

Year-4 Progress Report on Numerical Methods for BGK-Type Kinetic Equations

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Abstract

This Year-Four progress report presents ongoing research, supported by subcontracts from Oak Ridge National Laboratory (ORNL), on the design and analysis of numerical methods for multi-species kinetic equations. Rather than summarizing only recent developments, this cumulative report builds upon prior work and serves as a resource for training new graduate students and postdoctoral researchers. Three new sections have been added. First, a comprehensive chapter on the multi-species Boltzmann equation addresses gaps in the literature and offers a modern, pedagogical introduction to this fundamental kinetic framework. Second, we introduce a novel iterative solver for moment equations derived from the space-homogeneous multi-species BGK model, laying the groundwork for more advanced numerical solvers. Third, we provide an overview of the Ellipsoidal Statistical BGK (ES-BGK) model, which improves upon the basic BGK model by better capturing fluid dynamics in the Navier–Stokes and Euler limits. The report also reviews recent progress on the numerical solution of BGK-type kinetic equations, highlighting the challenges posed by high-dimensional phase space, nonlocal particle interactions, and numerical stiffness. To address these, we describe strategies including high-order finite volume methods, implicit-explicit (IMEX) time integrators, adaptive multi-level methods, discrete velocity schemes, and moment-based approaches. Preliminary implementations are developed in MATLAB for prototyping, with plans to migrate to modern production software. The report concludes with a summary of achieved milestones and outlines directions for future work, particularly in developing robust solvers for the ES-BGK model.

Key words: Boltzmann equation, BGK and ES-BGK approximations, multi-species BGK and ES-BGK models, finite volume schemes, MUSCL methods, numerically stiff equations, implicit-explicit time stepping strategies, discrete velocity methods, Runge–Kutta methods, moment equations, asymptotic relaxation.

Contents

Executive Summary	2
0.1 Milestones	3
1 Introduction and Report Organization	5
1.1 The Unary Boltzmann Equation	6
1.2 The BGK Approximation Model	7
1.3 Organization	10
1.4 Disclaimer	11
2 Multi-Species Boltzmann Equations	12
2.1 The Binary Collision Transformation	12
2.2 The Boltzmann Collision Operator	16
2.3 Collision Invariants	22
2.4 Information, Entropy, and Boltzmann's H-Theorem	27
2.5 Moments and Moment Equations	35
2.6 The Maxwellian and Maximal Entropy States	39
2.7 Space-Homogeneous Model	46
3 Single-Species BGK Kinetic Models	48
3.1 Basic Properties of Solutions	48
3.1.1 Collision Invariants	49
3.1.2 Space-Homogeneous Problem	53
3.1.3 The H-Theorem	55
3.2 Discrete-Velocity BGK Models	59
3.2.1 Discrete-Velocity BGK Model in One Space Dimension	59
3.2.2 Space-Homogeneous Discrete-Velocity Model	67

4	Numerics for the Single-Species BGK Model	70
4.1	Finite Volume Space and Velocity Discretization	70
4.2	Implicit-Explicit Runge–Kutta Time Stepping	74
4.3	Fully Discrete Scheme	76
4.4	Poisson Solver for Vlasov–Poisson–BGK Equation	77
4.5	Sample Computations and Accuracy Tests	79
5	Discrete-Velocity Numerical Methods for the Single-Species BGK Problem	92
5.1	A Fully Explicit Scheme	92
5.2	An Explicit Scheme for the Space-Homogeneous Case	95
5.3	An Implicit Scheme for the space-homogeneous Case	97
6	Multi-Species BGK Equations	100
6.1	Formulation and Properties	100
6.2	Numerical Approximation	104
7	Asymptotic Relaxation and Numerics of Multi-Species Moment Equations	106
7.1	Model Equations	107
7.1.1	Model Properties	108
7.1.2	Moment Equations	109
7.2	Properties of the ODE system	111
7.2.1	Positivity of the Temperature	111
7.2.2	Velocity Bounds	113
7.2.3	Existence and Uniqueness	114
7.3	Long-time Behavior	116
7.3.1	Null Spaces of $D - A$, Z , $F - B$, and $\hat{Z}$	118
7.3.2	Velocity Relaxation Proof	118
7.3.3	Energy Relaxation Proof	120
7.3.4	Temperature Relaxation	122
7.4	Numerical Confirmation of Theory	123
7.5	A Novel Nonlinear GST Iterative Solver	127
7.5.1	Sod problem with two identical species	128
7.5.2	Three Species Mixture: Ar–Kr–Xe	130
7.6	Conclusions	133

8	ES-BGK Models and Numerics	135
8.1	Introduction	135
8.2	Single-Species ES-BGK Model – A First Look	135
8.2.1	Model Overview	136
8.2.2	Conservation Laws and Moment ODE System	137
8.2.3	Numerical Time Update in Semi-Implicit Setting	138
8.3	Single-Species ES-BGK Model Fluid Limits	140
8.4	Numerical Demonstration of Implicit-Explicit Numerical Method	146
8.5	Multi-Species Models	149
8.5.1	Multi-Species BGK Model	149
8.5.2	Multi-Species ES-BGK Model	151
8.5.3	Multi-Species ES-BGK Model – Restricted Tensor Expression	156
8.5.4	Multi-Species ES-BGK Model – General Tensor Expression	160
9	Progress Summary and Next Steps	165
9.1	Summary	165
9.2	Next Steps	166
	Acknowledgements	168
A	An Important Integral	169
B	Picard–Lindelöf Theorem	171
C	Bounding the Eigenvalues of Z and $\hat{Z}$	172
D	Null Space Components of $\widetilde{W}$ and $\widetilde{\xi}$	174
E	1x1v Prototype Code	175
E.1	Main Driver: vlasovPoissonBGKMain.m	175
E.2	vlasovPoissonBGKSolver.m	182
E.3	BGKCollision.m	186
E.4	divFlux.m	189
E.5	slopeReconstruction.m	191
E.6	minMod.m	192
E.7	sodSoln.m	193
E.8	pStarSolve.m	195

F Bibliography

196

Executive Summary

In this Year-Four progress report we describe our research, which has been supported by subcontracts from Oak Ridge National Laboratory (ORNL), on the design and analysis of numerical methods for multi-species kinetic equations. Like the last progress report, we have decided to build upon our last progress report rather than to draft a new, separate document that merely summarizes the work done since the last. This cumulative document can be—and is now being, to good effect—used in the training of new graduate students and post doctoral researchers that join the project.

We have added three new import chapters/sections to the report. First, we add a new chapter that reviews the multi-species Boltzmann equation. This material is fundamental since all kinetic models, essentially, must conform to the same basic theoretical framework that holds for the Boltzmann system. Many of the details for the multi-species Boltzmann equation, which are taken for granted in the literature, are, in fact, difficult to find in existing textbooks. It has been our experience that many of the classic works that are cited and assumed to contain the theory and development of the multi-species Boltzmann equation, do not, in fact, give a clear, modern introduction. We sought to remedy the situation herein, or, at least, we have made an earnest attempt to do so.

Second, we report, for the first time, on a new iterative solver for the moment equations for multi-species BGK model in the space-homogeneous setting. The multi-species BGK model is an important approximate model for the Boltzmann system, in some ways the simplest. Our new solver is expected to be a springboard for sophisticated numerical solvers for the full multi-species BGK and ES-BGK models.

Third, and finally, regarding the latter model, we have added a new chapter outlining some facts about the Ellipsoidal Statistical BGK (ES-BGK) model. The ES-BGK model adds some approximation capabilities that are missing from the simple BGK models. In particular, it can more accurately capture the Navier–Stokes and Euler equations in the appropriate fluid limits.

After the new chapter on the multi-species Boltzmann equation, we review the basic unary BGK model, which is the simplest approximation model for the Boltzmann equation.

Specifically, we review some work on the numerical solution of single- and multi-species BGK-type kinetic equations of particle transport. Such equations model the motion of fluid particles via a density field when the kinetic theory of rarefied gases must be used in place of the continuum limit Navier–Stokes and Euler equations.

The Boltzmann and BGK-type equations (and kinetic models, more generally) describe a fluid in terms of phase space variables, and, in three space dimensions, require 6 independent phase-space variables (3 for space and 3 for velocity) for each species for accurate simulation. This requires sophisticated numerical algorithms and efficient code to realize predictions over desired space and time scales. In particular, stable numerical methods must be designed to handle potential discontinuities (shocks) and rarefaction waves in the solutions coming from conservative advection terms and, in addition, numerical stiffness owing to diffusive particle collision terms. Furthermore, the particle interaction terms are nonlocal in nature, adding yet another layer of complexity, and the interaction length scales of the nonlocal terms may be orders of magnitude different, when multiple particle species are involved.

In this report, we outline strategies for generating efficient and stable numerical algorithms and code, including the use of (i) stable high-order finite volume methods, (ii) fully implicit and implicit-explicit (IMEX) time integration techniques, (iii) adaptive time-phase-space multi-level methods, (iv) discrete velocity methods, and (v) moment equation methods. The preliminary codes, which will be demonstrated herein, are built in the commercial software package MATLAB for quick and easy prototyping, but will later be translated into production software using modern open languages.

At the end of this report, we provide a quick overview of the ES-BGK models, both unary and multi-species. These are almost as simple as the BGK models but add a few more parameters that help to make the resulting approximations more accurate. In particular, we discuss how these models better capture the fluid limits (Navier–Stokes and Euler equations) as the collision frequency becomes large. We will describe some ideas about future work involving numerical solvers for the ES-BGK models in this report.

We conclude the report with a full summary of work-goals that have been accomplished and what we think will be important for the future.

0.1 Milestones

There are four major milestones of this research effort that we would like to highlight.

1. This year (2025), we published

E. Habbershaw, R.S. Glasby, J.R. Haack, C.D. Hauck, and S.M. Wise, *Asymptotic Relaxation of Moment Equations for a Multi-species, Homogeneous BGK Model*, SIAP (SIAM J. Appl. Math.) 85 (2025) 294–313.

<https://doi.org/10.1137/23M1596314>

This paper, which appears in the prestigious *SIAM Journal on Applied Mathematics*, described long-time dynamics of the moment equations for the multi-species BGK model. Understanding these model characteristics are vital for designing and implementing sophisticated numerical approximation methods.

2. In the same year, we published

E. Habbershaw, C.D. Hauck, and S.M. Wise, *Implicit Update of the Moment Equations for a Multi-Species, Homogeneous BGK Model*, SINUM (SIAM J. Numer. Anal.) 63 (2025) 881–907.

<https://doi.org/10.1137/24M165421X>

This paper, which appears in the equally prestigious *SIAM Journal on Numerical Analysis*, described our novel iteration solver for the moment equations for the multi-species, spatially homogeneous BGK model. We prove several facts about our numerical solver therein, including stability, well-posedness and convergence. This iterative solver will be the basis of future sophisticated solvers for the full multi-species BGK and ES-BGK models that we are developing.

3. We have graduated one PhD student from the project. Evan Habbershaw officially graduated in August 2025, defending the thesis *Numerical Methods for Multi-Species Kinetic Models with Approximate Collision Operators*. Dr. Habbershaw is now a post-doctoral researcher at the Pennsylvania State University and a co-author of this report.
4. We have recently recruited two new UTK Math graduate students to work on this project, Jack Haight and Daniel Bond. And, we have developed a training infrastructure, based in part on this evolving document and also a new graduate course that Prof. Wise has developed in the UTK Mathematics Department called *Non-Equilibrium Thermodynamics*. The course will run for the first time in Spring Semester 2026.

Chapter 1

Introduction and Report Organization

The Navier–Stokes and Euler equations, with which most computational fluid dynamicists are intimately familiar, are used to describe the evolution of a fluid under the assumption that the constituent particles move in, essentially, lock-step motion. In other words, fluid particles with small space separation are assumed to have nearly identical velocity vectors. We refer these models as the fluid limits, or continuum limits.

To be precise, suppose that the mean free path (diffusion length scale) of particles is denoted λ , and the characteristic spatial size of the problem is denoted L . The *Knudsen number* is defined as $K_n = \lambda/L$. When $K_n \ll 1$, the diffusion length scale is too small to resolve accurately, and, in fact, the individual motions and interactions of constituent particles can be coarse-grained (averaged out) without significant loss of fidelity [44]. Indeed, the Navier–Stokes equation, which is applicable in this physical regime, is a highly successful and accurate model.

However, when $K_n = \mathcal{O}(1)$, the Navier–Stokes equation is no longer valid, and particle collisions/interactions must be taken into account. Particles with small space separation could move in entirely contrary directions, and, in this regime, the Boltzmann transport equation is an important model of particle evolution [44]. It describes the distribution of particles as a function of time, space ($d = 3$ dimensions), and velocity ($d = 3$ dimensions). The three dimensions of space and three dimensions of velocity comprise what is known as *phase space*. The Boltzmann equation is complicated not only by the high dimensionality of phase space but also the highly nonlinear, highly nonlocal nature of the collision (particle interaction) operator.

1.1 The Unary Boltzmann Equation

The *Vlasov–Boltzmann equation* for a single-species dilute gas is given as follows:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{a} \cdot \nabla_{\mathbf{v}} f = Q[f, f](\mathbf{x}, \mathbf{v}, t), \quad (1.1)$$

where f is the density of particles at position $\mathbf{x}$ with velocity $\mathbf{v}$ at time t ; and $\mathbf{a}$ is a particle acceleration determined by an external field, for example, an electric or magnetic field. The *Boltzmann transport equation* results from setting $\mathbf{a} \equiv \mathbf{0}$. The derivation of the equation is a straightforward exercise using the chain rule. In particular, the total time derivative of the distribution f can be realized as

$$\begin{aligned} \frac{d}{dt} f(\mathbf{x}, \mathbf{v}, t) &= \sum_{i=1}^d \frac{\partial f}{\partial x_i} \frac{dx_i}{dt} + \sum_{i=1}^d \frac{\partial f}{\partial v_i} \frac{dv_i}{dt} + \frac{\partial f}{\partial t} \\ &= \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{a} \cdot \nabla_{\mathbf{v}} f + \frac{\partial f}{\partial t}, \end{aligned}$$

where $d = 3$ for the standard model. Thus, the Vlasov–Boltzmann equation may be constructed via the following law: the total time rate of change of the distribution is equal to the collision (frequency) operator. In other words,

$$\frac{d}{dt} f(\mathbf{x}, \mathbf{v}, t) = Q[f, f](\mathbf{x}, \mathbf{v}, t).$$

The *Boltzmann collision operator*, $Q[f, f]$, requires much more physical insight for a clear derivation [44], involving certain conservation principles, in particular. Therefore, we will content ourselves by only stating its generic form in three dimensions for the moment:

$$Q[f, f](\mathbf{x}, \mathbf{v}, t) = \frac{1}{m} \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} [f' f'_* - f f_*] B(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) d\boldsymbol{\sigma} d\mathbf{v}_*,$$

where

$$\begin{aligned} f' &:= f(\mathbf{x}, \mathbf{v}', t), & f'_* &:= f(\mathbf{x}, \mathbf{v}'_*, t), \\ f &:= f(\mathbf{x}, \mathbf{v}, t), & f_* &:= f(\mathbf{x}, \mathbf{v}_*, t); \end{aligned}$$

m is the mass of an individual particle; B is the collision kernel describing binary collisions between particles; $\boldsymbol{\sigma}$ is a unit vector called the apse direction; and the primed coordinates are

computed via the transformation

$$\mathbf{v}' = \mathbf{v} - \boldsymbol{\sigma} \cdot (\mathbf{v} - \mathbf{v}_*), \quad (1.2)$$

$$\mathbf{v}'_* = \mathbf{v}_* + \boldsymbol{\sigma} \cdot (\mathbf{v} - \mathbf{v}_*). \quad (1.3)$$

The computation of the Boltzmann collision operator is very expensive. For the 3D case, the (5 dimensional) integral must be computed at every value of $(\mathbf{x}, \mathbf{v})$ in phase space. Additionally, the integral cannot be evaluated analytically, except for the simplest of cases (e.g., Maxwell molecules, with carefully prepared initial conditions). Thus, computation of the collision operator is usually the most expensive part of computing numerical solutions of the Boltzmann equation. For this reason, Monte Carlo (MC) methods are generally preferred over direct numerical simulation [36]. Unfortunately, MC methods are slow to converge, as is well known. What is worse, for the N -species case, there are N^2 collision operators that must be considered. Thus, a simpler, less costly BGK-type approximation is often implemented. BGK stands for the names Bhatnagar, Gross, and Krook, who introduced the approximation in 1954 [2], and we now explain this methodology.

1.2 The BGK Approximation Model

The *Vlasov–BGK equation* is a model derived by approximating the Boltzmann collision operator with a simpler nonlinear, nonlocal relaxation operator of the form

$$Q^{BGK}[f](\mathbf{x}, \mathbf{v}, t) = \lambda(M_f(\mathbf{x}, \mathbf{v}, t) - f(\mathbf{x}, \mathbf{v}, t)), \quad (1.4)$$

where $\lambda = \frac{1}{\tau}$ is the collision frequency between particles, $\tau > 0$ is a characteristic time, and M_f is the *Maxwellian*, which is constructed using the first three integral moments of f ,

$$n(\mathbf{x}, t) := \int_{\mathbb{R}^d} f \, d\mathbf{v}, \quad \mathbf{u}(\mathbf{x}, t) := \frac{1}{n} \int_{\mathbb{R}^d} f \mathbf{v} \, d\mathbf{v}, \quad \theta(\mathbf{x}, t) := \frac{m}{nd} \int_{\mathbb{R}^d} f |\mathbf{v} - \mathbf{u}|^2 \, d\mathbf{v}, \quad (1.5)$$

and is defined as

$$M_f(\mathbf{x}, \mathbf{v}, t) := M[f](\mathbf{x}, \mathbf{v}, t) := n \left(\frac{m}{2\pi\theta} \right)^{d/2} \exp \left(-\frac{m|\mathbf{v} - \mathbf{u}|^2}{2\theta} \right). \quad (1.6)$$

The space-time fields n , $\mathbf{u}$, and θ , are the macroscopic (coarse grained) number density, bulk velocity, and temperature, respectively. The following macroscopic variables are also of

interest: the (kinetic) energy density is given by

$$\omega(\mathbf{x}, t) := \frac{m}{2} \int_{\mathbb{R}^d} f |\mathbf{v}|^2 d\mathbf{v}, \quad (1.7)$$

and the internal energy density is defined as

$$e(\mathbf{x}, t) := \frac{m}{2} \int_{\mathbb{R}^d} f |\mathbf{v} - \mathbf{u}|^2 d\mathbf{v}. \quad (1.8)$$

We observe that the temperature and the internal energy are related via

$$\theta(\mathbf{x}, t) = \frac{2}{d} \frac{e(\mathbf{x}, t)}{n(\mathbf{x}, t)}.$$

Using the BGK approximation drastically reduces the computational cost of the simulation of dilute gases, and recovers both equilibrium and streaming behavior of the Boltzmann equation in collision-dominated, and collision-free limits. The BGK collision operator also satisfies conservation and entropy properties of the Boltzmann operator, as we show below. Of course, the basic design and principle of the BGK approximation is that the density, f , should relax over time toward the Maxwellian, and, clearly, at this state, the collision operator gives a zero contribution.

However, the BGK collision operator does not capture some important properties. First, it fails to capture the correct Prandtl number (essentially the ratio of viscosity to thermal conductivity), largely because the collision rate is velocity independent. As a result, the model may not agree with the compressible Navier–Stokes Equations that are derived from the Boltzmann equation in high collision regimes. A number of generalizations of the BGK model have been proposed to deal with this shortcoming. These include the ES-BGK [21] and Shakov [41] models, which incorporate extra degrees of freedom. The model of Mieussens and Struchtrup [31] incorporates a velocity dependent collision rate, which improves the capture of the correct Prandtl number. These models give a more physically realistic model, but cause a substantial increase to computational costs.

To summarize, the single-species Vlasov–BGK equation has the form

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{a} \cdot \nabla_{\mathbf{v}} f = \lambda (M_f(\mathbf{x}, \mathbf{v}, t) - f(\mathbf{x}, \mathbf{v}, t)), \quad (1.9)$$

and, in analogy to the previous setting, the *single-species BGK equation* results from setting $\mathbf{a} \equiv \mathbf{0}$. When, in equation (1.9), the acceleration is determined by an electric field, according

to the model

$$\mathbf{a}(\mathbf{x}, t) = -\chi \nabla_{\mathbf{x}} \Phi(\mathbf{x}, t),$$

where $\chi > 0$ is a constant, and

$$-\Delta \Phi(\mathbf{x}, t) = n(\mathbf{x}, t),$$

the resulting model is known as the *Vlasov–Poisson–BGK equation*.

Numerical methods for the BGK family of equations have been proposed and analyzed extensively. The discretization of phase space is costly, and there are challenges that occur in high-collision regimes. First, the BGK operator becomes stiff as the collision frequency becomes large, so an implicit approach is desired for this term, to avoid unacceptably small time steps. In a seminal paper [9], it was shown that a Backward Euler step could be applied in an explicit manner, allowing stable time stepping for a wide range of collisional regimes. Taking advantage of this, the paper [36] introduced an implicit-explicit (IMEX) Runge–Kutta scheme based on [33], treating the convection term explicitly and the collision term implicitly. Second, stable and accurate high-order conservation schemes are required for the convection terms. For example, Pieraccini and Puppo [36] use a high-order weighted essentially non-oscillatory (WENO) finite volume scheme, though high-order flux-limited schemes perform well, as we show, and are easily scaled to higher dimensions.

Most of the numerical schemes for the BGK equation, including the one that we focus on here from [36], lose the exact conservation of mass, momentum and energy at the discrete level, and, additionally, the entropy dissipation at the discrete level. This shortcoming is overcome in the work by Mieussens [29, 30]. Exact conservation is obtained by computing a discrete equilibrium function, which requires the solution of a nonlinear system of 5 equations for the BGK model and a nonlinear system of 10 equations for the ES-BGK model at each grid point in space. Another challenge is to recover consistent numerical solutions of the Euler and Navier–Stokes Equations for compressible flows, which can be derived from the BGK model using a Chapman–Enskog expansion [44].

In some situations, an explicit treatment of the advection terms in the BGK equation—even while giving the collision operator an implicit treatment—can lead to a method that requires excessively small time steps for stability and accuracy [12]. This can happen when there are long time scales that lead to incompressible equations in the high collision limit, or in problems for which the maximum velocity in the computational domain is significantly larger than the fluid speed of sound. A fully implicit approach can be taken to address these issues. This is common for time dependent kinetic equations in radiation transport contexts, and has

been considered for electron transport problems [12]. Fully implicit methods for dilute gases and collisionless plasmas have been proposed in [12]. These approaches use sophisticated iterative methods to manage the cost and memory requirements of the implicit update.

1.3 Organization

In Chapter 2, we give a fairly in-depth review of the multi-species Boltzmann equation. Our review is more thorough than most we have found in the literature, and it contains many details that are missing from the textbooks. We find that this overview is especially important for understanding aspects of our BGK-type approximations that come later, since those approximations inherit many of the properties of the original system.

In this progress report, some background for BGK-type models is presented. We do not conduct an extensive review of the models and literature but give the reader (especially those unfamiliar with kinetic equations) a gentle, albeit brief, introduction. In Chapter 3 we introduce the single-species BGK Equation. We describe some basic theory, deriving conservation and (mathematical) entropy dissipation properties.

Finite volume implicit-explicit (IMEX) Runge–Kutta (RK) numerical methods are presented in Chapter 4. We give some preliminary simulation results for basic problems, including the Sod shock tube benchmark and two-stream instability. In Chapter 5 we describe some numerical methods based on discrete-velocity models, which were described earlier in Chapter 3.

In Chapter 6, we give a brief introduction to multi-species BGK models in order to explain some numerical challenges for such equations. Chapter 7 describes asymptotic dynamics of the space-homogeneous multi-species BGK equation. In this chapter, we also summarize our recent numerical analysis for this model.

In Chapter 8 we describe a preliminary analysis of the Ellipsoidal Statistical BGK (ES-BGK) model, both unary and multi-species types.

The ES-BGK models can more accurately capture realistic Prandtl numbers of gases than the simpler BGK-type models. As a consequence, they provides more accurate hydrodynamic limits (Navier–Stokes–Fourier system) than the standard BGK models. At the same time, ES-BGK models retains the computational tractability of their BGK relatives.

We conclude the report with a brief summary of preliminary work and near and long-term future work in Chapter 9.

Several appendices are included that contain tedious calculations that we wished to keep out of the main text. A prototype $1x1v$ MATLAB code for the Sod shock tube problem is

contained in Appendix E.

1.4 Disclaimer

The information in this report has been collected from several sources. We have done our best to make certain that all of the important works have been appropriately cited. Some information in this report may be inaccurate. There are very likely many inadvertent typos and transcription errors. While we have done our best to check all of the claims, proofs, and equations, this report has not undergone external review. We have provided some sample codes in this report. We make no claims about the accuracy of those codes. They should be used at the risk of the reader and are provided for educational purposes only. Neither The University of Tennessee nor Oak Ridge National Laboratory can be held responsible for decisions made based on information in this report or the output from the codes in the appendix.

Chapter 2

Multi-Species Boltzmann Equations

Our primary objective in this document is to model the interaction of dilute mixtures of particles (gas mixtures). The most accurate kinetic model for such mixtures is a multi-species Boltzmann system, which we will now try to understand. Typically, the direct approximation of multi-species Boltzmann equations is intractable. We will ultimately turn to BGK-type approximations of the Boltzmann models, but we must understand some aspects of the Boltzmann model in order to effectively design and use the approximations.

In compiling the material for this chapter, we have found the thesis by Marlies Pirner [37] especially useful. The books [6, 19] also have short, readable descriptions of the multi-species Boltzmann system. The book by Kremer [28] has a fairly in-depth and modern account of the multi-species Boltzmann equation, and the notes by Alberto Bressan [5] were helpful in understanding the basics of the unary Boltzmann model as well as its mathematical analysis.

2.1 The Binary Collision Transformation

Definition 2.1.1. Let $m_i, m_j > 0$ be the masses of particles of species i and j , respectively, $i, j \in \{1, 2, \dots, N\}$. Fix a unit vector $\sigma \in \mathbb{S}^2$. The transformation $T_{\sigma}^{ij}(\mathbf{v}, \mathbf{v}_*) = (\mathbf{v}', \mathbf{v}'_*)$, which maps $\mathbb{R}^3 \times \mathbb{R}^3$ into $\mathbb{R}^3 \times \mathbb{R}^3$, is defined via

$$\mathbf{v}' = \mathbf{v} - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2m_j}{m_i + m_j} \sigma, \quad (2.1)$$

$$\mathbf{v}'_* = \mathbf{v}_* + [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2m_i}{m_i + m_j} \sigma. \quad (2.2)$$

We will write

$$\mathbf{v}' = T_{\sigma,1}^{ij}(\mathbf{v}, \mathbf{v}_*) \quad \text{and} \quad \mathbf{v}'_* = T_{\sigma,2}^{ij}(\mathbf{v}, \mathbf{v}_*)$$

for the first and second components of the transformation, respectively. The mapping $T_{\sigma}^{i,j}$ is called a **binary collision transformation** and σ is called the **apse direction**. The un-primed coordinates $\mathbf{v}$ and $\mathbf{v}_*$ are called the **pre-collision velocities** and the primed coordinates $\mathbf{v}'$ and $\mathbf{v}'_*$ are called the **post-collision velocities**.

Proposition 2.1.2. Let $m_i, m_j > 0$ be the masses of particles of species i and j , respectively, $i, j \in \{1, 2, \dots, N\}$, and fix an apse direction $\sigma \in \mathbb{S}^2$. Suppose that $(\mathbf{v}', \mathbf{v}'_*) = T_{\sigma}^{i,j}(\mathbf{v}, \mathbf{v}_*)$. Then,

$$m_i \mathbf{v} + m_j \mathbf{v}_* = m_i \mathbf{v}' + m_j \mathbf{v}'_*, \quad (2.3)$$

$$\frac{m_i}{2} |\mathbf{v}|^2 + \frac{m_j}{2} |\mathbf{v}_*|^2 = \frac{m_i}{2} |\mathbf{v}'|^2 + \frac{m_j}{2} |\mathbf{v}'_*|^2. \quad (2.4)$$

Furthermore,

$$\sigma \cdot (\mathbf{v}' - \mathbf{v}'_*) = -\sigma \cdot (\mathbf{v} - \mathbf{v}_*) \quad (2.5)$$

and

$$|\mathbf{v}' - \mathbf{v}'_*| = |\mathbf{v} - \mathbf{v}_*|. \quad (2.6)$$

Proof. To get (2.3) add m_i times (2.1) to m_j times (2.2), and the result immediately follows. To get (2.4), square both (2.1) and (2.2) to obtain

$$\begin{aligned} |\mathbf{v}'|^2 &= |\mathbf{v}|^2 - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{4m_j}{m_i + m_j} \sigma \cdot \mathbf{v} + [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)]^2 \frac{4m_j^2}{(m_i + m_j)^2}, \\ |\mathbf{v}'_*|^2 &= |\mathbf{v}_*|^2 + [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{4m_i}{m_i + m_j} \sigma \cdot \mathbf{v}_* + [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)]^2 \frac{4m_i^2}{(m_i + m_j)^2}. \end{aligned}$$

Then,

$$\begin{aligned} m_i |\mathbf{v}'|^2 + m_j |\mathbf{v}'_*|^2 &= m_i |\mathbf{v}|^2 + m_j |\mathbf{v}_*|^2 \\ &\quad - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{4m_i m_j}{m_i + m_j} \sigma \cdot \mathbf{v} + [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{4m_i m_j}{m_i + m_j} \sigma \cdot \mathbf{v}_* \\ &\quad + [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)]^2 \frac{4m_i m_j^2}{(m_i + m_j)^2} + [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)]^2 \frac{4m_i^2 m_j}{(m_i + m_j)^2} \\ &= m_i |\mathbf{v}|^2 + m_j |\mathbf{v}_*|^2 \\ &\quad - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)]^2 \frac{4m_i m_j}{m_i + m_j} \\ &\quad + [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)]^2 \frac{4m_i m_j}{(m_i + m_j)^2} (m_i + m_j) \\ &= m_i |\mathbf{v}|^2 + m_j |\mathbf{v}_*|^2. \end{aligned}$$

The proofs of identities (2.5) and (2.6) are left as simple exercises. ■

Proposition 2.1.3. *Let $m_i, m_j > 0$ be the masses of particles of species i and j , respectively, $i, j \in \{1, 2, \dots, N\}$, and fix an apse direction $\sigma \in \mathbb{S}^2$. Then, T_σ^{ij} is a linear transformation, that is,*

$$T_\sigma^{ij}(\alpha(\mathbf{v}, \mathbf{v}_*) + \beta(\mathbf{w}, \mathbf{w}_*)) = \alpha T_\sigma^{ij}(\mathbf{v}, \mathbf{v}_*) + \beta T_\sigma^{ij}(\mathbf{w}, \mathbf{w}_*), \quad (2.7)$$

for all $\alpha, \beta \in \mathbb{R}$ and all $\mathbf{v}, \mathbf{w}, \mathbf{v}_*, \mathbf{w}_* \in \mathbb{R}^3$. Furthermore,

$$(\mathbf{v}, \mathbf{v}_*) = T_\sigma^{ij}(T_\sigma^{ij}(\mathbf{v}, \mathbf{v}_*)), \quad (2.8)$$

for all $\mathbf{v}, \mathbf{v}_* \in \mathbb{R}^3$. In other words,

$$I = T_\sigma^{ij} \circ T_\sigma^{ij}, \quad (2.9)$$

or, equivalently,

$$(T_\sigma^{ij})^{-1} = T_\sigma^{ij}. \quad (2.10)$$

Proof. The linearity of T_σ^{ij} is a simple demonstration and is left to the reader. To prove the identity (2.8), observe that

$$\begin{aligned} & T_{\sigma,1}^{ij}(T_\sigma^{ij}(\mathbf{v}, \mathbf{v}_*)) \\ &= \mathbf{v} - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2m_j}{m_i + m_j} \sigma \\ &\quad - \left[\sigma \cdot \left(\mathbf{v} - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2m_j}{m_i + m_j} \sigma - \mathbf{v}_* - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2m_i}{m_i + m_j} \sigma \right) \right] \frac{2m_j}{m_i + m_j} \sigma \\ &= \mathbf{v} - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2m_j}{m_i + m_j} \sigma \\ &\quad - \left[\sigma \cdot \left((\mathbf{v} - \mathbf{v}_*) - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2(m_i + m_j)}{m_i + m_j} \sigma \right) \right] \frac{2m_j}{m_i + m_j} \sigma \\ &= \mathbf{v} - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2m_j}{m_i + m_j} \sigma \\ &\quad - [\sigma \cdot ((\mathbf{v} - \mathbf{v}_*) - 2[\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \sigma)] \frac{2m_j}{m_i + m_j} \sigma \\ &= \mathbf{v} - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2m_j}{m_i + m_j} \sigma + [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2m_j}{m_i + m_j} \sigma \\ &= \mathbf{v}. \end{aligned}$$

A similar calculation shows that

$$T_{\sigma,2}^{ij}(T_\sigma^{ij}(\mathbf{v}, \mathbf{v}_*)) = \mathbf{v}_*.$$

■

Proposition 2.1.4. *Let $m_i, m_j > 0$ be the masses of particles of species i and j , respectively, $i, j \in \{1, 2, \dots, N\}$, and fix an apse direction $\sigma \in \mathbb{S}^2$. Then,*

$$T_{\sigma,1}^{ij}(\mathbf{v}_*, \mathbf{v}) = T_{\sigma,2}^{ji}(\mathbf{v}, \mathbf{v}_*), \quad (2.11)$$

$$T_{\sigma,2}^{ij}(\mathbf{v}_*, \mathbf{v}) = T_{\sigma,1}^{ji}(\mathbf{v}, \mathbf{v}_*). \quad (2.12)$$

Proof. Let $\mathbf{v}, \mathbf{v}_* \in \mathbb{R}^3$ be arbitrary. Then,

$$\begin{aligned} T_{\sigma,1}^{ij}(\mathbf{v}_*, \mathbf{v}) &= \mathbf{v}_* - [\sigma \cdot (\mathbf{v}_* - \mathbf{v})] \frac{2m_j}{m_i + m_j} \sigma \\ &= \mathbf{v}_* + [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2m_j}{m_i + m_j} \sigma \\ &= T_{\sigma,2}^{ji}(\mathbf{v}, \mathbf{v}_*). \end{aligned}$$

Similarly,

$$\begin{aligned} T_{\sigma,2}^{ij}(\mathbf{v}_*, \mathbf{v}) &= \mathbf{v} + [\sigma \cdot (\mathbf{v}_* - \mathbf{v})] \frac{2m_i}{m_i + m_j} \sigma \\ &= \mathbf{v} - [\sigma \cdot (\mathbf{v} - \mathbf{v}_*)] \frac{2m_i}{m_i + m_j} \sigma \\ &= T_{\sigma,1}^{ji}(\mathbf{v}, \mathbf{v}_*). \end{aligned}$$

■

Proposition 2.1.5. *Let $m_i, m_j > 0$ be the masses of particles of species i and j , respectively, $i, j \in \{1, 2, \dots, N\}$, and fix an apse direction $\sigma \in \mathbb{S}^2$. Suppose that $f : \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{R}$ is integrable, that is,*

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |f(\mathbf{v}, \mathbf{v}_*)| \, d\mathbf{v} d\mathbf{v}_* < \infty.$$

Then, $f \circ T_{\sigma}^{ij} : \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{R}$ is integrable, and

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} f(\mathbf{v}, \mathbf{v}_*) \, d\mathbf{v} d\mathbf{v}_* = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} f(T_{\sigma}^{ij}(\mathbf{v}, \mathbf{v}_*)) \, d\mathbf{v} d\mathbf{v}_*. \quad (2.13)$$

Proof. This follows from the standard change of variable formula and the fact that $T_{\sigma}^{ij}(\mathbf{v}, \mathbf{v}_*)$ is a linear transformation with the property that

$$|\det(T_{\sigma}^{ij})| = 1.$$



2.2 The Boltzmann Collision Operator

Definition 2.2.1. Let $m_i, m_j > 0$ be the masses of particles of species i and j , respectively, $i, j \in \{1, 2, \dots, N\}$. Suppose that $f_i, f_j : \mathbb{R}^3 \rightarrow [0, \infty)$ are integrable kinetic distributions. The **general binary i, j collision operator** is defined as

$$Q_{i,j}[f_i, f_j](\mathbf{v}) := \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{j,*} - f_i f_{j,*}] B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) d\boldsymbol{\sigma} d\mathbf{v}_*, \quad (2.14)$$

where

$$\begin{aligned} f'_i &:= f_i(\mathbf{x}, \mathbf{v}', t), & f'_{j,*} &:= f_j(\mathbf{x}, \mathbf{v}'_*, t), \\ f_i &:= f_i(\mathbf{x}, \mathbf{v}, t), & f_{j,*} &:= f_j(\mathbf{x}, \mathbf{v}_*, t); \end{aligned}$$

and the primed coordinates are given precisely by the transformation

$$(\mathbf{v}', \mathbf{v}'_*) = T_{\boldsymbol{\sigma}}^{i,j}(\mathbf{v}, \mathbf{v}_*).$$

$B_{i,j} : \mathbb{R}^3 \times \mathbb{S}^2 \rightarrow [0, \infty)$ is the **collision kernel**, and we say that $B_{i,j}$ has **proper structure** iff

1. for all $i, j \in \{1, 2, \dots, N\}$, for all $\boldsymbol{\sigma} \in \mathbb{S}^2$ and all $\mathbf{w} \in \mathbb{R}^3$,

$$B_{i,j}(\mathbf{w}, \boldsymbol{\sigma}) = b_{i,j}(|\mathbf{w} \cdot \boldsymbol{\sigma}|, |\mathbf{w}|), \quad (2.15)$$

2. and, for $i \neq j$,

$$\frac{1}{m_i} B_{i,j}(\mathbf{w}, \boldsymbol{\sigma}) = \frac{1}{m_j} B_{j,i}(\mathbf{w}, \boldsymbol{\sigma}), \quad (2.16)$$

for all $\mathbf{w} \in \mathbb{R}^3$ and all $\boldsymbol{\sigma} \in \mathbb{S}^2$.

Proposition 2.2.2. Suppose that the collision kernel $B_{i,j} : \mathbb{R}^3 \times \mathbb{S}^2 \rightarrow [0, \infty)$ has proper structure. Let $\mathbf{v}, \mathbf{v}_* \in \mathbb{R}^3$ be arbitrary and set

$$(\mathbf{v}', \mathbf{v}'_*) = T_{\boldsymbol{\sigma}}^{i,j}(\mathbf{v}, \mathbf{v}_*),$$

as usual. Then,

$$B_{i,j}(\mathbf{v}' - \mathbf{v}'_*, \boldsymbol{\sigma}) = B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}). \quad (2.17)$$

Proof. Recall (2.5) and (2.6), respectively,

$$\boldsymbol{\sigma} \cdot (\mathbf{v}' - \mathbf{v}'_*) = -\boldsymbol{\sigma} \cdot (\mathbf{v} - \mathbf{v}_*) \quad \text{and} \quad |\mathbf{v}' - \mathbf{v}'_*| = |\mathbf{v} - \mathbf{v}_*|. \quad (2.18)$$

Then,

$$\begin{aligned} B_{ij}(\mathbf{v}' - \mathbf{v}'_*, \boldsymbol{\sigma}) &= b_{ij}(|(\mathbf{v}' - \mathbf{v}'_*) \cdot \boldsymbol{\sigma}|, |\mathbf{v}' - \mathbf{v}'_*|) \\ &= b_{ij}(|-(\mathbf{v} - \mathbf{v}_*) \cdot \boldsymbol{\sigma}|, |\mathbf{v} - \mathbf{v}_*|) \\ &= b_{ij}(|(\mathbf{v} - \mathbf{v}_*) \cdot \boldsymbol{\sigma}|, |\mathbf{v} - \mathbf{v}_*|) \\ &= B_{ij}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}), \end{aligned}$$

which establishes (2.17). ■

Definition 2.2.3. Let $\Omega \subset \mathbb{R}^3$ be a bounded open set. We say that the kinetic distributions $f_i : \Omega \times \mathbb{R}^3 \times [0, T] \rightarrow [0, \infty)$, $i = 1, \dots, N$, satisfy the **multi-species Boltzmann equation** iff, for all $\mathbf{x} \in \Omega$, $\mathbf{v} \in \mathbb{R}^3$, and $t \in (0, T]$,

$$\partial_t f_i(\mathbf{x}, \mathbf{v}, t) + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i(\mathbf{x}, \mathbf{v}, t) = Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t), \quad (2.19)$$

where $Q_i[f_i, \mathbf{f}]$, the **cumulative binary collision operator**, is defined as

$$Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t) := \sum_{j=1}^N Q_{ij}[f_i, f_j](\mathbf{x}, \mathbf{v}, t). \quad (2.20)$$

We often assume that the physical boundary conditions are of the **specular reflection type**, that is, for all $(\mathbf{x}, \mathbf{v}) \in \Gamma_{\text{in}}$, where

$$\Gamma_{\text{in}} := \{(\mathbf{x}, \mathbf{v}) \in \partial\Omega \times \mathbb{R}^3 \mid \mathbf{v} \cdot \mathbf{n}(\mathbf{x}) < 0\},$$

and for all $t \in (0, T]$,

$$f_i(\mathbf{x}, \mathbf{v}, t) = f_i(\mathbf{x}, \mathbf{R}(\mathbf{x}, \mathbf{v}), t),$$

where

$$\mathbf{R}(\mathbf{x}, \mathbf{v}) := \mathbf{v} - 2[\mathbf{v} \cdot \mathbf{n}(\mathbf{x})] \mathbf{n}(\mathbf{x}),$$

and $\mathbf{n}(\mathbf{x})$ is the outward-pointing unit normal vector on the boundary at $\mathbf{x} \in \partial\Omega$.

Remark 2.2.4. In the following two results, we will assume that the kinetic distributions are functions only of velocity. This simplification reduces the number of independent variables

that must be carried about. However, we lose no generality with these assumptions. More typically, the distributions are functions of space ($\mathbf{x}$) and time (t) as well.

Proposition 2.2.5. Suppose that $f_i : \mathbb{R}^3 \rightarrow [0, \infty)$ and $\psi : \mathbb{R}^3 \rightarrow \mathbb{R}$ are given and integrable. Then, assuming the collision kernel $B_{i,i}$ has proper structure,

$$\begin{aligned} & \int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i](\mathbf{v}) \psi(\mathbf{v}) d\mathbf{v} \\ &= \frac{1}{4m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{i,*} - f_i f_{i,*}] B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [\psi + \psi_* - \psi' - \psi'_*] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v}, \end{aligned} \quad (2.21)$$

where the primed coordinates are determined via

$$(\mathbf{v}', \mathbf{v}'_*) = T_{\boldsymbol{\sigma}}^{i,i}(\mathbf{v}, \mathbf{v}_*),$$

and, for shorthand

$$f_i := f_i(\mathbf{v}), \quad f_{i,*} := f_i(\mathbf{v}_*), \quad f'_i := f_i(\mathbf{v}'), \quad f'_{i,*} := f_i(\mathbf{v}'_*),$$

and

$$\psi := \psi(\mathbf{v}), \quad \psi_* := \psi(\mathbf{v}_*), \quad \psi' := \psi(\mathbf{v}'), \quad \psi'_* := \psi(\mathbf{v}'_*),$$

Proof. Let us set

$$J = \int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i](\mathbf{v}) \psi(\mathbf{v}) d\mathbf{v}.$$

Then, by definition,

$$\begin{aligned} J &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{i,*} - f_i f_{i,*}] B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(T_{\boldsymbol{\sigma},1}^{i,i}(\mathbf{v}, \mathbf{v}_*)) f_i(T_{\boldsymbol{\sigma},2}^{i,i}(\mathbf{v}, \mathbf{v}_*)) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_i(\mathbf{v}_*) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v}. \end{aligned} \quad (2.22)$$

The integration variables are dummy variables and may be interchanged. Doing so, we obtain

$$\begin{aligned} J &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(T_{\boldsymbol{\sigma},1}^{i,i}(\mathbf{v}_*, \mathbf{v})) f_i(T_{\boldsymbol{\sigma},2}^{i,i}(\mathbf{v}_*, \mathbf{v})) B_{i,i}(\mathbf{v}_* - \mathbf{v}, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v} d\mathbf{v}_* \\ &\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}_*) f_i(\mathbf{v}) B_{i,i}(\mathbf{v}_* - \mathbf{v}, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v} d\mathbf{v}_* \\ &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(T_{\boldsymbol{\sigma},1}^{i,i}(\mathbf{v}_*, \mathbf{v})) f_i(T_{\boldsymbol{\sigma},2}^{i,i}(\mathbf{v}_*, \mathbf{v})) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \end{aligned}$$

$$- \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_i(\mathbf{v}_*) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v},$$

where we have used (2.15). Observe that, using (2.11) and (2.12) (with $i = j$),

$$\begin{aligned} T_{\boldsymbol{\sigma},1}^{i,i}(\mathbf{v}_*, \mathbf{v}) &= T_{\boldsymbol{\sigma},2}^{i,i}(\mathbf{v}, \mathbf{v}_*), \\ T_{\boldsymbol{\sigma},2}^{i,i}(\mathbf{v}_*, \mathbf{v}) &= T_{\boldsymbol{\sigma},1}^{i,i}(\mathbf{v}, \mathbf{v}_*), \end{aligned}$$

so that

$$\begin{aligned} J &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(T_{\boldsymbol{\sigma},2}^{i,i}(\mathbf{v}, \mathbf{v}_*)) f_i(T_{\boldsymbol{\sigma},1}^{i,i}(\mathbf{v}, \mathbf{v}_*)) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_i(\mathbf{v}_*) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}') f_i(\mathbf{v}') B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_i(\mathbf{v}_*) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}') f_i(\mathbf{v}') B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_i(\mathbf{v}_*) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f_i' f_{i,*}' - f_i f_{i,*}] B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v}. \end{aligned} \tag{2.23}$$

Next, using the change of variables formula in Proposition 2.1.5 and the fact that $l = T_{\boldsymbol{\sigma}}^{i,i} \circ T_{\boldsymbol{\sigma}}^{i,i}$, where l is the identity transformation, we have

$$\begin{aligned} J &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(T_{\boldsymbol{\sigma},1}^{i,i}(\mathbf{v}, \mathbf{v}_*)) f_i(T_{\boldsymbol{\sigma},2}^{i,i}(\mathbf{v}, \mathbf{v}_*)) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_i(\mathbf{v}_*) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_i(\mathbf{v}_*) B_{i,i}(\mathbf{v}' - \mathbf{v}'_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}') f_i(\mathbf{v}'_*) B_{i,i}(\mathbf{v}' - \mathbf{v}'_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v}. \end{aligned}$$

Using (2.17), we find

$$\begin{aligned} J &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_i(\mathbf{v}_*) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\ &\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}') f_i(\mathbf{v}'_*) B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \end{aligned}$$

$$= -\frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{i,*} - f_i f_{i,*}] B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v}. \quad (2.24)$$

Finally, with (2.23) as the starting point, using the change of variables formula in Proposition 2.1.5, using the fact that $I = T_{\boldsymbol{\sigma}}^{i,i} \circ T_{\boldsymbol{\sigma}}^{i,i}$, and using the identity (2.17), we deduce that

$$J = -\frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{i,*} - f_i f_{i,*}] B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v}. \quad (2.25)$$

The combination of identities (2.22) – (2.25) gives the desired result. $\blacksquare$

Proposition 2.2.6. *For $i \neq j$, if $f_i, f_j : \mathbb{R}^3 \rightarrow [0, \infty)$ and $\psi : \mathbb{R}^3 \rightarrow \mathbb{R}$ are given and integrable, then, assuming the collision kernel $B_{i,j}$ has proper structure,*

$$\begin{aligned} & \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j](\mathbf{v}) \psi(\mathbf{v}) d\mathbf{v} \\ &= \frac{1}{4m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{j,*} - f_i f_{j,*}] B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [\psi - \psi'] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}), \\ &+ \frac{1}{4m_j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_j f'_{i,*} - f_j f_{i,*}] B_{j,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [\psi_* - \psi'_*] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{j,i}), \end{aligned} \quad (2.26)$$

where, to be precise, for the first integral the primed coordinates are determined via

$$(\mathbf{v}', \mathbf{v}'_*) = T_{\boldsymbol{\sigma}}^{i,j}(\mathbf{v}, \mathbf{v}_*),$$

and, in shorthand,

$$f_i := f_i(\mathbf{v}), \quad f_{j,*} := f_j(\mathbf{v}_*), \quad f'_i := f_i(\mathbf{v}'), \quad f'_{j,*} := f_j(\mathbf{v}'_*), \quad \psi := \psi(\mathbf{v}), \quad \psi' := \psi(\mathbf{v}'),$$

and, for the second integral the primed coordinates are determined via

$$(\mathbf{v}', \mathbf{v}'_*) = T_{\boldsymbol{\sigma}}^{j,i}(\mathbf{v}, \mathbf{v}_*),$$

and, in shorthand,

$$f_j := f_j(\mathbf{v}), \quad f_{i,*} := f_i(\mathbf{v}_*), \quad f'_j := f_j(\mathbf{v}'), \quad f'_{i,*} := f_i(\mathbf{v}'_*), \quad \psi_* := \psi(\mathbf{v}_*), \quad \psi'_* := \psi(\mathbf{v}'_*).$$

Proof. The steps are similar to those in the proof of the previous result. As before, let us set

$$J = \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j](\mathbf{v}) \psi(\mathbf{v}) d\mathbf{v}.$$

Then, by definition,

$$\begin{aligned}
J &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{j,*} - f_i f_{j,*}] B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\
&= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(T_{\boldsymbol{\sigma},1}^{i,j}(\mathbf{v}, \mathbf{v}_*)) f_j(T_{\boldsymbol{\sigma},2}^{i,j}(\mathbf{v}, \mathbf{v}_*)) B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\
&\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_j(\mathbf{v}_*) B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}). \tag{2.27}
\end{aligned}$$

Interchanging the integration variables $\mathbf{v}$ and $\mathbf{v}_*$, we obtain

$$\begin{aligned}
J &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(T_{\boldsymbol{\sigma},1}^{i,j}(\mathbf{v}_*, \mathbf{v})) f_j(T_{\boldsymbol{\sigma},2}^{i,j}(\mathbf{v}_*, \mathbf{v})) B_{i,j}(\mathbf{v}_* - \mathbf{v}, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v} d\mathbf{v}_* \\
&\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}_*) f_j(\mathbf{v}) B_{i,j}(\mathbf{v}_* - \mathbf{v}, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v} d\mathbf{v}_* \\
&= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_j(T_{\boldsymbol{\sigma},2}^{i,j}(\mathbf{v}_*, \mathbf{v})) f_i(T_{\boldsymbol{\sigma},1}^{i,j}(\mathbf{v}_*, \mathbf{v})) B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\
&\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_j(\mathbf{v}) f_i(\mathbf{v}_*) B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v},
\end{aligned}$$

where we have used (2.15). Observe that, using (2.11) and (2.12) (with $i \neq j$) and (2.16), we find that

$$\begin{aligned}
J &= \frac{1}{m_j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_j(T_{\boldsymbol{\sigma},1}^{j,i}(\mathbf{v}, \mathbf{v}_*)) f_i(T_{\boldsymbol{\sigma},2}^{j,i}(\mathbf{v}, \mathbf{v}_*)) B_{j,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\
&\quad - \frac{1}{m_j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_j(\mathbf{v}) f_i(\mathbf{v}_*) B_{j,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\
&= \frac{1}{m_j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_j f'_{i,*} - f_j f_{i,*}] B_{j,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}_*) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{j,i}). \tag{2.28}
\end{aligned}$$

Next, using the change of variables formula in Proposition 2.1.5 and the fact that $I = T_{\boldsymbol{\sigma}}^{i,j} \circ T_{\boldsymbol{\sigma}}^{j,i}$, where I is the identity transformation, we have

$$\begin{aligned}
J &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(T_{\boldsymbol{\sigma},1}^{i,j}(\mathbf{v}, \mathbf{v}_*)) f_j(T_{\boldsymbol{\sigma},2}^{i,j}(\mathbf{v}, \mathbf{v}_*)) B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\
&\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_j(\mathbf{v}_*) B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}) d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\
&= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_j(\mathbf{v}_*) B_{i,j}(\mathbf{v}' - \mathbf{v}'_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\
&\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}') f_j(\mathbf{v}'_*) B_{i,j}(\mathbf{v}' - \mathbf{v}'_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v}.
\end{aligned}$$

Using (2.17), we then find

$$\begin{aligned}
J &= \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}) f_j(\mathbf{v}_*) B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\
&\quad - \frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} f_i(\mathbf{v}') f_j(\mathbf{v}_*) B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \\
&= -\frac{1}{m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{j,*} - f_i f_{j,*}] B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}). \quad (2.29)
\end{aligned}$$

Finally, with (2.28) as the starting point, using the change of variables formula in Proposition 2.1.5, using the fact that $I = T_{\boldsymbol{\sigma}}^{j,i} \circ T_{\boldsymbol{\sigma}}^{i,j}$, and using the identity (2.17), we deduce that

$$J = -\frac{1}{m_j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_j f'_{i,*} - f_j f_{i,*}] B_{j,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) \psi(\mathbf{v}') d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{j,i}). \quad (2.30)$$

The combination of identities (2.27) – (2.30) gives the desired result. $\blacksquare$

2.3 Collision Invariants

Proposition 2.3.1. *Suppose that $f_i : \mathbb{R}^3 \rightarrow [0, \infty)$ is given and integrable. Then, assuming the collision kernel $B_{i,i}$ has proper structure, it follows that*

$$\int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i](\mathbf{v}) d\mathbf{v} = 0, \quad (2.31)$$

$$\int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i](\mathbf{v}) \mathbf{v} d\mathbf{v} = \mathbf{0}, \quad (2.32)$$

$$\int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i](\mathbf{v}) |\mathbf{v}|^2 d\mathbf{v} = 0. \quad (2.33)$$

Proof. These results follow from identity (2.21) in Proposition 2.2.5 and the transformation invariants (binary collision invariants) in Proposition 2.1.2 for the case that $i = j$. $\blacksquare$

Definition 2.3.2. *Suppose that $f_i : \mathbb{R}^3 \rightarrow [0, \infty)$ is given and integrable. Any function $\psi : \mathbb{R}^3 \rightarrow \mathbb{R}$ with the property that*

$$\int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i](\mathbf{v}) \psi(\mathbf{v}) d\mathbf{v} = 0 \quad (2.34)$$

*is called a **species i collisional invariant** or a **unary collisional invariant**.*

If the collision kernel $B_{i,i}$ has proper structure, then $\psi \equiv 1$, $\psi(\mathbf{v}) = \mathbf{v}$, and $\psi(\mathbf{v}) = |\mathbf{v}|^2$

are unary collisional invariants.

Proposition 2.3.3. *For $i \neq j$, if $f_i, f_j : \mathbb{R}^3 \rightarrow [0, \infty)$ are given and integrable, then, assuming the collision kernel $B_{i,j}$ has proper structure, it follows that*

$$\int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j](\mathbf{v}) d\mathbf{v} = 0, \quad (2.35)$$

$$m_i \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j](\mathbf{v}) \mathbf{v} d\mathbf{v} + m_j \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i](\mathbf{v}) \mathbf{v} d\mathbf{v} = \mathbf{0}, \quad (2.36)$$

$$m_i \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j](\mathbf{v}) |\mathbf{v}|^2 d\mathbf{v} + m_j \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i](\mathbf{v}) |\mathbf{v}|^2 d\mathbf{v} = 0. \quad (2.37)$$

Proof. The identity (2.35) follows from (2.26) with $\psi \equiv 1$. Using $\psi(\mathbf{v}) = \mathbf{v}$ in (2.26), we find that

$$\begin{aligned} & m_i \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j](\mathbf{v}) \mathbf{v} d\mathbf{v} + m_j \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i](\mathbf{v}) \mathbf{v} d\mathbf{v} \\ &= \frac{m_i}{4m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{j,*} - f_i f_{j,*}] B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [\mathbf{v} - \mathbf{v}'] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}), \\ &+ \frac{m_i}{4m_j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_j f'_{i,*} - f_j f_{i,*}] B_{j,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [\mathbf{v}_* - \mathbf{v}'] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{j,i}), \\ &+ \frac{m_j}{4m_j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_j f'_{i,*} - f_j f_{i,*}] B_{j,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [\mathbf{v} - \mathbf{v}'] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{j,i}), \\ &+ \frac{m_j}{4m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{j,*} - f_i f_{j,*}] B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [\mathbf{v}_* - \mathbf{v}'] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}) \\ &= \mathbf{0}, \end{aligned} \quad (2.38)$$

where we have used the following binary momentum invariants from Proposition 2.1.2:

$$m_i \mathbf{v} + m_j \mathbf{v}_* = m_i \mathbf{v}' + m_j \mathbf{v}'_* \iff m_i(\mathbf{v} - \mathbf{v}') = m_j(\mathbf{v}'_* - \mathbf{v}_*) \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}), \quad (2.39)$$

$$m_j \mathbf{v} + m_i \mathbf{v}_* = m_j \mathbf{v}' + m_i \mathbf{v}'_* \iff m_j(\mathbf{v} - \mathbf{v}') = m_i(\mathbf{v}'_* - \mathbf{v}_*) \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{j,i}). \quad (2.40)$$

Using $\psi(\mathbf{v}) = |\mathbf{v}|^2$ in (2.26) and the appropriate binary kinetic energy invariants from Proposition 2.1.2, the identity (2.37) immediately follows. $\blacksquare$

Proposition 2.3.4. *Suppose that $i, j \in \{1, \dots, N\}$ are arbitrary and $f_i, f_j : \mathbb{R}^3 \rightarrow [0, \infty)$ are given and integrable. Assume that the collision kernel $B_{i,j}$ has proper structure. Recall our definition*

$$Q_i[f_i, \mathbf{f}](\mathbf{v}) := \sum_{j=1}^N Q_{i,j}[f_i, f_j](\mathbf{v}). \quad (2.41)$$

Then,

$$\int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{v}) d\mathbf{v} = 0, \quad (2.42)$$

$$\sum_{i=1}^N m_i \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{v}) \mathbf{v} d\mathbf{v} = \mathbf{0}, \quad (2.43)$$

$$\sum_{i=1}^N m_i \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{v}) |\mathbf{v}|^2 d\mathbf{v} = 0. \quad (2.44)$$

Proof. We prove only (2.43). The other two identities are proved similarly. Set

$$J = \sum_{i=1}^N m_i \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{v}) \mathbf{v} d\mathbf{v}.$$

Then,

$$\begin{aligned} J &= \sum_{i=1}^N m_i \int_{\mathbb{R}^3} \sum_{j=1}^N Q_{ij}[f_i, f_j](\mathbf{v}) \mathbf{v} d\mathbf{v} \\ &= \sum_{i=1}^N \sum_{j=1}^N m_i \int_{\mathbb{R}^3} Q_{ij}[f_i, f_j](\mathbf{v}) \mathbf{v} d\mathbf{v} \\ &= \sum_{i=2}^N \sum_{j=1}^i \left(m_i \int_{\mathbb{R}^3} Q_{ij}[f_i, f_j](\mathbf{v}) \mathbf{v} d\mathbf{v} + m_j \int_{\mathbb{R}^3} Q_{ji}[f_j, f_i](\mathbf{v}) \mathbf{v} d\mathbf{v} \right) \\ &\quad + \sum_{i=1}^N m_i \int_{\mathbb{R}^3} Q_{ii}[f_i, f_i](\mathbf{v}) \mathbf{v} d\mathbf{v} \\ &= \mathbf{0}, \end{aligned}$$

where we have use (2.32) for the diagonal terms and (2.36) for the off-diagonal terms. $\blacksquare$

With the next result, we show that all unary collisional invariants have special structure.

Proposition 2.3.5. *Suppose that $\psi \in C^2(\mathbb{R}^3; \mathbb{R})$ has the property that*

$$\psi(\mathbf{v}) + \psi(\mathbf{v}_*) = \psi(T_{\sigma,1}^{i,i}(\mathbf{v}, \mathbf{v}_*)) + \psi(T_{\sigma,2}^{i,i}(\mathbf{v}, \mathbf{v}_*)), \quad (2.45)$$

for all $\mathbf{v}, \mathbf{v}_* \in \mathbb{R}^3$ and all $\sigma \in \mathbb{S}^2$. Then, there exist constants $A, C \in \mathbb{R}$ and $\mathbf{B} \in \mathbb{R}^3$, such that

$$\psi(\mathbf{v}) = \frac{m_i A}{2} |\mathbf{v}|^2 + m_i \mathbf{B} \cdot \mathbf{v} + C. \quad (2.46)$$

In other words, ψ is a velocity-space quadratic function.

Proof. This proof is from [5]. See [19] for another. Define

$$\begin{aligned}\frac{m_i A}{2} &= \frac{1}{6} \Delta \psi(\mathbf{0}), \\ m_i \mathbf{B} &= \nabla \psi(\mathbf{0}), \\ C &= \psi(\mathbf{0}).\end{aligned}$$

Set

$$\phi(\mathbf{v}) = \psi(\mathbf{v}) - \left(\frac{m_i A}{2} |\mathbf{v}|^2 + m_i \mathbf{B} \cdot \mathbf{v} + C \right), \quad \forall \mathbf{v} \in \mathbb{R}^3.$$

Then $\phi \in C^2(\mathbb{R}^3; \mathbb{R})$ is a unary collisional invariant, that is,

$$\int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i] \phi(\mathbf{v}) \, d\mathbf{v} = 0,$$

with the further property that

$$\phi(\mathbf{0}) = 0, \quad \nabla \phi(\mathbf{0}) = \mathbf{0}, \quad \Delta \phi(\mathbf{0}) = 0.$$

Now, suppose that $\mathbf{v}_* \in \mathbb{R}^3 \setminus \{\mathbf{0}\}$ is fixed but, otherwise, arbitrary. Suppose $\boldsymbol{\sigma} \in \mathbb{S}^2$ is perpendicular to $\mathbf{v}_*$, that is,

$$\boldsymbol{\sigma} \cdot \mathbf{v}_* = 0.$$

Set, for $s \in \mathbb{R} \setminus \{0\}$,

$$\mathbf{v} = s\boldsymbol{\sigma}.$$

Then, under the transformation $T_{\boldsymbol{\sigma}}^{i,i}$,

$$\begin{aligned}\mathbf{v}' &:= T_{\boldsymbol{\sigma},1}^{i,i}(\mathbf{v}, \mathbf{v}_*) \\ &= \mathbf{v} - \boldsymbol{\sigma} \cdot (\mathbf{v} - \mathbf{v}_*) \frac{2m_i}{m_i + m_i} \boldsymbol{\sigma} \\ &= \mathbf{v} - s\boldsymbol{\sigma} \\ &= \mathbf{0}.\end{aligned}$$

Furthermore,

$$\mathbf{v}'_* := T_{\boldsymbol{\sigma},2}^{i,i}(\mathbf{v}, \mathbf{v}_*) = \mathbf{v}_* + s\boldsymbol{\sigma}.$$

Thus,

$$\begin{aligned}
 \phi(s\sigma) + \phi(\mathbf{v}_*) &= \phi(\mathbf{v}) + \phi(\mathbf{v}_*) \\
 &= \phi(\mathbf{v}') + \phi(\mathbf{v}_*) \\
 &= \phi(\mathbf{0}) + \phi(\mathbf{v}_* + s\sigma) \\
 &= \phi(\mathbf{v}_* + s\sigma).
 \end{aligned}$$

Equivalently,

$$\phi(s\sigma) = \phi(\mathbf{v}_* + s\sigma) - \phi(\mathbf{v}_*).$$

Using l'Hôpital's rule and the fact that $\phi(\mathbf{0}) = 0$ and $\nabla\phi(\mathbf{0}) = \mathbf{0}$, it follows that

$$\sigma \cdot \nabla\phi(\mathbf{v}_*) = 0.$$

Since $\mathbf{v}_* \in \mathbb{R}^3 \setminus \{\mathbf{0}\}$ and $\sigma \in \mathbb{S}^2$ are perpendicular but otherwise arbitrary, it must be that

$$\phi(\mathbf{v}) = g(|\mathbf{v}|), \quad \forall \mathbf{v} \in \mathbb{R}^3,$$

that is, ϕ is radially symmetric.

Next, assume that $\mathbf{n} \in \mathbb{S}^2$ is arbitrary. Set

$$\mathbf{v} = s\mathbf{n} \quad \text{and} \quad \mathbf{v}_* = r\mathbf{n},$$

where

$$0 \leq s < r.$$

Pick $\sigma \in \mathbb{S}^3$ such that

$$\sigma \cdot \mathbf{n} = \pm \frac{1}{\sqrt{2}}.$$

With this particular choice,

$$\begin{aligned}
 \mathbf{v}' &= s\mathbf{n} - (s - r) \frac{\pm 1}{\sqrt{2}} \sigma, \\
 \mathbf{v}'_* &= r\mathbf{n} + (s - r) \frac{\pm 1}{\sqrt{2}} \sigma,
 \end{aligned}$$

and

$$|\mathbf{v}'|^2 = \frac{s^2 + r^2}{2},$$

$$|\mathbf{v}'_\star|^2 = \frac{s^2 + r^2}{2}.$$

Since

$$\phi(\mathbf{v}) + \phi(\mathbf{v}_\star) = \phi(\mathbf{v}') + \phi(\mathbf{v}'_\star),$$

and ϕ is radially symmetric, we have

$$g(s) + g(r) = 2g\left(\sqrt{\frac{s^2 + r^2}{2}}\right).$$

It follows that, upon differentiating with respect to s ,

$$\begin{aligned} g''(s) &= g''\left(\sqrt{\frac{s^2 + r^2}{2}}\right) \sqrt{\frac{2}{s^2 + r^2}} s + g'\left(\sqrt{\frac{s^2 + r^2}{2}}\right) \sqrt{\frac{2}{s^2 + r^2}} \\ &\quad - g'\left(\sqrt{\frac{s^2 + r^2}{2}}\right) \left(\frac{2}{s^2 + r^2}\right)^{3/2} \frac{s^2}{2}. \end{aligned}$$

Finally, for any $r > 0$,

$$0 = g''(s)|_{s=0} = g'\left(\frac{r}{\sqrt{2}}\right) \frac{\sqrt{2}}{r},$$

which implies that $g'\left(\frac{r}{\sqrt{2}}\right) = 0$, for any $r > 0$. The only possibility is that $g \equiv 0$. ■

2.4 Information, Entropy, and Boltzmann's H-Theorem

Definition 2.4.1. Suppose that $f_1, \dots, f_N : \Omega \times \mathbb{R}^3 \times [0, T] \rightarrow [0, \infty)$ are kinetic distributions that satisfy the multi-species Boltzmann equation. The quantity $h : \Omega \times [0, T] \rightarrow \mathbb{R}$, defined via

$$h(\mathbf{x}, t) := \sum_{i=1}^N \int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) \ln(f_i(\mathbf{x}, \mathbf{v}, t)) \, d\mathbf{v},$$

is called the **information density** of the multi-species mixture. The quantity

$$H(t) = \int_{\Omega} h(\mathbf{x}, t) \, d\mathbf{x}$$

is called the **total information** of the mixture. The quantity $s : \Omega \times [0, T] \rightarrow \mathbb{R}$ defined via

$$s(\mathbf{x}, t) := - \sum_{i=1}^N \int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) \ln(f_i(\mathbf{x}, \mathbf{v}, t)) \, d\mathbf{v} = -h(\mathbf{x}, t),$$

is called the **entropy density** of the multi-species mixture. The quantity

$$S(t) = \int_{\Omega} s(\mathbf{x}, t) d\mathbf{x} = -H(t)$$

is called the **total entropy** of the mixture.

We will need the following technical lemma.

Lemma 2.4.2. For any $x, y \in (0, \infty)$,

$$(\ln(x) - \ln(y))(x - y) \geq 0, \quad (2.47)$$

with equality iff $x = y$.

Proof. Observe that the function $q(x) = x \ln(x)$ is strictly convex on $[0, \infty)$. In fact, for any $x \in (0, \infty)$,

$$q''(x) = \frac{1}{x} > 0.$$

By Taylor's theorem, for any $x, y \in (0, \infty)$, $x \neq y$,

$$x \ln(x) = y \ln(y) + (\ln(y) + 1)(x - y) + \frac{1}{2} \frac{1}{\xi} (x - y)^2 > y \ln(y) + (\ln(y) + 1)(x - y),$$

for some ξ between x and y . The inequality above can be rewritten as

$$x \ln(x) - x \ln(y) > x - y.$$

Reversing the roles of x and y , we have

$$y \ln(y) - y \ln(x) > y - x.$$

Adding the inequalities, we have

$$(x - y)(\ln(x) - \ln(y)) > 0. \quad (2.48)$$

If $x = y$, then, clearly,

$$(\ln(x) - \ln(y))(x - y) = 0.$$

Conversely, suppose that

$$(\ln(x) - \ln(y))(x - y) = 0.$$

We get a clear contradiction, unless $x = y$, because of the strict inequality (2.48). ■

Proposition 2.4.3 (H-Theorem). *Suppose that $f_1, \dots, f_N : \Omega \times \mathbb{R}^3 \times [0, T] \rightarrow [0, \infty)$ are kinetic distributions that satisfy the multi-species Boltzmann equation with specular reflection-type boundary conditions. Assume that the collision kernels $B_{i,j}$ have proper structure. Then,*

$$\partial_t h(\mathbf{x}, t) + \nabla_{\mathbf{x}} \cdot \mathbf{J}_h(\mathbf{x}, t) = \sigma_h(\mathbf{x}, t) \leq 0, \quad (2.49)$$

where $\mathbf{J}_h$ is the **information flux**, given by

$$\mathbf{J}_h(\mathbf{x}, t) := \sum_{i=1}^N \int_{\mathbb{R}^3} \mathbf{v} f_i(\mathbf{x}, \mathbf{v}, t) \ln(f_i(\mathbf{x}, \mathbf{v}, t)) \, d\mathbf{v},$$

and σ_h is the **information loss rate**, defined via

$$\sigma_h(\mathbf{x}, t) := \sum_{i=1}^N \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t) \ln(f_i(\mathbf{x}, \mathbf{v}, t)) \, d\mathbf{v}.$$

The total information satisfies

$$d_t H(t) = \int_{\Omega} \sigma_h(\mathbf{x}, t) \, d\mathbf{x} \leq 0, \quad (2.50)$$

since, for specular reflection-type boundary conditions, it holds that

$$\mathbf{n}(\mathbf{x}) \cdot \mathbf{J}_h(\mathbf{x}, t) = 0, \quad \forall \mathbf{x} \in \partial\Omega, \quad (2.51)$$

where $\mathbf{n}(\mathbf{x})$ is the outward point unit normal on $\partial\Omega$ at the physical boundary point $\mathbf{x}$. Similarly,

$$\partial_t s(\mathbf{x}, t) + \nabla_{\mathbf{x}} \cdot \mathbf{J}_s(\mathbf{x}, t) = \sigma_s(\mathbf{x}, t) \geq 0, \quad (2.52)$$

where $\mathbf{J}_s$ is the **entropy flux**, given by

$$\mathbf{J}_s := - \sum_{i=1}^N \int_{\mathbb{R}^3} \mathbf{v} f_i(\mathbf{x}, \mathbf{v}, t) \ln(f_i(\mathbf{x}, \mathbf{v}, t)) \, d\mathbf{v} = -\mathbf{J}_h,$$

and σ_s is the **entropy production rate**, defined via

$$\sigma_s(\mathbf{x}, t) := - \sum_{i=1}^N \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t) \ln(f_i(\mathbf{x}, \mathbf{v}, t)) \, d\mathbf{v} = -\sigma_h(\mathbf{x}, t).$$

The total entropy satisfies

$$d_t S(t) = \int_{\Omega} \sigma_s(\mathbf{x}, t) d\mathbf{x} \geq 0, \quad (2.53)$$

since

$$\mathbf{n}(\mathbf{x}) \cdot \mathbf{J}_s(\mathbf{x}, t) = 0, \quad \forall \mathbf{x} \in \partial\Omega. \quad (2.54)$$

Proof. Let us multiply the i^{th} equation of multi-species Boltzmann system (2.19) by $\ln(f_i) + 1$, integrate in velocity space, and sum on i . We clearly obtain (2.49) after using (2.42).

Next, we want to show that

$$\sigma_h(\mathbf{x}, t) = \sum_{i=1}^N \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t) \ln(f_i(\mathbf{x}, \mathbf{v}, t)) d\mathbf{v} \leq 0, \quad \forall \mathbf{x} \in \Omega, \quad \forall t \geq 0.$$

Let us write this as the sum of sums, a diagonal sum and an off-diagonal sum:

$$\begin{aligned} \sigma_h &= \sum_{i=1}^N \int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i] \ln(f_i) d\mathbf{v} \\ &\quad + \sum_{i=2}^N \sum_{j=1}^i \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j] \ln(f_i) d\mathbf{v} + \sum_{j=2}^N \sum_{i=1}^j \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j] \ln(f_j) d\mathbf{v} \\ &= \sum_{i=1}^N \int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i] \ln(f_i) d\mathbf{v} \\ &\quad + \sum_{i=2}^N \sum_{j=1}^i \left[\int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j] \ln(f_i) d\mathbf{v} + \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i] \ln(f_j) d\mathbf{v} \right]. \end{aligned} \quad (2.55)$$

Let us tackle the diagonal terms first. Observe that, using (2.21),

$$\begin{aligned} &\int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i] \ln(f_i) d\mathbf{v} \\ &= \frac{1}{4m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{i,*} - f_i f_{i,*}] B_{i,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [L_i + L_{i,*} - L'_i - L'_{i,*}] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,i}), \end{aligned} \quad (2.56)$$

where

$$L_i := \ln(f_i), \quad L_{i,*} := \ln(f_{i,*}), \quad L'_i = \ln(f'_i), \quad L'_{i,*} = \ln(f'_{i,*}).$$

Now, observe that

$$L_i + L_{i,*} - L'_i - L'_{i,*} = \ln(f_i f_{i,*}) - \ln(f'_i f'_{i,*}).$$

Using estimate (2.47), it follows that

$$[f'_i f'_{i,*} - f_i f_{i,*}] [L_i + L_{i,*} - L'_i - L'_{i,*}] \leq 0,$$

for each $\mathbf{x} \in \Omega$, every $\mathbf{v} \in \mathbb{R}^3$, and every $t \geq 0$. Since $B_{i,i}(\mathbf{w}, \boldsymbol{\sigma}) \geq 0$, for all $\mathbf{w} \in \mathbb{R}^3$ and $\boldsymbol{\sigma} \in \mathbb{S}^2$, it follows that

$$\int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i] \ln(f_i) d\mathbf{v} \leq 0$$

for each $\mathbf{x} \in \Omega$ and every $t \geq 0$. As a consequence,

$$\sum_{i=1}^N \int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i] \ln(f_i) d\mathbf{v} \leq 0.$$

Next we address the off-diagonal sum in (2.55). Using (2.26), for $i > j$,

$$\begin{aligned} & \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j](\mathbf{v}) \ln(f_i(\mathbf{v})) d\mathbf{v} \\ &= \frac{1}{4m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{j,*} - f_i f_{j,*}] B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [L_i - L'_i] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}) \\ &+ \frac{1}{4m_j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_j f'_{i,*} - f_j f_{i,*}] B_{j,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [L_{i,*} - L'_{i,*}] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{j,i}), \end{aligned}$$

and

$$\begin{aligned} & \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i](\mathbf{v}) \ln(f_j(\mathbf{v})) d\mathbf{v} \\ &= \frac{1}{4m_j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_j f'_{i,*} - f_j f_{i,*}] B_{j,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [L_j - L'_j] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{j,i}) \\ &+ \frac{1}{4m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{j,*} - f_i f_{j,*}] B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [L_{j,*} - L'_{j,*}] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}). \end{aligned}$$

Thus, for $i > j$,

$$\begin{aligned} & \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j](\mathbf{v}) \ln(f_i(\mathbf{v})) d\mathbf{v} + \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i](\mathbf{v}) \ln(f_j(\mathbf{v})) d\mathbf{v} \\ &= \frac{1}{4m_i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_i f'_{j,*} - f_i f_{j,*}] B_{i,j}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [L_i - L'_i + L_{j,*} - L'_{j,*}] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}) \\ &+ \frac{1}{4m_j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f'_j f'_{i,*} - f_j f_{i,*}] B_{j,i}(\mathbf{v} - \mathbf{v}_*, \boldsymbol{\sigma}) [L_{i,*} - L'_{i,*} + L_j - L'_j] d\boldsymbol{\sigma} d\mathbf{v}_* d\mathbf{v} \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{j,i}). \end{aligned} \tag{2.57}$$

Using the logarithmic estimate (2.47) and the fact that $B_{i,j}, B_{j,i} \geq 0$, we conclude that

$$\int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j](\mathbf{v}) \ln(f_i(\mathbf{v})) d\mathbf{v} + \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i](\mathbf{v}) \ln(f_j(\mathbf{v})) d\mathbf{v} \leq 0.$$

Both terms in (2.55) are non-positive, and we conclude that $\sigma_h \leq 0$. The estimate (2.49) is proven.

To prove (2.50), integrate (2.49) over Ω , use the Divergence Theorem, the specular boundary condition (2.51), and the fact that $\sigma_h \leq 0$, point-wise.

The results for the entropy density and the total entropy are simple consequences of the corresponding results for the information density and total information, noting only that $s = -h$ and $S = -H$. ■

Proposition 2.4.4. *Suppose that $f_1, \dots, f_N : \Omega \times \mathbb{R}^3 \times [0, T] \rightarrow [0, \infty)$ are kinetic distributions. Assume that the collision kernels $B_{i,j}$ have proper structure. Then,*

$$\sigma_h(\mathbf{x}, t) := \sum_{i=1}^N \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t) \ln(f_i(\mathbf{x}, \mathbf{v}, t)) d\mathbf{v} = 0 \quad (2.58)$$

iff, for $i = 1, \dots, N$,

$$\ln(f_i(\mathbf{x}, \mathbf{v}, t)) = \frac{m_i A(\mathbf{x}, t)}{2} |\mathbf{v}|^2 + m_i \mathbf{B}(\mathbf{x}, t) \cdot \mathbf{v} + C_i(\mathbf{x}, t), \quad (2.59)$$

where A and $\mathbf{B}$ are independent of i and $\mathbf{v}$.

Proof. We have seen from the proof of the last proposition that

$$\begin{aligned} \sigma_h &= \sum_{i=1}^N \int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i] \ln(f_i) d\mathbf{v} \\ &\quad + \sum_{i=2}^N \sum_{j=1}^i \left[\int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j] \ln(f_i) d\mathbf{v} + \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i] \ln(f_j) d\mathbf{v} \right] \\ &\leq 0. \end{aligned} \quad (2.60)$$

More specifically,

$$\int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i] \ln(f_i) d\mathbf{v} \leq 0, \quad i \in \{1, \dots, N\},$$

and

$$\int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j] \ln(f_i) d\mathbf{v} + \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i] \ln(f_j) d\mathbf{v} \leq 0, \quad i, j \in \{1, \dots, N\}, \quad i > j.$$

If (2.59) holds, then $\sigma_h = 0$, using (2.31) – (2.33) ($i = j$) and (2.35) – (2.37) ($i > j$). Specifically, for the latter case ($i > j$), observe that

$$\begin{aligned} & \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j] \ln(f_i) d\mathbf{v} + \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i] \ln(f_j) d\mathbf{v} \\ &= \frac{A(\mathbf{x}, t)}{2} \left(m_i \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j] |\mathbf{v}|^2 d\mathbf{v} + m_j \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i] |\mathbf{v}|^2 d\mathbf{v} \right) \\ &+ \mathbf{B}(\mathbf{x}, t) \cdot \left(m_i \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j] \mathbf{v} d\mathbf{v} + m_j \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i] \mathbf{v} d\mathbf{v} \right) \\ &+ \left(C_i(\mathbf{x}, t) \int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j] d\mathbf{v} + C_j(\mathbf{x}, t) \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i] d\mathbf{v} \right) \\ &= 0, \end{aligned}$$

thanks to (2.35) – (2.37).

Conversely, if $\sigma_h(\mathbf{x}, t) = 0$ at a particular point $(\mathbf{x}, t) \in \Omega \times [0, \infty)$, then it must be that

$$\int_{\mathbb{R}^3} Q_{i,i}[f_i, f_i] \ln(f_i) d\mathbf{v} = 0, \quad \forall i \in \{1, \dots, N\}, \quad (2.61)$$

and

$$\int_{\mathbb{R}^3} Q_{i,j}[f_i, f_j] \ln(f_i) d\mathbf{v} + \int_{\mathbb{R}^3} Q_{j,i}[f_j, f_i] \ln(f_j) d\mathbf{v} = 0, \quad \forall i, j \in \{1, \dots, N\}, \quad i > j. \quad (2.62)$$

Using Equation (2.61), Equation (2.56), and Lemma 2.4.2, it must be that

$$L_i + L_{i,\star} - L'_i - L'_{i,\star} = 0 \quad (' \leftrightarrow T_{\sigma}^{i,i}),$$

for all $\mathbf{v}$, $\mathbf{v}_{\star}$, and σ . Invoking Proposition 2.3.5, it follows that, for $i = 1, \dots, N$, for all $\mathbf{v} \in \mathbb{R}^3$,

$$L_i = \ln(f_i(\mathbf{x}, \mathbf{v}, t)) = \frac{m_i A_i(\mathbf{x}, t)}{2} |\mathbf{v}|^2 + m_i \mathbf{B}_i(\mathbf{x}, t) \cdot \mathbf{v} + C_i(\mathbf{x}, t). \quad (2.63)$$

Here, A_i and $\mathbf{B}_i$ are independent of $\mathbf{v}$, but we leave open the possibility that A_i and $\mathbf{B}_i$ depend upon i .

Next, using Equation (2.62), Equation (2.57), and Lemma 2.4.2, it must be that

$$L_i - L'_i + L_{j,\star} - L'_{j,\star} = 0 \quad (' \leftrightarrow T_{\sigma}^{j,i})$$

and

$$L_{i,\star} - L'_{i,\star} + L_j - L'_j = 0 \quad (' \leftrightarrow T_{\sigma}^{j,i}),$$

for all $\mathbf{v}$, $\mathbf{v}_*$, and $\boldsymbol{\sigma}$. We now insert (2.63)—dropping the $\mathbf{x}$ and t dependencies, since these points are fixed—into the last two equations, to obtain

$$\begin{aligned} & \frac{m_i A_i}{2} |\mathbf{v}|^2 - \frac{m_i A_i}{2} |\mathbf{v}'|^2 + \frac{m_j A_j}{2} |\mathbf{v}_*|^2 - \frac{m_j A_j}{2} |\mathbf{v}'_*|^2 \\ & + m_i \mathbf{B}_i \cdot \mathbf{v} - m_i \mathbf{B}_i \cdot \mathbf{v}' + m_j \mathbf{B}_j \cdot \mathbf{v}_* - m_j \mathbf{B}_j \cdot \mathbf{v}'_* = 0 \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}) \end{aligned}$$

and

$$\begin{aligned} & \frac{m_i A_i}{2} |\mathbf{v}_*|^2 - \frac{m_i A_i}{2} |\mathbf{v}'_*|^2 + \frac{m_j A_j}{2} |\mathbf{v}|^2 - \frac{m_j A_j}{2} |\mathbf{v}'|^2 \\ & + m_i \mathbf{B}_i \cdot \mathbf{v}_* - m_i \mathbf{B}_i \cdot \mathbf{v}'_* + m_j \mathbf{B}_j \cdot \mathbf{v} - m_j \mathbf{B}_j \cdot \mathbf{v}' = 0 \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{j,i}), \end{aligned}$$

for all $\mathbf{v}$, $\mathbf{v}_*$, and $\boldsymbol{\sigma}$. Now, we invoke the particle transformation invariances, (2.3) and (2.4), to obtain

$$(A_j - A_i) \left(\frac{m_j}{2} |\mathbf{v}_*|^2 - \frac{m_j}{2} |\mathbf{v}'_*|^2 \right) + (\mathbf{B}_j - \mathbf{B}_i) \cdot (m_j \mathbf{v}_* - m_j \mathbf{v}'_*) = 0 \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}), \quad (2.64)$$

for all $\mathbf{v}$, $\mathbf{v}_*$, and $\boldsymbol{\sigma}$, and

$$(A_j - A_i) \left(\frac{m_j}{2} |\mathbf{v}|^2 - \frac{m_j}{2} |\mathbf{v}'|^2 \right) + (\mathbf{B}_j - \mathbf{B}_i) \cdot (m_j \mathbf{v} - m_j \mathbf{v}') = 0 \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{j,i}), \quad (2.65)$$

for all $\mathbf{v}$, $\mathbf{v}_*$, and $\boldsymbol{\sigma}$.

Let us examine Equation (2.64). Recall, from the transformation $T_{\boldsymbol{\sigma}}^{i,j}$,

$$\mathbf{v}'_* = \mathbf{v}_* + [\boldsymbol{\sigma} \cdot (\mathbf{v} - \mathbf{v}_*)] \mu_{i,j} \boldsymbol{\sigma}, \quad \mu_{i,j} := \frac{2m_i}{m_i + m_j}.$$

Let $\mathbf{v}_*$ be an arbitrary, non-zero vector. Choose

$$\mathbf{v} = \frac{\mu_{i,j} - 2}{\mu_{i,j}} \mathbf{v}_*, \quad \boldsymbol{\sigma} = \frac{\mathbf{v}_*}{|\mathbf{v}_*|}.$$

Then, it follows that $\mathbf{v}'_* = -\mathbf{v}_*$. Thus, (2.64) indicates that

$$(\mathbf{B}_j - \mathbf{B}_i) \cdot \mathbf{v}_* = 0.$$

Since $\mathbf{v}_*$ was arbitrary, $\mathbf{B}_j = \mathbf{B}_i$. Since i and j are also arbitrary, it must be that $\mathbf{B}_i = \mathbf{B}$, for all i , for some vector $\mathbf{B}$ that is i -independent. Thus, (2.64) is equivalent to

$$(A_j - A_i) \left(\frac{m_j}{2} |\mathbf{v}_*|^2 - \frac{m_j}{2} |\mathbf{v}'_*|^2 \right) = 0 \quad (' \leftrightarrow T_{\boldsymbol{\sigma}}^{i,j}),$$

for all $\mathbf{v}$, $\mathbf{v}_*$, and $\boldsymbol{\sigma}$. Again, let $\mathbf{v}_*$ be an arbitrary, non-zero vector. Choose

$$\mathbf{v} = \frac{\mu_{i,j} - 2}{\mu_{i,j}} \mathbf{v}_*, \quad \boldsymbol{\sigma} = \frac{\mathbf{v}_*}{|\mathbf{v}_*|}.$$

Then, it follows that $\mathbf{v}'_* = \mathbf{0}$. Thus,

$$(A_j - A_i)|\mathbf{v}_*|^2 = 0.$$

As above, it must be that $A_i = A$, for all i , where A is i -independent. ■

2.5 Moments and Moment Equations

In this section, we develop the macroscopic moment equations from the Boltzmann equations.

Definition 2.5.1. Suppose that $f_i : \Omega \times \mathbb{R}^3 \times [0, \infty) \rightarrow [0, \infty)$, $i = 1, \dots, N$ are kinetic distributions with the property that

$$\int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) |\mathbf{v}|^k d\mathbf{v} < \infty, \quad k = 0, 1, 2, \quad (2.66)$$

for each $\mathbf{x} \in \Omega$ and every $t \geq 0$. Assume that m_i , the **mass of the i^{th} particle**, is a positive real number. The quantity

$$n_i(\mathbf{x}, t) := \int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} \quad (2.67)$$

is called the **number density of the i^{th} species**, while

$$\rho_i(\mathbf{x}, t) := m_i n_i(\mathbf{x}, t) \quad (2.68)$$

is called the **mass density of the i^{th} species**. The quantity

$$\mathbf{u}_i(\mathbf{x}, t) := \frac{1}{n_i(\mathbf{x}, t)} \int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) \mathbf{v} d\mathbf{v} \quad (2.69)$$

is called the **bulk velocity of the i^{th} species**. The **total mass density of the mixture** is defined as

$$\rho(\mathbf{x}, t) := \sum_{i=1}^N \rho_i(\mathbf{x}, t). \quad (2.70)$$

The quantity

$$\mathbf{q}(\mathbf{x}, t) := \sum_{i=1}^N \rho_i(\mathbf{x}) \mathbf{u}_i(\mathbf{x}, t) \quad (2.71)$$

is called the **total momentum density of the mixture**. The **bulk mass-averaged velocity** is defined as

$$\mathbf{u}(\mathbf{x}, t) := \frac{\mathbf{q}(\mathbf{x}, t)}{\rho(\mathbf{x}, t)}. \quad (2.72)$$

The **kinetic energy density of the i^{th} species** is defined as

$$\omega_i(\mathbf{x}, t) := \frac{m_i}{2} \int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) |\mathbf{v}|^2 d\mathbf{v}. \quad (2.73)$$

The **total kinetic energy density** is defined as

$$\omega(\mathbf{x}, t) := \sum_{i=1}^N \omega_i(\mathbf{x}, t). \quad (2.74)$$

The **internal energy density of the i^{th} species** is defined via

$$e_i(\mathbf{x}, t) := \frac{m_i}{2} \int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) |\mathbf{v} - \mathbf{u}_i(\mathbf{x}, t)|^2 d\mathbf{v}. \quad (2.75)$$

The **total internal energy density** is defined as

$$e(\mathbf{x}, t) := \sum_{i=1}^N e_i(\mathbf{x}, t). \quad (2.76)$$

Finally, the **temperature of the i^{th} species** is defined via

$$\theta_i(\mathbf{x}, t) := \frac{2}{3} \frac{e_i(\mathbf{x}, t)}{n_i(\mathbf{x}, t)}, \quad (2.77)$$

so that, after some simple manipulation,

$$\theta_i(\mathbf{x}, t) = \frac{m_i}{3n_i(\mathbf{x}, t)} \int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) |\mathbf{v} - \mathbf{u}_i(\mathbf{x}, t)|^2 d\mathbf{v}. \quad (2.78)$$

Remark 2.5.2. Clearly, θ_i , the temperature of the i^{th} species is non-negative, provided f_i is non-negative.

Remark 2.5.3. The quantities ρ_i , $\mathbf{u}_i$, and θ_i are sometimes referred to, collectively, as the **first three moments of f_i** . Other authors use the collection ρ_i , $\rho_i \mathbf{u}_i$, and ω_i to stand for first three moments of f_i . Observe that the collections $(\rho_i, \mathbf{u}_i, \theta_i)$ and $(\rho_i, \rho_i \mathbf{u}_i, \omega_i)$ are essentially equivalent. One collection of variables can be derived from the other and vice versa.

Let us define a few more bulk/macroscopic quantities.

Definition 2.5.4. Suppose that $f_i : \Omega \times \mathbb{R}^3 \times [0, \infty) \rightarrow [0, \infty)$, $i = 1, \dots, N$ are kinetic distributions with the properties

$$\int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) |\mathbf{v}|^k d\mathbf{v} < \infty, \quad k = 0, 1, 2, 3, \quad (2.79)$$

for each $\mathbf{x} \in \Omega$ and every $t \geq 0$. The **energy flow of the i^{th} species** is defined as

$$\mathbf{r}_i(\mathbf{x}, t) := \frac{m_i}{2} \int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) \mathbf{v} |\mathbf{v}|^2 d\mathbf{v}. \quad (2.80)$$

The i^{th} **momentum flow tensor** is defined as

$$\mathbf{M}_i(\mathbf{x}, t) := m_i \int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) \mathbf{v} \otimes \mathbf{v} d\mathbf{v}. \quad (2.81)$$

The i^{th} **deviation velocity** is defined as

$$\mathbf{c}_i(\mathbf{x}, \mathbf{v}, t) := \mathbf{v} - \mathbf{u}_i(\mathbf{x}, t). \quad (2.82)$$

The **pressure tensor of the i^{th} species** is defined as

$$\mathbf{P}_i(\mathbf{x}, t) := m_i \int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) \mathbf{c}_i(\mathbf{x}, \mathbf{v}, t) \otimes \mathbf{c}_i(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}. \quad (2.83)$$

Define the i^{th} **heat flux** via

$$\boldsymbol{\chi}_i(\mathbf{x}, t) := \frac{m_i}{2} \int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) \mathbf{c}_i(\mathbf{x}, \mathbf{v}, t) |\mathbf{c}_i(\mathbf{x}, \mathbf{v}, t)|^2 d\mathbf{v}. \quad (2.84)$$

Next, we list some elementary identities that relate our defined bulk/macroscopic quantities.

Proposition 2.5.5. Suppose that $f_i : \Omega \times \mathbb{R}^3 \times [0, \infty) \rightarrow [0, \infty)$, $i = 1, \dots, N$, are kinetic distributions with the properties

$$\int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) |\mathbf{v}|^k d\mathbf{v} < \infty, \quad k = 0, 1, 2, 3, \quad (2.85)$$

for each $\mathbf{x} \in \Omega$ and every $t \geq 0$. Then, we have the following identities:

$$\omega_i(\mathbf{x}, t) = \frac{\rho_i(\mathbf{x}, t)}{2} |\mathbf{u}_i(\mathbf{x}, t)|^2 + e_i(\mathbf{x}, t); \quad (2.86)$$

$$\mathbf{M}_i(\mathbf{x}, t) = \rho_i(\mathbf{x}, t) \mathbf{u}_i(\mathbf{x}, t) \otimes \mathbf{u}_i(\mathbf{x}, t) + \mathbf{P}_i(\mathbf{x}, t); \quad (2.87)$$

and

$$\mathbf{r}_i(\mathbf{x}, t) = \omega_i(\mathbf{x}, t) \mathbf{u}_i(\mathbf{x}, t) + \boldsymbol{\chi}_i(\mathbf{x}, t) + \mathbf{P}_i(\mathbf{x}, t) \mathbf{u}_i(\mathbf{x}, t). \quad (2.88)$$

Proof. The proofs are straightforward and are skipped for brevity. ■

Finally, we can state the basic moment equations for the multi-species Boltzmann system.

Proposition 2.5.6. *Suppose that $f_i : \Omega \times \mathbb{R}^3 \times [0, \infty) \rightarrow [0, \infty)$, $i = 1, \dots, N$, are kinetic distributions that satisfy the multi-species Boltzmann system,*

$$\partial_t f_i(\mathbf{x}, \mathbf{v}, t) + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i(\mathbf{x}, \mathbf{v}, t) = Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t), \quad (2.89)$$

where $Q_i[f_i, \mathbf{f}]$ is the cumulative binary collision operator

$$Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t) := \sum_{j=1}^N Q_{i,j}[f_i, f_j](\mathbf{x}, \mathbf{v}, t). \quad (2.90)$$

Assume that

$$\int_{\mathbb{R}^3} f_i(\mathbf{x}, \mathbf{v}, t) |\mathbf{v}|^k d\mathbf{v} < \infty, \quad k = 0, 1, 2, 3, \quad (2.91)$$

for each $\mathbf{x} \in \Omega$ and every $t \geq 0$. Suppose that the collision kernels, $B_{i,j}$ have proper structure. Then, for all $\mathbf{x} \in \Omega$ and $t \geq 0$, and for each $i = 1, \dots, N$,

$$\partial_t \rho_i + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{u}_i) = 0, \quad (2.92)$$

$$\partial_t (\rho_i \mathbf{u}_i) + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i + \mathbf{P}_i) = m_i \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t) \mathbf{v} d\mathbf{v}, \quad (2.93)$$

and

$$\begin{aligned} \partial_t \left(\frac{\rho_i}{2} |\mathbf{u}_i|^2 + e_i \right) + \nabla_{\mathbf{x}} \cdot \left[\left(\frac{\rho_i}{2} |\mathbf{u}_i|^2 + e_i \right) \mathbf{u}_i \right] + \nabla_{\mathbf{x}} \cdot (\boldsymbol{\chi}_i + \mathbf{P}_i \mathbf{u}_i) \\ = \frac{m_i}{2} \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t) |\mathbf{v}|^2 d\mathbf{v}. \end{aligned} \quad (2.94)$$

Consequently, using the collisional invariants,

$$\partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u}) = 0, \quad (2.95)$$

$$\partial_t (\rho \mathbf{u}) + \nabla_{\mathbf{x}} \cdot \sum_{i=1}^N (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i + \mathbf{P}_i) = 0, \quad (2.96)$$

and

$$\partial_t \sum_{i=1}^N \left(\frac{\rho_i}{2} |\mathbf{u}_i|^2 + e_i \right) + \nabla_{\mathbf{x}} \cdot \sum_{i=1}^N \left[\left(\frac{\rho_i}{2} |\mathbf{u}_i|^2 + e_i \right) \mathbf{u}_i + \boldsymbol{\chi}_i + \mathbf{P}_i \mathbf{u}_i \right] = 0. \quad (2.97)$$

Proof. To prove the first three identities, multiply (2.89) by, respectively, m_i , $m_i \mathbf{v}$, and $\frac{m_i}{2} |\mathbf{v}|^2$ and integrate over velocity space. The last three are obtained by summing the first three on i and using the usual collision invariants (2.42) – (2.44).

Here we will prove only identities (2.93) and (2.94) in detail. First, multiply (2.89) by $m_i \mathbf{v}$ and integrate over velocity space to obtain

$$\begin{aligned} m_i \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t) \mathbf{v} d\mathbf{v} &= \partial_t (\rho_i \mathbf{u}_i) + m_i \int_{\mathbb{R}^3} \mathbf{v} \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i d\mathbf{v} \\ &= \partial_t (\rho_i \mathbf{u}_i) + \nabla_{\mathbf{x}} \cdot \mathbf{M}_i \\ &= \partial_t (\rho_i \mathbf{u}_i) + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i + \mathbf{P}_i), \end{aligned}$$

where we have used identity (2.87). Thus, we have identity (2.93).

Next, multiply (2.89) by $\frac{m_i}{2} |\mathbf{v}|^2$ and integrate over velocity space to obtain

$$\begin{aligned} \frac{m_i}{2} \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{x}, \mathbf{v}, t) |\mathbf{v}|^2 d\mathbf{v} &= \partial_t \omega_i + \nabla_{\mathbf{x}} \cdot \mathbf{r}_i \\ &= \partial_t \omega_i + \nabla_{\mathbf{x}} \cdot (\omega_i \mathbf{u}_i + \boldsymbol{\chi}_i + \mathbf{P}_i \mathbf{u}_i) \\ &= \partial_t \left(\frac{\rho_i}{2} |\mathbf{u}_i|^2 + e_i \right) + \nabla_{\mathbf{x}} \cdot \left[\left(\frac{\rho_i}{2} |\mathbf{u}_i|^2 + e_i \right) \mathbf{u}_i \right] \\ &\quad + \nabla_{\mathbf{x}} \cdot (\boldsymbol{\chi}_i + \mathbf{P}_i \mathbf{u}_i), \end{aligned}$$

using (2.88) and (2.86), which gives the identity (2.94). ■

2.6 The Maxwellian and Maximal Entropy States

In this section, we will do our calculations in a physical space of generic dimension $d \in \mathbb{N}$, to maintain some generality.

Definition 2.6.1. Suppose that $\Omega \subset \mathbb{R}^d$ is an open, bounded set and $f : \Omega \times \mathbb{R}^d \times [0, \infty) \rightarrow [0, \infty)$ is a kinetic distribution of particles of mass $m > 0$, with the property

$$\int_{\mathbb{R}^d} f(\mathbf{x}, \mathbf{v}, t) |\mathbf{v}|^k d\mathbf{v} < \infty, \quad k = 0, 1, 2, \quad (2.98)$$

for each $\mathbf{x} \in \Omega$ and every $t \geq 0$. The **Maxwellian distribution of f** is defined as

$$M_f(\mathbf{x}, \mathbf{v}, t) := M[f](\mathbf{x}, \mathbf{v}, t) := n \left(\frac{m}{2\pi\theta} \right)^{d/2} \exp \left(-\frac{m|\mathbf{v} - \mathbf{u}|^2}{2\theta} \right), \quad (2.99)$$

using the first three integral moments of f ,

$$n(\mathbf{x}, t) := \int_{\mathbb{R}^d} f \, d\mathbf{v}, \quad \mathbf{u}(\mathbf{x}, t) := \frac{1}{n} \int_{\mathbb{R}^d} f \mathbf{v} \, d\mathbf{v}, \quad \theta(\mathbf{x}, t) := \frac{m}{d n} \int_{\mathbb{R}^d} f |\mathbf{v} - \mathbf{u}|^2 \, d\mathbf{v}. \quad (2.100)$$

For convenience, we define the bracket notation, $\langle \cdot \rangle : L^1(\mathbb{R}^d; \mathbb{R}^p) \rightarrow \mathbb{R}^p$, by

$$\langle \mathbf{g} \rangle = \int_{\mathbb{R}^d} \mathbf{g}(\mathbf{v}) \, d\mathbf{v}.$$

Therefore, we have the usual definitions

$$\begin{bmatrix} \rho(\mathbf{x}, t) \\ \rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \\ \omega(\mathbf{x}, t) \end{bmatrix} = \left\langle f(\mathbf{x}, \mathbf{v}, t) \begin{bmatrix} m \\ m\mathbf{v} \\ \frac{m}{2} |\mathbf{v}|^2 \end{bmatrix} \right\rangle,$$

where $m > 0$ is the mass of the particles with kinetic distribution f .

For convenience, let us define

$$\boldsymbol{\rho}(\mathbf{x}, t) := [\rho, \rho \mathbf{u}^\top, \omega]^\top : \mathbb{R}^d \times \mathbb{R}^+ \rightarrow \mathbb{R}^{d+2}; \quad (2.101)$$

$$\mathbf{m}(\mathbf{v}) := \left[m, m\mathbf{v}^\top, \frac{m}{2} |\mathbf{v}|^2 \right]^\top : \mathbb{R}^d \rightarrow \mathbb{R}^{d+2}; \quad (2.102)$$

and

$$\boldsymbol{\alpha}(\mathbf{x}, t) := \frac{1}{m} \left[\ln \left(\frac{n}{(2\pi\theta/m)^{d/2}} \right) - \frac{m|\mathbf{u}|^2}{2\theta}, \frac{m\mathbf{u}^\top}{\theta}, -\frac{m}{\theta} \right]^\top : \mathbb{R}^d \times \mathbb{R}^+ \rightarrow \mathbb{R}^{d+2}. \quad (2.103)$$

Then, succinctly,

$$\boldsymbol{\rho} = \langle f \mathbf{m} \rangle, \quad \text{and} \quad M_f = \exp(\boldsymbol{\alpha} \cdot \mathbf{m}(\mathbf{v})). \quad (2.104)$$

Indeed,

$$\begin{aligned} \exp(\boldsymbol{\alpha} \cdot \mathbf{m}) &= \exp \left(\ln \left(\frac{n}{(2\pi\theta/m)^{d/2}} \right) - \frac{m|\mathbf{u}|^2}{2\theta} \right) \exp \left(\frac{m\mathbf{u} \cdot \mathbf{v}}{\theta} \right) \exp \left(-\frac{m}{2\theta} |\mathbf{v}|^2 \right) \\ &= n \left(\frac{m}{2\pi\theta} \right)^{d/2} \exp \left(-\frac{m|\mathbf{u}|^2}{2\theta} \right) \exp \left(\frac{m\mathbf{u} \cdot \mathbf{v}}{\theta} \right) \exp \left(-\frac{m}{2\theta} |\mathbf{v}|^2 \right) \end{aligned}$$

$$\begin{aligned}
&= n \left(\frac{m}{2\pi\theta} \right)^{d/2} \exp \left(-\frac{m}{2\theta} |\mathbf{u} - \mathbf{v}|^2 \right) \\
&= M_f.
\end{aligned}$$

The next result indicates that the first three moments of f and its associated Maxwellian are exactly the same.

Lemma 2.6.2. *Suppose that $f : \mathbb{R}^d \rightarrow [0, \infty)$ is a kinetic distribution of particles of mass $m > 0$, with the property*

$$\int_{\mathbb{R}^d} f(\mathbf{v}) |\mathbf{v}|^k d\mathbf{v} < \infty, \quad k = 0, 1, 2. \quad (2.105)$$

The following equality holds:

$$\langle (M_f - f) \mathbf{m} \rangle = \left\langle \begin{bmatrix} m \\ m\mathbf{v} \\ \frac{m}{2} |\mathbf{v}|^2 \end{bmatrix} (M_f - f) \right\rangle = \mathbf{0}. \quad (2.106)$$

Proof. 1. First we show that

$$\int_{\mathbb{R}^d} M_f d\mathbf{v} = \int_{\mathbb{R}^d} f d\mathbf{v}. \quad (2.107)$$

By definition,

$$\begin{aligned}
\int_{\mathbb{R}^d} M_f d\mathbf{v} &= \int_{\mathbb{R}^d} \frac{n}{(2\pi\theta/m)^{\frac{d}{2}}} \exp \left(-\frac{m|\mathbf{v} - \mathbf{u}|^2}{2\theta} \right) d\mathbf{v} \\
&= \frac{n}{(2\pi\theta/m)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \exp \left(-\left| \frac{\mathbf{v} - \mathbf{u}}{(2\theta/m)^{\frac{1}{2}}} \right|^2 \right) d\mathbf{v}.
\end{aligned} \quad (2.108)$$

Consider the substitution

$$\mathbf{s} = \frac{\mathbf{v} - \mathbf{u}}{(2\theta/m)^{\frac{1}{2}}} \implies d\mathbf{s} = \left(\frac{1}{(2\theta/m)^{\frac{1}{2}}} \right)^d d\mathbf{v} \implies d\mathbf{v} = (2\theta/m)^{\frac{d}{2}} d\mathbf{s}. \quad (2.109)$$

The integral becomes

$$\begin{aligned}
\int_{\mathbb{R}^d} M_f d\mathbf{v} &= \frac{n}{(2\pi\theta/m)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \exp(-|\mathbf{s}|^2) (2\theta/m)^{\frac{d}{2}} d\mathbf{s} \\
&= \frac{n(2\theta/m)^{\frac{d}{2}}}{\pi^{\frac{d}{2}} (2\theta/m)^{\frac{d}{2}}} \int_{\mathbb{R}^d} e^{-|\mathbf{s}|^2} d\mathbf{s}
\end{aligned}$$

$$\begin{aligned}
&= \frac{n}{\pi^{\frac{d}{2}}} \cdot \pi^{\frac{d}{2}} \\
&= \int_{\mathbb{R}^d} f \, d\mathbf{v},
\end{aligned} \tag{2.110}$$

as desired. Note that we have used the definition $n = \int_{\mathbb{R}^d} f \, d\mathbf{v}$, and the fact that in d dimensions, the integral $\int_{\mathbb{R}^d} e^{-|\mathbf{x}|^2} \, d\mathbf{x} = \pi^{\frac{d}{2}}$. We will use this frequently.

2. Next we show that

$$\int_{\mathbb{R}^d} \mathbf{v} M_f \, d\mathbf{v} = \int_{\mathbb{R}^d} \mathbf{v} f \, d\mathbf{v}. \tag{2.111}$$

Following a similar line of work, we have

$$\begin{aligned}
\int_{\mathbb{R}^d} \mathbf{v} M_f \, d\mathbf{v} &= \int_{\mathbb{R}^d} \frac{n}{(2\pi\theta/m)^{\frac{d}{2}}} \mathbf{v} \exp\left(-\frac{|\mathbf{v} - \mathbf{u}|^2}{2\theta/m}\right) \, d\mathbf{v} \\
&= \frac{n}{(2\pi\theta/m)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \mathbf{v} \exp\left(-\left|\frac{\mathbf{v} - \mathbf{u}}{(2\theta/m)^{\frac{1}{2}}}\right|^2\right) \, d\mathbf{v}.
\end{aligned} \tag{2.112}$$

Using the substitution in (2.109), the integral becomes

$$\begin{aligned}
\int_{\mathbb{R}^d} \mathbf{v} M_f \, d\mathbf{v} &= \frac{n}{(2\pi\theta/m)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \left((2\theta/m)^{\frac{1}{2}} \mathbf{s} + \mathbf{u}\right) \exp(-|\mathbf{s}|^2) \cdot (2\theta/m)^{\frac{d}{2}} \, d\mathbf{s} \\
&= \frac{n(2\theta/m)^{\frac{d}{2}}}{\pi^{\frac{d}{2}}(2\theta/m)^{\frac{d}{2}}} \left[(2\theta/m)^{\frac{1}{2}} \int_{\mathbb{R}^d} \mathbf{s} e^{-|\mathbf{s}|^2} \, d\mathbf{s} + \mathbf{u} \int_{\mathbb{R}^d} e^{-|\mathbf{s}|^2} \, d\mathbf{s} \right] \\
&= \frac{n}{\pi^{\frac{d}{2}}} \left[(2\theta/m)^{\frac{1}{2}} \int_{\mathbb{R}^d} \mathbf{s} e^{-|\mathbf{s}|^2} \, d\mathbf{s} + \mathbf{u} \int_{\mathbb{R}^d} e^{-|\mathbf{s}|^2} \, d\mathbf{s} \right].
\end{aligned} \tag{2.113}$$

Let us deal with the first term in (2.113). One can easily show that

$$\int_{-\infty}^{\infty} x e^{-x^2} \, dx = 0 \implies \int_{\mathbb{R}^d} \mathbf{s} e^{-|\mathbf{s}|^2} \, d\mathbf{s} = \mathbf{0}.$$

Therefore, we have

$$\int_{\mathbb{R}^d} \mathbf{v} M_f \, d\mathbf{v} = \frac{n}{\pi^{\frac{d}{2}}} \cdot \mathbf{u} \int_{\mathbb{R}^d} e^{-|\mathbf{s}|^2} \, d\mathbf{s} = \frac{n\mathbf{u}}{\pi^{\frac{d}{2}}} \cdot \pi^{\frac{d}{2}} = n\mathbf{u} = \int_{\mathbb{R}^d} \mathbf{v} f \, d\mathbf{v}.$$

3. Finally, we show that

$$\int \frac{|\mathbf{v}|^2}{2} M_f \, d\mathbf{v} = \int \frac{|\mathbf{v}|^2}{2} f \, d\mathbf{v}. \tag{2.114}$$

First, observe that

$$\int_{\mathbb{R}^d} |\mathbf{s}|^2 e^{-|\mathbf{s}|^2} d\mathbf{s} = \frac{d}{2} \pi^{\frac{d}{2}}. \quad (2.115)$$

(To see how to prove such results, see Appendix A). Now, using the substitution in (2.109), and the same integration techniques on the LHS of (2.114),

$$\begin{aligned} \int \frac{|\mathbf{v}|^2}{2} M_f d\mathbf{v} &= \frac{1}{2} \frac{n}{(2\pi\theta/m)^{\frac{d}{2}}} \int |\mathbf{v}|^2 e^{-\frac{|\mathbf{v}-\mathbf{u}|^2}{2\theta/m}} d\mathbf{v} \\ &= \frac{1}{2} \frac{n}{(2\pi\theta/m)^{\frac{d}{2}}} \int |\mathbf{u} + (\mathbf{v} - \mathbf{u})|^2 e^{-\frac{|\mathbf{v}-\mathbf{u}|^2}{2\theta/m}} d\mathbf{v} \\ &= \frac{n}{2(2\pi\theta/m)^{\frac{d}{2}}} \int (-|\mathbf{u}|^2 + 2\mathbf{u}^\top \mathbf{v} + |\mathbf{v} - \mathbf{u}|^2) e^{-\frac{|\mathbf{v}-\mathbf{u}|^2}{2\theta/m}} d\mathbf{v} \\ &= \frac{-n|\mathbf{u}|^2}{2(2\pi\theta/m)^{\frac{d}{2}}} (2\theta/m)^{\frac{d}{2}} \int_{\mathbb{R}^d} e^{-|\mathbf{s}|^2} d\mathbf{s} \\ &\quad + \frac{2n(2\theta/m)^{\frac{d}{2}}}{2(2\pi\theta/m)^{\frac{d}{2}}} \mathbf{u}^\top \int_{\mathbb{R}^d} [\mathbf{u} + (2\theta/m)^{\frac{1}{2}} \mathbf{s}] e^{-|\mathbf{s}|^2} d\mathbf{s} \\ &\quad + \frac{n(2\theta/m)^{\frac{d}{2}+1}}{2(2\pi\theta/m)^{\frac{d}{2}}} \int_{\mathbb{R}^d} |\mathbf{s}|^2 e^{-|\mathbf{s}|^2} d\mathbf{s} \\ &= \frac{-n|\mathbf{u}|^2}{2\pi^{\frac{d}{2}}} \pi^{\frac{d}{2}} + \frac{n|\mathbf{u}|^2}{\pi^{\frac{d}{2}}} \pi^{\frac{d}{2}} + 0 + \frac{2n\theta/m}{2\pi^{\frac{d}{2}}} \frac{d}{2} \pi^{\frac{d}{2}} \\ &= \frac{1}{2} n|\mathbf{u}|^2 + \frac{d}{2} n\theta/m \\ &= \int_{\mathbb{R}^d} \frac{|\mathbf{v}|^2}{2} f d\mathbf{v}, \end{aligned} \quad (2.116)$$

where the final line follows from identity (2.86) (with d and 3 interchanged).

The proof is complete. ■

We need the following simple result.

Lemma 2.6.3. *Suppose that $f : \mathbb{R}^d \rightarrow [0, \infty)$ is a kinetic distribution of particles of mass $m > 0$, with the property*

$$\int_{\mathbb{R}^d} f(\mathbf{v}) |\mathbf{v}|^k d\mathbf{v} < \infty, \quad k = 0, 1, 2. \quad (2.117)$$

The function $\ln(M_f)$ is a Maxwellian invariant, namely,

$$\int_{\mathbb{R}^d} \ln(M_f(\mathbf{v})) (M_f(\mathbf{v}) - f(\mathbf{v})) d\mathbf{v} = \langle \ln(M_f)(M_f - f) \rangle = 0.$$

Proof. From the last result, we already know that, for any $C_0, C_2 \in \mathbb{R}$, and any $\mathbf{C}_1 \in \mathbb{R}^d$,

$$\langle (C_0 + \mathbf{C}_1 \cdot \mathbf{v} + C_2 |\mathbf{v}|^2)(M_f - f) \rangle = 0.$$

Clearly,

$$\ln(M_f) = \ln(\exp(\boldsymbol{\alpha} \cdot \mathbf{m})) = \boldsymbol{\alpha} \cdot \mathbf{m},$$

is a linear combination of 1, $\mathbf{v}$, and $|\mathbf{v}|^2$. It follows that $\ln(M_f)$ is also a Maxwellian invariant, that is, $\langle \ln(M_f)(M_f - f) \rangle = 0$. ■

The Maxwellian is the least information, or information minimizing (entropy maximizing), state. Consider the following result.

Theorem 2.6.4. *Suppose that*

$$f_\star : \mathbb{R}^d \rightarrow [0, \infty)$$

is a given kinetic distribution. Let

$$\boldsymbol{\rho}_\star = [\rho_\star, \rho_\star \mathbf{u}_\star^\top, \omega_\star]^\top,$$

be the vector comprised of the first three moments of $f_\star$, that is,

$$\boldsymbol{\rho}_\star = \begin{bmatrix} \rho_\star \\ \rho_\star \mathbf{u}_\star \\ \omega_\star \end{bmatrix} = \left\langle f_\star(\mathbf{v}) \begin{bmatrix} m \\ m\mathbf{v} \\ \frac{m}{2} |\mathbf{v}|^2 \end{bmatrix} \right\rangle.$$

The temperature, $\theta_\star$, is defined via

$$\omega_\star = \frac{\rho_\star}{2} |\mathbf{u}_\star|^2 + e_\star = \frac{\rho_\star}{2} |\mathbf{u}_\star|^2 + \frac{d}{2} n_\star \theta_\star.$$

The Maxwellian, as usual, is defined using the macroscopic densities as

$$M_\star(\mathbf{x}, \mathbf{v}) := n_\star \left(\frac{m}{2\pi\theta_\star} \right)^{d/2} \exp \left(-\frac{m|\mathbf{v} - \mathbf{u}_\star|^2}{2\theta_\star} \right).$$

Consider the admissible class of distribution functions, defined as

$$\mathcal{A}_\star := \left\{ g : \mathbb{R}^d \rightarrow \mathbb{R} \mid g \geq 0 \quad \text{and} \quad \langle m\mathbf{g} \rangle = \boldsymbol{\rho}_\star \right\},$$

where, recall,

$$\mathbf{m}(\mathbf{v}) := \left[m, m\mathbf{v}^\top, \frac{m}{2}|\mathbf{v}|^2 \right]^\top : \mathbb{R}^d \rightarrow \mathbb{R}^{d+2}.$$

Then, $M_\star, f_\star \in \mathcal{A}_\star$. In other words, $\mathcal{A}_\star$ is non-empty. For every $g \in \mathcal{A}_\star$,

$$h[M_\star] \leq h[g],$$

where $h[g]$ is the information content of g , defined as

$$h[g] := \int_{\mathbb{R}^d} g(\mathbf{v}) \ln(g(\mathbf{v})) \, d\mathbf{v}.$$

In other words, the Maxwellian is the minimum information distribution out of the set of admissible distributions that gives rise to the macroscopic density $\rho_\star$.

Proof. Let us first show that $M_\star \in \mathcal{A}_\star$. Clearly $M_\star$ is non-negative. The fact that $\langle \mathbf{m} M_\star \rangle = \rho_\star$ follows from Lemma 2.6.2. Thus $M_\star \in \mathcal{A}_\star$.

Next, we prove the inequality. Let $g \in \mathcal{A}_\star$ be arbitrary. We may write $M_\star = M_g$, since g gives rise to the same macroscopic fields as $f_\star$. Define $\hat{h}(s) := s \ln(s)$. This function $\hat{h}$ is convex on $(0, \infty)$, as is easy to show. Its first two derivatives are

$$\hat{h}'(s) = \ln(s) + 1, \quad \hat{h}''(s) = \frac{1}{s} > 0, \quad \forall s > 0.$$

Thus,

$$\hat{h}(s) \geq \hat{h}(t) + \hat{h}'(t)(s - t), \quad \forall s, t \in (0, \infty).$$

It follows that, point-wise in $\mathbf{v}$,

$$\begin{aligned} \hat{h}(g) &\geq \hat{h}(M_g) + \hat{h}'(M_g)(g - M_g) \\ &= \hat{h}(M_g) + \ln(M_g)(g - M_g) + g - M_g. \end{aligned}$$

By Lemma 2.6.3,

$$\int_{\mathbb{R}^d} \hat{h}(g) \, d\mathbf{v} \geq \int_{\mathbb{R}^d} \hat{h}(M_g) \, d\mathbf{v} + \int_{\mathbb{R}^d} \ln(M_g)(g - M_g) \, d\mathbf{v} + \int_{\mathbb{R}^d} (g - M_g) \, d\mathbf{v} = \int_{\mathbb{R}^d} \hat{h}(M_g) \, d\mathbf{v}.$$

This shows that,

$$h[g] \geq h[M_g] = h[M_\star],$$

and the result is proven. ■

2.7 Space-Homogeneous Model

Definition 2.7.1. We say that the kinetic distributions $f_i : \mathbb{R}^3 \times [0, T] \rightarrow [0, \infty)$, $i = 1, \dots, N$, satisfy the **space-homogeneous multi-species Boltzmann equation** iff, for all $\mathbf{v} \in \mathbb{R}^3$ and $t \in (0, T]$,

$$\partial_t f_i(\mathbf{v}, t) = Q_i[f_i, \mathbf{f}](\mathbf{v}, t), \quad (2.118)$$

where $Q_i[f_i, \mathbf{f}]$, the **cumulative binary collision operator**, is defined as

$$Q_i[f_i, \mathbf{f}](\mathbf{v}, t) := \sum_{j=1}^N Q_{i,j}[f_i, f_j](\mathbf{v}, t). \quad (2.119)$$

For the space-homogeneous model, the approach of the system to the equilibrium Maxwellian states is clear.

Proposition 2.7.2 (H-Theorem). Suppose that $f_1, \dots, f_N : \mathbb{R}^3 \times [0, T] \rightarrow [0, \infty)$ are kinetic distributions that satisfy the space-homogeneous multi-species Boltzmann equation. Assume that the collision kernels $B_{i,j}$ have proper structure. Then,

$$\partial_t h(t) = \sigma_h(t) \leq 0, \quad (2.120)$$

where h is the **information content**, defined as

$$h(t) := \sum_{i=1}^N \int_{\mathbb{R}^3} f_i(\mathbf{v}, t) \ln(f_i(\mathbf{v}, t)) \, d\mathbf{v},$$

and σ_h is the **information loss rate**, defined via

$$\sigma_h(t) := \sum_{i=1}^N \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{v}, t) \ln(f_i(\mathbf{v}, t)) \, d\mathbf{v}.$$

Proof. The result follows from the proof of Proposition 2.4.3. ■

The following also follows from a previously-established result.

Proposition 2.7.3. Suppose that $f_i : \mathbb{R}^3 \times [0, \infty) \rightarrow [0, \infty)$, $i = 1, \dots, N$, are kinetic distributions with the properties

$$\int_{\mathbb{R}^3} f_i(\mathbf{v}, t) |\mathbf{v}|^k \, d\mathbf{v} < \infty, \quad k = 0, 1, 2, 3, \quad (2.121)$$

for every $t \geq 0$. Assume that the kinetic distributions satisfy the space-homogeneous multi-species Boltzmann system. Then, for all $t \geq 0$, and for each $i = 1, \dots, N$,

$$d_t \rho_i(t) = 0, \quad (2.122)$$

$$\rho_i d_t \mathbf{u}_i(t) = m_i \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{v}, t) \mathbf{v} d\mathbf{v}, \quad (2.123)$$

and

$$d_t \left(\frac{\rho_i}{2} |\mathbf{u}_i(t)|^2 + e_i(t) \right) = \frac{m_i}{2} \int_{\mathbb{R}^3} Q_i[f_i, \mathbf{f}](\mathbf{v}, t) |\mathbf{v}|^2 d\mathbf{v}. \quad (2.124)$$

Consequently, using the collisional invariants,

$$d_t \rho(t) = 0, \quad (2.125)$$

$$\rho d_t \mathbf{u}(t) = 0, \quad (2.126)$$

and

$$d_t \omega(t) = d_t \sum_{i=1}^N \left(\frac{\rho_i}{2} |\mathbf{u}_i(t)|^2 + e_i(t) \right) = 0. \quad (2.127)$$

Remark 2.7.4. It can be proven that solutions to the space-homogeneous multi-species Boltzmann equation dissipate the information content,

$$h(t) := \sum_{i=1}^N \int_{\mathbb{R}^3} f_i(\mathbf{v}, t) \ln(f_i(\mathbf{v}, t)) d\mathbf{v},$$

until the system reaches an equilibrium state (at $t = \infty$) characterized by

$$0 = [\sigma_h]_\infty := \sum_{i=1}^N \int_{\mathbb{R}^3} Q_i[f_{i,\infty}, \mathbf{f}_\infty](\mathbf{v}) \ln(f_{i,\infty}(\mathbf{v})) d\mathbf{v}.$$

The kinetic distributions evolve in such a way that ρ_i is time invariant, and the total momentum and energy are conserved. At equilibrium, the kinetic distributions will be Maxwellians, as guaranteed by Proposition 2.4.4. The particle temperatures will equilibrate to same temperatures, that is,

$$\lim_{t \rightarrow \infty} \theta_i(t) = \theta_\infty > 0, \quad i = 1, \dots, N.$$

Chapter 3

Single-Species BGK Kinetic Models

In this chapter, we describe some basic theory for the single-species BGK equation [2, 44], namely,

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \lambda (M_f - f). \quad (3.1)$$

It is clear to see why the BGK model is attractive. The collision term is much easier to compute than that of the Boltzmann equation. Furthermore, solutions are attracted to the Maxwellian states.

The existence of non-negative solutions to the (single-species) BGK equation was proved for $\mathbf{x} \in \mathbb{R}^d$ by Perthame (1989) [35], and on bounded domains by Ringeissen (1991) [39]. Uniqueness of mild solutions for the (single-species) spatially periodic case was shown by Perthame and Pulvirenti (1993) [34], and extended to the full space, $\mathbf{x} \in \mathbb{R}^d$, by Mischler (1996) [32].

Beyond questions about existence and uniqueness of solutions, it is important to have a firm grasp of the properties of solutions to BGK-type equations, since it is vital to build numerical approximation schemes that respect analogous features at the fully discrete level. Herein, we review conservation and entropy dissipation solution properties, and, later, we discuss how these are used in the design of numerical schemes.

3.1 Basic Properties of Solutions

Since we are examining the single-species case first, that is, the unary case, we can simplify our discussion slightly by setting the mass to be one, $m = 1$. We recall that the Maxwellian

is constructed using the first three integral moments of the kinetic distribution, f , that is,

$$n(\mathbf{x}, t) := \int_{\mathbb{R}^d} f \, d\mathbf{v}, \quad \mathbf{u}(\mathbf{x}, t) := \frac{1}{n} \int_{\mathbb{R}^d} f \mathbf{v} \, d\mathbf{v}, \quad \theta(\mathbf{x}, t) := \frac{1}{nd} \int_{\mathbb{R}^d} f |\mathbf{v} - \mathbf{u}|^2 \, d\mathbf{v}, \quad (3.2)$$

and is defined as

$$M_f(\mathbf{x}, \mathbf{v}, t) := M[f](\mathbf{x}, \mathbf{v}, t) := n \left(\frac{1}{2\pi\theta} \right)^{d/2} \exp \left(-\frac{|\mathbf{v} - \mathbf{u}|^2}{2\theta} \right). \quad (3.3)$$

The space-time fields n , $\mathbf{u}$, and θ , are the macroscopic (coarse grained) number density, bulk velocity, and temperature, respectively. The macroscopic kinetic energy density is given by

$$\omega(\mathbf{x}, t) := \frac{1}{2} \int_{\mathbb{R}^d} f |\mathbf{v}|^2 \, d\mathbf{v}, \quad (3.4)$$

and the internal energy density is defined as

$$e(\mathbf{x}, t) := \frac{1}{2} \int_{\mathbb{R}^d} f |\mathbf{v} - \mathbf{u}|^2 \, d\mathbf{v}. \quad (3.5)$$

We observe that the temperature and the internal energy are related via

$$\theta(\mathbf{x}, t) = \frac{2}{d} \frac{e(\mathbf{x}, t)}{n(\mathbf{x}, t)}.$$

3.1.1 Collision Invariants

Again, we define $\langle \cdot \rangle : L^1(\mathbb{R}^d; \mathbb{R}^p) \rightarrow \mathbb{R}^p$ by

$$\langle \mathbf{g} \rangle = \int_{\mathbb{R}^d} \mathbf{g}(\mathbf{v}) \, d\mathbf{v}.$$

Therefore,

$$\begin{bmatrix} n(\mathbf{x}, t) \\ n(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \\ \omega(\mathbf{x}, t) \end{bmatrix} = \left\langle f(\mathbf{x}, \mathbf{v}, t) \begin{bmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2} |\mathbf{v}|^2 \end{bmatrix} \right\rangle.$$

Thus, the macroscopic density, n , momentum, $\mathbf{p} := n\mathbf{u}$, and energy density, ω , may be viewed as the first three moments of the particle distribution function f . The first three moments of the collision operator are equal to zero. This gives us some conservation properties, as we show below.

For convenience, let us define

$$\boldsymbol{\rho}(\mathbf{x}, t) := [n, n\mathbf{u}^\top, \omega]^\top : \mathbb{R}^d \times \mathbb{R}^+ \rightarrow \mathbb{R}^{d+2}; \quad (3.6)$$

$$\mathbf{m}(\mathbf{v}) := \left[1, \mathbf{v}^\top, \frac{1}{2}|\mathbf{v}|^2\right]^\top : \mathbb{R}^d \rightarrow \mathbb{R}^{d+2}; \quad (3.7)$$

and

$$\boldsymbol{\alpha}(\mathbf{x}, t) := \left[\ln \left(\frac{n}{(2\pi\theta)^{d/2}} \right) - \frac{|\mathbf{u}|^2}{2\theta}, \frac{\mathbf{u}^\top}{\theta}, -\frac{1}{\theta} \right]^\top : \mathbb{R}^d \times \mathbb{R}^+ \rightarrow \mathbb{R}^{d+2}. \quad (3.8)$$

Then, succinctly,

$$\boldsymbol{\rho} = \langle f \mathbf{m} \rangle, \quad \text{and} \quad M_f = \exp(\boldsymbol{\alpha} \cdot \mathbf{m}(\mathbf{v})). \quad (3.9)$$

We summarize some facts that we have already established in the previous chapter.

Lemma 3.1.1. *The following equality holds:*

$$\langle (M_f - f) \mathbf{m} \rangle = \left\langle \begin{bmatrix} 1 \\ \mathbf{v} \\ \frac{|\mathbf{v}|^2}{2} \end{bmatrix} (M_f - f) \right\rangle = \mathbf{0}. \quad (3.10)$$

Definition 3.1.2. *We say that a function $g(\mathbf{v})$ is a **BGK collision invariant** iff*

$$\langle g(\mathbf{v}) (M_f - f) \rangle = \int_{\mathbb{R}^d} g(\mathbf{v}) (M_f - f) \, d\mathbf{v} = 0.$$

From the last Lemma, we observe that 1 , $\mathbf{v}$ and $|\mathbf{v}|^2$ are BGK collision invariant. Of course, any linear combination of these functions will also be collision invariant. We will use this fact later.

Multiplying the BGK Equation by the vector $\mathbf{m} = [1, \mathbf{v}^\top, \frac{1}{2}|\mathbf{v}|^2]^\top$ and integrating, we get expressions for the conservation of mass, momentum, and energy, respectively.

Lemma 3.1.3. *Suppose that f is a non-negative solution to the BGK equation (3.1). The following conservation equations hold:*

$$\frac{\partial}{\partial t} n + \nabla_{\mathbf{x}} \cdot (n\mathbf{u}) = 0, \quad (3.11)$$

$$\frac{\partial}{\partial t} (n\mathbf{u}) + \nabla_{\mathbf{x}} \cdot (n\mathbf{u} \otimes \mathbf{u} + \mathbf{P}) = \mathbf{0}, \quad (3.12)$$

$$\frac{\partial}{\partial t} \omega + \nabla_{\mathbf{x}} \cdot (\omega\mathbf{u} + \mathbf{P}\mathbf{u} + \mathbf{q}) = 0, \quad (3.13)$$

where

$$\mathbf{P} := \int_{\mathbb{R}^d} (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v}$$

is the pressure tensor and

$$\mathbf{q} := \frac{1}{2} \int_{\mathbb{R}^d} |\mathbf{v} - \mathbf{u}|^2 (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v}$$

is the heat flux.

Proof. The proof is more or less the same as that for the multi-species Boltzmann equation that we exhibited in the previous chapter. Multiplying the BGK equation by 1 and integrating, we have

$$\int_{\mathbb{R}^d} \left[\frac{\partial f}{\partial t} + \nabla_x \cdot (\mathbf{v} f) \right] d\mathbf{v} = \int_{\mathbb{R}^d} \lambda (M_f - f) d\mathbf{v} \quad (3.14)$$

$$\implies \frac{\partial}{\partial t} \left(\int_{\mathbb{R}^d} f \, d\mathbf{v} \right) + \nabla_x \cdot \left(\int_{\mathbb{R}^d} \mathbf{v} f \, d\mathbf{v} \right) = 0 \quad (3.15)$$

$$\implies \frac{\partial}{\partial t} n + \nabla_x \cdot (n\mathbf{u}) = 0. \quad (3.16)$$

This verifies the first equation, which is an expression for the conservation of mass.

Next, multiplying by $\mathbf{v}$ and integrating, we have

$$\int_{\mathbb{R}^d} \left[\mathbf{v} \frac{\partial f}{\partial t} + \nabla_x \cdot (\mathbf{v} \otimes \mathbf{v} f) \right] d\mathbf{v} = \int_{\mathbb{R}^d} \mathbf{v} \lambda (M_f - f) d\mathbf{v} \quad (3.17)$$

$$\implies \frac{\partial}{\partial t} \left(\int_{\mathbb{R}^d} \mathbf{v} f \, d\mathbf{v} \right) + \nabla_x \cdot \left(\int_{\mathbb{R}^d} \mathbf{v} \otimes \mathbf{v} f \, d\mathbf{v} \right) = \mathbf{0}. \quad (3.18)$$

The first term is equal to $\partial_t(n\mathbf{u})$, as desired. It remains to show that

$$\int_{\mathbb{R}^d} \mathbf{v} \otimes \mathbf{v} f \, d\mathbf{v} = n\mathbf{u} \otimes \mathbf{u} + \mathbf{P}.$$

Writing $\mathbf{v} = \mathbf{u} + (\mathbf{v} - \mathbf{u})$, gives

$$\begin{aligned} \int_{\mathbb{R}^d} \mathbf{v} \otimes \mathbf{v} f \, d\mathbf{v} &= \int_{\mathbb{R}^d} [\mathbf{u} + (\mathbf{v} - \mathbf{u})] \otimes [\mathbf{u} + (\mathbf{v} - \mathbf{u})] f \, d\mathbf{v} \\ &= \int_{\mathbb{R}^d} [\mathbf{u} \otimes \mathbf{u} + \mathbf{u} \otimes (\mathbf{v} - \mathbf{u}) + (\mathbf{v} - \mathbf{u}) \otimes \mathbf{u} + (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u})] f \, d\mathbf{v} \\ &= n\mathbf{u} \otimes \mathbf{u} + \mathbf{P} + \int_{\mathbb{R}^d} \mathbf{u} \otimes (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} + \int_{\mathbb{R}^d} (\mathbf{v} - \mathbf{u}) \otimes \mathbf{u} f \, d\mathbf{v}. \end{aligned} \quad (3.19)$$

The last two terms in the above expression are equal to zero:

$$\mathbf{u} \otimes \int_{\mathbb{R}^d} (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} = \mathbf{u} \otimes \left[\int_{\mathbb{R}^d} \mathbf{v} f \, d\mathbf{v} - \mathbf{u} \int_{\mathbb{R}^d} f \, d\mathbf{v} \right] = \mathbf{u} \otimes [n\mathbf{u} - n\mathbf{u}] = \mathbf{0}.$$

Putting it all together, we obtain the second equation, an expression for the conservation of momentum.

Finally, multiplying by $\frac{1}{2}|\mathbf{v}|^2$ and integrating, gives

$$\int_{\mathbb{R}^d} \frac{1}{2} |\mathbf{v}|^2 \left(\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{v} f) \right) d\mathbf{v} = \int_{\mathbb{R}^d} \frac{1}{2} |\mathbf{v}|^2 \lambda(M_f - f) d\mathbf{v} \quad (3.20)$$

$$\implies \frac{\partial}{\partial t} \left(\int_{\mathbb{R}^d} \frac{1}{2} |\mathbf{v}|^2 f \, d\mathbf{v} \right) + \nabla_{\mathbf{x}} \cdot \left(\int_{\mathbb{R}^d} \frac{1}{2} |\mathbf{v}|^2 \mathbf{v} f \, d\mathbf{v} \right) = 0. \quad (3.21)$$

The first term is equal to $\partial_t \omega$, as desired. It remains to show that

$$\int_{\mathbb{R}^d} \frac{1}{2} |\mathbf{v}|^2 \mathbf{v} f \, d\mathbf{v} = \omega \mathbf{u} + \mathbf{P} \mathbf{u} + \mathbf{q}.$$

Writing $\mathbf{v} = \mathbf{u} + (\mathbf{v} - \mathbf{u})$, gives

$$\begin{aligned} \int_{\mathbb{R}^d} \frac{1}{2} |\mathbf{v}|^2 \mathbf{v} f \, d\mathbf{v} &= \frac{1}{2} \int_{\mathbb{R}^d} |\mathbf{v}|^2 [\mathbf{u} + (\mathbf{v} - \mathbf{u})] f \, d\mathbf{v} \\ &= \mathbf{u} \int_{\mathbb{R}^d} \frac{1}{2} |\mathbf{v}|^2 f \, d\mathbf{v} + \frac{1}{2} \int_{\mathbb{R}^d} |\mathbf{v}|^2 (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} \\ &= \omega \mathbf{u} + \frac{1}{2} \int_{\mathbb{R}^d} [\mathbf{u} + (\mathbf{v} - \mathbf{u})]^\top [\mathbf{u} + (\mathbf{v} - \mathbf{u})] (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} \\ &= \omega \mathbf{u} + \frac{1}{2} \int_{\mathbb{R}^d} [|\mathbf{u}|^2 + 2\mathbf{u}^\top (\mathbf{v} - \mathbf{u}) + |\mathbf{v} - \mathbf{u}|^2] (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} \\ &= \omega \mathbf{u} + \frac{|\mathbf{u}|^2}{2} \int_{\mathbb{R}^d} (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} + \int_{\mathbb{R}^d} \mathbf{u}^\top (\mathbf{v} - \mathbf{u}) (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} + \frac{1}{2} \int_{\mathbb{R}^d} |\mathbf{v} - \mathbf{u}|^2 (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} \\ &= \omega \mathbf{u} + \mathbf{q} + \frac{1}{2} |\mathbf{u}|^2 \left(\int_{\mathbb{R}^d} \mathbf{v} f \, d\mathbf{v} - \mathbf{u} \int_{\mathbb{R}^d} f \, d\mathbf{v} \right) + \int_{\mathbb{R}^d} \mathbf{u}^\top (\mathbf{v} - \mathbf{u}) (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} \\ &= \omega \mathbf{u} + \mathbf{q} + \frac{1}{2} |\mathbf{u}|^2 (n\mathbf{u} - n\mathbf{u}) + \int_{\mathbb{R}^d} \mathbf{u}^\top (\mathbf{v} - \mathbf{u}) (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} \\ &= \omega \mathbf{u} + \mathbf{q} + \int_{\mathbb{R}^d} \mathbf{u}^\top (\mathbf{v} - \mathbf{u}) (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v}. \end{aligned} \quad (3.22)$$

It should be easy to see that

$$\mathbf{u}^\top (\mathbf{v} - \mathbf{u}) (\mathbf{v} - \mathbf{u}) = [(\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u})] \mathbf{u}.$$

Thus, the final term in the above Equation is

$$\begin{aligned}
 \int_{\mathbb{R}^d} \mathbf{u}^\top (\mathbf{v} - \mathbf{u})(\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} &= \int_{\mathbb{R}^d} [(\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u})] \mathbf{u} f \, d\mathbf{v} \\
 &= \left(\int_{\mathbb{R}^d} (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} \right) \mathbf{u} \\
 &= \mathbf{P} \mathbf{u}.
 \end{aligned} \tag{3.23}$$

Putting it all together gives the third equation, which is an expression for the conservation of energy. The proof is complete. $\blacksquare$

The conservation laws/properties above are reminiscent of those involved with the derivations of the Navier–Stokes and Euler equations. In fact, using the Chapman–Enskog expansion method one can show that in the limit as $\lambda \rightarrow \infty$, or $\tau \rightarrow 0$, one recovers macroscopic Navier–Stokes and/or Euler equations as formal limits, under certain assumptions [40, 48, 46, 44]. These limits can even guide in the design of stable numerical methods for the macroscopic models [48].

3.1.2 Space-Homogeneous Problem

Suppose that the density function is spatially homogeneous and/or particle advection may be neglected in the system. In this case, the distribution function f satisfies the space-homogeneous problem

$$\frac{\partial f}{\partial t} = \lambda(M_f - f). \tag{3.24}$$

This is a first order integro-differential equation (IDE), which can be solved using the integrating factor method.

Lemma 3.1.4. *Suppose that f is a solution to the space-homogeneous problem (3.24). Then*

$$f(\mathbf{x}, \mathbf{v}, t) = e^{-\lambda t} f(\mathbf{x}, \mathbf{v}, 0) + (1 - e^{-\lambda t}) M_f(\mathbf{x}, \mathbf{v}, 0). \tag{3.25}$$

Proof. We begin by proving that $\frac{\partial n}{\partial t} = 0 = \frac{\partial \theta}{\partial t}$, $\frac{\partial \mathbf{u}}{\partial t} = \mathbf{0}$, and $\frac{\partial M_f}{\partial t} = 0$. We will make frequent use of Lemma 3.1.1.

First, we show that $\frac{\partial n}{\partial t} = 0$. Utilizing the IDE,

$$\frac{\partial}{\partial t} n = \frac{\partial}{\partial t} \int_{\mathbb{R}^d} f \, d\mathbf{v} = \int_{\mathbb{R}^d} \frac{\partial f}{\partial t} \, d\mathbf{v} = \int_{\mathbb{R}^d} \lambda(M_f - f) \, d\mathbf{v} \stackrel{\text{Lem. 3.1.1}}{=} 0. \tag{3.26}$$

Next, we show that $\frac{\partial \mathbf{u}}{\partial t} = \mathbf{0}$. Using the quotient rule on the definition of $\mathbf{u} = \frac{1}{n} \int_{\mathbb{R}^d} f \, d\mathbf{v}$, and the fact that $\frac{\partial n}{\partial t} = 0$ gives

$$\frac{\partial \mathbf{u}}{\partial t} = \frac{\partial}{\partial t} \frac{1}{n} \int_{\mathbb{R}^d} f \mathbf{v} \, d\mathbf{v} = \frac{(n) \int_{\mathbb{R}^d} \frac{\partial f}{\partial t} \mathbf{v} \, d\mathbf{v} - 0}{n^2} = \frac{1}{n} \int_{\mathbb{R}^d} \lambda(M_f - f) \mathbf{v} \, d\mathbf{v} \stackrel{\text{Lem. 3.1.1}}{=} \mathbf{0}. \quad (3.27)$$

Next, we show that $\frac{\partial \theta}{\partial t} = 0$. Recall that

$$\frac{d}{2} n \theta = \omega - \frac{1}{2} n |\mathbf{u}|^2 \quad \Longleftrightarrow \quad \theta = \frac{2\omega}{nd} - \frac{1}{d} |\mathbf{u}|^2.$$

Using the quotient rule, and the fact that $\frac{\partial n}{\partial t} = 0$ and $\frac{\partial \mathbf{u}}{\partial t} = \mathbf{0}$, gives

$$\frac{\partial \theta}{\partial t} = \frac{2}{d} \frac{\left(\frac{\partial \omega}{\partial t}\right) (n) - 0}{n^2} - \frac{2}{d} \mathbf{u}^\top \frac{\partial \mathbf{u}}{\partial t} = \frac{2}{nd} \int_{\mathbb{R}^d} \frac{|\mathbf{v}|^2}{2} \lambda(M_f - f) \, d\mathbf{v} \stackrel{\text{Lem. 3.1.1}}{=} 0. \quad (3.28)$$

Next, to show $\frac{\partial M_f}{\partial t} = 0$, we use the temporal invariance of n , $\mathbf{u}$, and θ , as shown above,

$$\begin{aligned} \frac{\partial}{\partial t} M_f(\mathbf{x}, \mathbf{v}, t) &= (2\pi)^{-\frac{d}{2}} \frac{\partial}{\partial t} \left[n(\mathbf{x}, t) \theta(\mathbf{x}, t)^{-\frac{d}{2}} \exp \left(-\frac{1}{2} |\mathbf{v} - \mathbf{u}(\mathbf{x}, t)|^2 \theta(\mathbf{x}, t)^{-1} \right) \right] \\ &= (2\pi)^{-\frac{d}{2}} \left[\frac{\partial n}{\partial t} \theta^{-\frac{d}{2}} \exp \left(-\frac{1}{2} |\mathbf{v} - \mathbf{u}|^2 \theta^{-1} \right) \right. \\ &\quad + n(\mathbf{x}, t) \left(-\frac{d}{2} \right) \theta^{-\frac{d+2}{2}} \frac{\partial \theta}{\partial t} \exp \left(-\frac{1}{2} |\mathbf{v} - \mathbf{u}|^2 \theta^{-1} \right) \\ &\quad \left. + n \theta^{-\frac{d}{2}} \exp \left(-\frac{1}{2} |\mathbf{v} - \mathbf{u}|^2 \theta^{-1} \right) \frac{\partial}{\partial t} \left[-\frac{1}{2} |\mathbf{v} - \mathbf{u}|^2 \theta^{-1} \right] \right] \\ &= 0. \end{aligned} \quad (3.29)$$

So far, we have $\frac{\partial n}{\partial t} = 0 = \frac{\partial \theta}{\partial t}$, $\frac{\partial \mathbf{u}}{\partial t} = \mathbf{0}$, and $\frac{\partial M_f}{\partial t} = 0$. To finish, we use these properties to solve the IDE. Rearranging (3.24), gives

$$\frac{df}{dt} + \lambda f = \lambda M.$$

Multiplying by the integrating factor, $e^{\lambda t}$, and applying the product rule in reverse, gives

$$\frac{d}{dt} (e^{\lambda t} f) = \lambda M_f e^{\lambda t}.$$

Integrating with respect to t , we have

$$e^{\lambda t} f = C + \lambda \int e^{\lambda t} M_f(\mathbf{x}, \mathbf{v}, t) \, dt,$$

Since $M_f = M_f(\mathbf{x}, \mathbf{v}, t)$ is constant with respect to t , $M_f(\mathbf{x}, \mathbf{v}, t) = M_f(\mathbf{x}, \mathbf{v}, 0)$. Hence, it can be pulled through the integral sign:

$$\begin{aligned} e^{\lambda t} f &= C + \lambda M_f(\mathbf{x}, \mathbf{v}, 0) \int e^{\lambda t} dt \\ &= C + M_f(\mathbf{x}, \mathbf{v}, 0) e^{\lambda t}. \end{aligned} \quad (3.30)$$

Plugging in $t = 0$, and rearranging gives an expression for the constant term:

$$e^0 f(\mathbf{x}, \mathbf{v}, 0) = C + e^0 M(\mathbf{x}, \mathbf{v}, 0) \quad (3.31)$$

$$\implies C = f(\mathbf{x}, \mathbf{v}, 0) - M(\mathbf{x}, \mathbf{v}, 0). \quad (3.32)$$

Putting everything together, and multiplying by $e^{-\lambda t}$, we have the following solution to the space-homogeneous problem:

$$\begin{aligned} f(\mathbf{x}, \mathbf{v}, t) &= e^{-\lambda t} (f(\mathbf{x}, \mathbf{v}, 0) - M_f(\mathbf{x}, \mathbf{v}, 0)) + M_f(\mathbf{x}, \mathbf{v}, 0) \\ &= e^{-\lambda t} f(\mathbf{x}, \mathbf{v}, 0) + (1 - e^{-\lambda t}) M_f(\mathbf{x}, \mathbf{v}, 0). \end{aligned} \quad (3.33)$$

■

Since we have the true solution to this space-homogeneous problem, this allows us to test the accuracy of the code on the right hand side source term. Initial tests are performed in Section 4.5.

3.1.3 The H-Theorem

In this section, we discuss a very important solution property for the BGK equation, namely the entropy dissipation property. This is a key stability concept that should, in some way, be preserved in numerical approximations. We start off this section with a definition.

Definition 3.1.5. Suppose that $f : \Omega \times \mathbb{R}^d \times [0, \infty) \rightarrow [0, \infty)$ is a particle distribution function. The object

$$H[f](\mathbf{x}, t) := \int_{\mathbb{R}^d} f(\mathbf{x}, \mathbf{v}, t) \ln(f(\mathbf{x}, \mathbf{v}, t)) d\mathbf{v}$$

is called the **H functional** or **kinetic entropy**. We say that a flow is **entropy-dissipative** iff,

for every $0 \leq t_1 \leq t_2 < \infty$,

$$\int_{\Omega} H[f](\mathbf{x}, t_2) d\mathbf{x} \leq \int_{\Omega} H[f](\mathbf{x}, t_1) d\mathbf{x}.$$

Remark 3.1.6. *We should point out that workers in equilibrium thermodynamics and non-equilibrium thermodynamics generally prefer a definition of entropy that sees the entropy increasing as a function of time. But, for historical reasons, in the mathematical and numerical theory of the Boltzmann and the BGK equations, the prevailing definition of entropy is such that it is decreasing in time. We have chosen to use the mathematics standard for the rest of the report. Note that we used the physics convention in the last chapter. In any case, this is simply a matter of a sign difference.*

Remark 3.1.7. *The mathematical dissipation property is an important marker for the design of numerical methods. In particular, a numerical approximation scheme should satisfy, if possible, some discrete form of entropy dissipation. However, designing fully discrete approximation schemes that theoretically satisfy discrete dissipation (as determined by a rigorous proof) is a challenging task. The papers [29, 30] address this issue for the single-species BGK equation, but, this dissipation property comes at a rather high computational cost. Thus, it is not clear from the outset that it is practical to pursue this property from the theoretical point of view. On the other hand, checking the dissipation property numerically for benchmark simulations is certainly a worthwhile endeavor.*

Theorem 3.1.8. *Suppose that $f : \Omega \times \mathbb{R}^d \times [0, \infty) \rightarrow [0, \infty)$ is a solution to the spatially homogeneous BGK problem, that is,*

$$\frac{\partial f}{\partial t} = \frac{1}{\tau} (M_f - f),$$

where $\tau > 0$ is a constant. Then

$$\frac{d}{dt} H[f] \leq 0.$$

Proof. Observe that

$$\begin{aligned} \frac{d}{dt} H[f](t) &= \int_{\mathbb{R}^d} \frac{\partial f}{\partial t} (\ln(f) + 1) d\mathbf{v} \\ &= \frac{1}{\tau} \int_{\mathbb{R}^d} (M_f - f) (\ln(f) + 1) d\mathbf{v} \\ &= \frac{1}{\tau} \int_{\mathbb{R}^d} \ln(f) (M_f - f) d\mathbf{v} \end{aligned}$$

To finish the proof, we use that fact that $\ln(M_f)$ is a BGK collision invariant, that is

$$\int_{\mathbb{R}^d} \ln(M_f) (M_f - f) d\mathbf{v} = 0.$$

Thus

$$\begin{aligned} \frac{d}{dt} H[f](t) &= \frac{1}{\tau} \int_{\mathbb{R}^d} (\ln(f) - \ln(M_f)) (M_f - f) d\mathbf{v} \\ &= -\frac{1}{\tau} \int_{\mathbb{R}^d} (\ln(M_f) - \ln(f)) (M_f - f) d\mathbf{v} \leq 0, \end{aligned}$$

where in the last step we used Lemma 2.4.2. ■

More generally, we have

Theorem 3.1.9. *Suppose that $f : \Omega \times \mathbb{R}^d \times [0, \infty) \rightarrow [0, \infty)$ is an Ω -periodic (spatially periodic) solution to the BGK equation, that is,*

$$\partial_t f + \mathbf{v} \cdot \nabla_x f = \frac{1}{\tau} (M_f - f),$$

where $\tau > 0$ is constant. Then

$$\partial_t \langle f \ln(f) \rangle + \nabla_x \cdot \langle \mathbf{v} f \ln(f) \rangle \leq 0.$$

and

$$\frac{d}{dt} \int_{\Omega} H[f] d\mathbf{x} \leq 0.$$

In other words, solutions of the BGK equation are entropy dissipative.

Proof. Similar to the last proof, but using Lemma 3.1.3, we have

$$\begin{aligned} \frac{\partial}{\partial t} H[f](t) &= \int_{\mathbb{R}^d} \frac{\partial f}{\partial t} (\ln(f) + 1) d\mathbf{v} \\ &= \int_{\mathbb{R}^d} \frac{\partial f}{\partial t} \ln(f) d\mathbf{v} + \frac{\partial n}{\partial t} \\ &= \frac{1}{\tau} \int_{\mathbb{R}^d} (M_f - f) \ln(f) d\mathbf{v} - \int_{\mathbb{R}^d} \mathbf{v} \cdot \nabla_x f \ln(f) d\mathbf{v} + \frac{\partial n}{\partial t} \\ &= \frac{1}{\tau} \int_{\mathbb{R}^d} (M_f - f) \ln(f) d\mathbf{v} - \nabla_x \cdot \int_{\mathbb{R}^d} \mathbf{v} f \ln(f) d\mathbf{v} + \int_{\mathbb{R}^d} \mathbf{v} f \cdot \nabla_x (\ln(f)) d\mathbf{v} + \frac{\partial n}{\partial t} \\ &= \frac{1}{\tau} \int_{\mathbb{R}^d} \ln(f) (M_f - f) d\mathbf{v} - \nabla_x \cdot \int_{\mathbb{R}^d} \mathbf{v} f \ln(f) d\mathbf{v} + \frac{\partial n}{\partial t} + \nabla_x \cdot (n\mathbf{u}) \\ &= \frac{1}{\tau} \int_{\mathbb{R}^d} \ln(f) (M_f - f) d\mathbf{v} - \nabla_x \cdot \int_{\mathbb{R}^d} \mathbf{v} f \ln(f) d\mathbf{v}. \end{aligned}$$

Therefore,

$$\partial_t \int_{\mathbb{R}^d} f \ln(f) d\mathbf{v} + \nabla_{\mathbf{x}} \cdot \int_{\mathbb{R}^d} \mathbf{v} f \ln(f) d\mathbf{v} = -\frac{1}{\tau} \int_{\mathbb{R}^d} (f - M_f)(\ln(f) - \ln(M_f)) d\mathbf{v} \leq 0.$$

In other words,

$$\partial_t \langle f \ln(f) \rangle + \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} f \ln(f) \rangle \leq 0.$$

Using the Ω -periodicity of f and integrating over Ω , we have

$$d_t \int_{\Omega} \int_{\mathbb{R}^d} f \ln(f) d\mathbf{v} d\mathbf{x} = -\frac{1}{\tau} \int_{\Omega} \int_{\mathbb{R}^d} (f - M_f)(\ln(f) - \ln(M_f)) d\mathbf{v} d\mathbf{x} \leq 0,$$

and the proof is complete. ■

Finally, we have

Theorem 3.1.10. *Suppose that*

$$f_{\star} : \Omega \times \mathbb{R}^d \rightarrow [0, \infty)$$

is a given Ω -periodic distribution. Let

$$\boldsymbol{\rho}_{\star} = [n_{\star}, n_{\star} \mathbf{u}_{\star}^{\top}, \omega_{\star}]^{\top},$$

be the vector comprised of the first three moments of $f_{\star}$, that is,

$$\boldsymbol{\rho}_{\star}(\mathbf{x}) = \begin{bmatrix} n_{\star}(\mathbf{x}) \\ n_{\star}(\mathbf{x}) \mathbf{u}_{\star}(\mathbf{x}) \\ \omega_{\star}(\mathbf{x}) \end{bmatrix} = \left\langle f_{\star}(\mathbf{x}, \mathbf{v}) \begin{bmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2} |\mathbf{v}|^2 \end{bmatrix} \right\rangle, \quad \forall \mathbf{x} \in \Omega.$$

The Ω -periodic temperature, $\theta_{\star}$, is defined via

$$\omega_{\star}(\mathbf{x}) = \frac{1}{2} n_{\star}(\mathbf{x}) |\mathbf{u}_{\star}(\mathbf{x})|^2 + \frac{d}{2} n_{\star}(\mathbf{x}) \theta_{\star}(\mathbf{x}).$$

The Maxwellian, as usual, is defined using the macroscopic densities as

$$M_{\star}(\mathbf{x}, \mathbf{v}) := n_{\star} \left(\frac{1}{2\pi\theta_{\star}} \right)^{d/2} \exp \left(-\frac{|\mathbf{v} - \mathbf{u}_{\star}|^2}{2\theta_{\star}} \right).$$

Consider the admissible class of distribution functions defined as

$$\mathcal{A}_* := \left\{ g : \Omega \times \mathbb{R}^d \rightarrow \mathbb{R} \mid g \text{ is } \Omega\text{-periodic, } g \geq 0, \text{ and } \langle \mathbf{m}g \rangle = \boldsymbol{\rho}_* \right\},$$

where, recall,

$$\mathbf{m}(\mathbf{v}) := \left[1, \mathbf{v}^\top, \frac{1}{2}|\mathbf{v}|^2 \right]^\top : \mathbb{R}^d \rightarrow \mathbb{R}^{d+2}.$$

Then, $M_*, f_* \in \mathcal{A}_*$. In other words, $\mathcal{A}_*$ is non-empty. For every $g \in \mathcal{A}_*$,

$$H[M_*](\mathbf{x}) \leq H[g](\mathbf{x}), \quad \forall \mathbf{x} \in \Omega.$$

In other words, the Maxwellian is the minimum information distribution out of the set of admissible distributions that gives rise to the macroscopic density $\boldsymbol{\rho}_*$.

Proof. This was proved in the last chapter. ■

3.2 Discrete-Velocity BGK Models

Discrete velocity BGK models are constructed under the assumption that the velocity space is partitioned into discrete, allowable states. This discretized velocity space could be finite or countably infinite, in principle. But, typically the velocity space is constructed so that it is finite and approximates well the density of particles, f , for a given physical case, meaning that the velocity points might clustered around particular velocity values. To make the discussion simple, we will restrict our attention to the $d = 1$ case. The general case is constructed similarly.

3.2.1 Discrete-Velocity BGK Model in One Space Dimension

Let us make an analog model in one space dimension ($d = 1$) with discrete, rather than continuous, velocities, along the lines of the papers [29, 30]. Suppose that $h_v \in (0, 1)$ and $J \in \mathbb{N}$. Set

$$\mathcal{V}_{\mathcal{J}} := \left\{ v_j = h_v \cdot \left(j - \frac{1}{2} \right) \mid j \in \mathcal{J} \right\},$$

where

$$\mathcal{J} := \{-J + 1, \dots, J\}.$$

Note that the simple structure of $\mathcal{V}_{\mathcal{J}}$, with uniformly spaced points arranged symmetrically about 0, is used only for simplicity, and we may choose it in a more general fashion. In any

case, set

$$\mathbf{m}_{\mathcal{J}}(\mathbf{j}) := \left[1, v_{\mathbf{j}}, \frac{1}{2}|v_{\mathbf{j}}|^2 \right]^{\top}, \quad \forall \mathbf{j} \in \mathcal{J}.$$

Define, for $\mathbf{g} : \mathcal{J} \rightarrow \mathbb{R}^d$

$$\langle \mathbf{g} \rangle_{\mathcal{J}} := \sum_{\mathbf{j} \in \mathcal{J}} \mathbf{g}_{\mathbf{j}} h_{\mathbf{j}}.$$

Let us define the admissible class of solutions.

Definition 3.2.1. Suppose that $\Omega = [a, b] \subset \mathbb{R}$ and

$$f_{\mathcal{J},*} : \Omega \times \mathcal{J} \rightarrow [0, \infty)$$

is a given Ω -periodic discrete-velocity distribution. Let

$$\boldsymbol{\rho}_{\mathcal{J},*} = [n_{\mathcal{J},*}, n_{\mathcal{J},*} u_{\mathcal{J},*}, E_{\mathcal{J},*}]^{\top},$$

be the vector comprised of the first three discrete-velocity moments of $f_{\mathcal{J},*}$, that is,

$$\boldsymbol{\rho}_{\mathcal{J},*}(x) = \begin{bmatrix} n_{\mathcal{J},*}(x) \\ n_{\mathcal{J},*}(x) u_{\mathcal{J},*}(x) \\ E_{\mathcal{J},*}(x) \end{bmatrix} = \langle f_{\mathcal{J},*}(x, \cdot) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}}, \quad \forall x \in \Omega. \quad (3.34)$$

The **admissible class of discrete-velocity distribution functions**, subordinate to $\boldsymbol{\rho}_{\mathcal{J},*}$ or $f_{\mathcal{J},*}$ is defined as the set

$$\mathcal{A}_{\mathcal{J},*} := \{g_{\mathcal{J}} : \Omega \times \mathcal{J} \rightarrow \mathbb{R} \mid g_{\mathcal{J}} \text{ is } \Omega\text{-periodic, } g_{\mathcal{J}} \geq 0, \text{ and } \langle \mathbf{m}_{\mathcal{J}} g_{\mathcal{J}} \rangle_{\mathcal{J}} = \boldsymbol{\rho}_{\mathcal{J},*}\}.$$

We need the following technical lemma.

Lemma 3.2.2. Suppose that the moment vector $\boldsymbol{\rho}_{\mathcal{J},*}$ is realized from an Ω -periodic discrete-velocity density as above. Fix $x \in \Omega = [a, b]$, and define the function $K : \mathbb{R}^3 \rightarrow \mathbb{R}$ via

$$K(\boldsymbol{\beta}) = K_x(\boldsymbol{\beta}) := \langle \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \rangle_{\mathcal{J}} - \boldsymbol{\beta} \cdot \boldsymbol{\rho}_{\mathcal{J},*}(x), \quad \forall \boldsymbol{\beta} \in \mathbb{R}^3.$$

$K(\cdot)$ is smooth, convex, and coercive and, therefore, has a unique minimizer, $\boldsymbol{\beta}_* \in \mathbb{R}^3$, which satisfies the nonlinear equation

$$\langle \exp(\boldsymbol{\beta}_* \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} = \boldsymbol{\rho}_{\mathcal{J},*}(x).$$

Proof. Clearly, K is smooth. To see that it is convex, consider the first two functional derivatives. The first derivative is computed via

$$\begin{aligned} \frac{d}{ds} K(\boldsymbol{\beta} + s\boldsymbol{\eta}) &= \frac{d}{ds} \langle \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \exp(s\boldsymbol{\eta} \cdot \mathbf{m}_{\mathcal{J}}) \rangle_{\mathcal{J}} - \frac{d}{ds} (\boldsymbol{\beta} + s\boldsymbol{\eta}) \cdot \boldsymbol{\rho}_{\mathcal{J},*}(x) \\ &= \langle \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \boldsymbol{\eta} \cdot \mathbf{m}_{\mathcal{J}} \exp(s\boldsymbol{\eta} \cdot \mathbf{m}_{\mathcal{J}}) \rangle_{\mathcal{J}} - \boldsymbol{\eta} \cdot \boldsymbol{\rho}_{\mathcal{J},*}(x). \end{aligned}$$

Thus,

$$\begin{aligned} \left. \frac{d}{ds} K(\boldsymbol{\beta} + s\boldsymbol{\eta}) \right|_{s=0} &= \langle \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \boldsymbol{\eta} \cdot \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} - \boldsymbol{\eta} \cdot \boldsymbol{\rho}_{\mathcal{J},*}(x) \\ &= \boldsymbol{\eta} \cdot \{ \langle \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} - \boldsymbol{\rho}_{\mathcal{J},*}(x) \}, \end{aligned}$$

and we can write

$$\nabla K(\boldsymbol{\beta}) = \langle \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} - \boldsymbol{\rho}_{\mathcal{J},*}(x).$$

Further,

$$\begin{aligned} \frac{d^2}{ds^2} K(\boldsymbol{\beta} + s\boldsymbol{\eta}) &= \frac{d}{ds} \langle \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \boldsymbol{\eta} \cdot \mathbf{m}_{\mathcal{J}} \exp(s\boldsymbol{\eta} \cdot \mathbf{m}_{\mathcal{J}}) \rangle_{\mathcal{J}} \\ &= \langle \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) (\boldsymbol{\eta} \cdot \mathbf{m}_{\mathcal{J}})^2 \exp(s\boldsymbol{\eta} \cdot \mathbf{m}_{\mathcal{J}}) \rangle_{\mathcal{J}} \\ &= \boldsymbol{\eta}^{\top} [\langle \mathbf{m}_{\mathcal{J}} \mathbf{m}_{\mathcal{J}}^{\top} \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \exp(s\boldsymbol{\eta} \cdot \mathbf{m}_{\mathcal{J}}) \rangle_{\mathcal{J}}] \boldsymbol{\eta}. \end{aligned}$$

Thus,

$$\left. \frac{d^2}{ds^2} K(\boldsymbol{\beta} + s\boldsymbol{\eta}) \right|_{s=0} = \boldsymbol{\eta}^{\top} [\langle \mathbf{m}_{\mathcal{J}} \mathbf{m}_{\mathcal{J}}^{\top} \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \rangle_{\mathcal{J}}] \boldsymbol{\eta},$$

and we write

$$H_K(\boldsymbol{\beta}) = \langle \mathbf{m}_{\mathcal{J}} \mathbf{m}_{\mathcal{J}}^{\top} \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \rangle_{\mathcal{J}},$$

which is the 3×3 Hessian matrix, of course. This matrix is positive definite, since

$$\boldsymbol{\eta}^{\top} H_K(\boldsymbol{\beta}) \boldsymbol{\eta} = \langle (\boldsymbol{\eta} \cdot \mathbf{m}_{\mathcal{J}})^2 \exp(\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \rangle_{\mathcal{J}} > 0,$$

for every $\boldsymbol{\beta} \in \mathbb{R}^3$, for every $\boldsymbol{\eta} \in \mathbb{R}_*^3 := \mathbb{R}^3 \setminus \{\mathbf{0}\}$. It follows that K is convex.

Now, let us prove that K is coercive. Assume that $\boldsymbol{\beta} \in S^2 := \{\mathbf{x} \in \mathbb{R}^3 \mid \|\mathbf{x}\|_2 = 1\}$. To be precise, we will show the following: for every $M > 0$, there exists a number $R = R(M) > 0$, independent of $\boldsymbol{\beta}$, such that if s is any number satisfying $s > R$, then it follows that

$$K(s\boldsymbol{\beta}) > M,$$

where, of course,

$$K(s\boldsymbol{\beta}) := \langle \exp(s\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}) \rangle_{\mathcal{J}} - s\boldsymbol{\beta} \cdot \boldsymbol{\rho}_{\mathcal{J},*}(x).$$

Fix a vector $\boldsymbol{\beta} \in S^2$, and suppose that for this vector, for some $j_0 \in \mathcal{J}$,

$$\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}(j_0) > 0.$$

Then,

$$K(s\boldsymbol{\beta}) \geq h_v \exp(s\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}(j_0)) - s\boldsymbol{\beta} \cdot \boldsymbol{\rho}_{\mathcal{J},*}(x) \xrightarrow{s \rightarrow +\infty} +\infty.$$

In fact, by continuity, there is an $\varepsilon_{\boldsymbol{\beta}} > 0$ and a constant $C_1 > 0$, such that, if $\boldsymbol{\alpha} \in B(\boldsymbol{\beta}, \varepsilon_{\boldsymbol{\beta}})$ then,

$$\boldsymbol{\alpha} \cdot \mathbf{m}_{\mathcal{J}}(j_0) \geq C_1 > 0,$$

so that

$$K(s\boldsymbol{\alpha}) \geq h_v \exp(sC_1) - s\boldsymbol{\alpha} \cdot \boldsymbol{\rho}_{\mathcal{J},*}(x) \xrightarrow{s \rightarrow +\infty} +\infty.$$

To sum up, given any $M > 0$, there is an $R_{\boldsymbol{\beta}} = R_{\boldsymbol{\beta}}(M)$, such that, if $s > R_{\boldsymbol{\beta}}$, then

$$K(s\boldsymbol{\alpha}) > M,$$

for all $\boldsymbol{\alpha} \in B(\boldsymbol{\beta}, \varepsilon_{\boldsymbol{\beta}})$.

Again, fix a vector $\boldsymbol{\beta} \in S^2$, and suppose that for this vector, for all $j \in \mathcal{J}$,

$$\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}(j) \leq 0.$$

Now, we know that

$$\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}(j) = 0, \quad \forall j \in \mathcal{J} \quad \Longleftrightarrow \quad \boldsymbol{\beta} = \mathbf{0},$$

but $\boldsymbol{\beta} \neq \mathbf{0}$, since $\|\boldsymbol{\beta}\|_2 = 1$. Therefore, for some $j_1 \in \mathcal{J}$,

$$\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}(j_1) < 0.$$

It follows from (3.34) that

$$\boldsymbol{\beta} \cdot \boldsymbol{\rho}_{\mathcal{J},*}(x) < 0.$$

Consequently,

$$K(s\boldsymbol{\beta}) \geq h_v \exp(s\boldsymbol{\beta} \cdot \mathbf{m}_{\mathcal{J}}(j_1)) - s\boldsymbol{\beta} \cdot \boldsymbol{\rho}_{\mathcal{J},*}(x) \xrightarrow{s \rightarrow +\infty} +\infty.$$

In fact, there is an $\varepsilon_\beta > 0$, such that, if $\alpha \in B(\beta, \varepsilon_\beta)$, then

$$\alpha \cdot m_{\mathcal{J}}(j_1) \leq C_2 < 0,$$

and

$$\alpha \cdot \rho_{\mathcal{J},*}(x) \leq C_3 < 0.$$

Hence,

$$K(s\alpha) \geq -sC_3 \xrightarrow{s \rightarrow +\infty} +\infty.$$

To sum up this second case, given any $M > 0$, there is an $R_\beta = R_\beta(M)$, such that, if $s > R_\beta$, then

$$K(s\alpha) > M,$$

for all $\alpha \in B(\beta, \varepsilon_\beta)$.

Observe that

$$S^2 \subset \bigcup_{\beta \in S^2} B(\beta, \varepsilon_\beta),$$

the object on the right being an open cover. Since S^2 is compact, there is a finite sub-cover. In other words, there are finite points $\beta_1, \dots, \beta_N \in S^2$ such that

$$S^2 \subset \bigcup_{i=1}^N B(\beta_i, \varepsilon_{\beta_i}).$$

Let $M > 0$ be given. Set

$$R(M) = \max_{i=1}^N R_{\beta_i}(M).$$

If $s > R(M)$, it follows that

$$K(s\beta) > M,$$

for all $\beta \in S^2$. Since $R(M)$ is independent of β , K is coercive.

Since K is smooth, strictly convex, and coercive, it has a unique minimizer, $\beta_* \in \mathbb{R}^3$ that satisfies

$$\nabla K(\beta_*) = \langle \exp(\beta_* \cdot m_{\mathcal{J}}) m_{\mathcal{J}} \rangle_{\mathcal{J}} - \rho_{\mathcal{J},*}(x) = \mathbf{0}.$$

The proof is complete. ■

Remark 3.2.3. *The compactness argument is required above because, without it, it is not clear that*

$$R(M) = \sup_{\beta \in S^2} R_\beta$$

is finite, which is needed for our definition of coercivity.

Lemma 3.2.4. Suppose that $\Omega = [a, b] \subset \mathbb{R}$ and

$$f_{\mathcal{J}} : \Omega \times \mathcal{J} \rightarrow [0, \infty)$$

is a given Ω -periodic discrete-velocity distribution. Let

$$\boldsymbol{\rho}_{\mathcal{J}} = [n_{\mathcal{J}}, n_{\mathcal{J}} u_{\mathcal{J}}, E_{\mathcal{J}}]^{\top},$$

be the vector comprised of the first three discrete-velocity moments of $f_{\mathcal{J}}$, that is,

$$\boldsymbol{\rho}_{\mathcal{J}}(x) = \begin{bmatrix} n_{\mathcal{J}}(x) \\ n_{\mathcal{J}}(x) u_{\mathcal{J}}(x) \\ E_{\mathcal{J}}(x) \end{bmatrix} = \langle f_{\mathcal{J}}(x, \cdot) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}}, \quad \forall x \in \Omega. \quad (3.35)$$

Fix $x \in [a, b]$, and define

$$\mathcal{M}_{\mathcal{J},f}(x, j) = \exp(\boldsymbol{\alpha}_{\mathcal{J},f}(x) \cdot \mathbf{m}_{\mathcal{J}}(j)), \quad \forall j \in \mathcal{J},$$

where $\boldsymbol{\alpha}_{\mathcal{J},f}(x) \in \mathbb{R}^3$ is the solution to

$$\langle \exp(\boldsymbol{\alpha}_{\mathcal{J},f}(x) \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} = \boldsymbol{\rho}_{\mathcal{J}}(x),$$

which is guaranteed to exist, uniquely, by Lemma 3.2.2. Then

$$0 = \sum_{j \in \mathcal{J}} h_v (\mathcal{M}_{\mathcal{J},f}(x, j) - f_{\mathcal{J}}(x, j)), \quad (3.36)$$

$$0 = \sum_{j \in \mathcal{J}} h_v v_j (\mathcal{M}_{\mathcal{J},f}(x, j) - f_{\mathcal{J}}(x, j)), \quad (3.37)$$

$$0 = \sum_{j \in \mathcal{J}} h_v \frac{1}{2} |v_j|^2 (\mathcal{M}_{\mathcal{J},f}(x, j) - f_{\mathcal{J}}(x, j)). \quad (3.38)$$

This may be expressed succinctly as

$$\langle \mathbf{m}_{\mathcal{J}} (\mathcal{M}_{\mathcal{J},f}(x, \cdot) - f_{\mathcal{J}}(x, \cdot)) \rangle_{\mathcal{J}} = \mathbf{0}. \quad (3.39)$$

Furthermore, the function $\ln(\mathcal{M}_{\mathcal{J},f})$ is a discrete-velocity collision invariant, that is

$$\langle \ln(\mathcal{M}_{\mathcal{J},f}) (\mathcal{M}_{\mathcal{J},f} - f_{\mathcal{J}}) \rangle_{\mathcal{J}} = 0. \quad (3.40)$$

Proof. Identities (3.36) – (3.38) follow immediately from the definition. Since

$$\ln(\mathcal{M}_{\mathcal{J},f}(x, j)) = \ln(\exp(\boldsymbol{\alpha}_{\mathcal{J},f}(x) \cdot \mathbf{m}_{\mathcal{J}}(j))) = \boldsymbol{\alpha}_{\mathcal{J},f}(x) \cdot \mathbf{m}_{\mathcal{J}}(j),$$

identity (3.40) also follows. ■

Theorem 3.2.5. *Define, for all $f : \Omega \times \mathcal{J} \rightarrow [0, \infty)$, the discrete-velocity entropy functional*

$$H_{\mathcal{J}}[f](\cdot) := \langle f \ln(f) \rangle_{\mathcal{J}} : \Omega \rightarrow [0, \infty).$$

Let $\mathcal{A}_{\mathcal{J},}$ be the admissible class of discrete-velocity distribution functions, subordinate to a given discrete-velocity distribution $f_{\mathcal{J},*} : \Omega \times \mathcal{J} \rightarrow [0, \infty)$, so that $\mathcal{A}_{\mathcal{J},*}$ is non-empty. Then, there is a unique function $\mathcal{M}_{\mathcal{J},*} \in \mathcal{A}_{\mathcal{J},*}$ such that*

$$H_{\mathcal{J}}[\mathcal{M}_{\mathcal{J},*}](x) \leq H_{\mathcal{J}}[g](x), \quad (3.41)$$

for all $g \in \mathcal{A}_{\mathcal{J},}$, for all $x \in \Omega$. Furthermore, at every point $x \in \Omega$, there is a unique vector $\boldsymbol{\alpha}_{\mathcal{J},*}(x) \in \mathbb{R}^3$ such that*

$$\mathcal{M}_{\mathcal{J},*}(x, j) = \exp(\boldsymbol{\alpha}_{\mathcal{J},*}(x) \cdot \mathbf{m}_{\mathcal{J}}(j)), \quad \forall j \in \mathcal{J}.$$

Proof. Fix $x \in [a, b]$. Define

$$\mathcal{M}_{\mathcal{J},*}(x, j) = \exp(\boldsymbol{\alpha}_{\mathcal{J},*}(x) \cdot \mathbf{m}_{\mathcal{J}}(j)), \quad \forall j \in \mathcal{J},$$

where $\boldsymbol{\alpha}_{\mathcal{J},*}(x) \in \mathbb{R}^3$ is the solution to

$$\langle \exp(\boldsymbol{\alpha}_{\mathcal{J},*}(x) \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} = \boldsymbol{\rho}_{\mathcal{J},*}(x),$$

which is guaranteed to exist, uniquely, by Lemma 3.2.2. This definition shows that the function $\mathcal{M}_{\mathcal{J},*} \in \mathcal{A}_{\mathcal{J},*}$. Thus, to conclude, we need only show that

$$H_{\mathcal{J}}[\mathcal{M}_{\mathcal{J},*}](x) \leq H_{\mathcal{J}}[g](x),$$

for all $g \in \mathcal{A}_{\mathcal{J},*}$. The proof follows that of the continuous-velocity case.

Let $g \in \mathcal{A}_{\mathcal{J},*}$ be arbitrary. We may write $\mathcal{M}_{\mathcal{J},*} = \mathcal{M}_{\mathcal{J},g}$, since g gives rise to the same macroscopic, discrete-velocity fields as $f_{\mathcal{J},*}$. Define $h(s) := s \ln(s)$. This function h is convex

on $(0, \infty)$, and it follows that

$$\begin{aligned} h(g) &\geq h(\mathcal{M}_{\mathcal{J},g}) + h'(\mathcal{M}_{\mathcal{J},g})(g - \mathcal{M}_{\mathcal{J},g}) \\ &= h(\mathcal{M}_{\mathcal{J},g}) + \ln(\mathcal{M}_{\mathcal{J},g})(g - \mathcal{M}_{\mathcal{J},g}) + g - \mathcal{M}_{\mathcal{J},g}. \end{aligned}$$

By Lemma 3.2.4,

$$\langle h(g) \rangle_{\mathcal{J}} \geq \langle h(\mathcal{M}_{\mathcal{J},g}) \rangle_{\mathcal{J}} + \langle \ln(\mathcal{M}_{\mathcal{J},g})(g - \mathcal{M}_{\mathcal{J},g}) \rangle_{\mathcal{J}} + \langle g - \mathcal{M}_{\mathcal{J},g} \rangle_{\mathcal{J}} = \langle h(\mathcal{M}_{\mathcal{J},g}) \rangle_{\mathcal{J}}.$$

This shows that, point-wise in Ω ,

$$H_{\mathcal{J}}[g] \geq H_{\mathcal{J}}[\mathcal{M}_{\mathcal{J},g}] = H_{\mathcal{J}}[\mathcal{M}_{\mathcal{J},*}],$$

and the result is proven. ■

Definition 3.2.6. *The 1+1-dimensional discrete-velocity BGK model is defined as follows: given an $[a, b]$ -periodic function $f_0 : [a, b] \times \mathcal{J} \rightarrow (0, \infty)$, find $f : [a, b] \times \mathcal{J} \times [0, T] \rightarrow (0, \infty)$ such that $f(\cdot, \cdot, 0) = f_0$ and*

$$\partial_t f(x, j, t) + v_j \partial_x f(x, j, t) = \lambda (\mathcal{M}_{\mathcal{J},f}(x, j, t) - f(x, j, t)), \quad \forall j \in \mathcal{J}, \quad \forall x \in [a, b], \quad (3.42)$$

where

$$\mathcal{M}_{\mathcal{J},f}(x, j, t) = \exp(\alpha_{\mathcal{J},f}(x, t) \cdot \mathbf{m}_{\mathcal{J}}(j)), \quad \forall j \in \mathcal{J},$$

and $\alpha_{\mathcal{J},f}(x, t) \in \mathbb{R}^3$ is the solution to

$$\langle \exp(\alpha_{\mathcal{J},f}(x, t) \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} = \langle f(x, \cdot, t) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}}.$$

We have the following result concerning the solutions of the discrete-velocity model.

Theorem 3.2.7. *Suppose that $\Omega = [a, b] \subset \mathbb{R}$ and*

$$f : \Omega \times \mathcal{J} \times [0, \infty) \rightarrow [0, \infty)$$

is a given Ω -periodic solution to the discrete-velocity BGK model. Define, for all $x \in [a, b]$ and $t \geq 0$, the discrete-velocity entropy density via

$$H_{\mathcal{J}}[f](x, t) := \langle f(x, \cdot, t) \ln(f(x, \cdot, t)) \rangle_{\mathcal{J}}.$$

Then, for all $x \in [a, b]$ and $t \geq 0$,

$$\frac{\partial}{\partial t} \langle \mathbf{m}_{\mathcal{J}} f(x, \cdot, t) \rangle_{\mathcal{J}} + \frac{\partial}{\partial x} \langle v(\cdot) \mathbf{m}_{\mathcal{J}} f(x, \cdot, t) \rangle_{\mathcal{J}} = \mathbf{0}; \quad (3.43)$$

and

$$\frac{\partial}{\partial t} \langle f(x, \cdot, t) \ln(f(x, \cdot, t)) \rangle_{\mathcal{J}} + \frac{\partial}{\partial x} \langle v(\cdot) f(x, \cdot, t) \ln(f(x, \cdot, t)) \rangle_{\mathcal{J}} \leq 0. \quad (3.44)$$

Consequently,

$$\frac{d}{dt} \int_{\Omega} H_{\mathcal{J}}[f](x, t) dx \leq 0. \quad (3.45)$$

Proof. The proofs are analogous to the continuous-velocity cases. Equation (3.43) follows directly from (3.39). To prove inequality (3.44), observe that

$$\begin{aligned} \frac{\partial}{\partial t} H_{\mathcal{J}}[f] &= \left\langle \frac{\partial f}{\partial t} (\ln(f) + 1) \right\rangle_{\mathcal{J}} \\ &= \left\langle \frac{\partial f}{\partial t} \ln(f) \right\rangle_{\mathcal{J}} + \frac{\partial}{\partial t} \langle f \rangle_{\mathcal{J}} \\ &= \frac{1}{\tau} \langle (\mathcal{M}_{\mathcal{J},f} - f) \ln(f) \rangle_{\mathcal{J}} - \langle v \partial_x f \ln(f) \rangle_{\mathcal{J}} - \partial_x \langle v f \rangle_{\mathcal{J}} \\ &= \frac{1}{\tau} \langle \ln(f) (\mathcal{M}_{\mathcal{J},f} - f) \rangle_{\mathcal{J}} - \partial_x \langle v f \ln(f) \rangle_{\mathcal{J}} \\ &= \frac{1}{\tau} \langle (\ln(f) - \ln(\mathcal{M}_{\mathcal{J},f})) (\mathcal{M}_{\mathcal{J},f} - f) \rangle_{\mathcal{J}} - \partial_x \langle v f \ln(f) \rangle_{\mathcal{J}} \\ &= -\frac{1}{\tau} \langle (\ln(\mathcal{M}_{\mathcal{J},f}) - \ln(f)) (\mathcal{M}_{\mathcal{J},f} - f) \rangle_{\mathcal{J}} - \partial_x \langle v f \ln(f) \rangle_{\mathcal{J}} \\ &\leq -\partial_x \langle v f \ln(f) \rangle_{\mathcal{J}}, \end{aligned}$$

where we used Lemma 2.4.2. Finally, using the Ω -periodicity of f and integrating over Ω , gives (3.45). ■

3.2.2 Space-Homogeneous Discrete-Velocity Model

Similar to the continuous velocity case, we can make the following definition:

Definition 3.2.8. *The **space-homogeneous, 1-dimensional discrete-velocity BGK model** is defined as follows: given the function $f_0 : \mathcal{J} \rightarrow (0, \infty)$, find $f : \mathcal{J} \times [0, T] \rightarrow (0, \infty)$ such that $f(\cdot, 0) = f_0$ and*

$$\partial_t f(j, t) = \lambda (\mathcal{M}_{\mathcal{J},f}(j, t) - f(j, t)), \quad \forall j \in \mathcal{J}, \quad (3.46)$$

where

$$\mathcal{M}_{\mathcal{J},f}(\mathbf{j}, t) = \exp(\boldsymbol{\alpha}_{\mathcal{J},f}(t) \cdot \mathbf{m}_{\mathcal{J}}(\mathbf{j})), \quad \forall \mathbf{j} \in \mathcal{J}, \quad (3.47)$$

and $\boldsymbol{\alpha}_{\mathcal{J},f}(t) \in \mathbb{R}^3$ is the solution to

$$\langle \exp(\boldsymbol{\alpha}_{\mathcal{J},f}(t) \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} = \langle f(\cdot, t) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}}. \quad (3.48)$$

Theorem 3.2.9. *Suppose that*

$$f : \mathcal{J} \times [0, \infty) \rightarrow (0, \infty)$$

is a given solution to the space-homogeneous discrete-velocity BGK model. Define, for all $t \geq 0$, the discrete-velocity entropy via

$$H_{\mathcal{J}}[f](t) := \langle f(\cdot, t) \ln(f(\cdot, t)) \rangle_{\mathcal{J}}.$$

Then, for all $t \geq 0$,

$$\frac{\partial}{\partial t} \langle \mathbf{m}_{\mathcal{J}} f(\cdot, t) \rangle_{\mathcal{J}} = \mathbf{0}; \quad (3.49)$$

and

$$\frac{\partial}{\partial t} \langle f(\cdot, t) \ln(f(\cdot, t)) \rangle_{\mathcal{J}} \leq 0. \quad (3.50)$$

Consequently,

$$\frac{\partial}{\partial t} \mathcal{M}_{\mathcal{J},f}(\mathbf{j}, t) = 0, \quad \forall \mathbf{j} \in \mathcal{J}. \quad (3.51)$$

Proof. The proofs are again analogous to the continuous-velocity cases. Equation (3.49) follows directly from (3.39). To prove inequality (3.50), observe that

$$\begin{aligned} \frac{\partial}{\partial t} H_{\mathcal{J}}[f] &= \left\langle \frac{\partial f}{\partial t} (\ln(f) + 1) \right\rangle_{\mathcal{J}} \\ &= \left\langle \frac{\partial f}{\partial t} \ln(f) \right\rangle_{\mathcal{J}} + \frac{\partial}{\partial t} \langle f \rangle_{\mathcal{J}} \\ &= \frac{1}{\tau} \langle (\mathcal{M}_{\mathcal{J},f} - f) \ln(f) \rangle_{\mathcal{J}} \\ &= \frac{1}{\tau} \langle \ln(f) (\mathcal{M}_{\mathcal{J},f} - f) \rangle_{\mathcal{J}} \\ &= \frac{1}{\tau} \langle (\ln(f) - \ln(\mathcal{M}_{\mathcal{J},f})) (\mathcal{M}_{\mathcal{J},f} - f) \rangle_{\mathcal{J}} \\ &= -\frac{1}{\tau} \langle (\ln(\mathcal{M}_{\mathcal{J},f}) - \ln(f)) (\mathcal{M}_{\mathcal{J},f} - f) \rangle_{\mathcal{J}} \\ &\leq 0, \end{aligned}$$

where we used Lemma 2.4.2. Finally, (3.51) follows from (3.47) and (3.48), using (3.49). ■

Chapter 4

Numerics for the Single-Species BGK Model

In this chapter, we consider the numerical approximation of the BGK model for the $d = 1$ case. Therefore, phase space is two-dimensional, with one dimension for physical space and one for velocity space. It is not necessary to equate the dimensions of velocity and physical space, but this is a common practice, and, for the purpose of describing the numerical methods, one does not lose much generality using such simplifying assumptions. We call the present case the $1 \times 1v$ case. The methods that we describe in this section are scalable, meaning that, as more phase-space dimensions are added, the methods themselves change only slightly. The biggest obstacle for high-dimensional numerical simulation is the added number of degrees of freedom that accompany an increase in phase-space dimensions. Of course, this increase can be significant, since real-world phase space has 6 dimensions in the model.

4.1 Finite Volume Space and Velocity Discretization

Since the Vlasov–BGK equation is a nonlinear conservation-like law, shocks (discontinuities) and rarefaction waves can form and propagate in the solution. Thus, the integro-differential equation does not necessarily hold in the classical (strong) sense. In this case, finite volume methods, which are based on the integral form of the differential equation, are typically more appropriate and simpler to use.

First, we truncate the velocity space so that it is finite in size: $V = [-v_{\max}, v_{\max}]$, where $v_{\max} > 0$. This limits the range of velocities that may be approximated, but, as we will see, does not generally affect the accuracy of approximation as long as $v_{\max}$ is chosen sufficiently large. We note that it is not necessary to make a symmetric truncation about zero velocity,

and sometimes it is not advantageous to do so. This is only done for simplicity of presentation. In similar fashion, let us assume that $\Omega = [-L, L]$, with $L > 0$.

Let us define

$$h_x := \frac{2L}{N_x} \quad \text{and} \quad h_v := \frac{2v_{\max}}{N_v},$$

and then set

$$x_\ell := -L + (\ell - 1/2)h_x \quad \text{and} \quad v_\ell := -v_{\max} + (\ell - 1/2)h_v,$$

where ℓ can take integer and half-integer values. To discretize phase space, we break the rectangular 1×1 domain, $\Omega \times V$, into a two dimensional grid of cells with finite volume, and approximate the cell average of the function. $\Omega \times V \subset \mathbb{R}^2$ can be written as the union of the cells:

$$\Omega \times V = \bigcup_{i,j=1}^{N_x, N_v} C_{i,j} = \bigcup_{i,j=1}^{N_x, N_v} C_i^x \times C_j^v = \bigcup_{i,j=1}^{N_x, N_v} \left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}} \right] \times \left[v_{j-\frac{1}{2}}, v_{j+\frac{1}{2}} \right], \quad (4.1)$$

with the point (x_i, v_j) at the center of cell $C_{i,j} = C_i^x \times C_j^v$. Next, we define

$$\bar{f}_{i,j}(t) := \bar{f}(x_i, v_j, t) := \frac{1}{|C_i^x \times C_j^v|} \int_{C_i^x \times C_j^v} f(x, v, t) dx dv. \quad (4.2)$$

The integral form of the Vlasov–BGK equation is

$$\partial_t \bar{f}_{i,j}(t) + \frac{1}{|C_{i,j}|} \int_{C_{i,j}} (\partial_x(vf) + \partial_v(a(x, t)f)) dx dv = \frac{\lambda}{|C_{i,j}|} \int_{C_{i,j}} M_f(x, v, t) dx dv - \lambda \bar{f}_{i,j}(t), \quad (4.3)$$

where we have assumed that the acceleration of particles due to the external field, a , is independent of velocity. Let us define the flux function, $\mathbf{F}$, via

$$\mathbf{F}(x, v, t) := [vf(x, v, t), a(x, t)f(x, v, t)]^\top := [F(x, v, t), G(x, v, t)]^\top,$$

where

$$F(x, v, t) := vf(x, v, t), \quad G(x, v, t) := a(x, t)f(x, v, t).$$

Define

$$\bar{M}_{i,j}(t) := \frac{1}{|C_{i,j}|} \int_{C_{i,j}} M_f(x, v, t) dx dv.$$

Applying the Divergence Theorem,

$$\partial_t \bar{f}_{i,j}(t) + \lambda \bar{f}_{i,j}(t) - \lambda \bar{M}_{i,j}(t) = -\frac{1}{h_x h_v} \int_{C_j^v} (F(x_{i+1/2}, v, t) - F(x_{i-1/2}, v, t)) dv$$

$$- \frac{1}{h_x h_v} \int_{C_i^x} (G(x, v_{j+1/2}, t) - G(x, v_{j-1/2}, t)) dx. \quad (4.4)$$

Now, (4.4) is exact. To gain a practical numerical method, we must make some approximations. Let us first approximate the flux integrals:

$$\frac{1}{h_x h_v} \int_{C_j^v} (F(x_{i+1/2}, v, t) - F(x_{i-1/2}, v, t)) dv \approx \frac{F(x_{i+1/2}, v_j, t) - F(x_{i-1/2}, v_j, t)}{h_x}, \quad (4.5)$$

$$\frac{1}{h_x h_v} \int_{C_i^x} (G(x, v_{j+1/2}, t) - G(x, v_{j-1/2}, t)) dx \approx \frac{G(x_i, v_{j+1/2}, t) - G(x_i, v_{j-1/2}, t)}{h_v}. \quad (4.6)$$

To approximate the density function on the cell $C_{i,j}$, we use piecewise linear reconstructions:

$$p_{i,j}(x, v, t) = \bar{f}_{i,j}(t) + \sigma_{i,j}^x(x - x_i) + \sigma_{i,j}^v(v - v_j),$$

with the θ -minmod slope limiter,

$$\sigma_{i,j}^x = \text{minmod} \left(\left(\frac{\bar{f}_{i+1,j} - \bar{f}_{i-1,j}}{2h_x} \right), \theta^x \left(\frac{\bar{f}_{i,j} - \bar{f}_{i-1,j}}{h_x} \right), \theta^x \left(\frac{\bar{f}_{i+1,j} - \bar{f}_{i,j}}{h_x} \right) \right), \quad (4.7)$$

$$\sigma_{i,j}^v = \text{minmod} \left(\left(\frac{\bar{f}_{i,j+1} - \bar{f}_{i,j-1}}{2h_v} \right), \theta^v \left(\frac{\bar{f}_{i,j} - \bar{f}_{i,j-1}}{h_v} \right), \theta^v \left(\frac{\bar{f}_{i,j+1} - \bar{f}_{i,j}}{h_v} \right) \right), \quad (4.8)$$

where $\theta^x, \theta^v \in [1, 2]$. Note that for three *real* arguments, the minmod function is defined by

$$\text{minmod}(x, y, z) := \begin{cases} \min\{x, y, z\} & \text{if } x, y, z \geq 0 \\ \max\{x, y, z\} & \text{if } x, y, z \leq 0 \\ 0 & \text{otherwise} \end{cases}$$

The reconstructions make the density approximation multi-valued at the cell edges, a fact that we use to our advantage in the numerical approximation. Using the reconstructions, we define the density at the midpoints of each cell edge as follows:

$$f_{i+1/2,j}^-(t) := p_{i,j}(x_{i+1/2}, v_j, t), \quad f_{i+1/2,j}^+(t) := p_{i+1,j}(x_{i+1/2}, v_j, t),$$

and, likewise,

$$f_{i,j+1/2}^-(t) := p_{i,j}(x_i, v_{j+1/2}, t), \quad f_{i,j+1/2}^+(t) := p_{i,j+1}(x_i, v_{j+1/2}, t).$$

Next, the exact fluxes are replaced by numerical fluxes of the form

$$F(x_{i+1/2}, v_j, t) \approx \tilde{F}(f_{i+1/2,j}^+(t), f_{i+1/2,j}^-(t)) =: \hat{F}_{i+1/2,j}(t)$$

and

$$G(x_i, v_{j+1/2}, t) \approx \tilde{G}(f_{i,j+1/2}^+(t), f_{i,j+1/2}^-(t)) =: \hat{G}_{i,j+1/2}(t).$$

We use a simple upwind strategy to construct the numerical fluxes:

$$\hat{F}_{i+1/2,j}(t) = \tilde{F}(f_{i+1/2,j}^+(t), f_{i+1/2,j}^-(t)) = \begin{cases} v_j f_{i+1/2,j}^-(t) & \text{if } v_j \geq 0 \\ v_j f_{i+1/2,j}^+(t) & \text{if } v_j < 0 \end{cases}, \quad (4.9)$$

$$\hat{G}_{i,j+1/2}(t) = \tilde{G}(f_{i,j+1/2}^+(t), f_{i,j+1/2}^-(t)) = \begin{cases} a(x_i, t) f_{i,j+1/2}^-(t) & \text{if } a(x_i, t) \geq 0 \\ a(x_i, t) f_{i,j+1/2}^+(t) & \text{if } a(x_i, t) < 0 \end{cases}. \quad (4.10)$$

We can write the approximation scheme to this point as follows:

$$\begin{aligned} \partial_t \bar{f}_{i,j}(t) + \lambda \bar{f}_{i,j}(t) - \lambda \bar{M}_{i,j}(t) = & - \frac{\hat{F}_{i+1/2,j}(t) - \hat{F}_{i-1/2,j}(t)}{h_x} \\ & - \frac{\hat{G}_{i,j+1/2}(t) - \hat{G}_{i,j-1/2}(t)}{h_v} + \tilde{E}_{i,j}(t), \end{aligned} \quad (4.11)$$

where $\tilde{E}_{i,j}(t)$ is a local truncation (approximation) error.

Finally, to complete the spatial discretization of the Vlasov–BGK equation, we need to approximate the Maxwellian. For this we use the following:

$$n_i(t) = h_v \sum_{j=1}^{N_v} \bar{f}_{i,j}(t), \quad (4.12)$$

$$u_i(t) = \frac{h_v}{n_i(t)} \sum_{j=1}^{N_v} v_j \bar{f}_{i,j}(t), \quad (4.13)$$

$$\theta_i(t) = \frac{h_v}{n_i(t)} \sum_{j=1}^{N_v} |v_j|^2 \bar{f}_{i,j}(t) - |u_i(t)|^2, \quad (4.14)$$

$$\bar{M}_{i,j}(t) \approx \hat{M}_{i,j}(t) = \frac{n_i(t)}{(2\pi\theta_i(t))^{1/2}} \exp\left(-\frac{(v_j - u_i(t))^2}{2\theta_i(t)}\right). \quad (4.15)$$

Since we are replacing integrations by midpoint quadratures, we lose the collision invariances that we enjoyed at the continuum level. But, for the purpose of approximation, we will continue to assume that these invariances still exist at the discrete level.

We conclude this section by stating the spatially discrete approximation to the Vlasov–BGK equation:

$$\begin{aligned} d_t \bar{f}_{i,j}(t) + \lambda \bar{f}_{i,j}(t) - \lambda \hat{M}_{i,j}(t) = & - \frac{\hat{F}_{i+1/2,j}(t) - \hat{F}_{i-1/2,j}(t)}{h_x} \\ & - \frac{\hat{G}_{i,j+1/2}(t) - \hat{G}_{i,j-1/2}(t)}{h_y} + \hat{E}_{i,j}(t), \end{aligned} \quad (4.16)$$

where $\hat{E}_{i,j}(t)$ is a local truncation (approximation) error.

4.2 Implicit-Explicit Runge–Kutta Time Stepping

In this section we introduce an implicit-explicit (IMEX) Runge–Kutta (RK) method for integration in time that was proposed in [36]. The convection part is treated using an explicit method, while the collision part is solved using a diagonally implicit method. We will work with the phase-space continuous problem first, in order to take advantage of the collision invariants, before moving to the phase-space discrete problem. Let us rewrite the original Vlasov–BGK equation as

$$\frac{\partial}{\partial t} f(x, v, t) = T[f](x, v, t) + Q[f](x, v, t)$$

where T represents the transport term, and Q represents the collision term:

$$T[f](x, v, t) := -v \partial_x f(x, v, t) - a(x, t) \partial_v f(x, v, t), \quad (4.17)$$

$$Q[f](x, v, t) := \lambda (M_f(x, v, t) - f(x, v, t)). \quad (4.18)$$

The general ν -stage IMEX Runge–Kutta scheme (diagonally implicit) is one of the form

$$y^{(s)} = y^n + \Delta t \sum_{r=1}^{s-1} \tilde{a}_{s,r} T[y^{(r)}] + \Delta t \sum_{r=1}^s a_{s,r} Q[y^{(r)}], \quad s \in \{1, \dots, \nu\}, \quad (4.19)$$

$$y^{n+1} = y^n + \Delta t \sum_{s=1}^{\nu} \tilde{b}_s T[y^{(s)}] + \Delta t \sum_{s=1}^{\nu} b_s Q[y^{(s)}], \quad (4.20)$$

where $\tilde{a}_{s,r}$, $\tilde{b}_s$, $a_{s,r}$, b_s are taken from the following Butcher tables, respectively:

$$\begin{array}{c|c} \tilde{c} & \tilde{A} \\ \hline & \tilde{b}^\top \end{array} \qquad \begin{array}{c|c} c & A \\ \hline & b^\top \end{array}. \quad (4.21)$$

The matrix $\tilde{\mathbf{A}}$, for the explicit part, is strictly lower triangular, and $\mathbf{A}$ is lower triangular.

To run the algorithm, for each stage, we first calculate

$$\hat{y}^{(s-1)} := y^n + \Delta t \sum_{r=1}^{s-1} \tilde{a}_{s,r} T[y^{(r)}] + \Delta t \sum_{r=1}^{s-1} a_{s,r} Q[y^{(r)}]. \quad (4.22)$$

We then rearrange the terms in the final sum to find an expression for $y^{(s)}$:

$$\begin{aligned} y^{(r)} &= \hat{y}^{(s-1)} + \Delta t a_{s,s} Q[y^{(s)}] \\ &= \hat{y}^{(s-1)} + \Delta t a_{s,s} \lambda (M_{y^{(s)}} - y^{(s)}) \end{aligned} \quad (4.23)$$

$$\iff (1 + \Delta t a_{s,s} \lambda) y^{(s)} = \hat{y}^{(s-1)} + \Delta t a_{s,s} \lambda M_{y^{(s)}} \quad (4.24)$$

$$\iff y^{(s)} = \frac{1}{1 + \Delta t a_{s,s} \lambda} \hat{y}^{(s-1)} + \frac{\Delta t a_{s,s} \lambda}{1 + \Delta t a_{s,s} \lambda} M_{y^{(s)}}. \quad (4.25)$$

Note that we need to compute the Maxwellian $M_{y^{(s)}}$, which involves the current stage. This seems to present an issue. However, using the collision invariances properties in (3.1.1), we can circumvent this. In particular,

$$\begin{aligned} \int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ \mathbf{v} \\ |\mathbf{v}|^2 \end{pmatrix} y^{(s)} d\mathbf{v} &= \int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ \mathbf{v} \\ |\mathbf{v}|^2 \end{pmatrix} \hat{y}^{(s-1)} d\mathbf{v} + \Delta t a_{s,s} \lambda \int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ \mathbf{v} \\ |\mathbf{v}|^2 \end{pmatrix} (M_{y^{(s)}} - y^{(s)}) d\mathbf{v} \\ &= \int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ \mathbf{v} \\ |\mathbf{v}|^2 \end{pmatrix} \hat{y}^{(s-1)} d\mathbf{v}. \end{aligned} \quad (4.26)$$

Since the first, second, and third moments of $\hat{y}^{(s-1)}$ are equal to those of $y^{(s)}$, the two Maxwellians at these stages are equal:

$$M_{y^{(s)}} = M_{\hat{y}^{(s-1)}}.$$

Therefore, we have the explicit update formula

$$y^{(s)} = \frac{1}{1 + \Delta t a_{s,s} \lambda} \hat{y}^{(s-1)} + \frac{\Delta t a_{s,s} \lambda}{1 + \Delta t a_{s,s} \lambda} M_{\hat{y}^{(s-1)}}. \quad (4.27)$$

With the above expression for $y^{(s)}$, a convex combination of $\hat{y}^{(s-1)}$ and $M_{\hat{y}^{(s-1)}}$, the IMEX-RK scheme can be completed without any complicated inversions.

4.3 Fully Discrete Scheme

When we discretize velocity space, we lose the collision invariances at the discrete level; this is because velocity integrals are replaced with midpoint rule quadrature, in addition to the fact that the velocity space is truncated. It follows that (4.27) breaks down. Nevertheless, we will assume that the phase-space discrete analog to (4.27) holds so that stages may be updated in an explicit fashion.

Suppose that $f_{i,j}^n$ is an approximation of the cell average of the density field over cell $C_{i,j}$ at time $t^n := t^{n-1} + \Delta t$. Similarly, we denote by $f_{i,j}^{(\ell)}$ the ℓ^{th} stage of the IMEX-RK scheme with respect to $f_{i,j}^n$. Define

$$T_{i,j}^\square := -\frac{\widehat{F}_{i+1/2,j}^\square - \widehat{F}_{i-1/2,j}^\square}{h_x} - \frac{\widehat{G}_{i,j+1/2}^\square - \widehat{G}_{i,j-1/2}^\square}{h_v}, \quad (4.28)$$

$$Q_{i,j}^\square := \lambda(M_{i,j}^\square - f_{i,j}^\square), \quad (4.29)$$

where the fluxes $\widehat{F}_{i+1/2,j}^\square$ and $\widehat{G}_{i,j+1/2}^\square$ are computed with respect to the cell-centered approximation $f_{i,j}^\square$ and $\square$ is a stage iteration or a time step index. The fully discrete Maxwellian is computed via

$$n_i^\square = h_v \sum_{j=1}^{N_v} f_{i,j}^\square, \quad (4.30)$$

$$u_i^\square = \frac{h_v}{n_i^\square} \sum_{j=1}^{N_v} v_j f_{i,j}^\square, \quad (4.31)$$

$$\theta_i^\square = \frac{h_v}{n_i^\square} \sum_{j=1}^{N_v} |v_j|^2 f_{i,j}^\square - |u_i^\square|^2, \quad (4.32)$$

$$M_{i,j}^\square = \frac{n_i^\square}{(2\pi\theta_i^\square)^{1/2}} \exp\left(-\frac{(v_j - u_i^\square)^2}{2\theta_i^\square}\right). \quad (4.33)$$

Then we compute

$$\widehat{f}_{i,j}^{(s-1)} := f_{i,j}^n + \Delta t \sum_{r=1}^{s-1} \widetilde{a}_{s,r} T_{i,j}^{(r)} + \Delta t \sum_{r=1}^{s-1} a_{s,r} Q_{i,j}^{(r)}, \quad (4.34)$$

$$f_{i,j}^{(s)} = \frac{1}{1 + \Delta t a_{s,s} \lambda} \widehat{f}_{i,j}^{(s-1)} + \frac{\Delta t a_{s,s} \lambda}{1 + \Delta t a_{s,s} \lambda} \widehat{M}_{i,j}^{(s-1)}, \quad (4.35)$$

$$f_{i,j} = f_{i,j}^n + \Delta t \sum_{s=1}^{\nu} \widetilde{b}_s T_{i,j}^{(s)} + \Delta t \sum_{s=1}^{\nu} b_s Q_{i,j}^{(s)}, \quad (4.36)$$

where $\widehat{M}_{i,j}^{(s-1)}$ is the discrete Maxwellian computed with respect to the fully discrete approximation $\widehat{f}_{i,j}^{(s-1)}$. This completes the description of the fully discrete scheme.

4.4 Poisson Solver for Vlasov–Poisson–BGK Equation

For the Vlasov–Poisson–BGK equation the acceleration a is determined by an electric field as follows:

$$a(x, t) = -\chi \partial_x \Phi,$$

where $\chi > 0$ is a physical constant and Φ is the electric potential determined via

$$-\partial_{xx} \Phi(x, t) = n(x, t),$$

subject to appropriate boundary conditions.

First let us consider *Dirichlet boundary conditions*:

$$\Phi(x_{1/2} = -L) = \alpha, \quad \Phi(x_{N_x+1/2} = L) = \beta. \quad (4.37)$$

Using the standard three-point stencil approximation, we have, for $i = 2, \dots, N_x - 1$,

$$-\frac{1}{h_x^2} [\Phi_{i+1} - 2\Phi_i + \Phi_{i-1}] = n_i. \quad (4.38)$$

The boundary conditions are specified at the peripheral edges of the domain, $-L = x_{1/2}$ and $L = x_{N_x+1/2}$. As is standard, we use the average of the ghost cell and neighboring interior cell. That is, we use the approximations

$$\frac{\Phi_0 + \Phi_1}{2} = \alpha, \quad \implies \Phi_0 = 2\alpha - \Phi_1, \quad (4.39)$$

and we cancel the term Φ_0 in the stencil approximation. The first equation in the approximation thus becomes

$$-\Phi_2 + 3\Phi_1 = h_x^2 n_1 + 2\alpha. \quad (4.40)$$

Using a similar procedure for right boundary condition, we have

$$\Phi_{N_x+1} = 2\beta - \Phi_{N_x}, \implies -\Phi_{N_x-1} + 3\Phi_{N_x} = h_x^2 n_{N_x} + 2\beta. \quad (4.41)$$

Putting this all into a matrix system, we must solve

$$\begin{pmatrix} 3 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 3 \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_{N_x-1} \\ \Phi_{N_x} \end{pmatrix} = \begin{pmatrix} h_x^2 n_1 + 2\alpha \\ h_x^2 n_2 \\ \vdots \\ h_x^2 n_{N_x-1} \\ h_x^2 n_{N_x} + 2\beta \end{pmatrix}. \quad (4.42)$$

This system is symmetric positive definite (SPD) and always has a unique solution.

Next, we turn our attention to the case of *Neumann boundary conditions*:

$$\frac{d\Phi}{dx}(-L) = \alpha, \quad \frac{d\Phi}{dx}(L) = \beta. \quad (4.43)$$

In this case, using a second-order approximation at the boundary, we must solve matrix system

$$\begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_{N_x-1} \\ \Phi_{N_x} \end{pmatrix} = \begin{pmatrix} h_x^2 n_1 - h_x \alpha \\ h_x^2 n_2 \\ \vdots \\ h_x^2 n_{N_x-1} \\ h_x^2 n_{N_x} + h_x \beta \end{pmatrix}. \quad (4.44)$$

This is a symmetric positive semi-definite (SPSD) system. It has a unique mean-zero solution, that is, a solution satisfying

$$h_x \sum_{i=1}^{N_x} \Phi_i = 0, \quad \text{if and only if} \quad h_x \sum_{i=1}^{N_x} n_i = \alpha - \beta.$$

This is the discrete analog of the standard continuous compatibility conditions for unique solvability.

Given $f_{i,j}^\square$, we compute the accompanying macroscopic density,

$$n_i^\square = h_v \sum_{j=1}^{N_v} f_{i,j}^\square,$$

and then the associated electric potential $\Phi_i^\square$, as described above. Once the discrete potential

is available, the acceleration may be approximated via

$$a_{i+1/2}^{\square} = -\chi \frac{\Phi_{i+1}^{\square} - \Phi_i^{\square}}{h_x}.$$

4.5 Sample Computations and Accuracy Tests

In this section, we report on several numerical tests showing accuracy of the numerical implementation.

Relaxation Test 1

This first test is designed to confirm that the BGK operator is calculated correctly for the single-species case. We consider, in particular, the space-homogeneous case: the IPDE becomes the following IODE:

$$\begin{cases} \frac{df}{dt} = \lambda(M_f - f), & (x, v, t) \in \Omega \times V \times [0, \infty), \\ f(x, v, 0) = f_0(x, v), & (x, v, t) \in \Omega \times V \times \{t = 0\}. \end{cases} \quad (4.45)$$

Recall that as shown in Section 3.1.2, the exact solution is

$$f(x, v, t) = e^{-\lambda t} f(x, v, 0) + (1 - e^{-\lambda t}) M_f(x, v, 0). \quad (4.46)$$

For the first test, we chose a function of the form $f_0(x, v) = b(v)g(x)$, where $b(v)$ is a compactly supported C^∞ function, with nonzero values on $v \in (-2, 2)$. In particular, we use the function $g(x) = e^{-|x|}$. Consider the function

$$f(x, v, 0) = \begin{cases} e^{-|x|} \frac{5(v^2+4) \exp\left(\frac{5v}{v^2-4}\right)}{(v^2-4)^2 \left(1 + \exp\left(\frac{5v}{v^2-4}\right)\right)^2}, & \text{if } v \in (-2, 2), \\ 0, & \text{otherwise.} \end{cases} \quad (4.47)$$

Observe that

$$n = \int_V f(x, v) dv = g(x) \int_V b(v) dv = g(x) = e^{-|x|}.$$

Note that $b(v)$ is an even function:

$$\begin{aligned}
 b(-v) &= \frac{5((-v)^2 + 4) \exp\left(\frac{5(-v)}{(-v)^2 - 4}\right)}{((-v)^2 - 4)^2 \left(1 + \exp\left(\frac{5(-v)}{(-v)^2 - 4}\right)\right)^2} \\
 &= \frac{5(v^2 + 4) \exp\left(-\frac{5v}{v^2 - 4}\right)}{(v^2 - 4)^2 \left(1 + \exp\left(-\frac{5v}{v^2 - 4}\right)\right)^2} \cdot \frac{\exp\left(\frac{10v}{v^2 - 4}\right)}{\left[\exp\left(\frac{5v}{v^2 - 4}\right)\right]^2} \\
 &= \frac{5(v^2 + 4) \exp\left(\frac{5v}{v^2 - 4}\right)}{(v^2 - 4)^2 \left(\exp\left(\frac{5v}{v^2 - 4}\right) + 1\right)^2} \\
 &= b(v).
 \end{aligned}$$

Therefore, the function $h(v) = vb(v)$ is odd. Recall that when integrating an odd function over an interval that is symmetric about the origin, one obtains a zero integral. This means that $u = \frac{1}{n} \int_V vf dv \equiv 0$.

The energy density moment is not as easy to compute analytically, so we have found a numerical approximation:

$$E = \frac{1}{2} \int_V v^2 f dv \approx 0.3713094964845e^{-|x|}.$$

The code is run with $\lambda = 1$ up to a final time $t_f = 1$. The error is calculated by taking the difference of the true solution minus the computed solution. The initial distribution is given in Figure 4.1a, and the computational solution is given in Figure 4.1b. The error in Figure 4.2 is calculated by taking the difference of the true solution minus the computed solution. The errors are on the order of 10^{-5} when a mesh of size $N_x = N_v = 128$ is used.

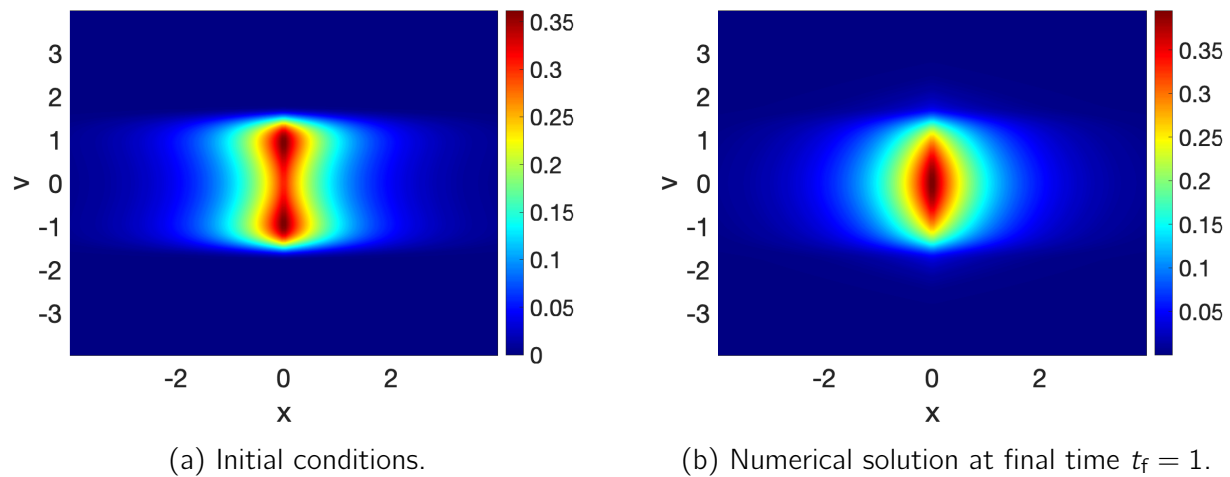


Figure 4.1: Relaxation Example 1: Initial and final time solutions are given for the space-homogeneous BGK model (3.24) using the initial conditions given in (4.47).

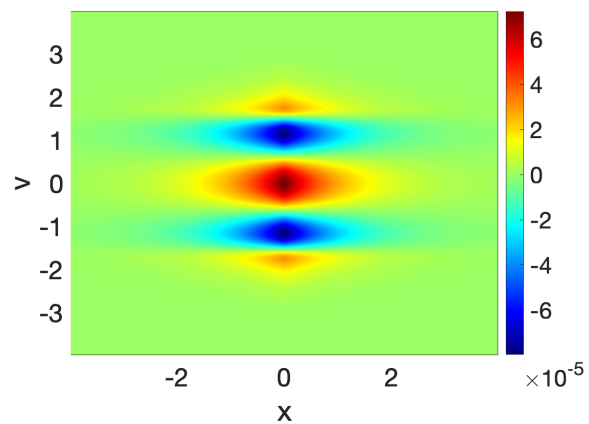


Figure 4.2: Relaxation Example 1: The error between the theoretical and numerical solution at the final time $t_f = 1$ is given for the space-homogeneous BGK model (3.24) using the initial conditions given in (4.47).

Relaxation Test 2

For the second test, we set $f_0(x, v)$ to be the sum of four Gaussians, centered at $(x, v) \in \{(\pm 2, \pm 2)\}$:

$$f_0(x, v) = e^{-2(x-2)^2-2(v-2)^2} + e^{-2(x-2)^2-2(v+2)^2} + e^{-2(x+2)^2-2(v-2)^2} + e^{-2(x+2)^2-2(v+2)^2}. \quad (4.48)$$

See Figure 4.3a. The trapezoidal rule is used for the initial moments. The code is run with $\lambda = 1$ up to time $t_f = 2$. The error is calculated by taking the difference of the true solution minus the computed solution. The initial and final computed solutions are given in Figures 4.3, and the errors are shown in Figure 4.4.

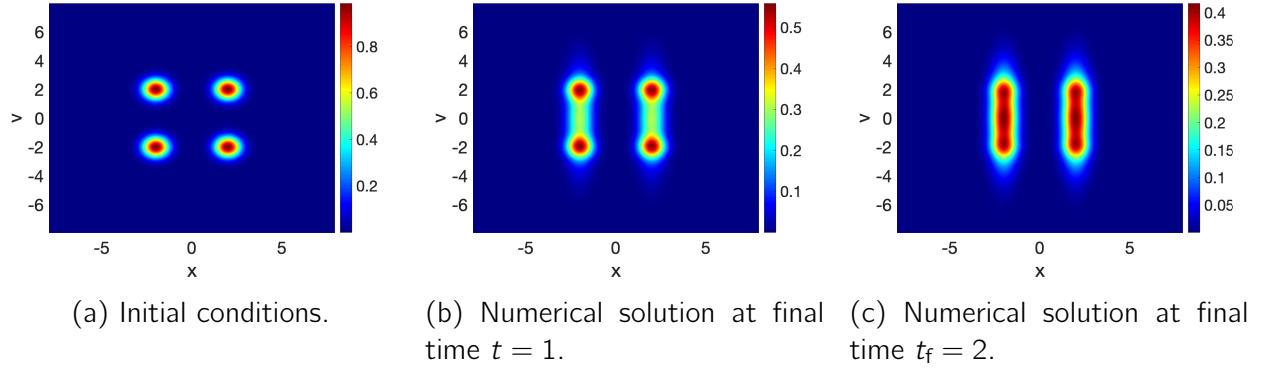


Figure 4.3: Relaxation Example 2: Initial and final time solutions are given for the space-homogeneous BGK model (3.24) using the initial conditions given in (4.48).

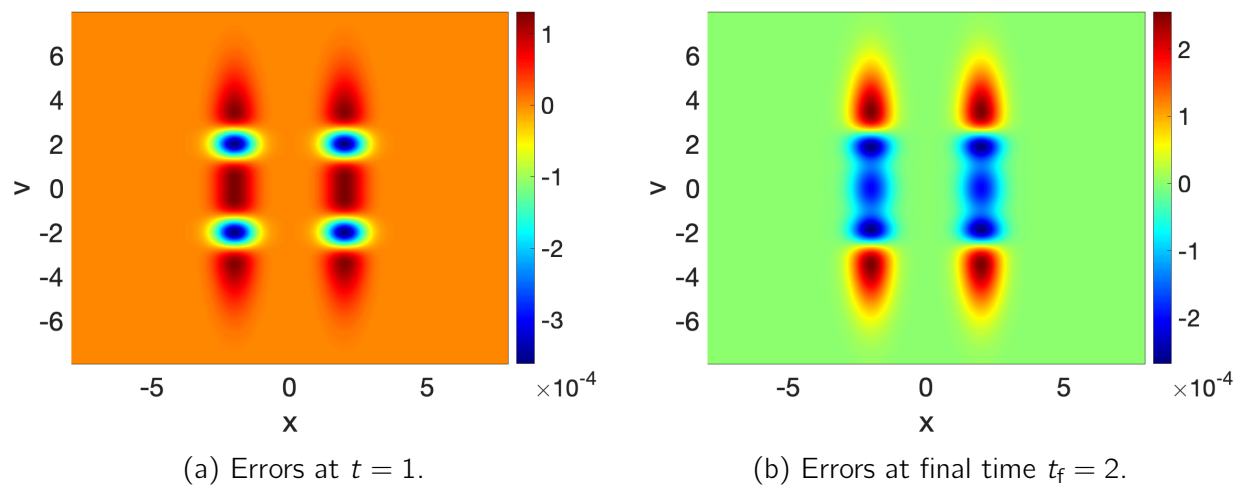


Figure 4.4: Relaxation Example 2: The error between the theoretical and numerical solution at the time $t = 1$ and $t_f = 2$ is given for the space-homogeneous BGK model (3.24) using the initial conditions given in (4.48).

Sod Shock Tube (Euler Equation Limit of BGK)

The Sod shock tube test is a standard test. Formally, in the collision limit as $\lambda \rightarrow \infty$, the BGK equation is asymptotically equivalent to the Euler Equations. (That is, f converges to the Maxwellian M_f , and the moments $n, \mathbf{u}, \theta$ follow the Euler equations.) Thus, we may test the ability of the code to solve the Sod shock tube problem, by letting λ be large (or equivalently, letting $\tau = \lambda^{-1}$ be small), and setting the initial conditions appropriately. For the test, we set $\lambda = 10^4$ ($\tau = 10^{-4}$).

The BGK equation in 1 dimension is

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} = \lambda(M_f - f). \quad (4.49)$$

To test our IMEX code, we compared the profiles of the number density ($n = \int f dv$), bulk velocity ($u = (\int v f dv)/n$), pressure ($P = n\theta$), and internal energy ($E = \frac{1}{2}\theta$) to the theoretical solution, worked out using the book by Toro [45]. We set the phase-space domain equal to $\Omega \times V = [-0.75, 0.75] \times [-10, 10]$. Since the moments are calculated over $\mathbb{R}^d$, then we must have a function that integrates to approximately the same value, when restricting $\mathbb{R}^d$ to the computational velocity domain (in this case, $[-10, 10] \subset \mathbb{R}$). That is, we must ensure that

$$\int_{\mathbb{R}^d} f(x, v, t) dv \approx \int_V f(x, v, t) dv,$$

where V is the truncated velocity domain. Using $[-10, 10]$ gives a reasonable approximation, as we show.

The setup for the Sod problem is a contact discontinuity separating gases of differing density and temperature, and zero velocity. Thus, for the Sod problem, the initial condition for the particle density is a piecewise Maxwellian with the following values:

$$\begin{pmatrix} n_L \\ u_L \\ \theta_L \end{pmatrix} = \begin{pmatrix} 1.0 \\ 0.0 \\ 1.0 \end{pmatrix}, \quad x \in (-0.75, 0), \quad \begin{pmatrix} n_R \\ u_R \\ \theta_R \end{pmatrix} = \begin{pmatrix} 0.125 \\ 0.0 \\ 0.8 \end{pmatrix}, \quad x \in (0, 0.75). \quad (4.50)$$

That is, the initial condition function (contour plot shown in Figure 4.5a) is given by

$$f_0(x, v) = \begin{cases} \frac{1.0}{\sqrt{2\pi(1.0)}} \exp\left(-\frac{|v-0.0|^2}{2(1.0)}\right), & x \in [-0.75, 0], v \in [-10, 10], \\ \frac{0.125}{\sqrt{2\pi(0.8)}} \exp\left(-\frac{|v-0.0|^2}{2(0.8)}\right), & x \in (0, 0.75], v \in [-10, 10]. \end{cases} \quad (4.51)$$

Figure 4.6 shows the moments of the numerical/computed solution at time $t_f = 0.20$.

The profiles of the macroscopic quantities follow the correct values (as computed using [45] for reference). The final distribution solution is shown in Figure 4.5b

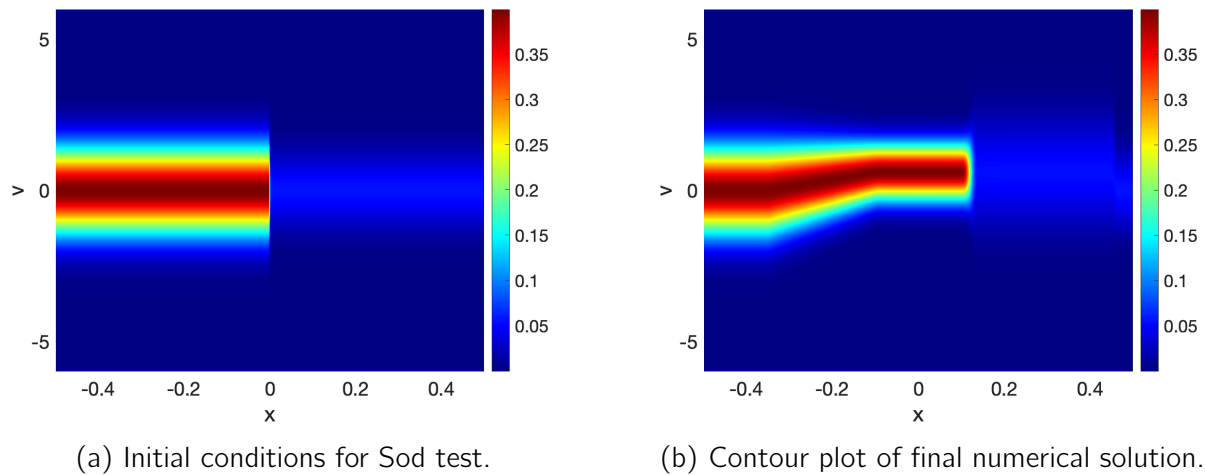


Figure 4.5: Initial conditions, and phase space solution of BGK Equation with $\tau = 0.0001$ at $t_f = 0.2$

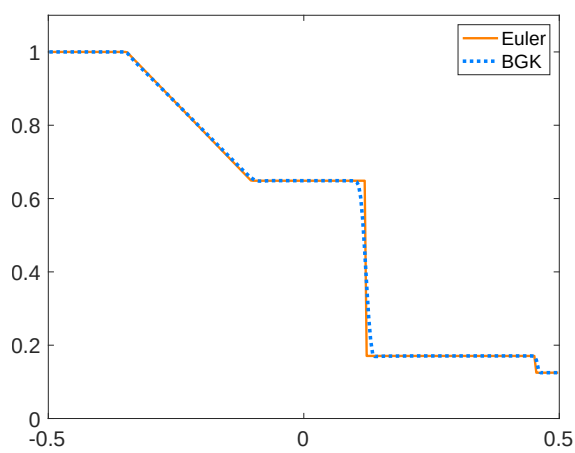
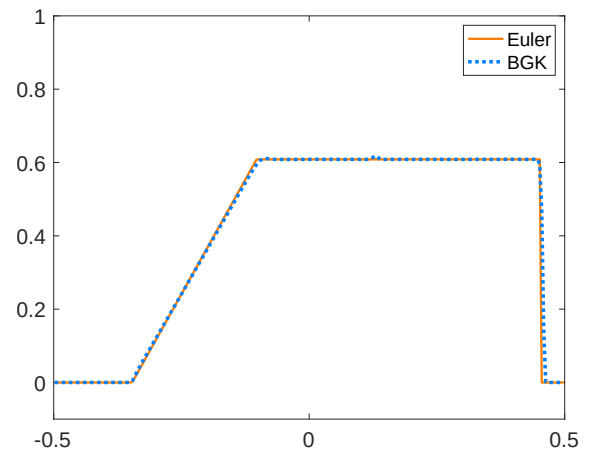
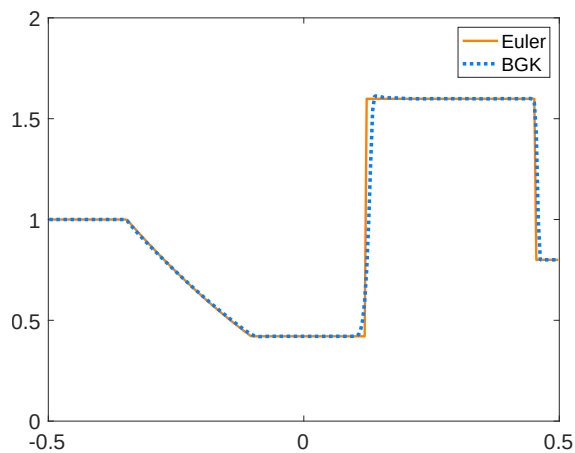
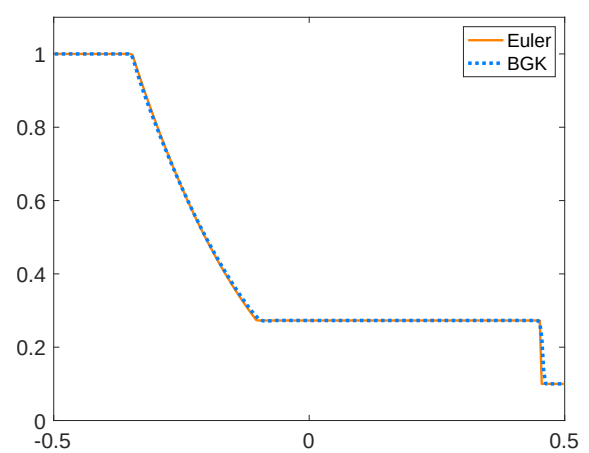
(a) Number density, n (b) Bulk velocity, u (c) Temperature, θ (d) Pressure, $p = n\theta$

Figure 4.6: The number density, bulk velocity, temperature, and pressure are compared to the solution of the Euler equations at time $t_f = 0.2$, with $\tau = 10^{-4}$.

Square Pulse Rotation

Consider the Vlasov Equation in 1 dimension:

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + a \frac{\partial f}{\partial v} = 0 \quad (4.52)$$

Setting the acceleration term to $a = -x$ results in a system where an initial distribution is advected counterclockwise, along circular characteristics around the origin. For constructing the characteristics curves, we have the system of ODEs:

$$\frac{dt}{ds} = 1 \quad (4.53)$$

$$\frac{dx}{ds} = v \quad (4.54)$$

$$\frac{dv}{ds} = -x. \quad (4.55)$$

The first equation gives $t = s$, and the remaining two form a system of two coupled ODEs:

$$\dot{x} = v \quad (4.56)$$

$$\dot{v} = -x. \quad (4.57)$$

Taking the derivative of the first equation, and plugging in the second equation, we have

$$\ddot{x} = \dot{v} = -x \iff \ddot{x} + x = 0. \quad (4.58)$$

The solution of this equation is

$$x(t) = c_1 \cos(t) + c_2 \sin(t). \quad (4.59)$$

Thus,

$$\dot{v} = -x = -c_1 \cos(t) - c_2 \sin(t). \quad (4.60)$$

Integrating gives

$$v(t) = -c_1 \sin(t) + c_2 \cos(t). \quad (4.61)$$

Putting these together, we have

$$x(t) = c_1 \cos(t) + c_2 \sin(t) \quad (4.62)$$

$$v(t) = -c_1 \sin(t) + c_2 \cos(t). \quad (4.63)$$

This is a circle of radius $\sqrt{c_1^2 + c_2^2}$, traversed clockwise around the origin in the (x, v) -plane. Figure 4.7 shows an image of four square pulses rotated counterclockwise to time $t_f = \frac{\pi}{2}$ (quarter rotation) and $t_f = 2\pi$ (full rotation), using a $N_x \times N_v = 400 \times 400$ grid on $\Omega \times V = [-3, 3] \times [-3, 3]$.

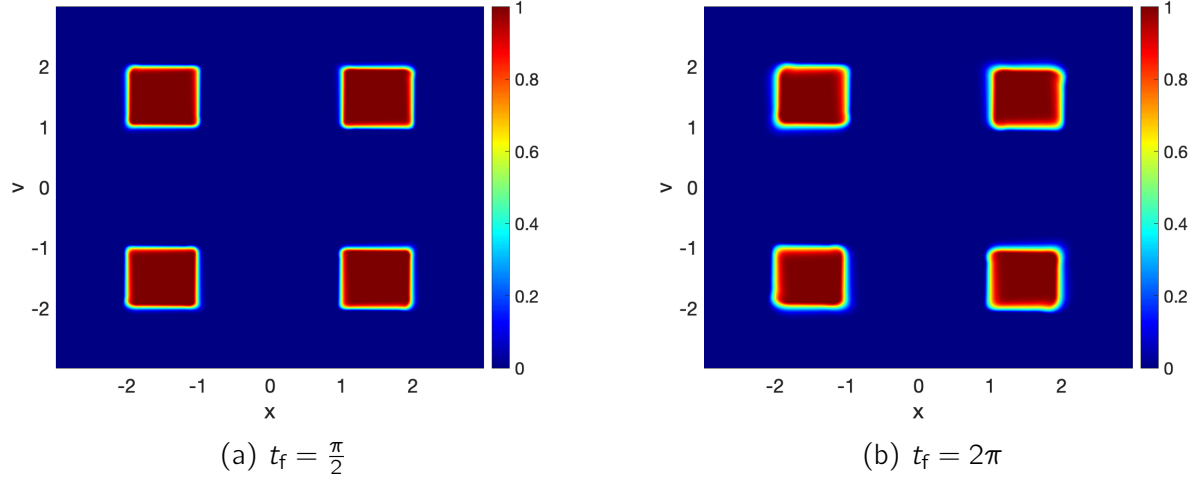


Figure 4.7: Rotation Problem: $\frac{\partial}{\partial t} f + v \frac{\partial}{\partial x} f - x \frac{\partial}{\partial v} f = 0$. Grid: $N_v = N_x = 400$.

Two Stream Instability (Vlasov–Poisson)

The next test that we performed is known as the *Two-Stream Instability Test*, and the present version is taken from Section 5.1.2 of [12]. In this test, two streams of electrons interact and create a highly filamented vortex. The test is designed to assess the code's ability to capture fine structure and examines only the advection piece of our equation (the Vlasov–Poisson equation):

$$\partial_t f + v \partial_x f + E \partial_v f = 0, \quad (x, v, t) \in [-2\pi, 2\pi] \times [-2\pi, 2\pi] \times [0, \infty) \quad (4.64)$$

where

$$-\partial_{xx}\Phi = \frac{e}{\epsilon_0}(n - \bar{n}), \quad E = -\partial_x\Phi, \quad n = \int f dv, \quad \bar{n} = \frac{1}{|V|} \int_V f dv. \quad (4.65)$$

For our test runs, we used $\frac{e}{\epsilon_0} = 1$. The initial condition function for the test is

$$f(x, v, 0) = \frac{v^2}{\sqrt{8\pi}} \left(2 - \cos\left(\frac{x}{2}\right) \right) e^{-\frac{v^2}{2}}. \quad (4.66)$$

The test uses periodic boundary conditions in x , and zero flow boundary conditions in v .

Figure 4.8 shows the results of running the code until $t_f = 5$ and $t_f = 45$. For these plots, we used 800^2 grid points; this is twice the number of grid points as in the paper (400^2). We find good agreement with the computed solutions.

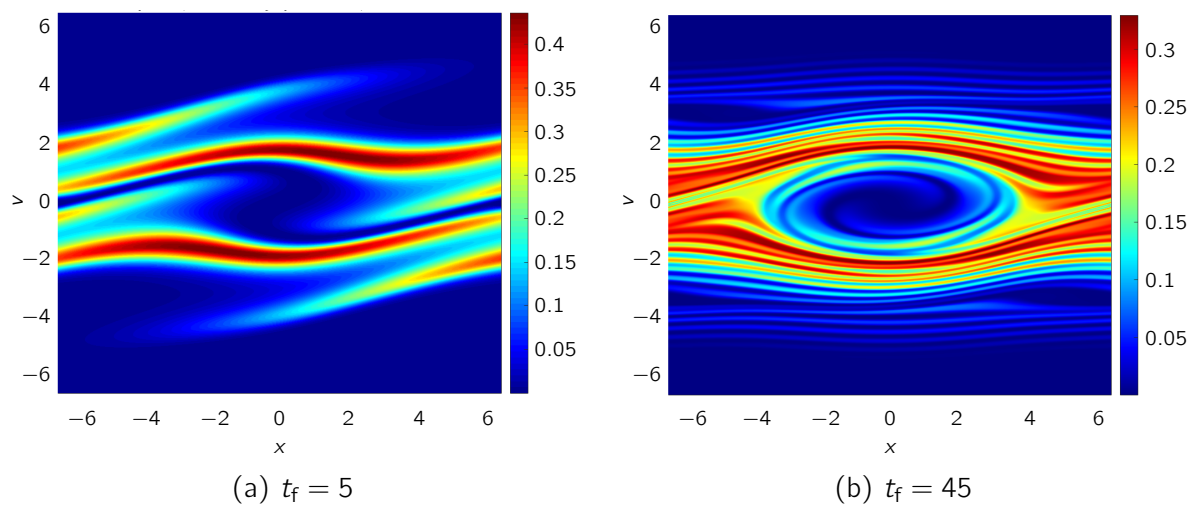


Figure 4.8: Two-Stream instability. The numerical solution is shown at $t_f = 5$ (left) and $t_f = 45$ (right). The numerical grid has $N_v \times N_x = 800 \times 800$ cells on the grid $\Omega \times V = [-2\pi, 2\pi] \times [-2\pi, 2\pi]$. The fine filamentation of the particle streams is adequately resolved and captured.

Landau Damping (Vlasov–Poisson)

This test is from Section 5.1.3 of [12]. To perform the test, the Vlasov–Poisson equation is solved and the L^2 norm of the electric field is computed at each time step. The initial condition function is

$$f(x, v, 0) = \frac{1}{\sqrt{2\pi}} (1 + \alpha \cos(kx)) e^{-\frac{v^2}{2}}, \quad (4.67)$$

where $\alpha = 0.01$, $k = 0.5$. According to [12], with these parameters, the L^2 norm of the electric field should decay exponentially at a rate of -0.1533 . Figure 4.9 demonstrates that the methods developed in the preceding sections successfully recover the correct decay rate of the L^2 norm of the electric field.

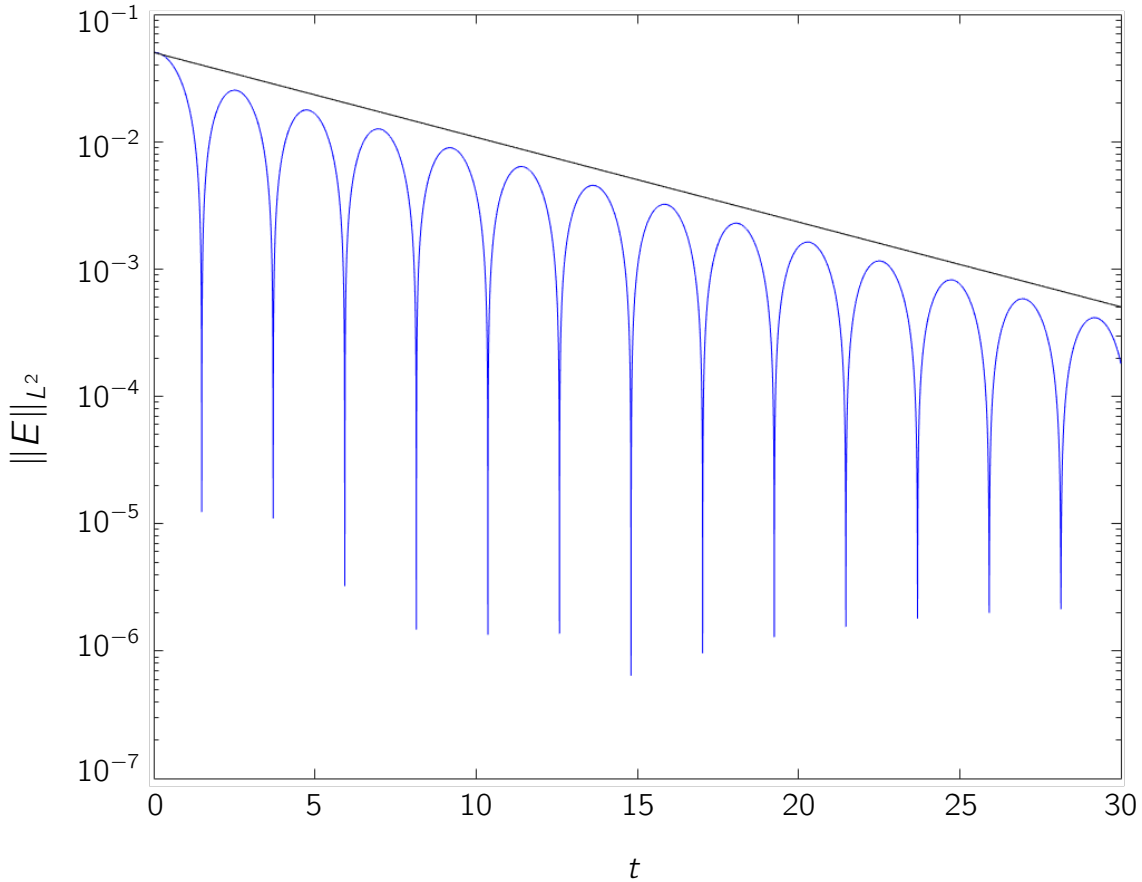


Figure 4.9: The L^2 norm of the electric field decays at an exponential decay rate of -0.1533 .

Chapter 5

Discrete-Velocity Numerical Methods for the Single-Species BGK Problem

In this chapter, we will describe numerical methods based on the discrete-velocity BGK model that we introduced in a previous chapter. Let us start with the standard discrete-velocity BGK problem first. After that, we will consider the space-homogeneous case.

5.1 A Fully Explicit Scheme

Let us again consider the $d = 1$ case. In other words, for simplicity, we will assume that the dimension of physical space is one and the dimension of velocity space is one. We will work under the assumption that velocity space is discrete and the discrete-velocity Maxwellian is computed via optimization. In other words, our starting model is the following:

$$\partial_t f(x, j, t) + v_j \partial_x f(x, j, t) = \lambda (\mathcal{M}_{\mathcal{J}, f}(x, j, t) - f(x, j, t)), \quad \forall j \in \mathcal{J}, \quad \forall x \in [a, b], \quad (5.1)$$

where

$$\mathcal{M}_{\mathcal{J}, f}(x, j, t) = \exp(\boldsymbol{\alpha}_{\mathcal{J}, f}(x, t) \cdot \mathbf{m}_{\mathcal{J}}(j)), \quad \forall j \in \mathcal{J},$$

and $\boldsymbol{\alpha}_{\mathcal{J}, f}(x, t) \in \mathbb{R}^3$ is the solution to

$$\langle \exp(\boldsymbol{\alpha}_{\mathcal{J}, f}(x, t) \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} = \langle f(x, \cdot, t) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}}.$$

For simplicity, we assume that the discrete velocities satisfy

$$v_j = h_v \cdot \left(j - \frac{1}{2} \right), \quad j \in \mathcal{J}, \quad \mathcal{J} := \{-J+1, \dots, J\}.$$

Definition 5.1.1. *The first-order explicit discrete-velocity scheme is defined as follows:*

$$f_{i,j}^{n+1} = f_{i,j}^n - \frac{\Delta t}{h_x} \left(\widehat{F}(x_{i+1/2}, v_j, t^n) - \widehat{F}(x_{i-1/2}, v_j, t^n) \right) + \frac{\Delta t}{\tau} (\mathcal{M}_{i,j}^n - f_{i,j}^n)$$

where

$$\mathcal{M}_{i,j}^n = \exp(\alpha_i^n \cdot \mathbf{m}_{\mathcal{J}}(j)),$$

and $\alpha_i^n \in \mathbb{R}^3$ is the solution to

$$\langle \exp(\alpha_i^n \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} = \langle f_{i,\cdot}^n \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}}.$$

The first-order numerical flux is obtained via a simple upwind methodology:

$$\widehat{F}(x_{i+1/2}, v_j, t^n) = \begin{cases} v_j f_{i,j}^n & \text{if } v_j \geq 0, \\ v_j f_{i,j+1}^n & \text{if } v_j < 0. \end{cases}$$

Based on our construction, we have the following result:

Theorem 5.1.2. *Suppose that $f_{i,j}^0 > 0$, for all $j \in \mathcal{J}$, and all $1 \leq i \leq N_x$. Then, for all $\mathbf{n} \in \mathbb{N}$,*

$$h_x \sum_{i=1}^{N_x} \langle \mathbf{m}_{\mathcal{J}}(\cdot) f_{i,\cdot}^n \rangle_{\mathcal{J}} = h_x \sum_{i=1}^{N_x} \langle \mathbf{m}_{\mathcal{J}}(\cdot) f_{i,\cdot}^0 \rangle_{\mathcal{J}}. \quad (5.2)$$

Additionally, provided that the CFL condition

$$\Delta t \left(\frac{1}{\tau} + \max_{j \in \mathcal{J}} \frac{|v_j|}{h_x} \right) \leq 1$$

holds, it follows that, for all $\mathbf{n} \in \mathbb{N}$, $j \in \mathcal{J}$, and $i \in \{1, 2, \dots, N_x\}$, $f_{i,j}^n > 0$. Furthermore, for all $\mathbf{n} \in \mathbb{N}$,

$$h_x \sum_{i=1}^{N_x} \langle \ln(f_{i,\cdot}^n) f_{i,\cdot}^n \rangle_{\mathcal{J}} \leq h_x \sum_{i=1}^{N_x} \langle \ln(f_{i,\cdot}^{n-1}) f_{i,\cdot}^{n-1} \rangle_{\mathcal{J}}. \quad (5.3)$$

In other words, the scheme is entropy-stable.

Proof. For $v_j > 0$, the scheme can be written as

$$\begin{aligned} f_{i,j}^{n+1} &= f_{i,j}^n - \frac{\Delta t v_j}{h_x} (f_{i,j}^n - f_{i,j-1}^n) + \frac{\Delta t}{\tau} (\mathcal{M}_{i,j}^n - f_{i,j}^n) \\ &= \left(1 - \frac{\Delta t v_j}{h_x} - \frac{\Delta t}{\tau} \right) f_{i,j}^n + \frac{\Delta t v_j}{h_x} f_{i,j-1}^n + \frac{\Delta t}{\tau} \mathcal{M}_{i,j}^n \end{aligned}$$

$$= \left(1 - \frac{\Delta t |v_j|}{h_x} - \frac{\Delta t}{\tau}\right) f_{i,j}^n + \frac{\Delta t |v_j|}{h_x} f_{i,j-1}^n + \frac{\Delta t}{\tau} \mathcal{M}_{i,j}^n.$$

For $v_j < 0$, the scheme is

$$\begin{aligned} f_{i,j}^{n+1} &= f_{i,j}^n - \frac{\Delta t v_j}{h_x} (f_{i,j+1}^n - f_{i,j}^n) + \frac{\Delta t}{\tau} (\mathcal{M}_{i,j}^n - f_{i,j}^n) \\ &= \left(1 + \frac{\Delta t v_j}{h_x} - \frac{\Delta t}{\tau}\right) f_{i,j}^n - \frac{\Delta t v_j}{h_x} f_{i,j+1}^n + \frac{\Delta t}{\tau} \mathcal{M}_{i,j}^n \\ &= \left(1 - \frac{\Delta t |v_j|}{h_x} - \frac{\Delta t}{\tau}\right) f_{i,j}^n + \frac{\Delta t |v_j|}{h_x} f_{i,j+1}^n + \frac{\Delta t}{\tau} \mathcal{M}_{i,j}^n. \end{aligned}$$

The composite scheme can be written as

$$f_{i,j}^{n+1} = \left(1 - \frac{\Delta t |v_j|}{h_x} - \frac{\Delta t}{\tau}\right) f_{i,j}^n + \frac{\Delta t (|v_j| - v_j)}{2h_x} f_{i,j+1}^n + \frac{\Delta t (|v_j| + v_j)}{2h_x} f_{i,j-1}^n + \frac{\Delta t}{\tau} \mathcal{M}_{i,j}^n,$$

which is a convex combination of $f_{i,j}^n$, $f_{i,j-1}^n$, $f_{i,j+1}^n$, and $\mathcal{M}_{i,j}^n$. If all of these values are positive, then $f_{i,j}^{n+1}$ is positive. Since the function $x \ln(x)$ is convex, it follows that, if $\alpha \in (0, 1)$ and $x \neq y$, $x, y \in (0, \infty)$, then

$$(\alpha x + (1 - \alpha)y) \ln(\alpha x + (1 - \alpha)y) \leq \alpha x \ln(x) + (1 - \alpha)y \ln(y).$$

Thus,

$$\begin{aligned} f_{i,j}^{n+1} \ln(f_{i,j}^{n+1}) &\leq \left(1 - \frac{\Delta t |v_j|}{h_x} - \frac{\Delta t}{\tau}\right) f_{i,j}^n \ln(f_{i,j}^n) + \frac{\Delta t (|v_j| - v_j)}{2h_x} f_{i,j+1}^n \ln(f_{i,j+1}^n) \\ &\quad + \frac{\Delta t (|v_j| + v_j)}{2h_x} f_{i,j-1}^n \ln(f_{i,j-1}^n) + \frac{\Delta t}{\tau} \mathcal{M}_{i,j}^n \ln(\mathcal{M}_{i,j}^n). \end{aligned}$$

Summing on k , we have

$$\begin{aligned} \langle f_{i,\cdot}^{n+1} \ln(f_{i,\cdot}^{n+1}) \rangle_{\mathcal{J}} &\leq \left\langle \left(1 - \frac{\Delta t |v_{\cdot}|}{h_x} - \frac{\Delta t}{\tau}\right) f_{i,\cdot}^n \ln(f_{i,\cdot}^n) \right\rangle_{\mathcal{J}} \\ &\quad + \left\langle \frac{\Delta t (|v_{\cdot}| - v_{\cdot})}{2h_x} f_{i+1,\cdot}^n \ln(f_{i+1,\cdot}^n) \right\rangle_{\mathcal{J}} \\ &\quad + \left\langle \frac{\Delta t (|v_{\cdot}| + v_{\cdot})}{2h_x} f_{i-1,\cdot}^n \ln(f_{i-1,\cdot}^n) \right\rangle_{\mathcal{J}} + \left\langle \frac{\Delta t}{\tau} \mathcal{M}_{i,\cdot}^n \ln(\mathcal{M}_{i,\cdot}^n) \right\rangle_{\mathcal{J}}, \end{aligned}$$

We next invoke the minimization property in (3.41): for all i ,

$$\langle f_{i,\cdot}^{n+1} \ln(f_{i,\cdot}^{n+1}) \rangle_{\mathcal{J}} \leq \left\langle \left(1 - \frac{\Delta t |v_{\cdot}|}{h_x} - \frac{\Delta t}{\tau}\right) f_{i,\cdot}^n \ln(f_{i,\cdot}^n) \right\rangle_{\mathcal{J}}$$

$$\begin{aligned}
& + \left\langle \frac{\Delta t(|v| - v.)}{2h_x} f_{i+1,\cdot}^n \ln(f_{i+1,\cdot}^n) \right\rangle_{\mathcal{J}} \\
& + \left\langle \frac{\Delta t(|v| + v.)}{2h_x} f_{i-1,\cdot}^n \ln(f_{i-1,\cdot}^n) \right\rangle_{\mathcal{J}} + \left\langle \frac{\Delta t}{\tau} f_{i,\cdot}^n \ln(f_{i,\cdot}^n) \right\rangle_{\mathcal{J}} \\
& = \left\langle \left(1 - \frac{\Delta t|v|}{h_x}\right) f_{i,\cdot}^n \ln(f_{i,\cdot}^n) \right\rangle_{\mathcal{J}} \\
& + \left\langle \frac{\Delta t(|v| - v.)}{2h_x} f_{i+1,\cdot}^n \ln(f_{i+1,\cdot}^n) \right\rangle_{\mathcal{J}} \\
& + \left\langle \frac{\Delta t(|v| + v.)}{2h_x} f_{i-1,\cdot}^n \ln(f_{i-1,\cdot}^n) \right\rangle_{\mathcal{J}},
\end{aligned}$$

Summing on i and using the spatial periodicity, completes the proof of (5.3). The proof of (5.2) is an easy exercise. $\blacksquare$

5.2 An Explicit Scheme for the Space-Homogeneous Case

In this section, we will explore an explicit scheme for the space-homogeneous, discrete-velocity BGK problem. Recall that the one-dimensional, space-homogeneous, discrete-velocity model is as follows:

$$\partial_t f(j, t) = \lambda (\mathcal{M}_{\mathcal{J},f}(j, t) - f(j, t)), \quad \forall j \in \mathcal{J}, \quad (5.4)$$

where

$$\mathcal{M}_{\mathcal{J},f}(j, t) = \exp(\alpha_{\mathcal{J},f}(t) \cdot \mathbf{m}_{\mathcal{J}}(j)), \quad \forall j \in \mathcal{J},$$

and $\alpha_{\mathcal{J},f}(t) \in \mathbb{R}^3$ is the solution to

$$\langle \exp(\alpha_{\mathcal{J},f}(t) \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} = \langle f(\cdot, t) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}}.$$

As before, it may be useful to suppose that the discrete velocities satisfy

$$v_j = h_v \cdot \left(j - \frac{1}{2}\right), \quad j \in \mathcal{J}, \quad \mathcal{J} := \{-J+1, \dots, J\},$$

though this can be generalized without any difficulty. The explicit scheme for the space-homogeneous case is given by the following:

Definition 5.2.1. *The first-order explicit discrete-velocity scheme is defined as follows:*

$$f_j^{n+1} = f_j^n + \frac{\Delta t}{\tau} (\mathcal{M}_j^n - f_j^n),$$

where

$$\mathcal{M}_j^n = \exp(\boldsymbol{\alpha}^n \cdot \mathbf{m}_{\mathcal{J}}(j)), \quad (5.5)$$

and $\boldsymbol{\alpha}^n \in \mathbb{R}^3$ is the solution to

$$\langle \exp(\boldsymbol{\alpha}^n \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} = \langle f^n \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}}. \quad (5.6)$$

We have the following result, which shows that an explicit scheme will always have a time step restriction owing to the stiffness of the BGK problem:

Theorem 5.2.2. *Suppose that $f_j^0 > 0$, for all $j \in \mathcal{J}$. Then, for all $n \in \mathbb{N}$,*

$$\langle \mathbf{m}_{\mathcal{J}}(\cdot) f^n \rangle_{\mathcal{J}} = \langle \mathbf{m}_{\mathcal{J}}(\cdot) f^0 \rangle_{\mathcal{J}}. \quad (5.7)$$

Additionally, provided that the condition

$$\frac{\Delta t}{\tau} \leq 1$$

holds, it follows that, for all $n \in \mathbb{N}$ and $j \in \mathcal{J}$, $f_j^n > 0$. Furthermore, for all $n \in \mathbb{N}$,

$$\langle \ln(f^n) f^n \rangle_{\mathcal{J}} \leq \langle \ln(f^{n-1}) f^{n-1} \rangle_{\mathcal{J}}. \quad (5.8)$$

In other words, the scheme is entropy-stable. Finally,

$$\mathcal{M}_j^n = \mathcal{M}_j^0, \quad \forall j \in \mathcal{J}, \quad (5.9)$$

for all $n \in \mathbb{N}$.

Proof. The scheme can be written as

$$f_j^{n+1} = \left(1 - \frac{\Delta t}{\tau}\right) f_j^n + \frac{\Delta t}{\tau} \mathcal{M}_j^n,$$

which is a convex combination of f_j^n and $\mathcal{M}_j^n$. Clearly, f_j^{n+1} is positive. Since the function $x \ln(x)$ is convex, it follows that

$$f_j^{n+1} \ln(f_j^{n+1}) \leq \left(1 - \frac{\Delta t}{\tau}\right) f_j^n \ln(f_j^n) + \frac{\Delta t}{\tau} \mathcal{M}_j^n \ln(\mathcal{M}_j^n).$$

Summing on j , we have

$$\langle f_i^{n+1} \ln(f_i^{n+1}) \rangle_{\mathcal{J}} \leq \left\langle \left(1 - \frac{\Delta t}{\tau}\right) f_i^n \ln(f_i^n) \right\rangle_{\mathcal{J}} + \left\langle \frac{\Delta t}{\tau} \mathcal{M}_i^n \ln(\mathcal{M}_i^n) \right\rangle_{\mathcal{J}},$$

Using the minimization property in (3.41), we find that,

$$\begin{aligned} \langle f_i^{n+1} \ln(f_i^{n+1}) \rangle_{\mathcal{J}} &\leq \left\langle \left(1 - \frac{\Delta t}{\tau}\right) f_i^n \ln(f_i^n) \right\rangle_{\mathcal{J}} + \left\langle \frac{\Delta t}{\tau} \mathcal{M}_i^n \ln(\mathcal{M}_i^n) \right\rangle_{\mathcal{J}} \\ &\leq \left\langle \left(1 - \frac{\Delta t}{\tau}\right) f_i^n \ln(f_i^n) \right\rangle_{\mathcal{J}} + \left\langle \frac{\Delta t}{\tau} f_i^n \ln(f_i^n) \right\rangle_{\mathcal{J}} \\ &= \langle f_i^n \ln(f_i^n) \rangle_{\mathcal{J}}. \end{aligned}$$

The proof of (5.7) is an easy exercise and is skipped for brevity. The proof of (5.9) follows from (5.7), (5.5), and (5.6). ■

5.3 An Implicit Scheme for the space-homogeneous Case

In the last section, we learned that an explicit scheme for the space-homogeneous case still requires a potentially restrictive time step constraint for stability. But, this can be easily overcome in the space-homogeneous case.

Definition 5.3.1. *The first-order implicit discrete-velocity scheme is defined as follows:*

$$f_j^{n+1} = f_j^n + \frac{\Delta t}{\tau} (\mathcal{M}_j^n - f_j^{n+1}),$$

where

$$\mathcal{M}_j^n = \exp(\boldsymbol{\alpha}^n \cdot \mathbf{m}_{\mathcal{J}}(j)), \quad (5.10)$$

and $\boldsymbol{\alpha}^n \in \mathbb{R}^3$ is the solution to

$$\langle \exp(\boldsymbol{\alpha}^n \cdot \mathbf{m}_{\mathcal{J}}) \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}} = \langle f_i^n \mathbf{m}_{\mathcal{J}} \rangle_{\mathcal{J}}. \quad (5.11)$$

Technically, the last scheme is an IMEX scheme, but we will stick to our definition, since we can show that, actually, $\mathcal{M}_j^n = \mathcal{M}_j^{n+1}$. Specifically, we have the following result:

Theorem 5.3.2. *Suppose that $f_j^0 > 0$, for all $j \in \mathcal{J}$. Then, for all $n \in \mathbb{N}$,*

$$\langle \mathbf{m}_{\mathcal{J}}(\cdot) f_i^n \rangle_{\mathcal{J}} = \langle \mathbf{m}_{\mathcal{J}}(\cdot) f_i^0 \rangle_{\mathcal{J}}. \quad (5.12)$$

Additionally, for all $\mathbf{n} \in \mathbb{N}$ and $j \in \mathcal{J}$, $f_j^n > 0$, and for all $\mathbf{n} \in \mathbb{N}$,

$$\langle \ln(f^n) f^n \rangle_{\mathcal{J}} \leq \langle \ln(f^{n-1}) f^{n-1} \rangle_{\mathcal{J}}. \quad (5.13)$$

In other words, the scheme is entropy-stable. Finally,

$$\mathcal{M}_j^n = \mathcal{M}_j^0, \quad \forall j \in \mathcal{J}, \quad (5.14)$$

for all $\mathbf{n} \in \mathbb{N}$. All of these properties hold unconditionally.

Proof. The scheme can be written as

$$\left(1 + \frac{\Delta t}{\tau}\right) f_j^{n+1} = f_j^n + \frac{\Delta t}{\tau} \mathcal{M}_j^n,$$

or, equivalently, as

$$f_j^{n+1} = \frac{1}{\left(1 + \frac{\Delta t}{\tau}\right)} f_j^n + \frac{\frac{\Delta t}{\tau}}{\left(1 + \frac{\Delta t}{\tau}\right)} \mathcal{M}_j^n, \quad (5.15)$$

which is again a convex combination of f_j^n and $\mathcal{M}_j^n$. Clearly, f_j^{n+1} is positive, provided f_j^n and $\mathcal{M}_j^n$ are positive. Let us write, for simplicity,

$$\alpha := \frac{1}{1 + \frac{\Delta t}{\tau}} \quad \text{and} \quad \beta := \frac{\frac{\Delta t}{\tau}}{1 + \frac{\Delta t}{\tau}}.$$

Since the function $x \ln(x)$ is convex, it follows that

$$f_j^{n+1} \ln(f_j^{n+1}) \leq \alpha f_j^n \ln(f_j^n) + \beta \mathcal{M}_j^n \ln(\mathcal{M}_j^n).$$

Summing on j , we have

$$\langle f^{n+1} \ln(f^{n+1}) \rangle_{\mathcal{J}} \leq \langle \alpha f^n \ln(f^n) \rangle_{\mathcal{J}} + \langle \beta \mathcal{M}^n \ln(\mathcal{M}^n) \rangle_{\mathcal{J}},$$

Using the minimization property in (3.41), we find that,

$$\begin{aligned} \langle f^{n+1} \ln(f^{n+1}) \rangle_{\mathcal{J}} &\leq \langle \alpha f^n \ln(f^n) \rangle_{\mathcal{J}} + \langle \beta \mathcal{M}^n \ln(\mathcal{M}^n) \rangle_{\mathcal{J}} \\ &\leq \langle \alpha f^n \ln(f^n) \rangle_{\mathcal{J}} + \langle \beta f^n \ln(f^n) \rangle_{\mathcal{J}} \\ &= \langle f^n \ln(f^n) \rangle_{\mathcal{J}}. \end{aligned}$$

Next, summing $\mathbf{m}_{\mathcal{J}}(\cdot)$ times (5.15) on j , we have

$$\begin{aligned}\langle \mathbf{m}_{\mathcal{J}}(\cdot) f^{\mathbf{n}+1} \rangle_{\mathcal{J}} &= \langle \alpha \mathbf{m}_{\mathcal{J}}(\cdot) f^{\mathbf{n}} \rangle_{\mathcal{J}} + \langle \beta \mathbf{m}_{\mathcal{J}}(\cdot) \mathcal{M}^{\mathbf{n}} \rangle_{\mathcal{J}} \\ &= \langle \alpha \mathbf{m}_{\mathcal{J}}(\cdot) f^{\mathbf{n}} \rangle_{\mathcal{J}} + \langle \beta \mathbf{m}_{\mathcal{J}}(\cdot) f^{\mathbf{n}} \rangle_{\mathcal{J}} \\ &= \langle \mathbf{m}_{\mathcal{J}}(\cdot) f^{\mathbf{n}} \rangle_{\mathcal{J}},\end{aligned}$$

which proves (5.12), and, finally, (5.14) follows directly from (5.12). ■

Chapter 6

Multi-Species BGK Equations

In the present chapter, we describe a relatively recent BGK-type model for the multi-species setting [15]. This model, which generalizes the one-species case, satisfies a multi-species analog of Boltzmann's H-Theorem [15]. In the multi-species setting, the locally conserved quantities are the species number $m_i \langle f_i \rangle$, the total momentum $\sum_i m_i \langle \mathbf{v} f_i \rangle$, and the total energy $\sum_i m_i \langle |\mathbf{v}|^2 f_i \rangle$; and the dissipated entropy (Lyapunov functional) is the total (mathematical) entropy $\sum_i \eta(f_i)$, where $\eta(f) := f \ln(f) - f$ is the kinetic entropy density. In the zero-relaxation-time limit, hydrodynamic equations can be derived along the lines of the single-species BGK equation [15]. Other consistent multi-species models can be found in [13, 18, 26, 4].

6.1 Formulation and Properties

Suppose that there are $N \in \mathbb{N}$ ($N \geq 2$) species of particles in a mixture of gases. For each species, $i \in \{1, \dots, N\}$, denote the kinetic distribution of particles with mass m_i , by $f_i(\mathbf{x}, \mathbf{v}, t)$, so that $f_i(\mathbf{x}, \mathbf{v}, t)$ describes the density of species- i particles at $\mathbf{x} \in \Omega \subset \mathbb{R}^d$, with microscopic velocity $\mathbf{v} \in \mathbb{R}^d$, at time $t \geq 0$, with respect to the measure $d\mathbf{v} d\mathbf{x}$. Define the *number density* n_i , *bulk velocity* $\mathbf{u}_i$, and *temperature* T_i , via

$$n_i = \int_{\mathbb{R}^d} f_i d\mathbf{v}, \quad \mathbf{u}_i = \frac{1}{n_i} \int_{\mathbb{R}^d} f_i \mathbf{v} d\mathbf{v}, \quad T_i = \frac{m_i}{n_i d} \int_{\mathbb{R}^d} f_i |\mathbf{u}_i - \mathbf{v}|^2 d\mathbf{v}, \quad (6.1)$$

and the *mass density* ρ_i , *momentum density* $\mathbf{k}_i$, and *energy density* E_i by

$$\rho_i = m_i n_i \quad \mathbf{k}_i = \rho_i \mathbf{u}_i \quad E_i = \frac{1}{2} \rho_i |\mathbf{u}_i|^2 + \frac{d}{2} n_i T_i. \quad (6.2)$$

The *multi-species Vlasov–BGK equation* models the evolution of the distribution fields $f_i(\mathbf{x}, \mathbf{v}, t)$, $i = 1, \dots, N$, via the system

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i + \mathbf{a}_i \cdot \nabla_{\mathbf{v}} f_i = \sum_{j=1}^N \lambda_{i,j} (M_{i,j} - f_i), \quad i = 1, \dots, N, \quad (6.3)$$

where $\mathbf{a}_i$ describes the acceleration of particles of species i , $\lambda_{i,j}$ is the collision frequency between species i and j , and the Maxwellian distribution $M_{i,j}$ is defined as

$$M_{i,j} = M_{i,j}[f_i, f_j](\mathbf{x}, \mathbf{v}, t) = n_i \left(\frac{m_i}{2\pi T_{i,j}} \right)^{\frac{d}{2}} \exp \left(-\frac{m_i |\mathbf{v} - \mathbf{u}_{i,j}|^2}{2T_{i,j}} \right), \quad (6.4)$$

using the *mixture velocities* and *mixture temperatures*,

$$\mathbf{u}_{i,j} = \frac{\lambda_{i,j} \rho_i \mathbf{u}_i + \lambda_{j,i} \rho_j \mathbf{u}_j}{\lambda_{i,j} \rho_i + \lambda_{j,i} \rho_j} \quad (6.5a)$$

$$T_{i,j} = \frac{\lambda_{i,j} n_i T_i + \lambda_{j,i} n_j T_j}{\lambda_{i,j} n_i + \lambda_{j,i} n_j} + \frac{\lambda_{i,j} \rho_i (|\mathbf{u}_i|^2 - |\mathbf{u}_{i,j}|^2) + \lambda_{j,i} \rho_j (|\mathbf{u}_j|^2 - |\mathbf{u}_{j,i}|^2)}{d(\lambda_{i,j} n_i + \lambda_{j,i} n_j)}. \quad (6.5b)$$

The mixture velocities and temperatures, $\mathbf{u}_{i,j}$ and $T_{i,j}$, are chosen so that certain collision invariances hold, as we show momentarily. The existence and uniqueness of non-negative mild solutions to the multi-species BGK equation was proved by Klingenberg & Pirner (2018) [25], for periodic physical space and under certain restrictions on the collision frequencies.

It is straightforward to check that the proposed system satisfies the usual conservation properties and an entropy dissipation property via an H-Theorem-like result. See [15] for details. In this next computation, we show that the system, as defined above, satisfies certain collision invariances.

Lemma 6.1.1. *If the mixture velocities $\mathbf{u}_{i,j}$ and the mixture temperatures $T_{i,j}$ are as given in (6.5), then the multi-species BGK collision operators*

$$Q_{i,j}[f_i, f_j] = \lambda_{i,j} (M_{i,j} - f_i) \quad (6.6)$$

satisfy the following conservation properties, which correspond to the conservation of mass, total momentum, and total energy: for any $i, j \in \{1, \dots, N\}$,

$$\int_{\mathbb{R}^d} \lambda_{i,j} (M_{i,j} - f_i) d\mathbf{v} = 0, \quad (6.7a)$$

$$m_i \int_{\mathbb{R}^d} \lambda_{i,j} (M_{i,j} - f_i) \mathbf{v} d\mathbf{v} + m_j \int_{\mathbb{R}^d} \lambda_{j,i} (M_{j,i} - f_j) \mathbf{v} d\mathbf{v} = \mathbf{0}, \quad (6.7b)$$

$$m_i \int_{\mathbb{R}^d} \lambda_{i,j} (M_{i,j} - f_i) |\mathbf{v}|^2 d\mathbf{v} + m_j \int_{\mathbb{R}^d} \lambda_{j,i} (M_{j,i} - f_j) |\mathbf{v}|^2 d\mathbf{v} = 0. \quad (6.7c)$$

Proof. Note that using the substitution

$$\mathbf{s} = \frac{\mathbf{v} - \mathbf{u}_{i,j}}{\left(\frac{2T_{i,j}}{m_i}\right)^{\frac{1}{2}}} \implies d\mathbf{s} = \left(\frac{m_i}{2T_{i,j}}\right)^{\frac{d}{2}} d\mathbf{v}, \quad (6.8)$$

and the fact that

$$\int_{\mathbb{R}^d} \exp(-|\mathbf{s}|^2) d\mathbf{s} = \pi^{\frac{d}{2}}, \quad \int_{\mathbb{R}^d} \mathbf{s} \exp(-|\mathbf{s}|^2) d\mathbf{s} = \mathbf{0}, \quad \int_{\mathbb{R}^d} |\mathbf{s}|^2 \exp(-|\mathbf{s}|^2) d\mathbf{s} = \frac{d}{2} \pi^{\frac{d}{2}}, \quad (6.9)$$

straightforward computations show that the moments of the Maxwellian $M_{i,j}$ satisfy

$$\int_{\mathbb{R}^d} M_{i,j} d\mathbf{v} = n_i, \quad \int_{\mathbb{R}^d} \mathbf{v} M_{i,j} d\mathbf{v} = n_i \mathbf{u}_{i,j}, \quad \int_{\mathbb{R}^d} |\mathbf{v}|^2 M_{i,j} d\mathbf{v} = n_i |\mathbf{u}_{i,j}|^2 + dn_i \frac{T_{i,j}}{m_i}. \quad (6.10)$$

Using these identities, the collision invariance properties of (6.7) follow. First, note that

$$I_1 := \int_{\mathbb{R}^d} Q_{i,j}^{BGK} d\mathbf{v} = \lambda_{i,j} \int_{\mathbb{R}^d} M_{i,j} d\mathbf{v} - \lambda_{i,j} \int_{\mathbb{R}^d} f_i d\mathbf{v} = \lambda_{i,j} n_i - \lambda_{i,j} n_i = 0, \quad (6.11)$$

which establishes (6.7a). To prove (6.7b), note that

$$\begin{aligned} I_2 &:= \int_{\mathbb{R}^d} Q_{i,j}^{BGK} m_i \mathbf{v} d\mathbf{v} + \int_{\mathbb{R}^d} Q_{j,i}^{BGK} m_j \mathbf{v} d\mathbf{v} \\ &= m_i \lambda_{i,j} \int_{\mathbb{R}^d} M_{i,j} \mathbf{v} d\mathbf{v} - m_i \lambda_{i,j} \int_{\mathbb{R}^d} f_i \mathbf{v} d\mathbf{v} + m_j \lambda_{j,i} \int_{\mathbb{R}^d} M_{j,i} \mathbf{v} d\mathbf{v} - m_j \lambda_{j,i} \int_{\mathbb{R}^d} f_j \mathbf{v} d\mathbf{v} \\ &= \rho_i \lambda_{i,j} \mathbf{u}_{i,j} - \lambda_{i,j} \rho_i \mathbf{u}_i + \rho_j \lambda_{j,i} \mathbf{u}_{j,i} - \rho_j \lambda_{j,i} \mathbf{u}_j. \end{aligned} \quad (6.12)$$

Rearranging this, and using the symmetry assumption, $\mathbf{u}_{i,j} = \mathbf{u}_{j,i}$ the result follows:

$$\mathbf{u}_{i,j} = \frac{\lambda_{i,j} \rho_i \mathbf{u}_i + \lambda_{j,i} \rho_j \mathbf{u}_{j,i}}{\lambda_{i,j} \rho_i + \lambda_{j,i} \rho_j} \implies (\lambda_{i,j} \rho_i + \lambda_{j,i} \rho_j) \mathbf{u}_{i,j} - \lambda_{i,j} \rho_i \mathbf{u}_i - \lambda_{j,i} \rho_j \mathbf{u}_j = I_2 = \mathbf{0}. \quad (6.13)$$

Finally, for (6.7c), note that

$$\begin{aligned}
I_3 &= \int_{\mathbb{R}^d} Q_{i,j}^{BGK} m_i |\mathbf{v}|^2 d\mathbf{v} + \int_{\mathbb{R}^d} Q_{j,i}^{BGK} m_j |\mathbf{v}|^2 d\mathbf{v} \\
&= m_i \lambda_{i,j} \int_{\mathbb{R}^d} M_{i,j} |\mathbf{v}|^2 d\mathbf{v} - m_i \lambda_{i,j} \int_{\mathbb{R}^d} f_i |\mathbf{v}|^2 d\mathbf{v} + m_j \lambda_{j,i} \int_{\mathbb{R}^d} M_{j,i} |\mathbf{v}|^2 d\mathbf{v} - m_j \lambda_{j,i} \int_{\mathbb{R}^d} f_j |\mathbf{v}|^2 d\mathbf{v} \\
&= m_i \lambda_{i,j} \left(n_i |\mathbf{u}_{i,j}|^2 + d n_i \frac{T_{i,j}}{m_i} \right) - m_i \lambda_{i,j} \left(n_i |\mathbf{u}_i|^2 + d n_i \frac{T_i}{m_i} \right) \\
&\quad + m_j \lambda_{j,i} \left(n_j |\mathbf{u}_{j,i}|^2 + d n_j \frac{T_{j,i}}{m_j} \right) - m_j \lambda_{j,i} \left(n_j |\mathbf{u}_j|^2 + d n_j \frac{T_j}{m_j} \right) \\
&= \rho_i \lambda_{i,j} [|\mathbf{u}_{i,j}|^2 - |\mathbf{u}_i|^2] + \rho_j \lambda_{j,i} [|\mathbf{u}_{j,i}|^2 - |\mathbf{u}_j|^2] + d n_i \lambda_{i,j} [T_{i,j} - T_i] + d n_j \lambda_{j,i} [T_{j,i} - T_j]. \quad (6.14)
\end{aligned}$$

Using symmetry assumptions $\mathbf{u}_{i,j} = \mathbf{u}_{j,i}$ and $T_{i,j} = T_{j,i}$, and gathering terms as in (6.13),

$$\begin{aligned}
T_{i,j} &= \frac{n_i \lambda_{i,j} T_i + n_j \lambda_{j,i} T_j}{n_i \lambda_{i,j} + n_j \lambda_{j,i}} + \frac{\rho_i \lambda_{i,j} (|\mathbf{u}_i|^2 - |\mathbf{u}_{i,j}|^2) + \rho_j \lambda_{j,i} (|\mathbf{u}_j|^2 - |\mathbf{u}_{j,i}|^2)}{d(n_i \lambda_{i,j} + d n_j \lambda_{j,i})} \\
\Rightarrow T_{i,j} d[n_i \lambda_{i,j} + n_j \lambda_{j,i}] &= d[n_i \lambda_{i,j} T_i + n_j \lambda_{j,i} T_j] + \rho_i \lambda_{i,j} [|\mathbf{u}_i|^2 - |\mathbf{u}_{i,j}|^2] + \rho_j \lambda_{j,i} [|\mathbf{u}_j|^2 - |\mathbf{u}_{j,i}|^2] \\
\Rightarrow I_3 &= 0. \quad (6.15)
\end{aligned}$$

The proof is complete. ■

The converse of the last result is also true, as is easy to show. We omit the proof for the sake of brevity.

Lemma 6.1.2. *Suppose that, for any $i, j \in \{1, \dots, N\}$, the following collision invariances hold:*

$$\int_{\mathbb{R}^d} \lambda_{i,j} (M_{i,j} - f_i) d\mathbf{v} = 0, \quad (6.16)$$

$$m_i \int_{\mathbb{R}^d} \lambda_{i,j} (M_{i,j} - f_i) \mathbf{v} d\mathbf{v} + m_j \int_{\mathbb{R}^d} \lambda_{j,i} (M_{j,i} - f_j) \mathbf{v} d\mathbf{v} = \mathbf{0}, \quad (6.17)$$

$$m_i \int_{\mathbb{R}^d} \lambda_{i,j} (M_{i,j} - f_i) |\mathbf{v}|^2 d\mathbf{v} + m_j \int_{\mathbb{R}^d} \lambda_{j,i} (M_{j,i} - f_j) |\mathbf{v}|^2 d\mathbf{v} = 0. \quad (6.18)$$

Consequently, it must be that the mixture velocities and temperatures satisfy

$$\mathbf{u}_{i,j} = \frac{\lambda_{i,j} \rho_i \mathbf{u}_i + \lambda_{j,i} \rho_j \mathbf{u}_j}{\lambda_{i,j} \rho_i + \lambda_{j,i} \rho_j} \quad (6.19)$$

$$T_{i,j} = \frac{\lambda_{i,j} n_i T_i + \lambda_{j,i} n_j T_j}{\lambda_{i,j} n_i + \lambda_{j,i} n_j} + \frac{\lambda_{i,j} \rho_i (|\mathbf{u}_i|^2 - |\mathbf{u}_{i,j}|^2) + \lambda_{j,i} \rho_j (|\mathbf{u}_j|^2 - |\mathbf{u}_{j,i}|^2)}{d(\lambda_{i,j} n_i + \lambda_{j,i} n_j)}. \quad (6.20)$$

6.2 Numerical Approximation

For certain parameter regimes, the problem may become numerically stiff, requiring prohibitively small time steps to resolve the dynamics of the particle interactions. To enable taking larger time steps, we aim to develop implicit and semi-implicit methods for the multi-species problem, wherein the collision term is computed implicitly. Thus, to see what difficulties lie ahead for the numerical analysis of the multi-species case, let us first examine the space-homogeneous problem,

$$\frac{\partial f_i}{\partial t} = \sum_{j=1}^N \lambda_{ij}(M_{ij} - f_i), \quad \text{for } i \in \{1, \dots, N\}. \quad (6.21)$$

As a prototype for the implicit treatment of the collision term, we discretize using the Backward Euler method:

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} = \sum_{j=1}^N \lambda_{ij}(M_{ij}^{n+1} - f_i^{n+1}) \quad (6.22)$$

$$\iff f_i^{n+1} = f_i^n + \Delta t \sum_{j=1}^N \lambda_{ij} M_{ij}^{n+1} - \Delta t f_i^{n+1} \sum_{j=1}^N \lambda_{ij} \quad (6.23)$$

$$\iff f_i^{n+1} \left(1 + \Delta t \sum_{j=1}^N \lambda_{ij} \right) = f_i^n + \Delta t \sum_{j=1}^N \lambda_{ij} M_{ij}^{n+1} \quad (6.24)$$

$$\iff f_i^{n+1} = \frac{f_i^n + \Delta t \sum_{j=1}^N \lambda_{ij} M_{ij}^{n+1}}{1 + \Delta t \sum_{j=1}^N \lambda_{ij}}. \quad (6.25)$$

Note that (6.25) has the terms M_{ij}^{n+1} , defined at the t^{n+1} time step. Recall that for the space-homogeneous, single-species model, the Maxwellian is time invariant (see (3.29)), so that $M^n = M^{n+1}$. This temporal invariance does not hold in the multi-species case, and this represents a significant numerical challenge. Care must be taken to give a proper implicit update for the collision operator.

As with fluid equations, spatially adaptive meshes are a requirement for highly efficient simulations of flows with fine-scale structures in phase space. However, kinetic equations also require adaptivity, not only for the resolution of fine scale structures, but also to address the fact that the effective support of the kinetic distribution may vary dramatically in phase space. Typically the size of the domain is based on the temperature of the distribution; for multi-species problems, each species may have its own temperature, which adds a complication not found in the single-species setting. In other words, the target Maxwellians in the model

may require different phase space resolutions. One way that this can be addressed is by defining the Maxwellians on different compatible grids that adequately resolve their individual supports.

Chapter 7

Asymptotic Relaxation and Numerics of Multi-Species Moment Equations

This chapter is based on two recently published papers:

1. Reference [16]: **E. Habbershaw**, R.S. Glasby, J.R. Haack, C.D. Hauck, and **S.M. Wise**, *Asymptotic Relaxation of Moment Equations for a Multi-species, Homogeneous BGK Model*, SIAP (SIAM J. Appl. Math.) 85 (2025) 294–313.
<https://doi.org/10.1137/23M1596314>

This paper, which appears in the prestigious *SIAM Journal on Applied Mathematics*, described certain dynamics of the multi-species BGK model. Understanding these model characteristics are vital for designing and implementing sophisticated numerical approximation methods.

2. Reference [17]: **E. Habbershaw**, C.D. Hauck, and **S.M. Wise**, *Implicit Update of the Moment Equations for a Multi-Species, Homogeneous BGK Model*, SINUM (SIAM J. Numer. Anal.) 63 (2025) 881–907.
<https://doi.org/10.1137/24M165421X>

This paper, which appears in the equally prestigious *SIAM Journal on Numerical Analysis*, described our novel iteration solver for the multi-species, spatially homogeneous BGK model. We prove several facts about our numerical solver therein. This iterative solver will be the basis of future sophisticated solvers for the full multi-species BGK and ES-BGK models that we are developing.

We study the space-homogeneous, multi-species BGK equations from [15], which can be understood as a special, illustrative case of the equations in [4] or [26]. We do so in the

context of collision frequencies that are independent of the phase-space velocity, but depend on both number density and temperature. In particular, we analyze the ODE system for the momentum and energy moments (the number density evolution is trivial), which is important for asymptotic analysis and for the development of numerical methods.

Indeed, many numerical simulations of the full BGK system (including phase-space advection) rely on implicit-explicit (IMEX) methods that treat the space-homogeneous component implicitly. In this setting, the result of solving the associated moments equations first is to effectively linearize and diagonalize (with respect to the phase-space velocity) the required implicit solve, yielding a significant reduction in computational cost. (See [9, 36] for applications to the single-species case and [38, Section 4] for an extension to the multi-species setting when the collision frequencies depend only on the number densities.)

In this chapter, we first establish existence and uniqueness of the momentum-energy ODE system, which follows from standard theory once a lower positive bound can be established on the species temperatures. We show monotonicity of the minimum temperature envelope as well as upper and lower bounds on the bulk velocity. We then prove exponential decay of the species momenta and energies to their steady state values, thereby generalizing some of the results in [10] to a system with an arbitrary number of species.

7.1 Model Equations

Here we recap the multi-species BGK equation, specifically for the case that the collision frequencies are dependent upon species temperatures. We denote by f_i the kinetic distribution of particles of species $i \in \{1, \dots, N\}$ having mass m_i . More specifically, $f_i(\mathbf{x}, \mathbf{v}, t)$ is the density of species i particles at the point $\mathbf{x} \in \Omega \subset \mathbb{R}^d$, with microscopic velocity $\mathbf{v} \in \mathbb{R}^d$, at time $t \geq 0$, with respect to the measure $d\mathbf{v} d\mathbf{x}$. Associated to each f_i are the species number density n_i , mass density ρ_i , bulk velocity $\mathbf{u}_i$, and temperature T_i , defined by

$$\rho_i = m_i n_i = m_i \int_{\mathbb{R}^d} f_i d\mathbf{v}, \quad \mathbf{u}_i = \frac{1}{\rho_i} \int_{\mathbb{R}^d} m_i \mathbf{v} f_i d\mathbf{v}, \quad T_i = \frac{m_i}{n_i d} \int_{\mathbb{R}^d} |\mathbf{v} - \mathbf{u}_i|^2 f_i d\mathbf{v}. \quad (7.1)$$

The species momentum densities $\mathbf{k}_i$ and species energy densities E_i are given by

$$\mathbf{k}_i = \rho_i \mathbf{u}_i \quad \text{and} \quad E_i = \frac{1}{2} \rho_i |\mathbf{u}_i|^2 + \frac{d}{2} n_i T_i. \quad (7.2)$$

BGK models are expressed in terms of Maxwellian distributions that depend on these moments.

Definition 7.1.1. Given $n > 0$, $\mathbf{u} \in \mathbb{R}^d$, $\theta > 0$, a Maxwellian $M_{n,\mathbf{u},\theta}$ is a function of the form

$$M_{n,\mathbf{u},\theta}(\mathbf{v}) = \frac{n}{(2\pi\theta)^{\frac{d}{2}}} \exp\left(-\frac{|\mathbf{v} - \mathbf{u}|^2}{2\theta}\right). \quad (7.3)$$

Straightforward computations show that the moments of a Maxwellian satisfy

$$\int_{\mathbb{R}^d} M_{n,\mathbf{u},\theta} d\mathbf{v} = n, \quad \int_{\mathbb{R}^d} \mathbf{v} M_{n,\mathbf{u},\theta} d\mathbf{v} = n\mathbf{u}, \quad \int_{\mathbb{R}^d} |\mathbf{v}|^2 M_{n,\mathbf{u},\theta} d\mathbf{v} = n|\mathbf{u}|^2 + dn\theta. \quad (7.4)$$

We consider in this chapter the multi-species BGK equation from [15], given by

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_x f_i = \frac{1}{\varepsilon} \sum_j \lambda_{i,j} (M_{i,j} - f_i), \quad \forall i \in \{1, \dots, N\}, \quad (7.5)$$

where $\varepsilon > 0$ is the Knudsen number, $\lambda_{i,j} > 0$ is the (nondimensional) frequency of collisions between species i and j (independent of $\mathbf{v}$), and

$$M_{i,j}(\mathbf{v}) = M_{n_i, \mathbf{u}_{i,j}, T_{i,j}/m_i}(\mathbf{v})$$

is a Maxwellian defined by (7.3), using the mixture velocities and temperatures

$$\mathbf{u}_{i,j} = \frac{\rho_i \lambda_{i,j} \mathbf{u}_i + \rho_j \lambda_{j,i} \mathbf{u}_j}{\rho_i \lambda_{i,j} + \rho_j \lambda_{j,i}}, \quad T_{i,j} = \frac{n_i \lambda_{i,j} T_i + n_j \lambda_{j,i} T_j}{n_i \lambda_{i,j} + n_j \lambda_{j,i}} + \frac{1}{d} \frac{\rho_i \rho_j \lambda_{i,j} \lambda_{j,i}}{\rho_i \lambda_{i,j} + \rho_j \lambda_{j,i}} \frac{|\mathbf{u}_i - \mathbf{u}_j|^2}{n_i \lambda_{i,j} + n_j \lambda_{j,i}}. \quad (7.6)$$

The existence and uniqueness of non-negative mild solutions to (a more general) multi-species BGK equation was proved in [25] for periodic spatial domains and the collision frequencies that depend on the number densities.

7.1.1 Model Properties

The BGK collision operators in (7.5) satisfy the following invariance properties: For any i, j ,

$$\int_{\mathbb{R}^d} \lambda_{i,j} (M_{i,j} - f_i) d\mathbf{v} = 0 \quad (7.7)$$

$$m_i \int_{\mathbb{R}^d} \lambda_{i,j} (M_{i,j} - f_i) \mathbf{v} d\mathbf{v} + m_j \int_{\mathbb{R}^d} \lambda_{j,i} (M_{j,i} - f_j) \mathbf{v} d\mathbf{v} = \mathbf{0} \quad (7.8)$$

$$m_i \int_{\mathbb{R}^d} \lambda_{i,j} (M_{i,j} - f_i) |\mathbf{v}|^2 d\mathbf{v} + m_j \int_{\mathbb{R}^d} \lambda_{j,i} (M_{j,i} - f_j) |\mathbf{v}|^2 d\mathbf{v} = 0, \quad (7.9)$$

corresponding to conservation of species mass, total momentum, and total energy, respectively. Furthermore, an entropy dissipation condition is satisfied: For a spatially homogeneous

mixture, the entropy function $\mathcal{H} = \sum_i \int_{\mathbb{R}^d} f_i \ln f_i d\mathbf{v}$ satisfies $\frac{d}{dt}\mathcal{H} \leq 0$. Moreover, $\frac{d}{dt}\mathcal{H} = 0$ if and only if $f_i = M_{n_i, \mathbf{u}_{\text{eq}}, T_{\text{eq}}/m_i}(\mathbf{v})$ for all $i \in \{1, \dots, N\}$, where $\mathbf{u}_{\text{eq}}$ and T_{eq} are the equilibrium bulk velocity and temperature, respectively, which are common to all species [15].

The collision frequencies $\lambda_{i,j}$ are typically expressed as functions of the species moments given in (7.1). To define these collision frequencies, [15] presents a recipe based on matching either momentum or energy relaxation rates of the Boltzmann equation, given either a differential cross section or a momentum transfer cross section. In this paper, we consider the case of hard sphere collisions, for which the momentum transfer cross section is independent of microscopic velocity and given by [3]

$$\sigma_{\text{MT}} = \pi \left(\frac{d_i + d_j}{2} \right)^2 = \pi d_{ij}^2, \quad (7.10)$$

where d_i and d_j are reference diameters for the particles of species i and j ; reference diameters for several species are given in [3] and [7]. Following the recipe for matching energy relaxation rates from Section 4.3 of [15], we obtain the following collision frequencies for hard sphere interactions:

$$\lambda_{i,j}^{\text{HS}} = \frac{32\pi^2}{3(2\pi)^{3/2}} \frac{m_i m_j}{(m_i + m_j)^2} (d_i + d_j)^2 n_j \sqrt{\frac{T_i}{m_i} + \frac{T_j}{m_j}}. \quad (7.11)$$

While the formula in (7.11) is specific to the physically relevant case $d = 3$, collision frequencies can be derived in arbitrary dimensions in a similar fashion.

The dependence of the collision frequencies on the temperature makes the BGK model considered here more complicated than many models considered in the literature which assume that $\lambda_{i,j}$ is a constant or depends only on n_j . This is largely due to the non-Lipschitz nature of the square root function near zero and the fact that the frequencies are time-dependent functions. While we focus on the hard spheres model in this paper for simplicity, the analysis provided here is readily applied to other models in the literature [3].

7.1.2 Moment Equations

The focus of the present work is the space-homogeneous multi-species BGK equation, obtained by removing the advection terms from (7.5). In this case $f_i = f_i(\mathbf{v}, t)$ satisfies

$$\frac{\partial f_i}{\partial t} = \frac{1}{\varepsilon} \sum_j \lambda_{i,j} (M_{i,j} - f_i), \quad i \in \{1, \dots, N\}. \quad (7.12)$$

Multiplication of (7.12) by m_i , $m_i \mathbf{v}$, and $m_i |\mathbf{v}|^2$, followed by integration with respect to $\mathbf{v}$, gives equations for the mass density, momentum density, and energy density of each species

$$\frac{d\rho_i}{dt} = 0, \quad (7.13a)$$

$$\frac{d(\rho_i \mathbf{u}_i)}{dt} = \frac{1}{\varepsilon} \sum_j A_{ij} (\mathbf{u}_j - \mathbf{u}_i), \quad (7.13b)$$

$$\frac{dE_i}{dt} = \frac{1}{\varepsilon} \sum_j B_{ij} \left(\frac{E_j}{n_j} - \frac{E_i}{n_i} \right) + \frac{1}{2\varepsilon} \sum_j B_{ij} S_{ij} (m_i - m_j), \quad (7.13c)$$

where the equations for $\rho_i \mathbf{u}_i$ and E_i are derived using the definitions for $\mathbf{u}_{i,j}$ and $T_{i,j}$ from (7.6) and we define $N \times N$ matrices A , B , C , D , F , G , and S by

$$[A]_{ij} = \frac{\rho_i \rho_j \lambda_{i,j} \lambda_{j,i}}{\rho_i \lambda_{i,j} + \rho_j \lambda_{j,i}}, \quad [B]_{ij} = \frac{n_i n_j \lambda_{i,j} \lambda_{j,i}}{n_i \lambda_{i,j} + n_j \lambda_{j,i}}, \quad [S]_{ij} = |\mathbf{u}_{i,j}|^2, \quad [C]_{ij} = B_{ij} S_{ij}, \quad (7.14a)$$

$$[D]_{ij} = \left(\sum_k A_{i,k} \right) \delta_{ij}, \quad [F]_{ij} = \left(\sum_k B_{i,k} \right) \delta_{ij}, \quad [G]_{ij} = \left(\sum_k C_{i,k} \right) \delta_{ij}. \quad (7.14b)$$

According to (7.13a), each individual species mass density ρ_i (or, equivalently, number density n_i) is conserved (i.e., constant in time). However, only the *total* momentum and energy are conserved. Indeed, summing (7.13b) and (7.13c) over all species yields:

$$\sum_{i=1}^N \frac{d(\rho_i \mathbf{u}_i)}{dt} = \mathbf{0} \quad \text{and} \quad \sum_{i=1}^N \frac{dE_i}{dt} = 0, \quad (7.15)$$

respectively.

In terms of the vectorized quantities

$$\mathbf{U} = [\mathbf{u}_1, \dots, \mathbf{u}_N]^\top \in \mathbb{R}^{N \times d} \quad \text{and} \quad \mathbf{E} = [E_1, \dots, E_N]^\top \in \mathbb{R}^N, \quad (7.16)$$

the equations in (7.13) take the form

$$P \frac{d\mathbf{U}}{dt} = -\frac{1}{\varepsilon} (D - A) \mathbf{U}, \quad (7.17a)$$

$$\frac{d\mathbf{E}}{dt} = -\frac{1}{\varepsilon} (F - B) Q^{-1} \mathbf{E} + \frac{1}{2\varepsilon} (G - C) M \mathbf{1}, \quad (7.17b)$$

where $P = \text{diag}\{\rho_k\} \in \mathbb{R}^{N \times N}$, $Q = \text{diag}\{n_k\} \in \mathbb{R}^{N \times N}$, and $M = \text{diag}\{m_k\} \in \mathbb{R}^{N \times N}$. To simplify the analysis later, it will be convenient to introduce variables

$$\mathbf{W} = P^{\frac{1}{2}} \mathbf{U} \in \mathbb{R}^{N \times d} \quad \text{and} \quad \boldsymbol{\xi} = Q^{-\frac{1}{2}} \mathbf{E} \in \mathbb{R}^N. \quad (7.18)$$

In terms of $\mathbf{W}$ and $\boldsymbol{\xi}$, (7.17) takes the form

$$\frac{d\mathbf{W}}{dt} = -\frac{1}{\varepsilon} \mathbf{Z} \mathbf{W}, \quad (7.19a)$$

$$\frac{d\boldsymbol{\xi}}{dt} = -\frac{1}{\varepsilon} \widehat{\mathbf{Z}} \boldsymbol{\xi} + \frac{1}{2\varepsilon} Q^{-\frac{1}{2}} (G - C) M \mathbf{1}, \quad (7.19b)$$

where

$$\mathbf{Z} = P^{-\frac{1}{2}} (D - A) P^{-\frac{1}{2}} \in \mathbb{R}^{N \times N} \quad \text{and} \quad \widehat{\mathbf{Z}} = Q^{-\frac{1}{2}} (F - B) Q^{-\frac{1}{2}} \in \mathbb{R}^{N \times N}. \quad (7.20)$$

7.2 Properties of the ODE system

The main result of this section is to show that there is a unique solution to the ODE system (7.17) for all physically meaningful initial conditions. When the collision frequencies are constant in time, such a result follows directly from the standard ODE theory for systems with Lipschitz dynamics. However, because the collision frequencies in (7.11) depend on $\sqrt{T_i}$, only a local Lipschitz condition can be obtained for the right-hand side of (7.17). Thus the key step is to show that the species temperatures are bounded below away from zero. This bound will also be important for establishing exponential decay to steady-state in Section 7.3. We also establish upper and lower bounds on the bulk velocity components that will be used in the decay estimates.

7.2.1 Positivity of the Temperature

To make the following proofs easier to manage, we introduce the parameters

$$\alpha_{i,j} = \frac{\rho_i \lambda_{i,j}}{\rho_i \lambda_{i,j} + \rho_j \lambda_{j,i}} \quad \text{and} \quad \beta_{i,j} = \frac{n_i \lambda_{i,j}}{n_i \lambda_{i,j} + n_j \lambda_{j,i}}, \quad (7.21)$$

which satisfy the conditions $\alpha_{i,j} + \alpha_{j,i} = 1 = \beta_{i,j} + \beta_{j,i}$. With these parameters, the mixture values in (7.6) can be expressed as

$$\mathbf{u}_{i,j} = \alpha_{i,j} \mathbf{u}_i + \alpha_{j,i} \mathbf{u}_j \quad \text{and} \quad T_{i,j} = \beta_{i,j} T_i + \beta_{j,i} T_j + \frac{1}{d} m_i \alpha_{j,i} \beta_{i,j} |\mathbf{u}_i - \mathbf{u}_j|^2. \quad (7.22)$$

Lemma 7.2.1. *The temperatures T_i , $i \in \{1, \dots, N\}$, satisfy the ODE*

$$\frac{dT_i}{dt} = \frac{1}{\varepsilon} \sum_j \lambda_{i,j} \beta_{j,i} (T_j - T_i) + \frac{1}{\varepsilon d} \sum_j \lambda_{i,j} m_i \alpha_{j,i} (\alpha_{j,i} + \beta_{i,j}) |\mathbf{u}_i - \mathbf{u}_j|^2. \quad (7.23)$$

Proof. The proof is a direct calculation. From (7.13b) and the fact that $A_{i,j} = \alpha_{j,i}\rho_i\lambda_{i,j}$, it follows that

$$\rho_i \frac{d}{dt} |\mathbf{u}_i|^2 = \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{i,j} (2\alpha_{j,i} \langle \mathbf{u}_i, \mathbf{u}_j \rangle - 2\alpha_{j,i} |\mathbf{u}_i|^2), \quad (7.24)$$

where $\langle \cdot, \cdot \rangle$ denotes the standard Euclidean inner product on $\mathbb{R}^d$. The equation in (7.23) can be obtained by (i) using (7.2) to express (7.13c) in terms of the temperatures and velocities; (ii) invoking (7.24) to eliminate the time derivative of $|\mathbf{u}_i|^2$; (iii) using the formula in (7.22) to replace $\mathbf{u}_{i,j}$ wherever it appears; and (iv) applying the elementary relations $\alpha_{j,i}^2 = \alpha_{j,i} - \alpha_{i,j}\alpha_{j,i} = 2\alpha_{j,i} + \alpha_{i,j}^2 - 1$. ■

Theorem 7.2.2. *Suppose that for some $t_f > 0$, there exists a local solution $\mathbf{U} \in C^1([0, t_f]; \mathbb{R}^{N \times d})$ and $\mathbf{E} \in C^1([0, t_f]; \mathbb{R}^N)$ to the system given by (7.17), with initial conditions $\mathbf{U}(0)$ and $\mathbf{E}(0)$ such that $T_i(0) > 0$ for all $i \in \{1, \dots, N\}$. Then $T_i(t) \geq T_{\min} := \min_k \{T_k(0)\}$ for all $t \in [0, t_f]$ and all $i \in \{1, \dots, N\}$.*

Proof. The proof relies on an integrating factor technique that yields a Grönwall-type estimate. Define a lower temperature envelope $T_*(t) = \min_k \{T_k(t)\}$. From (7.23) it follows that, for $i \in \{1, \dots, N\}$,

$$\frac{dT_i}{dt} + c_i(t)T_i(t) \geq c_i(t)T_*(t), \quad \text{where} \quad c_i(t) = \frac{1}{\varepsilon} \sum_j \lambda_{i,j}(t)\beta_{j,i}(t). \quad (7.25)$$

Let $a_i(t) = \int_0^t c_i(s) ds$. Then $a_i'(t) = c_i(t)$ and

$$\frac{d}{dt} (e^{a_i(t)} T_i(t)) = e^{a_i(t)} \left[\frac{d}{dt} T_i(t) + c_i(t) T_i(t) \right] \stackrel{(7.25)}{\geq} e^{a_i(t)} c_i(t) T_*(t) = \frac{d}{dt} (e^{a_i(t)} T_*(t)). \quad (7.26)$$

For each $\gamma > 0$, define the set

$$S_\gamma = \left\{ t \in [0, t_f] \mid T_*(t) < \frac{1}{1+\gamma} T_*(0) \right\}. \quad (7.27)$$

We now argue by contradiction. Assume that S_γ is nonempty and let $t_* = \inf S_\gamma$. Then by definition,

$$T_*(t_*) \leq \frac{1}{1+\gamma} T_*(0) < T_*(0). \quad (7.28)$$

However, because T_i is continuous on $[0, t_f]$, it follows that $T_*(t) \geq T_*(t_*)$ for every $t \in [0, t_*]$

which, along with (7.26), implies that

$$\frac{d}{dt} (e^{a_i(t)} T_i(t)) \geq \frac{d}{dt} (e^{a_i(t)} T_*(t_*)), \quad \forall t \in [0, t_*]. \quad (7.29)$$

Integrating both sides of (7.29) from $[0, t_*]$ and then multiplying the result by $e^{-a_i(t_*)} \geq 0$ gives

$$T_i(t_*) \geq T_i(0)e^{-a_i(t_*)} + T_*(t_*) (1 - e^{-a_i(t_*)}) \geq T_*(0)e^{-a_i(t_*)} + T_*(t_*) (1 - e^{-a_i(t_*)}). \quad (7.30)$$

Define i_* such that $T_{i_*}(t_*) = T_*(t_*)$. If $i = i_*$, then (7.30) becomes

$$T_*(t_*) \equiv T_{i_*}(t_*) \geq T_*(0)e^{-a_{i_*}(t_*)} + T_*(t_*) (1 - e^{-a_{i_*}(t_*)}), \quad (7.31)$$

which, after some simple algebra, implies that $T_*(t_*) \geq T_*(0)$. However this results contradicts (7.28) which means that no such t_* exists and the set S_γ must be empty. As a consequence, $T_*(t) \geq \frac{1}{1+\gamma} T_*(0)$ for all $t \in [0, t_f]$. Since $\gamma > 0$ is arbitrary, the limit $\gamma \rightarrow 0$ yields $T_*(t) \geq T_*(0) = T_{\min}$ for all $t \in [0, t_f]$. The proof is complete. ■

7.2.2 Velocity Bounds

For each component $j \in \{1, \dots, d\}$, define the lower and upper velocity envelopes

$$\underline{u}_k(t) = \min_j \{U_{j,k}(t)\}, \quad \bar{u}_k(t) = \max_j \{U_{j,k}(t)\}, \quad (7.32)$$

and the components of the vector $\mathbf{u}_{\max} \in \mathbb{R}^d$

$$[\mathbf{u}_{\max}(t)]_k = \max \{|\underline{u}_k(t)|, |\bar{u}_k(t)|\}. \quad (7.33)$$

Theorem 7.2.3. *Suppose that the assumptions of Theorem 7.2.2 hold. Then for each $j \in \{1, \dots, d\}$, the velocity components follow the inequalities*

$$\underline{u}_k(0) \leq \underline{u}_k(t) \leq U_{i,k}(t) \leq \bar{u}_k(t) \leq \bar{u}_k(0) \quad (7.34)$$

for all $t \in [0, t_f]$ and all $i \in \{1, \dots, N\}$. Further, for any $t \in [0, t_f]$, and all $i \in \{1, \dots, N\}$,

$$\|\mathbf{u}_i(t)\|_2 \leq \|\mathbf{u}_{\max}(t)\|_2 \leq \|\mathbf{u}_{\max}(0)\|_2 =: u_{\max}. \quad (7.35)$$

Proof. The proof of the inequalities in (7.34) are similar to the proof of the temperature

lower bound given in Theorem 7.2.2. From the velocity equation, (7.13b),

$$\frac{d}{dt} \mathbf{u}_{i,k} + \left(\frac{1}{\varepsilon} \sum_j \lambda_{ij} \alpha_{j,i} \right) \mathbf{u}_{i,k} = \frac{1}{\varepsilon} \sum_j \lambda_{ij} \alpha_{j,i} \mathbf{u}_{j,k}, \quad (7.36)$$

we obtain, using the definitions $\mathbf{u}_{j,k}(t) \leq \bar{u}_k(t)$, and $c_i = \frac{1}{\varepsilon} \sum_j \lambda_{ij} \alpha_{j,i}$,

$$\frac{d}{dt} \mathbf{u}_{i,k} + c_i(t) \mathbf{u}_{i,k} \leq c_i(t) \bar{u}_k(t). \quad (7.37)$$

From this point the proof of the upper bound in (7.34) follows that of Theorem 7.2.2, with (7.37) being the analog of (7.25). The proof of the lower bound is even more similar.

Finally, the bound in (7.35) follows from (7.34). Specifically, if a , b , and c are real-valued scalars such that $a \leq b \leq c$, then $|b| \leq \max\{|a|, |c|\}$. Hence

$$\|\mathbf{u}_i\|_2^2 = \sum_{k=1}^d \mathbf{u}_{i,k}^2 \leq \sum_{k=1}^d \max\{|\underline{u}_k(0)|, |\bar{u}_k(0)|\}^2 = \|\mathbf{u}_{\max}(0)\|_2^2 = u_{\max}^2. \quad (7.38)$$

■

7.2.3 Existence and Uniqueness

According to (7.13a), the number densities n_i and mass densities ρ_i are non-negative constants in time:

$$n_i(0) = n_i(t), \quad \rho_i(0) = \rho_i(t) = m_i n_i(t), \quad \forall i \in \{1, \dots, N\}, \quad t \in [0, t_f]. \quad (7.39)$$

To avoid any degenerate cases, we assume that $n_{\min} := \min_j n_j(0) > 0$ and $\rho_{\min} := \min_j \rho_j(0) > 0$. Then, given any velocity-energy pair $(\mathbf{u}_i, E_i)$, the associated temperature T_i is given by (cf. (7.1))

$$T_i = \vartheta_i(\mathbf{u}_i, E_i) := \frac{2}{dn_i} E_i - \frac{m_i}{d} |\mathbf{u}_i|^2, \quad (7.40)$$

and the set of all realizable velocity and energy states is given by

$$\mathcal{R} = \left\{ (\mathbf{U}, \mathbf{E}) \in \mathbb{R}^{N \times d} \times \mathbb{R}^N \mid \vartheta_i(\mathbf{u}_i, E_i) \geq 0, \forall i \in \{1, \dots, N\} \right\}, \quad (7.41)$$

where ϑ_i is defined in (7.40). Given positive scalars $T_{\min} \in (0, \infty)$ and $E_{\text{tot}} \in (0, \infty)$, let

$$\mathcal{D}(T_{\min}, E_{\text{tot}}) = \left\{ (\mathbf{U}, \mathbf{E}) \in \mathcal{R} \left| \sum_{i=1}^N E_i = E_{\text{tot}} \quad \text{and} \quad \vartheta_i(\mathbf{u}_i, E_i) \geq T_{\min}, \quad \forall i \in \{1, \dots, N\} \right. \right\}. \quad (7.42)$$

Recall that by Theorem 7.2.3, $|\mathbf{u}_i| \leq u_{\max} =: \|\mathbf{u}_{\max}(0)\|_2 \leq \sqrt{\frac{2E_{\text{tot}}}{\rho_{\min}}}$ for all $(\mathbf{U}, \mathbf{E}) \in \mathcal{D}(T_{\min}, E_{\text{tot}})$. Thus $\mathcal{D}(T_{\min}, E_{\text{tot}})$ is a closed and bounded subset of $\mathbb{R}^{N \times d} \times \mathbb{R}^N$.

Lemma 7.2.4. *Let $T_{\min} \in (0, \infty)$ and $E_{\text{tot}} \in (0, \infty)$ be given. Suppose that for some $t_f > 0$, there exists a local solution $\mathbf{U} \in C^1([0, t_f]; \mathbb{R}^{N \times d})$ and $\mathbf{E} \in C^1([0, t_f]; \mathbb{R}^N)$ of the system in (7.17) with initial condition $(\mathbf{U}^0, \mathbf{E}^0) \in \mathcal{D}(T_{\min}, E_{\text{tot}})$. Then $(\mathbf{U}(t), \mathbf{E}(t)) \in \mathcal{D}(T_{\min}, E_{\text{tot}})$ for all $t \in [0, t_f]$. In particular, $T_{\min} \leq T_i(t) \leq T_{\max} := \frac{2}{dn_{\min}} E_{\text{tot}}$ for all $t \in [0, t_f]$.*

Proof. To conclude that $(\mathbf{U}(t), \mathbf{E}(t)) \in \mathcal{D}$ for all $t \in [0, t_f]$, two conditions must be satisfied. The first condition:

$$\sum_{i=1}^N E_i(t) = \sum_{i=1}^N E_i(0) = E_{\text{tot}}, \quad \forall t \in [0, t_f], \quad (7.43)$$

follows immediately from (7.15), and the upper bound $T_i(t) \leq T_{\max}$ follows:

$$T_i(t) = \frac{2}{dn_i} E_i \leq \frac{2}{dn_{\min}} E_{\text{tot}} = T_{\max}. \quad (7.44)$$

The second condition:

$$T_{\min} \leq T_i(t) = \vartheta(\mathbf{u}_i(t), E_i(t)), \quad \forall t \in [0, t_f], \quad (7.45)$$

is a direct consequence of Theorem 7.2.2. ■

Theorem 7.2.5. *Suppose that $m_i > 0$ and $n_i > 0$ for all $i \in \{1, \dots, N\}$. Then for any $(\mathbf{U}^0, \mathbf{E}^0) \in \text{int } \mathcal{R}$, there exists a global, unique solution $(\mathbf{U}, \mathbf{E}) \in C^1([0, \infty); \mathcal{R})$ of the system (7.17) with the initial conditions $(\mathbf{U}(0), \mathbf{E}(0)) = (\mathbf{U}^0, \mathbf{E}^0)$. Moreover, the associated temperatures $T_i(t) = \vartheta_i(\mathbf{u}_i(t), E_i(t))$ are bounded below by their initial values; that is*

$$\min_i T_i(t) \geq \min_i T_i(0), \quad \forall t > 0. \quad (7.46)$$

Proof. The system (7.17) can be written as

$$\frac{d}{dt} \begin{pmatrix} \mathbf{U} \\ \mathbf{E} \end{pmatrix} = \mathbf{f}(\mathbf{U}, \mathbf{E}) \quad \text{where} \quad \mathbf{f}(\mathbf{U}, \mathbf{E}) := \begin{pmatrix} -\frac{1}{\varepsilon} P^{-1}(D - A)\mathbf{U} \\ -\frac{1}{\varepsilon}(F - B)Q^{-1}\mathbf{E} + \frac{1}{2\varepsilon}(G - C)M\mathbf{1} \end{pmatrix}. \quad (7.47)$$

Let $T_{\min} = \min_i T_i(0)$ and $E_{\text{tot}} = \sum_i E_i(0)$. Since $(\mathbf{U}, \mathbf{E}) \in \text{int } \mathcal{R}$, it follows that $T_{\min} > 0$ and $E_{\text{tot}} > 0$. Moreover, there exists an $\epsilon > 0$ such that the closed ϵ -neighborhood of $\mathcal{D}(T_{\min}, E_{\text{tot}})$, denoted by $\mathcal{D}_\epsilon(T_{\min}, E_{\text{tot}})$, is contained in $\text{int } \mathcal{R}$, i.e., $\mathcal{D}_\epsilon(T_{\min}, E_{\text{tot}}) \subset \text{int } \mathcal{R}$. In particular, $\min_i T_i = \min_i \vartheta(\mathbf{u}_i, E_i)$ is bounded below on $\mathcal{D}_\epsilon(T_{\min}, E_{\text{tot}})$. Hence, f is Lipschitz on $\mathcal{D}_\epsilon(T_{\min}, E_{\text{tot}})$ with Lipschitz constant $L > 0$ and bound $\|\mathbf{f}(\mathbf{U}, \mathbf{E})\|_2 \leq \mathcal{M} < \infty$. Since $(\mathbf{U}^0, \mathbf{E}^0) \in \mathcal{D}$, there is a number $\beta = \beta(\epsilon) > 0$, independent of the point $(\mathbf{U}^0, \mathbf{E}^0)$, such that the closed ball $\overline{B}((\mathbf{U}, \mathbf{E}), \beta) \subset \mathcal{D}_\epsilon$. Appealing to the Picard–Lindelöf Theorem B.0.1, there exists a unique solution on the interval $[0, \delta]$, where $\delta = \min(\frac{1}{2L}, \frac{\beta}{\mathcal{M}})$. By Lemma 7.2.4, $(\mathbf{U}(t), \mathbf{E}(t)) \in \mathcal{D}$, for all $t \in [0, \delta]$. Since $(\mathbf{U}(\delta), \mathbf{E}(\delta)) \in \mathcal{D}$, we can apply the Picard–Lindelöf Theorem to (7.17) again, but with the initial condition $= (\mathbf{U}(\delta), \mathbf{E}(\delta))$, and thereby extend the unique solution to the interval $[0, 2\delta]$. Again, $(\mathbf{U}(2\delta), \mathbf{E}(2\delta)) \in \mathcal{D}$, and the process can be continued indefinitely, with, crucially, no degradation of $\delta > 0$, since $\mathcal{M}$ and L cannot grow larger and β does not shrink. The result follows. ■

7.3 Long-time Behavior

Having proven the existence of unique, global, physically realizable solutions for (7.17), we now seek to characterize the asymptotic behavior of those solutions. In particular, we want to show that solutions converge to

$$\mathbf{U}^\infty(t) = \mathbf{1}(\mathbf{u}^\infty)^\top \quad \text{and} \quad \mathbf{E}^\infty(t) = \frac{|\mathbf{u}^\infty(t)|^2}{2} P\mathbf{1} + \frac{dT^\infty(t)}{2} Q\mathbf{1}, \quad (7.48)$$

where

$$\mathbf{u}^\infty(t) = \frac{\sum_i \rho_i \mathbf{u}_i(t)}{\sum_i \rho_i} \quad \text{and} \quad T^\infty(t) = \frac{\sum_i n_i T_i(t)}{\sum_i n_i} + \frac{\sum_i \rho_i (|\mathbf{u}_i(t)|^2 - |\mathbf{u}^\infty(t)|^2)}{d \sum_i n_i}. \quad (7.49)$$

are constant functions of time.

Proposition 7.3.1. *Suppose that $(\mathbf{U}, \mathbf{E}) \in C^1([0, \infty); \mathcal{R})$ is a unique global-in-time solution to the system (7.17a)–(7.17b) with assumptions as given in Theorem 7.2.5. Further let $\mathbf{T} \in C^1([0, \infty); \mathbb{R}^N)$ be the associated temperature vector, whose components satisfy (7.23). Then $\mathbf{u}^\infty$, T^∞ , and $\mathbf{E}^\infty$ are time invariant quantities, and $T^\infty > 0$.*

Proof. By conservation of mass, (7.13a), and total momentum, (7.15), $\sum_i \rho_i$ and $\sum_i \rho_i \mathbf{u}_i$ are constant. Thus $\mathbf{u}^\infty$ is time invariant. To show that T^∞ is constant in time, multiply

(7.49) by the expression $\frac{d}{2} \sum_i n_i$, which is constant by (7.13a), to obtain

$$\frac{d}{2} \left(\sum_i n_i \right) T^\infty = \sum_i \left[\frac{d}{2} n_i T_i + \frac{1}{2} \rho_i |\mathbf{u}_i|^2 \right] - \frac{1}{2} \left(\sum_i \rho_i \right) |\mathbf{u}^\infty|^2 = \sum_i E_i - \frac{1}{2} \left(\sum_i \rho_i \right) |\mathbf{u}^\infty|^2. \quad (7.50)$$

The first term on the right-hand side of (7.50) is constant by conservation of total energy, (7.15); the second term is constant by conservation of species mass, (7.13a), and the fact that $\mathbf{u}^\infty$ is constant. Thus T^∞ is time invariant. It follows immediately from (7.48) that $\mathbf{E}^\infty$ is also time invariant.

Since $(\mathbf{U}(t), \mathbf{E}(t)) \in \mathcal{R}$ for all $t > 0$, it follows that $T_i(t) = \vartheta(\mathbf{u}_i(t), E_i(t)) \geq 0$ for all $t > 0$. Thus to show that $T^\infty > 0$, it is sufficient to show that $\sum_i \rho_i (|\mathbf{u}_i|^2 - |\mathbf{u}^\infty|^2) \geq 0$. Let $r_i = \frac{\rho_i}{\sum_k \rho_k} > 0$. Then $\sum_i r_i = 1$ and $|\mathbf{u}^\infty|^2 = (\sum_i r_i \mathbf{u}_i)^\top (\sum_j r_j \mathbf{u}_j) = \sum_i \sum_j r_i r_j \mathbf{u}_i^\top \mathbf{u}_j$. Therefore

$$\sum_i \rho_i (|\mathbf{u}_i|^2 - |\mathbf{u}^\infty|^2) = \sum_k \rho_k \left[\sum_{i,j} r_i r_j |\mathbf{u}_i|^2 - \sum_{i,j} r_i r_j \mathbf{u}_i^\top \mathbf{u}_j \right] = \frac{1}{2} \sum_k \rho_k \sum_{i,j} r_i r_j |\mathbf{u}_i - \mathbf{u}_j|^2 \geq 0. \quad (7.51)$$

■

Remark 7.3.2. The quantities $\mathbf{u}^\infty$ and T^∞ were referred to as the mixture mean velocity and mixture temperature, respectively, in [14]. However, in this paper, we reserve these terms for the quantities $\mathbf{u}_{i,j}$ and $T_{i,j}$, respectively.

The convergence of $\mathbf{u}_i$, T_i , and $\mathbf{E}$ as $t \rightarrow \infty$ is established by the following result, the proof of which is the focus of the rest of this section.

Theorem 7.3.3. Under the assumptions of Proposition 7.3.1, for all $i \in \{1, \dots, N\}$,

$$\lim_{t \rightarrow \infty} \mathbf{u}_i(t) = \mathbf{u}^\infty, \quad \lim_{t \rightarrow \infty} T_i(t) = T^\infty, \quad \text{and} \quad \lim_{t \rightarrow \infty} \mathbf{E}(t) = \mathbf{E}^\infty, \quad (7.52)$$

and bounds for the decay rates of the bulk velocities and energies are given by

$$\|\mathbf{u}_i(t) - \mathbf{u}^\infty\|_2 \leq C_U \exp\left(-\frac{z_{\min}}{\varepsilon} t\right), \quad i \in \{1, \dots, N\} \quad (7.53)$$

$$\|\mathbf{E}(t) - \mathbf{E}^\infty\|_2 \leq C_1 e^{-\frac{\hat{z}_{\min}}{\varepsilon} t} + C_2 \frac{e^{-\frac{z_{\min}}{\varepsilon} t} - e^{-\frac{\hat{z}_{\min}}{\varepsilon} t}}{\hat{z}_{\min} - z_{\min}}, \quad (7.54)$$

where $z_{\min} > 0$ and $\hat{z}_{\min} > 0$ are lower bounds on the positive eigenvalues of Z and $\hat{Z}$,

respectively, and $C_U > 0$, $C_1 > 0$, and $C_2 > 0$ are constants depending only on the initial conditions of the system.

7.3.1 Null Spaces of $D - A$, Z , $F - B$, and $\hat{Z}$

To prove Theorem 7.3.3, we first characterize the null spaces of the matrices $D - A$, Z , $F - B$, and $\hat{Z}$, which are defined in (7.14), and (7.20).

Lemma 7.3.4. *The matrices $D - A$ and Z are symmetric positive semi-definite (SPSD), each with a one dimensional null space. In particular, $\mathcal{N}(D - A) = \text{span}(\{\mathbf{1}\})$ and $\mathcal{N}(Z) = \text{span}\left(\left\{P^{\frac{1}{2}}\mathbf{1}\right\}\right)$. Moreover, the null space and range space of Z are invariant with respect to time.*

Proof. Clearly $D - A$ and Z are symmetric by inspection. For any $\mathbf{y} \in \mathbb{R}^N$,

$$\mathbf{y}^\top (D - A) \mathbf{y} = \frac{1}{2} \sum_{i,j} A_{i,j} (y_i - y_j)^2 \geq 0. \quad (7.55)$$

Moreover, since $A_{i,j} > 0$, $\frac{1}{2} \sum_{i,j} A_{i,j} (y_i - y_j)^2 = 0$ if and only if $y_i = y_j$ for all i and j , in which case $\mathbf{y} = c\mathbf{1}$ for some $c \in \mathbb{R}$. Thus $D - A$ is SPD, with a one-dimensional null space spanned by the eigenvector $\mathbf{1}$. Similarly $\mathbf{y}^\top Z \mathbf{y} = (P^{-\frac{1}{2}}\mathbf{y})^\top (D - A) (P^{-\frac{1}{2}}\mathbf{y}) \geq 0$, and $Z\mathbf{y} = \mathbf{0} \iff P^{-\frac{1}{2}}\mathbf{y} = c\mathbf{1} \iff \mathbf{y} = cP^{\frac{1}{2}}\mathbf{1}$, for some $c \in \mathbb{R}$. Thus Z is SPD, with a one dimensional null space spanned by the eigenvector $P^{\frac{1}{2}}\mathbf{1}$. By conservation of mass, (7.13a), $P^{\frac{1}{2}}\mathbf{1}$ is independent of time. Thus the null space of Z is invariant with respect to time. The symmetry of Z implies that $\mathcal{R}(Z) = \mathcal{N}(Z)^\perp$ is also invariant. ■

Lemma 7.3.5. *The matrices $F - B$ and $\hat{Z}$ are symmetric positive semi-definite (SPSD). In particular $\mathcal{N}(F - B) = \text{span}(\{\mathbf{1}\})$ and $\mathcal{N}(\hat{Z}) = \text{span}\left(\left\{Q^{\frac{1}{2}}\mathbf{1}\right\}\right)$. Moreover, the null space and range space of $\hat{Z}$ are invariant with respect to time.*

Proof. The proof follows closely that of Lemma 7.3.4. Details are left to the reader. ■

7.3.2 Velocity Relaxation Proof

Theorem 7.3.6. *Under the assumptions of Proposition 7.3.1, $\lim_{t \rightarrow \infty} \mathbf{u}_i(t) = \mathbf{u}^\infty$ and*

$$\|\mathbf{u}_i(t) - \mathbf{u}^\infty\|_2 \leq C_U \exp\left(-\frac{z_{\min}}{\varepsilon} t\right), \quad i = 1, \dots, N, \quad (7.56)$$

where $C_U > 0$ is a constant that depends on the initial conditions of the system and $z_{\min} > 0$ is a lower bound on the positive eigenvalues of Z .

Proof. The proof is based on (7.19a) which is equivalent to (7.17a). Let $\mathbf{W}^\infty = P^{\frac{1}{2}} \mathbf{U}^\infty$, where $\mathbf{U}^\infty = \mathbf{1} (\mathbf{u}^\infty)^\top$ is given in (7.48). Then Lemma 7.3.4 implies that $Z\mathbf{W}^\infty = \mathbf{0} \in \mathbb{R}^{N \times d}$. Moreover, since P and $\mathbf{U}^\infty$ are independent of time, so too is $\mathbf{W}^\infty$. Thus in terms of $\widetilde{\mathbf{W}} := \mathbf{W} - \mathbf{W}^\infty$, (7.19a) takes the form

$$\frac{d\widetilde{\mathbf{W}}}{dt} = -\frac{1}{\varepsilon} Z \widetilde{\mathbf{W}}. \quad (7.57)$$

Write the element $\widetilde{\mathbf{W}}$ as a sum of the null and range space components with respect to Z : $\widetilde{\mathbf{W}} = \widetilde{\mathbf{W}}_{\mathcal{R}} + \widetilde{\mathbf{W}}_{\mathcal{N}}$. As shown in Appendix D, $\widetilde{\mathbf{W}}_{\mathcal{N}} = \mathbf{0}$. Hence $\widetilde{\mathbf{W}} = V\mathbf{A}$, where the columns of $V = [\mathbf{v}_1, \dots, \mathbf{v}_{N-1}] \in \mathbb{R}^{N \times (N-1)}$ are a set of orthonormal eigenvectors of Z that span $\mathcal{R}(Z)$ and $\mathbf{A} = [\mathbf{a}_1, \dots, \mathbf{a}_d] \in \mathbb{R}^{(N-1) \times d}$. Using this formulation, the ODE system (7.57) becomes

$$\frac{d\mathbf{A}}{dt} = -\frac{1}{\varepsilon} V^\top Z V \mathbf{A}. \quad (7.58)$$

The eigenvalues of $V^\top Z V$ are strictly positive and bounded below by the quantity $z_{\min} := N \max\{\rho_k\}^{-1} \min_{i,j} A_{i,j}$ (see Appendix C). Thus $(\mathbf{A}, V^\top Z V \mathbf{A})_{\text{F}} \geq z_{\min} \|\mathbf{A}\|_{\text{F}}^2$, where $\|\cdot\|_{\text{F}}$ is the Frobenius norm. Let $s(t) = \|\mathbf{A}\|_{\text{F}}^2$. Then, using (7.58),

$$\frac{1}{2} \frac{ds}{dt} = \left(\mathbf{A}, \frac{d\mathbf{A}}{dt} \right)_{\text{F}} = \left(\mathbf{A}, -\frac{1}{\varepsilon} V^\top Z V \mathbf{A} \right)_{\text{F}} \leq -\frac{z_{\min}}{\varepsilon} \|\mathbf{A}\|_{\text{F}}^2 = -\frac{z_{\min}}{\varepsilon} s \quad (7.59)$$

which implies that

$$\|\mathbf{A}(t)\|_{\text{F}}^2 \leq \|\mathbf{A}(0)\|_{\text{F}}^2 e^{-\frac{2z_{\min}}{\varepsilon} t}. \quad (7.60)$$

Since $V^\top V = I_{N-1}$, it follows then $\|\widetilde{\mathbf{W}}\|_{\text{F}}^2 = \|V\mathbf{A}\|_{\text{F}}^2 = \|\mathbf{A}\|_{\text{F}}^2$. Thus, (7.60) becomes

$$\|\mathbf{W}(t) - \mathbf{W}^\infty\|_{\text{F}}^2 \leq \|\mathbf{W}(0) - \mathbf{W}^\infty\|_{\text{F}}^2 e^{-\frac{2z_{\min}}{\varepsilon} t}. \quad (7.61)$$

Since $\mathbf{W} = P^{\frac{1}{2}} \mathbf{U}$, it follows that

$$\|\mathbf{W} - \mathbf{W}^\infty\|_{\text{F}}^2 = \sum_{k=1}^d \sum_{j=1}^N [\rho_j ((\mathbf{u}_j)_k - \mathbf{u}_k^\infty)^2] = \sum_{j=1}^N \rho_j \|\mathbf{u}_j - \mathbf{u}^\infty\|_2^2 \geq \min\{\rho_k\} \|\mathbf{u}_i - \mathbf{u}^\infty\|_2^2, \quad (7.62)$$

for any $i \in \{1, \dots, N\}$. Thus, (7.61) gives the decay bound

$$\|\mathbf{u}_i(t) - \mathbf{u}^\infty\|_2^2 \leq \frac{1}{\min\{\rho_k\}} \|\mathbf{W}(t) - \mathbf{W}^\infty\|_{\text{F}}^2 \leq \frac{1}{\min\{\rho_k\}} \|\mathbf{W}^0 - \mathbf{W}^\infty\|_{\text{F}}^2 e^{-\frac{2z_{\min}}{\varepsilon} t} =: C_{\mathbf{U}}^2 e^{-\frac{2z_{\min}}{\varepsilon} t}, \quad (7.63)$$

and $\lim_{t \rightarrow \infty} \mathbf{u}_i = \mathbf{u}^\infty$, as desired. ■

7.3.3 Energy Relaxation Proof

Theorem 7.3.7. *With the same assumptions as in Proposition 7.3.1, $\lim_{t \rightarrow \infty} \mathbf{E}(t) = \mathbf{E}^\infty$ and*

$$\|\mathbf{E}(t) - \mathbf{E}^\infty\|_2 \leq C_1 e^{-\frac{\hat{z}_{\min}}{\varepsilon} t} + C_2 \frac{e^{-\frac{z_{\min}}{\varepsilon} t} - e^{-\frac{\hat{z}_{\min}}{\varepsilon} t}}{\hat{z}_{\min} - z_{\min}}, \quad (7.64)$$

where $C_1 > 0$ and $C_2 > 0$ are constants that depend on the initial conditions of the system (7.17) and $\hat{z}_{\min}$ is a lower bound on the positive eigenvalues of $\hat{Z}$.

Proof. The proof is based on (7.19), which is equivalent to (7.17). Set $\boldsymbol{\xi}^\infty := Q^{-\frac{1}{2}} \mathbf{E}^\infty$, and note that

$$\hat{Z} \boldsymbol{\xi}^\infty = \frac{|\mathbf{u}^\infty|^2}{2} Q^{-\frac{1}{2}} (F - B) M \mathbf{1}. \quad (7.65)$$

Since Q and $\mathbf{E}^\infty$ are time invariant, so too is $\boldsymbol{\xi}^\infty$. Hence $\tilde{\boldsymbol{\xi}} := \boldsymbol{\xi} - \boldsymbol{\xi}^\infty$ satisfies the ODE

$$\frac{d\tilde{\boldsymbol{\xi}}}{dt} = -\frac{1}{\varepsilon} \hat{Z} \tilde{\boldsymbol{\xi}} + \frac{1}{2\varepsilon} Q^{-\frac{1}{2}} [(G - C) - |\mathbf{u}^\infty|^2 (F - B)] M \mathbf{1}. \quad (7.66)$$

Consider the null and range space components of $\tilde{\boldsymbol{\xi}}$ with respect to $\hat{Z}$: $\tilde{\boldsymbol{\xi}} = \tilde{\boldsymbol{\xi}}_{\mathcal{R}} + \tilde{\boldsymbol{\xi}}_{\mathcal{N}}$. It can be shown that $\tilde{\boldsymbol{\xi}}_{\mathcal{N}} \equiv \mathbf{0}$. (See Appendix D.) Therefore $\tilde{\boldsymbol{\xi}} = \tilde{\boldsymbol{\xi}}_{\mathcal{R}} = \hat{V} \mathbf{b}$, where $\hat{V} = [\hat{\mathbf{v}}_1, \dots, \hat{\mathbf{v}}_{N-1}] \in \mathbb{R}^{N \times (N-1)}$ is a matrix whose columns form an orthonormal basis for the range of $\hat{Z}$ and $\mathbf{b} = \hat{V}^\top \tilde{\boldsymbol{\xi}} \in \mathbb{R}^{N-1}$. Multiplication of (7.66) by $\mathbf{b}^\top \hat{V}^\top$ gives

$$\frac{1}{2} \frac{d}{dt} \|\mathbf{b}\|_2^2 = -\frac{1}{\varepsilon} \mathbf{b}^\top \hat{V}^\top \hat{Z} \hat{V} \mathbf{b} + \frac{1}{2\varepsilon} \mathbf{b}^\top \hat{V}^\top Q^{-\frac{1}{2}} [(G - C) - |\mathbf{u}^\infty|^2 (F - B)] M \mathbf{1}. \quad (7.67)$$

The eigenvalues of $\hat{V}^\top \hat{Z} \hat{V}$ are strictly positive and bounded below by $\hat{z}_{\min} := N \max\{n_k\}^{-1} \min_{i,j} B_{i,j}$ (see Appendix C), which gives the bound $\mathbf{b}^\top \hat{V}^\top \hat{Z} \hat{V} \mathbf{b} \geq \hat{z}_{\min} \|\mathbf{b}\|_2^2$ for any $\mathbf{b} \in \mathbb{R}^{N-1}$. With this bound and an application of the Cauchy–Schwarz inequality, (7.67) becomes

$$\frac{d}{dt} \|\mathbf{b}\|_2^2 \leq -\frac{2\hat{z}_{\min}}{\varepsilon} \|\mathbf{b}\|_2^2 + \frac{1}{\varepsilon} \|\mathbf{b}\|_2 \frac{1}{\min\{n_k\}^{\frac{1}{2}}} \left\| [(G - C) - |\mathbf{u}^\infty|^2 (F - B)] M \mathbf{1} \right\|_2. \quad (7.68)$$

The next step is to bound the source term in (7.68). Standard norm inequalities and the

definitions in (7.14), and Appendix C, give

$$\|[(G - C) - |\mathbf{u}^\infty|^2(F - B)] M\mathbf{1}\|_2 \leq 2 \max\{m_k\} \sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^N B_{\max} \left| |\mathbf{u}_{i,j}|^2 - |\mathbf{u}^\infty|^2 \right|. \quad (7.69)$$

Meanwhile, to bound $|S_{i,j} - |\mathbf{u}^\infty|^2|$, we use (i) the decay bound in (7.56), (ii) the definitions of $\mathbf{u}_{i,j}$ and $\mathbf{u}^\infty$, (iii) the triangle inequality and Cauchy Schwarz inequality, (iv) the fact that $\alpha_{i,j} + \alpha_{j,i} = 1$, and (v) the fact that $|\mathbf{u}_{i,j}| \leq \max_{i,j}\{|\mathbf{u}_i|, |\mathbf{u}_j|\} \leq u_{\max}$ to obtain

$$\begin{aligned} \left| |\mathbf{u}_{i,j}|^2 - |\mathbf{u}^\infty|^2 \right| &= |(\mathbf{u}_{i,j} + \mathbf{u}^\infty)^\top (\mathbf{u}_{i,j} - \mathbf{u}^\infty)| \leq 2u_{\max} \|\mathbf{u}_{i,j} - \mathbf{u}^\infty\|_2 \\ &\leq 2u_{\max} (\alpha_{i,j} \|\mathbf{u}_i - \mathbf{u}^\infty\|_2 + \alpha_{j,i} \|\mathbf{u}_j - \mathbf{u}^\infty\|_2) \leq 2C_U u_{\max} \exp\left(-\frac{z_{\min}}{\varepsilon} t\right). \end{aligned} \quad (7.70)$$

Together (7.69) and (7.70) give

$$\|[(G - C) - |\mathbf{u}^\infty|^2(F - B)] M\mathbf{1}\|_2 \leq 4N(N-1)C_U u_{\max} B_{\max} \max\{m_k\} e^{-\frac{z_{\min}}{\varepsilon} t}, \quad (7.71)$$

and (7.68) becomes, after dividing through by $\|\mathbf{b}\|_2$,

$$\frac{d}{dt} \|\mathbf{b}\|_2 \leq -\frac{\hat{z}_{\min}}{\varepsilon} \|\mathbf{b}\|_2 + \frac{1}{\varepsilon} C_0 e^{-\frac{z_{\min}}{\varepsilon} t}, \quad (7.72)$$

where $C_0 = \frac{1}{2} \frac{4N(N-1)C_U u_{\max} B_{\max} \max\{m_k\}}{\min\{n_k\}^{\frac{1}{2}}}$, or equivalently,

$$\frac{d}{dt} \left(\|\mathbf{b}\|_2 e^{\frac{\hat{z}_{\min}}{\varepsilon} t} \right) \leq \frac{C_0}{\varepsilon} e^{\frac{\hat{z}_{\min} - z_{\min}}{\varepsilon} t}. \quad (7.73)$$

Integrating both sides above in t gives

$$\|\mathbf{b}\|_2 \leq \|\mathbf{b}^0\|_2 e^{-\frac{\hat{z}_{\min}}{\varepsilon} t} + \frac{C_0}{\varepsilon} \frac{\varepsilon}{\hat{z}_{\min} - z_{\min}} \left(e^{-\frac{z_{\min}}{\varepsilon} t} - e^{-\frac{\hat{z}_{\min}}{\varepsilon} t} \right). \quad (7.74)$$

Since $\hat{V}^\top \hat{V} = I_{N-1}$, it follows that $\|\tilde{\boldsymbol{\xi}}\|_2^2 = \|\hat{V}\mathbf{b}\|_2^2 = \|\mathbf{b}\|_2^2$. Thus, (7.74) becomes

$$\|\boldsymbol{\xi} - \boldsymbol{\xi}^\infty\|_2 \leq \|\boldsymbol{\xi}^0 - \boldsymbol{\xi}^\infty\|_2 e^{-\frac{\hat{z}_{\min}}{\varepsilon} t} + C_0 \frac{e^{-\frac{z_{\min}}{\varepsilon} t} - e^{-\frac{\hat{z}_{\min}}{\varepsilon} t}}{\hat{z}_{\min} - z_{\min}}. \quad (7.75)$$

Further, since

$$\|\boldsymbol{\xi} - \boldsymbol{\xi}^\infty\|_2^2 = \|Q^{-\frac{1}{2}}(\mathbf{E} - \mathbf{E}^\infty)\|_2^2 = \sum_{i=1}^N n_i^{-1} |E_i - E_i^\infty|^2 \geq \frac{1}{\max\{n_k\}} \|\mathbf{E} - \mathbf{E}^\infty\|_2^2, \quad (7.76)$$

it follows that

$$\|\mathbf{E}(t) - \mathbf{E}^\infty\|_2 \leq \max\{n_k\}^{\frac{1}{2}} \left(\|\boldsymbol{\xi}^0 - \boldsymbol{\xi}^\infty\|_2 e^{-\frac{\hat{z}_{\min}}{\epsilon} t} + C_0 \frac{e^{-\frac{z_{\min}}{\epsilon} t} - e^{-\frac{\hat{z}_{\min}}{\epsilon} t}}{\hat{z}_{\min} - z_{\min}} \right), \quad (7.77)$$

which recovers (7.64) with $C_1 := \max\{n_k\}^{\frac{1}{2}} \|\boldsymbol{\xi}^0 - \boldsymbol{\xi}^\infty\|_2$ and $C_2 := C_0 \max\{n_k\}^{\frac{1}{2}}$. Thus $\lim_{t \rightarrow \infty} \mathbf{E}(t) = \mathbf{E}^\infty$, as desired. $\blacksquare$

7.3.4 Temperature Relaxation

Corollary 7.3.7.1. *With the same assumptions as in Proposition 7.3.1, for each species $i \in \{1, \dots, N\}$, $\lim_{t \rightarrow \infty} T_i(t) = T^\infty$, and*

$$|T_i - T^\infty| \leq \frac{2}{d \min\{n_k\}} \left[C_1 e^{-\frac{\hat{z}_{\min}}{\epsilon} t} + C_2 \frac{e^{-\frac{z_{\min}}{\epsilon} t} - e^{-\frac{\hat{z}_{\min}}{\epsilon} t}}{\hat{z}_{\min} - z_{\min}} \right] + \frac{\max\{m_k\}}{d} 2u_{\max} C_U e^{-\frac{z_{\min}}{\epsilon} t}. \quad (7.78)$$

Proof. For each i ,

$$T_i = \frac{2}{dn_i} E_i - \frac{m_i}{d} |\mathbf{u}_i|^2 \quad \text{and} \quad T^\infty = \frac{2}{dn_i} E_i^\infty - \frac{m_i}{d} |\mathbf{u}^\infty|^2. \quad (7.79)$$

Therefore

$$|T_i - T^\infty| \leq \frac{2}{d \min\{n_k\}} |E_i - E_i^\infty| + \frac{\max\{m_k\}}{d} \left| |\mathbf{u}^\infty|^2 - |\mathbf{u}_i|^2 \right|. \quad (7.80)$$

The velocity decay bound (7.56), gives

$$\left| |\mathbf{u}^\infty|^2 - |\mathbf{u}_i|^2 \right| \leq 2u_{\max} \|\mathbf{u}^\infty - \mathbf{u}_i\|_2 \leq 2u_{\max} C_U e^{-\frac{z_{\min}}{\epsilon} t}. \quad (7.81)$$

Using this and the energy decay bound (7.64), the result follows. $\blacksquare$

Remark 7.3.8. *The result in Corollary 7.3.7.1 can also be verified directly, using the formulation of the temperature equation (7.23) and an approach similar to the proof of Theorem 7.3.7. The difference in the proofs comes from the fact that the nullspace component analogous to $\tilde{\boldsymbol{\xi}}_{\mathcal{N}}$ is no longer zero when using (7.23).*

7.4 Numerical Confirmation of Theory

In this section, we compute temperature and velocity profiles using a fully implicit (backward) Euler time stepping scheme.¹ We assume a slab geometry in the x_1 direction. Thus while $d = 3$, the quantities of interest depend only on x_1 . Moreover the bulk velocities in the x_2 and x_3 direction are identically zero, i.e., $U_{ij} = 0$ for all $j \in \{2, 3\}$.

We consider systems with three different gas species chosen from a collection of four possible elements: Helium (He), Argon (Ar), Krypton (Kr), and Xenon (Xe). The masses and diameters of these elements are taken from [7] and are given below in SI units:

$$\begin{pmatrix} m_{\text{He}} \\ m_{\text{Ar}} \\ m_{\text{Kr}} \\ m_{\text{Xe}} \end{pmatrix} = \begin{pmatrix} 6.6464731 \\ 66.335209 \\ 139.14984 \\ 218.01714 \end{pmatrix} \times 10^{-27} \text{ kg}, \quad \begin{pmatrix} d_{\text{He}} \\ d_{\text{Ar}} \\ d_{\text{Kr}} \\ d_{\text{Xe}} \end{pmatrix} = \begin{pmatrix} 2.193 \\ 3.659 \\ 4.199 \\ 4.939 \end{pmatrix} \times 10^{-10} \text{ m}. \quad (7.82)$$

In all of the examples below, the monotonicity of the minimum temperature (Theorem 7.2.2) and the upper and lower bounds on the bulk velocities (Theorem 7.2.3) are respected.

Example 1: Temperature Decay, Ar–Kr–Xe Mixture. The purpose of this example is to demonstrate temperature relaxation when the bulk velocities are zero. The initial number densities, velocities, and temperatures are given by

$$\begin{pmatrix} n_{\text{Ar}}^0 \\ n_{\text{Kr}}^0 \\ n_{\text{Xe}}^0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \times 10^{28} \text{ m}^{-3}, \quad \mathbf{U}^0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \text{ m/s}, \quad \mathbf{T}^0 = \begin{pmatrix} 1000 \\ 2000 \\ 3000 \end{pmatrix} \text{ K}. \quad (7.83)$$

Figure 7.1 shows the relaxation of the temperatures to their steady state value. In this case the decay rate established in (7.78) is fairly sharp, even though the temperatures may not approach steady state monotonically.

Example 2: Velocity Decay, Ar–Kr–Xe Mixture. The purpose of this example is to demonstrate the velocity relaxation, with minimal effects from the temperature. A positive velocity is given to one particle type, and each temperature is set to the same constant. The

¹The Backward Euler method preserves the monotonicity properties of the temperature and bulk velocity established in Section 7.2. This fact will be proved in future work.

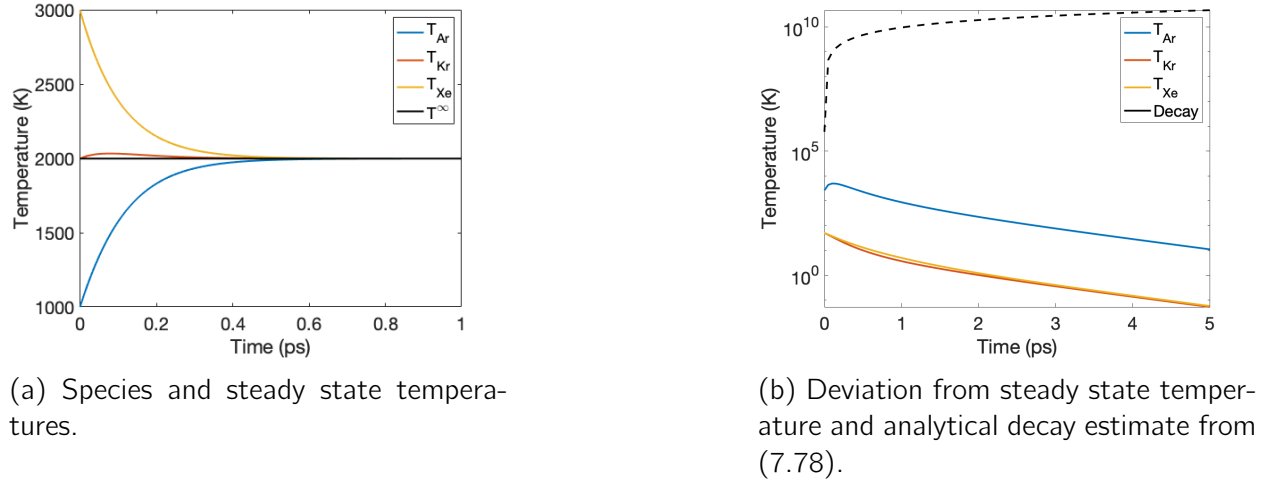


Figure 7.1: Temperature Decay of Ar-Kr-Xe Mixture in Example 1.

initial number densities, velocities, and temperatures are given by

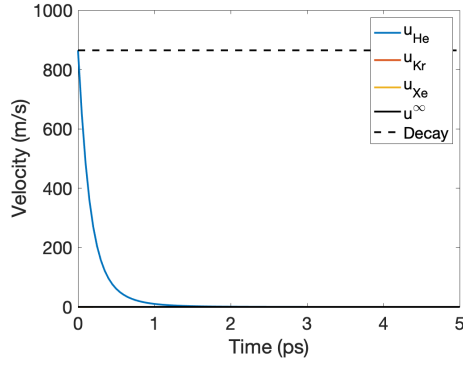
$$\begin{pmatrix} n_{Ar}^0 \\ n_{Kr}^0 \\ n_{Xe}^0 \end{pmatrix} = \begin{pmatrix} 3 \\ 2 \\ 1 \end{pmatrix} \times 10^{28} \text{ m}^{-3}, \quad \mathbf{U}^0 = \begin{pmatrix} 100 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \text{ m/s}, \quad \mathbf{T}^0 = \begin{pmatrix} 1000 \\ 1000 \\ 1000 \end{pmatrix} \text{ K.} \quad (7.84)$$

Figure 7.2 shows the relaxation of the velocities and temperatures to the steady state values. The decay rate established for the velocities and temperatures in (7.56) and (7.78) underestimate the true decay rates in the example. The results also demonstrate that, unlike the two-species case, particle velocities may not converge to the steady-state value monotonically.

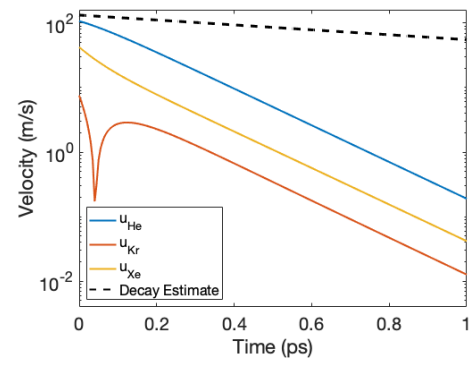
Example 3: Velocity-Temperature Relaxation, He-Kr-Xe Mixture This test case exercises the model due to the large kinetic energy differences between the species. The initial number densities, velocities, and temperatures are given by

$$\begin{pmatrix} n_{He}^0 \\ n_{Kr}^0 \\ n_{Xe}^0 \end{pmatrix} = \begin{pmatrix} 0.01 \\ 1 \\ 1 \end{pmatrix} \times 10^{28} \text{ m}^{-3}, \quad \mathbf{U}^0 = \begin{pmatrix} 864.8 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \text{ m/s}, \quad \mathbf{T}^0 = \begin{pmatrix} 3000 \\ 300 \\ 300 \end{pmatrix} \text{ K.} \quad (7.85)$$

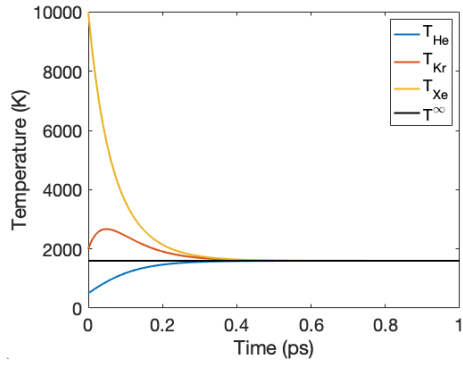
The momentum equilibration has a corresponding kinetic energy redistribution which causes non-monotonic changes in the temperature profile, as seen in Figure 7.3c. Because of the large differences in the particle masses and number densities, the estimates for the decay



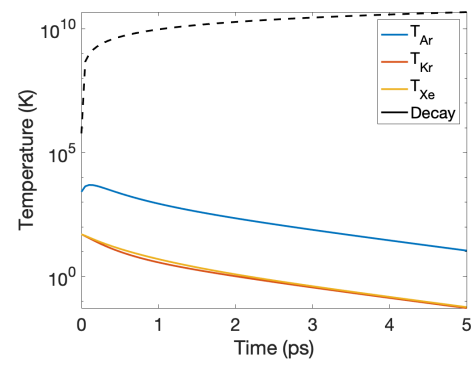
(a) Species and steady state velocities.



(b) Deviation from steady state velocity and analytical decay estimate from (7.56).



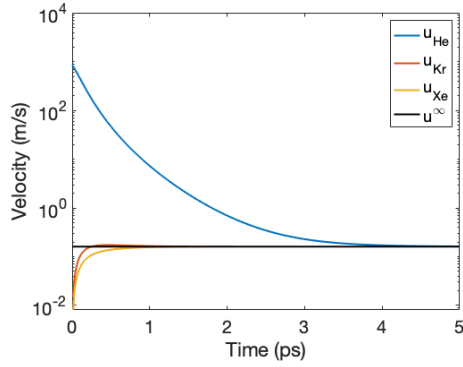
(c) Species and steady state temperatures.



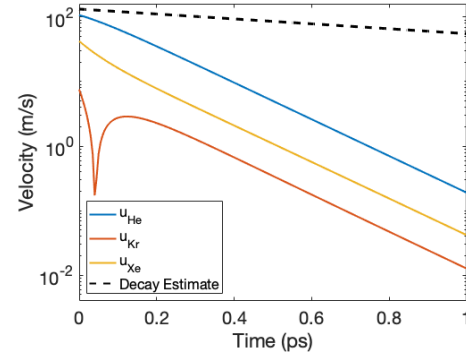
(d) Deviation from steady state velocity and analytical decay estimate from (7.78).

Figure 7.2: Velocity and Temperature Decay of Ar–Kr–Xe Mixture in Example 2.

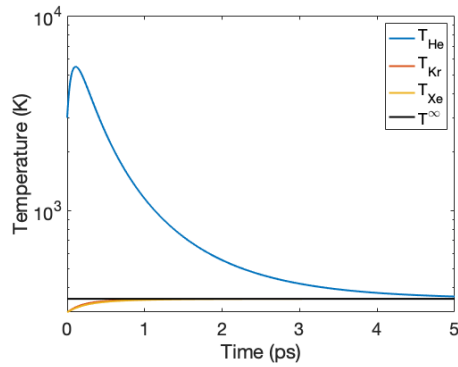
rates established in (7.56) and (7.78) are very weak.



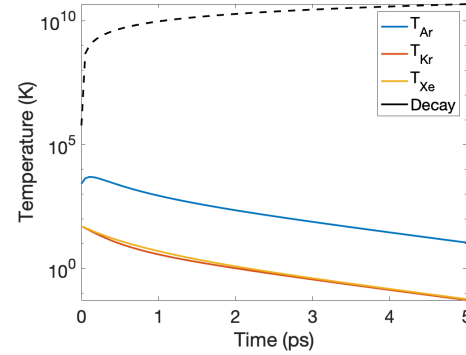
(a) Species and steady state velocities.



(b) Deviation from steady state velocity and analytical decay estimate from (7.56).



(c) Species and steady state temperatures.



(d) Deviation from steady state velocity and analytical decay estimate from (7.78).

Figure 7.3: Velocity and Temperature Decay of He–Kr–Xe Mixture in Example 3.

7.5 A Novel Nonlinear GST Iterative Solver

This section is based on our recent paper [17]:

E. Habbershaw, C.D. Hauck, and S.M. Wise, *Implicit Update of the Moment Equations for a Multi-Species, Homogeneous BGK Model*, SINUM (SIAM J. Numer. Anal.) 63 (2025) 881–907.

<https://doi.org/10.1137/24M165421X>

There we derived and analyzed a new nonlinear Gauss–Seidel-type (GST) solver for the space-homogeneous, multi-species BGK model. We will not give the tedious details of the method or the analyses in this document. Rather, we will content ourselves with some numerical simulations using the GST iterative method.

We first consider a slab geometry, in which the distribution functions f_i are invariant in the x_2 and x_3 direction. In this setting, the multi-species BGK equation takes the form

$$\frac{\partial f_i}{\partial t} + v_1 \partial_x f_i = \frac{1}{\varepsilon} \sum_j \lambda_{ij} (M_{ij} - f_i) \quad \forall i \in \{1, \dots, N\}, \quad (7.86)$$

where $[\mathbf{u}_{i,j}]_2 = [\mathbf{u}_{i,j}]_3 = 0$, and to simplify the notation, we let $x_1 = x$, $[\mathbf{u}_i]_1 = u_i$, and $[\mathbf{u}_{i,j}]_1 = u_{i,j}$. Rather than solve (7.86) in the full three-dimensional velocity space, we apply a multi-species extension of Chu reduction [8]. For each $i \in \{1, \dots, N\}$, let

$$g_i(x, v_1, t) = \int_{\mathbb{R}^2} f_i(x, \mathbf{v}, t) dv_2 dv_3, \quad (7.87a)$$

$$h_i(x, v_1, t) = \int_{\mathbb{R}^2} (v_2^2 + v_3^2) f_i(x, \mathbf{v}, t) dv_2 dv_3. \quad (7.87b)$$

Then (7.86) can be reduced to a system of equations for g_i and h_i :

$$\frac{\partial g_i}{\partial t} + v_1 \frac{\partial g_i}{\partial x} = \frac{1}{\varepsilon} \sum_j \lambda_{ij} (G_{ij} - g_i), \quad (7.88a)$$

$$\frac{\partial h_i}{\partial t} + v_1 \frac{\partial h_i}{\partial x} = \frac{1}{\varepsilon} \sum_j \lambda_{ij} (H_{ij} - h_i), \quad (7.88b)$$

where $G_{ij}(v_1) = M_{n_i, u_{i,j}, T_{i,j}/m_i}^{(1)}(v_1)$ is a Maxwellian with $d = 1$, $H_{ij} = 2 \frac{T_{i,j}}{m_i} G_{ij}$, and

$$n_i = \int_{\mathbb{R}} g_i dv_1, \quad n_i u_i = \int_{\mathbb{R}} v_1 g_i dv_1, \quad \frac{3n_i}{m_i} T_i = \int_{\mathbb{R}} (v_1 - u_i)^2 g_i dv_1 + \int_{\mathbb{R}} h_i dv_1. \quad (7.89)$$

We use the IMEX approach outlined in [17] to solve (7.88). The Butcher tableaux for

the IMEX method is taken from Table II of [33]. The implicit step takes the form of a backward Euler method. The nonlinear GST method still forms the key component of the implicit step. The spatial discretization of the advection operator uses a second-order finite volume scheme with minmod-type slope limiters, as described in earlier chapters. The velocity is discretized using standard discrete velocity models based on evenly spaced points and a midpoint quadrature rule. Details of these discretizations can be found in Chapter 4. The strategy for selecting the time step is to use the natural hyperbolic restriction of the advection operators in the equations. In practice, we observe that the GST method converges without onerous restrictions. However, for general problems, these restrictions provide a rigorous fall-back whenever the GST method fails to converge at the hyperbolic time step [17].

Anderson Acceleration (AA) [47] is a commonly used method to speed up fixed point iterative methods. We wrap the GST method with an Anderson Acceleration loop, and find that using this method decreases the iteration counts required for convergence of the method.

7.5.1 Sod problem with two identical species

To verify the multi-species code, we perform a simulation of the Sod shock tube problem [43], a Riemann problem for the compressible Euler equations of a perfect gas. The initial data are $(n_L, \mathbf{u}_L, T_L) = (1, \mathbf{0}, 1)$ for $x \leq 0$, and $(n_R, \mathbf{u}_R, T_R) = (0.125, \mathbf{0}, 0.8)$ for $x \geq 0$. An analytical solution for the Riemann problem can be found in [45]. For small values of ε , both the single-species BGK equation [9] and multi-species BGK (M-BGK) equations [15] with properly initialized data formally recover the Sod solution. Because the slab problem (7.86) is formulated in three velocity dimensions, the adiabatic index for the limiting Euler equations is $\gamma = 5/3$.

In the current test, we treat the left- and right-hand side of the domain as different particle species, each having mass $m_i = 1$. The kinetic initial data is

$$f_1(x, \mathbf{v}, 0) = \begin{cases} M_{n_L, \mathbf{u}_L, T_L}^{(3)}, & x \leq 0, \\ M_{0.001, \mathbf{u}_R, T_R}^{(3)}, & x > 0, \end{cases} \quad \text{and} \quad f_2(x, \mathbf{v}, 0) = \begin{cases} M_{0.001, \mathbf{u}_L, T_L}^{(3)}, & x \leq 0, \\ M_{n_R, \mathbf{u}_R, T_R}^{(3)}, & x > 0, \end{cases} \quad (7.90)$$

where $M_{n, \mathbf{u}, \theta}^{(d)}$ denotes the d -dimensional Maxwellian, defined in (7.3). Trace densities are used in (7.90) instead of voids in order to avoid negativity in the numerical solutions.

The numerical solution is computed on a discretization of the phase space $X \times V = [-1, 1] \times [-10, 10]$, using periodic boundary conditions and a mesh with $N_x = 256$ by $N_v = 192$ cells of uniform size. The time step selection is driven by the advection in (7.88):

$\Delta t = 0.9 \frac{2/Nx}{2 \max\{|v_i|\}}$. Figure 7.4 shows single- and multi-species simulations of the model with $\varepsilon = 10^{-4}$, run to a final time of $t_f = 0.2$, compared with the Sod solution for the associated Euler equations. The results show that both BGK and M-BGK models perform well as numerical solvers for the Sod problem in this highly collisional regime.

Figure 7.5 contains a comparison of the iteration counts required for convergence at a tolerance of 10^{-8} . The iteration count for the GST method ranges from one to five over the simulation, with an average of approximately 1.982 iterations, and the Anderson Acceleration method reduces the number of iterations to a range of one to four, with an average of approximately 1.943 iterations.

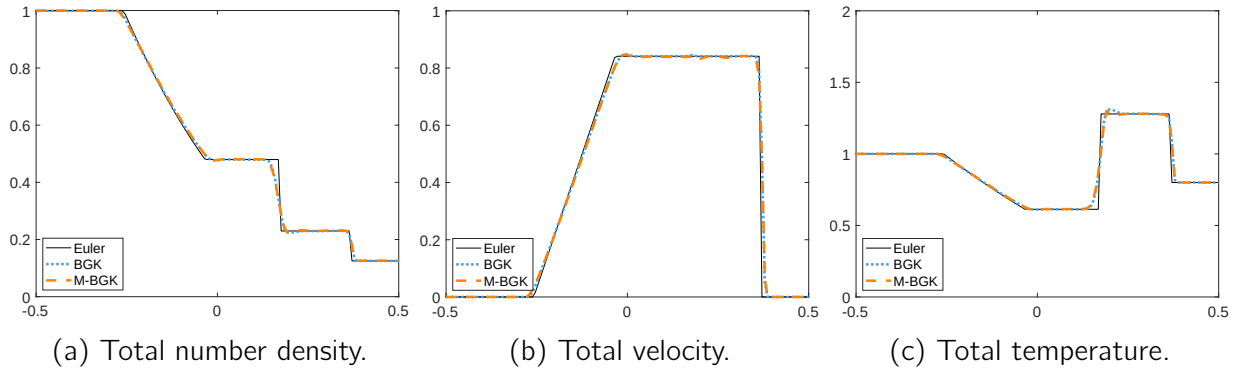


Figure 7.4: The total density, total bulk velocity, and total temperature moments are compared to the solution of the Euler equations at time $t = 0.2$, with $\varepsilon = 10^{-4}$.

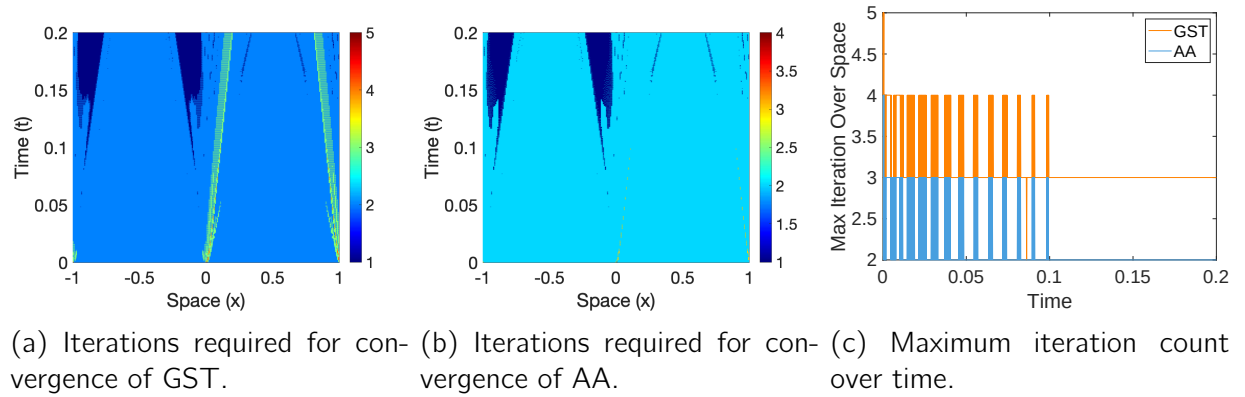


Figure 7.5: The number of iterations required for convergence is decreased by the application of Anderson Acceleration (AA) to the GST algorithm. The maximum iteration number over the spatial grid is strictly greater for the GST algorithm, compared to the Anderson Acceleration approach.

7.5.2 Three Species Mixture: Ar–Kr–Xe

The goal of this test is to demonstrate the benefits of the IMEX method when the problem becomes stiff (i.e., as $\varepsilon \rightarrow 0$). The following CFL-type conditions on the time step are required for the explicit and IMEX methods (which use a minmod-type slope limiter in the flux computation) to ensure stability and positivity of the numerical solution:

$$\Delta t^n \leq \begin{cases} \frac{\varepsilon \Delta x}{2\varepsilon \max\{|v_i|\} + \Delta x \Lambda^n} =: \Delta t_{\text{EX}}^n, \\ \frac{\Delta x}{2 \max\{|v_i|\}} =: \Delta t_{\text{IMEX}}, \end{cases} \quad \text{where} \quad \Lambda^n = \max_{i=1}^N \left\{ \max_{\kappa} \left\{ \sum_{j=1}^N \lambda_{i,j}^n(x_{\kappa}) \right\} \right\}. \quad (7.91)$$

As $\varepsilon \rightarrow 0$, the condition on Δt_{EX}^n becomes restrictive.

To compare the methods, we simulate an interface problem, with a mixture of Argon, Krypton, and Xenon; the masses and diameters of these particle species are taken from [7] and are given below in SI units:

$$\begin{pmatrix} m_{\text{Ar}} \\ m_{\text{Kr}} \\ m_{\text{Xe}} \end{pmatrix} = \begin{pmatrix} 6.6335209 \\ 13.914984 \\ 21.801714 \end{pmatrix} \times 10^{-26} \text{ kg}, \quad \begin{pmatrix} d_{\text{Ar}} \\ d_{\text{Kr}} \\ d_{\text{Xe}} \end{pmatrix} = \begin{pmatrix} 3.659 \\ 4.199 \\ 4.939 \end{pmatrix} \times 10^{-10} \text{ m}. \quad (7.92)$$

The setup for the test is similar to that of Section 7.5.1: a mixture of gases at rest is initialized with a high temperature on the left, and a low temperature on the right of the domain. Specifically, the mixture of Ar, Kr, and Xe is initialized on the left half of the one-dimensional spatial domain with number densities $(n_{\text{Ar}}^0, n_{\text{Kr}}^0, n_{\text{Xe}}^0) = (5, 5, 0.5) \times 10^{25} \text{ m}^{-3}$, and common temperature $T_L = 10$; on the right half, the mixture is initialized with number densities $(n_{\text{Ar}}^0, n_{\text{Kr}}^0, n_{\text{Xe}}^0) = (0.5, 0.5, 5) \times 10^{25} \text{ m}^{-3}$, and the common temperature $T_R = 1$. The initial kinetic distributions are given by

$$f_{\text{Ar}}(x, \mathbf{v}, 0) = \chi_{[-1,0]}(x) M_{5,0,10/m_{\text{Ar}}}^{(3)}(\mathbf{v}) + \chi_{(0,1]}(x) M_{0.5,0,1/m_{\text{Ar}}}^{(3)}(\mathbf{v}), \quad (7.93a)$$

$$f_{\text{Kr}}(x, \mathbf{v}, 0) = \chi_{[-1,0]}(x) M_{5,0,10/m_{\text{Kr}}}^{(3)}(\mathbf{v}) + \chi_{(0,1]}(x) M_{0.5,0,1/m_{\text{Kr}}}^{(3)}(\mathbf{v}), \quad (7.93b)$$

$$f_{\text{Xe}}(x, \mathbf{v}, 0) = \chi_{[-1,0]}(x) M_{0.5,0,10/m_{\text{Xe}}}^{(3)}(\mathbf{v}) + \chi_{(0,1]}(x) M_{5,0,1/m_{\text{Xe}}}^{(3)}(\mathbf{v}), \quad (7.93c)$$

where χ_S is the indicator function on the set S , and $M_{n,u,\theta}^{(d)}$ denotes the d -dimensional Maxwellian, defined in (7.3).

The numerical solution is computed on a discretization of the phase space $X \times V = [-1, 1] \times [-30, 30]$, using reflective boundaries; the mesh consists of $N_x = 256 \times N_v = 192$ cells of uniform size. The IMEX method (using the GST solver) uses a time step of size

$\Delta t = 0.9\Delta t_{\text{IMEX}}$, and the fully explicit method uses a time step of size $\Delta t^n = 0.9\Delta t_{\text{EX}}^n$; the simulation is run to a final time of $t_f = 1 \mu\text{s}$.

Moment plots for numerical solutions computed with the IMEX and fully explicit method are compared in Figure 7.6 for $\varepsilon \approx 0.001$. The computed solutions align closely. However, the explicit method requires 7089 time steps, while the IMEX method only requires 854 steps. In practice, as ε decreases, the number of time steps for the explicit method grows, slowing the simulation, while the IMEX method experiences no slow down in computation time.

Figure 7.7 contains a comparison of the iteration counts required for convergence at a tolerance of 10^{-8} . The iteration count for the GST method ranges from two to five during the simulation, with an average of approximately 2.0989 iterations, and the Anderson Acceleration method reduces the number of iterations to a range of two to four, with an average of approximately 2.0001 iterations.

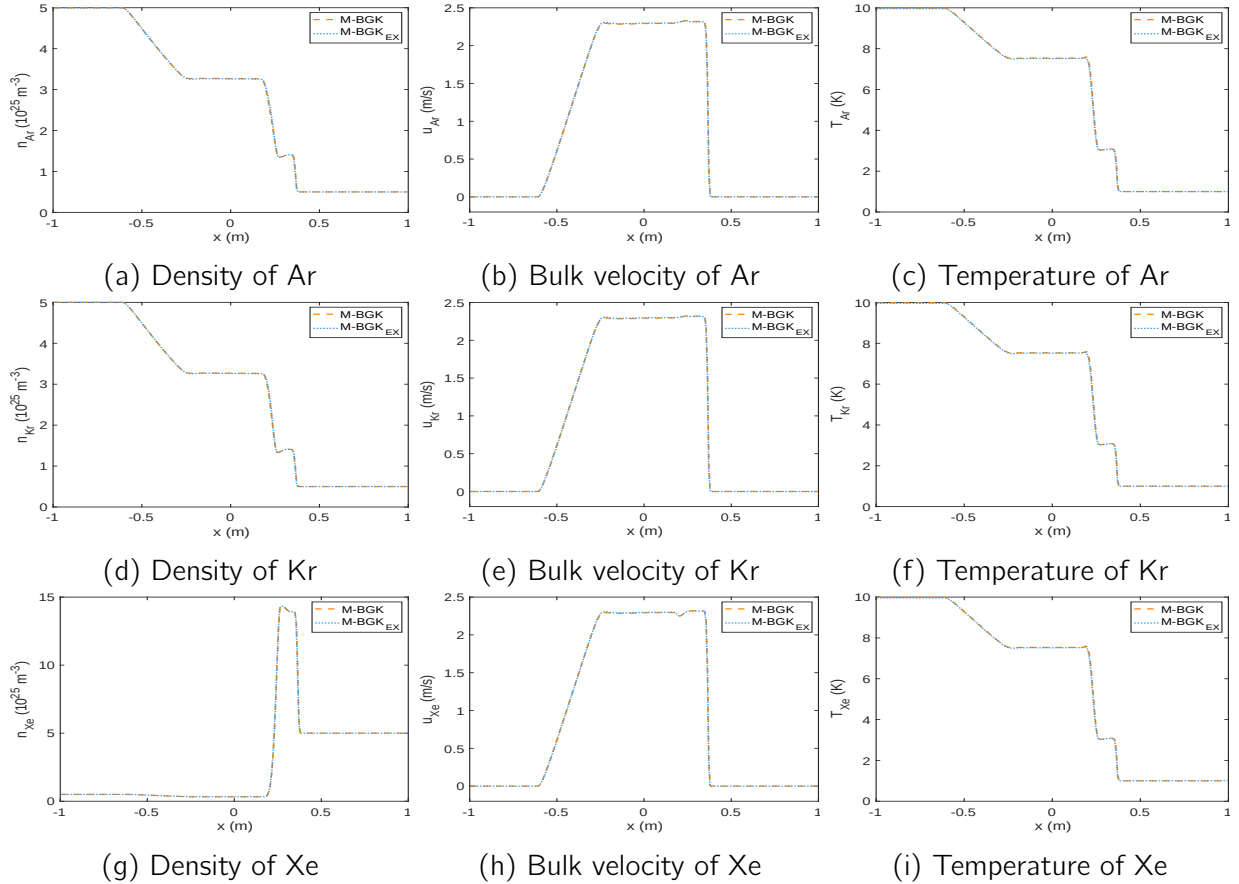


Figure 7.6: Noble gas mixture of Ar, Kr, and Xe: Moment plots of species number density, bulk velocity, and temperature, are given at $t_f = 1 \mu\text{s}$, for a mixture with $\varepsilon \approx 0.00103$. M-BGK uses the GST algorithm for the moment solve. M-BGK_EX uses a fully explicit method.

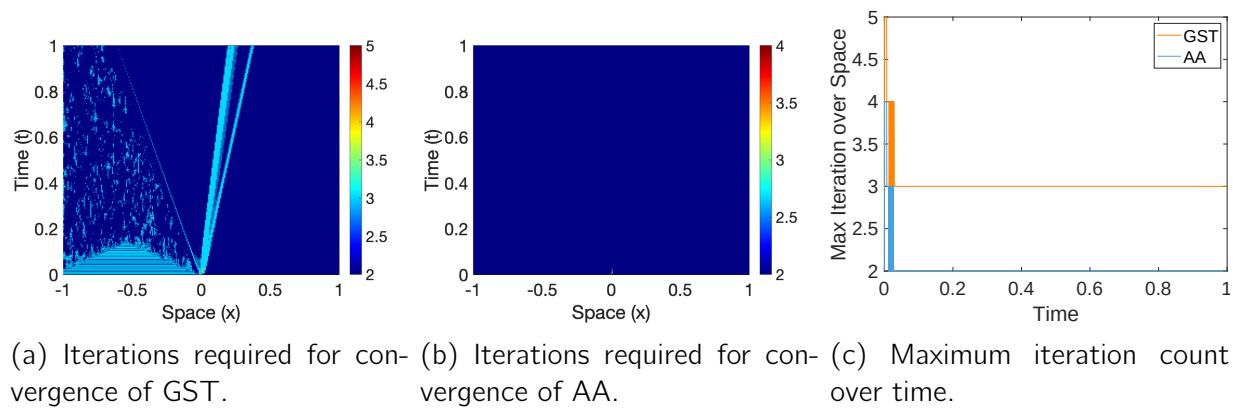


Figure 7.7: The number of iterations required for convergence is decreased by the application of Anderson Acceleration (AA) to the GST algorithm. The maximum iteration number over the spatial grid is strictly greater for the GST algorithm, compared to the Anderson Acceleration approach.

7.6 Conclusions

In this chapter, we have studied the moment equations associated to a recently developed multi-species BGK kinetic model for rarefied gas dynamics in the spatially homogeneous setting. The model includes collision frequencies that, unlike most models in the literature, depend on the species temperatures. This fact complicates the analysis of the moment equations and subsequent numerical tools. We have proven that all species temperatures are bounded below by a positive, non-decreasing temperature envelope, thus establishing that species temperatures always remain positive. We have also established upper and lower bounds on the components of the bulk velocity that are in terms of the initial data.

Using the lower bound on the species temperatures, we have shown that the moments always stay within a bounded, time-invariant set of physically realizable states, which, in turn, leads to the existence of global unique solutions. Finally, we have proved that unique equilibria exist for the moment equations, and solutions converge to these equilibria exponentially in time. In addition, we have established bounds on the convergence rates to equilibria. We concluded the examination of the space-homogeneous problem with some basic numerical simulations that demonstrate some of the established theoretical behavior.

The numerical results in this chapter are computed with a backward Euler method, using an iterative scheme to solve the relevant nonlinear algebraic equations at each time-step. In future work, we will describe the scheme more fully and prove convergence under a suitable time step restriction that does not require resolution of the parameter ε . We will use the backward Euler method as a component in an IMEX scheme for simulating multi-species BGK models that include phase-space advection.

In our paper [17], we presented a simple iterative approach for solving a set of implicit moment equations as part of a larger IMEX-based strategy for computing solutions of a multi-species BGK model. The main challenge is that the collision frequencies in the moment equations themselves depend on the moments in a complicated way. The key contribution is a rigorous contraction mapping proof, which shows that the iterative method converges to a unique solution under reasonable time steps that do not degenerate to zero when the collision parameter $\varepsilon \rightarrow 0$. This implicit solve is a key component in the IMEX discretization of the multi-species BGK model, the implementation of which is performed in slab geometry but closed in three-dimensional velocity space using a Chu reduction technique [8].

In future work, we will examine similar problems for multi-species ellipsoidal statistical models (ES-BGK) [22, 1] that, unlike standard BGK models, recover in highly collisional regimes, the correct Prandtl number for the compressible Navier–Stokes equations. We will

also extend the current code structure used here to generate results for more general problems in multi-dimensional domains. The ES-BGK model is the subject of the next chapter.

Chapter 8

ES-BGK Models and Numerics

8.1 Introduction

In this chapter, we discuss single- and multi-species ellipsoidal-statistical Bhatnagar–Gross–Krook (ES-BGK) models and their numerical time integration. These models replace the (isotropic) Maxwellian target distribution of the standard BGK model with an anisotropic Gaussian target that introduces adjustable stress tensor components into the target distribution, enabling resolution of the correct viscosity transport coefficients of the particle distributions.

Of particular interest are semi-implicit and fully implicit numerical strategies that enable large time steps in numerically stiff problems approaching the hydrodynamic (fluid) limit.

In Section 8.2, a single-species ES-BGK model is presented, along with an approach for a semi-implicit numerical time-stepping update. In Section 8.3, a Chapman–Enskog expansion of the model is given to derive fluid limits for the ES-BGK model. In Section 8.4, the semi-implicit numerical method described in Section 8.2 is applied in a $1 \times 2 \nu$ slab geometry, using techniques introduced in Chapter 4. In Section 8.5, multi-species BGK (M-BGK) and multi-species ES-BGK (M-ES-BGK) models for particle mixtures are considered; properties of some M-ES-BGK models are presented, and a numerical strategy that follows [17] is developed for the semi-implicit update of these multi-species models.

8.2 Single-Species ES-BGK Model – A First Look

To gain an understanding of the modeling framework of interest, we first examine the single-species model.

8.2.1 Model Overview

Suppose that f is a kinetic distribution of particles with mass $m_f > 0$. The number density, n_f , mass density, ρ_f , bulk velocity, $\mathbf{u}_f$, and temperature, T_f , are defined by

$$\rho_f = m_f n_f = m_f \int_{\mathbb{R}^d} f \, d\mathbf{v}, \quad \mathbf{u}_f = \frac{1}{n_f} \int_{\mathbb{R}^d} \mathbf{v} f \, d\mathbf{v}, \quad \text{and} \quad T_f = \frac{m_f}{n_f d} \int_{\mathbb{R}^d} |\mathbf{v} - \mathbf{u}_f|^2 f \, d\mathbf{v}, \quad (8.1)$$

where $d \in \mathbb{N}$ is the dimension of the microscopic velocity vector $\mathbf{v} \in \mathbb{R}^d$ ($d = 3$ in the standard physical setting). The energy density is

$$E_f = \frac{m_f}{2} \int_{\mathbb{R}^d} |\mathbf{v}|^2 f \, d\mathbf{v} = \frac{1}{2} \rho_f |\mathbf{u}_f|^2 + \frac{d}{2} \rho_f \theta_f, \quad \text{where} \quad \theta_f = \frac{T_f}{m_f} \quad (8.2)$$

and the pressure tensor

$$\mathbb{P}_f = m_f \int_{\mathbb{R}^d} (\mathbf{v} - \mathbf{u}_f) \otimes (\mathbf{v} - \mathbf{u}_f) f \, d\mathbf{v}, \quad \mathbf{a}_1 \otimes \mathbf{a}_2 = \mathbf{a}_1 \mathbf{a}_2^\top, \quad (8.3)$$

satisfies

$$m_f \int_{\mathbb{R}^d} \mathbf{v} \otimes \mathbf{v} f \, d\mathbf{v} = \rho_f \mathbf{u}_f \otimes \mathbf{u}_f + \mathbb{P}_f \quad \text{and} \quad \text{tr}(\mathbb{P}_f) = m_f \int_{\mathbb{R}^d} f \sum_{k=1}^d (v_k - [\mathbf{u}_f]_k)^2 \, d\mathbf{v} = d n_f T_f. \quad (8.4)$$

It will also be convenient to consider the trace-free pressure tensor $\boldsymbol{\sigma}_f$, defined via

$$\boldsymbol{\sigma}_f = m_f \int_{\mathbb{R}^d} \left[(\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) - \frac{1}{d} |\mathbf{v} - \mathbf{u}|^2 I_{d \times d} \right] f \, d\mathbf{v} = \mathbb{P}_f - \rho_f \theta_f I_{d \times d}, \quad (8.5)$$

and note that $\text{tr}(\boldsymbol{\sigma}) = 0$.

Definition 8.2.1. *The ellipsoidal-statistical BGK (ES-BGK) model is given by*

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\varepsilon} (G[f] - f) =: \frac{1}{\varepsilon} Q^{\text{ES-BGK}}, \quad (8.6)$$

where G is a Gaussian defined by

$$G[f](\mathbf{x}, \mathbf{v}, t) = G_{n_f, \mathbf{u}_f, T_f} := \frac{n_f}{\sqrt{\det(2\pi \mathcal{T}_f)}} \exp \left(-\frac{1}{2} (\mathbf{v} - \mathbf{u}_f) \cdot \mathcal{T}_f^{-1} (\mathbf{v} - \mathbf{u}_f) \right), \quad (8.7)$$

and

$$\mathcal{T}_f := (1 - \nu) \frac{T_f}{m_f} I_{d \times d} + \nu \frac{\mathbb{P}_f}{\rho_f}, \quad (8.8)$$

and $\nu \in [-\frac{1}{2}, 1]$ is related to the viscosity.

Lemma 8.2.2. *The Gaussian G from (8.7) has the following properties*

$$\int_{\mathbb{R}^d} G_{n,u,\mathcal{T}} \begin{pmatrix} 1 \\ \mathbf{v} \\ \mathbf{v} \otimes \mathbf{v} \\ |\mathbf{v}|^2 \\ |\mathbf{v} - \mathbf{u}|^2 \\ (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) \end{pmatrix} d\mathbf{v} = \begin{pmatrix} n \\ n\mathbf{u} \\ n\mathbf{u} \otimes \mathbf{u} + n\mathcal{T} \\ n|\mathbf{u}|^2 + n\text{tr}(\mathcal{T}) \\ n\text{tr}(\mathcal{T}) \\ n\mathcal{T} \end{pmatrix}. \quad (8.9)$$

Remark 8.2.3. *The parameter ν is related to the Prandtl number Pr , via $\nu = 1 - \frac{1}{\text{Pr}}$ [44]. Thus, when $\nu = -\frac{1}{2}$, the case of $\text{Pr} = \frac{2}{3}$ is recovered (which is relevant for monoatomic gases). If the pressure tensor (8.8) is isotropic ($\nu = 0$), then*

$$\mathcal{T}_f = \frac{T_f}{m_f} I_{d \times d}, \quad (8.10)$$

and the standard BGK model [2] is recovered.

Remark 8.2.4. *With $\mathcal{T}_f$ defined as in (8.8), $\text{tr}(\mathcal{T}_f) = d \frac{T_f}{m_f}$, so that with $\phi(\mathbf{v}) = m(1, \mathbf{v}, |\mathbf{v}|^2)$, utilizing (8.9) gives*

$$\int_{\mathbb{R}^d} G[f] \phi(\mathbf{v}) d\mathbf{v} = \int_{\mathbb{R}^d} f \phi(\mathbf{v}) d\mathbf{v} \iff \int_{\mathbb{R}^d} \phi(\mathbf{v}) \mathcal{Q}^{\text{ES-BGK}} d\mathbf{v} = \mathbf{0}. \quad (8.11)$$

Remark 8.2.5. *For clarity and conciseness, we will frequently suppress subscripts in the notation of macroscopic quantities when the underlying distribution function f is unambiguous from context.*

8.2.2 Conservation Laws and Moment ODE System

Multiply (8.6) by m , $m\mathbf{v}$, and $\frac{m}{2}|\mathbf{v}|^2$, and integrate using (8.9) and (8.11) to obtain expressions for the conservation of mass, momentum, and energy:

$$\partial_t \rho + \nabla_x \cdot (\rho \mathbf{u}) = 0, \quad (8.12a)$$

$$\partial_t (\rho \mathbf{u}) + \nabla_x \cdot (\rho \mathbf{u} \otimes \mathbf{u} + \mathbb{P}) = \mathbf{0}, \quad (8.12b)$$

$$\partial_t (E) + \nabla_x \cdot (E \mathbf{u} + \mathbb{P} \mathbf{u} + \mathbf{q}) = 0, \quad (8.12c)$$

where

$$\mathbf{q} = \frac{m}{2} \int_{\mathbb{R}^d} |\mathbf{v} - \mathbf{u}|^2 (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v} \quad (8.13)$$

is the heat flux. If we multiply (8.6) by $m\mathbf{v} \otimes \mathbf{v}$ and integrate, we can obtain an equation describing the evolution of the pressure tensor, $\mathbb{P}$, in terms of higher order moment $\mathbf{r}$ (defined below):

$$\frac{\partial}{\partial t} \left[m \int_{\mathbb{R}^d} \mathbf{v} \otimes \mathbf{v} f \, d\mathbf{v} \right] + \nabla_{\mathbf{x}} \cdot \left[m \int_{\mathbb{R}^d} \mathbf{v} \otimes \mathbf{v} \otimes \mathbf{v} f \, d\mathbf{v} \right] = \frac{m}{\varepsilon} \left(\int_{\mathbb{R}^d} \mathbf{v} \otimes \mathbf{v} G \, d\mathbf{v} - \int_{\mathbb{R}^d} \mathbf{v} \otimes \mathbf{v} f \, d\mathbf{v} \right) \quad (8.14a)$$

$$\iff \frac{\partial}{\partial t} (\rho \mathbf{u} \otimes \mathbf{u} + \mathbb{P}) + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u} \otimes \mathbf{u} \otimes \mathbf{u} + 3\mathbf{u} \otimes \mathbb{P} + \mathbf{r}) = \frac{1}{\varepsilon} (\rho \mathcal{T} - \mathbb{P}), \quad (8.14b)$$

where

$$\mathbf{r} = m \int_{\mathbb{R}^d} (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) f \, d\mathbf{v}. \quad (8.15)$$

The energy equation (8.12c) can be derived by taking the trace of (8.14b).

8.2.3 Numerical Time Update in Semi-Implicit Setting

In this subsection, we consider a system near the hydrodynamic (fluid) limit, characterized by a small Knudsen number ($\varepsilon \lesssim 0.01$), and evolving at non-relativistic speeds. Under these conditions, the advection term in the ES-BGK model can be evaluated using the hyperbolic time scaling. Thus, the numerical time update of (8.6) may be performed using a methodology similar to the implicit-explicit (IMEX) Runge–Kutta (RK) update in Chapter 4 for the single-species BGK model, wherein the advection term is updated explicitly and the collision term is updated implicitly via a moment-based construction of the target distribution, avoiding the need for a fully nonlinear solve. The explicit advection update can be treated in the same manner as in Chapter 4. Thus, the focus of this subsection is the implicit update of the space-homogeneous equation

$$\frac{\partial f}{\partial t} = \frac{1}{\varepsilon} (G[f] - f). \quad (8.16)$$

The implicit Euler update of (8.16) is

$$\frac{f^{n+1} - f^n}{\Delta t} = \frac{1}{\varepsilon} (G^{n+1} - f^{n+1}) \iff f^{n+1} = \frac{\varepsilon}{\varepsilon + \Delta t} f^n + \frac{\Delta t}{\varepsilon + \Delta t} G^{n+1}. \quad (8.17)$$

Since $G^{n+1} = G[f^{n+1}]$ is defined in terms of n^{n+1} , $\mathbf{u}^{n+1}$, and $\mathcal{T}^{n+1}$ (see (8.7)), our approach will be to determine the quantities n^{n+1} , $\mathbf{u}^{n+1}$, and $\mathcal{T}^{n+1}$, with which to define the target Gaussian, G^{n+1} .

Definition 8.2.6 (Backward Euler). *The implicit Euler update for the spatially homogeneous moment system (i.e., (8.12) and (8.14b), with the spatial derivatives removed) is given by*

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} = 0, \quad (8.18a)$$

$$\frac{\rho^{n+1} \mathbf{u}^{n+1} - \rho^n \mathbf{u}^n}{\Delta t} = \mathbf{0}, \quad (8.18b)$$

$$\frac{\rho^{n+1} |\mathbf{u}^{n+1}|^2 + d n^{n+1} \mathcal{T}^{n+1} - (\rho^n |\mathbf{u}^n|^2 + d n^n \mathcal{T}^n)}{\Delta t} = 0, \quad (8.18c)$$

$$\frac{\rho^{n+1} \mathbf{u}^{n+1} \otimes \mathbf{u}^{n+1} - \rho^n \mathbf{u}^n \otimes \mathbf{u}^n}{\Delta t} + \frac{\mathbb{P}^{n+1} - \mathbb{P}^n}{\Delta t} = \frac{1}{\varepsilon} (\rho^{n+1} \mathcal{T}^{n+1} - \mathbb{P}^{n+1}). \quad (8.18d)$$

Remark 8.2.7. *By observation of (8.18a), (8.18b), and (8.18c), it follows that*

$$(n^{n+1}, \mathbf{u}^{n+1}, \mathcal{T}^{n+1}) = (n^n, \mathbf{u}^n, \mathcal{T}^n), \quad (8.19)$$

and thus the terms in (8.18d) involving the bulk velocity cancel so that, using the definition of $\mathcal{T}$ in (8.8), (8.18d) simplifies to

$$\frac{\mathbb{P}^{n+1} - \mathbb{P}^n}{\Delta t} = \frac{1}{\varepsilon} [(1-\nu) n^{n+1} \mathcal{T}^{n+1} I_{d \times d} + \nu \mathbb{P}^{n+1} - \mathbb{P}^{n+1}] = \frac{1}{\varepsilon} (1-\nu) (n^{n+1} \mathcal{T}^{n+1} I_{d \times d} - \mathbb{P}^{n+1}) \quad (8.20a)$$

$$\iff \mathbb{P}^{n+1} = \frac{\varepsilon}{\varepsilon + \Delta t(1-\nu)} \mathbb{P}^n + \frac{\Delta t(1-\nu)}{\varepsilon + \Delta t(1-\nu)} n^n \mathcal{T}^n I_{d \times d}. \quad (8.20b)$$

Proposition 8.2.8. *The implicit temporal update of the space-homogeneous, single-species ES-BGK equation (8.16) (with time discretization (8.17)) can be performed as follows:*

(i) *Update the pressure tensor using (8.20)*

$$\mathbb{P}^{n+1} = \frac{\varepsilon}{\varepsilon + \Delta t(1-\nu)} \mathbb{P}^n + \frac{\Delta t(1-\nu)}{\varepsilon + \Delta t(1-\nu)} n^n \mathcal{T}^n I_{d \times d}. \quad (8.21)$$

(ii) *Use (8.21) and (8.19) to define G^{n+1} via*

$$G^{n+1} = \frac{n^n}{\sqrt{\det(2\pi \mathcal{T}^{n+1})}} \exp \left(-\frac{1}{2} (\mathbf{v} - \mathbf{u}^n) \cdot (\mathcal{T}^{n+1})^{-1} (\mathbf{v} - \mathbf{u}^n) \right), \quad (8.22a)$$

$$\text{where} \quad \mathcal{T}^{n+1} = (1 - \nu) \frac{T^n}{m} I_{d \times d} + \nu \frac{\mathbb{P}^{n+1}}{\rho^n}. \quad (8.22b)$$

(iii) Compute f^{n+1} via (8.17), using (8.22):

$$f^{n+1} = \frac{\varepsilon}{\varepsilon + \Delta t} f^n + \frac{\Delta t}{\varepsilon + \Delta t} G^{n+1}. \quad (8.23)$$

8.3 Single-Species ES-BGK Model Fluid Limits

In this section, we will examine the Chapman–Enskog expansion for the ES-BGK model.

Consider the equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{\lambda}{\varepsilon} (G_f - f), \quad (8.24)$$

where λ is a (scaled) collision frequency ($\lambda = \mathcal{O}(1)$, with respect to ε), and the target Gaussian $G_f = \tilde{\mathcal{G}}[f]$ is defined as above.

Since the target Gaussian is defined in terms of the full second order tensor, it will be necessary¹ to expand both the distribution f and the target Gaussian G_f in powers of ε :

$$f = \sum_{k \geq 0} \varepsilon^k \varphi_k \quad \text{and} \quad G_f = \sum_{k \geq 0} \varepsilon^k \psi_k, \quad (8.25)$$

where each φ_k and ψ_k are functions, to be determined. Since the local equilibrium is characterized by the local Maxwellian (H-Theorem), this serves as the zeroth-order term in the expansion (i.e., $\psi_0 = M_{n_f, u_f, \theta_f}$, as demonstrated below).

Define the moments of the functions φ_k as

$$\rho^{(k)} = m_f \int_{\mathbb{R}^d} \varphi_k \, d\mathbf{v}, \quad (\rho \mathbf{u})^{(k)} = m_f \int_{\mathbb{R}^d} \mathbf{v} \varphi_k \, d\mathbf{v}, \quad E^{(k)} = \frac{m_f}{2} \int_{\mathbb{R}^d} |\mathbf{v}|^2 \varphi_k \, d\mathbf{v}. \quad (8.26)$$

Assume that each order of the expansion satisfies the conservation laws (8.12). That is, for any $N \in \mathbb{N} \cup \{0\}$, the function $F_N = \sum_{k=0}^N \varepsilon^k \varphi_k$ must satisfy (8.12) (or, equivalently,

¹In the BGK model, the target Maxwellian function depends only on the conserved variables, and thus as a direct result of compatibility conditions (8.27), the target Maxwellian need not be expanded in powers of ε . Here, the dependence on the full second order tensor moment, and in particular $\boldsymbol{\sigma}$, requires that the target Gaussian in the ES-BGK model be expanded.

(8.11)). This leads to² the compatibility conditions,

$$\begin{pmatrix} \rho \\ \rho \mathbf{u} \\ E \end{pmatrix} := m \int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2}|\mathbf{v}|^2 \end{pmatrix} f \, d\mathbf{v} = m \int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2}|\mathbf{v}|^2 \end{pmatrix} \varphi_0 \, d\mathbf{v} =: \begin{pmatrix} \rho^{(0)} \\ (\rho \mathbf{u})^{(0)} \\ E^{(0)} \end{pmatrix}, \quad (8.27a)$$

$$\text{and} \quad \begin{pmatrix} \rho^{(k)} \\ (\rho \mathbf{u})^{(k)} \\ E^{(k)} \end{pmatrix} := \int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2}|\mathbf{v}|^2 \end{pmatrix} \varphi_k \, d\mathbf{v} = \mathbf{0}, \quad \forall k \geq 1. \quad (8.27b)$$

We use an expansion in ε to write the trace-free pressure tensor $\boldsymbol{\sigma} = \mathbb{P} - \frac{1}{d}\text{tr}(\mathbb{P})I_{d \times d} = \mathbb{P} - \rho\theta I_{d \times d}$, and heat flux $\mathbf{q}$. Since $\psi_0 = M_{n_f, \mathbf{u}_f, \theta_f}$, the local Maxwellian, the zeroth order term in the expansion for $\boldsymbol{\sigma}$ and $\mathbf{q}$ are zero, and we write

$$\boldsymbol{\sigma} = \sum_{k \geq 1} \varepsilon^k \boldsymbol{\sigma}^{(k)} = \sum_{k \geq 1} \varepsilon^k m \int_{\mathbb{R}^d} [(\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) - \frac{1}{d}|\mathbf{v} - \mathbf{u}|^2] \varphi_k \, d\mathbf{v} = \sum_{k \geq 1} \varepsilon^k [\mathbb{P}^{(k)} - (\rho\theta)^{(k)} I_{d \times d}], \quad (8.28a)$$

$$\mathbf{q} = \sum_{k \geq 1} \varepsilon^k \mathbf{q}^{(k)} = \sum_{k \geq 1} \varepsilon^k \frac{m}{2} \int_{\mathbb{R}^d} |\mathbf{v} - \mathbf{u}|^2 (\mathbf{v} - \mathbf{u}) \varphi_k \, d\mathbf{v}. \quad (8.28b)$$

Remark 8.3.1. The compatibility conditions imply that $\boldsymbol{\sigma}^{(0)} = \mathbb{P}^{(0)} - \rho\theta I_{d \times d}$, and $\mathbb{P}^{(k)} = \boldsymbol{\sigma}^{(k)}$ for $k \geq 1$. As is demonstrated below, the zeroth order approximation is the local Maxwellian, $\varphi_0 = M_{n_f, \mathbf{u}_f, \theta_f}$, so that $\mathbb{P}^{(0)} = m_f \langle (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) M_{n_f, \mathbf{u}_f, \theta_f} \rangle = \rho_f \theta_f I_{d \times d}$ and we may conclude that $\boldsymbol{\sigma}^{(0)} = \mathbf{0}$ and $\mathbf{q}^{(0)} = \mathbf{0}$.

To develop a first-order expansion of the target Gaussian around the local Maxwellian $\psi_0 = M_{n_f, \mathbf{u}_f, \theta_f}$, we use the following

Lemma 8.3.2. Up to first order in ε , the tensor $\mathcal{T} = (1 - \nu)\theta I_{d \times d} + \nu \frac{\mathbb{P}}{\rho}$ satisfies

$$\mathcal{T} = \theta I_{d \times d} + \varepsilon \frac{\nu}{\rho} \boldsymbol{\sigma}^{(1)} + \mathcal{O}(\varepsilon^2), \quad (8.29a)$$

$$\det(\mathcal{T}) = \theta^d + \mathcal{O}(\varepsilon^2), \quad (8.29b)$$

$$\mathcal{T}^{-1} = \frac{1}{\theta} I_{d \times d} - \varepsilon \frac{\nu}{\rho \theta^2} \boldsymbol{\sigma}^{(1)} + \mathcal{O}(\varepsilon^2). \quad (8.29c)$$

Proof. Using the expansion of the term $\boldsymbol{\sigma}$ given in (8.28), the tensor $\mathcal{T}$ can be written

$$\mathcal{T} = (1 - \nu)\theta I_{d \times d} + \nu \frac{\mathbb{P}}{\rho} = \theta I_{d \times d} + \nu \frac{1}{\rho} \boldsymbol{\sigma} = \theta I_{d \times d} + \varepsilon \frac{\nu}{\rho} \boldsymbol{\sigma}^{(1)} + \mathcal{O}(\varepsilon^2). \quad (8.30)$$

²We require that each term must have the same moments with respect to $m(1, \mathbf{v}^\top, \frac{1}{2}|\mathbf{v}|^2)^\top$.

Factoring θ and applying the first order determinant expansion gives

$$\det(\mathcal{T}) = \theta^d \det\left(1 + \varepsilon \frac{\nu}{\rho\theta} \boldsymbol{\sigma}^{(1)} + \mathcal{O}(\varepsilon^2)\right) = \theta^d \left(1 + \varepsilon \frac{\nu}{\rho\theta} \text{tr}(\boldsymbol{\sigma}^{(1)}) + \mathcal{O}(\varepsilon^2)\right) = \theta^d + \mathcal{O}(\varepsilon^2), \quad (8.31)$$

where we have used the trace-free property of $\boldsymbol{\sigma}^{(1)}$. Finally, write

$$\mathcal{T} = \theta \left(I_{d \times d} + \varepsilon B + \mathcal{O}(\varepsilon^2) \right), \quad \text{where} \quad B := \frac{\nu}{\rho\theta} \boldsymbol{\sigma}^{(1)}, \quad (8.32)$$

and note that

$$(I_{d \times d} + \varepsilon B + \mathcal{O}(\varepsilon^2)) (I_{d \times d} - \varepsilon B) = I_{d \times d} - \varepsilon^2 B^2 + \mathcal{O}(\varepsilon^2) = I_{d \times d} + \mathcal{O}(\varepsilon^2), \quad (8.33a)$$

$$\iff (I_{d \times d} + \varepsilon B + \mathcal{O}(\varepsilon^2))^{-1} = I_{d \times d} - \varepsilon B + \mathcal{O}(\varepsilon^2). \quad (8.33b)$$

It therefore follows that

$$\mathcal{T}^{-1} = \left(\theta (I_{d \times d} + \varepsilon B + \mathcal{O}(\varepsilon^2)) \right)^{-1} = \frac{1}{\theta} (I_{d \times d} - \varepsilon B + \mathcal{O}(\varepsilon^2)) = \frac{1}{\theta} I_{d \times d} - \varepsilon \frac{\nu}{\rho\theta^2} \boldsymbol{\sigma}^{(1)} + \mathcal{O}(\varepsilon^2). \quad (8.34)$$

■

Lemma 8.3.3. *Up to first order in ε , the target Gaussian can be represented as*

$$G = \psi_0 + \varepsilon \psi_1 + \mathcal{O}(\varepsilon^2), \quad (8.35)$$

$$\text{where } \psi_0 = M_{n,u,\theta} \quad \text{and} \quad \psi_1 = M_{n,u,\theta} \frac{\nu}{2\rho\theta^2} \left((\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}), \boldsymbol{\sigma}^{(1)} \right)_{\mathbb{F}}. \quad (8.36)$$

Proof. Using Lemma 8.3.2 and the Taylor expansion of the exponential

$$\exp(\varepsilon \alpha + \mathcal{O}(\varepsilon^2)) = 1 + \varepsilon \alpha + \mathcal{O}(\varepsilon^2), \quad \text{for } \alpha \in \mathbb{R}, \quad (8.37)$$

the Gaussian $G_{n,u,\mathcal{T}}$ can be written as

$$\begin{aligned} G_{n,u,\mathcal{T}} &= \frac{n}{\sqrt{\det(2\pi\mathcal{T})}} \exp\left(-\frac{1}{2}(\mathbf{v} - \mathbf{u}) \cdot \mathcal{T}^{-1}(\mathbf{v} - \mathbf{u})\right) \\ &= \frac{n}{(2\pi)^{d/2} \sqrt{\theta^d + \mathcal{O}(\varepsilon^2)}} \exp\left(-\frac{1}{2}(\mathbf{v} - \mathbf{u}) \cdot \left[\frac{1}{\theta} I_{d \times d} - \varepsilon \frac{\nu}{\rho\theta^2} \boldsymbol{\sigma}^{(1)} + \mathcal{O}(\varepsilon^2)\right] (\mathbf{v} - \mathbf{u})\right) \\ &= \frac{n}{(2\pi\theta)^{d/2}} \exp\left(-\frac{|\mathbf{v} - \mathbf{u}|^2}{2\theta}\right) \exp\left(+\varepsilon \frac{\nu}{2\rho\theta^2} (\mathbf{v} - \mathbf{u}) \cdot \boldsymbol{\sigma}^{(1)} (\mathbf{v} - \mathbf{u})\right) + \mathcal{O}(\varepsilon^2) \\ &= M_{n,u,\theta} \left[1 + \varepsilon \frac{\nu}{2\rho\theta^2} (\mathbf{v} - \mathbf{u}) \cdot \boldsymbol{\sigma}^{(1)} (\mathbf{v} - \mathbf{u})\right] + \mathcal{O}(\varepsilon^2) \end{aligned}$$

$$= M_{n,u,\theta} + \varepsilon M_{n,u,\theta} \frac{\nu}{2\rho\theta^2} \left((\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}), \boldsymbol{\sigma}^{(1)} \right)_{\mathbb{F}} + \mathcal{O}(\varepsilon^2). \quad (8.38)$$

■

Since the first order approximation of the target Gaussian requires knowledge of the term $\boldsymbol{\sigma}^{(1)}$, we must solve a system of PDEs that describes this moment. Thus, to obtain the Navier–Stokes equations, we will need to expand the PDEs that govern the macroscopic moments. To do so, let us consider an expansion of the time derivative as

$$\frac{\partial}{\partial t} = \sum_{k \geq 0} \varepsilon^k \frac{\partial^{(k)}}{\partial t}, \quad (8.39)$$

where, for each $k \in \mathbb{N} \cup \{0\}$, $\frac{\partial^{(k)}}{\partial t} = \partial_t^{(k)}$ denotes the time derivative for the k^{th} order term in the expansion.

Lemma 8.3.4. *It holds that*

$$\frac{\partial^{(0)} n}{\partial t} = -\partial_{x_j}(nu_j), \quad \text{and} \quad \frac{\partial^{(k)} n}{\partial t} = 0, \quad \forall k \geq 1, \quad (8.40a)$$

$$\frac{\partial^{(0)} u_i}{\partial t} = -u_j \partial_{x_j} u_i - \frac{1}{\rho} \partial_{x_j} (\rho \theta \delta_{ij} + \boldsymbol{\sigma}_{ij}^{(0)}), \quad \text{and} \quad \frac{\partial^{(k)} u_i}{\partial t} = -\frac{1}{\rho} \partial_{x_j} \boldsymbol{\sigma}_{ij}^{(k)}, \quad \forall k \geq 1, \quad (8.40b)$$

$$\begin{aligned} \frac{\partial^{(0)} \theta}{\partial t} &= -u_j (\partial_{x_j} \theta) - \frac{2}{d\rho} \left[\partial_{x_j} q_j^{(0)} + (\rho \theta \delta_{ij} + \boldsymbol{\sigma}_{ij}^{(0)}) \partial_{x_j} u_i \right], \\ \text{and} \quad \frac{\partial^{(k)} \theta}{\partial t} &= -\frac{2}{d\rho} \left[\partial_{x_j} q_j^{(k)} + \boldsymbol{\sigma}_{ij}^{(k)} \partial_{x_j} (u_i) \right], \quad \forall k \geq 1, \end{aligned} \quad (8.40c)$$

where we have used Einstein summation notation for repeated indices.

Proof. The verification of (8.40) requires application of (8.39) to (8.12), and then careful bookkeeping of each derivative term.

First, applying (8.39) to (8.12a) gives

$$\sum_{k \geq 0} \varepsilon^k \partial_t^{(k)} \rho + \nabla_x \cdot (\rho \mathbf{u}) = 0. \quad (8.41)$$

The identity (8.40a) follows upon comparing powers of ε and using compatibility conditions (8.27).

Next, each component of the momentum equation can be written (using Einstein sum-

mation notation)

$$\sum_{k \geq 0} \varepsilon^k \partial_t^{(k)}(\rho u_i) + \partial_{x_j} \left(\rho u_i u_j + \rho \theta \delta_{ij} + \sum_{k \geq 0} \varepsilon^k \sigma_{ij}^{(k)} \right) = 0. \quad (8.42)$$

Use the product rule for the time derivative and the space derivative of the term $\rho u_i u_j$, apply (8.40a), rearrange terms, and compare powers of ε to obtain (8.40b).

Finally, to obtain (8.40c), note that applying the product rule and using (8.12a) and (8.12b), it follows that

$$\mathbb{P}_{ij} \partial_{x_j} u_i = \partial_t \left(\frac{1}{2} \rho |\mathbf{u}|^2 \right) + \partial_{x_j} \left(\frac{1}{2} \rho |\mathbf{u}|^2 u_j \right) + \partial_{x_j} (u_i \mathbb{P}_{ij}), \quad (8.43)$$

so that, canceling terms, (8.12c) can be written

$$\partial_t \left(\frac{d}{2} \rho \theta \right) + \partial_{x_j} \left(\frac{d}{2} \rho \theta u_j + q_j \right) + \mathbb{P}_{ij} \partial_{x_j} u_i = 0. \quad (8.44)$$

Recalling that $\sigma = -\rho \theta I_{d \times d} + \sum_{k \geq 0} \varepsilon^k \mathbb{P}^{(k)}$, then (8.40c) can be written

$$\sum_{k \geq 0} \varepsilon^k \partial_k \left(\frac{d}{2} \rho \theta \right) + \partial_{x_j} \left(\frac{d}{2} \rho \theta u_j + \sum_{k \geq 0} \varepsilon^k q_j^{(k)} \right) + \left(\rho \theta \delta_{ij} + \sum_{k \geq 0} \varepsilon^k \sigma_{ij}^{(k)} \right) \partial_{x_j} (u_i) = 0. \quad (8.45)$$

Applying the product rule, rearranging terms, and comparing powers of ε , the final identity (8.40c) follows. ■

Now, assume that the distribution function f depends on the position and time only through the macroscopic variables and their space derivatives, i.e. for each $k \in \mathbb{N} \cup \{0\}$,

$$\varphi_k = \varphi_k[\boldsymbol{\rho}, \nabla_x \boldsymbol{\rho}, \dots, \nabla_x^k \boldsymbol{\rho}](\mathbf{v}), \quad (8.46)$$

but φ_k does not depend on higher order spatial derivatives $\nabla_x^{k+\ell} \boldsymbol{\rho}, \ell \geq 1$, where $\boldsymbol{\rho} := \langle (1, \mathbf{v}^\top, \frac{1}{2} |\mathbf{v}|^2)^\top f \rangle \in \mathbb{R}^{d+2}$ is indexed as

$$\boldsymbol{\rho}_r = \begin{cases} \rho, & r = 1, \\ \rho u_i, & r = 1 + i, i = 1, \dots, d, \\ E, & r = d + 2. \end{cases} \quad (8.47)$$

The model equation can be expanded using the chain rule to write

$$\partial_t f + \mathbf{v} \cdot \nabla_x = \frac{\lambda}{\varepsilon} (G - f) \iff \sum_{k \geq 0} \varepsilon^k \left(\frac{\partial_k f}{\partial t} + \mathbf{v} \cdot \nabla_x \varphi_k \right) = \lambda \sum_{k \geq 0} \varepsilon^{k-1} (\psi_k - \varphi_k), \quad (8.48)$$

where

$$\frac{\partial_k f}{\partial t} = \sum_{\substack{m+\ell=k \\ m, \ell \geq 0}} \left[\sum_{r=1}^{d+2} \frac{\partial \varphi_m}{\partial \mathbf{p}_r} \partial_t^{(\ell)} \mathbf{p}_r + \sum_{r=1}^{d+2} \frac{\partial \varphi_m}{\partial (\nabla_x \mathbf{p}_r)} \partial_t^{(\ell)} (\nabla_x \mathbf{p}_r) + \cdots + \sum_{r=1}^{d+2} \frac{\partial \varphi_m}{\partial (\nabla_x^m \mathbf{p}_r)} \partial_t^{(\ell)} (\nabla_x^m \mathbf{p}_r) \right], \quad (8.49a)$$

$$\frac{\partial \varphi_k}{\partial x_j} = \sum_{r=1}^{d+2} \frac{\partial \varphi_k}{\partial \mathbf{p}_r} \frac{\partial \mathbf{p}_r}{\partial x_j} + \sum_{r=1}^{d+2} \frac{\partial \varphi_k}{\partial (\nabla_x \mathbf{p}_r)} \frac{\partial (\nabla_x \mathbf{p}_r)}{\partial x_j} + \cdots + \sum_{r=1}^{d+2} \frac{\partial \varphi_k}{\partial (\nabla_x^k \mathbf{p}_r)} \frac{\partial (\nabla_x^k \mathbf{p}_r)}{\partial x_j}, \quad (8.49b)$$

and we assume the property

$$\partial_t^{(k)} (\nabla_x^m \mathbf{p}_r) = \nabla_x^m \partial_t^{(k)} \mathbf{p}_r. \quad (8.50)$$

Remark 8.3.5. *In the present work, we expand the model equations up to the Navier–Stokes equations, which requires only the first term in the expansion of these equations. The full generality is shown in (8.49) to give an indication of how an expansion to higher order might be accomplished. See [49, 44].*

Euler equations

Examining (8.48) to order $\mathcal{O}(\varepsilon^{-1})$ yields the Euler equations in (8.40), and gives

$$\varphi_0 = \psi_0 = M_{n_f, u_f, \theta_f} \quad \text{and} \quad [\boldsymbol{\sigma}^{(0)}]_{ij} = 0 = [\mathbf{q}^{(0)}]_i \quad \forall i, j \in \{1, \dots, d\}. \quad (8.51)$$

Navier–Stokes equations

Examining (8.48) to $\mathcal{O}(\varepsilon^0)$ gives

$$\frac{\partial_0 f}{\partial t} + \mathbf{v} \cdot \nabla_x \varphi_0 = \lambda (\psi_1 - \varphi_1) \iff \varphi_1 = \psi_1 - \frac{1}{\lambda} \left(\frac{\partial_0 f}{\partial t} + \mathbf{v} \cdot \nabla_x \varphi_0 \right). \quad (8.52)$$

We can write

$$\varphi_1 = M_{n, u, \theta} \frac{\nu}{2\rho\theta^2} \sum_{i,j=1}^d (v_i - u_i)(v_j - u_j) \boldsymbol{\sigma}_{ij}^{(1)} \quad (8.53)$$

$$- \frac{M_{n,u,\theta}}{\lambda} \left\{ \sum_{i,j=1}^d \left[\frac{(v_i - u_i)(v_j - u_j)}{\theta} - \frac{|\mathbf{v} - \mathbf{u}|^2}{d\theta} \right] \frac{\partial u_i}{\partial x_j} + \left(\frac{|\mathbf{v} - \mathbf{u}|^2}{2\theta} - \frac{d+2}{2} \right) \sum_{j=1}^d \frac{v_j - u_j}{\theta} \frac{\partial \theta}{\partial x_j} \right\}, \quad (8.54)$$

where

$$\sigma_{ij}^{(1)} = -\frac{2}{1-\nu} \frac{\rho\theta}{\lambda} \frac{\partial u_{\langle i}}{\partial x_{j\rangle}} \quad \text{and} \quad \mathbf{q}^{(1)} = -\frac{d+2}{2} \frac{\rho\theta}{\lambda} \nabla_x \theta, \quad (8.55)$$

and $\frac{\partial u_{\langle i}}{\partial x_{j\rangle}}$ denotes the symmetric, trace-free part of the velocity gradient tensor:

$$\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{d} \left(\sum_{k=1}^d \frac{\partial u_k}{\partial x_k} \right) \delta_{ij}. \quad (8.56)$$

8.4 Numerical Demonstration of Implicit-Explicit Numerical Method

In this section, we give simple numerical examples to demonstrate the time stepping method described in Section 8.2.3. Specifically, we simulate a Riemann problem in a $1 \times 2\nu$ phase space (cf. [11, Section 3]) for the model equation³

$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} = \frac{\lambda}{\varepsilon} (G[f] - f), \quad x \in [-1, 2], \quad (v_x, v_y) \in [-15, 15]^2, \quad (8.57)$$

using a finite volume discretization and an implicit-explicit Runge–Kutta time stepping method. The implicit part of the time update is computed using the moment-based formulation of Proposition 8.2.8, which is applied at each Runge–Kutta stage. The initial conditions are given by piecewise Maxwellian distributions according to

$$f(x, v_x, v_y, t=0) = M_{n_L, \mathbf{u}_L, \theta_L}(v_x, v_y) \chi_{[-1,0)}(x) + M_{n_R, \mathbf{u}_R, \theta_R}(v_x, v_y) \chi_{[0,2]}(x), \quad (8.58a)$$

$$\text{where } n_L = 1, \mathbf{u}_L = (2.5\sqrt{2}, 0)^\top, \theta_L = 1, \quad \text{and} \quad n_R = 1, \mathbf{u}_R = (0, 0)^\top, \theta_R = 1.05, \quad (8.58b)$$

and χ_S denotes the indicator function on the set S .

³This $1 \times 2\nu$ slab geometry reduction assumes translational invariance in the y -direction, so that $\frac{\partial f}{\partial y} = 0$. The distribution function, however, retains full dependence on (v_x, v_y) , allowing for transverse momentum and temperature anisotropy to be represented. As a result, the transport operator reduces from $\mathbf{v} \cdot \nabla_x f = v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y}$ to $v_x \frac{\partial f}{\partial x}$, and we write $f = f(x, v_x, v_y, t)$.

Spatial discretization. The physical domain $\Omega_x = [-1, 2]$ is partitioned into $N_x = 300$ uniform finite volumes of width $\Delta x = |\Omega_x|/N_x = 1/100$. Second order spatial accuracy is obtained using piecewise linear slope reconstructions with a θ -minmod slope limiter as in Chapter 4. Numerical fluxes at cell interfaces are computed using upwind data determined by the sign of v_x .

Velocity grid and quadrature. The velocity domain $V = [-15, 15]^2 \subset \mathbb{R}^2$ is discretized with a uniform Cartesian grid of $N_{v_x} \times N_{v_y} = 80 \times 80$ discrete velocities, with spacing $\Delta v = 30/N_{v_x}$. Velocity moments are computed using a midpoint quadrature rule over cells centered at $(v_{x,p}, v_{y,q})$.

Time integration. The explicit transport operator and implicit collision operator are coupled using a two-stage second-order implicit-explicit Runge–Kutta method. The implicit collision terms are updated following Proposition 8.2.8 of Section 8.2.3. The method updates the pressure tensor using explicit moment data, and then constructs the target Gaussian using these updated quantities; this approach avoids a nonlinear solve by computing the implicit collision step using fully explicit data.

Collision frequency and ES-BGK simulation parameters. As in [11], to obtain the desired Prandtl number and viscosity coefficient, the parameter for the anisotropic tensor in the target Gaussian is $\nu = \frac{1}{2}$, and the collision frequency is taken to be

$$\lambda(x, t) = \frac{3\pi}{\sqrt{2}} \frac{1}{1 - \nu} (0.436) n(x, t), \quad (8.59)$$

where $n(x, t)$ is the number density obtained from kinetic density f , and the factor 0.436 is chosen (as in [11]) to match a prescribed viscosity coefficient. We report below results for Knudsen number $\varepsilon = 10^{-3}$ at a final time of $t_F = 0.25$.

Boundary conditions. Far-field inflow boundary conditions are imposed at the edges of the domain by specifying the ghost cells as the left and right initial Maxwellian conditions of (8.58); that is, inflow at $x = -1$ is given by M_{n_L, u_L, θ_L} , and inflow at $x = 2$ is given by M_{n_R, u_R, θ_R} .

Time step selection. The time step is restricted by the hyperbolic CFL condition determined by the spatial grid size and maximum computational (microscopic) velocity, and is

given by⁴

$$\Delta t = 0.9 \cdot \Delta t_* = 0.9 \cdot \frac{\Delta x}{2 \max_{\ell} \{|v_{x,\ell}|\}} = \frac{0.9(1/100)}{2(15)}. \quad (8.60)$$

Preliminary Simulation Results Figure 8.1 gives the preliminary simulation results obtained using the methodology described above.

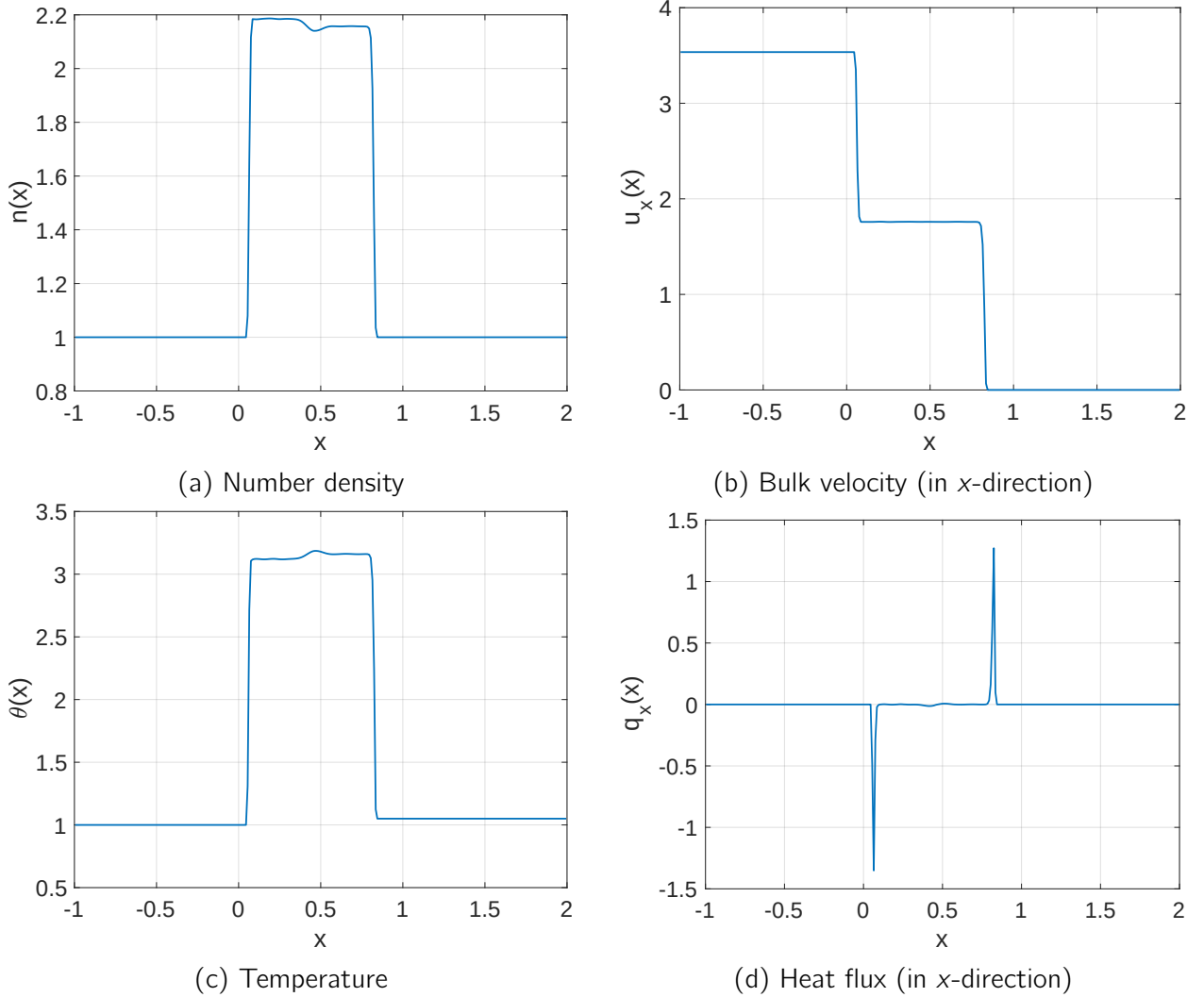


Figure 8.1: Moment profiles for number density, bulk velocity, temperature, and heat flux are given for a simulation, in a $1 \times 2\nu$ slab geometry, of the ES-BGK model with $\varepsilon = 0.001$, at time $t_F = 0.25$.

⁴The extra factor of 2 in this time step restriction appears as a result of the minmod slope limiters used for flux computations.

8.5 Multi-Species Models

Now that the single-species case has been reviewed, and a numerical approach for the temporal update has been presented, let us start developing a multi-species modeling framework. Since the ES-BGK model can be considered as a generalization of the BGK model, we will first present a multi-species BGK model which will provide the base for the multi-species ES-BGK model we develop.

8.5.1 Multi-Species BGK Model

Denote by f_i the kinetic distribution of particles of species $i \in \{1, \dots, N\}$, with mass m_i . Associated to each f_i are the species number density n_i , mass density ρ_i , bulk velocity $\mathbf{u}_i$, and temperature T_i , defined by

$$\rho_i = m_i n_i = m_i \int_{\mathbb{R}^d} f_i d\mathbf{v}, \quad \mathbf{u}_i = \frac{1}{\rho_i} \int_{\mathbb{R}^d} m_i \mathbf{v} f_i d\mathbf{v}, \quad T_i = \frac{m_i}{n_i d} \int_{\mathbb{R}^d} |\mathbf{v} - \mathbf{u}_i|^2 f_i d\mathbf{v}. \quad (8.61)$$

The species energy densities E_i are given by

$$E_i = \frac{1}{2} \int_{\mathbb{R}^d} m_i |\mathbf{v}|^2 f_i d\mathbf{v} = \frac{1}{2} \rho_i |\mathbf{u}_i|^2 + \frac{d}{2} n_i T_i, \quad (8.62)$$

and the species pressure tensors

$$\mathbb{P}_i = \int_{\mathbb{R}^d} m_i (\mathbf{v} - \mathbf{u}_i) \otimes (\mathbf{v} - \mathbf{u}_i) f_i d\mathbf{v}, \quad (8.63)$$

have the following properties: for every $i \in \{1, \dots, N\}$,

$$m_i \int_{\mathbb{R}^d} f_i \mathbf{v} \otimes \mathbf{v} d\mathbf{v} = \rho_i \mathbf{u}_i \otimes \mathbf{u}_i + \mathbb{P}_i \quad \text{and} \quad \text{tr}(\mathbb{P}_i) = \int_{\mathbb{R}^d} m_i f_i \sum_{k=1}^d (v_k - [\mathbf{u}_i]_k)^2 d\mathbf{v} = d n_i T_i. \quad (8.64)$$

Definition 8.5.1. For $n > 0$, $\mathbf{u} \in \mathbb{R}^d$, and $\theta > 0$, define the Maxwellian

$$M_{n,\mathbf{u},\theta} = \frac{n}{(2\pi\theta)^{d/2}} \exp\left(-\frac{|\mathbf{v} - \mathbf{u}|^2}{2\theta}\right). \quad (8.65)$$

Lemma 8.5.2. A general Maxwellian $M_{n,\mathbf{u},\theta}$ has the following properties:

$$\int_{\mathbb{R}^d} M_{n,\mathbf{u},\theta} d\mathbf{v} = n, \quad \int_{\mathbb{R}^d} \mathbf{v} M_{n,\mathbf{u},\theta} d\mathbf{v} = n\mathbf{u}, \quad \int_{\mathbb{R}^d} |\mathbf{v}|^2 M_{n,\mathbf{u},\theta} d\mathbf{v} = n|\mathbf{u}|^2 + dn\theta. \quad (8.66)$$

Definition 8.5.3. Let f_i denote the mass- m_i kinetic distribution of particle species $i \in \{1, \dots, N\}$. The (space-homogeneous) multi-species BGK (M-BGK) model is

$$\frac{\partial f_i}{\partial t} = \frac{1}{\varepsilon} \sum_j \lambda_{i,j} (M_{i,j} - f_i) =: \frac{1}{\varepsilon} \sum_j \mathcal{Q}_{i,j}^{\text{BGK}}, \quad i \in \{1, \dots, N\}, \quad (8.67)$$

where $\varepsilon > 0$ is the Knudsen number, and the Maxwellian

$$M_{i,j} := M_{n_i, \mathbf{u}_{i,j}, T_{i,j}/m_i} \quad (8.68)$$

is defined using the mixture velocities and temperatures

$$\mathbf{u}_{i,j} = \alpha_{i,j} \mathbf{u}_i + (1 - \alpha_{i,j}) \mathbf{u}_j, \quad 0 \leq \alpha_{i,j} \leq 1, \quad (8.69a)$$

$$T_{i,j} = \beta_{i,j} T_i + (1 - \beta_{i,j}) T_j + \frac{1}{d} \gamma_{i,j} |\mathbf{u}_i - \mathbf{u}_j|^2, \quad 0 \leq \beta_{i,j} \leq 1, \quad \gamma_{i,j} \geq 0. \quad (8.69b)$$

Lemma 8.5.4. The conservation of pairwise momentum and pairwise energy

$$\mathbf{0} = m_i \int_{\mathbb{R}^d} \phi(\mathbf{v}) \mathcal{Q}_{i,j}^{\text{BGK}} d\mathbf{v} + m_j \int_{\mathbb{R}^d} \phi(\mathbf{v}) \mathcal{Q}_{j,i}^{\text{BGK}} d\mathbf{v}, \quad \text{for} \quad \phi(\mathbf{v}) = (\mathbf{v}, |\mathbf{v}|^2), \quad (8.70)$$

implies that

$$\mathbf{u}_{j,i} = \alpha_{j,i} \mathbf{u}_j + (1 - \alpha_{j,i}) \mathbf{u}_i, \quad (8.71a)$$

$$T_{j,i} = \beta_{j,i} T_j + (1 - \beta_{j,i}) T_i + \frac{1}{d} \gamma_{j,i} |\mathbf{u}_i - \mathbf{u}_j|^2, \quad (8.71b)$$

where

$$\alpha_{j,i} = 1 - \frac{\rho_i \lambda_{i,j}}{\rho_j \lambda_{j,i}} (1 - \alpha_{i,j}) \iff \rho_i \lambda_{i,j} (1 - \alpha_{i,j}) = \rho_j \lambda_{j,i} (1 - \alpha_{j,i}), \quad (8.72a)$$

$$\beta_{j,i} = 1 - \frac{n_i \lambda_{i,j}}{n_j \lambda_{j,i}} (1 - \beta_{i,j}) \iff n_i \lambda_{i,j} (1 - \beta_{i,j}) = n_j \lambda_{j,i} (1 - \beta_{j,i}), \quad (8.72b)$$

$$\begin{aligned} \gamma_{j,i} &= \frac{1}{n_j \lambda_{j,i}} [\rho_i \lambda_{i,j} (1 - \alpha_{i,j}) (\alpha_{i,j} + \alpha_{j,i}) - n_i \lambda_{i,j} \gamma_{i,j}] \\ &\iff n_i \lambda_{i,j} \gamma_{i,j} + n_j \lambda_{j,i} \gamma_{j,i} = \rho_i \lambda_{i,j} (1 - \alpha_{i,j}) (\alpha_{i,j} + \alpha_{j,i}). \end{aligned} \quad (8.72c)$$

Lemma 8.5.5. *To ensure positivity of the source term, $\gamma_{j,i}$, we must constrain $\gamma_{i,j}$:*

$$\gamma_{j,i} \geq 0 \iff m_i n_i \lambda_{i,j} (1 - \alpha_{i,j}) (\alpha_{i,j} + \alpha_{j,i}) \geq n_i \lambda_{i,j} \gamma_{i,j} \iff \gamma_{i,j} \leq m_i (1 - \alpha_{i,j}) (\alpha_{i,j} + \alpha_{j,i}). \quad (8.73)$$

Since the RHS of this also must be nonnegative, we must constrain $\alpha_{i,j}$:

$$\frac{\rho_i \lambda_{i,j} - \rho_j \lambda_{j,i}}{\rho_i \lambda_{i,j} + \rho_j \lambda_{j,i}} \leq \alpha_{i,j} \leq 1. \quad (8.74)$$

To ensure that $0 \leq \alpha_{j,i} \leq 1$, we must require that

$$0 \leq \alpha_{j,i} = 1 - \frac{\rho_i \lambda_{i,j}}{\rho_j \lambda_{j,i}} (1 - \alpha_{i,j}) \leq 1 \iff 1 - \frac{\rho_j \lambda_{j,i}}{\rho_i \lambda_{i,j}} = \frac{\rho_i \lambda_{i,j} - \rho_j \lambda_{j,i}}{\rho_i \lambda_{i,j}} \leq \alpha_{i,j} \leq 1, \quad (8.75)$$

and to ensure that $0 \leq \beta_{j,i} \leq 1$, we must require that

$$0 \leq \beta_{j,i} = 1 - \frac{n_i \lambda_{i,j}}{n_j \lambda_{j,i}} (1 - \beta_{i,j}) \leq 1 \iff 1 - \frac{n_j \lambda_{j,i}}{n_i \lambda_{i,j}} = \frac{n_i \lambda_{i,j} - n_j \lambda_{j,i}}{n_i \lambda_{i,j}} \leq \beta_{i,j} \leq 1. \quad (8.76)$$

Remark 8.5.6. *The restriction (8.74) is weaker than (8.75), in the sense that*

$$\frac{\rho_i \lambda_{i,j} - \rho_j \lambda_{j,i}}{\rho_i \lambda_{i,j} + \rho_j \lambda_{j,i}} < \frac{\rho_i \lambda_{i,j} - \rho_j \lambda_{j,i}}{\rho_i \lambda_{i,j}} \iff \rho_i \lambda_{i,j} (\rho_i \lambda_{i,j} - \rho_j \lambda_{j,i}) < (\rho_i \lambda_{i,j} + \rho_j \lambda_{j,i}) (\rho_i \lambda_{i,j} - \rho_j \lambda_{j,i}). \quad (8.77)$$

In the case where $\rho_i \lambda_{i,j} - \rho_j \lambda_{j,i} \leq 0$, the requirement that $\alpha_{i,j} \in (0, 1)$ already restricts the parameter sufficiently. When this term is positive, we can cancel it from (8.77) and obtain the following equation which always holds:

$$\rho_i \lambda_{i,j} < \rho_i \lambda_{i,j} + \rho_j \lambda_{j,i}. \quad (8.78)$$

This implies that $\gamma_{i,j} \geq 0$, provided that (8.75) holds.

8.5.2 Multi-Species ES-BGK Model

In this section, we extend the multi-species BGK framework of Section 8.5.1 to a multi-species ellipsoidal-statistical BGK (M-ES-BGK) model. The definition of the mixture velocity $\mathbf{u}_{i,j}$ in the M-ES-BGK model remains the same as for the M-BGK model. However, the mixture temperatures $T_{i,j}$ in the M-BGK model must be expanded to tensors, $\mathcal{T}_{i,j} \in \mathbb{R}^{d \times d}$ that take the place of $\mathcal{T}$ in the single-species model (cf. (8.8)). In the following sections, we distinguish between two formulations of the mixture target Gaussian tensors $\mathcal{T}_{i,j}$: (i) a restricted form,

which depends on the pressure tensor of species i and the mixture temperature $T_{i,j}$, discussed in Section 8.5.3; and (ii) a general form, which couples the pressure tensors of both species and the mixture temperature $T_{i,j}$, discussed in Section 8.5.4.

For a first look, we will examine the space-homogeneous model; doing so, allows us to focus on the analysis of the collision term, which is useful for developing semi-implicit methods for the numerical time integration of the equations. In particular, a fully implicit update of the collision term can be used as part of an implicit-explicit Runge–Kutta formulation, as in Chapter 4.

M-ES-BGK Model Equations

Definition 8.5.7. Let f_i denote the mass- m_i kinetic distribution of particle species $i \in \{1, \dots, N\}$. The (space-homogeneous) multi-species ellipsoidal-statistical BGK (M-ES-BGK) model is

$$\frac{\partial f_i}{\partial t} = \frac{1}{\varepsilon} \sum_j \lambda_{i,j} (G_{i,j} - f_i) =: \frac{1}{\varepsilon} \sum_j \mathcal{Q}_{i,j}^{\text{ES}}, \quad i \in \{1, \dots, N\}, \quad (8.79)$$

where $\varepsilon > 0$ is the Knudsen number, and $G_{i,j}$ is a Gaussian defined by

$$G_{i,j}(\mathbf{v}) = \frac{n_i}{\sqrt{\det\left(2\pi \frac{\mathcal{T}_{i,j}}{m_i}\right)}} \exp\left(-\frac{1}{2}(\mathbf{v} - \mathbf{u}_{i,j}) \cdot \left(\frac{\mathcal{T}_{i,j}}{m_i}\right)^{-1} (\mathbf{v} - \mathbf{u}_{i,j})\right), \quad (8.80)$$

where $\mathbf{u}_{i,j} = \alpha_{i,j} \mathbf{u}_i + (1 - \alpha_{i,j}) \mathbf{u}_j$ is defined as in (8.69), and the tensor $\mathcal{T}_{i,j}$ is to be defined.

The Gaussian, $G_{i,j}$, in (8.80) has the properties

$$\int_{\mathbb{R}^d} m_i G_{i,j} \begin{pmatrix} 1 \\ \mathbf{v} \\ \mathbf{v} \otimes \mathbf{v} \\ |\mathbf{v}|^2 \\ |\mathbf{v} - \mathbf{u}_{i,j}|^2 \\ (\mathbf{v} - \mathbf{u}_{i,j}) \otimes (\mathbf{v} - \mathbf{u}_{i,j}) \end{pmatrix} d\mathbf{v} = \begin{pmatrix} \rho_i \\ \rho_i \mathbf{u}_{i,j} \\ \rho_i \mathbf{u}_{i,j} \otimes \mathbf{u}_{i,j} + n_i \mathcal{T}_{i,j} \\ \rho_i |\mathbf{u}_{i,j}|^2 + n_i \text{tr}(\mathcal{T}_{i,j}) \\ n_i \text{tr}(\mathcal{T}_{i,j}) \\ n_i \mathcal{T}_{i,j} \end{pmatrix}. \quad (8.81)$$

Implicit Numerical Update for Space-Homogeneous M-ES-BGK Model

To obtain a semi-implicit numerical method for this model using the same implicit-explicit Runge–Kutta framework previously discussed, we discretize the space homogeneous model

(8.79) in time and obtain

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} = \frac{1}{\varepsilon} \sum_j \lambda_{ij} (G_{ij}^{n+1} - f_i^{n+1}) \iff f_i^{n+1} = \frac{\varepsilon}{\varepsilon + \Delta t \sum_j \lambda_{ij}} \left(f_i^n + \sum_j \lambda_{ij} G_{ij}^{n+1} \right). \quad (8.82)$$

This has a similar form to the update of Section 8.2.3 for the single-species model, but with collisions scaled by inter- and intra-species collision frequencies (cf. (8.17)). However, because of the interactions between particles of different species, momenta and energies are exchanged, and the properties of (8.19) do not hold (i.e., $\mathbf{u}_i^{n+1} \neq \mathbf{u}_i^n$ and $T_i^{n+1} \neq T_i^n$). As a result, the pressure tensor may not be updated analogously to (8.20), and a result akin to Proposition 8.2.8 is unavailable. Instead, to define the target Gaussians G_{ij}^{n+1} , a multi-species moment system must first be updated, to obtain the quantities $\mathbf{u}_i^{n+1}$, T_i^{n+1} , and $\mathbb{P}_i^{n+1}$. We consider this problem below for two cases of target Gaussian tensors $\mathcal{T}_{ij}$, and develop a method for the implicit update of the collision operator. To maintain the ability to define collision frequencies in terms of higher order moments (e.g., species temperatures), we will adapt the Gauss–Seidel-type iterative method of [17].

First, we discuss some properties of the model, and describe the moment systems that we seek to compute implicit updates for.

M-ES-BGK Model Properties

Lemma 8.5.8. *The conservation of pairwise momentum and pairwise energy*

$$\mathbf{0} = m_i \int_{\mathbb{R}^d} \mathbf{v} \mathcal{Q}_{ij}^{\text{ES}} d\mathbf{v} + m_j \int_{\mathbb{R}^d} \mathbf{v} \mathcal{Q}_{ji}^{\text{ES}} d\mathbf{v}, \quad (8.83a)$$

$$0 = m_i \int_{\mathbb{R}^d} |\mathbf{v}|^2 \mathcal{Q}_{ij}^{\text{ES}} d\mathbf{v} + m_j \int_{\mathbb{R}^d} |\mathbf{v}|^2 \mathcal{Q}_{ji}^{\text{ES}} d\mathbf{v}, \quad (8.83b)$$

hold if and only if

$$\mathbf{u}_{j,i} = \alpha_{j,i} \mathbf{u}_j + (1 - \alpha_{j,i}) \mathbf{u}_i, \quad (8.84a)$$

$$T_{j,i} = \beta_{j,i} T_j + (1 - \beta_{j,i}) T_i + \frac{1}{d} \gamma_{j,i} |\mathbf{u}_i - \mathbf{u}_j|^2, \quad (8.84b)$$

where $\alpha_{j,i}$, $\beta_{j,i}$, and $\gamma_{j,i}$ are given in (8.72).

Proof. Using (8.61) and (8.81) on (8.83a) gives

$$\rho_i \lambda_{ij} \mathbf{u}_{i,j} + \rho_j \lambda_{ji} \mathbf{u}_{j,i} = \rho_i \lambda_{ij} \mathbf{u}_i + \rho_j \lambda_{ji} \mathbf{u}_j, \quad (8.85)$$

and using (8.69a) to isolate $\mathbf{u}_{j,i}$ gives

$$\mathbf{u}_{j,i} = \alpha_{j,i} \mathbf{u}_j + (1 - \alpha_{j,i}) \mathbf{u}_i, \quad (8.86)$$

where $\alpha_{j,i}$ is defined in (8.72a).

Using (8.61), (8.81), and (8.98), on (8.83b) gives

$$\begin{aligned} 0 &= \lambda_{i,j} \int_{\mathbb{R}^d} m_i G_{i,j} |\mathbf{v}|^2 d\mathbf{v} - \lambda_{i,j} \int_{\mathbb{R}^d} m_i f_i |\mathbf{v}|^2 d\mathbf{v} + \lambda_{j,i} \int_{\mathbb{R}^d} m_j G_{j,i} |\mathbf{v}|^2 d\mathbf{v} - \lambda_{j,i} \int_{\mathbb{R}^d} m_j f_j |\mathbf{v}|^2 d\mathbf{v} \\ &= \lambda_{i,j} [\rho_i |\mathbf{u}_{i,j}|^2 + dn_i T_{i,j}] - \lambda_{i,j} [\rho_i |\mathbf{u}_i|^2 + dn_i T_i] + \lambda_{j,i} [\rho_j |\mathbf{u}_{j,i}|^2 + dn_j T_{j,i}] - \lambda_{j,i} [\rho_j |\mathbf{u}_j|^2 + dn_j T_j] \end{aligned} \quad (8.87a)$$

$$\begin{aligned} \iff dn_i \lambda_{i,j} T_{i,j} + dn_j \lambda_{j,i} T_{j,i} &= dn_i \lambda_{i,j} T_i + dn_j \lambda_{j,i} T_j \\ &\quad - \rho_i \lambda_{i,j} (|\mathbf{u}_{i,j}|^2 - |\mathbf{u}_i|^2) - \rho_j \lambda_{j,i} (|\mathbf{u}_{j,i}|^2 - |\mathbf{u}_j|^2) - n_i \lambda_{i,j} \gamma_{i,j} |\mathbf{u}_i - \mathbf{u}_j|^2. \end{aligned} \quad (8.87b)$$

Rearranging (8.87b) to isolate $T_{j,i}$ and using (8.69b), the result follows. ■

M-ES-BGK Moment System of Equations

Multiply (8.79) by $m_i(1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v})^\top$, integrate with respect to $\mathbf{v}$, and use (8.61), (8.64), and (8.81) to obtain the following equations. (For the momentum equation (8.88b), use the definition of $\mathbf{u}_{i,j}$ from (8.69a) to write the given equation.)

$$\frac{\partial}{\partial t} \rho_i = 0 \quad (8.88a)$$

$$\frac{\partial}{\partial t} (\rho_i \mathbf{u}_i) = \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{i,j} (1 - \alpha_{i,j}) (\mathbf{u}_j - \mathbf{u}_i) \quad (8.88b)$$

$$\frac{\partial}{\partial t} (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i + \mathbb{P}_i) = \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{i,j} (\mathbf{u}_{i,j} \otimes \mathbf{u}_{i,j} - \mathbf{u}_i \otimes \mathbf{u}_i) + \frac{1}{\varepsilon} \sum_j \lambda_{i,j} (n_i \mathcal{T}_{i,j} - \mathbb{P}_i). \quad (8.88c)$$

Taking the trace of (8.88c) and using (8.64) and (8.98) gives an equation for the energy densities E_i (see (8.62)):

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_i |\mathbf{u}_i|^2 + dn_i T_i) &= \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{i,j} (|\mathbf{u}_{i,j}|^2 - |\mathbf{u}_i|^2) + \frac{1}{\varepsilon} \sum_j n_i \lambda_{i,j} \gamma_{i,j} |\mathbf{u}_i - \mathbf{u}_j|^2 \\ &\quad + \frac{d}{\varepsilon} \sum_j n_i \lambda_{i,j} (1 - \beta_{i,j}) (T_j - T_i). \end{aligned} \quad (8.89)$$

Lemma 8.5.9. *The moment system (8.88) – (8.89) conserves total momentum and total*

energy:

$$\sum_i \frac{\partial(\rho_i \mathbf{u}_i)}{\partial t} = \mathbf{0} \quad \text{and} \quad \sum_i \frac{\partial E_i}{\partial t} = 0. \quad (8.90)$$

Proof. Sum (8.88b) over all species $i \in \{1, \dots, N\}$ and use the symmetry of (8.72a) to obtain

$$\sum_i \frac{\partial(\rho_i \mathbf{u}_i)}{\partial t} = \frac{1}{2\varepsilon} \sum_{i,j} [\rho_i \lambda_{i,j}(1 - \alpha_{i,j}) - \rho_j \lambda_{j,i}(1 - \alpha_{j,i})](\mathbf{u}_j - \mathbf{u}_i) = \mathbf{0}. \quad (8.91)$$

To confirm the conservation of total energy, first sum (8.89) over all species $i \in \{1, \dots, N\}$ to obtain

$$\sum_i \frac{\partial E_i}{\partial t} = \frac{1}{\varepsilon} \sum_{i,j} [\rho_i \lambda_{i,j}(|\mathbf{u}_{i,j}|^2 - |\mathbf{u}_i|^2) + n_i \lambda_{i,j} \gamma_{i,j} |\mathbf{u}_i - \mathbf{u}_j|^2] + \frac{d}{\varepsilon} \sum_{i,j} n_i \lambda_{i,j} (1 - \beta_{i,j})(T_j - T_i). \quad (8.92)$$

Using the definition of $\mathbf{u}_{i,j}$ and the symmetries in (8.72a) and (8.72c), the first sum on the right hand side of (8.92) is

$$\begin{aligned} & \frac{1}{\varepsilon} \sum_{i,j} \rho_i \lambda_{i,j} (|\mathbf{u}_{i,j}|^2 - |\mathbf{u}_i|^2) + n_i \lambda_{i,j} \gamma_{i,j} |\mathbf{u}_i - \mathbf{u}_j|^2 \\ &= \frac{1}{2\varepsilon} \sum_{i,j} \rho_i \lambda_{i,j} (|\mathbf{u}_{i,j}|^2 - |\mathbf{u}_i|^2) + \rho_j \lambda_{j,i} (|\mathbf{u}_{j,i}|^2 - |\mathbf{u}_j|^2) + (n_i \lambda_{i,j} \gamma_{i,j} + n_j \lambda_{j,i} \gamma_{j,i}) |\mathbf{u}_i - \mathbf{u}_j|^2 = 0. \end{aligned} \quad (8.93)$$

The remaining term is also zero, by the symmetry (8.72b):

$$\frac{d}{\varepsilon} \sum_{i,j} n_i \lambda_{i,j} (1 - \beta_{i,j})(T_j - T_i) = \frac{d}{2\varepsilon} \sum_{i,j} [n_i \lambda_{i,j} (1 - \beta_{i,j}) - n_j \lambda_{j,i} (1 - \beta_{j,i})](T_j - T_i) = 0. \quad (8.94)$$

■

Remark 8.5.10. Previous work suggests using a Gauss–Seidel-type iterative approach (cf. [17]) to update the velocity-energy system (8.88b) and (8.89). If the collision frequencies depend only on the temperatures, then they can be updated at this point. More effort is needed to address the pressure tensor update, which is relegated to next subsection.

Remark 8.5.11. It is convenient to express the mixture pressure tensors $\mathcal{T}_{i,j}$ in their traceless formulation. Thus, we give the following definition, which will be used in the following discussion.

Definition 8.5.12. *The traceless part of a matrix $X \in \mathbb{R}^{d \times d}$ is defined as*

$$\text{tl}(X) := X - \frac{1}{d} \text{tr}(X) I_{d \times d}, \quad (8.95)$$

where $\text{tr}(X) = \sum_{k=1}^d [X]_{k,k}$ is the trace of X .

8.5.3 Multi-Species ES-BGK Model – Restricted Tensor Expression

Now, let us examine an ellipsoidal-statistical model presented in [27, Section 2.2], with the (restricted) tensor ansatz $\mathcal{T}_{i,j}$ given by Equation (22) and (23) of [27].

Using Definition 8.5.12 and (8.4), note that

$$\text{tl}(\mathbb{P}_i) = \mathbb{P}_i - n_i T_i I_{d \times d} \iff \mathbb{P}_i = n_i T_i I_{d \times d} + \text{tl}(\mathbb{P}_i). \quad (8.96)$$

Thus, the (restricted) tensor $\mathcal{T}_{i,j}$ used in Equation (22) and (23) of [27] can be written using our notation and Definition 8.5.12 as

$$\mathcal{T}_{i,j} = \beta_{i,j} \frac{\mathbb{P}_i}{n_i} + (1 - \beta_{i,j}) T_j I_{d \times d} + \frac{\gamma_{i,j}}{d} |\mathbf{u}_i - \mathbf{u}_j|^2 I_{d \times d} = T_{i,j} I_{d \times d} + \beta_{i,j} \text{tl}\left(\frac{\mathbb{P}_i}{n_i}\right), \quad (8.97)$$

and using (8.64), it follows that

$$\text{tr}(\mathcal{T}_{i,j}) = d\beta_{i,j} T_i + d(1 - \beta_{i,j}) T_j + \gamma_{i,j} |\mathbf{u}_i - \mathbf{u}_j|^2 = dT_{i,j}. \quad (8.98)$$

Remark 8.5.13. *The justification (as given in [27]) for using the mixture tensor (8.97) quotes the theory of “persistence of velocity”, and cites a paper and book by Jeans ([23, 24], 1904).*

Remark 8.5.14. *With $\mathcal{T}_{i,j}$ defined as in (8.97), the model retains desirable symmetries and conservation properties: (i) Lemma 8.5.8 holds, and the parameters $\alpha_{i,j}$, $\beta_{i,j}$, and $\gamma_{i,j}$ enjoy the symmetries of (8.71), and (ii) the conservation of total momentum and total energy hold (Lemma 8.5.9).*

Pressure Tensor Equation for Restricted Tensor

Using the definition for $\mathcal{T}_{i,j}$ in (8.97), the equation for the pressure tensor (8.88c) can be written

$$\frac{\partial}{\partial t} (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i + \mathbb{P}_i) = \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{i,j} \{ \mathbf{u}_{i,j} \otimes \mathbf{u}_{i,j} - \mathbf{u}_i \otimes \mathbf{u}_i \} + \frac{1}{\varepsilon d} \sum_j n_i \lambda_{i,j} \gamma_{i,j} |\mathbf{u}_i - \mathbf{u}_j|^2 I_{d \times d}$$

$$+ \frac{1}{\varepsilon} \sum_j n_i \lambda_{ij} (1 - \beta_{ij}) (T_j - T_i) I_{d \times d} - \frac{1}{\varepsilon} \sum_j n_i \lambda_{ij} (1 - \beta_{ij}) \text{tl} \left(\frac{\mathbb{P}_i}{n_i} \right), \quad (8.99)$$

and using traceless matrices and (8.89) to remove the diagonal terms, we can write

$$\frac{\partial}{\partial t} \left(\text{tl}(\rho_i \mathbf{u}_i \otimes \mathbf{u}_i) + \text{tl}(\mathbb{P}_i) \right) = \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{ij} [\text{tl}(\mathbf{u}_{ij} \otimes \mathbf{u}_{ij}) - \text{tl}(\mathbf{u}_i \otimes \mathbf{u}_i)] - \frac{1}{\varepsilon} \sum_j n_i \lambda_{ij} (1 - \beta_{ij}) \text{tl} \left(\frac{\mathbb{P}_i}{n_i} \right). \quad (8.100)$$

Numerical Update of Moment Equations (Restricted Tensor)

In this subsection, we present a staged iterative approach similar to that of [17], using a nonlinear Gauss–Seidel-type (GST) iterative method. Once the moments are updated they can be used to define the target Gaussians, $G_{i,j}$, in the kinetic model.

Discretizing (8.88a) in time gives $n_i^{n+1} = n_i^n$; thus we suppress superscripts on species densities and only consider the moment update for velocities, temperatures/energies, and pressure tensors.

Definition 8.5.15 (Backward Euler, Restricted Tensor Ansatz). *The implicit Euler update of the moment equations (8.88b), (8.89), and (8.100) is given by*

$$\rho_i \frac{\mathbf{u}_i^{n+1} - \mathbf{u}_i^n}{\Delta t} = \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{ij}^{n+1} (1 - \alpha_{ij}) (\mathbf{u}_j^{n+1} - \mathbf{u}_i^{n+1}), \quad (8.101a)$$

$$\begin{aligned} \rho_i \frac{|\mathbf{u}_i^{n+1}|^2 - |\mathbf{u}_i^n|^2}{\Delta t} + d n_i \frac{T_i^{n+1} - T_i^n}{\Delta t} &= \frac{d}{\varepsilon} \sum_j n_i \lambda_{ij}^{n+1} (1 - \beta_{ij}) (T_j^{n+1} - T_i^{n+1}) \\ &+ \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{ij}^{n+1} (|\mathbf{u}_{ij}^{n+1}|^2 - |\mathbf{u}_i^{n+1}|^2) + n_i \lambda_{ij}^{n+1} \gamma_{ij} |\mathbf{u}_i^{n+1} - \mathbf{u}_j^{n+1}|^2, \end{aligned} \quad (8.101b)$$

$$\begin{aligned} \rho_i \frac{\text{tl}(\mathbf{u}_i^{n+1} \otimes \mathbf{u}_i^{n+1}) - \text{tl}(\mathbf{u}_i^n \otimes \mathbf{u}_i^n)}{\Delta t} &+ \frac{\text{tl}(\mathbb{P}_i^{n+1}) - \text{tl}(\mathbb{P}_i^n)}{\Delta t} \\ &= \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{ij}^{n+1} [\text{tl}(\mathbf{u}_{ij}^{n+1} \otimes \mathbf{u}_{ij}^{n+1}) - \text{tl}(\mathbf{u}_i^{n+1} \otimes \mathbf{u}_i^{n+1})] - \frac{1}{\varepsilon} \left(\sum_j \lambda_{ij}^{n+1} (1 - \beta_{ij}) \right) \text{tl}(\mathbb{P}_i^{n+1}), \end{aligned} \quad (8.101c)$$

where the diagonal component of the final equation is removed using (8.101b).

The pressure tensor equation (8.101c) can be written

$$\begin{aligned} \text{tl}(\mathbb{P}_i^{n+1}) \left(1 + \frac{\Delta t}{\varepsilon} \sum_j \lambda_{ij}^{n+1} (1 - \beta_{ij}) \right) &= \text{tl}(\mathbb{P}_i^n) - \rho_i [\text{tl}(\mathbf{u}_i^{n+1} \otimes \mathbf{u}_i^{n+1}) - \text{tl}(\mathbf{u}_i^n \otimes \mathbf{u}_i^n)] \\ &\quad + \frac{\Delta t}{\varepsilon} \sum_j \rho_i \lambda_{ij}^{n+1} [\text{tl}(\mathbf{u}_{ij}^{n+1} \otimes \mathbf{u}_{ij}^{n+1}) - \text{tl}(\mathbf{u}_i^{n+1} \otimes \mathbf{u}_i^{n+1})]. \end{aligned} \quad (8.102)$$

A Gauss–Seidel-type iterative method can be derived from this backward Euler step: For iteration index $\ell = 0, 1, 2, \dots$,

$$\mathbf{U}^{\ell+1} = \mathcal{F}^\ell(\mathbf{U}^n), \quad (8.103a)$$

$$\mathbf{T}^{\ell+1} = \mathcal{G}^\ell(\mathbf{U}^{\ell+1}, \mathbf{U}^n, \mathbf{T}^n), \quad (8.103b)$$

$$\mathbb{P}_i^{\ell+1} = \mathcal{H}_i^\ell(\mathbf{U}^{\ell+1}, \mathbf{T}^{\ell+1}, \mathbb{P}_i^n) \quad \text{for } i \in \{1, \dots, N\}, \quad (8.103c)$$

$$\lambda_{ij}^{\ell+1} = \mathcal{I}(n^n, \mathbf{U}^{\ell+1}, \mathbf{T}^{\ell+1}, \{\mathbb{P}_k^{\ell+1}\}_{k=1}^N), \quad (8.103d)$$

where the superscript ℓ on the functions $\mathcal{F}$, $\mathcal{G}$, and $\mathcal{H}$ denotes the dependence on the collision frequencies, λ_{ij}^ℓ , and we have used the vectorized notation

$$\mathbf{U}^{\ell+1} = [\mathbf{u}_1^{\ell+1}, \dots, \mathbf{u}_N^{\ell+1}]^\top \in \mathbb{R}^{N \times d}, \quad \mathbf{T}^{\ell+1} = (T_1^{\ell+1}, \dots, T_N^{\ell+1})^\top \in \mathbb{R}_+^N, \quad (8.104)$$

with $\mathbb{R}_+ = (0, \infty)$. With this formulation, the collision frequencies can depend on species densities, momenta, temperatures/energies, and even pressure tensors.

Definition 8.5.16 (GST Method, Restricted Tensor Ansatz). *Let $\mathbf{u}_i^{n+1,0} = \mathbf{u}_i^n$ and $T_i^{n+1,0} = T_i^n$ be given. For $\ell \in \{0, 1, 2, \dots\}$, let $\mathbf{u}_i^{n+1,\ell+1}$ and $T_i^{n+1,\ell+1}$ be given by*

$$\rho_i \frac{\mathbf{u}_i^{\ell+1} - \mathbf{u}_i^n}{\Delta t} = \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{ij}^\ell (1 - \alpha_{ij}) (\mathbf{u}_j^{\ell+1} - \mathbf{u}_i^{\ell+1}) \quad (8.105a)$$

$$\begin{aligned} \rho_i \frac{|\mathbf{u}_i^{\ell+1}|^2 - |\mathbf{u}_i^n|^2}{\Delta t} + dn_i \frac{T_i^{\ell+1} - T_i^n}{\Delta t} &= \frac{d}{\varepsilon} \sum_j n_i \lambda_{ij}^\ell (1 - \beta_{ij}) (T_j^{\ell+1} - T_i^{\ell+1}) \\ &\quad + \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{ij}^\ell (|\mathbf{u}_{ij}^{\ell+1}|^2 - |\mathbf{u}_i^{\ell+1}|^2) + n_i \lambda_{ij}^\ell \gamma_{ij} |\mathbf{u}_i^{\ell+1} - \mathbf{u}_j^{\ell+1}|^2 \end{aligned} \quad (8.105b)$$

$$\begin{aligned} &\rho_i \frac{\text{tl}(\mathbf{u}_i^{\ell+1} \otimes \mathbf{u}_i^{\ell+1}) - \text{tl}(\mathbf{u}_i^n \otimes \mathbf{u}_i^n)}{\Delta t} + \frac{\text{tl}(\mathbb{P}_i^{\ell+1}) - \text{tl}(\mathbb{P}_i^n)}{\Delta t} \\ &= \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{ij}^\ell [\text{tl}(\mathbf{u}_{ij}^{\ell+1} \otimes \mathbf{u}_{ij}^{\ell+1}) - \text{tl}(\mathbf{u}_i^{\ell+1} \otimes \mathbf{u}_i^{\ell+1})] - \frac{1}{\varepsilon} \left(\sum_j \lambda_{ij}^\ell (1 - \beta_{ij}) \right) \text{tl}(\mathbb{P}_i^{\ell+1}). \end{aligned} \quad (8.105c)$$

We can rearrange the tensor equation (8.105c) to write the equation for the traceless

tensor as

$$\begin{aligned} \text{tl}(\mathbb{P}_i^{\ell+1}) = \frac{\varepsilon}{\varepsilon + \Delta t \sum_j \lambda_{i,j}^\ell (1 - \beta_{i,j})} & \left[\text{tl}(\mathbb{P}_i^n) - \rho_i [\text{tl}(\mathbf{u}_i^{\ell+1} \otimes \mathbf{u}_i^{\ell+1}) - \text{tl}(\mathbf{u}_i^n \otimes \mathbf{u}_i^n)] \right. \\ & \left. + \frac{\Delta t}{\varepsilon} \sum_j \rho_i \lambda_{i,j}^\ell [\text{tl}(\mathbf{u}_{i,j}^{\ell+1} \otimes \mathbf{u}_{i,j}^{\ell+1}) - \text{tl}(\mathbf{u}_i^{\ell+1} \otimes \mathbf{u}_i^{\ell+1})] \right], \end{aligned} \quad (8.106)$$

and then define the tensor $\mathbb{P}_i^{\ell+1}$ via

$$\mathbb{P}_i^{\ell+1} = n_i T_i^{\ell+1} I_{d \times d} + \text{tl}(\mathbb{P}_i^{\ell+1}) =: \mathcal{H}_i^\ell(\mathbf{U}^{\ell+1}, \mathbf{T}^{\ell+1}, \mathbb{P}_i^n). \quad (8.107)$$

Proposition 8.5.17. *The vectorized update can be written*

$$\mathbf{U}^{\ell+1} = \left(I_{d \times d} + \frac{\Delta t}{\varepsilon} P^{-1} (D^\ell - A^\ell) \right)^{-1} \mathbf{U}^n, \quad (8.108a)$$

$$\mathbf{T}^{\ell+1} = \left(I_{d \times d} + \frac{\Delta t}{\varepsilon} Q^{-1} (F^\ell - B^\ell) \right)^{-1} \left[\mathbf{T}^n + \frac{1}{d} \mathbf{s}^{(1),\ell+1} + \frac{\Delta t}{\varepsilon} \mathbf{s}^{(2),\ell+1,\ell} \right], \quad (8.108b)$$

$$\mathbb{P}_i^{\ell+1} = n_i T_i^{\ell+1} I_{d \times d} + \frac{\varepsilon}{\varepsilon + \Delta t \sum_j \lambda_{i,j}^\ell (1 - \beta_{i,j})} \left[\text{tl}(\mathbb{P}_i^n) + \mathbf{s}_i^{(3),\ell+1} + \frac{\Delta t}{\varepsilon} \mathbf{s}_i^{(4),\ell+1,\ell} \right], \quad (8.108c)$$

where we define

$$P = \text{diag}\{\rho_k\}, \quad Q = \text{diag}\{n_k\}, \quad M = \text{diag}\{m_k\}, \quad (8.109a)$$

$$A_{i,j}^\ell = \rho_i \lambda_{i,j}^\ell (1 - \alpha_{i,j}), \quad B_{i,j}^\ell = n_i \lambda_{i,j}^\ell (1 - \beta_{i,j}), \quad D_{i,j}^\ell = \delta_{i,j} \left(\sum_k A_{i,k}^\ell \right), \quad F_{i,j}^\ell = \delta_{i,j} \left(\sum_k B_{i,k}^\ell \right), \quad (8.109b)$$

and

$$\mathbf{s}^{(1),\ell+1} = M(\mathbf{s}^n - \mathbf{s}^{\ell+1}), \quad \mathbf{s} = (|\mathbf{u}_1|^2, \dots, |\mathbf{u}_N|^2)^\top, \quad (8.110a)$$

$$[\mathbf{s}^{(2),\ell+1,\ell}]_i = \sum_j m_i \lambda_{i,j}^\ell (|\mathbf{u}_{i,j}^{\ell+1}|^2 - |\mathbf{u}_i^{\ell+1}|^2) + \lambda_{i,j}^\ell \gamma_{i,j} |\mathbf{u}_i^{\ell+1} - \mathbf{u}_j^{\ell+1}|^2, \quad (8.110b)$$

$$\mathbf{s}_i^{(3),\ell+1} = \rho_i [\text{tl}(\mathbf{u}_i^n \otimes \mathbf{u}_i^n) - \text{tl}(\mathbf{u}_i^{\ell+1} \otimes \mathbf{u}_i^{\ell+1})], \quad (8.110c)$$

$$\mathbf{s}_i^{(4),\ell+1,\ell} = \sum_j \rho_i \lambda_{i,j}^\ell [\text{tl}(\mathbf{u}_{i,j}^{\ell+1} \otimes \mathbf{u}_{i,j}^{\ell+1}) - \text{tl}(\mathbf{u}_i^{\ell+1} \otimes \mathbf{u}_i^{\ell+1})]. \quad (8.110d)$$

8.5.4 Multi-Species ES-BGK Model – General Tensor Expression

In this section, we consider an ellipsoidal-statistical model similar to the more general model from [27, Section 2.2; Equations (18) and (19)]; i.e., with $\mathcal{T}_{i,j}$ defined by

$$\begin{aligned}\mathcal{T}_{i,j} &= (1 - \mu_{i,j})(\beta_{i,j}T_i + (1 - \beta_{i,j})T_j)I_{d \times d} + \mu_{i,j} \left[\beta_{i,j} \frac{\mathbb{P}_i}{n_i} - (1 - \beta_{i,j}) \frac{\mathbb{P}_j}{n_j} \right] + \frac{\gamma_{i,j}}{d} |\mathbf{u}_i - \mathbf{u}_j|^2 I_{d \times d} \\ &= T_{i,j} I_{d \times d} + \mu_{i,j} \left[\beta_{i,j} \text{tl} \left(\frac{\mathbb{P}_i}{n_i} \right) + (1 - \beta_{i,j}) \text{tl} \left(\frac{\mathbb{P}_j}{n_j} \right) \right].\end{aligned}\quad (8.111)$$

Remark 8.5.18. With $\mathcal{T}_{i,j}$ defined as in (8.111), the model retains desirable symmetries and conservation properties: As in (8.98), $\text{tr}(\mathcal{T}_{i,j}) = dT_{i,j}$, so that (i) Lemma 8.5.8 holds, and the parameters $\alpha_{i,j}$, $\beta_{i,j}$, and $\gamma_{i,j}$ still enjoy the symmetries of (8.71), and (ii) the conservation of total momentum and total energy still hold (Lemma 8.5.9).

Pressure Tensor Equation for General Tensor

Using the definition for $\mathcal{T}_{i,j}$ in (8.111), the equation for the pressure tensor, (8.88c), can also be written

$$\begin{aligned}\frac{\partial}{\partial t} \left(\rho_i \mathbf{u}_i \otimes \mathbf{u}_i + \mathbb{P}_i \right) &= \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{i,j} \{ \mathbf{u}_{i,j} \otimes \mathbf{u}_{i,j} - \mathbf{u}_i \otimes \mathbf{u}_i \} + \sum_j n_i \lambda_{i,j} \left(\mathcal{T}_{i,j} - \frac{\mathbb{P}_i}{n_i} \right) \\ &= \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{i,j} \{ \mathbf{u}_{i,j} \otimes \mathbf{u}_{i,j} - \mathbf{u}_i \otimes \mathbf{u}_i \} + \frac{1}{\varepsilon d} \sum_j n_i \lambda_{i,j} \gamma_{i,j} |\mathbf{u}_i - \mathbf{u}_j|^2 I_{d \times d} \\ &\quad + \frac{1}{\varepsilon} \sum_j n_i \lambda_{i,j} (1 - \beta_{i,j}) (T_j - T_i) I_{d \times d} \\ &\quad + \frac{1}{\varepsilon} \sum_j n_i \lambda_{i,j} (1 - \beta_{i,j}) \mu_{i,j} \left[\text{tl} \left(\frac{\mathbb{P}_j}{n_j} \right) - \text{tl} \left(\frac{\mathbb{P}_i}{n_i} \right) \right] - \frac{1}{\varepsilon} \sum_j n_i \lambda_{i,j} (1 - \beta_{i,j}) \text{tl} \left(\frac{\mathbb{P}_i}{n_i} \right),\end{aligned}\quad (8.112)$$

and using traceless matrices for all terms,

$$\begin{aligned}\frac{\partial}{\partial t} \left(\frac{1}{d} \rho_i |\mathbf{u}_i|^2 + n_i T_i \right) I_{d \times d} &+ \frac{\partial}{\partial t} \left(\text{tl}(\rho_i \mathbf{u}_i \otimes \mathbf{u}_i) + \text{tl}(\mathbb{P}_i) \right) \\ &= \frac{1}{\varepsilon d} \sum_j \lambda_{i,j} \left[\rho_i (|\mathbf{u}_{i,j}|^2 - |\mathbf{u}_i|^2) + n_i \gamma_{i,j} |\mathbf{u}_i - \mathbf{u}_j|^2 \right] I_{d \times d} \\ &\quad + \frac{1}{\varepsilon} \sum_j n_i \lambda_{i,j} (1 - \beta_{i,j}) (T_j - T_i) I_{d \times d}\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{i,j} [\text{tl}(\mathbf{u}_{i,j} \otimes \mathbf{u}_{i,j}) - \text{tl}(\mathbf{u}_i \otimes \mathbf{u}_i)] - \frac{1}{\varepsilon} \sum_j n_i \lambda_{i,j} (1 - \beta_{i,j}) \text{tl} \left(\frac{\mathbb{P}_i}{n_i} \right) \\
& + \frac{1}{\varepsilon} \sum_j n_i \lambda_{i,j} (1 - \beta_{i,j}) \mu_{i,j} \left[\text{tl} \left(\frac{\mathbb{P}_j}{n_j} \right) - \text{tl} \left(\frac{\mathbb{P}_i}{n_i} \right) \right]. \tag{8.113}
\end{aligned}$$

Note that $\frac{1}{d} \rho_i |\mathbf{u}_i|^2 + n_i T_i = (2/d) E_i$, so, as above, the energy terms will cancel, if updated first. Thus, subtracting $((1/d) I_{d \times d})$ times the energy equation (8.89) from this equation yields

$$\begin{aligned}
\frac{\partial}{\partial t} \left(\text{tl}(\rho_i \mathbf{u}_i \otimes \mathbf{u}_i) + \text{tl}(\mathbb{P}_i) \right) &= \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{i,j} [\text{tl}(\mathbf{u}_{i,j} \otimes \mathbf{u}_{i,j}) - \text{tl}(\mathbf{u}_i \otimes \mathbf{u}_i)] \\
& - \frac{1}{\varepsilon} \sum_j n_i \lambda_{i,j} (1 - \beta_{i,j}) \text{tl} \left(\frac{\mathbb{P}_i}{n_i} \right) \\
& + \frac{1}{\varepsilon} \sum_j n_i \lambda_{i,j} (1 - \beta_{i,j}) \mu_{i,j} \left[\text{tl} \left(\frac{\mathbb{P}_j}{n_j} \right) - \text{tl} \left(\frac{\mathbb{P}_i}{n_i} \right) \right] \tag{8.114}
\end{aligned}$$

Remark 8.5.19. *The moment equations for the traceless pressure tensors, given in (8.100) and (8.113) are structurally similar; the latter differs only by the addition of the final term, which accounts for the difference between species pressure tensors when the general tensor expression (8.111) for $\mathcal{T}_{i,j}$ is used in place of the restricted form (8.97).*

Numerical Update of Moment Equations (General Tensor)

Similarly to the numerical update for the restricted tensor, considered above, a Gauss–Seidel-type (GST) iterative method can be used to update the moment equations. The updated moments can then, be used to define the target Gaussians in the kinetic model for the implicit update of the collision operator.

Remark 8.5.20. *For the general tensor $\mathcal{T}_{i,j}$ in (8.111), the update equations for the momenta and temperatures/energies are identical to those for the restricted tensor (8.97) (and are given in (8.101a) and (8.101b)), and thus, we will consider only the pressure tensor moment equation (8.114).*

Definition 8.5.21 (Backward Euler, General Tensor Ansatz). *The implicit Euler step of the pressure tensor equation (8.114) is given by*

$$\rho_i \frac{\text{tl}(\mathbf{u}_i^{n+1} \otimes \mathbf{u}_i^{n+1}) - \text{tl}(\mathbf{u}_i^n \otimes \mathbf{u}_i^n)}{\Delta t} + \frac{\text{tl}(\mathbb{P}_i^{n+1}) - \text{tl}(\mathbb{P}_i^n)}{\Delta t}$$

$$\begin{aligned}
&= \frac{1}{\varepsilon} \sum_j \rho_i \lambda_{i,j}^{n+1} [\text{tl}(\mathbf{u}_{i,j}^{n+1} \otimes \mathbf{u}_{i,j}^{n+1}) - \text{tl}(\mathbf{u}_i^{n+1} \otimes \mathbf{u}_i^{n+1})] \\
&\quad - \frac{1}{\varepsilon} \sum_j n_i \lambda_{i,j}^{n+1} (1 - \beta_{i,j}) \text{tl} \left(\frac{\mathbb{P}_i^{n+1}}{n_i} \right) \\
&\quad + \frac{1}{\varepsilon} \sum_j n_i \lambda_{i,j}^{n+1} (1 - \beta_{i,j}) \mu_{i,j} \left[\text{tl} \left(\frac{\mathbb{P}_j^{n+1}}{n_j} \right) - \text{tl} \left(\frac{\mathbb{P}_i^{n+1}}{n_i} \right) \right] \quad (8.115)
\end{aligned}$$

Similarly to Section 8.5.3, we aim to describe an iterative approach similar to (8.103). Due to the inclusion of the interaction term between pressure tensors, the update is far less straightforward. Thus, it may be convenient to consider a vectorized formulation of the pressure tensor equation (8.114), and perform a Backward Euler step on the resulting equation.

Lemma 8.5.22. *The pressure tensor equation (8.114) can be written as,*

$$\begin{aligned}
&M \boxtimes I_{d \times d} \partial_t (\vec{X}) + (I_{N \times N} \boxtimes I_{d \times d}) \overrightarrow{\text{tl}(\mathbb{P}/n)} \\
&= \frac{1}{\varepsilon} \mathbf{s}^{(4)}(\mathbf{U}) - \frac{1}{\varepsilon} (\hat{B} \boxtimes I_{d \times d}) \overrightarrow{\text{tl}(\mathbb{P}/n)} - \frac{1}{\varepsilon} [Q^{-1}(\tilde{F} - \tilde{B}) \boxtimes I_{d \times d}] \overrightarrow{\text{tl}(\mathbb{P}/n)}, \quad (8.116)
\end{aligned}$$

and the resulting backward Euler time discretization is

$$\begin{aligned}
&M \boxtimes I_{d \times d} \frac{\vec{X}^{n+1} - \vec{X}^n}{\Delta t} + \frac{\overrightarrow{\text{tl}(\mathbb{P}/n)^{n+1}} - \overrightarrow{\text{tl}(\mathbb{P}/n)^n}}{\Delta t} \\
&= \frac{1}{\varepsilon} \mathbf{s}^{(4),n+1} - \frac{1}{\varepsilon} (\hat{B}^{n+1} \boxtimes I_{d \times d}) \overrightarrow{\text{tl}(\mathbb{P}/n)^{n+1}} - \frac{1}{\varepsilon} [Q^{-1}(\tilde{F}^{n+1} - \tilde{B}^{n+1}) \boxtimes I_{d \times d}] \overrightarrow{\text{tl}(\mathbb{P}/n)^{n+1}} \quad (8.117a)
\end{aligned}$$

$$\begin{aligned}
&\iff \left\{ \left(I_{N \times N} + \frac{\Delta t}{\varepsilon} \hat{B}^{n+1} + \frac{\Delta t}{\varepsilon} Q^{-1}(\tilde{F}^{n+1} - \tilde{B}^{n+1}) \right) \boxtimes I_{d \times d} \right\} \overrightarrow{\text{tl}(\mathbb{P}/n)^{n+1}} \\
&= \overrightarrow{\text{tl}(\mathbb{P}/n)^n} + \mathbf{s}^{(3),n+1} + \frac{\Delta t}{\varepsilon} \mathbf{s}^{(4),n+1,n+1}, \quad (8.117b)
\end{aligned}$$

where $A_1 \boxtimes A_2$ denotes the Kronecker product of matrices A_1 and A_2 ,

$$M = \text{diag}\{m_k\} \in \mathbb{R}^{N \times N}, \quad (8.118a)$$

$$\overrightarrow{\text{tl}(\mathbb{P}/n)^{\ell+1}} := \begin{bmatrix} \text{tl}(\mathbb{P}_1^{\ell+1}/n_1) \\ \vdots \\ \text{tl}(\mathbb{P}_N^{\ell+1}/n_N) \end{bmatrix} \in \mathbb{R}^{Nd \times d}, \quad (8.118b)$$

$$\vec{X}^{\ell+1} := \begin{bmatrix} \text{tl}(\mathbf{u}_1^{\ell+1} \otimes \mathbf{u}_1^{\ell+1}) \\ \vdots \\ \text{tl}(\mathbf{u}_N^{\ell+1} \otimes \mathbf{u}_N^{\ell+1}) \end{bmatrix} \in \mathbb{R}^{Nd \times d}, \quad (8.118c)$$

$$\tilde{B}_{i,j}^\ell := n_i \lambda_{i,j}^\ell (1 - \beta_{i,j}) \mu_{i,j} = B_{i,j}^\ell \mu_{i,j} \implies \tilde{B} \in \mathbb{R}^{N \times N}, \quad (8.118d)$$

$$\tilde{F}_{i,j}^\ell := \delta_{i,j} \left(\sum_k \tilde{B}_{i,k}^\ell \right) \implies \tilde{F} \in \mathbb{R}^{N \times N}, \quad (8.118e)$$

$$\hat{B}^\ell := \text{diag} \left\{ \sum_j \lambda_{i,j}^\ell (1 - \beta_{i,j}) \right\} \in \mathbb{R}^{N \times N}, \quad (8.118f)$$

$$\mathbf{s}^{(3),\ell+1} := \mathbf{s}^{(3)}(\mathbf{U}^{\ell+1}) = M \boxtimes I_{d \times d} (\vec{X}^{\mathbf{n}} - \vec{X}^{\mathbf{n}+1}) \in \mathbb{R}^{Nd \times d}, \quad (8.118g)$$

$$\mathbf{s}^{(4),\ell+1,\ell} := \mathbf{s}^{(4)}(\mathbf{U}^{\ell+1}, \lambda_{i,j}^\ell) = \begin{bmatrix} \sum_j m_1 \lambda_{1,j}^\ell [\text{tl}(\mathbf{u}_{1,j}^{\ell+1} \otimes \mathbf{u}_{1,j}^{\ell+1}) - \text{tl}(\mathbf{u}_1^{\ell+1} \otimes \mathbf{u}_1^{\ell+1})] \\ \vdots \\ \sum_j m_N \lambda_{N,j}^\ell [\text{tl}(\mathbf{u}_{N,j}^{\ell+1} \otimes \mathbf{u}_{N,j}^{\ell+1}) - \text{tl}(\mathbf{u}_N^{\ell+1} \otimes \mathbf{u}_N^{\ell+1})] \end{bmatrix} \in \mathbb{R}^{Nd \times d}. \quad (8.118h)$$

From the backward Euler update of (8.101a), (8.101b), and (8.117), we obtain the following vectorized version of the GST iterative method:

Proposition 8.5.23 (GST Method, General Tensor Ansatz). *The vectorized GST update can be written as*

$$\mathbf{U}^{\ell+1} = \left(I_{d \times d} + \frac{\Delta t}{\varepsilon} P^{-1} (D^\ell - A^\ell) \right)^{-1} \mathbf{U}^{\mathbf{n}} \quad (8.119a)$$

$$\mathbf{T}^{\ell+1} = \left(I_{d \times d} + \frac{\Delta t}{\varepsilon} Q^{-1} (F^\ell - B^\ell) \right)^{-1} \left[\mathbf{T}^{\mathbf{n}} + \frac{1}{d} \mathbf{s}^{(1),\ell+1} + \frac{\Delta t}{\varepsilon} \mathbf{s}^{(2),\ell+1,\ell} \right] \quad (8.119b)$$

$$\begin{aligned} \overrightarrow{(\mathbb{P}/n)}^{\ell+1} &= \vec{\mathbf{T}}^{\ell+1} + \overrightarrow{\text{tl}(\mathbb{P}/n)}^{\ell+1} \\ &= \vec{\mathbf{T}}^{\ell+1} + (Z^\ell)^{-1} \left[\overrightarrow{\text{tl}(\mathbb{P}/n)}^{\mathbf{n}} + \mathbf{s}^{(3),\ell+1} + \mathbf{s}^{(4),\ell+1,\ell} \right], \end{aligned} \quad (8.119c)$$

where

$$\vec{\mathbf{T}}^{\ell+1} = \begin{pmatrix} T_1 I_{d \times d} \\ \vdots \\ T_N I_{d \times d} \end{pmatrix} \quad \text{and} \quad Z^\ell = \left\{ \left(I_{N \times N} + \frac{\Delta t}{\varepsilon} \hat{B}^\ell + \frac{\Delta t}{\varepsilon} Q^{-1} (\tilde{F}^\ell - \tilde{B}^\ell) \right) \boxtimes I_{d \times d} \right\}. \quad (8.120)$$

Proof. The expressions in (8.119a) and (8.119b) are a restatement of the corresponding expressions in (8.108) and can be derived directly from (8.101) and (8.105). To verify (8.119c), first recall from (8.96) that for each i , $\mathbb{P}_i/n_i = T_i I_{d \times d} + \text{tl}(\mathbb{P}_i/n_i)$. Stacking these

terms, gives

$$\overrightarrow{(\mathbb{P}/n)}^{\ell+1} = \overrightarrow{\mathcal{T}}^{\ell+1} + \text{tl}(\overrightarrow{(\mathbb{P}/n)})^{\ell+1}. \quad (8.121)$$

Expressing (8.117b) as an iteration scheme, isolating $\overrightarrow{\text{tl}(\mathbb{P}/n)}^{\ell+1}$, and substituting the result into (8.121), the result follows. ■

Chapter 9

Progress Summary and Next Steps

9.1 Summary

This Year-Four progress report presents a review of basic background on the theory of the multi-species Boltzmann equation and two associated, approximating models, the multi-species BGK and the multi-species ES-BGK models. The BGK equations, which simplify their Boltzmann equation counterparts, are highly nonlinear, nonlocal, and high-dimensional models of particle kinetics in rarefied gases and plasmas. We discuss both single-species models and self-consistent extensions to multi-species BGK models. Preliminary work toward the efficient numerical simulation of BGK-type kinetic equations is presented via several benchmark problems.

Theoretical aspects of single-species BGK kinetic models have been presented in order to motivate and describe the types of numerical methods used. In particular, conservation and entropy dissipation properties were presented, along with an analysis of the space-homogeneous (no advection) problem. Numerical methods must be sophisticated enough to respect these conservation and dissipation properties at the fully discrete level. A stable finite volume numerical approximation framework has been outlined to capture potential discontinuities in the approximate solutions. Since the problem can be numerically stiff for some parameter regimes, implicit and semi-implicit time integration schemes are of particular importance for stability. Particular focus is given to implicit-explicit Runge–Kutta (IMEX-RK) time stepping methods, as they give a reasonable balance between accuracy, efficiency, and stability. However, in some cases, fully implicit integration strategies are demanded, and the work here is a stepping stone toward developing such algorithms and codes.

Several numerical benchmark problems and tests of the prototype MATLAB codes are presented, including the Sod shock tube and two-stream instability test cases. The tests are

presented for $1 \times 1 \nu$ phase spaces, but code is currently under development for more realistic higher-dimensional cases. In particular, $1 \times 3 \nu$ and $2 \times 3 \nu$ codes for “slab geometries” will be designed and benchmarked in the near future. The numerical methods that are presented are inherently scalable, and, thus, the only impediment for efficient and stable numerical simulation is the increased number of degrees of freedom. An example $1 \times 1 \nu$ code, used for numerical solutions of the Sod shock tube problem, is given in Appendix E. This work is done to address the goal of developing practical stable and efficient semi-implicit and fully implicit time integrator strategies for the problem.

An introduction to a particular self-consistent BGK-type model for multi-species particle kinetics is given. The combinatorial complexity of the model grows with the addition of distinct chemical constituents, making such multi-species models even more challenging for numerical solution. We have discussed the moment equations for the multi-species case, as the moments can be used to update the Maxwellians in an IMEX approach. We have studied the asymptotic relaxation behavior of the moment equations and have proven that the temperatures always remain positive, which guarantees the existence and uniqueness of the moment equations [16].

We have developed a nonlinear Gauss–Seidel-type iterative solver for the numerical approximation of the moment equations of a space-homogeneous multi-species BGK model. Solving the moment equation system is a fundamental bridge toward an efficient IMEX scheme for the multi-species case. A sophisticated fixed point iterative scheme has been developed to address this issue in computing the implicit update for the moment equations. The scheme is designed to relax the implicit updates of the velocity and temperature to appropriate values, depending on collisional frequencies that themselves depend on the implicit moments. This allows for the desired implicit update of the BGK collision operators. Time discretization is performed by a backward Euler method so as to overcome stability and accuracy issues. We have provided some sample numerical simulations from our recent paper describing and analyzing our solver [16].

9.2 Next Steps

There are several outstanding issues that this work will address in the future. In particular, as in the single-species case, an implicit (or, at least, semi-implicit) approach is desired for the computation of the stiff collision operators in the multi-species case to achieve numerical stability. However, the procedures used in the single-species case do not work directly in the multi-species case. A sophisticated solver for the full multi-species BGK is currently being

developed and analyzed.

Beyond the multi-species BGK model presented, we will continue to examine a multi-species ellipsoidal statistical BGK model (ES-BGK), that allows for simulation with the correct Prandtl number, and captures anisotropic effects in the flow behavior. We have outlined some very preliminary ideas in the last chapter of this report. We will examine the moment system for this model, and develop iterative methods akin to the ones currently in development, to update the moment system. A hybrid numerical method inspired by the work in [20, 42] is currently in development for the multi-species ES-BGK model.

In the longer term, in addition to semi- and fully-implicit solvers, this work will focus on the design of fast adaptive phase-space methods and block-structured adaptive mesh refinement (AMR) that will efficiently accommodate disparate scales that are inherent in multi-species problems, owing, for example, to disparate particle sizes and temperatures. Incorporating implicit solver technology with AMR, especially in the context of such highly nonlinear and nonlocal models is expected to be challenging. We will also develop efficient discrete velocity methods for multi-species BGK and ES-BGK models, extending the framework that we outlined herein for the single-species case.

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Appendix A

An Important Integral

We need to compute the following generalized Gaussian integral in several places in the report.

Lemma A.0.1.

$$\int_{\mathbb{R}^d} |\mathbf{s}|^2 e^{-|\mathbf{s}|^2} d\mathbf{s} = \frac{d}{2} \pi^{\frac{d}{2}}. \quad (\text{A.1})$$

Proof.

$$\begin{aligned} \int_{\mathbb{R}^d} |\mathbf{s}|^2 e^{-|\mathbf{s}|^2} d\mathbf{s} &= \int_{\mathbb{R}^d} (s_1^2 + \dots + s_d^2) e^{-(s_1^2 + \dots + s_d^2)} d\mathbf{s} \\ &= \int_{\mathbb{R}^d} \left(\sum_{j=1}^d s_j^2 \right) \prod_{k=1}^d e^{-s_k^2} d\mathbf{s} \\ &= \int_{\mathbb{R}^d} s_1^2 \prod_{k=1}^d e^{-s_k^2} d\mathbf{s} + \dots + \int_{\mathbb{R}^d} s_d^2 \prod_{k=1}^d e^{-s_k^2} d\mathbf{s} \\ &= \left(\prod_{\substack{k=1 \\ k \neq 1}}^d \int_{\mathbb{R}} e^{-s_k^2} ds_k \right) \int_{\mathbb{R}} s_1^2 e^{-s_1^2} ds_1 + \dots + \left(\prod_{\substack{k=1 \\ k \neq d}}^d \int_{\mathbb{R}} e^{-s_k^2} ds_k \right) \int_{\mathbb{R}} s_d^2 e^{-s_d^2} ds_d \\ &= \left(\pi^{\frac{1}{2}} \right)^{d-1} \int_{\mathbb{R}} s_1^2 e^{-s_1^2} ds_1 + \dots + \left(\pi^{\frac{1}{2}} \right)^{d-1} \int_{\mathbb{R}} s_d^2 e^{-s_d^2} ds_d \\ &= \pi^{\frac{d-1}{2}} \sum_{i=1}^d \int_{\mathbb{R}} s_i^2 e^{-s_i^2} ds_i, \end{aligned} \quad (\text{A.2})$$

where we have used many elementary integration techniques, and the fact that $\int_{\mathbb{R}} e^{-x^2} dx = \pi^{\frac{1}{2}}$. It remains to determine the value of the terms of the form $\int_{\mathbb{R}} s^2 e^{-s^2} ds$. To that end, utilizing integration by parts, with

$$u = s_i \implies du = ds_i \quad (\text{A.3})$$

$$dv = 2s_i e^{-s_i^2} ds_i \implies v = -e^{-s_i^2}, \quad (\text{A.4})$$

we have

$$\begin{aligned} \frac{1}{2} \int_{\mathbb{R}} 2s_i^2 e^{-s_i^2} ds_i &= \frac{1}{2} \left[\left[-s_i e^{-s_i^2} \right]_{-\infty}^{\infty} - \int_{\mathbb{R}} -e^{-s_i^2} ds_i \right] \\ &= \frac{1}{2} \int_{\mathbb{R}} e^{-s_i^2} ds_i \\ &= \frac{1}{2} \pi^{\frac{1}{2}}. \end{aligned} \quad (\text{A.5})$$

Thus, Equation (A.2) gives us

$$\int_{\mathbb{R}^d} |\mathbf{s}|^2 e^{-|\mathbf{s}|^2} d\mathbf{s} = \pi^{\frac{d-1}{2}} \sum_{i=1}^d \frac{1}{2} \pi^{\frac{1}{2}} = \pi^{\frac{d-1}{2}} \left(\frac{d}{2} \pi^{\frac{1}{2}} \right) = \frac{d}{2} \pi^{\frac{d}{2}}, \quad (\text{A.6})$$

as desired. ■

Appendix B

Picard–Lindelöf Theorem

We will make use of the following version of the Picard–Lindelöf Theorem for autonomous systems:

Theorem B.0.1. *Suppose that $\mathbf{u}_0 \in \mathbb{R}^d$ and $\mathbf{f} \in C(\overline{B}(\mathbf{u}_0, \beta); \mathbb{R}^d)$, where $B(\mathbf{u}_0, \beta)$ ($\overline{B}(\mathbf{u}_0, \beta)$) denotes the open (closed) Euclidean ball of radius β centered at $\mathbf{u}_0$. Suppose further that $\|\mathbf{f}(\mathbf{v})\|_2 \leq M$, for all $\mathbf{v} \in \overline{B}(\mathbf{u}_0, \beta)$, and $\mathbf{f}$ is Lipschitz continuous, with constant $L > 0$, on $\overline{B}(\mathbf{u}_0, \beta)$. Set $\delta = \min(\frac{1}{2L}, \frac{\beta}{M})$. Then the IVP $\mathbf{u}'(t) = \mathbf{f}(\mathbf{u}(t))$, $\mathbf{u}(t_0) = \mathbf{u}_0$ has a unique solution on the interval $[t_0 - \delta, t_0 + \delta]$.*

Appendix C

Bounding the Eigenvalues of Z and $\hat{Z}$

The matrices Z and $\hat{Z}$, defined in (7.20), play a key role in the dynamics of (7.17) and the equivalent system (7.19). In this appendix, we prove bounds on the eigenvalues of these matrices. With the collision frequencies defined in (7.11), the matrices A and B , defined in (7.14a), take the form

$$A_{i,j} = \frac{16}{3} \sqrt{\frac{\pi}{2}} \frac{m_i m_j (d_i + d_j)^2}{(m_i + m_j)^3} \rho_i \rho_j \sqrt{\frac{T_i}{m_i} + \frac{T_j}{m_j}}, \quad (\text{C.1})$$

$$B_{i,j} = \frac{8}{3} \sqrt{\frac{\pi}{2}} \frac{(d_i + d_j)^2}{(m_i + m_j)^2} \rho_i \rho_j \sqrt{\frac{T_i}{m_i} + \frac{T_j}{m_j}}. \quad (\text{C.2})$$

Since each value used to define the matrix elements is positive and bounded above and below (importantly, the temperature), then their values can be bounded as follows:

$$A_{\min}(t) := \min_{i,j} A_{i,j}(t) \leq A_{i,j}(t) \leq \max_{i,j} A_{i,j}(t) =: A_{\max}(t) \quad (\text{C.3})$$

$$B_{\min}(t) := \min_{i,j} B_{i,j}(t) \leq B_{i,j}(t) \leq \max_{i,j} B_{i,j}(t) =: B_{\max}(t) \quad (\text{C.4})$$

Theorem C.0.1 (Eigenvalue Bounds). *Let $A, B, D, F \in \mathbb{R}^{N \times N}$ be the matrices defined in (7.14), and let $A_{\min} = \min_{i,j} A_{i,j}$, $B_{\min} = \min_{i,j} B_{i,j}$, $A_{\max} = \max_{i,j} A_{i,j}$, and $B_{\max} = \max_{i,j} B_{i,j}$. Then the eigenvalues of the matrices $Z = P^{-\frac{1}{2}}(D - A)P^{-\frac{1}{2}}$ and $\hat{Z} = Q^{-\frac{1}{2}}(F - B)Q^{-\frac{1}{2}}$ satisfy*

$$0 = z_0 < z_{\min} \leq z_1 \leq \cdots \leq z_{N-1} \leq z_{\max}, \quad (\text{C.5})$$

$$0 = \hat{z}_0 < \hat{z}_{\min} \leq \hat{z}_1 \leq \cdots \leq \hat{z}_{N-1} \leq \hat{z}_{\max}, \quad (\text{C.6})$$

where

$$z_{\min} = \frac{A_{\min} N}{\max\{\rho_k\}}, \quad z_{\max} = \frac{A_{\max}(N-1)}{\min\{\rho_k\}}, \quad (\text{C.7})$$

$$\hat{z}_{\min} = \frac{B_{\min} N}{\max\{n_k\}}, \quad \hat{z}_{\max} = \frac{B_{\max}(N-1)}{\min\{n_k\}}. \quad (\text{C.8})$$

Proof. The proofs of (C.5) and (C.6) are similar; thus we prove (C.5) and leave the remaining details to the reader. The (single) zero eigenvalue of $(D - A)$ corresponds to the eigenvector, $\mathbf{1}$, spanning the null space of $(D - A)$. To find bounds on the other eigenvalues, let $\mathbf{y} \in \mathcal{R}(D - A) = \mathcal{N}(D - A)^\perp$, so that $\mathbf{y}^\top \mathbf{1} = \sum_i y_i = 0$. Recall that $\mathbf{y}^\top (D - A) \mathbf{y} = \frac{1}{2} \sum_i \sum_j A_{ij} (y_i - y_j)^2$. Using $\sum_i y_i = 0$,

$$\mathbf{y}^\top (D - A) \mathbf{y} \leq \frac{A_{\max}}{2} \sum_i \sum_j (y_i - y_j)^2 = \frac{A_{\max}}{2} \sum_i \sum_{j \neq i} (y_i^2 + y_j^2) = A_{\max}(N-1) \|\mathbf{y}\|_2^2. \quad (\text{C.9})$$

Thus if $\mathbf{y} = P^{-\frac{1}{2}} \mathbf{z}$, then

$$\mathbf{z}^\top Z \mathbf{z} \leq (N-1) A_{\max} \mathbf{z}^\top P^{-1} \mathbf{z} = (N-1) A_{\max} \sum_i \frac{1}{\rho_i} z_i^2 \leq \frac{(N-1) A_{\max}}{\min\{\rho_k\}} \|\mathbf{z}\|_2^2 =: z_{\max} \|\mathbf{z}\|_2^2, \quad (\text{C.10})$$

which gives the upper bound in (C.5). For the lower bound,

$$\mathbf{y}^\top (D - A) \mathbf{y} \geq \frac{A_{\min}}{2} \sum_{i=1}^N \sum_{j=1}^N (y_i^2 + y_j^2) = A_{\min} N \|\mathbf{y}\|_2^2. \quad (\text{C.11})$$

Thus if $\mathbf{y} = P^{-\frac{1}{2}} \mathbf{z}$, then

$$\mathbf{z}^\top Z \mathbf{z} \geq N A_{\min} \mathbf{z}^\top P^{-1} \mathbf{z} \geq \frac{N A_{\min}}{\max\{\rho_k\}} \|\mathbf{z}\|_2^2 =: z_{\min} \|\mathbf{z}\|_2^2. \quad (\text{C.12})$$

■

Appendix D

Null Space Components of $\widetilde{W}$ and $\widetilde{\xi}$

In this appendix, we show that $\widetilde{W}_{\mathcal{N}}$ (the projection of $\widetilde{W}$ onto $\mathcal{N}(Z)$) and $\widetilde{\xi}_{\mathcal{N}}$ (the projection of $\widetilde{\xi}$ onto $\mathcal{N}(\widehat{Z})$) are both zero. These results are used in the proofs of Theorems 7.3.6 and 7.3.7, respectively.

Lemma D.0.1. $\widetilde{W}_{\mathcal{N}} \equiv \mathbf{0}$.

Proof. Since the null space of Z is spanned by $P^{\frac{1}{2}}\mathbf{1}$, it is sufficient to show that $\widetilde{W}^{\top} P^{\frac{1}{2}}\mathbf{1} = \mathbf{0}$. Write $\mathbf{u}^{\infty} = \frac{\mathbf{U}^{\top} P\mathbf{1}}{\mathbf{1}^{\top} P\mathbf{1}}$ and $(\mathbf{U}^{\infty})^{\top} = \mathbf{u}^{\infty} \mathbf{1}^{\top}$, so that

$$\widetilde{W}^{\top} P^{\frac{1}{2}}\mathbf{1} = (\mathbf{W} - \mathbf{W}^{\infty})^{\top} P^{\frac{1}{2}}\mathbf{1} = \mathbf{U}^{\top} P\mathbf{1} - (\mathbf{U}^{\infty})^{\top} P\mathbf{1} = \mathbf{U}^{\top} P\mathbf{1} - \frac{\mathbf{U}^{\top} P\mathbf{1}}{\mathbf{1}^{\top} P\mathbf{1}} \mathbf{1}^{\top} P\mathbf{1} = \mathbf{0}. \quad (\text{D.1})$$

■

Lemma D.0.2. $\widetilde{\xi}_{\mathcal{N}} \equiv \mathbf{0}$.

Proof. Since the null space of $\widehat{Z}$ is spanned by $Q^{\frac{1}{2}}\mathbf{1}$, it is sufficient to show that $\widetilde{\xi}^{\top} Q^{\frac{1}{2}}\mathbf{1} = 0$. Recall that $\widetilde{\xi} = Q^{-\frac{1}{2}}(\mathbf{E} - \mathbf{E}^{\infty})$; hence

$$\widetilde{\xi}^{\top} Q^{\frac{1}{2}}\mathbf{1} = (\mathbf{E} - \mathbf{E}^{\infty})^{\top} \mathbf{1} = \sum_{i=1}^N E_i - \sum_{i=1}^N E_i^{\infty} = 0, \quad (\text{D.2})$$

where the fact that $\sum_i E_i = \sum_i E_i^{\infty}$ is a consequence of (7.50) in the proof of Proposition 7.3.1. ■

Appendix E

1x1v Prototype Code

The MATLAB code listed in this appendix is that used to generate the results of Section 4.5 for the Sod shock tube benchmark problem. This code is developed for prototyping and demonstration purposes only and is not meant to represent production-quality software.

E.1 Main Driver: vlasovPoissonBGKMain.m

```
% Script to solve Vlasov-Poisson-BGK Equation:
%
% 1X1V
%
%  $f_t + v * f_x + a * f_v = 1/\tau * (M-f)$ 
%
% This set of code is designed to solve the Sod Shock tube problem.
% In the limit as ( $\tau \rightarrow 0$ ) or ( $\lambda \rightarrow \infty$ ), BGK  $\rightarrow$  Euler.
% So, for the current test, set  $\tau=10^{-N}$ , set  $a = 0$ .
%
% Scheme:
% IMEX RK: Explicit Advection, Implicit Collision.
%
clear;
clc;
tic
%
% Number of ghost cells:
del = 1;
%
```

```

% Collision time:
tau = 10^(-4);
%
% Theta values for minmod:
thetaX = 2;
thetaV = 2;
%
% Spatial domain:
xL = -0.5;
xR = 0.5;
%
% Number of cells:
Nx = 256;
%
% Cell edge points:
x = linspace(xL,xR,Nx+1);
%
% Cell center points:
xC = x(1:end-1) + 0.5 * (x(2:end) - x(1:end-1));
xCenter = [xC(1:del) , xC , xC(end-del+1:end)];
hX = xC(2) - xC(1);
%
% Velocity domain:
vMin = -10;
vMax = 10;
%
% Number of cells:
Nv = 258;
%
% Cell edge points:
v = linspace(vMin,vMax,Nv+1);
%
% Cell center points:
vC = v(1:end-1) + 0.5 * (v(2:end) - v(1:end-1));
vCenter = [vC(1:del) , vC , vC(end-del+1:end)];
hV = vC(2) - vC(1);
%
% Define time levels:
tInit = 0;
tFin = 0.2;
%
% Vectors for ghost cells

```

```

gVx = [1,length(xC)]+del;
gVv = [1,length(vC)]+del;
%
tableNum = 8;
[Ae,be,ce,Ai,bi,ci] = butcherTable(tableNum);
butcher.Ae = Ae; butcher.Ai = Ai;
butcher.be = be; butcher.bi = bi;
butcher.ce = ce; butcher.ci = ci;
%
% Stiffness matrix for the Poisson solve...zero Dirichlet BC
% (as per the test problems). This is not needed for the Sod problem,
% but I kept it so I didn't have to change all my function
% dependencies.
%
temp = zeros(1,Nx);
temp(1)=2; temp(2)=-1;
A = toeplitz(temp);
A(1,1) = 3; A(end,end) = 3;
%
grid.del = del;
grid.gVx = gVx; grid.Nx = Nx; grid.xC = xC; grid.xCenter = xCenter;
grid.gVv = gVv; grid.Nv = Nv; grid.vC = vC; grid.vCenter = vCenter;
grid.hX = hX;
grid.hV = hV;
grid.xL = xL ; grid.xR = xR ;
grid.vMin = vMin; grid.vMax = vMax;
grid.tInit = tInit; grid.tFin = tFin;
grid.thetaX = thetaX;
grid.thetaV = thetaV;
%
testNum = 1;
[f] = initialCondition(testNum,grid);
%
[tVec,y,MAX] = vlasovPoissonBGKSolver(f,butcher,grid,tau,A,f);
%
figure(107)
pcolor(xC,vC,y);
title(['Contour plot of computed f, in the Velocity/Space', ...
      ' Domain, for Time t = ', num2str(tFin), ' '])
xlabel('x')
ylabel('v')
shading interp;

```

```

colormap(jet);
colorbar;
%
toc
%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
% Embedded functions below:
%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
function [f] = initialCondition(testNum,grid)
%
xC = grid.xC; xCenter = grid.xCenter;
vC = grid.vC; vCenter = grid.vCenter;
%
% Initialize solution array:
f = zeros(length(vC),length(xC),1);
%
switch testNum
    case 1 % tFin = 0.250
        nL = 1.00000; uL = 0.00000; thetaL = 0001.000;
        nR = 0.12500; uR = 0.00000; thetaR = 0000.800;
    case 2 % tFin = 0.150
        nL = 1.00000; uL = -2.00000; thetaL = 0000.400;
        nR = 1.00000; uR = 2.00000; thetaR = 0000.400;
    case 3 % tFin = 0.012
        nL = 1.00000; uL = 0.00000; thetaL = 1000.000;
        nR = 1.00000; uR = 0.00000; thetaR = 0000.010;
    case 4 % tFin = 0.035
        nL = 1.00000; uL = 0.00000; thetaL = 0000.010;
        nR = 1.00000; uR = 0.00000; thetaR = 0100.000;
    case 5 % tFin = 0.035
        nL = 5.99924; uL = 19.59750; thetaL = 0460.894;
        nR = 5.99242; uR = -6.19633; thetaR = 046.0950;
end
%
% Initial condition (make a separate function?):
%
for j = 1:length(vC)
    for i = 1:length(xC)
        if xCenter(i) <= 0.0

```

```

        f(j,i) = nL / sqrt(2*pi*thetaL) * exp(-(vC(j)-uL)^2 ...
            / (2*thetaL));
    else
        f(j,i) = nR / sqrt(2*pi*thetaR) * exp(-(vC(j)-uR)^2 ...
            / (2*thetaR));
    end
end
end
%
% %Plot the initial conditions....
% figure(110)
% % pcolor(x_c,v_c,f);
% surf(x_c,v_c,f); view(-30,50); zlim([0,2.1]);
% % title(['Contour plot of f, in the Velocity/Space Domain,' ...
% ' for Time t = ',num2str(0),' '])
% xlabel('x')
% ylabel('v')
% shading interp;
% colormap(jet);
% colorbar;
%
end
%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
function [Ae,be,ce,Ai,bi,ci] = butcherTable(table)
%
% Butcher Tableaux for the IMEX-RK scheme. Tables 2-6 come from
% the Pareschi & Russo paper. Table 7 is Backward Euler. Table 8
% (needs reference, from Cory).
%
switch table
case 2
    Ae = [0,0 ; 1,0];
    be = [0.5 ; 0.5];
    ce = [0 ; 1];
%
    gam = 1-1/sqrt(2);
    Ai = [gam,0 ; 1-2*gam,gam];
    bi = [0.5 ; 0.5];
    ci = [gam ; 1-gam];
%

```

```

case 3
    Ae = [0,0,0 ; 0,0,0 ; 0,1,0];
    be = [0 ; 0.5 ; 0.5];
    ce = [0 ; 0 ; 1];

%
    Ai = [0.5,0,0 ; -0.5,0.5,0 ; 0,0.5,0.5];
    bi = [0 ; 0.5 ; 0.5];
    ci = [0.5 ; 0 ; 1];

%
case 4
    Ae = [0,0,0 ; 0.5,0,0 ; 0.5,0.5,0];
    be = [1/3 ; 1/3 ; 1/3];
    ce = [0 ; 0.5 ; 1];

%
    Ai = [0.25,0,0 ; 0,0.25,0 ; 1/3,1/3,1/3];
    bi = [1/3 ; 1/3 ; 1/3];
    ci = [0.25 ; 0.25 ; 1];

%
case 5
    Ae = [0,0,0 ; 1,0,0 ; 0.25,0.25,0];
    be = [1/6 ; 1/6 ; 2/3];
    ce = [0 ; 1 ; 0.5];

%
    gam = 1-1/sqrt(2);
    Ai = [gam,0,0 ; 1-2*gam,gam,0 ; 0.5-gam,0,gam];
    bi = [1/6 ; 1/6 ; 2/3];
    ci = [gam ; 1-gam ; 0.5];

%
case 6
    Ae = [0,0,0,0 ; 0,0,0,0 ; 0,1,0,0 ; 0,0.25,0.25,0];
    be = [0 ; 1/6 ; 1/6 ; 2/3];
    ce = [0 ; 0 ; 1 ; 0.5];

%
    alpha = 0.24169426078821;
    beta = 0.06042356519705;
    eta = 0.12915286960590;
    Ai = [alpha,0,0,0; -alpha,alpha,0,0; 0,1-alpha,alpha,0; ...
        beta,eta,0.5-beta-eta-alpha,alpha];
    bi = [0 ; 1/6 ; 1/6 ; 2/3];
    ci = [alpha ; 0 ; 1 ; 0.5];

%
case 7

```

```
%  
% Forward Euler:  
    Ae = 0;  
    be = 1;  
    ce = 0;  
%  
% Backward Euler  
    Ai = 1;  
    bi = 1;  
    ci = 1;  
%  
case 8  
    gam = 1 - 1/sqrt(2);  
    deltax = 1 - 1/(2*gam);  
%  
    Ae = [0,0,0 ; gam,0,0 ; deltax,1-deltax,0];  
    be = [deltax;1-deltax;0];  
    ce = [0;gam;1];  
%  
    Ai = [0,0,0 ; 0,gam,0 ; 0,1-gam,gam];  
    bi = [0;1-gam;gam];  
    ci = [0;gam;1];  
end  
end
```

Listing E.1: Main driver: vlasovPoissonBGKMain.m.

E.2 vlasovPoissonBGKSolver.m

```

function [t,Z,M] = vlasovPoissonBGKSolver(y0,butcher,grid,tau,A,f)
%
% y0 = IC grid function (j,i) = (velocity,space)
% Ae, be, ce: Butcher Tableau for explicit solve
% Ai, bi, ci: Butcher tableau for implicit solve
%
Ai = butcher.Ai;
bi = butcher.bi;
ci = butcher.ci;
Ae = butcher.Ae;
be = butcher.be;
ce = butcher.ce;
%
gVx = grid.gVx; Nx = grid.Nx; hX = grid.hX;
gVv = grid.gVv; Nv = grid.Nv; hV = grid.hV;
%
% A is the stiffness matrix for the Poisson solve.
%
% Number of ghost cells
del = grid.del;
%
% Spatial domain:
xL = grid.xL; xR = grid.xR;
%
% Velocity domain:
vMin = grid.vMin; vMax = grid.vMax;
%
% Define CFL(s)
CFLMaxX = min(hX) / max(abs(vMax),abs(vMin));
CFLMaxV = min(hV) / max(abs(xL),abs(xR));
%
% Define initial/final time levels:
tCurrent = grid.tInit;
tFinal = grid.tFin;
%
% size of grid function array y including ghost cells:
d = size(y0)+2*del;
%

```

```

% Initialize array of solutions:
y = zeros([d,2]);
%
% Input initial conditions into solution vector
y(gVv(1):gVv(2),gVx(1):gVx(2),1) = f;
%
% Store appropriate initial values in ghost cells
for i = 1:del
    y(:,gVx(1)-i,1) = y(:,gVx(1),1);
    y(:,gVx(2)+i,1) = y(:,gVx(2),1);
end
for j = 1:del
    y(gVv(1)-j,(:,1) = y(gVv(1),(:,1);
    y(gVv(2)+j,(:,1) = y(gVv(2),(:,1);
end
%
% Number of stages of RK scheme:
s = length(ce);
%
% Initial vectors for RK scheme:
uo = zeros([d,s]);
fI = zeros([d,s]);
fE = zeros([d,s]);
M = zeros([d,s]);
%
redo = 0;
EMax = 1;
t = 1;
%
while tCurrent < tFinal
%
    dt = min(0.24 * min(CFLMaxX,CFLMaxV),tFinal-tCurrent) ...
        / (1 + (redo > 0));
%
% This flag indicates that the electric field gets bigger than E.max.
% If so, the step needs to recalculate.
    redo = 0;
%
    uo(:, :, :) = 0;
    uo(:, :, 1) = y(:, :, 1);
    [~,M(:, :, 1)] = BGKCollision(tCurrent,y(:, :, 1),grid,tau,tCurrent);
    u(:, :, 1) = (tau*uo(:, :, 1) + dt*Ai(1,1)*M(:, :, 1)) ...

```

```

    / (tau + dt*Ai(1,1));
fI(:, :, 1) = BGKCollision(tCurrent+ci(1)*dt,u(:, :, 1), grid, ...
    tau, tCurrent);
%
[fE(:, :, 1), re] = divFlux(tCurrent+ce(1)*dt,u(:, :, 1), grid, EMax, A);
redo = redo+re;

for r = 2:s
    uo(:, :, r) = y(:, :, 1) ...
        + dt * reshape(Ae(r, :) * reshape(permute(fE, [3, 1, 2]), s, ...
            (Nv+2*del)*(Nx+2*del)), Nv+2*del, Nx+2*del) ...
        + dt * reshape(Ai(r, :) * reshape(permute(fI, [3, 1, 2]), s, ...
            (Nv+2*del)*(Nx+2*del)), Nv+2*del, Nx+2*del);
%
[~, M(:, :, r)] = BGKCollision(tCurrent+ci(r)*dt,uo(:, :, r), ...
    grid, tau, tCurrent);
%
u(:, :, r) = (tau*uo(:, :, r) + dt*Ai(r, r)*M(:, :, r)) ...
    / (tau + dt*Ai(r, r));

[fE(:, :, r), re] = divFlux(tCurrent+ce(r)*dt,u(:, :, r), grid, EMax, A);
redo = redo+re;

fI(:, :, r) = BGKCollision(tCurrent+ci(r)*dt,u(:, :, r), ...
    grid, tau, tCurrent);
end
%
y(:, :, 2) = y(:, :, 1) ...
    + (dt * reshape(be' * reshape(permute(fE, [3, 1, 2]), s, ...
        (Nv+2*del)*(Nx+2*del)), Nv+2*del, Nx+2*del) ...
    + dt * reshape(bi' * reshape(permute(fI, [3, 1, 2]), s, ...
        (Nv+2*del)*(Nx+2*del)), Nv+2*del, Nx+2*del) ...
    ) * (1 - (redo > 0));
%
y(:, :, 1) = y(:, :, 2);
tCurrent = tCurrent + dt*(1 - (redo>0));
%
% This computes the moments and Maxwellian at the final time step.
if tCurrent == tFinal
    BGKCollision(tCurrent+ci(r)*dt,y(:, :, 1), grid, tau, tCurrent);
end
end

```

```
%  
% Return solution at final time  
Z = y(gVv(1):gVv(2),gVx(1):gVx(2),1);  
%  
end
```

Listing E.2: vlasovPoissonBGKSolver.m.

E.3 BGKCollision.m

```

function [z,M] = BGKCollision(t,y,grid,tau,tCurrent)
%
del = grid.del;
hx = grid.hX; gVx = grid.gVx; x = grid.xC;
hv = grid.hV; gVv = grid.gVv; v = grid.vC;
%
% Grid function array must have ghost cells already.
M = zeros(length(x)+2*del,length(v)+2*del);
nDens = zeros(1,length(x));
mDens = zeros(1,length(x));
EDens = zeros(1,length(x));

uDens = zeros(1,length(x));
theta = zeros(1,length(x));
%
% Moment integrals: n, n*u, and E.
nDens(1:length(x)) = hv * sum(y(gVv(1):gVv(2),1+del:length(x)+del));
mDens(1:length(x)) = hv * sum(v(:).*y(gVv(1):gVv(2), ...
    1+del:length(x)+del));
EDens(1:length(x)) = 0.5 * hv * sum(v(:).^2 .* y(gVv(1):gVv(2), ...
    1+del:length(x)+del));

uDens(:) = mDens(:)./nDens(:);

theta(:) = 2*EDens(:)./nDens(:)-uDens(:).^2;

M(gVx(1):gVx(2),gVv(1):gVv(2)) = nDens(:) ./ sqrt(2*pi*theta(:)) ...
    .* exp(-0.5 * abs(v - uDens(:)).^2 ./ theta(:));
%
% Ghost cells: zero flow boundaries.
for i = 1:del
    M(:,gVv(1)-i) = M(:,gVv(1));
    M(:,gVv(2)+i) = M(:,gVv(2));
end
for j = 1:del
    M(gVx(1)-j,:) = M(gVx(1),:);
    M(gVx(2)+j,:) = M(gVx(2),:);
end

```

```

%
if tCurrent == 0.2
%
% initial shock happens here.
x0 = 0;
gam = 3;
uL = [1,0,1]; uR = [0.125,0,0.1];
%
pDens = nDens .* theta;
%
[nSod,uSod,pSod,eSod] = sodSoln(x,tCurrent,uL,uR,gam,x0);
%
figure(1)
plot(x,nDens,'b','LineWidth',3)
hold on
plot(x,nSod,'LineWidth',3)
xlim([-0.5,0.5])
ylim([0,1])
set(gca,'fontsize',24)
legend('BGK','Euler')
hold off
%
figure(2)
plot(x,uDens,'b','LineWidth',3)
hold on
plot(x,uSod,'LineWidth',3)
xlim([-0.5,0.5])
ylim([0,1])
set(gca,'fontsize',24)
legend('BGK','Euler')
hold off
%
figure(3)
plot(x,theta,'b','LineWidth',3)
hold on
plot(x,2*eSod,'LineWidth',3)
xlim([-0.5,0.5])
ylim([0,2]) % may need to shift this
set(gca,'fontsize',24)
legend('BGK','Euler')
hold off
end

```

```
%  
z = (M'-y)/tau;  
%  
% M is a [Nv]X[Nx] array after transpose  
M = M';  
%  
end
```

Listing E.3: BGKCollision.m

E.4 divFlux.m

```

function [z,redo] = divFlux(t,y,grid,EMax,A)
%
% y = grid function of f_{ij}^k values for fixed k
%
del = grid.del;
hx = grid.hX; gVx = grid.gVx; x = grid.xCenter; thetaX = grid.thetaX;
hv = grid.hV; gVv = grid.gVv; v = grid.vCenter; thetaV = grid.thetaV;
%
fP = zeros(size(y));
fM = zeros(size(y));
gP = zeros(size(y));
gM = zeros(size(y));
%
% construct slopes
[sX(:, :), sV(:, :)] = slopeReconstruction(y,grid);
%
% % Spatial fluxes
fP(:,gVx(1):gVx(2)) = (y(:,gVx(1):gVx(2)) ...
    + 0.5*hx*sX(:,gVx(1):gVx(2))) .* v(:).*(v>0)' ...
    +(y(:,gVx(1)+1:gVx(2)+1) - 0.5*hx*sX(:,gVx(1)+1:gVx(2)+1)) ...
    .* v(:).*(v<=0)';
fM(:,gVx(1):gVx(2)) = (y(:,gVx(1)-1:gVx(2)-1) ...
    + 0.5*hx*sX(:,gVx(1)-1:gVx(2)-1)) .* v(:).*(v>0)' ...
    +(y(:,gVx(1):gVx(2)) - 0.5*hx*sX(:,gVx(1):gVx(2))) ...
    .* v(:).*(v<=0)';
%
% The electric field is unnecessary for this test, so we set it to
% zero here.
E = zeros(1,length(x));
redo = 0;

% % Velocity fluxes
gP(gVv(1):gVv(2), :) = (y(gVv(1):gVv(2), :) ...
    + 0.5*hv*sV(gVv(1):gVv(2), :)) .* E.*(E>0) ...
    + (y(gVv(1)+1:gVv(2)+1, :) - 0.5*hv*sV(gVv(1)+1:gVv(2)+1, :)) ...
    .* E.*(E<=0);
gM(gVv(1):gVv(2), :) = (y(gVv(1)-1:gVv(2)-1, :) ...
    + 0.5*hv*sV(gVv(1)-1:gVv(2)-1, :)) .* E.*(E>0) ...

```

```

+ (y(gVv(1):gVv(2),:) - 0.5*hv*sV(gVv(1):gVv(2),:)) ...
.* E.*(E<=0) ;

z = - (fP - fM)/hx - (gP - gM)/hv;

end

```

Listing E.4: divFlux.m

E.5 slopeReconstruction.m

```

function [sX,sV] = slopeReconstruction(y,grid)
%
sX = zeros(size(y));
sV = zeros(size(y));
%
del = grid.del;
hx = grid.hX; gVx = grid.gVx; thetaX = grid.thetaX;
hv = grid.hV; gVv = grid.gVv; thetaV = grid.thetaV;
%
SV(:, :, 1) = (y(gVv(1)+1:gVv(2)+1, gVx(1):gVx(2)) ...
    - y(gVv(1)-1:gVv(2)-1, gVx(1):gVx(2))) / 2 ;
SV(:, :, 2) = thetaV * (y(gVx(1):gVv(2), gVx(1):gVx(2)) ...
    - y(gVv(1)-1:gVv(2)-1, gVx(1):gVx(2))) ;
SV(:, :, 3) = thetaV * (y(gVx(1)+1:gVv(2)+1, gVx(1):gVx(2)) ...
    - y(gVv(1):gVv(2), gVx(1):gVx(2))) ;
%
sV(gVv(1):gVv(2), gVx(1):gVx(2)) = minMod(SV)/hv;
%
SX(:, :, 1) = (y(gVv(1):gVv(2), gVx(1)+1:gVx(2)+1) ...
    - y(gVv(1):gVv(2), gVx(1)-1:gVx(2)-1)) / 2 ;
SX(:, :, 2) = thetaX * (y(gVx(1):gVv(2), gVx(1):gVx(2)) ...
    - y(gVv(1):gVv(2), gVx(1)-1:gVx(2)-1)) ;
SX(:, :, 3) = thetaX * (y(gVx(1):gVv(2), gVx(1)+1:gVx(2)+1) ...
    - y(gVv(1):gVv(2), gVx(1):gVx(2))) ;
%
sX(gVv(1):gVv(2), gVx(1):gVx(2)) = minMod(SX)/hx;
%
for i = 1:del
    sX(:, gVx(1)-i) = sX(:, gVx(1));
    sX(:, gVx(2)+i) = sX(:, gVx(2));
end
for j = 1:del
    sV(gVv(1)-j, :) = sV(gVv(2), :);
    sV(gVv(2)+j, :) = sV(gVv(1), :);
end
%
end

```

Listing E.5: slopeReconstruction.m

E.6 minMod.m

```
function M = minMod(x)
%
M(:, :) = 0.25*abs(sign(x(:, :, 1))+sign(x(:, :, 2))) ...
    .* (sign(x(:, :, 1))+sign(x(:, :, 3))) .* min(abs(x), [], 3);
%
end
```

Listing E.6: minMod.m

E.7 sodSoln.m

```

function [n,u,p,e] = sodSoln(x,tCurrent,phiL,phiR,gam,x0)
%
% Script to compute theoretical sod solution at given time with
% given gamma.
%
%
% phiL and phiR are ordered as (n,u,p)
nL = phiL(1); uL = phiL(2); pL = phiL(3);
nR = phiR(1); uR = phiR(2); pR = phiR(3);
%
% This function does an iterative solve to compute the value of
% pStar.
pStar = pStarSolve(10^(-8));
thL = pL / nL;
thR = pR / nR;

aL = sqrt(3*thL);
aStarL = aL * (pStar/pL)^((gam-1)/(2*gam));
aR = sqrt(3*thR);

nFan = nL * (2/(gam+1) + (gam-1)*(uL-x/tCurrent) ...
    / (gam+1)/aL).^ (2/(gam-1));

nStarL = nL * (pStar/pL)^(1/gam);
nStarR = nR * ( (pStar/pR + (gam-1)/(gam+1)) ...
    / ((gam-1)*pStar/(gam+1)/pR + 1) );

uFan = 2/(gam+1) * (aL + (gam-1)*uL/2 + x/tCurrent);

uStar = uL - 2*aL / (gam-1) * ((pStar/pL)^((gam-1)/(2*gam)) - 1);

pFan = pL * (2/(gam+1) + (gam-1)*(uL-x/tCurrent) ...
    / (gam+1) / aL).^ (2*gam/(gam-1));

eL = 0.5*pL/nL;
eStarL = 0.5*pStar/nStarL;
eStarR = 0.5*pStar/nStarR;
eR = 0.5*pR/nR;

```

```

sHL = uL - aL;
sTL = uStar - aStarL;
%
% speed of the contact wave.
% lambda_2(U_star_L) = S_2 = lambda_2(U_star_R)
% Toro book: Equation 2.134, and page 96
sC = uStar; sR = uR + aR*( (gam+1)*pStar / (2*gam*pR) ...
    + 0.5*(gam-1)/gam)^(0.5);

nFunc = @(x) nL .* ((x<x0 + sHL*tCurrent)) ...
    + nFan .* ((x0 + sHL*tCurrent <= x) & (x < x0 + sTL*tCurrent)) ...
    + nStarL .* ((x0 + sTL*tCurrent <= x) & (x < x0 + sC*tCurrent)) ...
    + nStarR .* ((x0 + sC*tCurrent <= x) & (x < x0 + sR*tCurrent)) ...
    + nR .* ((x0 + sR*tCurrent <= x));

uFunc = @(x) uL .* ((x<x0 + sHL*tCurrent)) ...
    + uFan .* ((x0 + sHL*tCurrent <= x) & (x < x0 + sTL*tCurrent)) ...
    + uStar .* ((x0 + sTL*tCurrent <= x) & (x < x0 + sR*tCurrent)) ...
    + uR .* ((x0 + sR*tCurrent <= x));

pFunc = @(x) pL .* ((x<x0 + sHL*tCurrent)) ...
    + pFan .* ((x0 + sHL*tCurrent <= x) & (x < x0 + sTL*tCurrent)) ...
    + pStar .* ((x0 + sTL*tCurrent <= x) & (x < x0 + sR*tCurrent)) ...
    + pR .* ((x0 + sR*tCurrent <= x));

eFunc = @(x) eL .* ((x<x0 + sHL*tCurrent)) ...
    + (0.5*pFan./nFan) .* ((x0 + sHL*tCurrent <= x) ...
    & (x < x0 + sTL*tCurrent)) ...
    + eStarL .* ((x0 + sTL*tCurrent <= x) & (x < x0 + sC*tCurrent)) ...
    + eStarR .* ((x0 + sC*tCurrent <= x) & (x < x0 + sR*tCurrent)) ...
    + eR .* ((x0 + sR*tCurrent <= x));

n = nFunc(x);
u = uFunc(x);
p = pFunc(x);
e = eFunc(x);

end

```

Listing E.7: sodSoln.m

E.8 pStarSolve.m

```
function pStar = pStarSolve(TOL)
%
% Newton Raphson to compute the pressure in Sod problem.
%
ERR = 1;
%
% Initial guess.
pOld = 0.9;
k = 0;
%
while ERR > TOL
    pNew = pOld - (sqrt(3)*pOld^(1/3) - sqrt(3) + ...
        2*(pOld-0.1)/sqrt(pOld+0.05)) / (sqrt(3)*pOld^(-2/3)/3 ...
        + 2*(pOld+0.05)^(-0.5) - (pOld-0.1)*(pOld+0.05)^(-1.5));
    ERR = abs(pOld-pNew) / (0.5*(pOld+pNew));
    pOld = pNew;
    k = k+1;
end
%
pStar = pNew;
%
end
```

Listing E.8: pStarSolve.m

Appendix F

Bibliography

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