Accuracy of Discrete-Velocity BGK Models for the Simulation of the Incompressible Navier-Stokes Equations

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ABSTRACT

Two discretizations of a 9-velocity Boltzmann equation with a BGK collision operator are studied. A Chapman-Enskog expansion of the PDE system predicts that the macroscopic behavior corresponds to the incompressible Navier-Stokes equations with additional terms of order Mach number squared. We introduce a fourth-order scheme and compare results with those of the commonly used lattice Boltzmann discretization and with finite-difference schemes applied to the incompressible Navier-Stokes equations in primitive-variable form. We numerically demonstrate convergence of the BGK schemes to the incompressible Navier-Stokes equations and quantify the errors associated with compressibility and discretization effects. When compressibility error is smaller than discretization error, convergence in both grid spacing and time step is shown to be second-order for the LB method and is confirmed to be fourth-order for the fourth-order BGK solver. However, when the compressibility error is simultaneously reduced as the grid is refined, the LB method behaves as a first-order scheme in time.

1 Introduction

The Navier-Stokes equations of fluid mechanics may be derived as the macroscopic behavior of hard-sphere particles with a Maxwellian velocity distribution function whose evolution is governed by Boltzmann’s equation. However, vastly simpler kinetic models can result in the same macroscopic behavior. This idea led Frisch et al [1] to the invention of ‘minimalist’ models for the purpose of numerical computation of fluid flows. Pursuant to this work, a significant number of papers have been published concerning lattice gas automata (LGA) and the related lattice Boltzmann (LB) method. As a subset of these we reference here two collections of papers compiled by Doolen [2, 3].

The LB method was proposed by McNamara and Zanetti [4] as a derivative of LGA’s, but it may also be viewed as a finite-difference method for the numerical simulation of the discrete-velocity Boltzmann equation that makes use of a BGK relaxation term instead of the full nonlinear collision operator [5]. Macroscopic Navier-Stokes behavior
is obtained by stipulating that the BGK relaxation is towards an equilibrium velocity distribution function whose first several velocity moments match those of a Maxwellian distribution.

Although the LB method has been used to simulate many physical phenomena, its characterization as a numerical method has been primarily qualitative. Several researchers have made quantitative comparisons of LB results with traditional CFD methods \cite{6} \cite{7} \cite{8} \cite{9}. Comparisons of measured transport coefficients have frequently been made (e.g. reference \cite{10}) and there has been some recent work concerning quantification of global error and demonstration of convergence (e.g. reference \cite{11}).

In an effort to characterize the LB method and establish its validity as a Navier-Stokes solver, we numerically demonstrate convergence of a 9-velocity LB scheme to the incompressible Navier-Stokes equations. The order of the method is determined and errors associated with discretization and compressibility effects are identified. We also introduce a finite-difference Boltzmann (FDB) scheme by applying a fourth-order finite-difference method to the 9-velocity BGK model and demonstrate convergence of this scheme to Navier-Stokes behavior in the incompressible and continuum limits. Comparisons are also made with 2nd and 4th order finite-difference methods applied directly to the incompressible Navier-Stokes equations.

In section 2, we describe how the Chapman-Enskog expansion is used to determine the macroscopic behavior associated with the discrete-velocity BGK models. Error terms are discussed and the models are compared with traditional computational fluid dynamics methods. In section 3, the fourth-order finite difference Boltzmann scheme is introduced and its differences from the traditional LB method are highlighted. In Section 4 we present the convergence studies and discuss the results. We conclude with some comments regarding the overall accuracy, speed, and stability of the discrete-velocity BGK models in comparison with other CFD methods.

2 Discrete-Velocity BGK Macroscopic Behavior

We begin by presenting a discrete-velocity BGK model that uses nine velocities. The particle populations, $f_i$, are associated with a zero-velocity rest population, $f_0$, and with the set of discrete velocities given by $\mathbf{e}_i = c \{ \cos(\pi(i - 1)/2), \sin(\pi(i - 1)/2) \}$ for $i = 1, 2, 3, 4$ and $\mathbf{e}_i = \sqrt{2} c \{ \cos(\pi(i - 9/2)/2), \sin(\pi(i - 9/2)/2) \}$ for $i = 5, 6, 7, 8$. The parameter $c$ is the characteristic particle speed and is proportional to the speed of sound. The mass and momentum of the fluid at a site are obtained using the following sums over all nine velocities ($i = 0, 8$):

Mass:

$$n \equiv \sum_i f_i$$  \hfill (1)

Momentum:

$$n \mathbf{u} \equiv \sum_i f_i \mathbf{e}_i.$$  \hfill (2)

The BGK model presented here makes use of Boltzmann’s equation with the collision term replaced by a single-time relaxation towards an equilibrium population denoted $f_i^{eq}$ \cite{5}. The discrete-velocity model that describes the evolution of $f_i$ is written

$$\frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i = -\frac{1}{\tau} (f_i - f_i^{eq}).$$  \hfill (3)
The value of $\tau$ in this model is inversely proportional to density (assumed constant for incompressible flows) and is assumed to be small so that for small nonequilibrium populations, the right side of the above equation will be of $O(1)$. The equilibrium populations of this model are given in reference [8] as

$$f_{eq}^0 = \frac{4}{9}n - \frac{2}{3}nu^2$$

(4)

$$f_{eq}^i = \frac{1}{9}n + \frac{n}{3c^2}e_i \cdot u + \frac{n}{2c^4}(e_i \cdot u)^2 - \frac{n}{6c^2}u^2$$

(5)

for $i = 1, 2, 3, 4$ and

$$f_{eq}^i = \frac{1}{36}n + \frac{n}{12c^2}e_i \cdot u + \frac{n}{8c^4}(e_i \cdot u)^2 - \frac{n}{24c^2}u^2$$

(6)

for $i = 5, 6, 7, 8$.

A Chapman-Enskog procedure is applied to determine the macroscopic behavior of this model. Details of this procedure are provided in reference [12]. The resulting continuity and momentum equations follow.

$$\frac{\partial n}{\partial t} + \frac{\partial nu_\beta}{\partial x_\beta} + O(\varepsilon^2) = 0$$

(7)

$$n\frac{\partial u_\alpha}{\partial t} + nu_\beta \frac{\partial u_\alpha}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial}{\partial x_\beta}(\mu(\frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial u_\alpha}{\partial x_\beta})) + O(\varepsilon^2) + O(M^3)$$

(8)

where

$$\mu = \frac{\tau nc^2}{3}.$$ 

(9)

Characteristic dimensionless parameters are the Mach number, $M = \frac{\sqrt{\mu U}}{\varepsilon}$ where $U$ is a characteristic macroscopic flow speed, the Knudsen number which is proportional to $\varepsilon = \frac{c}{L}$, where $L$ is a macroscopic flow length, and the Reynolds number,

$$Re = \frac{nUL}{\mu} = \frac{\sqrt{3ML}}{\tau c}.$$ 

(10)

We note that the Knudsen number is proportional to the Mach number so that the $O(\varepsilon^2)$ terms are of $O(M^2)$. Thus, equations (7) and (8) are the compressible Navier-Stokes equations with additional terms that are of $O(M^2)$. Deviations from incompressible behavior are still present in the compressible Navier-Stokes equations. These deviations are associated with gradients of density and velocity field divergence and are also of $O(M^2)$ [8] [13]. We group all three types of terms; Knudsen number squared, Mach number cubed, and Navier-Stokes compressibility terms, into ‘compressibility error’. As the Mach number approaches zero, the above model should approach incompressible Navier-Stokes behavior.

Numerical simulations of the incompressible Navier-Stokes equations may be performed by discretizing equation (3). We note that convergence to the incompressible equations is obtained only if the compressibility errors are smaller than the discretization error. Here we discuss the commonly used LB discretization while in section 3 we introduce a fourth-order discretization.
The lattice Boltzmann discretization of equation (3) consists of a first order upwind discretization of the left side and the selection of the lattice spacing \( h \), and the time step \( \Delta t \), to provide an exact Lagrangian solution. This is accomplished by selecting \( \frac{h}{\Delta t} = c \) so that the discrete equation becomes

\[
f_i(x + e_i \Delta t, t + \Delta t) - f_i(x, t) = -\frac{\Delta t}{\tau} (f_i(x, t) - f^{(0)}_i(x, t)).
\]  

(11)

While this appears to be a first-order method, it is actually second-order if the second order terms in the truncation error are considered to represent artificial viscosity. More precisely, when a Taylor series expansion is performed on the first term in the above equation, all second order terms may be combined in a manner that the value of \( \tau \) in equation (9) may simply be replaced by \( \tau - \frac{\Delta t^2}{2} \) for the LB method.

The use of the second order discretization error to represent physics, leaves only third-order terms as the truncation error so that the method is effectively second order \cite{13} \cite{12}. Since the time step is proportional to the lattice spacing, the scheme is second order in both time and space (again, if compressibility effects are smaller than discretization error). These analytical trends are numerically studied and verified in Section 4 below.

### 3 Fourth Order Discrete Velocity BGK Model Solver

In this section we present a fourth order finite difference discretization of the discrete velocity BGK equation. In the previous section we described how the Chapman-Enskog expansion can be used to recover the incompressible Navier-Stokes equations from the BGK equation with a certain set of discrete velocities. We showed that if the Mach number is sufficiently small, a numerical solver that produces a higher order approximation to the Boltzmann equation will also produce a higher order approximation to the Navier-Stokes equations.

We seek to discretize

\[
\frac{\partial f_i}{\partial t} + \vec{e}_i \cdot \nabla f_i = -\frac{1}{\tau} (f_i - f^{eq}_i)
\]

(12)

We use centered differences to discretize the convective terms. This is done because of their simplicity to implement, and because they have lower truncation errors than upwind schemes of equal order. The fourth order approximation used for the convective term can be written as

\[
\frac{\partial f}{\partial x} \approx D^0_x f = \frac{-f(x + 2h) + 8f(x + h) - 8f(x - h) + f(x - 2h)}{12h}
\]

(13)

where \( h \) is the mesh width.

This produces a system of ordinary differential equations for the distributions at each point:

\[
\frac{\partial f_i(x, y, t)}{\partial t} = -\vec{e}_i \cdot (D^0_x f(x, y, t), D^0_y f(x, y, t)) - \frac{1}{\tau} (f_i(x, y, t) - f^{eq}_i(x, y, t))
\]

(14)

We discretize in time explicitly using the following fourth order Runge-Kutta method.

\[
\tilde{k}^0 = \Delta t G(\tilde{f}(t_n), t_n)
\]

(15)

\[
\tilde{k}^1 = \Delta t G(\tilde{f}(t_n) + \frac{1}{2} \tilde{k}^0, t_n + \frac{1}{2} \Delta t)
\]

(16)
\[ \vec{k}^2 = \Delta t G(\vec{f}(t_n) + \frac{1}{2}\vec{k}^1, t_n + \frac{1}{2}\Delta t) \]  
\[ \vec{k}^3 = \Delta t G(\vec{f}(t_n) + \vec{k}^2, t_n + \Delta t) \]  
\[ \bar{f}(t_{n+1}) = \bar{f}(t_n) + \frac{1}{6}(\vec{k}^0 + 2\vec{k}^1 + 2\vec{k}^2 + \vec{k}^3) \]

where \( G(\vec{x}, t) \) is the right hand side of equation (14). The use of centered differences on the convection term makes some commonly used marching procedures such as Euler’s and Heun’s method unstable in the absence of a dissipative term. However both third and fourth order Runge-Kutta methods have a region of stability that contains a portion of the imaginary axis in the complex plane and hence are stable for our discretization [16]. The larger stability region of the fourth order Runge-Kutta method makes the computation more efficient, and as a bonus we obtain fourth order accuracy in time.

This finite difference Boltzmann (FDB) scheme differs from the traditional LB scheme. The stream/collide process is replaced by the combination of a finite difference calculation of the convection terms and a four step Runge-Kutta process for advancement in time. A key difference is the value of the viscosity. Artificial viscosity produced by the grid is not used to represent physics as in the LB method, so the relationship between the relaxation parameter \( \tau \) and the physical parameters can be obtained directly from equation (10) as

\[ \tau = \frac{\sqrt{3}ML}{cRe} \]  

whereas for the LB method the relationship is

\[ \tau = \frac{\sqrt{3}ML}{cRe} + \frac{\Delta t}{2} \]

We must examine the stability of this numerical scheme. The value of the time step \( \Delta t \) is no longer set by the lattice size but is an independent numerical parameter. In the absence of a collision term the stability requirement for the convective term is [16]

\[ \Delta t < \frac{\sqrt{8h}}{e_{\max}} \]  

where \( e_{\max} \) is the maximum absolute value of the discrete velocities. However the collision term has an approximate stability condition that \( \Delta t < \tau \), which is consistent with the earlier statement that populations not be allowed to evolve far from equilibrium. This condition can be quite restrictive, since for high Reynolds numbers and low Mach numbers \( \tau \) can be quite small. One does not encounter this problem with the LB method because, as seen in equation (21), \( \Delta t \) is always of \( O(\tau) \) for small Mach number.

**4 Test Problem and Results**

We choose as our test problem the evolution of a decaying Taylor vortex in a \( 2\pi \) periodic domain. The exact solution for the flow satisfies

\[ u(x, y, t) = -\exp(-\nu t(w_1^2 + w_2^2)) \cos(w_1 x) \sin(w_2 y) \]  
\[ v(x, y, t) = \frac{w_1}{w_2} \exp(-\nu t(w_1^2 + w_2^2)) \sin(w_1 x) \cos(w_2 y) \]

\[ u(x, y, t) = -\exp(-\nu t(w_1^2 + w_2^2)) \cos(w_1 x) \sin(w_2 y) \]  
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\[ \bar{f}(t_{n+1}) = \bar{f}(t_n) + \frac{1}{6}(\vec{k}^0 + 2\vec{k}^1 + 2\vec{k}^2 + \vec{k}^3) \]  
\[ \vec{k}^2 = \Delta t G(\vec{f}(t_n) + \frac{1}{2}\vec{k}^1, t_n + \frac{1}{2}\Delta t) \]  
\[ \vec{k}^3 = \Delta t G(\vec{f}(t_n) + \vec{k}^2, t_n + \Delta t) \]  

Our tests were performed at $Re = 100$ with $w_1 = 3$ and $w_2 = 2$.

For LB and FDB calculations, we must specify how to initialize the populations $f_i$ from a given velocity field. First, a pressure field is generated from the velocity field by taking the divergence of the momentum equation and solving for the pressure. Since the velocity field is divergence free,

$$\nabla^2 p = -\nabla \cdot (u \cdot \nabla u). \quad (25)$$

We then use the equation of state to initialize the density to $\rho = \rho_0 + \frac{3p}{c_s^2}$. With the velocity and density specified, we investigated two methods of initializing the populations $f_i$. In the first, the populations are initialized to the equilibrium distributions. In the second method, we add the non-equilibrium populations to the equilibrium values using the formula (see also [11])

$$f_{i}^{\text{neq}} = -\tau \Delta t (\frac{\partial f_{i}^{\text{eq}}}{\partial t} + \bar{e}_{i} \cdot \nabla f_{i}^{\text{eq}}) \quad (26)$$

where the derivatives are evaluated analytically using the known exact solution for this flow.

### 4.1 Rate of Convergence

We first examine the spatial and temporal convergence rates for the LB and FDB methods. For a given Mach and Reynolds number, the Chapman-Enskog expansion yields the compressibility error discussed in Section 2 so that we are not exactly calculating the solution to the incompressible Navier-Stokes equations. However we expect that as we refine in time and space at a fixed Mach number, our methods will be converging to some solution. We first examine the speed at which convergence to this solution occurs.

We do not have an exact solution for the discrete velocity Boltzmann equation that is being simulated. However we can calculate convergence rates by looking at the difference in the values of solutions computed on successive grids. If we let

$$E(h) = \|U(2h) - U(h)\| \quad (27)$$

where $U(h)$ is the solution calculated on a grid with mesh width $h$, then the rate of convergence can be estimated by

$$\rho = \log_2 \frac{E(2h)}{E(h)} \quad (28)$$

In the remainder of this section we will use the $L^2$ norm to compute our differences. These differences will be evaluated at $t = 1$. We first show in Table 1 the convergence rates for the LB method when equilibrium populations are used for initialization. Spatial and temporal convergence are equivalent for this method because the time step is a linear function of the mesh size. The Mach numbers presented in the tables are based on the lattice speed instead of the sound speed and are therefore equal to the actual Mach number divided by $\sqrt{3}$. We see that one gets second order convergence, even for Mach numbers for which compressibility effects are significant.

One sees a different behavior when the second initialization method is used. This initialization appears to deteriorate convergence behavior, and we see less than second order accuracy. This failure to reach second order decreases as Mach number decreases,
so for very small Mach number second order accuracy does result. We note that a possible cause of the loss of accuracy is that the artificial viscosity from the grid that is used to attain second order accuracy is not taken into account in this initialization method.

Tables 3 and 4 show the space and time convergence behavior for the FDB method. We only present results at the relatively high Mach number \( M = 0.25 \), but one sees similar behavior throughout the entire range of Mach numbers. The fourth order convergence behavior is quite clear, and small errors are attained with much fewer lattice points than for the LB method.

### 4.2 Effect of Initialization

It was expected that with increasing time, the differences between the solutions calculated with either initialization method would decrease. However we see that this is not the case. As Table 5 shows, for a fixed grid size and Mach number, the difference between the LB solutions computed with the two initialization methods remains relatively constant for all time. However this difference decreases as the Mach number decreases and the mesh is refined. It appears that in the limit of zero Mach number and infinite
| Time Step | E(h)         | ρ         |
|-----------|--------------|-----------|
| .0025     | 5.14 × 10⁻³  |           |
| .00125    | 3.08 × 10⁻⁶  | 4.06      |
| .000625   | 1.90 × 10⁻⁷  | 4.02      |

Table 4: Convergence behavior in time for FDB

| Time | Grid Size | Mach | Difference |
|------|-----------|------|------------|
| .25  | 32 × 32   | 0.25 | .108       |
| 1.00 | 32 × 32   | 0.25 | .116       |
| .25  | 64 × 64   | 0.25 | .0482      |
| 1.00 | 64 × 64   | 0.25 | .0496      |
| .25  | 128 × 128 | 0.25 | .0268      |
| 1.00 | 128 × 128 | 0.25 | .0271      |
| .25  | 256 × 256 | 0.25 | .0184      |
| 1.00 | 256 × 256 | 0.25 | .0186      |
| .25  | 256 × 256 | 0.125| .00632     |
| 1.00 | 256 × 256 | 0.125| .00489     |
| .25  | 256 × 256 | 0.0625| .00250    |
| 1.00 | 256 × 256 | 0.0625| .00252    |

Table 5: Difference in solutions with different initialization methods

mesh the two methods of initialization give equal solutions. But if one is computing underresolved solutions, then it must be concluded that the evolution of the computed velocity field is a function not just of the initial velocity field but of the initial particle distribution at each point. Differences in initializations produce differences in the evolving velocity field that do not decay in time.

4.3 Convergence to Incompressible Navier-Stokes Solutions

We now investigate the convergence of the LB and FDB methods to the incompressible Navier-Stokes solutions to test problems. For this experiment we can now compare the numerical results to the known exact solutions. During simulation it was found that the error oscillated in time. In order to get a clear picture of the accuracy of the methods, we computed the error at small intervals up to $t = 1$ and then averaged to compute an average error. The average divergence was also computed to indicate the deviation from incompressibility.

Solutions were also calculated with a finite difference solver for the Navier-Stokes equations. Both a second and fourth order solver that employed the primitive variables (velocity and pressure) were used. These results allow us to compare the accuracy of the Boltzmann methods to methods that discretize the Navier-Stokes equations directly.

The results of this study are presented in figure 1. The dotted lines represent the errors of the LB simulations as the mesh is refined for fixed Mach numbers. The solid lines are the FDB errors for the same constant Mach numbers. The dash-dotted lines
represent the errors in the finite difference solutions to the incompressible Navier-Stokes equations.

We observe that convergence to the solution of the incompressible Navier-Stokes equations is only attained by simultaneously refining both the mesh size and decreasing the Mach number. As can be seen in figure 1, the error for the LB method saturates at a certain level as the mesh is refined. These deviations from the exact solutions are caused by the “compressibility errors” that were discussed in section 2. In table 6 we look at errors and divergences for calculations on a $512 \times 512$ lattice at various Mach numbers. At this lattice size the discretization error is quite small, and differences from incompressible Navier-Stokes behavior are due to compressibility effects that are of $O(M^2)$.

By simultaneously decreasing Mach number and mesh size, we can demonstrate convergence to Navier-Stokes solutions. (see table 7). The convergence is second order in space, because halving the grid size reduces the error by approximately a factor of four. However, the time step is also halved because it is proportional to the grid spacing, and the Mach number is halved to keep compressibility error of the same size as the discretization error. The lower Mach number requires an increase in the time needed for the same flow evolution to occur (eddy-turnover time). Thus, while the error is reduced by a factor of four, the number of time steps increases by a factor of four. Keeping compressibility error equal to discretization error makes the scheme effectively first-order in time.

Figure 1 also shows the more rapid convergence of the FLB method to Navier-Stokes solutions. One can obtain errors near those of the LB method with $\frac{1}{16}$ as many points. This rapid convergence leads to the dominance of compressibility errors at coarser grids than for the LB method.

Finally we present the errors from a second and fourth order finite difference method for the incompressible Navier-Stokes equations in both figure 1 and table 7. One sees that the fourth order scheme clearly outperforms all methods. The second order scheme produces errors slightly smaller than the LB method for an equal number of points. For
| Grid Size | Second Order | Fourth Order |
|-----------|--------------|--------------|
|           | error        | error        |
| 16 × 16   | .275         | .0652        |
| 32 × 32   | .0798        | .00464       |
| 64 × 64   | .0208        | .000299      |
| 128 × 128 | .00526       | .000019      |

Table 8: Convergence behavior for finite difference NS solvers

this method, an elliptic equation must be solved at each time step. However the time step of the calculation no longer is limited by the Mach number so many fewer time steps are needed.

5 Conclusions

Convergence of two different discretizations of a discrete-velocity BGK model to the incompressible Navier-Stokes equations has been numerically demonstrated. The model consists of PDEs that describe the evolution of the velocity distribution function associated with each discrete velocity. A Chapman-Enskog expansion predicts that the macroscopic behavior of the model corresponds to the incompressible Navier-Stokes equations with deviations of $O(M^2)$ that are referred to as ‘compressibility error’. Thus, if the Mach number is small enough, one should be able to discretize the PDE using any preferred finite-difference method and the convergence to incompressible Navier-Stokes behavior should occur at the rate corresponding to the order of the finite-difference method.

We introduced a fourth-order finite-difference Boltzmann method (FDB) and verified convergence to the exact solution of the Navier-Stokes equations for a decaying Taylor vortex flow. For small enough compressibility error, fourth-order convergence was confirmed. Similarly, the commonly used lattice Boltzmann discretization was confirmed to behave as a second order scheme in both time and space when compressibility error was smaller than discretization error and when the artificial viscosity associated with second order discretization error was taken to represent a physical viscosity.

The computational time of the LB and FDB methods is inversely proportional to the Mach number. Therefore, it is most efficient to choose the Mach number so that compressibility error is equal to discretization error. As the grid is refined, one must simultaneously decrease the Mach number as illustrated in table 7. With this approach, the LB scheme behaves as a first order scheme in time.

The stream/collide view of the LB scheme results in a naturally parallel algorithm that is easy to program and allows the use of particle reflection boundary conditions. However, with a small amount of additional effort, one may implement a higher-order scheme that allows coarser resolution for a given error or lower error for fixed resolution in comparison with the LB method. Stability requirements of the LB method are described in reference [12]. The stability requirements of the FDB method require that the time step be on the order of the BGK relaxation time. We hope to develop methods that have a less stringent stability requirement while retaining higher order accuracy. In addition, studies concerning the effect of boundary conditions on accuracy are needed to complete the numerical characterization of these methods.
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**Figure Captions**

Fig. 1: Error of Discrete-Velocity BGK Methods as function of Mach number and grid resolution. Dashed lines represent the error of the LB method for various Mach numbers. Solid lines represent the error of the FDB method. The dashed-dotted lines are the errors of the finite-difference Navier-Stokes solvers.