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SHOCK CAPTURING SCHEMES WITH GAS-KINETIC METHODS

A DISSERTATION
SUBMITTED TO THE DEPARTMENT OF AERONAUTICS AND ASTRONAUTICS
AND THE COMMITTEE ON GRADUATE STUDIES
OF STANFORD UNIVERSITY
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY

Yeefeng Ruan
June 2002
I certify that I have read this dissertation and that in my opinion it is fully adequate, in scope and quality, as dissertation for the degree of Doctor of Philosophy.

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Approved for the University Committee on Graduate Studies
ABSTRACT

The development of gas-kinetic methods for compressible flow simulations has attracted much attention in the last decade. Gas-kinetic schemes are based on the Boltzmann equation, which represents a better physical description of the behavior of the flows than either the Euler equations or the Navier-Stokes equations. Due to the complications of the collision integral term of the Boltzmann equation, most gas-kinetic schemes solve the collisionless Boltzmann equation instead by neglecting the collision integral term. The gas-kinetic Bhatnagar-Gross-Krook (BGK) method offers a simplified model by linearizing the collision integral term. Since the BGK model includes the collision term, which simulates flow transition from a non-equilibrium state to an equilibrium one, it is an excellent shock-capturing method, especially for multidimensional compressible flows and strong shock tubes, with only moderate extra effort on a computer.

A typical Godunov-type numerical scheme has two stages: the reconstruction stage for generating initial cell-averaged values at cell interfaces and the evolution stage for computing flow variables at later time by solving the physical governing equations. For the reconstruction stage, to avoid generating spurious oscillations in the solutions, Jameson developed the LED (local extremum diminishing) theory. Based on the LED principle, the limiter is used to interpolate cell interface variables for higher-order schemes. During the evolution stage, the simplified Boltzmann equation (BGK equation) is used as the flow solver in this research. It is superior to other Riemann solvers that use the Euler or the Navier-Stokes equations as the governing equations because the Boltzmann equation is not only good in smooth areas but also in areas having discontinuities such as shocks. It is also better than other collisionless gas-kinetic schemes such as the Kinetic Flux Vector Splitting (KFVS) scheme because the particle collision effect is taken into consideration in the gas evolution stage.

The objective of this dissertation is firstly to illustrate the robustness of the BGK scheme
and its accuracy on variety of shock applications, especially for three-dimensional transonic and supersonic wing computations that have not been done before. Some of the computational results are shown to compare well with the exact results, other existing numerical results, or experimental results. Secondly, the positivity properties of the first-order BGK method are analyzed in detail for the linear advection equation and the Euler equations. It is proved here that the gas-kinetic BGK scheme is a positivity-preserving scheme. The positivity conditions, which are dependent on the collision time, are also given here for these two governing equations. Lastly, some advantages and disadvantages of gas-kinetic BGK schemes will be discussed for future reference.
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accomplishment is made. I would also like to express my deep appreciation to my parents for their lifetime sacrifice and encouragement. I know that this Ph.D. degree means as much to them as to myself. I really wish my father could see this happening.
DEDICATION

The author wishes to dedicate this dissertation to my parents and my wife for their longtime supporting and understanding.
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CHAPTER 1
INTRODUCTION

1.1 History of Gas-Kinetic Methods

The development of numerical schemes based on kinetic theories for compressible flow simulations started in the 1960s. Chu's method[1], based on the gas-kinetic BGK model, with a discretized velocity space, is one of the earliest kinetic methods used for shock tube calculations. In the 1980's and 90's, many researchers have contributed to gas-kinetic schemes. Pullin[2] was the first to split the Maxwellian distribution into two parts and used the complete error function to obtain the numerical fluxes. The resulting scheme was named the Equilibrium Flux Method (EFM). By applying the upwind technique directly to the collisionless Boltzmann equation, Mandal[40] and Deshpande derived the same scheme, which they named Kinetic Flux Vector Splitting (KFVS). The KFVS Navier-Stokes solver, which was developed by Chou[5] and Baganoff, is a special case of the current gas-kinetic BGK method in which the particle collisional time is much larger than the time step.

A typical Godunov-type finite volume scheme has two stages: the reconstruction stage for generating initial cell-averaged values at cell interfaces and the evolution stage for computing flow variables at later times by solving the physical governing equations. Gas-kinetic schemes based on the Bhatnagar-Gross-Krook (BGK) model are new methods to model the gas evolution process by solving the simplified Boltzmann equation. BGK-type schemes are different from other Boltzmann-type schemes, which solve the collisionless Boltzmann equation by neglecting the collision term of the Boltzmann equation. Because of the inclusion of the collision term of the Boltzmann equation, BGK-type schemes take into account the particle collisions in the whole gas evolution process within a time step, from which the time-dependent gas distribution function and the
resulting numerical fluxes at the cell interface are obtained. Moreover, due to its specific governing equation, the BGK method gives Navier-Stokes solutions directly in smooth regions. In the discontinuous regions, the scheme provides a delicate dissipative mechanism to produce stable and crisp shock transitions. Since the gas evolution process is a relaxation process from a non-equilibrium state to an equilibrium one, the entropy condition is always satisfied by the BGK method. Due to the dissipative nature of BGK methods, rarefaction shocks, carbuncle phenomena or odd-even decoupling have never been observed, although they occasionally appear in other Godunov-type schemes. Finally, the gas-kinetic BGK scheme is positivity-preserving, which makes certain that only positive densities and pressures are obtained from numerical computations.

The development of gas-kinetic BGK methods for compressible flow simulations and other applications has attracted much attention and has matured in the last decade. In 1993, Prendergast\cite{25,33} and Xu first successfully used the gas-kinetic BGK method to solve the two-dimensional hydrodynamic equations. In 1995, Xu\cite{38,39,40} introduced Jameson's SLIP formulation\cite{9,10,11,12,13,14} to construct higher-order BGK schemes. In 1998, Kim\cite{16,17,18,19} and Jameson developed the LED-BGK solver on unstructured adaptive meshes. In 2000, Chae\cite{15} and Kim proposed the modified gas-kinetic BGK scheme by introducing a Prandtl number correction into the flux calculations. Lately, Xu\cite{34,35,36} has used the BGK scheme to solve the shallow water equations, the ideal MHD equations, and to compute flows with chemical reactions. In 1996, Balakrishnan\cite{60} and Agarwal used the BGK method to solve the Burnett equations for hypersonic flows. Another aspect of the gas-kinetic BGK scheme is its entropy condition and its positivity-preserving property. In 1997, Tang\cite{27} and Xu proved that the collisionless KFVS scheme, which is a special case of the BGK scheme as the collision coefficient goes to zero, is a positive scheme. Tang also suggested that the general gas-kinetic BGK scheme is a positivity-preserving scheme based on the computational experience, although he did not prove this property mathematically.
1.2 Objective of This Thesis

The theory and formulation of gas-kinetic BGK schemes have been well established in the last decade, and a lot of numerical applications have been carried to demonstrate the robustness and accuracy of the method. In order to enrich gas-kinetic BGK schemes, the author is trying to accomplish the following tasks in this thesis:

- To perform more numerical calculations for the linear advection equation, the nonlinear Burger's equation, the one-dimensional and two-dimensional Euler and Navier-Stokes equations in order to show that gas-kinetic BGK schemes are very good shock-capturing schemes.

- Because of the formulation complexity of BGK schemes, no one has used them for three-dimensional flow applications before. To prove the feasibility of gas-kinetic BGK schemes for three-dimensional transonic and supersonic wing calculations, the flux computation procedures for non-rectangular meshes will be given in detail.

- The improvement of the gas-kinetic BGK scheme over other collisionless kinetic schemes, such as the KFVS scheme, is that particle collisions are included in the evolution stage of the flux calculations. The numerical dissipation is determined by the collision time instead of the time step. The author will give the optimized collision time calculation for the three dimensional wing calculations based on numerous numerical experiments.

- Positivity of solutions from the gas-kinetic BGK method is guaranteed. This property might not be retained by other flux-splitting schemes. The author will prove for the linear advection equation and the one-dimensional Euler equations that the 1st-order BGK scheme is a positive scheme.
1.3 Thesis Outline

Following a brief introduction in Chapter 1, the fundamental concepts and governing equations that are prerequisite in understanding the present work are outlined in Chapter 2. Firstly, two ways describing flow motions are introduced in that chapter: the theory based on macroscopic quantities leads to the Euler and the Navier-Stokes equations; the theory based on microscopic quantities leads to the Boltzmann equation. Secondly, the relationship between macroscopic quantities and microscopic quantities are given. Finally, the Euler and the Navier-Stokes equations are derived from the Boltzmann equation using the Chapman-Enskog technique.

The detailed design process of the gas-kinetic BGK scheme is described in Chapter 3. Godunov-type schemes are first introduced, and the steps to build a Godunov-type scheme are also briefly outlined. The theory of LED (Local Extremum Diminishing), which was first developed by Jameson, is used to construct flow variables at cell interfaces for higher-order BGK schemes.

Chapter 4 is devoted to discussing the positivity property of BGK schemes. This property is proved for the first-order linear scalar equation and one-dimensional Euler equations: the gas-kinetic BGK scheme is a positive scheme as long as collision coefficients are within a limit and the standard CFL-like stability conditions are satisfied.

Chapter 5 gives results of numerical tests of gas-kinetic BGK schemes. These test problems include solving the scalar equations, the multi-dimensional Euler and Navier-Stokes equations, and demonstrate the stability and positivity properties of the gas-kinetic BGK scheme.

Lastly in Chapter 6, a few points of view on gas-kinetic BGK schemes from the author’s research experience are brought up for future reference.
CHAPTER 2

GAS KINETIC THEORY

There are two ways to describe fluid motions. The first one is based on macroscopic quantities, such as mass, momentum and energy density, as well as the physical laws governing these quantities, such as the Euler equations, the Navier-Stokes equations or higher order approximate equations provided by the equation of state. Another type of description comes from microscopic considerations, i.e. the gas kinetic theory. The fundamental quantity in this description is the particle distribution function $f(x,u,t)$, which gives the number density of molecules in six-dimensional phase space $(x,u) = (x_i,u_i)$, $i = 1,2,\cdots,6$. The governing equation for the gas distribution function $f(x,u,t)$ is called the Boltzmann equation. Physically, the gas kinetic equation provides more information about the gas flow and has larger applicability than its macroscopic counterparts.

These two governing equations are derived from two different methods: the continuum theory for the macroscopic model and the gas kinetic theory for the microscopic model. The validity of the two theories largely depends on the ratio of two representative length scales: the particle mean free path length and the macroscopic characteristic length. The particle mean free path length is defined as the average distance traveled by a molecule between successive collisions. The macroscopic characteristic length is the smallest physical length scale associated with the flow field. The ratio of the mean free path length to the macroscopic characteristic length is called the Knudsen number.

$$K_n \equiv \frac{\lambda}{l}$$

where $\lambda$ is the mean free path length and $l$ is a characteristic length in the flow field.
From the kinetic theory definition for $\lambda$, the Knudsen number can also be expressed as

$$K_n \approx \frac{M}{\text{Re}}$$

where $\text{Re}$ is the Reynolds number and $M$ is the Mach number.

As the Knudsen number becomes small, we say that the flow is approaching the inviscid flow limit. In this region, macroscopic models are used for flow simulations, and the governing equations are the Navier-Stokes equations. On the other hand, as the Knudsen number becomes very large, we say the flow is approaching the free molecule limit. In this region, microscopic models are used for flow simulations, and the governing equation is the Boltzmann equation. For the Knudsen numbers around 0.01, we say the flow is in the near continuum region. This is the region where the Navier-Stokes equations continue to agree with the Boltzmann equation. Figure 2.1 shows the validation of various equations as the Knudsen number is varied.

![Figure 2.1 Knudsen Number vs. Various Equations](image)

This chapter will first introduce the Navier-Stokes equations (and the Euler equations) from the continuum theory and the Boltzmann equation from the gas kinetic theory. Then the relationship between macroscopic quantities, which are governed by the Navier-
Stokes equations, and microscopic quantities, which are governed by the Boltzmann equation, are given. Finally, the continuous Euler and Navier-Stokes equations will be derived from the gas-kinetic BGK equation using the Chapman-Enskog technique.

2.1 The Navier-Stokes Equations

Consider an unsteady, compressible, viscous gas flow, the three-dimensional Navier-Stokes equations in conservative form in Cartesian coordinates can be written as:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = 0$$

(2.1)

where

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix}$$

(2.2)

$$F = F_I + F_v$$

$$G = G_I + G_v$$

$$H = H_I + H_v$$

$F_I$, $G_I$ and $H_I$ are inviscid fluxes in the $x$, $y$ and $z$ directions. $F_v$, $G_v$ and $H_v$ are viscous fluxes in the $x$, $y$ and $z$ directions. These fluxes are given by:

$$F_I = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ \rho uH \end{bmatrix}$$

(2.3)
\[
G_I = \begin{bmatrix}
\rho v \\
\rho u v \\
\rho v^2 + p \\
\rho v w \\
\rho w H
\end{bmatrix}
\] (2.4)

\[
H_I = \begin{bmatrix}
\rho w \\
\rho u w \\
\rho v w \\
\rho w^2 + p \\
\rho w H
\end{bmatrix}
\] (2.5)

\[
F_y = \begin{bmatrix}
0 \\
-\tau_{xx} \\
-\tau_{xy} \\
-\tau_{xz} \\
-\tau_{yx} u - \tau_{yy} v - \tau_{yz} w + q_x
\end{bmatrix}
\] (2.6)

\[
G_y = \begin{bmatrix}
0 \\
-\tau_{yx} \\
-\tau_{yy} \\
-\tau_{yz} \\
-\tau_{yz} u - \tau_{yy} v - \tau_{yz} w + q_y
\end{bmatrix}
\] (2.7)

\[
H_y = \begin{bmatrix}
0 \\
-\tau_{zx} \\
-\tau_{zy} \\
-\tau_{zz} \\
-\tau_{zx} u - \tau_{zy} v - \tau_{zz} w + q_z
\end{bmatrix}
\] (2.8)

In deriving the above equations, we are assuming that the flow is continuous with no dissociation and real gas effects, and the fluid is in a state of thermodynamic equilibrium. Body forces and heat sources have been neglected.

The basic variables that define the changes in the thermodynamic state of the fluid are the density $\rho$, the velocity components $u$, $v$, $w$, and the total specific energy $E$. To close
the system of equations, constitutive relationships that define the stress tensor \( \tau_{ij} \) and the heat flux vector \( q_j \) must be given, as well as an equation of state.

For Newtonian fluids, the stress tensor is linearly related to the rate of strain tensor:

\[
\nu_j = -p \delta_{ij} + \mu \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] + \lambda \delta_{ij} \frac{\partial u_k}{\partial x_k}
\]  
(2.9)

and the heat flux vector follows Fourier's law:

\[
q_j = -k \frac{\partial T}{\partial x_j}
\]  
(2.10)

We also assume that the fluid is a thermally and calorically perfect gas with constant specific heats, so the equations of state to be used are:

\[
p = (\gamma - 1) \rho E
\]  
(2.11)

\[
E = c_v T + \frac{1}{2} (u^2 + v^2 + w^2)
\]  
(2.12)

The viscosity of air may be determined from Sutherland's law for a gas, namely

\[
\frac{\mu}{\mu_0} = \left[ \frac{T}{T_0} \right]^{3/2} \left[ \frac{T_0 + 110^0 K}{T + 110^0 K} \right]
\]  
(2.13)

### 2.2 The Gas Kinetic Theory

Gas dynamics deals with macroscopic quantities, such as density, velocity and pressure. These quantities are perceived or measured in an average over a certain volume, or area, or interval of time. The governing equations for these quantities are expressions of very
broad laws of physics — the law of conservation of mass, Newton's law, and the law of conservation of energy.

In contrast with the treatment of gas dynamics on the basis of empirically determined bulk properties, it is the aim of kinetic theory to predict the dynamics of a gas on the basis of molecular mechanics and statistics. From knowledge of the forces between molecules, within the gas and at the boundaries, kinetic theory is capable, in principle, of computing the complete motions of gases. Thus it furnishes the link between the properties of matter in bulk and the properties of individual molecules and atoms. It explains the equations of state, and the concepts of temperature and of heat. Furthermore, the kinetic theory is expected to describe transport processes, that is, to furnish the general relations between stress and rate of strain and between heat flux and temperature gradient. From these it infers the range of applicability of the linear relations and hence of the Navier-Stokes equations.

2.2.1 The Boltzmann Equation

Classical kinetic theory leads to the Boltzmann equation, which is an integral-differential equation for the particle distribution function $f(\vec{x}, \vec{v}, t)$. Assuming that there is no external body force, the Boltzmann equation can be written as

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{x}} = Q(f, f)$$

(2.14)

where $Q(f, f)$ is the collision integral, or simply the collision term, $t$ is the time, $\vec{x} = (x, y, z)$ is the location of the particle, and $\vec{v} = (u, v, w)$ is the particle velocity with three components in the $x$, $y$, $z$ directions.

Since the macroscopic gas density is defined as a collection of individual particles, it can be written as an integral of the particle distribution function $f(\vec{x}, \vec{v}, t)$
\[ \rho = \int \int \int \int f \, dv \, dw \]  

(2.15)

From the physical constraints of the conservation of mass, momentum and energy during particle collisions, the following compatibility condition has to be satisfied,

\[ \int \psi_\alpha Q(\mathbf{f}, \mathbf{f}) \, d\Xi = 0 \]  

(2.16)

where \( d\Xi = dv \, dw \, d\xi_1 \, d\xi_2 \ldots d\xi_K \), and

\[ \psi_\alpha = \begin{pmatrix} 1 \\ u \\ v \\ w \\ \frac{1}{2}(u^2 + v^2 + w^2 + \xi^2) \end{pmatrix} \]  

(2.17)

\[ \xi^2 = \xi_1^2 + \xi_2^2 + \ldots + \xi_K^2 \]  

(2.18)

where \( K \) is the dimension of internal variables that represent particle rotations and vibrations, and it depends on the gas and the degrees of freedom of flow simulations.

The assumption for the Navier-Stokes equations is that the variation from an equilibrium state to a non-equilibrium state is small. We generally don’t know the non-equilibrium state distribution function \( f(\mathbf{x}, \mathbf{v}, t) \) (unknown of the Boltzmann equation), but we do know the equilibrium state distribution from the flow variables. We define \( g \) as the particle distribution function in an equilibrium state. The equilibrium distribution function, or the Maxwell-Boltzmann distribution \( g \), can be written as:

\[ g = \rho \left( \frac{2\pi}{\kappa} \right)^{\frac{K+1}{2}} e^{-\frac{1}{2}(u^2 + v^2 + w^2 + \xi^2)} \]  

(2.19)

where \( I = 3 \) for three-dimensional flows. The relationship between macroscopic and microscopic variables is given by moments of \( g \)
\[
\begin{pmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
\rho e
\end{pmatrix} = \int \begin{pmatrix}
1 \\
u \\
v \\
w \\
\frac{1}{2}(u^2 + v^2 + w^2 + \xi^2)
\end{pmatrix} gdu dv dw d\xi
\]  
(2.20)

The viscous stress tensor \(\sigma_v\) and the heat flux vector \(q_i\) in the Navier-Stokes equations can be obtained from the particle distribution function \(f\) as follows:

\[
\sigma_v = -\left(\int (u_i - U_i)(u_j - U_j) f dudvdwd\xi - p \delta_{ij}\right)
\]
(2.21)

\[
q_i = \frac{1}{2} \int (u_i - U_i)[(u - U)^2 + (v - V)^2 + (w - W)^2 + \xi^2] f dudvdwd\xi
\]
(2.22)

where \(p\) is the local pressure. The viscous stress and the heat flux will go to zero if the flow is in the equilibrium state.

2.2.2 The BGK Model

Because of the complex nonlinear structure of the collision integral \(Q(f, f)\), the Boltzmann equation is very difficult to solve and analyze. It is of interest to make a qualitative study of the properties of its solutions by use of simplified model equations. One of the simplified methods is the BGK model.

The BGK collision theory assumes that the effect of the collision term is to alter the distribution function from a non-equilibrium state to an equilibrium state. In the BGK model, the collision term will be modeled as

\[
Q(f, f) = \frac{f - g}{\tau}
\]
(2.23)
where $f$ is the particle distribution function at the non-equilibrium state, and $g$ is the particle distribution function at the equilibrium state. $\tau$ is the collision time from a non-equilibrium state to an equilibrium state.

The gas kinetic BGK model leads to the linearized Boltzmann equation, or the BGK equation. Since the BGK equation is a linear equation, an analytical solution for $f$ can be obtained. Moments of the distribution function yield the macroscopic flow fluxes. The detailed formulation of the integrations of the Maxwellian distribution function can be found in Appendix A.

2.3 Connection Between the BGK Equation and the Navier-Stokes Equations

A derivation of the Navier-Stokes equations from the Boltzmann equation can be found in Kogan, Chapman and Cowling\textsuperscript{[45]} and from the Bhatnagar-Gross-Krook equation in Cercignani\textsuperscript{[3]} and Vincenti and Kruger for the case of perfect monotonic gases. Here we reconsider the derivation of the Navier-Stokes and Euler equations from the BGK equation, right from the outset for polyatomic gases.

To derive the Navier-Stokes equations, let $\tau = \varepsilon \tilde{\tau}$ where $\varepsilon$ is a small dimensionless quantity, and suppose that $g$ has a Taylor series expansion about some point $(x_i, t)$. Since $\tau$ depends on the local thermodynamic variables, which are functions of moments of $g$, we may assume that $\tau$ and consequently $\tilde{\tau}$ can be expanded about the point $(x_i, t)$. Now consider the formal solution of the BGK equation for $f$, supposing that $g$ is known, and suppose that $t' >> \tau$; i.e. that the initial conditions were imposed many relaxation time ago. We can then ignore the initial value of $f$, and, with negligible error, the difference between $t' = 0$ and $t' = -\infty$ in the integral solution of the BGK model. It can be shown from the integral solution that the Taylor series expansion of $\tau$ and $g$
about \((x_i, t)\) may be written as power series in \(\varepsilon\). We can find the terms in the expansion from the formal solution for \(f\), or, more easily, by putting
\[
f = f_0 + \varepsilon f_1 + \varepsilon^2 f_2 + \cdots
\]
(2.24)
and plug in
\[
\tau = \varepsilon \hat{\tau}
\]
(2.25)
into the BGK equation directly. Let
\[
D_u = \frac{\partial}{\partial t} + u_i \frac{\partial}{\partial x_i}
\]
The BGK equation becomes
\[
\varepsilon \hat{\tau} D_u f + f - g = 0
\]
(2.26)
An expansion of this equation in terms of \(\varepsilon\) yields
\[
f = g - \varepsilon \hat{\tau} D_u g + \varepsilon^2 \hat{\tau} D_u (\hat{\tau} D_u g) + \cdots
\]
(2.27)
And the compatibility condition, after dividing by \(\varepsilon \hat{\tau}\), gives
\[
\int \psi_a D_u g d\Xi = \varepsilon \int \psi_a D_u (\hat{\tau} D_u g) d\Xi + O(\varepsilon^2)
\]
(2.28)
We define \(L_\alpha\) to be the integral on the left side of the equation, and \(R_\alpha\) to be the integral on the right side, so the equation can be written as
\[
L_\alpha = \varepsilon R_\alpha + O(\varepsilon^2)
\]
(2.29)
We show that this equation gives the Euler equations if we drop the terms of $O(\epsilon^1)$ and higher, and the Navier-Stokes equations if we drop terms of $O(\epsilon^3)$ and higher. To simplify the notation, let

$$<\psi_{\alpha}(\cdot\cdot\cdot) > \equiv \int \psi_{\alpha}(\cdot\cdot\cdot)d\Xi,$$  \hspace{0.5cm} (2.30)

and consider

$$L_{\alpha} \equiv \int \psi_{\alpha} D_x g d\Xi$$

$$= \int \psi_{\alpha} (g_j + u_t g_j) d\Xi$$

$$= <\psi_{\alpha} >_j + <\psi_{\alpha} u_t >_j$$  \hspace{0.5cm} (2.31)

since $\psi_{\alpha}$ is independent of $(x, t)$ . From equation we have

$$<\psi_{\alpha} >_j + <\psi_{\alpha} u_t >_j = O(\epsilon)$$  \hspace{0.5cm} (2.32)

for all $\alpha$, and therefore, in reducing $R_{\alpha}$ on the right hand side of the equation, which is already $O(\epsilon)$, we can drop $O(\epsilon)$ quantities and their derivatives.

We will show that $L_{\alpha} = 0 \ (\alpha = 1, 2, 3, 4, 5)$ represents the Euler equations. And then we use the fact that $L_{\alpha}$ is $O(\epsilon)$ to simplify $R_{\alpha}$, this assumption will lead to the Navier-Stokes equations.

The Euler equations follow from putting $L_{\alpha} = 0$. To see this, consider

$$L_1 = <\psi_1 >_j + <\psi_1 u_t >_j = \rho_j + (\rho U_t)_j$$  \hspace{0.5cm} (2.33)

since $\psi_1 = 1$; This is the continuity equation. For $\alpha = 2,3,4$, it is convenient to define $L_{\alpha}$ such that
\[ i = \alpha - 1 \text{ and to let } w_i = u_i - U_i. \text{ Then} \]
\[ L_i = \langle u_i \rangle_j + \langle u_i u_k \rangle_j = (\rho U_i)_j + [\rho U_i U_k + \langle w_i w_k \rangle_r]_r \]  
(2.34)

since all moments of \( g \) odd in \( w_i \) vanish. The pressure tensor is defined by
\[ p_{ik} = \langle w_i w_k \rangle = p \delta_{ik} \]

Then we have
\[ L_i = (\rho U_i)_j + [\rho U_i U_k + p \delta_{ik}]_r \]  
(2.35)

and \( L_i = 0 \) is the Euler equation for the conservation of momentum. For the energy equation we have
\[ L_5 = \frac{1}{2} \langle u_i^2 + \xi^2 \rangle_j + \frac{1}{2} \langle u_i (u_n^2 + \xi^2) \rangle_j \]  
(2.36)

or
\[ L_5 = \left( \frac{1}{2} \rho U_n^2 + \frac{K + 3}{2} p \right)_j + \left( \frac{1}{2} \rho U_k U_n^2 + \frac{K + 5}{2} p U_k \right)_k \]  
(2.37)

Setting \( L_5 = 0 \) gives the energy equation in the absence of dissipation.

Detailed derivations of the Navier-Stokes equations can be found in reference [29]
CHAPTER 3

NUMERICAL SCHEMES FOR
CONSERVATION LAWS

Godunov-type schemes are well known finite volume methods to obtain numerical solutions for hyperbolic conservation laws. The flux is discretized by the finite volume method, in which average values are calculated for the conserved quantities in each cell from the balance of the fluxes through the cell boundaries. In the original Godunov scheme, the solution is averaged in each cell to produce a piecewise constant states and the flux through the interface is derived from the solution of a Riemann problem. Higher order Godunov-type schemes use more accurate reconstruction methods to obtain better estimates of the left and right states for the Riemann problem at each interface. In the finite volume BGK scheme, we use gas kinetic theory to solve a Riemann problem at each cell interface. The Godunov-type scheme is illustrated in figure 3.1.

In this chapter, the detailed formulation of the BGK scheme will be outlined.

3.1 Godunov-Type Schemes

Godunov introduced an enlightening idea for this nonlinear system. The approach is to abandon finite differences or the interpolation in finite volume methods, since the solutions sought are singular ones. The focus is rather placed on the discontinuities of a step function, which is constant on a cell partition of the interval considered. The evolution of the discontinuities can be considered as an independent Riemann problem. The schemes developed based on this idea are called Godunov-type schemes.
Godunov Scheme: Piecewise constant
First order, no reconstruction
Riemann problem at each interface

Higher Order Scheme: Reconstruction of higher order left and right states
for Riemann problem
Piecewise linear
Reconstruction leads to oscillation unless limiters are introduced

Figure 3.1 Godunov-type Finite Volume Scheme
To illustrate this approach we consider the one-dimensional hyperbolic system of conservation laws

\[ u_t + f(u)_x = 0 \quad (3.1) \]

where \( u \) is the velocity and \( f \) is the flux.

In constructing a finite volume scheme, we proceed in two steps: first, we introduce a small spatial scale, \( \Delta x \), and we consider the corresponding average \( \bar{u}(x,t) \) inside each cell:

\[ x_i - \frac{\Delta x}{2} \leq x \leq x_i + \frac{\Delta x}{2} \]

to be

\[ \bar{u}_{i}(x,t) + \frac{1}{\Delta x} \left[ f(u(x+\frac{\Delta x}{2},t)) - f(u(x-\frac{\Delta x}{2},t)) \right] = 0 \quad (3.2) \]

Next, we introduce a small time-step, \( \Delta t \), and integrate over the slab \( t \leq \tau \leq t + \Delta t \). Hence

\[ \bar{u}(x,t + \Delta t) = \bar{u}(x,t) - \frac{1}{\Delta x} \left[ \int_{t}^{t+\Delta t} f(u(x+\frac{\Delta x}{2},\tau))d\tau - \int_{t}^{t+\Delta t} f(u(x-\frac{\Delta x}{2},\tau))d\tau \right] \quad (3.3) \]

We end up with an equivalent reformulation of the conservation law. The first step is the variable reconstruction stage and the second step is the flux evolution stage.
3.1.1 Reconstruction Stage

In the reconstruction stage, in order to avoid generating spurious oscillations in the solution, a limiter is used in the interpolation of cell interface variables for higher-order schemes. Jameson has developed a general Symmetric Limited Positive (SLIP) formulation for limiters\cite{9,10}. Define the limited average

\[ L(u, v) = \frac{1}{2} (u + v) \left( 1 - \frac{|u - v|}{|u| + |v|} \right) \]  

(3.4)

- For \( q = 1 \), the MinMod limiter is obtained
- For \( q = 2 \), Van Leer's limiter is obtained
- For \( q = 3 \) or larger, the higher-order SLIP method is obtained

Let \( x_j = j \Delta x \) be a uniform mesh and \( \Delta x \) the mesh size. \( W_j \), \( W_{j \pm 1} \) are cell-averaged variables and \( W_{j \frac{1}{2}}, W_{j \frac{3}{2}} \) are the interpolated values at the cell interface. To second order accuracy, the interpolated values at the left and right states of the interface (\( i = 1/2 \)) can be written as

\[
W_{j \frac{1}{2}}^L = W_j + \frac{1}{2} L(\Delta W_{j \frac{1}{2}}, \Delta W_{j \frac{3}{2}}) \\
W_{j \frac{1}{2}}^R = W_{j \frac{3}{2}} - \frac{1}{2} L(\Delta W_{j \frac{1}{2}}, \Delta W_{j \frac{3}{2}}) 
\]  

(3.5)

where \( L(u, v) \) is the nonlinear limiter. It is illustrated in Figure 3.2.
3.1.2 Evolution Stage

The evolution stage basically solves a Riemann problem. This area has been well established in the past decades. Some well-known Riemann solvers for the cell-interface flux estimations are:

- The exact iterative solver
- Roe's approximate solver
- The Harten-Lax-VanLeer Einfeldt (HLL) approximate solver

Each Riemann solver has its own limitations. The exact Riemann solver is too costly, and Roe's approximate solver permits unphysical solutions such as expansion shock waves. In this study, a robust and accurate high-order evolution method based on gas-kinetic theory
is used to construct the numerical fluxes across a cell interface via a solution of the Riemann problem. This gas-kinetic BGK scheme is not just a simple alternative to the Riemann solver or another upwinding method. It uses the Boltzmann equation as its governing equation. It has an analytical solution since it is the solution of a linear equation. It is based on the underlying physics of fluid flows, and perhaps provides better numerical solutions for compressible flows, especially for very strong shock flows and supersonic flows.

3.2 GAS-KINETIC BGK METHOD

3.2.1 Boltzmann Equation

Due to the unique form of the equilibrium distribution function $g$ in classical statistical physics, at each point in space and time, there is a one to one correspondence between $g$ and the macroscopic densities, e.g. mass, momentum and energy. Therefore, from macroscopic flow variables at any point in space and time, we can construct a unique equilibrium state. However, in the real physical situation, the gas does not necessarily stay in the local thermodynamic equilibrium state, such as gas inside a shock or boundary layer, even though we can construct a local equilibrium state there from the corresponding macroscopic flow variables. Usually, we do not know the explicit form of the gas distribution function $f$ in an extremely dissipative flow region, such as inside a strong shock wave. What we know is the time evolution of $f$, the so-called the Boltzmann Equation, for one-dimensional flow,

$$f_t + uf_x = Q(f,f)$$

Here $f$ is the real gas distribution function, and $Q(f,f)$ is the collision operator. From the physical constraints of the conservation of mass, momentum and energy during particle collisions, the following compatibility condition has to be satisfied,
\[ \int \psi_\alpha Q(f, f) dud\xi = 0 \] (3.7)

where \( \psi_\alpha \) is the vector of moments; its three-dimensional formula will be given later.

### 3.2.2 BGK Model of the Boltzmann Equation

One of the main functions of the particle collisions is to drive the gas distribution function \( f \) back to the equilibrium state \( g \) corresponding to the local values of \( \rho, \rho U \) and \( \rho e \). The collision theory assumes that during a time \( dt \), a fraction of \( dt / \tau \) of molecules in a given small volume undergo collisions, where \( \tau \) is the average time interval between successive particle collisions for the same particle. The collision term in the BGK model alters the velocity-distribution function from \( f \) to \( g \). This is equivalent to assuming that the rate of change \( (df / dt) \) of \( f \) due to collisions is \( -\frac{(f-g)}{\tau} \). So the Boltzmann equation becomes

\[
\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = -\frac{f-g}{\tau} \tag{3.8}
\]

At the same time, due to the mass, momentum and energy conservation in particle collisions, the collision term \( (g-f) / \tau \) satisfies the compatibility condition,

\[
\int \frac{g-f}{\tau} \psi_\alpha dud\xi = 0 \tag{3.9}
\]

The BGK model coincides in form with the equations in the theory of relaxation processes and is therefore sometimes called the relaxation model.

If \( \tau \) is a local constant, the solution may be written as

\[
f(x,t,u,\xi) = \frac{1}{\tau} \int g(x-u(t-t_0),t',u,\xi)e^{-(t-t')/\tau}dt' + e^{-(t-t')/\tau}f_0(x-u(t-t_0),t_0,u,\xi) \tag{3.10}
\]

23
where $f_0$ is the real gas distribution function $f$ at $t_0$, and $g$ is the equilibrium state in $(x,t)$.

### 3.3 The BGK Scheme for 3D Flows

In the finite volume method, the discretization is accomplished by dividing the flow into a large number of small sub-domains and by applying the conservation laws in the integral form

$$\frac{d}{dt} \int_{\Omega} U dV + \int_{\partial \Omega} F \cdot dS = 0 \quad (3.11)$$

to each sub-domain $\Omega$ with boundary $\partial \Omega$. In this equation $U$ is the macroscopic state vector, defined as

$$U = \begin{pmatrix} \rho \\ P_x \\ P_y \\ P_z \\ \varepsilon \end{pmatrix} \quad (3.12)$$

where $\rho$, $\vec{P}$ and $\varepsilon$ are the mass, momentum, and energy density, and $\vec{F}$ is the flux vector with components $F_x$, $F_y$ and $F_z$ in the three coordinate directions. In a gas-kinetic finite volume scheme the flux vectors across cell boundaries are constructed by computing the gas distribution function $f$. In three dimensions, the governing equation for $f$ is described by the BGK model, which is

$$f_t + uf_x + vf_y + w f_z = \frac{g - f}{\tau} \quad (3.13)$$
where $f$ is a function of space $(x, y, z)$, time $t$, particle velocity $(u, v, w)$, and internal variable $\xi$ with $K$ degrees of freedom (i.e., $K = 2$ for $\gamma = 1.4$ diatomic gases in 3D). The relations between mass $\rho$, momentum $\vec{P}$, and energy $\varepsilon$ densities and the distribution function $f$ are

\[
\begin{pmatrix}
\rho \\
\vec{P} \\
P_r \\
P_t \\
P_z \\
\varepsilon
\end{pmatrix} = \int \psi_\alpha f d\Xi
\]  

(3.14)

where $\psi_\alpha$ is the vector of moments

\[
\psi_\alpha = \begin{pmatrix}
1 \\
u \\
v \\
w \\
\frac{1}{2}(u^2 + v^2 + w^2 + \xi^2)
\end{pmatrix}
\]  

(3.15)

and $d\Xi = du dv dw d\xi$ is the volume element in the phase space. The equilibrium state $g$ in the BGK model has a Maxwellian distribution of

\[
g = A e^{-\frac{1}{2}[(u-U)^2 + (v-V)^2 + (w-W)^2 + \xi^2]} 
\]  

(3.16)

where $U$, $V$, and $W$ are macroscopic gas velocities, and $A$ is a constant. From the physical constraint of the conservation of mass, momentum and energy during particle collisions, the following compatibility condition has to be satisfied,

\[
\int \frac{(g - f)}{\tau} \psi_\alpha d\Xi = 0
\]  

(3.17)
at any point in space and time. This will lead to the three-dimensional Euler equations. Here \( \frac{g-f}{\tau} \) is the collision term of the Boltzmann equation, and \( \tau \) is the collision time.

The general solution for \( f \) in equation (3.3) in three dimensions at the position of \((x, y, z)\) and \(t\) is

\[
f(x, y, z, t, u, v, w, \xi) = \frac{1}{\tau} \int_0^1 g(x', y', z', t, u, v, w, \xi) e^{-\left(u(t-t')\right)/\tau} dt' + e^{-(t-t')/\tau} f_0(x - ut, y - vt, z - wt)
\]

(3.18)

where \( x' = x - u(t - t') \), \( y' = y - v(t - t') \), \( z' = z - w(t - t') \) are the trajectory of a particle, and \( f_0 \) is the initial non-equilibrium gas distribution \( f \) at the beginning of each step \((t = 0)\). Two unknowns \( g \) and \( f_0 \) must be determined in the above equation to obtain the solution \( f \). In order to calculate the evolution of the macroscopic quantities in equation (3.14), equation (3.13) can be integrated over \( u, v, w, x, y, z \), and \( t \) for a control volume defined by a mesh cell and a time step \( \Delta T \). This requires the evaluation of fluxes across a boundary separating two cells in the \( x \) direction and, to simplify the notation, the point for evaluating fluxes at the cell boundary will be assumed at \((x = 0, y = 0, z = 0)\).

Generally, \( f_0 \) and \( g \) can be expanded around the cell boundary as

\[
f_0 = \begin{cases} 
g'(1 + a'x + b'y + c'z), & x < 0 
g'(1 + a''x + b''y + c''z), & x > 0 \end{cases}
\]

(3.19)

and

\[
g = g_0(1 + \bar{a}x + \bar{b}y + \bar{c}z + \bar{d}t)
\]

(3.20)
where \( g', g', \) and \( g_0 \) are local Maxwellian distribution functions. The dependence of \( a', b', ..., \overline{A} \) on the particle velocity can be obtained from the Taylor expansions of a Maxwellian, which have the form

\[
a' = a'_1 + a'_2 u + a'_3 v + a'_4 w +
+ a'_5 (u^2 + v^2 + w^2 + \xi^2),
\]

\[...
\]

\[
a' = a'_1 + a'_2 u + a'_3 v + a'_4 w +
+ a'_5 (u^2 + v^2 + w^2 + \xi^2),
\]

\[...
\]

\[
\overline{A} = \overline{A}_1 + \overline{A}_2 u + \overline{A}_3 v + \overline{A}_4 w +
+ \overline{A}_5 (u^2 + v^2 + w^2 + \xi^2), \tag{3.21}
\]

where all coefficients of \( a_1, a_2, ..., \overline{A}_5 \) are local constants. The idea of interpolating \( f_0 \) separately in the regions of \( x < 0 \) and \( x > 0 \) follows from physical considerations: for a non-equilibrium gas flow, the physical quantities can change dramatically from place to place, such as across a shock front where the upstream and downstream gas distribution function \( f \) could be different Maxwellian functions.

In the following, the SLIP formulation, similar to that used for the linear advection equation, will be used for the interpolation of all initial mass, momentum, and energy densities in the \( x, y, \) and \( z \) directions, respectively. After implementing the limiters, the macroscopic variables can be obtained in the left and right sides of the interface separately,
\[
\begin{pmatrix}
\bar{\rho} \\
\bar{P}_x \\
\bar{P}_y \\
\bar{P}_z \\
\epsilon
\end{pmatrix} = 
\begin{pmatrix}
\rho_0 + \rho_1 x + \rho_2 y + \rho_3 z \\
P_{x0} + P_{x1} x + P_{x2} y + P_{x3} z \\
P_{y0} + P_{y1} x + P_{y2} y + P_{y3} z \\
P_{z0} + P_{z1} x + P_{z2} y + P_{z3} z \\
\epsilon_0 + \epsilon_1 x + \epsilon_2 y + \epsilon_3 z
\end{pmatrix}
\] (3.22)

where \( \rho_1, \rho_2, \ldots, \epsilon_3 \) are local constants. The equations (3.19) and (3.22) are substituted into the moment equation (3.14) to yield

\[
\begin{pmatrix}
\bar{\rho} \\
\bar{P}_x \\
\bar{P}_y \\
\bar{P}_z \\
\epsilon
\end{pmatrix} = \int \psi_a f_0 dE
\] (3.23)

All the coefficients in \( f_0 \) can be obtained directly. Then, \( g_0 \) in equation (3.20) at \( (x = 0, y = 0, z = 0) \) can be evaluated automatically by taking the limit of equation (3.18) as \( t \to 0 \) and substituting it into equation (3.17) to obtain

\[
\int g_0 \psi_a dE = \int_{x=0} \int g' \psi_a dE + \int_{y=0} \int g'' \psi_a dE
\] (3.24)

The other terms of \( \vec{a}, \vec{b}, \) and \( \vec{c} \) in equation (3.20) at \( t = 0 \) can be computed from the new mass, momentum, and energy interpolations that are continuous across the cell boundary in all three directions. Now, the only unknown term left in equation (3.20) is \( \vec{a} \). This can be evaluated as follows by substituting equation (3.19) and equation (3.20) into equation (3.18). We obtain

\[
f(0,0,0,t,u,v,w,\xi) = (1 - e^{-t/P}) g_0 + \tau(1 + e^{-t/P}) + te^{-t/P}(u\vec{a} + v\vec{b} + w\vec{c}) g
\]

\[
+ \tau(t - 1 + e^{-t/P}) \vec{a} g_0 + e^{-t/P} f_0 (-ut,-vt,-wt)
\] (3.25)

with
\[ f_0(-ut,-vt,-wt) = \begin{cases} g'(1-a'ut-b'vt-c'wt), u > 0 \\ g''(1-a'ut-b'vt-c'wt), u < 0 \end{cases} \quad (3.26) \]

Both \( f \) in equation (3.25) and \( g \) in equation (3.20) contain \( \overrightarrow{A} \). After applying the condition (3.17) at \( (x=0, y=0, z=0) \) and integrating it over the whole time step \( \Delta T \), such that

\[ \int_0^T \int (g-f) \psi_a d\Xi dt = 0 \quad (3.27) \]

Five moment equations of \( \overrightarrow{A} \) can be obtained, from which the five constants in \( \overrightarrow{A} \) of equation (3.21) can be uniquely determined. Finally, the time-dependent numerical fluxes in the x-direction across the cell boundary can be computed as

\[
F_x = \begin{pmatrix} F_p \\ F_{p_t} \\ F_{p_v} \\ F_{p_w} \\ F_e \end{pmatrix} = \int u \begin{pmatrix} 1 \\ u \\ v \\ w \\ \frac{1}{2} (u^2 + v^2 + w^2 + \xi^2) \end{pmatrix} f(0,0,0,t,u,v,w,\xi) d\Xi \quad (3.28)
\]

The corresponding fluxes \( F_y \) and \( F_z \) in the \( y \) and \( z \) directions are similarly obtained by taking moments with \( v \) and \( w \), respectively.

### 3.4 BGK Scheme for Scalar Equations

In gas-kinetic theory, it is assumed that the macroscopic fluid flow results from the collective motion of a large number of molecules. The complete description of a particle motion is described by the evolution equation of a particle distribution function \( f(\vec{x},t,\vec{u}) \), where \( \vec{x} \) is a space variable vector, \( t \) is a time and \( \vec{u} \) is a particle velocity vector in phase space. Since every macroscopic phenomenon is determined by the
integration of a single scalar distribution \( f(\vec{x},t,\vec{u}) \). This provides a unified numerical approach from a scalar conservation law to systems of equations.

### 3.4.1 The Gas-Kinetic BGK Scheme

Consider the linear advection equation

\[
U_t + aU_x = 0
\]  
(3.29)

where \( U \) is the dependent variable and \( a \) is the wave speed.

In order to approach Equation (3.29) from the gas kinetic theory, \( U \) must be considered as an average quantity of a group of microscopic particles. The dynamics of these particles can be described by a distribution function \( f(x,t,u) \), defined as

\[
U(x,t) = \int f(x,t,u) du
\]  
(3.30)

where \( u \) is the individual particle velocity. The evolution of \( f(x,t,u) \) is properly described by the Boltzmann equation, where molecule collisions are considered. However, due to the intrinsic difficulty of solving the collision term in the Boltzmann equation, the BGK model is used here. That is

\[
\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = \frac{g - f}{\tau}
\]  
(3.31)

where \( g(x,t,u) \) is an equilibrium distribution function. From the compatibility condition, we have Maxwellian function

\[
g(x,t,u) = \sqrt{\frac{\beta}{\pi}} U e^{-\frac{\beta(u-a)^2}{4}}
\]  
(3.32)
The solution of the BGK equation is given by

\[
 f(x_{j+1/2},t,u) = \frac{1}{\tau} \int_0^t g(x',t',u)e^{-\frac{(t-t')}{\tau}} \, dt' + e^{-\frac{t}{\tau}} f_0(x_{j+1/2} - ut)
\]  

(3.33)

where \( f_0 \) is the initial state distribution function.

In order to simplify the notation and without losing generality, we derive the formulas at the cell interface \( x_{j+1/2} = 0 \) using a cell size \( \Delta x=1 \).

\[
 f_0(x,0,u) = \begin{cases} 
 g_l(1 + a_l x), & x \leq 0 \\
 g_r(1 + a_r x), & x \geq 0 
\end{cases}
\]  

(3.34)

where

\[
 g_l = \sqrt{\frac{\beta}{\pi}} \overline{U} e^{-\beta(u-u_l)^2}; \\
 g_r = \sqrt{\frac{\beta}{\pi}} \overline{U} e^{-\beta(u-u_r)^2};
\]  

(3.35)

are left and right Maxwellians, and \( a_l \) and \( a_r \) are local slope constants to the left and right of the cell interface respectively. \( \overline{U}_l \) and \( \overline{U}_r \) are interpolated variables at the left and right of the cell interface. The SLIP construction is similar to that used in gas dynamics flows.

The distribution function \( g \) corresponding to the equilibrium state will be smoother than \( f \). Thus it can be expanded locally across the cell boundary as

\[
 g(x,t) = g_0(1 + \bar{a} x + \bar{A} t)
\]  

(3.36)

where \( g_0 \) is a local Maxwellian \( g_0 = \sqrt{\frac{\beta}{\pi}} \overline{U} e^{-\beta(u-u_0)^2} \), \( \bar{a} \) and \( \bar{A} \) are local constants.
In summary, the variables above can be expressed as

\[
\begin{align*}
\overline{U}_t &= U_j + L(\Delta U_{j+1/2}, \Delta U_{j-1/2}) \\
\overline{U}_r &= U_{j+1} - L(\Delta U_{j+3/2}, \Delta U_{j+1/2}) \\
a_t &= \frac{L(\Delta U_{j+1/2}, \Delta U_{j-1/2})}{\overline{U}_t} \\
a_r &= \frac{L(\Delta U_{j+3/2}, \Delta U_{j+1/2})}{\overline{U}_r} \\
\overline{U} &= \frac{1}{2} \overline{U}_t \text{erf}c(-\sqrt{\beta}a) + \frac{1}{2} \overline{U}_r \text{erf}c(\sqrt{\beta}a) \\
\overline{a} &= \frac{L(\Delta U_{j+1/2}, \Delta U_{j-1/2})}{\overline{U}} \\
\overline{A} &= b_1 + b_2 a \overline{a} + \frac{1}{2} b_3 \left\{ \frac{\overline{U}_t}{\overline{U}} \text{erf}c(-\sqrt{\beta}a) + \frac{\overline{U}_r}{\overline{U}} \text{erf}c(\sqrt{\beta}a) \right\} \\
&\quad + \frac{1}{2} b_4 \left\{ \frac{\overline{U}_t a_t}{\overline{U}} (\text{erf}c(-\sqrt{\beta}a)a + e^{-\beta^2 a^2}/\sqrt{\pi\beta}) + \frac{\overline{U}_r a_r}{\overline{U}} (\text{erf}c(\sqrt{\beta}a)a - e^{-\beta^2 a^2}/\sqrt{\pi\beta}) \right\}
\end{align*}
\]

where

\[
\begin{align*}
b_0 &= \Delta t - \tau(1 - e^{-\Delta t/\tau}) , \\
b_1 &= -(1 - e^{-\Delta t/\tau}) / b_0 \\
b_2 &= (-\Delta t + 2\tau(1 - e^{-\Delta t/\tau}) - \Delta t e^{-\Delta t/\tau}) / b_0 \\
b_3 &= (1 - e^{-\Delta t/\tau}) / b_0
\end{align*}
\]
\[ b_4 = \left( \Delta e^{-\Delta t} - \tau (1 - e^{-\Delta t}) \right) / b_0 \]

Having obtained a complete estimate of the distribution function \( f \) at the cell interface, we can write down the final expression for the time dependent numerical flux.

\[
F(x_{j+1/2} , t) = (\alpha_1 + \alpha_2 b_4) a \bar{U} \\
+ \left( \alpha_2 (a^2 + \frac{1}{2 \beta}) + \alpha_3 b_4 a^2 \right)a \bar{U} \\
+ \left[ \frac{a}{2} (\alpha_3 b_4 + \alpha_4) \text{erfc}(-\sqrt{\beta} a) + \frac{\alpha_4}{2 \sqrt{\pi \beta}} e^{-\beta t} \right] \bar{U}_l \\
+ \left[ \frac{a}{2} (\alpha_3 b_4 + \alpha_4) \text{erfc}(\sqrt{\beta} a) - \frac{\alpha_4}{2 \sqrt{\pi \beta}} e^{-\beta t} \right] \bar{U}_r \\
+ \left[ \frac{1}{2} (a^2 \alpha_4^2 b_4 - \alpha_5 (a^2 + \frac{1}{2 \beta})) \text{erfc}(\sqrt{\beta} a) + \frac{a}{2 \sqrt{\pi \beta}} (\alpha_3 b_4 + \alpha_3 e^{-\beta t}) \right] a_1 \bar{U}_l \\
+ \left[ \frac{1}{2} (a^2 \alpha_4^2 b_4 + \alpha_5 (a^2 + \frac{1}{2 \beta})) \text{erfc}(\sqrt{\beta} a) - \frac{a}{2 \sqrt{\pi \beta}} (\alpha_3 b_4 + \alpha_3 e^{-\beta t}) \right] a_1 \bar{U}_r 
\]

(3.37)

where

\[
\alpha_1 = (1 - e^{-\tau t}), \\
\alpha_2 = (\tau (-1 + e^{-\tau t}) + te^{-\tau t}), \\
\alpha_3 = \tau (t / \tau - 1 + e^{-\tau t}), \\
\alpha_4 = e^{-\tau t}, \\
\alpha_5 = -te^{-\tau t}
\]
Finally, the BGK scheme for the conservative scalar equation can be written as

$$U_{j}^{n+1} = U_{j}^{n} - \frac{\Delta t}{\Delta x} \left( \int F(x_{j+1/2}, t) dt - \int F(x_{j-1/2}, t) dt \right) \quad (3.38)$$

The numerical flux is exact for a uniform flow ($\overline{U} = \overline{U}_i = \overline{U}_r = \overline{U}$ and $\bar{a} = a_i = a_r = 0$), and therefore it satisfies the consistency condition $F(U, U) = aU$. 

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CHAPTER 4

POSITIVITY ANALYSIS OF THE GAS-KINETIC BGK METHOD

Positivity is an important property for any numerical scheme. For scalar equations, the positivity condition leads to LED schemes, which will not produce spurious oscillations. For the Euler and Navier-Stokes equations, the positivity condition means that only positive densities and pressures are obtained, which should be the basic requirement of all numerical schemes. Although positivity is a basic and natural requirement for any numerical scheme to be used in real engineering applications, there are not many schemes that satisfy this property. Currently, there are three schemes that can be proved to be positive, namely, the Godunov, Lax-Friedrichs, and Kinetic Flux Vector Splitting (KFVS) schemes. The positivity property of the gas-kinetic BGK scheme is proved in this thesis.

This chapter will first derive the positivity and stability conditions for the linear advection equation. Then similar conditions will be introduced for the one-dimensional Euler equations. All the derivations are for first order schemes.

From the analysis of this chapter, we will conclude that the collisional gas-kinetic BGK scheme is a positivity-preserving scheme as long as a standard Courant-Friedrichs-Lewy (CFL) condition is satisfied and the collision coefficient is within a pre-specified limit. For the collisionless scheme (KFVS), in which the collision coefficient is approaching zero, the scheme only needs to satisfy a standard CFL condition to be a positive scheme.
4.1 Three Gas-Kinetic Schemes

For the 1$^{st}$-order gas-kinetic BGK scheme, the particle distribution function $f$ can be expressed as

$$f = (1 - e^{-\Delta t / t})g + e^{-\Delta t / t} f_0$$

$$= \alpha \cdot g + \beta \cdot f_0$$

where $g$ is the equilibrium state distribution, which can be expressed as a Maxwellian function, and $f_0$ is the initial non-equilibrium state distribution, which will be constructed from initial flow variables. The collision coefficient, $\beta = e^{-\Delta t / t}$, ranges from 0 to 1. In the next two sections, the following three numerical schemes are analyzed to assess their positivity properties:

- Collisionless scheme, when $\alpha = 1$ and $\beta = 0$. This is one extreme case, which is also called the KFVS (Kinetic Flux Vector Splitting) scheme.

- Collisonal scheme, when $\alpha = 0$ and $\beta = 1$. This is the other extreme case of the BGK scheme.

- General BGK scheme, when $\alpha \neq 0$ and $\beta \neq 0$. This is a linear combination of the collisionless scheme and the collisional scheme.

The name of collisional and collisionless are defined as the result of the inclusion of the collision term of the Boltzmann equation. Numerically, the collisionless scheme has more dissipation and the collisional scheme has less dissipation. The gas-kinetic BGK scheme has the appropriate dissipation as the result of the inclusion of the collision effect. It has also been proved that the BGK scheme is a positivity-preserving scheme. So it is a very robust shock-capturing scheme.
4.2 Positivity of the Linear Scalar Equation

Consider the linear advection equation

$$U_t + aU_x = 0$$  \hspace{1cm} (4.1)

where $U$ is the solution and $a$ is the wave speed. The general flux of the BGK scheme at cell interfaces can be expressed as:

$$h(x_{j+1/2}, t) = \beta a \overline{U}_{j+1/2} + \alpha \left\{ \frac{a}{2} \text{erfc}(-\sqrt{\lambda}a) + \frac{e^{-\lambda a^2}}{2 \sqrt{\pi \lambda}} \right\} U_j + \alpha \left\{ \frac{a}{2} \text{erfc}(\sqrt{\lambda}a) - \frac{e^{-\lambda a^2}}{2 \sqrt{\pi \lambda}} \right\} U_{j+1}$$  \hspace{1cm} (4.2)

$$h(x_{j-1/2}, t) = \beta a \overline{U}_{j-1/2} + \alpha \left\{ \frac{a}{2} \text{erfc}(-\sqrt{\lambda}a) + \frac{e^{-\lambda a^2}}{2 \sqrt{\pi \lambda}} \right\} U_{j-1} + \alpha \left\{ \frac{a}{2} \text{erfc}(\sqrt{\lambda}a) - \frac{e^{-\lambda a^2}}{2 \sqrt{\pi \lambda}} \right\} U_j$$  \hspace{1cm} (4.3)

where

$$\alpha = (1 - e^{-\Delta t / \tau}),$$

$$\beta = e^{-\Delta t / \tau},$$

$$\overline{U}_{j+1/2} = \frac{1}{2} U_j \text{erfc}(-\sqrt{\lambda}a) + \frac{1}{2} U_{j+1} \text{erfc}(\sqrt{\lambda}a)$$

$$\overline{U}_{j-1/2} = \frac{1}{2} U_{j-1} \text{erfc}(-\sqrt{\lambda}a) + \frac{1}{2} U_j \text{erfc}(\sqrt{\lambda}a)$$

Hence, the BGK scheme for the conservative scalar equation can be written as

$$U_j^{n+1} = U_j^n - \frac{\Delta t}{\Delta x} (h_{j+1/2} - h_{j-1/2})$$  \hspace{1cm} (4.4)
For the first-order upwind scheme, from the above equations, the final fluxes are as follows:

\[
    h(x_{j+1/2},t) = \beta a \bar{U}_{j+1/2} + \alpha \left[ \frac{a}{2} \text{erfc}(-\sqrt{\lambda}a) + \frac{e^{-\sigma^2 \lambda}}{2\sqrt{\pi \lambda}} U_j + \alpha \left[ \frac{a}{2} \text{erfc}(\sqrt{\lambda}a) - \frac{e^{-\sigma^2 \lambda}}{2\sqrt{\pi \lambda}} U_{j+1} \right] \right]
\]

(4.5)

\[
    h(x_{j-1/2},t) = \beta a \bar{U}_{j-1/2} + \alpha \left[ \frac{a}{2} \text{erfc}(-\sqrt{\lambda}a) + \frac{e^{-\sigma^2 \lambda}}{2\sqrt{\pi \lambda}} U_{j-1} + \alpha \left[ \frac{a}{2} \text{erfc}(\sqrt{\lambda}a) - \frac{e^{-\sigma^2 \lambda}}{2\sqrt{\pi \lambda}} U_j \right] \right]
\]

(4.6)

Let \( \sigma = \frac{\Delta t}{\Delta x} \), hence we obtain the discrete form

\[
    U_j^{n+1} = U_j^n - \sigma \left( h(x_{j+1/2},t) - h(x_{j-1/2},t) \right)
\]

\[
    = \left[ -\sigma \beta a \left( \frac{a}{2} \text{erfc}(\sqrt{\lambda}a) + \frac{e^{-\sigma^2 \lambda}}{2\sqrt{\pi \lambda}} \right) \right] U_j^n
\]

\[
    + \left[ 1 + \sigma \beta a (1 - \text{erfc}(-\sqrt{\lambda}a)) + \sigma \alpha \left( \frac{a}{2} \text{erfc}(\sqrt{\lambda}a) - \frac{a}{2} \text{erfc}(-\sqrt{\lambda}a) - \frac{e^{-\sigma^2 \lambda}}{2\sqrt{\pi \lambda}} \right) \right] U_{j-1}^n
\]

\[
    + \left[ \sigma \beta a \frac{a}{2} \text{erfc}(-\sqrt{\lambda}a) + \sigma \alpha \left( \frac{a}{2} \text{erfc}(\sqrt{\lambda}a) + \frac{e^{-\sigma^2 \lambda}}{2\sqrt{\pi \lambda}} \right) \right] U_{j+1}^n
\]

(4.7)

To analyze the stability of 1st-order BGK scheme, we rewrite the above equation as

\[
    U_j^{n+1} = \sum_{k=-1}^{n} a_{j+k} U_{j+k}^n
\]

(4.8)

where

\[
    a_{j+1} = -\sigma \beta a \left( \frac{a}{2} \text{erfc}(\sqrt{\lambda}a) + \frac{e^{-\sigma^2 \lambda}}{2\sqrt{\pi \lambda}} \right)
\]
\[ a_j = 1 + \sigma \beta a \left[ 1 - \text{erfc}(\sqrt{\lambda a}) \right] + \sigma a \left[ \frac{a}{2} \text{erfc}(\sqrt{\lambda a}) - \frac{a}{2} \text{erfc}(\sqrt{\lambda a}) - \frac{e^{-\lambda a}}{\sqrt{\pi \lambda}} \right] \]

\[ a_{j-1} = \sigma \beta \frac{a}{2} \text{erfc}(\sqrt{\lambda a}) + \sigma a \left[ \frac{a}{2} \text{erfc}(\sqrt{\lambda a}) + \frac{e^{-\lambda a}}{2\sqrt{\pi \lambda}} \right] \]

(1) **Collisionless Method**

\[ \alpha = 1, \]
\[ \beta = 0 \]

For this choice of parameters

\[ a_{j+1} = \sigma a \left[ -\frac{1}{2} \text{erfc}(\sqrt{\lambda a}) + \frac{e^{-\lambda a}}{2\sqrt{\pi \lambda a}} \right] \]

\[ a_j = 1 - \alpha a - \sigma a \left[ -\text{erfc}(\sqrt{\lambda a}) + \frac{e^{-\lambda a}}{\sqrt{\pi \lambda a}} \right] \]

\[ a_{j-1} = \sigma a \left[ \frac{1}{2} \text{erfc}(\sqrt{\lambda a}) + \frac{e^{-\lambda a}}{2\sqrt{\pi \lambda a}} \right] \]

It can be shown that

\[ a \cdot \text{erfc}(\sqrt{\lambda a}) + \frac{e^{-\lambda a}}{\sqrt{\pi \lambda}} \geq 0 \]

\[ -a \cdot \text{erfc}(\sqrt{\lambda a}) + \frac{e^{-\lambda a}}{\sqrt{\pi \lambda}} \geq 0 \]

Hence, \( a_{j+1} \) and \( a_{j-1} \) are positive automatically. To make the \( a_j \) term positive, the following CFL-like condition must be satisfied:
\[
\sigma \leq \frac{1}{a + a[-\text{erfc}(\sqrt{\lambda}a) + \frac{e^{-\lambda a^2}}{\sqrt{\pi}a} ]}
\] (4.9)

The collisionless scheme is a positivity-preserving scheme if the CFL-like condition is satisfied.

(2) Collisional Method

\[
\begin{align*}
\alpha &= 0, \\
\beta &= 1
\end{align*}
\]

With this choice of parameters

\[
\begin{align*}
a_{j+1} &= -\alpha \frac{1}{2} \text{erfc}(\sqrt{\lambda}a) \\
a_j &= 1 + \alpha a - \alpha a \cdot \text{erfc}(\sqrt{\lambda}a) \\
a_{j-1} &= \alpha \frac{1}{2} \text{erfc}(-\sqrt{\lambda}a)
\end{align*}
\]

The coefficient \(a_{j+1}\) is always negative for a positive wave speed \(a\), hence this is not a positivity-preserving method.

(3) BGK Method

\[
\alpha = 1 - \beta, \quad \text{where} \quad 0 \leq \beta \leq 1
\]

As was shown above, the coefficients are:

\[
a_{j+1} = -\sigma \beta \frac{a}{2} \text{erfc}(\sqrt{\lambda}a) + \sigma (1 - \beta)\left[-\frac{a}{2} \text{erfc}(\sqrt{\lambda}a) + \frac{e^{-\lambda a^2}}{2\sqrt{\pi}a}\right]
\]
\[
a_j = 1 - \sigma[a - a \cdot \text{erfc}(-\sqrt{\lambda}a) + \frac{e^{-\lambda a^2}}{2\sqrt{\pi} \lambda}] + \sigma \beta \frac{e^{-\lambda a^2}}{2\sqrt{\pi} \lambda}
\]

\[
a_{j-1} = \sigma \left[ \frac{a}{2} \cdot \text{erfc}(-\sqrt{\lambda}a) + \frac{e^{-\lambda a^2}}{2\sqrt{\pi} \lambda} \right] - \sigma \beta \frac{e^{-\lambda a^2}}{2\sqrt{\pi} \lambda}
\]

To ensure that all coefficients \(a_{j+1}, a_{j-1}\) and \(a_j\) are positive, the following conditions must be satisfied:

- Collision coefficient \(\beta\) must be:

\[
\beta = e^{-\Delta t^*} \leq 1 - \frac{\frac{a}{2} \cdot \text{erfc}(\sqrt{\lambda}a)}{e^{-\lambda a^2}} \quad (4.10)
\]

- The CFL-like condition is also

\[
\sigma \leq \frac{1}{a + \left[ -a \cdot \text{erfc}(\sqrt{\lambda}a) + \frac{e^{-\lambda a^2}}{\sqrt{\pi} \lambda} \right] - \beta \frac{e^{-\lambda a^2}}{\sqrt{\pi} \lambda}} \quad (4.11)
\]

In conclusion, for the linear scalar equation, the collisionless method (KFVS scheme) is always positive as long as the general CFL condition is satisfied, and the collisional method is not positive. The 1st-order gas-kinetic BGK scheme is also a positive scheme as long as the collision coefficient \(\beta = e^{-\Delta t^*}\) is within the specified range and the general CFL condition is satisfied.
4.3 Positivity of the Euler Equations

We now consider the one-dimensional Euler equations of gas dynamics:

\[
\begin{align*}
\rho_t + m_x &= 0 \\
m_t + (mU + p)_x &= 0 \\
E_t + (EU + pU)_x &= 0
\end{align*}
\tag{4.12}
\]

where

- \( \rho \) is the density
- \( U \) is the velocity
- \( m = \rho U \) is the momentum
- \( E = \frac{1}{2} \rho U^2 + \rho e \) is the energy per unit
- \( e \) is the internal energy, and
- \( p \) is the pressure, and \( p = (\gamma - 1)\rho e \)

Rewrite the equation as:

\[
\begin{bmatrix}
\rho \\
m \\
E
\end{bmatrix}_t + \begin{bmatrix}
m \\
mu + p \\
EU + pU
\end{bmatrix}_x = 0
\]

We call it a positivity-preserving scheme for the Euler equations if the following conditions are satisfied:

- density is positive, \( \rho \geq 0 \)

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\begin{itemize}
\item internal energy is positive, \( \rho E - \frac{1}{2} m^2 \geq 0 \)
\end{itemize}

(1) Collisionless Method

Let \( \sigma = \frac{\Delta t}{\Delta x} \), hence the numerical formula becomes

\[
\begin{pmatrix}
\frac{\rho_j}{m_j} \\
\frac{E_j}{m_j}
\end{pmatrix}
= \begin{pmatrix}
\rho_j \\
m_j \\
E_j
\end{pmatrix}
+ \sigma \begin{pmatrix}
F_{\rho,j-1/2} - F_{\rho,j+1/2} \\
F_{m,j-1/2} - F_{m,j+1/2} \\
F_{E,j-1/2} - F_{E,j+1/2}
\end{pmatrix}
\]

\[
\begin{pmatrix}
\rho_j \\
m_j \\
E_j
\end{pmatrix}
= \begin{pmatrix}
\rho_j \\
m_j \\
E_j
\end{pmatrix}
+ \sigma \begin{pmatrix}
\int_{u < 0} u g_j \, dud\xi + \int_{u > 0} u g_{j-1} \, dud\xi - \int_{u < 0} u^2 g_{j+1} \, dud\xi - \int_{u > 0} u^2 g_{j-1} \, dud\xi \\
\int_{u < 0} u^2 g_j \, dud\xi + \int_{u > 0} u^2 g_{j-1} \, dud\xi - \int_{u < 0} u^2 g_{j+1} \, dud\xi - \int_{u > 0} u^2 g_{j-1} \, dud\xi \\
\int_{u < 0} \frac{u}{2} (u^2 + \xi^2) g_j \, dud\xi + \int_{u > 0} \frac{u}{2} (u^2 + \xi^2) g_{j+1} \, dud\xi - \int_{u < 0} \frac{u}{2} (u^2 + \xi^2) g_{j-1} \, dud\xi - \int_{u > 0} \frac{u}{2} (u^2 + \xi^2) g_{j-1} \, dud\xi
\end{pmatrix}
\]
\[
\begin{align*}
&\quad \left. \begin{array}{rl}
\int_{u<0} u g_{j-1} dud\xi - & \int_{u>0} u g_{j+1} dud\xi \\
\int_{u<0} u^2 g_{j-1} dud\xi - & \int_{u>0} u^2 g_{j+1} dud\xi \\
\left( \int_{u>0} \frac{u}{2}(u^2 + \xi^2) g_{j-1} dud\xi - \int_{u<0} \frac{u}{2}(u^2 + \xi^2) g_{j+1} dud\xi \right)
\end{array} \right) \\
+ \sigma
\end{align*}
\] 
(4.13)

- For density positivity

Assume the initial condition \( \rho_j \geq 0 \). From the definition, the Maxwellian function \( g \) is always positive, hence

\[
\tilde{\rho}_j = \rho_j + \sigma \left( \int_{u<0} u g_{j-1} dud\xi - \int_{u>0} u g_{j+1} dud\xi \right) + \sigma \left( \int_{u<0} u^2 g_{j-1} dud\xi - \int_{u>0} u^2 g_{j+1} dud\xi \right)
\]

\[
\geq \rho_j + \sigma \left( \int_{u<0} u g_{j-1} dud\xi - \int_{u>0} u g_{j+1} dud\xi \right)
\]

\[
= \rho_j - \sigma \rho_j \left( \frac{1}{2} U_j \alpha_j + \beta_j \right)
\]

where

\[
\alpha_j = \text{erfc}(\sqrt{\lambda_j} U_j) - \text{erfc}(\sqrt{\lambda_j} U_j)
\]

\[
\beta_j = \frac{e^{-\lambda_j U_j^2}}{2\pi^{1/2} \lambda_j}
\]

Since

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\[ \alpha_j = 2 - 2erfc(\sqrt{\lambda_j} U_j) \]
\[ \beta_j = \frac{e^{-\lambda_j U_j}}{\sqrt{\pi \lambda_j}} \leq \frac{1}{\sqrt{\pi \lambda_j}} \]

We conclude that

\[ \tilde{\rho}_j \geq \rho_j - \sigma \rho_j (\frac{1}{2} U_j \alpha_j + \beta_j) \]
\[ = \sigma \rho_j (\frac{1}{\sigma} - (\frac{1}{2} U_j \alpha_j + \beta_j)) \]

Hence, the density \( \tilde{\rho}_j \) is positive if the following CFL-like condition is satisfied:

\[ \sigma \leq \frac{1}{\max\{U_j + \frac{1}{\sqrt{\pi \lambda_j}} e^{-\lambda_j U_j} - U_j erfc(\sqrt{\lambda_j} U_j)\}} \] (4.14)

- **For internal energy positivity**

The numerical scheme (4.13) can be split into two steps. In the first step we only consider the case when there is only gas flowing out from the cell \((j)\). This gives that

\[
\begin{pmatrix}
\rho_j' \\
\rho_j' \\
E_j'
\end{pmatrix} = \begin{pmatrix}
\rho_j \\
\rho_j \\
E_j
\end{pmatrix} + \sigma \begin{pmatrix}
\int_{\alpha < 0} u g, dud\xi - \int_{\alpha > 0} u g, dud\xi \\
\int_{\alpha < 0} u^2 g, dud\xi - \int_{\alpha > 0} u^2 g, dud\xi \\
\int_{\alpha < 0} \frac{u}{2} (u^2 + \xi^2) g, dud\xi - \int_{\alpha > 0} \frac{u}{2} (u^2 + \xi^2) g, dud\xi
\end{pmatrix}
\] (4.15)

The second step is to add the correction terms:

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\[
\begin{pmatrix}
\dot{\rho}_j \\
\dot{m}_j \\
\dot{E}_j
\end{pmatrix} = \begin{pmatrix}
\rho_j \\
m_j \\
E_j
\end{pmatrix} + \begin{pmatrix}
\int_{u>0} u g_{j,i} dud\xi - \int_{u<0} u g_{j,i} dud\xi \\
\int_{u>0} u^2 g_{j,i} dud\xi - \int_{u<0} u^2 g_{j,i} dud\xi \\
\int_{u>0} \frac{u}{2} (u^2 + \xi^2) g_{j,i} dud\xi - \int_{u<0} \frac{u}{2} (u^2 + \xi^2) g_{j,i} dud\xi
\end{pmatrix}
\] (4.16)

The same methods are used to prove internal energy positivity of the scheme (4.15) and (4.16). The following is the proof of the positivity property of the above schemes.
Assume initially \( \rho_j E_j - \frac{1}{2} m_j^2 \geq 0 \), from the formula given, we have

\[
\rho_j^* E_j^* - \frac{1}{2} (m_j^*)^2 = [\rho_j - \sigma \rho_j \left( \frac{1}{2} U_j \alpha_j \right) + \beta_j)] [E_j - \sigma \rho_j \left( \frac{U_j^3}{4} + \frac{K + 3}{8 \lambda_j} \alpha_j \right) + \left( \frac{U_j^2}{2} + \frac{K + 2}{4 \lambda_j} \right) \beta_j)] \\
- \frac{1}{2} [m_j - \sigma \rho_j \left( \frac{U_j^2}{2} + \frac{1}{4 \lambda_j} \right) \alpha_j + U_j \beta_j)]^2 \\
= A \sigma^2 - B \sigma + C \tag{4.17}
\]

where

\[
A = \left( \frac{K + 1}{16 \lambda_j} \right) \rho_j^2 \alpha_j^2 + \frac{K + 2}{4 \lambda_j} \rho_j^2 \beta_j^2 + \frac{2K + 3}{8 \lambda_j} U_j \rho_j^2 \alpha_j \beta_j, \\
B = \frac{K + 1}{4 \lambda_j} \rho_j^2 U_j \alpha_j + \frac{2K + 3}{4 \lambda_j} \rho_j^2 \beta_j, \\
C = \rho E - \frac{1}{2} m^2 = \frac{K + 1}{4 \lambda_j} \rho_j^2
\] \tag{4.18}

It is obvious from above that \( C \geq 0 \). It can also be proved from Jensen's inequality that \( A, B \geq 0 \). Direct calculation shows that \( B^2 - 4AC \geq 0 \) which indicates there are two positive roots for the equation: \( A \sigma^2 - B \sigma + C = 0 \).

![Figure 4.1 Sketch of roots for internal energy](image)

Figure 4.1 Sketch of roots for internal energy

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The equation is always positive if \( \sigma = \frac{\Delta t}{\Delta x} \) is smaller than the smaller solution \( r_1 \). The smaller solution \( r_1 \) is

\[
r_1 = \frac{B - \sqrt{B^2 - 4AC}}{2A} = \frac{B - B(1 - \frac{4AC}{B^2})^{1/2}}{2A}
\]

\[
= \frac{B - B\{1 - \frac{4AC}{2B^2} - \frac{1}{8}(\frac{4AC}{B^2})^2 - \cdots\}}{2A}
\]

\[
= \frac{B}{2} \frac{4AC}{B^2} + \frac{B}{8}(\frac{4AC}{B^2})^2 + \cdots \quad \frac{B}{2} \frac{4AC}{B^2} = \frac{C}{B}
\]

\[
= \frac{1}{2} \frac{U_j}{\alpha_j} + \frac{2K + 3}{2K + 1} \beta_j \quad U_j - U_j,_{erfc}(\sqrt{\lambda_j} U_j) + \frac{2K + 3 e^{-\lambda_j U_j}}{2K + 2 \sqrt{\lambda_j} \pi}
\]

Hence, the internal energy is positive if the following CFL-like condition is satisfied:

\[
\sigma = \frac{\Delta t}{\Delta x} \leq r_1 = \frac{1}{\max\{U - U_{erfc}(\sqrt{\lambda U}) + \frac{2K + 3 e^{-\lambda U^2}}{2K + 2 \sqrt{\lambda} \pi}\}}
\]

(4.19)
(2) Collisional Method

From gas-kinetic BGK scheme, the cell interface values can be evaluated as:

\[
\begin{pmatrix}
\overline{\rho}_{j+1/2} \\
\overline{\rho}_{j+1/2} U_{j+1/2} \\
\frac{1}{2} \overline{\rho}_{j+1/2} \left(\overline{U}_{j+1/2} + \frac{K+1}{2\overline{l}_{j+1/2}}\right)
\end{pmatrix}
= \rho_j \begin{pmatrix}
\frac{1}{2} \text{erfc}(-\sqrt{\lambda_j} U_j) \\
\frac{1}{2} U_j \text{erfc}(-\sqrt{\lambda_j} U_j) + \frac{1}{2} \frac{e^{-\lambda_j U_j^2}}{\sqrt{\pi \lambda_j}} \\
\frac{1}{2} \left(\frac{U_j^2}{2} + \frac{K+1}{4\lambda_j}\right) \text{erfc}(-\sqrt{\lambda_j} U_j) + \frac{U_j}{2} \frac{e^{-\lambda_j U_j^2}}{\sqrt{\pi \lambda_j}}
\end{pmatrix}
\]

\[
+ \rho_{j+1} \begin{pmatrix}
\frac{1}{2} \text{erfc}(\sqrt{\lambda_{j+1}} U_{j+1}) \\
\frac{1}{2} U_{j+1} \text{erfc}(\sqrt{\lambda_{j+1}} U_{j+1}) - \frac{1}{2} \frac{e^{-\lambda_{j+1} U_{j+1}^2}}{\sqrt{\pi \lambda_{j+1}}} \\
\frac{1}{2} \left(\frac{U_{j+1}^2}{2} + \frac{K+1}{4\lambda_{j+1}}\right) \text{erfc}(\sqrt{\lambda_{j+1}} U_{j+1}) - \frac{U_{j+1}}{2} \frac{e^{-\lambda_{j+1} U_{j+1}^2}}{\sqrt{\pi \lambda_{j+1}}}
\end{pmatrix}
\] \tag{4.20}

The interface variables \(\overline{\rho}_{j+1/2}, \overline{U}_{j+1/2},\) and \(\overline{l}_{j+1/2}\) can be obtained from the above equation. Let \(\sigma = \frac{\Delta t}{\Delta x}\), the numerical formula becomes:

\[
\begin{pmatrix}
\tilde{\rho}_j \\
\tilde{m}_j \\
\tilde{E}_j
\end{pmatrix}
= \begin{pmatrix}
\rho_j \\
m_j \\
E_j
\end{pmatrix}
+ \sigma \begin{pmatrix}
F_{\rho,j-1/2} - F_{\rho,j+1/2} \\
F_{m,j-1/2} - F_{m,j+1/2} \\
F_{E,j-1/2} - F_{E,j+1/2}
\end{pmatrix}
\] \tag{4.21}
where

\[
\begin{pmatrix}
F'_{p,j+1/2} \\
F'_{m,j+1/2} \\
F'_{E,j+1/2}
\end{pmatrix}
= \bar{\rho}_{j+1/2}
\begin{pmatrix}
\bar{U}_{j+1/2} \\
\frac{1}{2\bar{\lambda}_{j+1/2}} \\
\frac{K+3}{4\bar{\lambda}_{j+1/2}} \bar{U}_{j+1/2}
\end{pmatrix}
\]

• For density positivity

Assume \( \rho_j \geq 0 \), we have

\[
\tilde{\rho}_j = \rho_j + \sigma \left( \frac{\rho_{j-1} U_{j-1}}{2} \text{erfc}(\sqrt{\bar{\lambda}_j} U_{j-1}) + \frac{\rho_{j-1} e^{-\bar{\lambda}_j U_{j-1}^2}}{2 \sqrt{\pi \bar{\lambda}_{j-1}}} \right)
\]

\[
+ \frac{\rho_j U_j}{2} \left( \text{erfc}(\sqrt{\bar{\lambda}_j} U_j) - \text{erfc}(\sqrt{\bar{\lambda}_j} U_j) - \rho_j \frac{e^{-\bar{\lambda}_j U_j^2}}{\sqrt{\pi \bar{\lambda}_j}} \right)
\]

\[
- \frac{\rho_{j+1} U_{j+1}}{2} \text{erfc}(\sqrt{\bar{\lambda}_{j+1}} U_{j+1}) + \frac{\rho_{j+1} e^{-\bar{\lambda}_{j+1} U_{j+1}^2}}{2 \sqrt{\pi \bar{\lambda}_{j+1}}} \}
\]

It can be proved that

\[
U \text{erfc}(\sqrt{\bar{\lambda}} U) + \frac{e^{-U^2}}{\sqrt{\pi \bar{\lambda}}} \geq 0, \text{ and}
\]

\[-U \text{erfc}(\sqrt{\bar{\lambda}} U) + \frac{e^{-U^2}}{\sqrt{\pi \bar{\lambda}}} \geq 0\]
Hence

\[ \tilde{\rho}_j \geq \rho_j + \sigma \rho_j \left\{ \frac{U_j}{2} \left( \text{erfc} \left( \sqrt{\lambda_j U_j} \right) - \text{erfc} \left( - \sqrt{\lambda_j U_j} \right) \right) - \frac{e^{-\lambda_j \mu_j^2}}{\sqrt{\pi \lambda_j}} \right\} \]

\[ = \rho_j + \sigma \rho_j \left\{ -U_j + U_j \text{erfc} \left( \sqrt{\lambda_j U_j} \right) - \frac{e^{-\lambda_j \mu_j^2}}{\sqrt{\pi \lambda_j}} \right\} \]

Hence, the density \( \tilde{\rho}_j \) is positive if the following CFL-like condition is satisfied:

\[ \sigma \leq \frac{1}{\max \left\{ U_j + \frac{1}{\sqrt{\pi \lambda_j}} e^{-\lambda_j \mu_j^2} - U_j \text{erfc} \left( \sqrt{\lambda_j U_j} \right) \right\}} \] (4.22)

- **For internal energy positivity**

Based on the conclusion from the linear scalar equation, the collisional method of the Euler equations may not be a positivity-preserving method. Actually, non-positive results have been observed in numerical tests. It is almost impossible to prove it theoretically because of the strong non-linearity of the formula. Since we have already proved that the density of the collision scheme is positive, only internal energy could be negative.

(3) **BGK Method**

The numerical formula of the BGK method can be written as the combination of the collisionless and collisional approaches:

\[
\begin{pmatrix}
\tilde{\rho}_j \\
\tilde{m}_j \\
\tilde{E}_j
\end{pmatrix}
= \begin{pmatrix}
\rho_j \\
m_j \\
E_j
\end{pmatrix}
+ \sigma \alpha \begin{pmatrix}
F_{\rho,j-1/2} - F_{\rho,j+1/2} \\
F_{m,j-1/2} - F_{m,j+1/2} \\
F_{E,j-1/2} - F_{E,j+1/2}
\end{pmatrix}
+ \sigma \beta \begin{pmatrix}
F'_{\rho,j-1/2} - F'_{\rho,j+1/2} \\
F'_{m,j-1/2} - F'_{m,j+1/2} \\
F'_{E,j-1/2} - F'_{E,j+1/2}
\end{pmatrix}
\] (4.23)
where \( \sigma = \frac{\Delta t}{\Delta x} \),

\[
\alpha = (1 - e^{-\Delta t/\tau}),
\]

\[
\beta = e^{-\Delta t/\tau},
\]

\( F^\rho, F^m, F^E \) are the fluxes of the collisionless scheme, and

\( F'^\rho, F'^m, F'^E \) are the fluxes of the collisionless scheme

- **For density positivity**

Assume initially that \( \rho_j \geq 0 \), we can use the conclusions drawn from the collisionless method and the collisional method

\[
\tilde{\rho} = \rho + \sigma \Delta F^\rho
\]

\[
= (\alpha + \beta) \rho + \sigma (\alpha \Delta F^{\text{collisionless}} + \beta \Delta F^{\text{collisional}})
\]

\[
= (\alpha \rho + \beta \rho) + \alpha \sigma \Delta F^{\text{collisionless}} + \beta \sigma \Delta F^{\text{collisional}}
\]

\[
= \alpha (\rho + \sigma \Delta F^{\text{collisionless}}) + \beta (\rho + \sigma \Delta F^{\text{collisional}})
\]

\[
\geq \alpha \cdot 0 + \beta \cdot 0 = 0
\]

Hence the density is positive.

- **For internal energy positivity**

Assume initially \( \rho_j E_j - \frac{1}{2} m_j^2 \geq 0 \), we rewrite the gas-kinetic BGK scheme for the Euler equations as:

\[
\begin{pmatrix}
\tilde{\rho}_j \\
\tilde{m}_j \\
\tilde{E}_j
\end{pmatrix} =
\begin{pmatrix}
\rho_j \\
m_j \\
E_j
\end{pmatrix} + \sigma \alpha 
\begin{pmatrix}
\Delta \rho_1 \\
\Delta m_1 \\
\Delta E_1
\end{pmatrix} + \sigma \beta 
\begin{pmatrix}
\Delta \rho_2 \\
\Delta m_2 \\
\Delta E_2
\end{pmatrix} =
\begin{pmatrix}
\rho_j \\
m_j \\
E_j
\end{pmatrix} + \sigma 
\begin{pmatrix}
\Delta \rho \\
\Delta m \\
\Delta E
\end{pmatrix}
\]

(4.24)
where

\[
\begin{pmatrix}
\Delta \rho_1 \\
\Delta m_1 \\
\Delta E_1
\end{pmatrix}
\]
is the vector of density, momentum, and energy of the collisionless scheme

\[
\begin{pmatrix}
\Delta \rho_2 \\
\Delta m_2 \\
\Delta E_2
\end{pmatrix}
\]
is the vector of density, momentum, and energy of the collisional scheme

So the internal energy becomes:

\[
\tilde{\rho E} - \frac{1}{2} \tilde{m}^2 = (\rho + \sigma \Delta \rho)(E + \sigma \Delta E) - \frac{1}{2} (m + \sigma \Delta m)^2
\]

\[
= (\rho E - \frac{1}{2} m^2) + (\Delta \rho \cdot E + \Delta E \cdot \rho - \Delta m \cdot m)\sigma + (\Delta \rho \Delta E - \frac{1}{2} (\Delta m)^2)\sigma^2
\]

\[
= A \sigma^2 - B \sigma + C
\]  \hfill (4.25)

From the initial condition \(\rho E - \frac{1}{2} m^2 \geq 0\), we conclude that \(C \geq 0\). Also

\[
A = \Delta \rho \Delta E - \frac{1}{2} \Delta m^2
\]

\[
= p_s \beta^2 - p_s \beta + (\Delta \rho, \Delta E, -\frac{1}{2} \Delta m^2)
\]  \hfill (4.26)

and

\[
B = \Delta \rho \cdot E + \Delta E \cdot \rho - \Delta m \cdot m
\]

\[
= q_s \beta + (\Delta \rho, E, \Delta E, \rho - \Delta m, m)
\]  \hfill (4.27)
If $\beta = 0$, then the coefficients $A, B$ of the BGK method become those of the collisionless method, which have been proven positive. Hence the constant terms of above two equations are always positive.

Coefficient $A$ is a quadratic function of $\beta$, and $0 \leq \beta \leq 1$. Since the constant part of the equation is positive, assume it is $p_c > 0$. Depending on the sign of $p_a$, the distributions of coefficient $A$ are as follows:

![Graph of coefficient A's distribution for the BGK method]

Figure 4.2 Coefficient $A$'s distribution for the BGK method

If we choose the collision term $\beta$ to be: $0 \leq \beta \leq \beta_1 = \min(r_1, r_2, 1)$, the coefficient $A$ will be positive.

The coefficient $B$ is a linear function of $\beta$. The constant part of the equation, or $q_c$, is also positive. Depending on the sign of $q_b$, the distributions of the coefficient $B$ are as
follows:

\[
\begin{align*}
B & \quad \beta \\
q_c & \quad 0
\end{align*}
\]

\[
\begin{align*}
B & \quad \beta \\
q_c & \quad 0
\end{align*}
\]

Figure 4.3 Coefficient $B$'s distribution for the BGK method

The collision coefficient $\beta$ is always positive, so for the case $q_b \geq 0$, coefficient $B$ is positive. For the case $q_b \leq 0$, the coefficient $B$ is positive if $0 \leq \beta \leq \beta_2 = \frac{-q_c}{q_b}$.

We have already shown that the coefficient $C$ is positive using initial conditions. Hence, all coefficients $A$, $B$, and $C$ of internal energy formula are positive. Using the same method for the collisionless case, we can prove that the internal energy is positive too as long as the following conditions are satisfied:

- The collision term

\[
\beta = e^{-\Delta t/\tau} \leq \min(\beta_1, \beta_2)
\] (4.28)

where $\beta_1$ and $\beta_2$ are calculated as above.

55
- The CFL-like condition of the BGK scheme is:

\[
\sigma \leq \frac{1}{\max\{U - U_{erf}(\sqrt{\lambda}U) + \frac{2K + 3e^{-\lambda U^2}}{2K + 2\sqrt{\lambda \pi}} + \frac{q_b}{c} \beta\}}
\]  

(4.29)

From above discussion we conclude that the collisionless scheme is a positive scheme and the collisional scheme is not. But the collisionless scheme adds too much dissipation, which makes it unattractive for some strong shock applications. Gas-kinetic BGK scheme not only is a positive scheme, it also introduces right amount of dissipation that is depending on the shock strength. Hence it is a very good shock-capturing scheme.
CHAPTER 5
RESULTS AND DISCUSSIONS

Gas-kinetic BGK schemes have been applied to many test cases ranging from the solution of the linear advection equation to unsteady hypersonic flow computations. This chapter is devoted to the investigation of the performance of BGK schemes in terms of their robustness, accuracy and efficiency. In all test cases, entropy-violating solutions have never been obtained using the BGK methods, which is an important property of the gas-kinetic BGK approach. For all the test examples here, the second order SLIP (Van Leer limiter) formulation is used for the construction of conservative variables inside each numerical cell unless stated otherwise.

5.1 Numerical Experiments of Scalar Equations

For the linear advection equation and Burger's equation, two different initial profiles are tested: a sine wave and a square wave.

Case 1: Find \( u(x, 0) \) where

\[
\begin{align*}
\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} &= 0 \\
u(x, 0) &= -\sin(\pi x)
\end{align*}
\]

which is a linear advection of one period of a sinusoid. Use 50 evenly spaced grid points and \( \lambda = \Delta t / \Delta x = 0.5 \). This test case has a completely smooth exact solution with no sonic points. The results of the BGK scheme are shown in Figure 5.2 to compare with the analytical solution. In the case of first-order BGK scheme, the sine wave is smeared due to large numerical diffusion. In the cases of the higher-order BGK scheme, the results with the Van Leer limiter are better than the results with the MinMod limiter for this
smooth flow because the higher-order SLIP method is used for variable reconstruction. The effect of limiters, i.e. the effect of interpolation techniques, is visible.

Case 2: Find \( u(x,30) \) where

\[
\frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial}{\partial x} (u^2) = 0
\]

\[
u(x,0) = \sin(\pi x)
\]

which is a Burgers' equation propagation of a one period of a sinusoid. Use 50 evenly spaced grid points and \( \lambda = \Delta t / \Delta x = 0.5 \). The results of the BGK scheme are shown in Figure 5.3 to compare with the analytical solution. It can be observed that the first-order BGK scheme and high-order BGK schemes all capture the discontinuity with one interior point.

Case 3: Find \( u(x,0.6) \)

\[
\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0
\]

\[
u(x,0) = \begin{cases} 
1 & \text{for } |x| < \frac{1}{3}, \\
0 & \text{for } \frac{1}{3} < |x| \leq 1
\end{cases}
\]

Use 60 evenly spaced grid points and \( \lambda = \Delta t / \Delta x = 0.5 \). The scalar conservation law is a linear advection equation and the initial condition is a square wave. The results of the BGK scheme are shown in Figure 5.4 to compare with the analytical solutions. Just as in case 1, the first-order BGK scheme is rather too diffusive, so it is not as good in capturing discontinuities as the second-order BGK scheme for the square wave.
Case 4: Find $u(x,0.6)$

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left( \frac{1}{2} u^2 \right) = 0$$

$$u(x,0) = \begin{cases} 1 & \text{for } |x| < \frac{1}{3}, \\ 0 & \text{for } \frac{1}{3} < |x| \leq 1 \end{cases}$$

Use 60 evenly spaced grid points and $\lambda = \Delta t / \Delta x = 0.5$. The scalar conservation law is Burgers' equation and the initial condition is a square wave. For this problem, an expansion fan is created at $x = -1/3$ and a shock wave is created at $x = 1/3$. The results of the BGK scheme are shown in Figure 5.5 to compare with the analytical solution. Similarly to case 2, the first-order BGK scheme is too diffusive but still captures the shock with two interior points. The high-order BGK schemes can capture the shock wave and the expansion fan better. From all these results of the BGK scheme for the scalar equations, it can be concluded that the BGK scheme doesn't produce oscillations near discontinuities and variable reconstructions with the SLIP method is necessary to produce better results.

5.2 The BGK Scheme for One-Dimensional Flows

From gas-kinetic theory, the collision time should depend on macroscopic flow variables, such as density and temperature. For shock-capturing calculations, a common practice is to use a collision time $\tau$ which is composed of two parts,

$$\tau = C_1 \Delta t + \Delta t \text{Min}(1,C)$$

where

$$C = C_2 \frac{\left| \rho/\lambda - \rho/\lambda_r \right|}{\left| \rho/\lambda + \rho/\lambda_r \right|}$$
and $\Delta t$ is the CFL time step. The first term on the right-hand side gives a limiting threshold for the collision time to stabilize the program, such as the evaluations of $\Delta t / \tau$ and $e^{-\Delta t / \tau}$, it also provides background dissipation for the numerical fluid. The second term is related to the pressure jump in the reconstructed initial data, which introduces additional artificial dissipation if a high pressure-gradient is present in the flow. For shock tube test cases, numerical results are not sensitive to the choices of the values of $C_1$ and $C_2$. In the following testing cases, $C_1 = 0.05$ and $C_2 = 5$ are chosen to do the computations.

Case 1: Shock Tube: Sod Case

This test case is a one-dimensional shock tube problem with two different initial constant states in the left and right parts of the tube. It is a standard Riemann problem with a similarity solution. The three waves: shock, contact discontinuity and rarefaction are emerging from the location of the initial discontinuity. Figure 5.6 compares the numerical results of the BGK scheme with the results of Roe's scheme. The initial test data are:

Length = 20.0  
CFL = 0.4  
Time = 4.0 sec.  
Speed = 1.2  
Number of elements = 200

$$\begin{pmatrix} \rho \\ \rho U \\ \rho e_T \end{pmatrix}_l = \begin{pmatrix} 1 \\ 0 \\ 2.5 \end{pmatrix}$$

$$\begin{pmatrix} \rho \\ \rho U \\ \rho e_T \end{pmatrix}_r = \begin{pmatrix} 0.125 \\ 0 \\ 0.25 \end{pmatrix}$$
It can be seen that the BGK scheme gives competitive numerical results for the Sod shock tub. It doesn’t need any entropy fix as Roe’s scheme (not required for this test case) because it satisfies the entropy condition automatically.

**Case 2: Shock Tube: Lax-Harten Case**

This is another Riemann problem, which gives much stronger shock waves and contact discontinuity than the Sod shock tube. The results of the BGK scheme are shown in Figure 5.7 to compare with the results of Roe’s scheme. The initial test data are:

- Length = 20.0
- CFL = 0.4
- Time = 2.0 sec.
- Speed = 2.65
- Number of elements = 200

\[
\begin{pmatrix}
\rho \\
\rho U \\
\rho e_r
\end{pmatrix}_{l} = \begin{pmatrix}
0.445 \\
0.311 \\
8.928
\end{pmatrix},
\]

\[
\begin{pmatrix}
\rho \\
\rho U \\
\rho e_r
\end{pmatrix}_{r} = \begin{pmatrix}
0.5 \\
0 \\
1.4275
\end{pmatrix}
\]

Just as case 1, the BGK scheme gives competitive numerical results for the Lax-Harten shock tube.

**Case 3: Woodward-Collela Shock Tube**

The initial condition consists of three constant states, each at rest between reflecting walls, separated by a distance of unity. Two strong blast waves develop and collide, producing new contact discontinuities. This test problem is used to illustrate the strong relationship between the accuracy of the overall flow solution and the thinness of
discontinuities on the grid. The results of the BGK scheme are shown in Figure 5.8. The initial test data are:

\[
\begin{align*}
\text{Length} = 1.0 \\
\text{CFL} = 0.4 \\
\text{Time} = 0.038 \text{ sec.} \\
\text{Number of elements} = 400 \text{ and } 600
\end{align*}
\]

\[
\begin{align*}
\begin{pmatrix}
\rho \\
\rho U \\
\rho \varepsilon_f
\end{pmatrix}
&= \begin{pmatrix}
1 \\
0 \\
2500
\end{pmatrix}, \text{for } 0 \leq x < 0.1 \\
\begin{pmatrix}
\rho \\
\rho U \\
\rho \varepsilon_f
\end{pmatrix}
&= \begin{pmatrix}
1 \\
0 \\
0.025
\end{pmatrix}, \text{for } 0.1 \leq x \leq 0.9 \\
\begin{pmatrix}
\rho \\
\rho U \\
\rho \varepsilon_f
\end{pmatrix}
&= \begin{pmatrix}
1 \\
0 \\
250
\end{pmatrix}, \text{for } 0.9 < x \leq 1
\end{align*}
\]

5.3 The BGK Scheme for Two-Dimensional Flows

The collision time of the gas-kinetic BGK scheme for the Navier-Stokes equations will be chosen according to the real physical viscosity coefficient \( \nu \), such that

\[
\tau = \frac{\nu \rho}{p},
\]

where \( \rho \) and \( p \) are local density and pressure.
Case 1: The interaction of an oblique shock wave with a laminar boundary layer

This is a classical shock and boundary layer interference problem that has attracted a lot of attention in the CFD community. It is supposed to calculate the two-dimensional viscous flow past a flat plate. An incident shock comes in from the top with an angle \( \theta \), and intersects with the boundary layer. The sketch of the flow is shown in Figure 5.9. The surface pressure and skin friction of the BGK scheme’s calculations are shown in Figures 5.10 and 5.11 to compare with the experimental data\(^{61}\). The results show that the gas-kinetic BGK scheme can capture the oblique shock and accurately predict the reverse flow inside the boundary layer.

Case 2: Double Mach reflection problem

It is generally known that schemes based on characteristic splitting with Roe averaging can produce the carbuncle phenomenon in steady or near-steady flows with a slowly moving shock. Increasing the artificial dissipation introduced with an entropy fix can cure this phenomenon. Gas-kinetic BGK schemes produced a result without any presence of the carbuncle phenomenon, which suggests that BGK fluxes provide an appropriate amount of numerical dissipation. The density and pressure contours of the BGK scheme for this problem are shown in Figure 5.12 and 5.13, respectively.

5.4 The BGK Scheme for Three-Dimensional Flows

The full gas-kinetic BGK scheme gives time-dependent fluxes, which may handicap the convergence of the scheme to a steady state. Thus, for steady-state calculations, the relaxation process must be simplified in order to yield time independent numerical fluxes. The easiest way to achieve this is to keep only the pointwise values and ignore all high-
order spatial and temporal slopes in the expansion of the distribution functions $f$ and $g$. The new solution of the BGK equation can be written as:

$$f = g_0 + \epsilon^{(2)}(f_0 - g_0)$$

where $\epsilon^{(2)}$ is the adaptive coefficient to control the dissipation in the scheme. It is the collision coefficient of the BGK scheme.

For three-dimensional wing calculations, the parameter $\epsilon^{(2)}$ is determined by a switching function calculated from local pressure gradients. Using subscripts $i$ and $j$ to label the neighbor cells, the switching function for fluxes in the $i$ direction is:

$$\epsilon^{(2)} = 1 - e^{-\alpha \max(P_{i+1}, P_i)}$$

where $\alpha$ is a constant,

$$P_i = \frac{|\Delta p_{i+1/2} - \Delta p_{i-1/2}|}{|\Delta p_{i+1/2}| + |\Delta p_{i-1/2}|}$$

and

$$\Delta p_{i+1/2} = p_{j+1} - p_i$$

The three-dimensional BGK scheme was implemented on Jameson's FLO87 code. In this three-dimensional Euler equation solver, the EFLUX and DFLUX subroutines were replaced by a new BGKFLUX subroutine. The flowchart of the BGK scheme is shown in Figure 5.1.
Extensive test cases have been run for wing calculations with a modification of Jameson's FLO87 program to incorporate the gas-kinetic BGK scheme. The program uses explicit multistage Runge-Kutta time stepping scheme and multigridding techniques to improve the converging speed. The problems range from transonic to supersonic flows for various angles of attack. Figure 5.14 shows the transonic flow pressure distributions and contour of a wing with the NACA0012 section on a 192x32x48 mesh. Figure 5.15 shows the comparison between results of the BGK scheme and the Jameson's CUSP scheme for the same wing. In order to reach the steady state solutions, the BGK scheme
used three stages, and each stage had 200 steps. The CPU time for each step was 72 seconds on . For the CUSP scheme, it also used three stages, and each stage only had 30 steps. The time for each step was 32 seconds. The BGK scheme successfully catches the strong normal shock at the upper surface and the trailing edge at all sections of the wing. Figure 5.16 and 5.17 show the results for supersonic flow over the NACA0012 wing. Shocks in front of the wing and behind the wing can be observed on the contour plot. Figures 5.18 to 5.21 show the similar results of transonic and supersonic flows for the ONERA M6 wing.

It can be concluded that the gas-kinetic BGK scheme is a very good shock-capturing scheme although it is not a very efficient scheme comparing to Jameson's CUSP scheme. The CUSP scheme is the fastest reported scheme, and some other Euler solvers need 500 or more steps to achieve steady-state solutions.

5.5 Stability and Positivity of the First-Order BGK Scheme

In this section, we investigate the stability and positivity properties of the first-order BGK scheme for the linear advection equation. By keeping all coefficients of BGK formula positive, we obtained the CFL-like condition and maximum collision coefficient requirement. Positivity property is a necessary condition for any shock-capturing scheme in order to get non-oscillated solutions at discontinuities.

To analyze the stability of 1st-order BGK scheme, we rewrite equation (4.8)

\[ U_j^{n+1} = \sum_k a_{j+k} U_{j+k}^n \]

where

\[ a_{j+1} = -\sigma \beta \frac{a}{2} \text{erfc}(\sqrt{\lambda} a) + \sigma (1 - \beta) \left[ -\frac{a}{2} \text{erfc}(\sqrt{\lambda} a) + \frac{e^{-ka^2}}{2\sqrt{\pi \lambda}} \right] \]

\[ a_j = 1 - \sigma [a - a \cdot \text{erfc}(\sqrt{\lambda} a) + \frac{e^{-ka^2}}{\sqrt{\pi \lambda}}] + \sigma \beta \frac{e^{-ka^2}}{\sqrt{\pi \lambda}} \]
\[ a_{j-1} = \sigma \left[ \frac{a}{2} \text{erfc}(-\sqrt{\lambda}a) + \frac{e^{-\lambda a^2}}{2\sqrt{\pi} \lambda} \right] - \sigma \beta \frac{e^{-\lambda a^2}}{2\sqrt{\pi} \lambda} \]

In order to ensure the 1\textsuperscript{st}-order BGK scheme is a positive scheme, two conditions must be satisfied:

- The collision coefficient

\[ \beta = e^{-\lambda a^2/\tau} \leq 1 - \frac{2}{\frac{e^{-\lambda a^2}}{2\sqrt{\pi} \lambda}} \]

- The CFL-like condition

\[ \sigma \leq \frac{1}{a + [-a \cdot \text{erfc}(-\sqrt{\lambda}a) + \frac{e^{-\lambda a^2}}{\sqrt{\pi} \lambda}] - \beta \frac{e^{-\lambda a^2}}{\sqrt{\pi} \lambda}} \]

**EXAMPLE:**

For Sine wave with \( a = 0.1 \), we choose \( \lambda = 100 \). So, in order to get a positive scheme, the following conditions must be satisfied:

1. \( \beta = e^{-\lambda a^2/\tau} \leq 1 - \frac{2}{\frac{e^{-\lambda a^2}}{2\sqrt{\pi} \lambda}} = 0.25 \)

Let \( \alpha = 1 - \beta \), so \( \alpha \geq 0.75 \)

2. \( \sigma \alpha \leq 0.98 \) for \( \beta = 0.2 \)
The test results are shown in Figure 5.22.

-- From results (c) and (d) we can see if \( \alpha \) doesn’t satisfy the first condition \( (\alpha = 0.7, \ \alpha = 0.2) \), it will cause oscillations at discontinuity. Because the oscillations are so small, they can hardly been observed in figure (c) or (d). These oscillations do exist and can be verified by checking the numerical data.

-- From results (e) and (f) we can see that if CFL-like condition and collision coefficient condition are satisfied, non-oscillated results are obtained.

-- From results (g) and (h) we can see that if CFL-like condition is violated, the results will either be oscillated (g) or diverged (h).
Figure 5.2 The Linear Advection Equation for Sine Wave
Figure 5.3 Burger’s Equation for Sine Wave
Figure 5.4 Linear Advection Equation for Square Wave
Figure 5.5 Burger’s Equation for Square Wave
Figure 5.6 Shock Tube: Sod Case
Figure 5.7 Shock Tube: Lax-Harten Case
Figure 5.8 Woodward-Colella Test Case
Figure 5.9 Sketch of Shock-Boundary Layer Interaction
Figure 5.10 Surface Pressure of Shock-Boundary Layer Interaction

Figure 5.11 Skin Friction of Shock-Boundary Layer Interaction
Figure 5.12 Density Distribution of Double Mach Reflection Problem

Figure 5.13 Pressure Distribution of Double Mach Reflection Problem
Figure 5.14 NACA0012 Wing Transonic Flow of the BGK Scheme

\[ M = 0.84, \, \alpha = 9^0 \]

Top: Pressures of Wing Upper & Lower Surfaces
Bottom Left: Tip-Section Pressure Distribution
Bottom Right: Tip-Section Pressure Contour
Figure 5.15 NACA0012 Wing Contours and Cp Distributions of Transonic Flow

Red: The BGK Scheme; Blue: The CUSP Scheme
Figure 5.16 NACA0012 Wing Supersonic Flow of the BGK Scheme

\[ M = 2, \alpha = 11^\circ \]

Top: Pressures of Wing Upper & Lower Surfaces
Bottom Left: Tip-Section Pressure Distribution
Bottom Right: Pressure Contour of Tip-Section
Figure 5.17 NACA0012 Wing Contours and Cp Distributions of Supersonic Flow
Red: The BGK Scheme; Blue: The CUSP Scheme

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Figure 5.18 ONERA M6 Wing Transonic Flow of the BGK Scheme

$M = 0.84$, $\alpha = 9^\circ$

Top: Pressures of Wing Upper & Lower Surfaces
Bottom Left: Tip-Section Pressure Distribution
Bottom Right: Pressure Contour of Tip-Section
Figure 5.19 ONERA M6 Wing Contours and Cp Distributions of Transonic Flow
Red: The BGK Scheme; Blue: The CUSP Scheme
Figure 5.20 ONERA M6 Wing Supersonic Flow of the BGK Scheme

$M = 2, \alpha = 9^\circ$

Top: Pressures of Wing Upper & Lower Surfaces
Bottom Left: Tip-Section Pressure Distribution
Bottom Right: Pressure Contour of Tip-Section
Figure 5.21 ONERA M6 Wing Contours and Cp Distributions of Supersonic Flow
Red: The BGK Scheme; Blue: The CUSP Scheme
Figure 5.22 Stability of the Linear Advection Equation
CHAPTER 6
CONCLUDING REMARKS AND FUTURE WORKS

Gas-kinetic schemes are based on the gas kinetic theory, which analyzes fluid flows from an alternative microscopic description. Since their governing equation is the Boltzmann equation, which can be used in a broader range of applications, gas-kinetic schemes are superior for complex flows. The collisional BGK scheme presented in this thesis is based on the gas-kinetic BGK model, which is distinguished from other gas-kinetic schemes, such as KFVS scheme, where the collisionless Boltzmann equation is solved in the gas evolution stage. The machinery of the BGK method consists of combining an explicit solution of the BGK model of the Boltzmann equation with the compatibility condition relating moments of the real distribution function to those of the equilibrium distribution towards which it continuously tends to relax.

The following conclusions are drawn from the research experiences:

(1) The gas-kinetic BGK scheme produces very accurate results for three-dimensional transonic and supersonic wing applications at high angle of attack.

(2) Gas-kinetic BGK schemes have very complicated formulation, which include computations of error function and exponential function. It is more costly than other simpler schemes, such as Jameson's CUSP scheme. But with the growth of computer resources, the implementations of BGK schemes become practical for three-dimensional flow simulations.

(3) The particle collision BGK scheme presented here automatically satisfies entropy condition, which guarantees transition from non-equilibrium state to equilibrium state. So no unphysical solutions such as expansion shock waves
will be allowed with the BGK scheme. It is also a positivity-preserving scheme, which ensures that only positive density and pressure are obtained in the numerical computations.

(4) Because of the inclusion of particle collision term, the gas-kinetic BGK scheme is an excellent shock-capturing scheme. It is demonstrated from extensive numerical experiments ranging from one-dimensional strong shock cases to three-dimensional supersonic wing calculations. The main reason for it is that inside each shock layer, the flow is so complicated and can be better described by microscopic quantity that is governed by the Boltzmann equation.

(5) Theoretically, the Navier-Stokes equations can be derived from the gas-kinetic BGK model due to the connection between the viscosity coefficient and the relaxation time. The Euler solutions are the limit cases when the viscosity coefficient is very small in the Navier-Stokes solutions.

Two main goals have been accomplished in this thesis: first, the gas-kinetic BGK scheme for three-dimensional compressible flows was proposed and successfully implemented on transonic and supersonic wing calculations. Secondly, the positivity property of the first-order BGK scheme was proved rigorously for the linear scalar equation and the one-dimensional Euler equations.

Considering the advantages and disadvantages of gas-kinetic BGK methods, future research subjects on BGK schemes are suggested as followings:

(1) The BGK scheme was successfully used on wing calculations for transonic and supersonic flows. To extend the computation to hypersonic flows at very high angle of attack, the original gas-kinetic BGK scheme may be a better choice and the collision time and fluxes should include the viscous effects.

(2) Based on the experiences of three-dimensional computations, the convergence time is slower than other schemes, such as Jameson's CUSP scheme. In order to
use the BGK scheme more efficiently, it would be ideal to use it with the parallel computing technology.

(3) Currently, extensions of gas-kinetic BGK schemes to multiphase, chemical reactive, relativistic, inhomogeneous, semiconductor, phase transition and other physical applications, have attracted much attention. They can be extended further to three-dimensional cases.

(4) Because the BGK scheme is based on the gas kinetic theory, it has the potential advantages for the treatment of rarefied flows. It can be used for rarefied gas flows in the future.
APPENDIX A:

MOMENTS OF THE MAXWELLIAN DISTRIBUTION FUNCTION

In the gas-kinetic scheme, we need to evaluate moments of the Maxwellian distribution function with bounded and unbounded integration limits.

In the 1-D case, the Maxwellian distribution function is

\[ g = \rho \left( \frac{\lambda}{\pi} \right)^{K+1} \frac{1}{2} e^{-\lambda (u-u')^2 + \xi^2} \]

where \( \xi \) has \( K \) degrees of freedom. With the introduction of following notation.

\[ \rho < \ldots > \equiv \int \int \ldots \int g dud \xi \]

the general integration formula becomes

\[ < u^n \xi^l > = < u^n > < \xi^l > \]

where \( n \) is an integer, and \( l \) is an even integer (owing to the symmetrical property of \( \xi \)).

The moments of \( < \xi^l > \) are:

\[ < \xi > = \frac{K}{2\lambda} \]

\[ < \xi^2 > = \frac{3K}{4\lambda^2} + \frac{K(K-1)}{4\lambda^2} \]

The values of \( < u^n > \) depend on the integration limits. If the limit is from \(-\infty\) to \(+\infty\),
we have

\[ <u^0 > = 1, \]

\[ <u^1 > = U, \]

\[ <u^2 > = \left(U^2 + \frac{1}{2\Lambda}\right) \]

\[ <u^3 > = \left(U^3 + 1.5 \frac{U}{\lambda}\right) \]

\[ <u^4 > = \left(U^4 + \frac{3U^2}{\lambda} + 0.75 \frac{U}{\lambda^2}\right) \]

\[ <u^5 > = \left(U^5 + 5 \frac{U^3}{\lambda} + 3.75 \frac{U}{\lambda^2}\right) \]

\[ \ldots \]

\[ <u^{n+2} > = U <u^{n+1} > + \frac{n+1}{2\Lambda} <u^n > \]

If the integration limit for \( u \) is from 0 to \(+\infty\), such as

\[ \rho <\ldots>_{\infty} = \int_0^{\infty} (\ldots) g(u) du \xi \]

or from \(-\infty\) to 0,

\[ \rho <\ldots>_{\infty} = \int_{-\infty}^0 (\ldots) g(u) du \xi \]

the error function and the complimentary error function have to be used. The moments for \( u^n \) in the half space are,
\[ <u^0>_{\sigma_0} = \frac{1}{2} \text{erfc}(\sqrt{\lambda} U) \]

\[ <u^1>_{\sigma_0} = U <u^0>_{\sigma_0} + \frac{1}{2} \frac{e^{-U^2}}{\sqrt{\pi \lambda}} \]

...

\[ <u^{n+2}>_{\sigma_0} = U <u^{n+1}>_{\sigma_0} + \frac{n+1}{2\lambda} <u^n>_{\sigma_0} \]

Similarly,

\[ <u^0>_{\omega_0} = \frac{1}{2} \text{erfc}(\sqrt{\lambda} U) \]

\[ <u^1>_{\omega_0} = U <u^0>_{\omega_0} - \frac{1}{2} \frac{e^{-U^2}}{\sqrt{\pi \lambda}} \]

...

\[ <u^{n+2}>_{\omega_0} = U <u^{n+1}>_{\omega_0} + \frac{n+1}{2\lambda} <u^n>_{\omega_0} \]

In the 2-D and 3-D cases, the equilibrium state can be decomposed into the form of the 1-D case, and the above integration formula can be used too. For example, in the 3-D case we have

\[ \rho <\ldots> = \int (...) g du dv dw d\xi, \]

and

\[ <u^m v^n w^p \xi^l> = <u^m> <v^n> <w^p> <\xi^l> \]

where the integration limits can be the whole or half velocity space.
BIBLIOGRAPHY


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[31] K. Xu, *Gas-Kinetic Schemes for Fluid Simulations*, Invited Lecture at 1st International Conference on Computational Fluid Dynamics, July 9-14, 2000, Kyoto, Japan


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