-1}{\tau} [f_\alpha(\mathbf{x}, t) - f_\alpha^{eq}(\mathbf{x}, t)], \quad (13)$$

where f_α^{eq} is the discretized equilibrium distribution function, and $\mathbf{c}_\alpha$ is the velocity set which forms the lattice on which the phase space is approximated. The details on the equilibrium distribution function discretization and corresponding weight coefficients for two-dimensional and three dimensional lattices (e.g. D2Q9 and D3Q19) are provided in many references (cf. [1], [20], and [21]) and are not repeated here.

The macroscopic properties, such as the fluid density and the flow momentum, are obtained from the moments of the distribution function. Despite the first order discretization of the equations, the lattice Boltzmann method is a second-order scheme in both time and space [22].

1.1.4. Implementation of the LBM—Solving the LBE equation, eq. (13), is straightforward. The LBM algorithm consists of three steps. The collision step involves the calculation of the distribution function following molecular collisions, as follows

$$\tilde{f}_\alpha(\mathbf{x}, t) = f_\alpha(\mathbf{x}, t) - \frac{1}{\tau} [f_\alpha(\mathbf{x}, t) - f_\alpha^{eq}(\mathbf{x}, t)]. \quad (14)$$

The streaming step involves propagating the distribution function to the neighboring lattice

$$f_\alpha(\mathbf{x} + \mathbf{c}_\alpha \Delta t, t + \Delta t) = \tilde{f}_\alpha(\mathbf{x}, t). \quad (15)$$

Finally, the reduction step involves the calculation of the macroscopic properties from the particle distribution functions

$$\rho = \sum_\alpha f_\alpha = \sum_\alpha f_\alpha^{eq} \quad (16)$$

$$\rho \mathbf{u} = \sum_\alpha \mathbf{c} f_\alpha = \sum_\alpha \mathbf{c} f_\alpha^{eq} \quad (17)$$

These calculations are performed at each time step for all nodes. However, the implementation of free-space boundaries is challenging. Consider a D2Q9 lattice node somewhere on the upper transverse boundary of a computational domain, as shown in Fig. 1. During the streaming step, this node (I, J_{max}) , shown by red circles, receives the particle distributions in the lattice directions 1 to 5 from nodes $(I-1, J_{max})$, $(I-1, J_{max}-1)$, $(I, J_{max}-1)$, $(I+1, J_{max}-1)$, and $(I+1, J_{max})$, respectively. However, there exists no node in the computational domain to supply distribution functions for lattice directions 6 to 8, and hence, they are shown by dashed arrows. A proper BC in LBM should supply the distribution functions for those lattice directions which do not receive data during the streaming step.

A somehow trivial method to solve this problem for transverse and inflow boundaries is to use the distribution functions which correspond to the free-stream properties. However, the boundary constructed by this method acts like the pressure release boundary of an open tube, and is highly reflective with respect to acoustic waves. Another method, which is commonly used for outlet boundaries, is the zero f gradient (ZG) boundary condition. In this method, the gradient of the distribution function along the direction normal to the boundary is set to zero. Although this method yields acceptable results for the mean flow, it yields a reflective boundary for CAA applications.

A more effective technique is the absorbing layer method, also referred to as *sponge layer*, which is often used for Navier-Stokes equations. In this method, a damping term is added to the lattice Boltzmann equation within a sponge zone right before the boundary to attenuate the disturbances from a prescribed mean flow [9]. Although the sponge layer method is fairly robust, the difference between the dispersion properties of the sponge zone and the computational domain results in wave reflection at their interface. To minimize this reflection, the damping coefficient should be increased gradually from the interface of the sponge zone and the interior domain which tends to increase the length of the sponge zone.

Another method of constructing an absorbing layer is the perfectly matched layer [10]. In this technique, an absorbing layer similar to the sponge zone is added to the computational

domain (cf. Fig. 2). However, the governing equations of the absorbing layer are constructed such that they perfectly match with the governing equations of the interior domain. In other words, the PML is constructed in such a way that outgoing waves will not cause any reflection at the interface between the PML and the interior domain for any frequency and angle of incidence. The theory of the PML for a linear hyperbolic system of equations is the subject of the next section.

2. Perfectly Matched Layer for Hyperbolic Systems of Equations

Consider the evolution of a linear hyperbolic system which is governed by the following system of equations:

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{U}}{\partial x} + \mathbf{B} \frac{\partial \mathbf{U}}{\partial y} + \mathbf{C} \frac{\partial \mathbf{U}}{\partial z} = 0, \quad (18)$$

where $\mathbf{U}$ is the m -vector of unknowns, and $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are $m \times m$ matrices.

These equations are first decomposed into a systems of equations, as follows

$$\frac{\partial \mathbf{U}_1}{\partial t} + \sigma_x \mathbf{U}_1 + \mathbf{A} \frac{\partial \mathbf{U}}{\partial x} = 0, \quad (19a)$$

$$\frac{\partial \mathbf{U}_2}{\partial t} + \sigma_y \mathbf{U}_2 + \mathbf{B} \frac{\partial \mathbf{U}}{\partial y} = 0, \quad (19b)$$

and

$$\frac{\partial \mathbf{U}_3}{\partial t} + \sigma_z \mathbf{U}_3 + \mathbf{C} \frac{\partial \mathbf{U}}{\partial z} = 0, \quad (19c)$$

where $\mathbf{U} = \mathbf{U}_1 + \mathbf{U}_2 + \mathbf{U}_3$, and σ_x , σ_y , and σ_z are positive damping coefficients. Collino and Tsogka [23] proved that this formulation results in an exponential decay of waves within the PML without reflection from the PML/interior domain interface. However, a single-equation form is more desirable for coding to preserve the intrinsic simplicity of LBM algorithm. Such form may be obtained by defining auxiliary variables [12]. Using

$$\mathbf{U} = \widehat{\mathbf{U}}(x, y) e^{-i\omega t} \quad (20)$$

the system of equations (19) can be written in the frequency domain

$$-i\omega \widehat{\mathbf{U}}_1 + \sigma_x \widehat{\mathbf{U}}_1 + \mathbf{A} \frac{\partial \widehat{\mathbf{U}}}{\partial x} = 0, \quad (21a)$$

$$-i\omega \widehat{\mathbf{U}}_2 + \sigma_y \widehat{\mathbf{U}}_2 + \mathbf{B} \frac{\partial \widehat{\mathbf{U}}}{\partial y} = 0, \quad (21b)$$

and

$$-i\omega\widehat{\mathbf{U}}_3 + \sigma_z\widehat{\mathbf{U}}_3 + \mathbf{C}\frac{\partial\widehat{\mathbf{U}}}{\partial z} = 0, \quad (21c)$$

Division of eq. (21) by $1 + i\sigma_a/\omega$ where $a = x, y, z$ yields

$$-i\omega\widehat{\mathbf{U}}_1 + \frac{1}{1 + \frac{i\sigma_x}{\omega}}\mathbf{A}\frac{\partial\widehat{\mathbf{U}}}{\partial x} = 0, \quad (22a)$$

$$-i\omega\widehat{\mathbf{U}}_2 + \frac{1}{1 + \frac{i\sigma_y}{\omega}}\mathbf{B}\frac{\partial\widehat{\mathbf{U}}}{\partial y} = 0, \quad (22b)$$

and

$$i\omega\widehat{\mathbf{U}}_3 + \frac{1}{1 + \frac{i\sigma_z}{\omega}}\mathbf{C}\frac{\partial\widehat{\mathbf{U}}}{\partial z} = 0. \quad (22c)$$

Summation of the above equations yields

$$-i\omega\widehat{\mathbf{U}} + \frac{1}{1 + \frac{i\sigma_x}{\omega}}\mathbf{A}\frac{\partial\widehat{\mathbf{U}}}{\partial x} + \frac{1}{1 + \frac{i\sigma_y}{\omega}}\mathbf{B}\frac{\partial\widehat{\mathbf{U}}}{\partial y} + \frac{1}{1 + \frac{i\sigma_z}{\omega}}\mathbf{C}\frac{\partial\widehat{\mathbf{U}}}{\partial z} = 0 \quad (23)$$

which can be recast as

$$\begin{aligned} -i\omega\widehat{\mathbf{U}} + \mathbf{A}\frac{\partial\widehat{\mathbf{U}}}{\partial x} + \mathbf{B}\frac{\partial\widehat{\mathbf{U}}}{\partial y} + \mathbf{C}\frac{\partial\widehat{\mathbf{U}}}{\partial z} = & -(\sigma_x + \sigma_y + \sigma_z)\widehat{\mathbf{U}} \\ & -(\sigma_x\sigma_y + \sigma_x\sigma_z + \sigma_y\sigma_z)\widehat{\mathbf{Q}}_1 \\ & -\sigma_x\sigma_y\sigma_z\widehat{\mathbf{Q}}_2 \\ & -\mathbf{A}\frac{\partial}{\partial x}\left[(\sigma_y + \sigma_z)\widehat{\mathbf{Q}}_1 + \sigma_y\sigma_z\widehat{\mathbf{Q}}_2\right] \\ & -\mathbf{B}\frac{\partial}{\partial y}\left[(\sigma_x + \sigma_z)\widehat{\mathbf{Q}}_1 + \sigma_x\sigma_z\widehat{\mathbf{Q}}_2\right] \\ & -\mathbf{C}\frac{\partial}{\partial z}\left[(\sigma_x + \sigma_y)\widehat{\mathbf{Q}}_1 + \sigma_x\sigma_y\widehat{\mathbf{Q}}_2\right], \end{aligned} \quad (24a)$$

where

$$\widehat{\mathbf{Q}}_1 = \frac{i}{\omega}\widehat{\mathbf{U}} \quad \widehat{\mathbf{Q}}_2 = \frac{-1}{\omega_2}\widehat{\mathbf{U}} = \frac{i}{\omega}\widehat{\mathbf{Q}}_1 \quad (24b)$$

Equations (24a) and (24b) are then transformed in the time domain to yield

$$\begin{aligned} \frac{\partial\mathbf{U}}{\partial t} + \mathbf{A}\frac{\partial\mathbf{U}}{\partial x} + \mathbf{B}\frac{\partial\mathbf{U}}{\partial y} + \mathbf{C}\frac{\partial\mathbf{U}}{\partial z} = & -(\sigma_x + \sigma_y + \sigma_z)\mathbf{U} \\ & -(\sigma_x\sigma_y + \sigma_x\sigma_z + \sigma_y\sigma_z)\mathbf{Q}_1 \\ & -\sigma_x\sigma_y\sigma_z\mathbf{Q}_2 \\ & -\mathbf{A}\frac{\partial}{\partial x}[(\sigma_y + \sigma_z)\mathbf{Q}_1 + \sigma_y\sigma_z\mathbf{Q}_2] \\ & -\mathbf{B}\frac{\partial}{\partial y}[(\sigma_x + \sigma_z)\mathbf{Q}_1 + \sigma_x\sigma_z\mathbf{Q}_2] \\ & -\mathbf{C}\frac{\partial}{\partial z}[(\sigma_x + \sigma_y)\mathbf{Q}_1 + \sigma_x\sigma_y\mathbf{Q}_2], \end{aligned} \quad (25a)$$

where

$$\frac{\partial \mathbf{Q}_1}{\partial t} = \mathbf{U}, \quad (26a)$$

and

$$\frac{\partial \mathbf{Q}_2}{\partial t} = \mathbf{Q}_1. \quad (26b)$$

Equation (25a) may be simplified for two-dimensional problems,

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{U}}{\partial x} + \mathbf{B} \frac{\partial \mathbf{U}}{\partial y} = -(\sigma_x + \sigma_y) \mathbf{U} - \sigma_x \sigma_y \mathbf{Q}_1 - \sigma_y \mathbf{A} \frac{\partial \mathbf{Q}_1}{\partial x} - \sigma_x \mathbf{B} \frac{\partial \mathbf{Q}_1}{\partial y}, \quad (27)$$

and there would be no need to calculate or store $\mathbf{Q}_2$.

3. PML formulation for LBM

3.1. Derivation

The BGK-Lattice Boltzmann equation, in two dimensions, may be written in the following vector form as

$$\frac{\partial \mathbf{f}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{f}}{\partial x} + \mathbf{B} \frac{\partial \mathbf{f}}{\partial y} + \mathbf{C} \frac{\partial \mathbf{f}}{\partial z} = -\frac{1}{\tau} (\mathbf{f} - \mathbf{f}^{eq}), \quad (28)$$

where $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are diagonal matrices with elements on the diagonal equal to the x , y , and z components of the lattice velocity vector (i.e. $A_{kk} = c_x^k$, $B_{kk} = c_y^k$, and $C_{kk} = c_z^k$).

The fluid density and flow velocity at each point are obtained from the moments of the equilibrium distribution function, $\mathbf{f}^{eq}$. The non-equilibrium distribution function takes the viscous effects into account and will be included later. Replacing $\mathbf{f}$ with $\mathbf{f}^{eq}$ in eq. (28) yields

$$\frac{\partial \mathbf{f}^{eq}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{f}^{eq}}{\partial x} + \mathbf{B} \frac{\partial \mathbf{f}^{eq}}{\partial y} + \mathbf{C} \frac{\partial \mathbf{f}^{eq}}{\partial z} = 0. \quad (29)$$

Decomposition of the equilibrium functions into the sum of a mean uniform component and an acoustic perturbation component yields

$$\mathbf{f}^{eq} = \overline{\mathbf{f}^{eq}} + \tilde{\mathbf{f}}^{eq} \quad (30)$$

where the overbar and the tilde denote the mean and the perturbed values, respectively. Whence, it can be directly concluded from eq. (29) that

$$\frac{\partial \tilde{\mathbf{f}}^{eq}}{\partial t} + \mathbf{A} \frac{\partial \tilde{\mathbf{f}}^{eq}}{\partial x} + \mathbf{B} \frac{\partial \tilde{\mathbf{f}}^{eq}}{\partial y} + \mathbf{C} \frac{\partial \tilde{\mathbf{f}}^{eq}}{\partial z} = 0. \quad (31)$$

Equation (31) has exactly the same form as eq. 18. Therefore, as outlined in the previous section, the PML formulation for three dimensional problems is

$$\begin{aligned} \frac{\partial \tilde{\mathbf{f}}^{eq}}{\partial t} + \mathbf{A} \frac{\partial \tilde{\mathbf{f}}^{eq}}{\partial x} + \mathbf{B} \frac{\partial \tilde{\mathbf{f}}^{eq}}{\partial y} + \mathbf{C} \frac{\partial \tilde{\mathbf{f}}^{eq}}{\partial z} = & -(\sigma_x + \sigma_y + \sigma_z) \tilde{\mathbf{f}}^{eq} \\ & -(\sigma_x \sigma_y + \sigma_x \sigma_z + \sigma_y \sigma_z) \mathbf{Q}_1 \\ & -\sigma_x \sigma_y \sigma_z \mathbf{Q}_2 \\ & -\mathbf{A} \frac{\partial}{\partial x} [(\sigma_y + \sigma_z) \mathbf{Q}_1 + \sigma_y \sigma_z \mathbf{Q}_2] \\ & -\mathbf{B} \frac{\partial}{\partial y} [(\sigma_x + \sigma_z) \mathbf{Q}_1 + \sigma_x \sigma_z \mathbf{Q}_2] \\ & -\mathbf{C} \frac{\partial}{\partial z} [(\sigma_x + \sigma_y) \mathbf{Q}_1 + \sigma_x \sigma_y \mathbf{Q}_2], \end{aligned} \quad (32a)$$

where

$$\frac{\partial \mathbf{Q}_1}{\partial t} = \tilde{\mathbf{f}}^{eq} \quad \frac{\partial \mathbf{Q}_2}{\partial t} = \mathbf{Q}_1 \quad (32b)$$

while the formulation for two dimensional problems is

$$\frac{\partial \tilde{\mathbf{f}}^{eq}}{\partial t} + \mathbf{A} \frac{\partial \tilde{\mathbf{f}}^{eq}}{\partial x} + \mathbf{B} \frac{\partial \tilde{\mathbf{f}}^{eq}}{\partial y} = - \left[\sigma_y \mathbf{A} \frac{\partial \mathbf{Q}}{\partial x} + \sigma_x \mathbf{B} \frac{\partial \mathbf{Q}}{\partial y} + (\sigma_x + \sigma_y) \tilde{\mathbf{f}}^{eq} + \sigma_x \sigma_y \mathbf{Q} \right], \quad (33a)$$

where

$$\frac{\partial \mathbf{Q}}{\partial t} = \tilde{\mathbf{f}}^{eq} = \mathbf{f}^{eq} - \overline{\mathbf{f}}^{eq}. \quad (33b)$$

Noting that

$$f = \tilde{f}^{eq} + \overline{\tilde{f}}^{eq} + f^{neq}, \quad (34)$$

the final result is obtained by summing eq. (32), or (33) in two dimensional problems, with the evolution equation for the non-equilibrium distribution function, given by

$$\frac{\partial \mathbf{f}^{neq}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{f}^{neq}}{\partial x} + \mathbf{B} \frac{\partial \mathbf{f}^{neq}}{\partial y} + \mathbf{C} \frac{\partial \mathbf{f}^{neq}}{\partial z} = - \frac{\mathbf{f}^{neq}}{\tau}. \quad (35)$$

The additional PML terms may be recast into an additional collision term in the Boltzmann equation,

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = \Omega_{BGK} + \Omega_{PML}, \quad (36)$$

where Ω_{BGK} is the BGK collision operator,

$$\Omega_{BGK} = - \frac{f - f^{eq}}{\tau}, \quad (37)$$

and Ω^{PML} is equal to the RHS of (33) and eq.'s (32), for two and three dimensional problems, respectively.

A stability analysis, presented in the appendix, shows that the above equations may become numerically unstable in some lattice directions. To overcome this problem, let us assume that $\sigma_x = \sigma_y = \sigma_z = \sigma$. Then for each lattice direction, eq.'s (32) and (33) reduce to

$$\frac{\partial \tilde{f}^{eq}}{\partial t} + \mathbf{c} \cdot \nabla \tilde{f}^{eq} = - \left[3\sigma \tilde{f}^{eq} + 3\sigma^2 Q_1 + \sigma^3 Q_2 + 2\sigma \mathbf{c} \cdot \nabla Q_1 + \sigma^2 \mathbf{c} \cdot \nabla Q_2 \right], \quad (38)$$

and

$$\frac{\partial \tilde{f}^{eq}}{\partial t} + \mathbf{c} \cdot \nabla \tilde{f}^{eq} = - \left[\sigma \mathbf{c} \cdot \nabla Q + 2\sigma \tilde{f}^{eq} + \sigma^2 Q \right], \quad (39)$$

respectively. The operator $\mathbf{c} \cdot \nabla$ can then be replaced by a central difference along the lattice direction. It can be shown that the resulting formulation is stable for all lattice directions (c.f. Appendix). Therefore, Ω^{PML} must be replaced by the RHS of eq.'s (39) and (38) to obtain a stable PML formulation. At boundary points, one-sided differences are used for lattice directions which point outside of the domain, and the differential terms for whose which point inside are set to zero to avoid downwind discretization.

The proposed PML formulation can be easily implemented by calculating and adding one additional term, Ω^{PML} , in the collision step of the conventional LBM scheme. It should be mentioned that the resulting PML formulation may be used to simulate viscous flows with arbitrary directions.

3.2. LBM-PML in macroscopic scale

It is beneficial to study the behavior of the suggested PML formulation for the Lattice Boltzmann Equations at the macroscopic scale. For simplicity, this analysis is restricted to two-dimensional problems, although a similar analysis holds for three-dimensional formulation as well.

By definition,

$$\rho = \int_{-\infty}^{\infty} f d^3 \mathbf{c} = \int_{-\infty}^{\infty} \tilde{f}^{eq} d^3 \mathbf{c}, \quad (40)$$

$$\rho u_i = \int_{-\infty}^{\infty} c_i f d^3 \mathbf{c} = \int_{-\infty}^{\infty} c_i \tilde{f}^{eq} d^3 \mathbf{c}, \quad (41)$$

$$p \delta_{ij} = \int_{-\infty}^{\infty} c_i c_j \tilde{f}^{eq} d^3 \mathbf{c}, \quad (42)$$

and

$$\rho e = \frac{1}{2} \int_{-\infty}^{\infty} \mathbf{c} \cdot \mathbf{c} f d^3 \mathbf{c} = \frac{1}{2} \int_{-\infty}^{\infty} \mathbf{c} \cdot \mathbf{c} \tilde{f}^{eq} d^3 \mathbf{c}. \quad (43)$$

The collision operator satisfies the following condition

$$\int_{-\infty}^{\infty} \Omega_{BGK} \begin{bmatrix} 1 \\ c_j \\ c_j c_j \end{bmatrix} d^3c = 0 \quad (44)$$

The conservation of mass, momentum, and energy may be obtained from moments of the Boltzmann equation in the velocity space. Similarly, the corresponding PML equations at the macroscopic scale can be obtained from the moments of the PML-Boltzmann equation, eq. (36). For example, the continuity equation is obtained from

$$\int_{-\infty}^{\infty} \frac{\partial f}{\partial t} d^3c + \int_{-\infty}^{\infty} c_j \frac{\partial f}{\partial x_j} d^3c = \int_{-\infty}^{\infty} \Omega_{BGK} d^3c + \int_{-\infty}^{\infty} \Omega_{PML} d^3c \quad (45)$$

which can be recast as

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = \int_{-\infty}^{\infty} \Omega_{PML} d^3c. \quad (46)$$

The effect of PML adds the first moment of Ω_{PML} to the continuity equation. Similarly, the second and third moments of Ω_{PML} are added to the conservation of momentum and energy. These moments are given in two dimensional problems by

$$\int_{-\infty}^{\infty} \Omega_{PML} \begin{bmatrix} 1 \\ c_j \\ c_j c_j \end{bmatrix} d^3c = \sigma_y \frac{\partial \tilde{\mathbf{Q}}_1}{\partial x} + \sigma_x \frac{\partial \tilde{\mathbf{Q}}_2}{\partial y} + (\sigma_x + \sigma_y) (\mathbf{U} - \bar{\mathbf{U}}) + \sigma_x \sigma_y \tilde{\mathbf{Q}}, \quad (47)$$

where

$$\mathbf{U} = [\rho \quad \rho u_j \quad \rho e]^T, \quad (48)$$

and

$$\frac{\partial \tilde{\mathbf{Q}}}{\partial t} = \mathbf{U} - \bar{\mathbf{U}}. \quad (50)$$

The $\tilde{\mathbf{Q}}_1$ and $\tilde{\mathbf{Q}}_2$ terms have slightly more complicated forms,

$$\frac{\partial \tilde{\mathbf{Q}}_i}{\partial t} = \int_{-\infty}^{\infty} c_i \begin{bmatrix} 1 \\ c_j \\ c_j c_j \end{bmatrix} \frac{\partial Q}{\partial t} d^3c = \int_{-\infty}^{\infty} c_i \begin{bmatrix} 1 \\ c_j \\ c_j c_j \end{bmatrix} [f^{eq} - \bar{f}^{eq}] d^3c \quad (51)$$

Using the definition of the peculiar velocity,

$$\tilde{c}_i = c_i - u_i, \quad (52)$$

eq. (51) can be written as

$$\frac{\partial \tilde{\mathbf{Q}}_i}{\partial t} = \int_{-\infty}^{+\infty} (\tilde{c}_i + u_i) \begin{bmatrix} 1 \\ \tilde{c}_j + u_j \\ (\tilde{c}_j + u_j)(\tilde{c}_j + u_j) \end{bmatrix} f^{eq} d^3 c - \int_{-\infty}^{+\infty} (\tilde{c}_i + \bar{u}_i) \begin{bmatrix} 1 \\ \tilde{c}_j + \bar{u}_j \\ (\tilde{c}_j + \bar{u}_j)(\tilde{c}_j + \bar{u}_j) \end{bmatrix} \bar{f}^{eq} d^3 c, \quad (53)$$

where over bar denotes mean properties, i.e. the ambient state. Assuming a monoatomic gas, the equation can be simplified as follows

$$\frac{\partial \tilde{\mathbf{Q}}_i}{\partial t} = \mathbf{F}_i(\mathbf{U}) - \mathbf{F}_i(\bar{\mathbf{U}}), \quad (54)$$

where

$$\mathbf{F}_i(\mathbf{U}) = \begin{bmatrix} \rho u_i \\ \rho u_i u_j + p \delta_{ij} \\ \rho u_i h \end{bmatrix}. \quad (55)$$

It is interesting to note that eq.'s (47), (50), and (55) are consistent with Hu's PML formulation for nonlinear Euler equations [15]. The reason that the above PML is recovered for Euler equations and not for full Navier-Stokes equations is because only the equilibrium components of the distribution functions, f^{eq} , were considered in the derivations. The derivation of a PML formulation which is perfectly matched with Navier-Stokes equations at the macroscopic scale requires taking both the equilibrium and the nonequilibrium part of the distribution function into account. This is the object of the future works.

4. Verification studies

In this section, the effectiveness of the PML in absorbing acoustic perturbations is demonstrated for the canonical Gaussian pulse propagation problem in two- and three-dimensional domains. The performance of the PML to minimize the spurious disturbances due to convected vortices are also demonstrated for an iso-thermal isolated vortex and vortex shedding by a bluff body in a 2D uniform flow.

4.1. Gaussian pulse propagation in two dimensions

An acoustic Gaussian pulse was generated using the initial conditions

$$\rho = 1 + \varepsilon \exp(-\ln 2 \frac{x^2 + y^2}{b^2}), \quad (56)$$

$$u = 0, \quad (57)$$

$$v = 0, \quad (58)$$

where $\varepsilon = 0.0005$ and $b = 3$. All macroscopic quantities are made dimensionless using lattice units. The pulse was initially located at the center of a 300×300 lattice grid. A 50-lattice wide PML was laid between the interior domain and the $y = 300$ boundary. Zero normal gradient (ZG) BCs were imposed on all other boundaries. The damping coefficient, σ , was varied from zero, at the interface with the computational domain, to 0.08, at the outer boundary, following a parabolic distribution. The attenuation of the wave in the PML region

is shown in Fig 3. The pressure time histories measured at $x = 150$ and $y = 200$ are shown in Fig. 4. Fig. 4.a shows that PML results a in much smaller reflection (almost indistinguishable) compared to the case where a ZG boundary condition was used. A baseline pressure history, obtained at the same location using a larger computational domain is also shown for comparison. The pressure history for a longer period of time is shown in Fig. 4.b to illustrate the stability of the PML formulation.

Figure 5.(a) shows the Fourier transform of the incident Gaussian pulse and the reflected waves measured by a virtual microphone at $x = 150$ and $y = 240$. The incident pulse is considered to be the reading obtained from the larger domain simulation which does not include any reflected wave. The reflected waves are obtained by subtracting the pressure at each instant of time from its corresponding value obtained from the large domain simulation. The Fourier transform of these signals were used to obtain the reflection factor from

$$R(f) = \frac{\widehat{p}_r(f)}{\widehat{p}_i(f)}, \quad (59)$$

where $\widehat{p}_i$ and $\widehat{p}_r$ are incident and reflected waves Fourier transforms, respectively. The reflection factor for the present test case is shown in Fig. 5.b. The reflection factor for the PML was around 5 times smaller than the that of the ZG for almost all frequencies. This ratio can be improved by adjusting the damping coefficient and thickness of the PML. The wave amplitudes decay exponentially within the PML according to [15]

$$p_a(x) \sim \exp\left(-\frac{k}{\omega} \int_{x_0}^x \sigma(x) dx\right). \quad (60)$$

A parametric study of the effect of increasing damping coefficient and PML thickness on the reflected pulse was performed. The reflected pulse waveforms are shown in Fig. 6. An increase in the damping coefficient and PML thickness tend to decrease the amplitude of the reflected pulse if modest values of damping coefficient and PML thickness are chosen. It was also observed that increasing the damping coefficient beyond a certain optimum value, which depends on the PML thickness, may result in the growth of spurious waves.

4.2. Gaussian pulse propagation in three dimensions

For verification of the three dimensional formulation, the Gaussian pulse propagation in a 3D domain of $200 \times 200 \times 150$ lattices was studied. The Gaussian pulse was generated at the center of the domain using the following initial conditions

$$\rho = 1 + \varepsilon \exp\left(-\ln 2 \frac{(x^2 + y^2 + z^2)^2}{b^2}\right), \quad (61)$$

$$u = 0, \quad (62)$$

$$v = 0, \quad (63)$$

$$w = 0, \quad (64)$$

where $\varepsilon = 0.001$ and $b = 5$. A 20-lattice wide PML was laid at the upper boundary with a parabolic distribution of damping coefficient, σ , from zero (at the interface with the computational domain) to 0.05 (at the upper boundary). Iso-pressure contours at the midsection of the domain are shown in Figure 7. Iso-pressure contours of a case where no PML was used are also presented for comparison. At time $t = 60\Delta t$ both domains exhibit similar spherical wave propagation as the wave has not yet reached the PML. Comparison of the pressure contours at $t = 120\Delta t$ demonstrate the attenuation effect of the PML on the incoming wave. This attenuation results in a weaker (and almost indistinguishable) wave reflection from the boundary as can be observed from the pressure contours at $t = 200\Delta t$. To better quantify the effect of PML, the time history of the pressure measured at (100, 100, 100) is shown in Fig. 8 for the domain with PML, for the domain without any PML, and for a larger domain (to avoid wave reflection from the boundary). For the case without the PML, the dashed dotted line, the incoming wave was strongly reflected from the outlet (zero gradient) boundary, while using PML yielded in negligible reflection from the boundary and almost the same pressure history as that obtained from a larger domain simulation.

4.3. Isothermal vortex advection in two dimensions

The PML can be an effective tool in absorbing the vortices before their exit through the boundaries and thus yielding low levels of acoustic reflection. Since the conventional LBM is formulated for isothermal flows, an isolated, isothermal vortex advection is considered as the test case.

The two-dimensional Euler equations support the following solution for an isolated vortex advecting with constant velocity (U_0, V_0) [14]:

$$\begin{bmatrix} \rho(\mathbf{x}, t) \\ u(\mathbf{x}, t) \\ v(\mathbf{x}, t) \end{bmatrix} = \begin{bmatrix} 0 \\ U_0 \\ V_0 \end{bmatrix} + \begin{bmatrix} \rho_r(r) \\ -u_r(r)\sin\theta \\ v_r(r)\cos\theta \end{bmatrix} \quad (65)$$

where

$$r = \sqrt{(x - x_0 - U_0 t)^2 + (y - y_0 - V_0 t)^2}. \quad (66)$$

The radial velocity, the density, and the pressure distributions satisfy the conservation of momentum in the following form

$$\frac{dp_r}{dr} = \rho_r(r) \frac{u_r(r)^2}{r}. \quad (67)$$

For an isothermal flow, where $p_r = \rho_r RT$, eq. (67) becomes

$$\frac{d\rho_r}{\rho_r} = \frac{1}{RT} \frac{u_r(r)^2}{r}. \quad (68)$$

Considering the radial velocity distribution of the form

$$u_r(r) = \frac{U_{max}}{b} r e^{\frac{1}{2} \left(1 - \frac{r^2}{b^2}\right)} \quad (69)$$

Integrating eq. (68) from infinity to r yields

$$\ln \frac{\rho_r(r)}{\rho_\infty} = -\frac{U_{max}^2}{2RT} e^{(1-r^2/b^2)}. \quad (70)$$

Equations (69) and (70) were used to initialize the flow field with $b = 10$, $U_{max} = 0.5 U_0$, and $(U_0, V_0) = (0.17, 0)$, where all macroscopic quantities are made dimensionless using lattice units. The computation domain consisted of 500×500 lattices. The PMLs spanned 50 lattices for all four boundaries of the domain. The absorption of vortex can be observed from the iso-vorticity and iso-transverse-velocity contours, v , as shown in Fig.'s 9 and 10, respectively.

Figure 11 compares the transverse velocity component from the numerical solution with PML and a reference solution obtained using a larger computational domain, along the centerline of the domain. This figure shows that the vortex is clearly absorbed with minimal reflection. In fact, the maximum amplitude of the reflected acoustic wave was found to be 8×10^{-4} times the mean pressure. The reflected pressure amplitude can be further decreased by increasing the PML thickness.

4.4. Flow around a bluff body at $Re = 224$

Another considered example was a flow around a square bluff body at $Re = 224$. The computational domain had 1200×900 lattices and the square bluff dimensions were equivalent to 66 lattices. A bounce-back scheme [24] was used to include the solid boundaries. The PML thickness was equal to 134 lattices on all sides except at the outlet. At the outlet the PML thickness was 268 lattices. A damping coefficient of $\sigma = 0.05$ was chosen for this example. In preliminary simulations, it was observed that spurious waves were not able to destabilize the vortices in the wake of the square to form von Karman vortex street, due to the attenuation of perturbation in the PML. Therefore, in the subsequent simulations, the inlet flow was forced by an acoustic fluctuation at a frequency near to the frequency of vortex shedding of a cylinder at the same Reynolds number to act as acoustic forcing.

Two snapshots of the flow field are shown in Fig. 12. Figure 12.a shows the flow field at $t = 800\Delta t$ where the initial pressure and shear wave has reached the PML. These waves are attenuated in the PML, while Fig. 12.b shows the flow field at $t = 35000\Delta t$. Two microphones were placed in the domain: one at $x = 800\Delta x$ in the wake of the square and the other at $x = 1150\Delta x$ just upstream of the outlet. Figure 13 shows the density fluctuation history measured by the two microphones. As it can be observed from Microphone 1 reading, the flow was forced by the incoming disturbance to form a von Karman vortex street. Comparing the reading from Microphone 1 with that of Microphone 2, it can be observed that fluctuations, including the vortices, are almost completely damped in the PML.

To demonstrate the fact that the present PML formulation is stable and effective for any mean flow direction, a similar case was simulated with mean flow direction having an angle 30 [deg] with respect to the x -axis. A snapshot of the flow field (iso-vorticity contours) is shown in Fig. 14.

5. Conclusions

In this study, the development of an absorbing boundary condition based on the Perfectly Matched Layer concept for the lattice Boltzmann method was investigated.

The PML formulation was derived by recasting the lattice Boltzmann equation in terms of acoustic distribution functions to obtain a linear homogeneous hyperbolic system of equations. It can be proven mathematically the PML formulation for such system leads to an exponential attenuation of the incoming waves, with no reflection from the interface of the PML with the computational domain. Unlike previous PML formulations for fluid flow simulations [15], for which the mean flow direction needs to be known a priori to formulate a stable PML, the present formulation is stable regardless of the mean flow direction and can also be used for viscous flow simulations. This is a significant achievement as this formulation can be used to construct robust, stable and effective absorbing boundary conditions for real-life CAA applications.

A Gaussian pulse propagation, and an isolated vortex advection were used to demonstrate the effectiveness of the proposed PML formulation in absorbing acoustic and vortical perturbations. The reflection factor, for the two dimensional case, was around 5 times smaller than for the ZG for almost all frequencies. This ratio can be improved by adjusting the damping coefficient and thickness of the PML. Vortex shedding from a bluff square in a 2D flow was simulated to demonstrate the performance of and stability of the PML.

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7. Appendix: The stability of PML

It is known that PML might result in exponential growth of errors and instabilities in some applications [12]. Recently, Bécache, Fauqueux and Joly [25] studied the well-posedness and the stability of perfectly matched layers for a general first-order evolution problem. The major results of their work are two remarkable theorems. Their first theorem addresses the well-posedness of a PML formulation and the second theorem provides a necessary condition for the stability of PMLs. These two theorems will be referred to as *BFJ Theorem 1* and *BFJ Theorem 2*. In what follows an outline of their analysis is presented and the stability of the present PML formulation for LBEs is analyzed. For simplicity, the analysis is presented for the two dimensional formulation only. Similar analysis and conclusions can also be made about the three dimensional formulation.

7.1. Well-posedness, Stability, and BFJ Theorems

7.1.1. Definitions

BFJ Theorems are proved based on a set of definitions and assumptions which are presented here for the ease of understanding the theorems and the analysis which will follow.

Definition—Consider a first-order system given by eq. (18). Such system is hyperbolic if for $\mathbf{k} = (k_x, k_y) \in \mathbb{R}^2$, the eigenvalues of $\mathbf{A}(\mathbf{k}) = k_x \mathbf{A} + k_y \mathbf{B}$ are real. This system is strongly hyperbolic if for all $\mathbf{k} = (k_x, k_y) \in \mathbb{R}^2$, $\mathbf{A}(\mathbf{k})$ can be diagonalized [26].

The first-order system given by eq. (18), admits the solution of the form

$$\mathbf{U}(\mathbf{x}, t) = \exp[i(\mathbf{k} \cdot \mathbf{x} - \omega t)] \quad (71)$$

if and only if $\vec{k}$ and ω satisfy the dispersion relation

$$F(\omega, \mathbf{k}) = \det(\omega \mathbf{I} - k_x \mathbf{A} - k_y \mathbf{B}) = 0 \quad (72)$$

The *group velocity* is then defined by

$$\vec{V}_g = \nabla_k \omega(k) = - \left(\frac{\partial F(\omega(k), k)}{\partial \omega} \right)^{-1} \nabla_k F(\omega, k) \quad (73)$$

Another important quantity is the slowness vector

$$\vec{S} = \frac{\vec{k}}{\omega}. \quad (74)$$

The slowness curve is then defined as the set of points in the slowness vector plane that satisfy the dispersion relation

$$F(\omega, \vec{k}) = F\left(1, \frac{\vec{k}}{\omega}\right) = F(1, \vec{S}) = 0. \quad (75)$$

Using the slowness vector definition, the group velocity can be rewritten as

$$\vec{V}_g = - \left(\frac{\partial F(1, \vec{S})}{\partial \omega} \right)^{-1} \nabla_k F(1, \vec{S}). \quad (76)$$

which also shows that the group velocity is always orthogonal to the slowness curve.

7.1.2. BFJ Theorems

The formal splitted-PML formulation for the general hyperbolic system (18) is given by eq. (19). However, for the sake of simplicity of analysis, assume that the PML is constructed in the x -direction (parallel to the y axis). Setting $\sigma_y = 0$ to obtain

$$\frac{\partial \mathbf{U}_1}{\partial t} + \sigma_x \mathbf{U}_1 + \mathbf{A} \frac{\partial \mathbf{U}}{\partial x} = 0, \quad (77a)$$

and

$$\frac{\partial \mathbf{U}_2}{\partial t} + \mathbf{B} \frac{\partial \mathbf{U}}{\partial y} = 0. \quad (77b)$$

Definition—The Cauchy problem, eq. (77), subject to the initial value $\mathbf{U}_0$ is well posed if for any $\mathbf{U}(\mathbf{x}, 0) = \mathbf{U}_0(\mathbf{x})$ in the Sobolev space H^s , $s \geq 0$,

$$\|\mathbf{U}(\mathbf{x}, t)\|_{L^2} \leq K e^{\alpha t} \|\mathbf{U}_0(\mathbf{x})\|_{H^s} \quad (78)$$

Furthermore, the system is said to be strongly well posed if $s = 0$.

BFJ Theorem 1: Assuming that

1. the unsplitted system eq. (18) is **strongly hyperbolic**, and
2. the dispersion relation can be written as

$$F(\omega, \vec{k}) = \omega_0^l \prod_{j=1}^{N_e} [\omega - \omega_j(\vec{k})] \quad (79)$$

where $\omega_j(\vec{k}) \neq 0$,

the PML formulation given by eq. (77) is well posed. The mode zero, $\omega = 0$, is called the non-propagating mode, whereas $\omega_j \neq 0$ are called the physical modes.

BFJ Theorem 2: Suppose that PML formulation given by eq. (77) satisfies the same two assumptions made in BFJ Theorem 1. The necessary condition to have stability at high frequency is that for all physical modes, $\omega_j \neq 0$, of eq. (18)

$$S_x(\vec{K}) \cdot (\vec{V}_g)_x \geq 0 \quad \forall \vec{K} = \frac{\vec{k}}{|\vec{k}|}, \quad (80)$$

where the subscript x denotes the x components of the slowness and group velocity vectors. Similarly, if a PML is constructed in y direction ($\sigma_x = 0$ and $\sigma_y \neq 0$), a necessary condition to have stability at high frequencies is

$$S_y(\vec{K}) \cdot (\vec{V}_g)_y \geq 0 \quad \forall \vec{K} = \frac{\vec{k}}{|\vec{k}|}, \quad (81)$$

7.2. Well-posedness and Stability of the PML for LBE

In this section, the BFJ theorems are used to study the well-posedness and the stability of the LBE-PML formulation. The present analysis is presented for D2Q9 lattices only. However, extension of the present analysis to other lattices is straightforward.

The dispersion relation for two-dimensional lattice Boltzmann equations, with a D2Q9 lattice, reads

$$F(\omega, \vec{k}) = \det \mathcal{A} \quad (82)$$

where $\mathcal{A}$ is a diagonal matrix given by

$$\mathcal{A} = \text{Diag} \begin{bmatrix} \omega \\ \omega - k_x \\ \omega - k_x - k_y \\ \omega - k_y \\ \omega + k_x - k_y \\ \omega + k_x \\ \omega + k_x + k_y \\ \omega + k_y \\ \omega - k_x + k_y \end{bmatrix}$$

The above system is *strongly hyperbolic*, and the dispersion relation can be rewritten as

$$F(\omega, \vec{k}) = \omega \prod_{\alpha=1}^8 \left(\omega_{\alpha} - \vec{k} \cdot \vec{c}_{\alpha} \right) = 0. \quad (83)$$

Therefore, the LBE satisfies both the BFJ assumptions. Thus, according to the BFJ first theorem, it can be concluded that the PML-LBEs formulation is well-posed.

The BJF second theorem determines the stability condition on each physical mode. It should be noted that each physical mode corresponds to a lattice direction in LBEs. Moreover, the group velocity for each physical mode is equal to the lattice velocity:

$$\vec{V}_g = \nabla_k \omega_{\alpha} = \vec{c}_{\alpha}. \quad (84)$$

Figure 15 illustrates the stability regions of each physical mode for a PML constructed in x -direction ($\sigma_x \neq 0, \sigma_y = 0$). The solid lines correspond to the slowness curves which are the locus of the endpoints of slowness vectors. Two slowness vectors, one in the stable region and one in the unstable region (if any), is shown with corresponding group velocities. The stable regions are those where the x components of the slowness vector and the group velocity (the lattice velocity) have the same direction, whereas the unstable regions are those where these vectors have different directions. As it can be observed, except modes 1, 3, 5, and 7, for which the lattice velocity has either a component in x or in y directions, other modes can become unstable depending on the wave propagation direction as was mentioned earlier in Sec. 3. Similar conclusion can be made about a PML constructed in the y -direction. Another way of explaining the possible instability of the mentioned modes is that depending on the wave propagation direction, the algorithm may encounter downwind discretization in certain lattice directions which results in the instability of the simulation.

One can overcome this problem by separating modes 2, 4, 6, and 8 from the stable modes and reformulate a PML in (1, 1) and (-1, 1) directions. This is basically rotating the frame of references in the slowness space by 45 degrees which makes these modes satisfy the stability condition. In other words, instead of calculating the spatial derivatives in x or y direction which might lead to downwind discretization for some lattice directions, the derivatives are calculated along characteristic directions using an upwind discretization. The new set of PML equations is completely similar to those of modes 1, 3, 5, and 7. The only difference lies in the direction of the Q derivatives. This means that for modes 2, 4, 6, and 8, the Q derivatives along the lattice directions will appear in the PML equations rather than the derivatives in x and y directions. This is basically the formulation suggested by eq. (39).

Figure 1. Schematic of a lattice node on the upper transverse boundary of a two dimensional computational domain.

Figure 2.
Schematic of computational domain for PML study in a two-dimensional simulation.

Figure 3. Acoustic pressure contours (level -0.003 to 0.003) of a Gaussian pulse propagation in a 300×300 domain; (a) $t = 0$; (b) $t = 130$; (c) $t = 230$; (d) $t = 350$. A 50-lattice wide PML is used in the upper transverse boundary. All dimensions are normalized by lattice units.

(a)

(b)

Figure 4.

Pressure measured at $x = 150$, and $y = 200$ for the case shown in Fig. 3; (a) results near the reflection waves arrival time; (b) results measured for a long period of time; solid line: PML; dashed line: zero gradient BC; symbols: pressure history obtained for a larger domain to eliminate reflection.

(a)

(b)

Figure 5. Frequency spectra of measured pressure signals shown in Fig. 4. (a) Fast Fourier Transform of the incident Gaussian pulse and the reflected pulses from the boundaries; (b) reflection factor as a function of frequency as defined by eq. (59).

(a)

(b)

Figure 6.

The effect of (a): PML thickness, and (b): damping coefficient on the reflected pulse measured at $x = 200$ and $y = 300$ in a 400 by 400 domain; the damping coefficient is $\sigma = 0.06$ for (a), and the PML thickness is $L = 20\Delta x$ in (b);

Figure 7.

Iso-pressure contours of a Gaussian pulse propagation in a $200 \times 200 \times 150$ domain.

(a)

Figure 8. Pressure measured at (100, 100, 100), for the case shown in Fig. 7; solid line: PML; dashed line: zero gradient BC; ○: pressure history obtained for a larger domain to eliminate reflection.

(a)

(b)

(c)

(d)

Figure 9.

Iso-vorticity contours for an isolated vortex advection in a 500×500 domain; (a) $t = 0$; (b) $t = 1200$; (c) $t = 1290$; (d) $t = 1500$. A 50-lattice wide PML is used. All dimensions are normalized by lattice units.

Figure 10.

Iso-transverse-velocity contours ($v \in [-0.08, 0.08]$) for an isolated vortex advection in a 500×500 domain; (a) $t = 0$; (b) $t = 1200$; (c) $t = 1300$; (d) $t = 1430$. A 50-lattice wide PML is used. All dimensions are normalized by lattice units.

Figure 11.

The transverse velocity component, v , in an isolated-vortex-propagation problem at (a); (a) $t = 10$; (b) $t = 1200$; (c) $t = 1500$; (d) $t = 1700$; (e) $t = 2000$; solid line: numerical results obtained with PML; symbols: solution in a larger domain; dashed line: the interface between PML and the computational domain. All dimensions are normalized by lattice units.

(a)

(b)

Figure 12. Iso-vorticity contours (level -10 to 10) of 2D flow around a bluff square; (a) $t = 800\Delta t$; (b) $t = 35000\Delta t$

Figure 13.
The density fluctuation history of the flow at the two microphones.

(b)

Figure 14. Iso-vorticity contours (level -10 to 10) of 2D flow around a bluff square with 30 [deg] angle of attack at (a) $t = 3500\Delta t$.

Figure 15.
Stability regions of D2Q9-LBEs physical modes.