A BGK-penalization based asymptotic-preserving scheme for the multispecies Boltzmann equation

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Abstract

An asymptotic preserving scheme is efficient in solving multiscale problems where kinetic and hydrodynamic regimes co-exist. In this paper we extend the BGK-penalization based asymptotic preserving scheme, originally introduced by Filbet and Jin for the single species Boltzmann equation [16], to its multispecies counterpart. For the multispecies Boltzmann equation the new difficulties arise due to: 1) the breaking down of the conservation laws for each species; 2) different convergence rates to equilibria for different species in disparate masses systems. To resolve these issues, we find a suitable penalty function – the local Maxwellian that is based on the mean velocity and mean temperature, and justify various asymptotic properties of this method. This asymptotic preserving scheme does not contain any nonlinear nonlocal implicit solver, yet can capture the fluid dynamic limit with time step and mesh size independent of the Knudsen number. Numerical examples demonstrate the correct asymptotic-behavior of the scheme.

1 Introduction

In kinetic theory, the Boltzmann equation is a fundamental equation to describe the evolution of rarefied gases. In this paper, we are interested in numerical solution of the Boltzmann equation for multispecies gas mixture. The most basic example is high altitude gas, which could be modeled as a binary mixture of Oxygen and Nitrogen. Other applications of gas mixture may come from nuclear engineering or evaporation-condensation.

One of the difficulties in numerically solving the Boltzmann equation comes from the varying Knudsen number, which describes the ratio of the mean free path over a typical length scale such as the domain size. If the Knudsen number is small, the collision term becomes numerically stiff. When using an explicit scheme, to guarantee the numerical stability, one has to resolve the small Knudsen number to avoid instability, and this causes a tremendous computational cost. On the other hand, it is very difficult to use implicit schemes because of the nonlinear and the nonlocal nature of the collision operator.

The Chapman-Enskog expansion for the Boltzmann equation yields the compressible Euler or Navier-Stokes equations in the limit of vanishing Knudsen number. Generally speaking, numerically solving the hydrodynamic system is much more efficient, so when the Knudsen number is small, one can just solve this set of equations in lower dimension. However, in zones where these macroscopic models break down, one has to come back to solve the Boltzmann equation. This domain decomposition approach has attracted a great amount of attentions [2, 3, 9, 10, 21, 24, 31, 33, 34, 40].

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main difficulty there is to determine the matching interface conditions between two different domains
in which different physical models are used.

Another approach, the one we are going to pursue in this paper, is called the asymptotic preserving
(AP) method. This method dates back to the 90s from the last century and has been widely used
in time dependent kinetic and hyperbolic systems since then. This approach looks for simple and
cheap solvers for the Boltzmann equation that can preserve asymptotic limits from the microscopic
to the macroscopic models in the discrete setting, which means that the numerical solution to the
Boltzmann equation should converge to that of the Euler equations when the Knudsen number van-
ishes. Compared with multiphysics domain decomposition methods, this framework only solves one
set of equation: the microscopic one. In the hydrodynamic regime, it becomes a robust hydrodynamic
solver automatically without resolving the small Knudsen number or switching to the macroscopic
model. As summarized by Jin [27], an AP scheme for kinetic equations should have the following
features:

• it preserves the discrete analogy of the Chapman-Enskog expansion, namely, it is a suitable
  scheme for the kinetic equation, yet, when holding the mesh size and time step fixed and letting
  the Knudsen number go to zero, the scheme becomes a suitable scheme for the limiting fluid
dynamic Euler equations;

• implicit collision terms can be implemented efficiently.

There are several variations of the AP property, including weakly-AP, relaxed-AP, and strongly-
AP, defined as follows (see [16] and also a recent review [28]):

• weakly-AP. If the data are within $O(\varepsilon)$ of the local equilibrium initially, they remain so for all
  future time steps;

• relaxed-AP. For non-equilibrium initial data, the solution will be projected to the local equilib-
  rium beyond an initial layer (after several time steps).

• strongly-AP. For non-equilibrium initial data, the solution will be projected to the local equi-
  librium immediately in one time step.

In general, the strongly-AP property is preferred, and was the designing principle of most of
the classical AP schemes [26, 5]. The relaxed-AP is a concept introduced recently in [16], which was
shown numerically to be sufficient to capture the hydrodynamic limit when the Knudsen number goes
to zero. The weakly-AP is often a necessary condition for the AP property. Many non-AP schemes
do not satisfy this property, namely solutions initially close to the local equilibrium can move away.
See discussion in [16].

Several AP schemes have recently been designed for the Boltzmann equation for monospecies.
One approach was to use the micro-macro decomposition method [35] (see its multispecies extension
in [29]), but the issue of designing an efficient implicit collision term, which is necessary for numerical
stability independent of the Knudsen number, is still unsolved. An earlier approach introduced
by Gabetta, Pareschi and Toscani uses the truncated Wild Sum for uniform numerical stability
of the collision term [18]. For a simple BGK model it was realized by Coron and Perthame in [8]
that an implicit BGK operator can be integrated explicitly, using the basic conservation properties
of the BGK operator. Utilizing this property, Filbet and Jin introduced the BGK penalization
method for the Boltzmann collision operator [16]. The main idea is to subtract the Boltzmann
operator by a BGK operator, and then add the BGK operator back. Only the latter BGK operator is
treated implicitly, while the complicated Boltzmann operator is solved explicitly. The entire scheme
is implemented explicitly, yet the numerical stability is independent of the Knudsen number and the relaxed AP property was achieved (which was verified numerically). Yan and Jin recently extended this approach to a positive and strongly-AP scheme by adding an extra relaxation step \[41\]. This BGK penalization idea, in the space homogeneous case, agrees with the Wild Sum approach \[18\], but they differ when the space is inhomogeneous. Another implementations can be found using the exponential Runge-Kutta method, see Dimarco and Pareschi \[13\], resulting a strongly AP scheme with positivity. A rigorous justification of the AP property of this methodology for hyperbolic systems with stiff relaxation was carried out recently in \[17\]. The BGK penalization method has also been extended to the Fokker-Planck-Laudau equation \[30\], the quantum Boltzmann equation \[15\], and the quantum Fokker-Planck-Landau equation \[25\].

In this article, we generalize the BGK-penalization idea of Filbet-Jin to the multispecies Boltzmann equation. Several new difficulties arise here. First there are several possible choices of the local Maxwellian and one has to determine the one that suits our needs. We found that a suitable choice is the local Maxwellian that depends on the mean velocity and mean temperature. Secondly, to justify various AP properties one needs to prove that the velocities and temperatures of different species equilibrate, a property one does not encounter for the single species Boltzmann equation. We justify this property for the proposed scheme, in the relaxed-AP sense. Finally we demonstrate that this method can also be used for gas mixtures with disparate masses, which arises in ion-electron evolution problem in plasma \[22\] \[41\] \[39\] \[6\].

This paper is organized as follows. We describe the Boltzmann equation for the multispecies system in section 2, including their theoretical properties. In section 3, we give details of the numerical scheme. This is followed by section 4 where we prove various AP properties of the scheme. In section 5, we discuss the disparate masses system. We show several numerical examples in section 6.

2 The multispecies models

2.1 The multispecies Boltzmann equation

The Boltzmann equation describes the evolution of the density distribution of rarefied gases. We use \( f_i(t, x, v) \) to represent the distribution function of the \( i \)th species at time \( t \) on the phase space \((x, v)\), and \( f = (f_1, f_2, \cdots, f_N)^T \). The Boltzmann equation for the multispecies system is given by \[13\]:

\[
\partial_t f_i + v \cdot \nabla_x f_i = Q_i(f, f), \quad t \geq 0, \quad (x, v) \in \mathbb{R}^d \times \mathbb{R}^d, \tag{2.1}
\]

with

\[
Q_i(f, f) = \sum_{k=1}^{N} Q_{ik}(f, f), \tag{2.2a}
\]

\[
Q_{ik}(f, f)(v) = \int_{S^{d-1}} \int_{\mathbb{R}^d} (f_i' f_k^* - f_i f_k^*) B_{ik}(|v - v_*|, \Omega) dv_* d\Omega, \tag{2.2b}
\]

where \( x \) is the position of the particle, \( B_{ik} \) is the collision kernel, and \( B_{ik} = B_{ki} \), (thus \( Q_{ik} = Q_{ki} \)); \( v, v_* \) are pre-collisional velocities; \( v' \) and \( v_*' \) are post-collisional velocities; \( f_i' = f_i(t, x, v') \) and \( f_k^* = f_k(t, x, v_*') \); \( \Omega \) is a unit vector, and \( S^{d-1}_+ \) is the semi-sphere defined by \( g \cdot \Omega \geq 0 \), where \( g \) is relative velocity

\[
g = v - v_*.
\]
There are many variations for the collision kernel $B_{ik}$. One of the simple cases is the Maxwell molecule when $B_{ik} = B_{ik} \left( \frac{g \cdot \Omega}{|g|} \right)$. The post-collisional velocities $v'$ and $v'_*$ satisfy:

$$v' = v - \frac{2\mu_{ik}}{m_i} (g \cdot \Omega) \Omega,$$

$$v'_* = v_* + \frac{2\mu_{ik}}{m_k} (g \cdot \Omega) \Omega,$$

with $\mu_{ik} = \frac{m_im_k}{m_i+m_k}$ being the reduced mass and $m_i$, $m_k$ being the mass for species $i$ and $k$ respectively. This deduction is based on momentum and energy conservations:

$$m_i v + m_k v_* = m_i v' + m_k v'_*,$$

$$m_i |v|^2 + m_k |v_*|^2 = m_i |v'|^2 + m_k |v'_*|^2.$$

### 2.2 Properties of the multispecies Boltzmann equation

In $d$-dimensional space, we define the macroscopic quantities for species $i$: $n_i$ is the number density; $\rho_i$ is the mass density; $u_i$ is the average velocity; $E_i$ is the total energy; $e_i$ is the specific internal energy; $T_i$ is the temperature; $S_i$ is the stress tensor; and $q_i$ is the heat flux vector, given by:

$$n_i = \int f_i dv, \quad \rho_i = m_i n_i,$$

$$\rho_i u_i = m_i \int v f_i dv,$$

$$E_i = \frac{1}{2} \rho_i u_i^2 + n_i e_i = \frac{1}{2} m_i \int |v|^2 f_i dv,$$

$$e_i = \frac{d}{2} T_i = \frac{m_i}{2n_i} \int f_i |v - u_i|^2 dv,$$

$$S_i = \int (v - u_i) \otimes (v - u_i) f_i dv,$$

$$q_i = \frac{1}{2} m_i \int (v - u_i) |v - u_i|^2 f_i dv.$$

We also have global quantities for the mixture: the total mass density $\rho$, the number density $n$, the mean velocity $\bar{u}$, the total energy $E$, the internal energy $n\bar{e}$ and the mean temperature $\bar{T} = \frac{2\bar{e}}{d}$ are defined by:

$$\rho = \sum_i \rho_i, \quad n = \sum_i n_i,$$

$$\rho \bar{u} = \sum_i \rho_i u_i,$$

$$E = n\bar{e} + \frac{1}{2} \rho |\bar{u}|^2 = \frac{d}{2} n \bar{T} + \frac{\rho}{2} |\bar{u}|^2 = \sum_i E_i.$$

### 2.2.1 Conservations

In the gas mixture system, for each species, the mass is conserved, but not the momentum and energy. This means that the first moment of the collision term is zero, but the second and the third are not. They are obtained by multiplying the collision term with $\phi = m_i \left( 1, v, \frac{1}{2} |v|^2 \right)^T$ and then integrating
with respect to \( v \). Usually explicit expressions for these moments cannot be obtained, but for some special case, for example, the Maxwell molecule, explicit expression is available:

\[
< m_i Q_i > = \int m_i Q_i(f) dv = 0,
\]

\[
< m_i v Q_i > = \int m_i v Q_i(f) dv = \sum_{k=1}^{n} 2\mu_{ik}\chi_{ik} n_i n_k [u_k - u_i],
\]

\[
< \frac{1}{2} m_i v^2 Q_i > = \int \frac{m_i}{2} [v^2 Q_i(f) dv
= \sum_{k=1}^{n} 2m_i \chi_{ik} n_i n_k \left[ \left( \frac{\mu_{ik}}{m_i} \right)^2 \left( |u_k - u_i|^2 + 2 \frac{e_k}{m_k} + 2 \frac{e_i}{m_i} \right) + \frac{\mu_{ik}}{m_i} \left( (u_k - u_i) \cdot u_i - 2 \frac{e_i}{m_i} \right) \right],
\]

where \( \chi_{ik} = \int (\cos \theta)^2 B_{ik}(\theta) d\theta \), with \( \theta = \arccos \left( \frac{g \Omega}{|g|} \right) \). One can check [20] for power law molecules.

Based on these formulas, when taking moments of the Boltzmann equation, one obtains the corresponding evolution of the macroscopic quantities. Taking the 1D Maxwell molecule for example:

\[
\partial_t \rho_i + \partial_x (\rho_i u_i) = < m_i Q_i > = 0, \quad \text{or} \quad \partial_t n_i + \partial_x (n_i u_i) = 0,
\]

\[
\partial_t (\rho_i u_i) + \partial_x (S_i + \rho_i u_i^2) = \frac{1}{\varepsilon} < m_i v Q_i > = \frac{1}{\varepsilon} \sum_{k=1}^{n} 2B_{ik} n_i n_k \mu_{ik} [u_k - u_i],
\]

\[
\partial_t E_i + \partial_x (E_i u_i + S_i u_i + q_i) = \frac{1}{\varepsilon} \frac{1}{2} m_i v^2 Q_i = \frac{1}{\varepsilon} \sum_{k=1}^{n} 2B_{ik} n_i n_k \left( \frac{\mu_{ik}^2}{m_i m_k} \right) (a + b),
\]

where \( a = (m_k u_k + m_i u_i) \cdot (u_k - u_i) \), \( b = 2(e_k - e_i) \). However, the total momentum and total energy are still conserved. By summing up the momentum and energy equations for all species, one obtains:

\[
\partial_t (\rho \bar{u}) + \partial_x \left( \sum_i S_i + \sum_i \rho_i u_i^2 \right) = \frac{1}{\varepsilon} \sum_i < m_i v_i Q_i > = 0,
\]

\[
\partial_t E + \partial_x \left( \sum_i E_i u_i + \sum_i S_i u_i + \sum_i q_i \right) = \frac{1}{\varepsilon} \sum_i < \frac{1}{2} m_i v_i^2 Q_i > = 0.
\]

These hold for all kinds of cross-sections.

### 2.2.2 The local Maxwellian

The local equilibrium is reached when the gaining part and losing part of collision terms balance out, namely \( Q_i(f) = 0 \) for each \( i \). It is given by [11]:

\[
f_i = M_i = n_i \left( \frac{m_i}{2\pi T} \right)^{d/2} e^{-m_i |v - \bar{u}|^2 / 2T},
\]

where \( T \) is the mean temperature and \( \bar{u} \) is mean velocity defined in (2.5). We call this Maxwellian the “unified Maxwellian” because the velocity \( \bar{u} \) and temperature \( T \) are given by those for the entire system instead of those for each single species.
2.2.3 The Euler limit

Expanding $f_i$ around the unified Maxwellian \ref{eq:2.9}, the standard Chapman-Enskog expansion shows that at the local equilibrium, the collision term vanishes, and the system yields its Euler limit \cite{1}:

\begin{align}
\partial_t \rho_i + \nabla \cdot (\rho_i \bar{u}) &= 0, \\
\partial_t (\rho \bar{u}) + \nabla \cdot (\rho \bar{u} \otimes \bar{u} + n \bar{T} I) &= 0, \\
\partial_t E + \nabla \cdot ((E + n \bar{T}) \bar{u}) &= 0.
\end{align} \tag{2.10}

Here $I$ is the identity matrix. Note that in the equation for $\rho_i$, we have $\bar{u}$ instead of $u_i$ as in \ref{eq:2.7}. This is because when $\varepsilon \to 0$, $u_i \to \bar{u}$ and $T_i \to \bar{T}$ for all $i$.

2.3 A BGK model

The BGK operator is a classical approximation for the Boltzmann collision operator. There are several BGK models, but most of them either suffer from the loss of positivity \cite{19}, or fail to satisfy the indifferentiability principle \cite{23}. The positivity guarantees that the distribution function is always positive, and indifferentiability requires that when different species share the same mass, equations of the system should be consistent with the single species Boltzmann equation. We choose the BGK model proposed by Andries, Aoki and Perthame \cite{1}, the one that guarantees both of these two properties.

The model reads:

\begin{align}
\partial_t f_i + v \cdot \nabla f_i = \frac{\nu_i}{\varepsilon} (\bar{M}_i - f_i), \tag{2.11}
\end{align}

with $\nu_i$ being collision frequency and $\bar{M}_i$ being a Maxwellian:

\begin{align}
\nu_i &= \sum_k n_k \chi_{ik}, \\
\bar{M}_i &= n_i \left( \frac{m_i}{2\pi T_i} \right)^{d/2} e^{-\frac{|v - u_i|^2}{2m_i T_i}}. \tag{2.12}
\end{align}

The way $\bar{M}$ is defined is to capture the moments of the collision $Q_i$, i.e. $\nu_i \left( \bar{M}_i - f_i \right)$ shares the same first five moments as $Q_i$. For the Maxwell molecule, explicit expressions are computed from \ref{eq:2.6}:

\begin{align}
\nu_i \bar{u}_i - \nu_i u_i &= \langle m_i v Q_i \rangle = \sum_{k=1}^n 2\mu_{ik} \chi_{ik} n_i n_k [u_k - u_i], \tag{2.13a} \\
\nu_i \bar{E}_i - \nu_i E_i &= \langle \frac{1}{2} m_i v^2 Q_i \rangle = \sum_{k=1}^n 2m_i \chi_{ik} n_i n_k \left[ \left( \frac{\mu_{ik}}{m_i} \right)^2 \left( |u_k - u_i|^2 + \frac{e_k}{m_k} + \frac{e_i}{m_i} \right) + \frac{\mu_{ik}}{m_i} \left( (u_k - u_i) \cdot u_i - \frac{e_i}{m_i} \right) \right], \tag{2.13b}
\end{align}

and $\bar{T}_i = \left( \frac{2\bar{E}_i - \rho_i \bar{u}_i^2}{n_i d} \right)$. Note that the right hand side of equation \ref{eq:2.13a} is just a linear operator of macroscopic velocities. Also, when $u$ is known, the right hand side of \ref{eq:2.13b} is linear on $e$. For later reference, we define a matrix $\mathbb{L}$ by:

\begin{equation}
(\mathbb{L})_{ij} = \begin{cases} 
2\mu_{ij} \chi_{ij} n_i n_j, & i \neq j, \\
-2 \sum_k \mu_{ik} \chi_{ik} n_i n_k, & i = j.
\end{cases} \tag{2.14}
\end{equation}
Apparently, \( L \) is a symmetric matrix with each row summing up to 0, and all non-diagonal entries are positive. Since \( L \) is a symmetric weakly diagonally dominant matrix, it is semi-negative definite, i.e. all its eigenvalues are non-positive. Under this definition, equation (2.13a) turns out to be \( \nu_i \rho_i \tilde{u}_i - \nu_i \rho_i u_i = Lu \). For later convenience, we denote \( \lambda(M) \) the spectral radius of matrix \( M \):

\[
\lambda(M) = \sup_i (|\lambda_i(M)|),
\]

(2.15)

where \( \lambda_i(M) \) are eigenvalues of \( M \).

We also mention another type of Maxwellian, which is defined by macroscopic quantities \( u_i \) and \( T_i \) for each species. We call it the “species Maxwellian”:

\[
M_i = n_i \left( \frac{m_i}{2\pi T_i}\right)^{d/2} e^{-\frac{m_i |v-u_i|^2}{2 T_i}}.
\]

(2.16)

Remark 1. \( M_i - f_i \) can not be used as a BGK operator. In the multispecies system, one has to introduce some mechanism into the collision term that captures the interactions between species. \( M_i - f_i \) gives no communication between the species, so it cannot be used to express the multispecies collision.

3 An AP scheme for the multispecies Boltzmann equation

In this chapter, we derive our AP scheme for the multispecies Boltzmann equation. Our idea is based on the BGK-penalization method proposed by Filbet and Jin [16].

3.1 The time discretization

Here we adopt the same strategy and write our scheme as:

\[
\frac{f_i^{l+1} - f_i^l}{\Delta t} + v \cdot \nabla_x f_i^l = Q_i(f_i^l) - P_i(f_i^l) + \frac{P_i(f_i^{l+1})}{\varepsilon}.
\]

(3.1)

The superscript \( l \) stands for the time step. Later we will use \( Q_i^l \triangleq Q_i(f_i^l), P_i^l \triangleq P_i(f_i^l) \) for convenience. \( P_i \) is chosen to be the BGK operator:

\[
P_i = \beta(M_i - f_i),
\]

(3.2)

where \( \beta \) is a positive constant chosen for stability and positivity, see section 3.4. A simple algebraic manipulation on (3.1) gives:

\[
f_i^{l+1} = \frac{\varepsilon f_i^l + \Delta t (Q_i^l - \beta (M_i^{l} - f_i^l)) - \varepsilon \Delta t v \cdot \nabla_x f_i^l + \beta^{l+1} \Delta t M_i^{l+1}}{\varepsilon + \beta^{l+1} \Delta t}.
\]

(3.3)

The computation of the collision term \( Q_i \) and the flux term \( v \cdot \nabla_x f \) is relatively classical and will be given later; \( M_i \) is defined in (2.9); and the choice of \( \beta \) is also going to be presented below.
3.2 The computation of $M^{l+1}$

Taking moments of (3.1), one gets:

$$n^l_{i} + 1 = n^l_i - \Delta t \int v \cdot \nabla_x f^l_i \, dv,$$

$$(\rho \bar{u})^l_{i+1} = (\rho \bar{u})^l_i - \Delta t \sum_i m_i \int v \otimes v \nabla_x f^l_i \, dv,$$

$$E^l_{i+1} = E^l_i - \Delta t \sum_i \frac{m_i}{2} |v|^2 v \cdot \nabla_x f^l_i \, dv,$$

and by the definition of $\bar{T}$ in (2.5c),

$$\bar{T}^l_{i+1} = \frac{2E^l_{i+1} - (\rho \bar{u}^2)^l_{i+1}}{dn^l_{i+1}}.$$

The discretization of the flux term will be discussed in section 3.5.

3.3 The collision term $Q$

We use the spectral method introduced in [38] to compute the collision term $Q_i$. Use a ball $B(0, S)$ to represent the domain of the compactly supported distribution $f$. Then we periodize $f$ on $v \in [-L, L]^d$ with $L \geq (3 + \sqrt{2})S$. $L$ is chosen much larger than $S$ to avoid non-physical collision at different periods of the periodized $f$. Define the Fourier transform as:

$$\hat{f}(x; p) = \int f(x; v) e^{-ip \cdot v} \, dv,$$

$$f(x; v) = \frac{1}{(2L)^d} \sum_p \hat{f}(x; p) e^{ik \cdot v}. \quad (3.4)$$

Plugging into the collision term (2.2b):

$$Q_{ik} = \iint B_{ik} \left[ f'_i f'_{k^*} - f_i f_{k^*} \right] \, dv_s d\Omega \equiv Q^+_{ik} - f_i Q^-_{ik},$$

where we define the gaining part and losing part as:

$$Q^+_{ik} = \iint B_{ik} \left( f'_i f'_{k^*} \right) \, dv_s d\Omega, \quad f_i Q^-_{ik} = \iint B_{ik} \left( f_i f_{k^*} \right) \, dv_s d\Omega = f_i \iint B_{ik} f_{k^*} \, dv_s d\Omega.$$

Using the Fourier transform (3.4), one gets:

$$Q^+_{ik} = \iint \frac{B_{ik}}{(2L)^d} \left[ \sum_p \sum_q \hat{f}_i(x; p) e^{ip \cdot v'} \hat{f}_k(x; q) e^{iq \cdot v'} \right] \, dv_s d\Omega.$$

For easier computation, one can rewrite equations (2.3) to:

$$v' = v - \frac{\mu_{ik}}{m_i} (g - |g| \omega), \quad v'_s = v_s + \frac{\mu_{ik}}{m_k} (g - |g| \omega) = v - g + \frac{\mu_{ik}}{m_k} (g - |g| \omega).$$

Note the domain for $\omega$ is the entire unit sphere $S^{d-1}$ instead of the semi-sphere for $\Omega$. Then:

$$Q^+_{ik} = \frac{1}{(2L)^d} \sum_{p,q} \hat{f}_i \hat{f}_k \iint B_{ik} e^{i(p \cdot v' + q \cdot v')} \, dv_s \, d\omega$$

$$= \frac{1}{(2L)^d} \sum_{p,q} \hat{f}_i \hat{f}_k \iint B_{ik} e^{i\lambda \cdot v + i|g| \gamma \omega} \, dv_s \, d\omega,$$
where \( \lambda = \frac{-m_k}{m_i+m_k} p + \frac{-m_k}{m_i+m_k} q \) and \( \gamma = \frac{m_k}{m_i+m_k} p - \frac{m_k}{m_i+m_k} q \). Given a specific \( B_{ik} \) one can analytically compute the integration above. The expression, however, can be very tedious, even in one dimensional space, especially when \( B_{ik} \) depends on \(|g|\). Note that the integration domain for \( g \) is not symmetric. But for the 1D Maxwell molecule, \( B_{ik} \) is a constant, and can be pulled out of the integral, making the computation much easier. We show examples for the 1D Maxwell molecule and leave other situations for further discussions. In this case,

\[
\begin{align*}
v' &= v - \frac{2m_k}{m_i+m_k} (v - v_s) = \frac{m_i - m_k}{m_i + m_k} v + \frac{2m_k}{m_i + m_k} v_s, \\
v' &= v + \frac{m_i - m_k}{m_i + m_k} (v - v_s) = \frac{2m_i}{m_i + m_k} v - \frac{m_i - m_k}{m_i + m_k} v_s.
\end{align*}
\]

Plugging in \( Q_{ik}^+ \), one gets:

\[
Q_{ik}^+ = \frac{B_{ik}}{(2L)^2} \sum_{p,q} \hat{f}_k^p \hat{f}_k^q e^{i \left( \frac{m_i-m_k}{m_i+m_k} p + \frac{2m_i}{m_i+m_k} q \right) v} \int e^{i \left( \frac{2m_k}{m_i+m_k} p - \frac{m_i-m_k}{m_i+m_k} q \right) v_s} dv_s.
\]

One can also write \( Q_{ik}^+ \) as a summation of its Fourier modes \( Q_{ik}^+(v) = \frac{1}{(2L)^2} \sum_l \hat{Q}_{ik}^l e^{ilv} \) where

\[
\hat{Q}_{ik}^l = \int Q_{ik}^+ e^{-ilv} dv
= \frac{B_{ik}}{(2L)^2} \sum_{p,q} \hat{f}_k^p \hat{f}_k^q \int e^{i \left( \frac{m_i-m_k}{m_i+m_k} p + \frac{2m_i}{m_i+m_k} q - l \right) v} \int e^{i \left( \frac{2m_k}{m_i+m_k} p - \frac{m_i-m_k}{m_i+m_k} q \right) v_s} dv_s
= B_{ik} \sum_{p,q} \hat{f}_k^p \hat{f}_k^q \text{sinc}(a) \text{sinc}(b),
\]

where \( a = \left( \frac{m_i-m_k}{m_i+m_k} p + \frac{2m_i}{m_i+m_k} q - l \right) L \), and \( b = \left( \frac{2m_k}{m_i+m_k} p - \frac{m_i-m_k}{m_i+m_k} q \right) L \). The FFT and the inverse FFT are used to speed up the computation.

The computation for \( f_l Q_{ik}^- \) is much simpler in this special case: \( f_l Q_{ik}^- = f_l \int B_{ik} f_k dv_k = f_l m_k B_{ik} \).

After getting all \( Q_{ik} \), \( Q_i = \sum_k Q_{ik} \).

### 3.4 The choice of the free parameter \( \beta \)

\( \beta \) should be chosen as the maximum value of the Frechet derivative \( \nabla Q_i(f) \) [16]. Numerically, to guarantee positivity, one can split the collision \( Q \) into the gaining part and the losing part \( Q_i = Q_i^+ - f_i Q_i^- \) by \( Q_i^+ = \sum_k Q_{ik}^+ \) and \( f_i Q_i^- = f_i \sum_k Q_{ik}^- \). Plug back in the scheme \( (3.3) \), one can rearrange the scheme:

\[
f_i^{l+1} = \frac{\varepsilon (f_i^l - \Delta t v \cdot \nabla x f_i^l) + \Delta t Q_i^+(f^l) + \left[ (\beta^l - Q_i^-(f^l)) f_i^l + \beta^l+1 M_i^{l+1} - \beta^l M_i^l \right] \Delta t}{\varepsilon + \beta^l+1 \Delta t}.
\]

To obtain positivity, it is sufficient to require the followings for all \( i \) [11]:

\[
\beta^l > Q_i^-(f^l), \quad \beta^l M_i^l > \beta^{l-1} M_i^{l-1}.
\]
3.5 The flux term $v \cdot \nabla_x f_i$

Here we give the numerical flux in 1D. Use $v \partial_x f_{i,j}$ to denote the flux term for species $i$ at the grid point $x_j$. A shock-capturing finite volume method we use is [36]:

$$v \partial_x f_{i,j} = \nu(f_{i,j} - f_{i,j-1}) - \frac{1}{2} \nu(\text{sgn}(\nu) - \nu)(h \sigma_{i,j} - h \sigma_{i,j-1}),$$

(3.6)

where $\nu = \frac{v}{h}$, $h$ is the mesh size. $j_1$ is chosen to be $j$ for $v > 0$ and $j + 1$ for $v < 0$. $\sigma_{i,j}$ is the slope limiter. For the van Leer limiter, it takes value as $\phi(\theta) = \frac{\theta + |\theta|}{\theta + 1}$ and $\theta_{i,j} = \frac{f_{i,j} - f_{i,j-1}}{f_{i,j+1} - f_{i,j}}$ reflects the smoothness around grid point $x_j$.

The discretization for the flux term in higher dimension uses the dimension-by-dimension approach.

4 The AP property of the time discretization

The time discrete scheme (3.1) is written as:

$$f_{i}^{l+1} - f_{i}^{l} + v \cdot \nabla_x f_{i}^{l} = \frac{Q_{i}^{l} - \beta(M_{i}^{l} - f_{i}^{l}) + \beta(M_{i}^{l+1} - f_{i}^{l+1})}{\varepsilon}.$$  

(4.1)

We will show below that this method is weakly-AP for the Maxwell molecule, and relaxed-AP for the BGK model given in section 2.3. Below we always assume that $\Delta t \gg \varepsilon$. Besides the definition for the linear operator $L$ in (2.14) and $\lambda(M)$ in (2.15), we also define:

$$\delta u_{i}^{l} = u_{i}^{l} - \bar{u}^{l}, \quad \delta T_{i}^{l} = T_{i}^{l} - \bar{T}^{l},$$  

(4.2)

and

$$\mathbb{D} = \begin{bmatrix} \rho_{1} & 0 & \ldots & 0 \\ 0 & \rho_{2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \ldots & \ldots & \rho_{N} \end{bmatrix}.$$  

(4.3)

4.1 Weakly-AP

Lemma 4.1. For the Maxwell molecule, if $\delta u_{i}^{l} = O(\varepsilon)$ and $\delta T_{i}^{l} = O(\varepsilon)$ for $\forall i$, then $\delta u_{i}^{l+1} = O(\varepsilon)$ and $\delta T_{i}^{l+1} = O(\varepsilon)$.

Proof. Rewrite scheme (4.1) as:

$$f_{i}^{l+1} - M_{i}^{l+1} = \frac{\varepsilon(-M_{i}^{l+1} + M_{i}^{l}) - \varepsilon \Delta t v \cdot \nabla_x f_{i}^{l}}{\varepsilon + \beta \Delta t} + \frac{\Delta t Q_{i}^{l}}{\varepsilon + \beta \Delta t} - \left(M_{i}^{l} - f_{i}^{l}\right).$$

(4.4)

Take the first moment on both sides. On the left hand side, one gets $(\rho_i u_i)^{l+1} - (\rho_i \bar{u})^{l+1}$, while on the right hand side, the first term is $O(\varepsilon)$. The second term gives:

$$\frac{\Delta t}{\varepsilon + \beta \Delta t} < m_i v Q_{i}^{l} > = \frac{\Delta t}{\varepsilon + \beta \Delta t} \sum_{k} 2 \chi_{ik} \mu_{ik} n_{i} n_{k} [u_{k}^{l} - u_{i}^{l}]$$

(4.5)

$$= \frac{\Delta t}{\varepsilon + \beta \Delta t} \sum_{k} 2 \chi_{ik} \mu_{ik} n_{i} n_{k} (\delta u_{k}^{l} - \delta u_{i}^{l}) = O(\varepsilon).$$
The third term gives:

\[ < m_i v (\overline{M}_i^l - f_i^l) > = \rho_i (\bar{u}^l - u_i^l) = O(\varepsilon). \]

So the entire right hand side is of \( O(\varepsilon) \), thus the term on the left hand side, \((\rho_i u_i)^{l+1} - (\rho_i \bar{u})^{l+1} = O(\varepsilon)\), i.e. \( \delta u_i^{l+1} = O(\varepsilon) \). Similar analysis can be carried out for \( T \).

\[ \square \]

**Remark 2.** In the proof, we used that the collision kernel is for the Maxwell molecule in (4.5). The proof can be extended to other collision kernels as long as one can show the moments of \( Q \) is of \( O(\varepsilon) \) whenever \( \delta u = O(\varepsilon) \).

**Theorem 4.1.** The method is weakly-AP; namely, if \( \overline{M}_i^l - f_i^l = O(\varepsilon) \), then \( \overline{M}_i^{l+1} - f_i^{l+1} = O(\varepsilon) \).

**Proof.** Since \( \overline{M}_i^l - f_i^l = O(\varepsilon) \), both \( P_i(f^l) \) and \( Q_i(f^l) \) are of \( O(\varepsilon) \). Plugging back into the scheme (4.4), one gets \( f_i^{l+1} - \overline{M}_i^{l+1} = O(\varepsilon) \).

\[ \square \]

### 4.2 Relaxed-AP

**Lemma 4.2.** For the Maxwell molecules, when \( \Delta t \ll 1 \), in the limit of \( \varepsilon \to 0 \), there \( \exists L \), such that \( \forall l > L, \delta u^l = O(\varepsilon) \), given big enough \( \beta \).

**Proof.** We prove the result for the 1D case. The proof for higher dimension can be carried out similarly. The proof follows that of [16]. One can take moments of numerical scheme (4.1):

\[
\frac{(\rho u)^{l+1} - (\rho u)^l}{\Delta t} + \partial_x \int v^2 m f^{l+1} dv = \frac{1}{\varepsilon} \left( L^l u^l + \beta^l D^l \delta u^l - \beta^{l+1} D^{l+1} \delta u^{l+1} \right),
\]

\[
\Rightarrow (\varepsilon + \beta^{l+1} \Delta t) D^{l+1} \delta u^{l+1} = \left( (\varepsilon + \beta^l \Delta t) D^l + \Delta t L^l \right) \delta u^l + \varepsilon \left( (\rho \bar{u})^l - (\rho u)^{l+1} \right) - \varepsilon \Delta t \partial_x \int v^2 m f^{l+1} dv,
\]

\[
\Rightarrow (\varepsilon + \beta^{l+1} \Delta t) \left( D^l + O(\Delta t) \right) \delta u^{l+1} = \left[ (\varepsilon + \beta^l \Delta t) D^l + \Delta t L^l \right] \delta u^l + O(\varepsilon),
\]

where \( L^l \bar{u} = 0 \) and \( D^{l+1} = D^l + O(\Delta t) \) were used.

After some simple algebra, one can rewrite the previous equation as:

\[
\delta u^{l+1} = \left[ \frac{\beta^l}{\beta^{l+1} + \frac{1}{\beta^{l+1}} (D^l)^{-1} L^l + O(\Delta t)} \right] \delta u^l + O(\varepsilon).
\]

Define \( A_u \) as:

\[
A_u = \left[ \frac{\beta^l}{\beta^{l+1} + \frac{1}{\beta^{l+1}} (D^l)^{-1} L^l + O(\Delta t)} \right].
\]

(4.6)

Since the eigenvalues for \( L \) are non-positive, if one chooses \( \beta^{l+1} + \beta^l > \lambda((D^l)^{-1} L^l) \), given small enough \( \Delta t, |\lambda(A_u)| < 1 \), thus in the limit of \( \varepsilon \to 1 \), \( \delta u \) would decrease to \( O(\varepsilon) \), and we get our conclusion.

\[ \square \]

The same analysis can be carried out for \( T \). We call this property proved above “macro-AP”.

**Remark 3.** The proof above is also valid for the BGK model in section 2.3. It can also be extended to other kinds of collision kernel, but the corresponding \( L \) may not be linear on \( u \), and the requirement on \( \beta \) may not have an explicit expression. In that case, one needs to define \( \lambda(L) \) as the spectrum of the nonlinear operator \( L \).
Theorem 4.2. If the problem is macro-AP, then, \( \exists L \) such that \( \forall l > L, M_l^i - \overline{M}_l^i = O(\varepsilon) \), and \( \overline{M}_l^i - M_l^i = O(\varepsilon) \).

Proof. It is a straightforward conclusion from the lemma above, and from the definition for \( \tilde{M} \) in (2.12).

Remark 4. Up to now, we have shown that \( M_i \) approaches to \( \overline{M}_i \) for the Boltzmann collision operator with the Maxwell molecule collision kernel. Rearranging scheme (4.1), one gets:

\[
    f^{l+1} - \overline{M}^{l+1} = \frac{(\varepsilon + \beta \Delta t)(f^l - \overline{M}^l) + \Delta t Q^l}{\varepsilon + \beta \Delta t} + \frac{\varepsilon(M^l - \overline{M}^l + 1)}{\varepsilon + \beta \Delta t} - \varepsilon \Delta t \nu \cdot \nabla_x f^l.
\]

(4.7)

The second term on the right is of \( O(\varepsilon) \). So, one can get relaxed-AP only if it can be shown that \( Q \) and \( f - \overline{M} \) have opposite signs. We can prove this for limited form of \( Q \), say the BGK operator introduced in section 2.3. Later in section 6 we will show that numerically the scheme is relaxed-AP for the general Boltzmann collision defined in (2.2).

Theorem 4.3. The scheme is relaxed-AP for the BGK operator \( Q = \nu(\tilde{M} - f) \) defined in section 2.3.

Proof. Plug in the definition for \( Q \), (4.7) writes:

\[
    f^{l+1} - \overline{M}^{l+1} = \frac{\varepsilon + \beta \Delta t - \nu \Delta t}{\varepsilon + \beta \Delta t} (f^l - \overline{M}^l) + \frac{\nu \Delta t (\overline{M}^l - \overline{M}^l)}{\varepsilon + \beta \Delta t} + O(\varepsilon)
\]

The second equality comes from Theorem 4.2 and Remark 3. Define:

\[
    \alpha = \frac{\varepsilon + \beta \Delta t - \nu \Delta t}{\varepsilon + \beta \Delta t},
\]

(4.8)

and we call it the convergent rate to the unified Maxwellian \( \overline{M} \). In the limit of \( \varepsilon \to 0 \), if one has \( \beta > \frac{\nu}{2} \), then \( |\alpha| < 1 \), thus \( |f - \overline{M}| \) keeps diminishing until reaching to \( O(\varepsilon) \), and we get the relaxed-AP.

5 Disparate masses

This section is for the system of gas mixture with disparate masses in the space homogeneous case. The mathematical problem was first pointed out by Grad [22], and has attracted great interests since then. The fundamental example is plasma, for which, the basic derivation can be found in [39, 4]. For these systems, it is the different time scalings for different species to reach to the equilibria that makes the problem difficult. Generally speaking, the light species should be able to get to the equilibrium faster, that is to say there is a time period when the light species is in hydrodynamic regime while the heavy species is, on the other hand, in kinetic regime. Analyses of the scalings of the collision operators have been done based on both postulate physical consideration [7, 32] and formal derivation [11, 12].
5.1 Theoretical rescaling analysis

In homogeneous space, the disparate masses system should be written as:

\[
\begin{align*}
\partial_t f_H &= Q_H = Q_{HH} + Q_{HL} = \int B_{HH}(f'_H f_H^* - f_H f_{H*}) \, dv_s + \int B_{HL}(f'_H f_L^* - f_H f_{L*}) \, dv_s, \\
\partial_t f_L &= Q_L = Q_{LL} + Q_{LH} = \int B_{LL}(f'_L f_L^* - f_L f_{L*}) \, dv_s + \int B_{LH}(f'_L f_H^* - f_H f_{L*}) \, dv_s.
\end{align*}
\] (5.1)

Now the small parameter that makes the collision term stiff is the ratio of mass \( \varepsilon = \sqrt{m_L/m_H} \) where the subindices \( H \) and \( L \) stand for heavy and light respectively. While assuming that the two species have densities and temperatures of the same order of magnitude, one could obtain that \( f_H \) is much narrower than \( f_L \) as shown in Figure 5.1. To analyze the magnitude of the collision terms, we define \( \tilde{f}_H(v) = f_H(\varepsilon v) \) to stretch \( f_H \) to a function that has comparable variance as \( f_L \). As derived in [11, 12], the scaling ratio of the two collision terms is \( Q_H/Q_L = O(\varepsilon) \), which means that the collision \( Q_L \) has stronger effect, and that the light species gets to the hydrodynamical regime much faster.

For convenience, we write both \( Q_H \) and \( Q_L \) as \( O(1) \) term, and put \( \varepsilon \) in front of \( Q_H \) to represent its magnitude. The system turns out to be:

\[
\begin{align*}
\partial_t f_H &= \varepsilon Q_H, \\
\partial_t f_L &= Q_L.
\end{align*}
\] (5.2)

One can also rescale the time by \( \tau \) and obtain:

\[
\begin{align*}
\partial_t f_H &= \frac{\varepsilon}{\tau} Q_H, \\
\partial_t f_L &= \frac{1}{\tau} Q_L.
\end{align*}
\] (5.3)

When \( \tau = O(\varepsilon) \), the light species is in hydrodynamic regime but the heavy one is still in kinetic regime; and when \( \tau = O(\varepsilon^2) \), both species should be close to the equilibria.

Remark 5. The inhomogeneous problem gets even harder to analyze, especially when the different species have different spatial rescaling coefficients. But numerically it makes very little difference: one simply needs to add the flux term \( v \cdot \nabla_x f \) to the homogeneous scheme.
5.2 The numerical scheme

The scheme we adopt for (5.2) is:

\[
\begin{align*}
\frac{f_{l,H}^{l+1} - f_{l,H}^l}{\Delta t} &= \frac{\varepsilon}{\tau} \left( Q_{l,H}^l - \beta \left( M_{l,H}^l - f_{l,H}^l \right) \right) + \frac{\beta \varepsilon}{\tau} \left( M_{H}^{l+1} - f_{H}^{l+1} \right), \\
\frac{f_{l,L}^{l+1} - f_{l,L}^l}{\Delta t} &= \frac{1}{\tau} \left( Q_{l,L}^l - \beta \left( M_{l,L}^l - f_{l,L}^l \right) \right) + \frac{\beta}{\tau} \left( M_{L}^{l+1} - f_{L}^{l+1} \right),
\end{align*}
\]

(5.4a) (5.4b)

where \( \beta = O(1). \)

**Theorem 5.1.** This scheme yields the following behavior at: \( O(\frac{1}{\varepsilon}) \) and \( O(\frac{1}{\varepsilon^2}) \).

- at \( \tau = O(\frac{1}{\varepsilon}) \), the scheme is first order consistent to \( \partial_t f_H = Q_H \), and \( f_L^l \) is an \( O(\varepsilon) \) approximation of \( \overline{M}_L \);
- at \( \tau = O(\frac{1}{\varepsilon^2}) \), both \( f_H^l \) and \( f_L^l \) are within \( O(\varepsilon) \) of the unified Maxwellians \( \overline{M}_H \) and \( \overline{M}_L \) respectively.

**Proof.** To prove the second statement:

At this time scale, \( \tau = O(\varepsilon^2) \), the system turns out to be:

\[
\begin{align*}
\partial_t f_H &= \frac{1}{\varepsilon} Q_H, \\
\partial_t f_L &= \frac{1}{\varepsilon^2} Q_L.
\end{align*}
\]

By the same arguments as in the previous sections, one gets:

\[
\begin{align*}
f_H^l - \overline{M}_H^l &= O(\varepsilon), \\
f_L^l - \overline{M}_L^l &= O(\varepsilon^2).
\end{align*}
\]

for \( l \) large enough.

To prove the first statement:

At this time scale, \( \tau = O(\varepsilon) \), system (5.3) can be written as:

\[
\begin{align*}
\partial_t f_H &= Q_H, \\
\partial_t f_L &= \frac{1}{\varepsilon} Q_L.
\end{align*}
\]

The scheme still gives \( f_L^l \rightarrow \overline{M}_L^l \). One just needs to show that the scheme gives a correct discretization of the equation for \( f_H \) too. Write (5.4a) as (set \( \tau = \varepsilon \)):

\[
\frac{f_{H}^{l+1} - f_{H}^l}{\Delta t} = Q_{H}^l - \beta (M_{H}^l - f_{H}^l) + \beta (M_{H}^{l+1} - f_{H}^{l+1}).
\]

Rearrange it, one gets:

\[
\frac{f_{H}^{l+1} - f_{H}^l}{\Delta t} = Q_{H}^l - \frac{\beta \Delta t}{1 + \beta \Delta t} Q_{H}^l + \frac{\beta}{1 + \beta \Delta t} \left( M_{H}^{l+1} - M_{H}^l \right).
\]

The second and the third terms on the right are both of order \( \Delta t \), i.e. the scheme gives a first order discretization to \( \partial_t f_H = Q_H \).

\[\square\]
6 Numerical examples

For comparison, the examples chosen are similar to those in [29]. We also perturb the data on the level of macroscopic quantities. For all the examples below: when \( \varepsilon \) is not very small so that solving the Boltzmann equation is still possible by using the basic explicit scheme with a resolved mesh, we compare our numerical results to those of the forward Euler, and when \( \varepsilon \) is unbearably small for the forward Euler, we compare our results to its Euler limit. To solve the Euler equations, we used the CLAWPACK Euler solver [37].

6.1 A stationary shock

In this example, we show numerical solution to a Riemann problem of two species. The analytical solution to the Euler equations is a stationary shock. Here the subscripts 1 and 2 stand for different species.

\[
\begin{align*}
m_1 &= 1, m_2 = 1.5, n_1 = n_2 = 1, u_1 = 1.8, u_2 = 1.3, T_1 = 0.3, T_2 = 0.35, & \text{if } x < 0; \\
m_1 &= 1, m_2 = 1.5, n_1 = n_2 = 1.401869, u_1 = u_2 = 1.07, T_1 = T_2 = 0.8605, & \text{if } x > 0.
\end{align*}
\]

The initial distribution for \( f \) is given by summation of two Gaussian functions, so it is far away from the unified Maxwellian \( M \):

\[
f(t = 0) = \sum_{i=1}^{2} A_i e^{-B_i(v-C_i)^2},
\]

where

\[
B_1 = B_2 = \frac{\rho}{4E - 2p\varepsilon^2(1 + \kappa^2)}, \quad A_1 = A_2 = \frac{n}{2} \sqrt{\frac{B_1}{\pi}} \quad \text{and} \quad C_1 - u = u - C_2 = \kappa u,
\]

i.e. the two Gaussian functions have the same height and variation, but their centers are \( 2\kappa u \) away from each other. In the numerical experiment, we choose \( \kappa = 0.2, \Delta x = 10^{-2} \) and \( \Delta t \) is chosen to satisfy the CFL condition: \( 10^{-3} \) in our simulation. Numerically we check whether the scheme gives the Euler limit when \( \varepsilon \) goes to zero; and whether it matches well with the forward Euler method with relatively fine mesh when \( \varepsilon \) is big. We first show in Figure 7.1 that as \( \varepsilon \) goes to zero, the numerical solution converges to the Euler limit, the stationary shock in this case. In Figure 7.2 we show that the AP scheme matches very well with the numerical results given by the forward Euler method for \( \varepsilon = 10^{-1} \). Then we show in Figure 7.3 that given an initial data far away from the unified Maxwellian \( M \), \( f \) gets close to \( M \) quickly with \( \varepsilon = 10^{-5} \). This verifies that the scheme is relaxed-AP numerically. Figure 7.4 shows that smaller \( \varepsilon \) gives faster convergence to the equilibria for macroscopic quantities.

6.2 A sod problem

In this example, we solve a Sod problem. The initial data are given by:

\[
\begin{align*}
m_1 &= m_2 = 1, n_1 = 1, n_2 = 1.2, u_1 = 0.6, u_2 = -0.5, T_1 = T_2 = 0.709, & \text{if } x < 0; \\
m_1 &= m_2 = 1, n_1 = 0.125, n_2 = 0.2, u_1 = -0.2, u_2 = 0.125, T_1 = T_2 = 0.075, & \text{if } x > 0.
\end{align*}
\]

The initial distribution is also given by (6.1) and (6.2) with \( \kappa = 0.2 \). For all \( \varepsilon \), we choose \( \Delta x = 10^{-2} \) and \( \Delta t = 10^{-3} \). In this problem, \( m_1 = m_2 \), so we first show the numerical indifferentiability in Figure 7.5 that is: computing the problem as a multispecies system gives the same result as computing the monospecies Boltzmann equation. In Figure 7.6 we show that as \( \varepsilon \) goes to zero, the numerical solution converges to the Euler limit. For \( \varepsilon \) as big as \( 10^{-1} \) and \( 10^{-2} \), we compare the results with those of the forward Euler with a fine mesh. They match well as shown in Figure 7.7. In Figure 7.8

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we show that for $\varepsilon = 10^{-4}$, although the initial $f$ is far away from the unified Maxwellian $M$, as time evolves, it converges to $M$. This numerically verifies the relaxed-AP property. In Figure 7.9, we show the evolution of $u$ with different $\varepsilon$. Apparently different species gradually share the same velocity, and the smaller $\varepsilon$ is, the faster the convergence is.

6.3 A disparate masses problem

In this example, we solve the disparate masses system. Define $\varepsilon = \sqrt{\frac{m_L}{m_H}}$, we want to verify that the light species gets close to the unified Maxwellian $M_L$ faster than the heavy one. We solve an inhomogeneous problem with the following initial data:

$m_H = 8, \quad m_L = 0.08, \quad u_H = 0, \quad u_L = 0.5, \quad T_H = T_L = 2.5, \quad n_H = 1, n_L = 1.2.$

The initial distribution functions are still given by the summation of two Gaussians as in (6.1), with parameters $A_1 = A_2$ and $B_1 = B_2$ defined in (6.2), and $C_1$ and $C_2$ defined by: $C_1 - u = u - C_2 = \kappa$. We choose $\kappa = 0.5$ for the heavy species and $\kappa = 4$ for the light one. In Figure 7.10 on the left we show the initial distribution functions for the two species, both of which are given by summation of two Gaussian functions and are far away from the Maxwellian. On the right we show several snapshots of the distribution functions as they evolve. In Figure 7.11, we show that as time evolves, the velocities converge toward each other. Note that the heavy species weighted more when computing for the mean velocity $\bar{u}$ as in (2.5b), thus its average velocity does not change much.

7 Conclusion

Motivated by the work of Filbet-Jin [16], we use an appropriate BGK operator that is defined by the common velocity and common temperature to penalize the stiff collision operator for multispecies Boltzmann equation, which yields an asymptotically preserving scheme. This scheme can capture the Euler limit with mesh size and time step independent of the Knudsen number, thus is suitable for simulating the multispecies Boltzmann equation efficiently in both the kinetic and fluid regimes. The BGK penalization allows one to avoid inverting the nonlinear Boltzmann collision operator in the fluid regime. This approach is also applied to system of gas mixture with disparate masses. Numerical results were used to demonstrate the validity of the scheme.

In the future we will extend and verify numerically this method to the case of more general collision kernels, and in higher space dimension.

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Figure 7.1: The Stationary Shock problem. As $\varepsilon \to 0$, solution of the Boltzmann equation goes to the Euler limit. $t = 0.1$.

Figure 7.2: The Stationary Shock Problem. $\varepsilon = 0.1$, $t = 0.1$. The dashed line is given by the AP scheme, and the solid line is given by the forward Euler with a fine mesh: $\Delta x = 0.01$ and $\Delta t = 0.0005$. 
Figure 7.3: The Stationary Shock Problem. $\varepsilon = 10^{-5}$, $\delta f = f_1 - \overline{M}_1$ diminishes as time evolves.

Figure 7.4: The Stationary Shock problem. $u_1$ and $u_2$ at $x = -0.5$ on the left and $T_1, T_2$ on the right, as functions of time, for $\varepsilon = 10^{-2}$ and $10^{-5}$ respectively. Note the different time scales for the two figures.
Figure 7.5: The Sod problem. Indifferentiability. \( t = 0.1 \). \( \rho \), \( u \) and \( T \) are computed using two species model ("o") and one species model (".").

Figure 7.6: The Sod problem. \( t = 0.1 \). As \( \varepsilon \to 0 \), the numerical results go to the Euler limit. Solid lines give the Euler limit computed by using [37].
Figure 7.7: The Sod problem. $t = 0.1$. For $\varepsilon = 0.1, 0.01$, we compare the results of the AP scheme, given by the circled lines, and the results of the forward Euler with a fine mesh, given by the solid lines.

Figure 7.8: The Sod problem. $\varepsilon = 10^{-4}$. $\delta f = f_1 - \overline{M}_1$. 

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Figure 7.9: The Sod problem. The three figures show velocities $u_1$ and $u_2$ at $x = -0.3$ as functions of time for $\varepsilon = 0.1, 0.01,$ and $10^{-5}$ respectively. Note different time scales for three figures.

Figure 7.10: The disparate masses problem. The left figure shows the initial distributions and the right figure shows the time evolutions of $f_H$ and $f_L$. $f_H$ is put at the top and $f_L$ is at the bottom. At $t = 0.007$, $f_L$ is close to $\bar{M}_L$ while $f_H$ is still far away from the equilibrium. Note the different scales for $v$. 
Figure 7.11: The disparate masses problem. The velocities for the two species converge to each other.

References


[28] ——, Asymptotic preserving (AP) schemes for multiscale kinetic and hyperbolic equations: a review, Lecture Notes for Summer School on “Methods and Models of Kinetic Theory” (M&MKT), Porto Ercole (Grosseto, Italy), June 2010.


