

Numerical approximation of the Boltzmann equation : moment closure

Citation for published version (APA):

Abdel Malik, M. R. A., & Brummelen, van, E. H. (2012). *Numerical approximation of the Boltzmann equation : moment closure*. (CASA-report; Vol. 1230). Technische Universiteit Eindhoven.

Document status and date:

Published: 01/01/2012

Document Version:

Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
- The final author version and the galley proof are versions of the publication after peer review.
- The final published version features the final layout of the paper including the volume, issue and page numbers.

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EINDHOVEN UNIVERSITY OF TECHNOLOGY
Department of Mathematics and Computer Science

CASA-Report 12-30
September 2012

Numerical approximation of the Boltzmann equation: Moment closure

by

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ISSN: 0926-4507

Numerical Approximation of the Boltzmann equation: Moment Closure

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Abstract

This work applies the moment method onto a generic form of kinetic equations to simplify kinetic models of particle systems. This leads to the moment closure problem which is addressed using entropy-based moment closure techniques utilizing entropy minimization. The resulting moment closure system forms a system of partial differential equations that retain structural features of the kinetic system in question. This system of partial differential equations generate balance laws for velocity moments of a kinetic density that are symmetric hyperbolic, implying well-posedness in finite time. In addition, the resulting moment closure system satisfies an analog of Boltzmann's H-Theorem, i.e. solutions of the moment closure system are entropy dissipative. Such a model provides a promising alternative to particle methods, such as the Monte Carlo approaches, which can be prohibitive with regard to computational costs and inefficient with regard to error decay. However, several challenges pertaining to the analytical formulation and computational implementation of the moment closure system arise that are addressed in this work.

The entropy minimization problem is studied in light of the classical results by Junk [18] showing that this technique suffers from a realizability problem, i.e. there exists realizable moments such that the entropy minimizer does not exist. Recent results by Hauck [17], Schneider [31] and Pavan [29] are used to investigate and circumvent this issue.

The resulting moment closure system involves moments of exponentials of polynomials of, in principle, arbitrary order. In the context of numerical approximations, this is regarded as a complication. A novel and mathematically tractable moment system is developed that is based on approximating the entropy minimizing distribution. It will be shown that the resulting system retains the same structural features of the kinetic system in question. This system can be seen as a refinement of Grad's original moment system [15, 32].

Finally, a numerical approximation of the resulting moment systems is devised using discontinuous Galerkin (DG) finite elements method. Energy analysis based on the work of Barth [1, 2] is employed to investigate energy stable numerical flux functions to be used for the DG discretization of the moment systems. In contrast to the work of Barth [1], the numerical flux function suggested for the tractable system does not require a simplified construction since it is computable. In addition, higher order (approximated) moment systems, beyond the 10-moment system investigated by Barth [1], can be considered.

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Chapter 1

Introduction

1. Motivation

A fluid dynamical description of gases is based on the assumption that a typical macroscopic length scale pertaining to the flow geometry is much larger than the mean free path of a fluid particle. This is quantified by the Knudsen number viz., the ratio of the mean free path to the macroscopic length scale of interest. Such a description suggests that the velocity distribution of these particles tends towards a local equilibrium that is parametrized by fluid variables (typically the mass density, fluid velocity and temperature). In the context of fluid dynamics, the evolution of fluid variables is governed by either the (compressible) Euler equations, which approximate the velocity by a local equilibrium, or the Navier-Stokes-Fourier (NSF) equations, which account for small deviations of the velocity distribution from a local equilibrium. As the Knudsen number grows, the basic assumption of fluid dynamics breaks down leading to what are known as rarefaction effects. Typical situations in which such effects take place include the following examples (see [9, 32] and references therein),

- At high altitudes (for example, in high altitude flights) and in near-vacuum applications, gas pressure and density are very low. Consequently, the mean free path becomes large enough such that the Knudsen number can not be neglected giving rise to rarefaction effects.
- Flow across small geometries such that the relevant length scales are so small that, even at normal pressure and densities, the Knudsen number becomes significant. Typical applications of such a situation include micro-channel flows or flow in porous media.
- Accounting for rarefied gas effects is required in order to understand the behavior of small particles in a fluid as well as their space-time distributions. Typical applications include environmental problems such as emission of particles from electric power plants, chemical plants or vehicles, as well as understanding the role such small particles play in fog or cloud formation and the release of radioactivity from nuclear reactor accidents

The significance of rarefaction effects is that the deviation of the velocity distribution from a local equilibrium may become large and the NSF equations can yield momentum and energy fluxes that are inconsistent with nonnegative particle densities and that may even be wrong by orders of magnitude [24].

In the context of kinetic theory, deviations of the velocity distribution of dilute gases from equilibrium can be described using kinetic equations that govern the evolution of single-particle phase-space densities (one for each species in the case of multi-component flows) rather than fluid dynamical variables. In the continuum limit, solutions of the kinetic system correspond to the solution of both the Euler and the NSF equations [30]. Furthermore, the NSF equations can be recovered in the fluid dynamical regime by using either a Hilbert or Chapman-Enskog expansion [32].

Kinetic equations pose a formidable challenge for numerical approximations methods, on account of their high dimensional phase-space setting: for a problem in N spatial dimensions, the single molecule phase-space is $2N$ dimensional. The corresponding computational complexity of conventional discretization methods for differential equations, such as finite-element methods with uniform meshes, is prohibitive. Away from the fluid dynamical regime numerical approximations of kinetic systems are predominantly based on particle methods, such as the Direct Simulation Monte Carlo (DSMC) method. However, the phase-space description of the system results in the prohibitive computational cost of DSMC in the fluid dynamical limit. Moreover, from an approximation perspective, DSMC can be inefficient since it is inherent to the Monte-Carlo process that the approximation error decays only as $n^{-\frac{1}{2}}$ for the number of simulation molecules n [21]. Hence, efficiently modeling gases in the transition regime between the free molecular flow and fluid dynamics remains difficult.

Physically, rather than solving the kinetic equations for particle phase-space density, it would be more interesting to solve for functions of this density that would, for example, correspond to some macroscopic properties of the gas. This implies that one would instead track weighted averages or moments of the particle phase-space density. Such an approximation can be achieved using the method of moments. A moment method is a statistical approximation technique which suggests that the unknown parameters should be estimated by matching population moments (which are functions of unknown parameters) with appropriate sample moments [25].

Grad's moment method [15] is based on an expansion of the one-molecule marginal using Hermite polynomials, modulated by the local equilibrium distribution. A deficiency of Grad's moment closure system is the potential occurrence of locally negative and therefore inadmissible phase-space distributions, and potential loss of hyperbolicity [7, 33]. Later, Levermore [23] developed a moment closure system based on entropy minimization, which leads to an exponential closure. However, it was subsequently shown by Junk [18] that Levermore's moment closure system suffers from a realizability problem, i.e. there exist moments for which the minimum entropy solution is undefined. On the other hand, results of recent work by Schneider [31] and Pavan [29], show that a relaxation of the entropy minimization problem does not suffer from non-realizability while retaining exponential closure.

Another fundamental complication pertaining to the implementation of the moment-closure systems based on exponential closure, is that the resulting formulation requires the evaluation of moments of exponentials of polynomials of, in principle, arbitrary orders. It is generally accepted that the derivation of closed-form expressions for such moments is intractable, and accurate approximation of the moments is a notoriously difficult problem [22].

This study investigates the application of the method of moments to a generic form of a kinetic system given by the Boltzmann equation and the resulting moment closure problem. Furthermore, the moment closure system is studied from the perspective of subspace approximations, based on the observation that taking moments of the kinetic system over some basis vectors can be viewed as a projection of the system onto the space spanned by the basis vectors. Moreover, this work attempts to develop a tractable approximation to Levermore's moment-closure by approximation (Taylor expansion) of the minimizing entropy distribution. It has been noted that Grad's moment closure can be perceived as a first order linearization of the Levermore's exponential closure [32]. The results of this study can be conceived as a refinement of Grad's moment system since it overcomes potentially negative densities and potential loss of hyperbolicity. In addition, the work of Barth [1] is extended to develop a discontinuous Galerkin approximation of the resulting approximate moment closure system.

2. The Boltzmann equation: Properties

This work involves describing a gas composed of a single species of identical classical particles, i.e. a monatomic gas, contained within a fixed spatial domain $\Omega \subset \mathbb{R}^D$. Through kinetic theory such a description involves the evolution of a non-negative (phase-space) density $f = f(t, \mathbf{x}, \mathbf{v})$ over a single particle phase $\Omega \times \mathbb{R}^D$. This evolution is governed by the (kinetic) Boltzmann equation expressed, using the Einstein summation convention, as

$$\partial_t f + v_j \partial_{x_j} f = \mathcal{C}(f) \quad (1.1)$$

where the collision operator $f \mapsto \mathcal{C}(f)$ acts only on the \mathbf{v} dependence of f locally at each (t, \mathbf{x}) . Let $\langle \cdot, \cdot \rangle$ denote \mathbf{v} -integrations, i.e. the integral of any scalar or vector valued measurable function over the D -dimensional Lebesgue measure $d^D \mathbf{v}$; thus,

$$\langle q, 1 \rangle \equiv \int_{\mathbb{R}^D} q(\mathbf{v}) d^D \mathbf{v} \quad (1.2)$$

Note that all function considered in this work are understood to be Lebesgue measurable in all variables.

The collision operator \mathcal{C} is assumed to be defined over the domain $\mathcal{D}(\mathcal{C})$ that is contained within the set of non-negative functions of \mathbf{v} . Furthermore, it is assumed that \mathcal{C} has the following properties: [23]

1. Conservation: Mass, Momentum and Energy

The operator \mathcal{C} is assumed to have $\gamma \in \{1, v_i, |\mathbf{v}|^2\}$, $i = 1, 2, \dots, D$ as locally conserved quantities; thus,

$$\langle \mathcal{C}(f), \gamma \rangle = 0, \quad \forall f \in \mathcal{D}(\mathcal{C}) \quad (1.3)$$

Note that equations (1.3) represent the physical laws of mass, momentum and energy conservation during collisions. Moreover, it is assumed that there are no other conservation laws and that every locally conserved quantity is a linear combination of these three, i.e. for any $g = g(\mathbf{v})$ the following statements are equivalent:

- (a) $\langle \mathcal{C}(f), g \rangle = 0, \quad \forall f \in \mathcal{D}(\mathcal{C})$
- (b) $g \in \mathcal{C} \equiv \text{span}\{1, v_1, v_2, \dots, v_D, |\mathbf{v}|^2\}$.

Note that \mathcal{C} denotes the collection of collision invariants.

2. Dissipation: H-Theorem

The operator \mathcal{C} is assumed to satisfy the local dissipation relation

$$\langle \mathcal{C}(f), \ln f \rangle \leq 0, \quad \forall f \in \mathcal{D}(\mathcal{C}) \quad (1.4)$$

The local equilibria of \mathcal{C} are assumed to be characterized by the vanishing of the local entropy dissipation rate and to be given by the class of Maxwellian densities for some $(\varrho, u, \eta) \in \mathbb{R}_+ \times \mathbb{R}^D \times \mathbb{R}_+$. More precisely, for every $f \in \mathcal{D}(\mathcal{C})$ the following statements are assumed to be equivalent

- (a) $\langle \mathcal{C}(f), \ln f \rangle = 0$
- (b) $\mathcal{C}(f) = 0$
- (c) f is a Maxwellian density i.e. it is given by the form

$$f = \mathcal{M}(\varrho, u, \eta) \equiv \frac{\varrho}{(2\pi\eta)^{\frac{D}{2}}} e^{-\frac{|\mathbf{v}-\mathbf{u}|^2}{2\eta}} \quad (1.5)$$

where ϱ is the mass density, $\varrho \mathbf{u}$ is the momentum density and μ is the rescaled temperature of the gas

It is worthy to note that, naturally, any modification of the assumption in the dissipation relation (1.4) should be consistent with the equivalence relation of the aforementioned statements.

3. Symmetry: Galilean Invariance

The operator \mathcal{C} is assumed to commute with translational and orthogonal transformations. Specifically, given any $g = g(\mathbf{v})$ then for every vector $\mathbf{u} \in \mathbb{R}^D$ and for every orthogonal matrix $O \in \mathbb{R}^{D \times D}$ define transformed functions $\mathcal{T}_u g$ and $\mathcal{T}_O g$ by

$$\begin{aligned}\mathcal{T}_u g &= \mathcal{T}_u g(\mathbf{v}) \equiv g(\mathbf{u} - \mathbf{v}) \\ \mathcal{T}_O g &= \mathcal{T}_O g(\mathbf{v}) \equiv g(O^\top \mathbf{v})\end{aligned}\tag{1.6}$$

Hence, equation (1.1) formally retains Galilean invariance, i.e. if f satisfies (1.1) so does every Galilean group acting on f . Physically, this implies the Galilean invariance of the microscopic collisional dynamics.

3. Moment Systems

Physically, one maybe more interested in functions of f , which would correspond to macroscopic properties, rather than in f itself. Such reasoning motivates deriving equations for functions of f instead. That is, rather than resolving equation (1.1) for f , one could resolve moment systems (or weighted averages) of f instead, which would govern the evolution of a finite set of velocity moments of f because it is the moments which are (at least in theory) experimentally measurable quantities [16]. In resolving the moment equations instead of (1.1), the velocity dependence of f is replaced by a finite number of parameters, thus, reducing the complexity of the problem [32].

To derive the moment equations, consider a finite linear subspace Θ of functions of \mathbf{v} (taken to be polynomials) with dimension θ and basis $\{\vartheta_i = \vartheta_i(\mathbf{v})\}_{i=1}^\theta$. Denote the column θ -vector of these basis elements by $\boldsymbol{\vartheta} = \boldsymbol{\vartheta}(\mathbf{v})$, so that every $\vartheta \in \Theta$ has a unique representation in the form $\vartheta(\mathbf{v}) = \boldsymbol{\alpha}^\top \boldsymbol{\vartheta}(\mathbf{v})$ for some $\boldsymbol{\alpha} \in \mathbb{R}^\theta$. Consider the space of phase-space density distributions given by

$$\mathcal{F} := \{f \in \mathbb{L}^1(\mathbb{R}^D) : f \geq 0 \text{ and } f\vartheta_i \in \mathbb{L}^1(\mathbb{R}^D)\}\tag{1.7}$$

Taking the moments, i.e. weighted average, of equation (1.1) over the vector $\boldsymbol{\vartheta}(\mathbf{v})$:

$$\partial_t \langle f, \boldsymbol{\vartheta} \rangle + \partial_{x_j} \langle f, v_j \boldsymbol{\vartheta} \rangle = \langle \mathcal{C}(f), \boldsymbol{\vartheta} \rangle\tag{1.8}$$

thus, equation (1.1) is formally expressed as a hierarchy of a system of partial differential equations in (1.8). It is not known whether the quantities appearing in this equation are well defined for every solution f of a given kinetic equation. Since, it has been shown that this is the case for the spatially homogenous equation [12], following Levermore [23] it shall be assumed here that these quantities are well defined. Furthermore, it is observed that in equations (1.8) the flux in one equation appears as the density in the subsequent one, i.e. the expansion at some order n contains the moments at orders $n \pm 1$. Moreover, the equations contain the production terms which are related to the distribution function f through the collision term $\mathcal{C}(f)$. Therefore, in order to have a complete set of equations for the moments, it is necessary to express the production and flux terms as functions of the density moments. Generally, this is achieved by finding a relation between the moments and the distribution function. Finding this relation is called the *moment closure problem*.

3.1 Moment Closure

The system (1.8) involves more dependent variables than equations, hence it is not closed. In order to close the system, constitutive relations are needed to express the above densities $\langle f, \boldsymbol{\vartheta} \rangle$, fluxes $\langle f, \mathbf{v} \boldsymbol{\vartheta} \rangle$ and collisional terms $\langle \mathcal{C}(f), \boldsymbol{\vartheta} \rangle$ as a function of θ variables, thus forming a closed system. This can be done if there exists a function \mathbf{F} (and is made known) such that $f(t, \mathbf{x}, \mathbf{v}) = \mathbf{F}(\langle f, \boldsymbol{\vartheta} \rangle, \mathbf{v})$. Then the

flux terms $\langle f, \mathbf{v}\boldsymbol{\vartheta} \rangle$ and the collision terms $\langle \mathcal{C}(f), \boldsymbol{\vartheta} \rangle$ can be related to the densities $\langle \mathbf{F}, \boldsymbol{\vartheta} \rangle$ to provide a closed system of the form

$$\partial_t \langle \mathbf{F}, \boldsymbol{\vartheta} \rangle + \partial_{x_j} \langle \mathbf{F}, v_j \boldsymbol{\vartheta} \rangle = \langle \mathcal{C}(\mathbf{F}), \boldsymbol{\vartheta} \rangle \quad (1.9)$$

Note that f is an element of an infinite dimensional vector space and typically cannot be expressed by any finite number of components. Therefore, any closure will require the approximation of f . The goal then is to devise an approximation that, in addition to providing well-posedness of (1.9), maintains the key physical and mathematical features of (1.1). Thus, closure should yield a system such that [23]:

1. Every member of the hierarchy is hyperbolic and has an entropy extension, i.e. it should satisfy some local dissipation relation. Thus, the resulting equations are formally well posed.
2. Collisional terms are approximated such that each member of the hierarchy beyond the second recovers the proper Navier-Stokes approximation.

To attain such steps it would be required that [23]

- i. $\text{span}\{1, \mathbf{v}, |\mathbf{v}|^2\} \equiv \mathcal{C} \subseteq \Theta$:

In this condition, the collection of collision invariants \mathcal{C} is retained within Θ . More specifically, the constant functions are included in Θ so that any moment closure will include the conservation law for mass. It also includes multiples of the polynomial \mathbf{v} , which gives a balance law for momentum. Multiples of $|\mathbf{v}|^2$ give a balance law for the energy and $|\mathbf{v}|^2 \in \Theta$. This is needed if any fluid dynamical approximation is to be recovered.

- ii. Θ is invariant under actions of \mathcal{T}_u and \mathcal{T}_o :

More specifically, this means that Θ is unchanged when $\mathbf{v} \mapsto O^\top \mathbf{v}$ or $\mathbf{v} \mapsto \mathbf{v} - \mathbf{u}$, for every vector $\mathbf{u} \in \mathbb{R}^D$ and for every orthogonal matrix $O \in \mathbb{R}^{D \times D}$. This is a prerequisite of classical dynamics, in particular, that Galilean invariance holds.

- iii. The set $\Theta_c \equiv \{\boldsymbol{\vartheta} \in \Theta : \langle e^\boldsymbol{\vartheta}, 1 \rangle < \infty\}$ has a nonempty interior in Θ :

This requires, at a minimum, that Θ contain suitable functions to ensure integrability. Considering a subspace of polynomials, this condition would imply that the set Θ_c contains only polynomials $\boldsymbol{\vartheta}(\mathbf{v})$ for which $\boldsymbol{\vartheta}(\mathbf{v}) \rightarrow -\infty$ as $|\mathbf{v}| \rightarrow \infty$. This implies that condition *iii.* is satisfied only for linear subspaces of polynomials over \mathbf{v} with even maximal degree.

All subspaces that satisfy conditions *i-iii* will be called *admissible* and all other subspaces *inadmissible*. Examples of admissible subspaces with maximal degree two are

$$\begin{aligned} \Theta &= \text{span}\{1, \mathbf{v}, |\mathbf{v}|^2\} \equiv \mathcal{C} \\ \Theta &= \text{span}\{1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}\} \end{aligned} \quad (1.10)$$

and with maximal degree four

$$\begin{aligned} \Theta &= \text{span}\{1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, |\mathbf{v}|^2 v_i, |\mathbf{v}|^4\} \\ \Theta &= \text{span}\{1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v} \otimes \mathbf{v} \otimes \mathbf{v}, |\mathbf{v}|^4\} \\ \Theta &= \text{span}\{1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v} \otimes \mathbf{v} \otimes \mathbf{v}, |\mathbf{v}|^2 \mathbf{v} \otimes \mathbf{v}\} \\ \Theta &= \text{span}\{1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v} \otimes \mathbf{v} \otimes \mathbf{v}, \mathbf{v} \otimes \mathbf{v} \otimes \mathbf{v} \otimes \mathbf{v}\} \end{aligned} \quad (1.11)$$

Note that considering three spatial dimensions, the aforementioned subspaces in (1.10) and (1.11) are 5, 10, 14, 21, 26, and 35 dimensional, respectively.

4. Thesis Outline

In summary, Chapter 1 is a review of the basic properties of a generic kinetic system given by the Boltzmann equation (1.1). Moreover, the notion of moment systems and its application to the Boltzmann equation are introduced. Finally, the resulting moment closure problem is presented, thereby providing a general framework for the subsequent theory. The remainder of this work is organized as follows.

Chapter 2 presents the details of closing the moment system (1.9) using entropy minimization. The properties of the resulting system are analyzed in light of the aforementioned properties of the Boltzmann equation. More specifically, properties pertaining to well-posedness and entropy dissipation are investigated. Within this context, the issue of realizability is introduced as well as recent results that involve modifying the closure procedure in order to circumvent this problem.

Chapter 3 introduces an analytical approximation of the moment closure system based on a linearization procedure that results in mathematically tractable relations. The properties of this linearized system are investigated for the properties of the full moment closure system. More specifically, properties involving well-posedness and entropy-dissipation are investigated.

Chapter 4 considers a numerical approximation of the resulting moment closure systems in the discontinuous Galerkin (DG) finite element framework. Energy analysis is employed to show stability of a class of energy stable numerical flux functions which are introduced for the DG discretization.

Finally, Chapter 5 gives a concluding summary of the work and prospects for future studies.

Chapter 2

Entropy Minimization Closure

For a system of identical particles, Boltzmann [3–5] described the micro-state of the system by particle arrangements in phase space, and the macro-state by macroscopic properties of the system while proceeding to explain entropy probabilistically. He characterized entropy by describing its dependence on the number of micro-states that are consistent with the macro-state of the system. Boltzmann's celebrated H -Theorem infers equilibria as the minimizers of entropy [3, 6]. Mathematically, this relates equilibria to the dissipation of an entropy-based Lyapunov function. Such a characterization of equilibrium motivates a choice for approximating f [23].

Denote the entropy by $\mathcal{H} = \mathcal{H}(f) := \langle f, \ln f - 1 \rangle$, the entropy flux by $\phi_j = \phi_j(f) := \langle f, v_j(\ln f - 1) \rangle$ and a dissipation term by $\sigma = \sigma(f) := \langle \mathcal{E}(f), \ln f \rangle$. Moreover, note that $\mathcal{H}(f)$ is a strictly convex functional since the second (functional) derivative

$$\left. \frac{d^2}{d\epsilon^2} \mathcal{H}(f + \epsilon\psi) \right|_{\epsilon=0} = \left\langle \frac{\psi^2}{f} \right\rangle > 0 \quad (2.1)$$

for all functions ψ . Note that relation (1.4) implies that solutions of the Boltzmann equation (1.1) formally satisfy the local dissipation law corresponding to entropy dissipation

$$\partial_t \mathcal{H} + \partial_{x_j} \phi_j = \sigma \leq 0 \quad (2.2)$$

Levermore [23] described a way of specifying \mathbf{F} that closes the moment system as in (1.9) by utilizing entropy minimization. Levermore proceeded to show that entropy dissipation is still satisfied if f is replaced by the minimum entropy distribution \mathbf{F} , if it exists. Formally, \mathbf{F} is defined as the minimizer for the entropy minimization problem:

$$\arg \min_{g \in \mathcal{F}} \{ \mathcal{H}(g) : \langle g, \boldsymbol{\vartheta} \rangle = \boldsymbol{\rho} \} \quad (2.3)$$

where $\boldsymbol{\rho} := \langle f, \boldsymbol{\vartheta} \rangle$. From an approximation perspective, the minimizer \mathbf{F} for (2.3) (if it exists) can be interpreted as an entropic projection [16] in the sense that it is a projection of f , parametrized by $\boldsymbol{\rho}$, from the velocity space onto a finite-dimensional subspace, thus providing a candidate for \mathbf{F} that closes the system (1.8). Such a closure, provided by entropy minimization, is called an *entropy-based closure*. Later in this chapter, it will be shown that the resulting moment system retains important properties of Boltzmann equation.

The formal solution of (2.3) is obtained by constrained optimization using Lagrange multipliers. Denote the vector of Lagrange multipliers by ζ and consider the Lagrange function

$$\mathcal{L}(g, \zeta) := \mathcal{H}(g) + \zeta \cdot (\rho - \langle g, \vartheta \rangle) \quad (2.4)$$

Note that the Lagrange multipliers ζ are subject to optimality conditions such that they satisfy the moment constraints $\rho = \langle f_\zeta, \vartheta \rangle$. Denote the extrema by f_ζ , that is, where all directional derivatives vanish. Thus

$$\delta \mathcal{L}(f_\zeta, \zeta) = \ln f_\zeta - \zeta \cdot \vartheta = 0 \quad (2.5)$$

This implies that

$$f_\zeta = e^{\zeta \cdot \vartheta} \quad (2.6)$$

Junk [18] has shown that when Lagrange multipliers that satisfy the aforementioned optimality conditions exist, the minimum entropy problem in (2.3) exhibits a unique solution of the form (2.6). The entropy minimizing distribution (2.6) is used to attain moment closure for the system in (1.9),

$$\mathbf{F}(\rho, \mathbf{v}) = f_{\zeta(\rho)}(\mathbf{v}) \quad (2.7)$$

Furthermore, recalling requirement (iii) for admissible subspaces, the Lagrange multipliers ζ should allow integrability of the distribution (2.6). It follows that the set of ζ for which $e^{\zeta(\rho) \cdot \vartheta(\mathbf{v})}$ is integrable, denoted by \mathcal{I}_ϑ , can be expressed as

$$\mathcal{I}_\vartheta \equiv \{ \zeta \in \mathbb{R}^\theta : \vartheta e^{\zeta \cdot \vartheta} \in \mathbb{L}^1(\mathbb{R}^\theta) \} \quad (2.8)$$

that is to say, $\vartheta(\mathbf{v}) = \zeta \cdot \vartheta$ lies in Θ_c . Using the minimum entropy distribution, the moment system (1.8) can be closed:

$$\partial_t \langle \mathbf{F}(\rho, \mathbf{v}), \vartheta(\mathbf{v}) \rangle + \partial_{x_j} \langle \mathbf{F}(\rho, \mathbf{v}), v_j \vartheta(\mathbf{v}) \rangle = \langle \mathcal{C}(\mathbf{F}(\rho, \mathbf{v})), \vartheta(\mathbf{v}) \rangle \quad (2.9)$$

It is understood that $\mathbf{F} \in \mathcal{F}_\vartheta$ given by

$$\mathcal{F}_\vartheta := \{ g \in \mathcal{F} : \langle g, \vartheta \rangle = \rho \} \quad (2.10)$$

and that $\mathcal{F}_\vartheta \subset \mathcal{F}$.

The main deficiency of the aforementioned entropy-based closures is that for useful choices of the basis vector $\vartheta(\mathbf{v})$ (in the sense that $\{\vartheta_i\}_{i=1}^\theta$ span some admissible subspace), the set defined by densities corresponding to physically realizable values of ρ for which a minimizer for (2.3) does not exist, is non-void [17, 20]. Such densities are called *degenerate*. It is important to note, however, that this does not mean that the moment-closure system (2.9) with exponential closure is ill posed; it merely implies that the exponential closure can not be obtained as the solution of the entropy-minimization problem (2.3).

1. Galerkin Projection

Levermore's approach [23] can be conceived of as a Galerkin approximation of (1.1). It is performed in two steps [31]:

1. Projecting equation (1.1) onto a given polynomial space Θ yielding the system (1.8). The highest order fluxes in the resulting system of moment equations are not yet defined, thus, the moment system is not closed.

2. Projecting f (belonging to the velocity space) onto a finite dimensional subspace by solving the minimization problem (2.3). That is, the non-linear projection of f is of the form $e^{\zeta \cdot \vartheta}$ and the complete approximation of (1.1) is expressed in (2.9). Physically, this can be interpreted as closure through constitutive relations which express fluxes and collisions of highest order as functions of moments of lower order. In the case of using entropy minimization such relations are obtained under the assumption that the density function is close to a local equilibrium function.

Given a space \mathcal{V} of functions $\mathbb{R}^D \rightarrow \mathbb{R}_+$, denote by $\mathcal{W}(\Omega \times (0, T); \mathcal{V})$ a suitable class of functions from the spatial domain Ω and the temporal interval $(0, T)$ into \mathcal{V} . Similarly, $\mathcal{W}(\Omega; \mathcal{V})$ denotes a class of functions from Ω into \mathcal{V} . Moreover, denote by $\mathcal{P}^n(\mathbb{R}^D)$ the set of D -variate polynomials of degree at most n and let \mathcal{V}^n denote a polynomial subspace such that $\mathcal{C} \subseteq \mathcal{V}^n \subseteq \mathcal{P}^n(\mathbb{R}^D)$, $n \geq 2$. Levermore's moment closure approximation of the Boltzmann equation can be written as

$$g \in \mathcal{W}(\Omega \times (0, T); \mathcal{V}^n) : \quad \partial_t \langle e^g, \psi \rangle + \partial_{x_j} \langle v_j e^g, \psi \rangle - \langle \mathcal{C}(e^g), \psi \rangle = 0 \\ \forall \psi \in \mathcal{W}(\Omega; \mathcal{V}^n), \text{ a.e. } t \in (0, T) \quad (2.11)$$

Equation (2.11) expresses Levermore's moment closure system from the perspective of a Galerkin approximation. Equation (2.11) reduces to equation (2.9) when $\mathcal{V}^n \equiv \Theta$ and noting that $\vartheta_i \in \mathcal{W}(\Omega; \Theta)$.

Remark. Another way to perceive the Galerkin approximation, is that (2.11) can be conceived of as a Galerkin projection of the renormalized Boltzmann equation conforming to $f = e^g$.

2. Entropy-based Moment Closure System: Properties

This section investigates the properties of the resulting entropy-based moment closure system (2.9). More specifically, it will be shown that system (2.9) is well-posed and that it retains the fundamental properties of the Boltzmann equation (1.1). In particular, it will be shown that

1. The moment closure system (2.9) is a symmetric hyperbolic system.
2. Solutions of the moment closure system (2.9) satisfy the dissipation relation (2.2).
3. Equality in the dissipation relation (2.2) is attained if and only if \mathbf{F} is an equilibrium density given by (1.5), i.e. $\mathcal{C}(\mathbf{F}) = 0$

Note that the moment closure system (2.9) retains conservation of mass, momentum and energy (collision invariance) as well as Galilean invariance since the finite linear subspace Θ is admissible.

2.1 Well-Posedness: Symmetric Hyperbolic System

Using the Einstein summation convention, consider a generic quasi-linear first order system of the type

$$A_0(\mathbf{u})\partial_t \mathbf{u} + A_i(\mathbf{u})\partial_{x_i} \mathbf{u} = \mathbf{f}(\mathbf{u}) \quad (2.12)$$

for the unknown m -column vector $\mathbf{u}(x, t) : \mathbf{u} \equiv (u_1, u_2, \dots, u_m)^\top$; $\mathbf{x} \in \mathbb{R}^n$; A_0, A_i are real $m \times m$ matrices which are functions of \mathbf{u} ; the source term $\mathbf{f}(\mathbf{u})$ is vector in \mathbb{R}^m ; $i = 1, 2, \dots, n$. By denoting the time t with x^0 it is possible to write the system in abbreviated form

$$A_\alpha(\mathbf{u})\partial_\alpha \mathbf{u} = \mathbf{f}(\mathbf{u}) \quad (\alpha = 0, 1, \dots, n) \quad (2.13)$$

For each $y \in \mathbb{R}^n$, set

$$A(\mathbf{x}, t; \mathbf{y}) := \sum_{j=1}^n y_j A_j \quad (x \in \mathbb{R}^n, t \geq 0) \quad (2.14)$$

DEFINITION 2.1 (Hyperbolicity). *The system (2.12) is hyperbolic if the matrix A_0 is invertible and the matrix A is diagonalizable for each $x, y \in \mathbb{R}^n$, $t \geq 0$*

DEFINITION 2.2 (Symmetric Hyperbolic Systems). *The system (2.12) is said to be symmetric hyperbolic if*

1. ${}^\alpha A = ({}^\alpha A)^\top$
2. ${}^0 A$ is positive definite

Remark. For hyperbolic systems, the corresponding Cauchy initial value problem is well posed [14], at least for finite time.

Equation (2.9) can be rewritten using the chain rule as

$$\langle \mathbf{F}, \boldsymbol{\vartheta} \boldsymbol{\vartheta}^\top \rangle \partial_t \boldsymbol{\zeta} + \langle \mathbf{F}, v_j \boldsymbol{\vartheta} \boldsymbol{\vartheta}^\top \rangle \partial_{x_j} \boldsymbol{\zeta} = \langle \mathcal{C}(\mathbf{F}), \boldsymbol{\vartheta} \rangle \quad (2.15)$$

The symmetry of the coefficient matrices is clear and thus, the first requirement of definition 2.2 is satisfied. The second requirement follows from the fact that for every $\boldsymbol{\gamma} \in \mathbb{R}^\theta$

$$\boldsymbol{\gamma}^\top \langle \mathbf{F}, \boldsymbol{\vartheta} \boldsymbol{\vartheta}^\top \rangle \boldsymbol{\gamma} = \langle \mathbf{F}, (\boldsymbol{\gamma} \cdot \boldsymbol{\vartheta})^2 \rangle \geq 0 \quad (2.16)$$

with the equality attained if and only if $\boldsymbol{\gamma} = 0$. Thus, the moment closure system (2.9) is a symmetric hyperbolic system.

2.2 Entropy Dissipation

Levermore [23] showed the existence of a convex entropy extension that is locally dissipated by multiplying (2.20) from the left by $\boldsymbol{\zeta}^\top$, yielding

$$\partial_t \langle \mathbf{F}, \boldsymbol{\zeta}^\top \boldsymbol{\vartheta} - 1 \rangle + \partial_{x_j} \langle \mathbf{F}, v_j (\boldsymbol{\zeta}^\top \boldsymbol{\vartheta} - 1) \rangle = \langle \mathcal{C}(\mathbf{F}), \boldsymbol{\zeta}^\top \boldsymbol{\vartheta} \rangle \quad (2.17)$$

Recalling that $\boldsymbol{\zeta}^\top \boldsymbol{\vartheta} = \ln \mathbf{F}$, equation (2.17) reads

$$\partial_t \langle \mathbf{F}, \ln \mathbf{F} - 1 \rangle + \partial_{x_j} \langle \mathbf{F}, v_j (\ln \mathbf{F} - 1) \rangle = \langle \mathcal{C}(\mathbf{F}), \ln \mathbf{F} \rangle \leq 0 \quad (2.18)$$

which is equivalent to the convex entropy extension expressed in equation (2.2) when evaluated at $f = \mathbf{F}$. Hence, the system (2.9) possesses a convex entropy extension expressed in (2.18). It is worthy to note that it is an assumption that an entropy pair $\{\mathcal{H}(\mathbf{F}(\boldsymbol{\rho}; \mathbf{v})), \phi(\mathbf{F}(\boldsymbol{\rho}; \mathbf{v}))\}$ exists such that the entropy inequality (2.18) holds. Implicit to this assumption, is that a solution to the entropy minimization problem (2.3) exists.

Remark. In light of the Galerkin projection relation in (2.11), a similar argument could be made when noting that $\ln \mathbf{F} = \boldsymbol{\zeta}^\top \boldsymbol{\vartheta} - 1$ resides in the test space of equation (2.11). Consequently setting $\psi = \boldsymbol{\zeta}^\top \boldsymbol{\vartheta} - 1$ in (2.11) yields

$$\partial_t \langle \mathbf{F}, \ln \mathbf{F} - 1 \rangle + \partial_{x_j} \langle \mathbf{F}, v_j (\ln \mathbf{F} - 1) \rangle = \langle \mathcal{C}(\mathbf{F}), \ln \mathbf{F} - 1 \rangle \quad (2.19)$$

Recalling collision invariance properties expressed in (1.4), equation (2.19) reduces to (2.18). Thus, there exists a convex entropy extension to the system (2.11), given by (2.18), that is locally dissipated which is obtained by choosing a suitable test function from the test space (in this case $\ln \mathbf{F} - 1$).

3. Realizability and the Domain of Definition of Levermore's Moment Closure System

Levermore's moment closure system, as discussed previously, retains the structural features of the Boltzmann equation and exhibits hyperbolicity for each member of the hierarchy implying well-posedness. These desirable properties all stem from the assumption that the minimum entropy distribution for a set of velocity moments given by the optimization problem (2.3) always exists. Junk [18–20], however, has shown that for any moment system that include super-quadratic polynomial moments the set containing all degenerate densities, i.e. for which a minimum entropy distribution function cannot be found, is non-empty. Moreover, the densities describing local thermodynamic equilibrium, given by Maxwellian distribution (1.5), always lies on the boundary of the set containing all degenerate densities.

This deficiency reveals a fundamental problem if weight functions of fourth (or higher) order are used. To explain this problem, consider the example given by Junk [20] for the 14-moment case. The minimum entropy distribution function has the structure

$$\mathbf{F}(\boldsymbol{\rho}, \mathbf{v}) = e^{\boldsymbol{\zeta}(\boldsymbol{\rho}) \cdot \boldsymbol{\vartheta}(\mathbf{v})} = e^{\zeta + \zeta_i v_i + \zeta_{ij} v_i v_j + \bar{\zeta}_i |\mathbf{v}|^2 v_i + \zeta_{14} |\mathbf{v}|^4} \quad (2.20)$$

Obviously, this distribution function is only integrable if either $\zeta_{14} < 0$ or if $\zeta_{14} = \bar{\zeta}_i = 0$ and ζ_{ij} is negative definite. Recall the set $\mathcal{I}_{\boldsymbol{\vartheta}}$ in (2.8) of $\boldsymbol{\zeta}$ for which $e^{\boldsymbol{\zeta}(\boldsymbol{\rho}) \cdot \boldsymbol{\vartheta}(\mathbf{v})}$ is integrable. The physical equilibrium states of the gas are given by Maxwellian states (1.5) which are of the form (2.20) with

$$\begin{aligned} \zeta^{\#} &= \ln \frac{\varrho}{(s\pi\eta)^{\frac{3}{2}}} - \frac{|\mathbf{u}|}{2\eta} \\ \zeta_i^{\#} &= \frac{u_i}{\eta} \\ \zeta_{ij}^{\#} &= -\frac{1}{2\eta} \delta_{ij} \\ \bar{\zeta}_i^{\#} &= \zeta_{14}^{\#} = 0 \end{aligned} \quad (2.21)$$

These states belong to $\partial\mathcal{I}_{\boldsymbol{\vartheta}}$ because any small deviation $\boldsymbol{\zeta}$ from $\boldsymbol{\zeta}^{\#}$ with $\zeta_{14} > 0$ does not belong to $\mathcal{I}_{\boldsymbol{\vartheta}}$. As a consequence, the equilibrium moments $\boldsymbol{\rho}^{\#}$ from the set

$$\mathcal{U}_{\boldsymbol{\vartheta}}^{\#} = \left\{ \left\langle \varrho (2\pi\eta)^{-\frac{d}{2}} e^{-\frac{|\mathbf{v}-\mathbf{u}|}{2\eta}}, \boldsymbol{\vartheta} \right\rangle : \varrho, T > 0, \mathbf{u} \in \mathbb{R}^{\theta} \right\} \quad (2.22)$$

are also on the boundary of the state space

$$\mathcal{U}_{\boldsymbol{\vartheta}} = \{ \langle e^{\boldsymbol{\zeta} \cdot \boldsymbol{\vartheta}}, \boldsymbol{\vartheta} \rangle : \boldsymbol{\zeta} \in \mathcal{I}_{\boldsymbol{\vartheta}} \} \quad (2.23)$$

which is the domain of definition of equation (2.9). In most practical applications, there are regions in the physical space where states are close to equilibrium. Hence, $\boldsymbol{\rho}(t, \mathbf{x})$ is at least very close to $\partial\mathcal{U}_{\boldsymbol{\vartheta}}$ for a certain t and \mathbf{x} . Junk [20] goes on to show that equilibrium states on the boundary $\partial\mathcal{U}_{\boldsymbol{\vartheta}}$ always appear when the set of weight functions contains functions with super-quadratic growth at infinity. Finally, Junk [20] concludes that Galilean invariance dictates the use of polynomials as weight functions, while on the other hand polynomial weight functions with super-quadratic growth at infinity lead to non-convexity of the state space (domain of definition) and the equilibrium states are located on the boundary.

In summary, it has been argued [18, 20] that there are indeed functions f whose moments cannot be realized by any exponential function, that is, for no value of $\boldsymbol{\zeta} \in \mathbb{R}^{\theta}$ does

$$\langle e^{\boldsymbol{\zeta} \cdot \boldsymbol{\vartheta}}, \boldsymbol{\vartheta} \rangle = \langle f, \boldsymbol{\vartheta} \rangle \quad (2.24)$$

Thus, the constraints of the minimization problem (2.3) can not be satisfied

Remark. It is proved in [27] that kinetic closures based on entropy minimization are formally equivalent to the systems derived from extended thermodynamics. Recall the minimization problem (2.3); if the minimizer exists, and if \mathcal{H} is differentiable at the solution, the standard Lagrange multiplier theory yields relation (2.7). However, this issue of non-realizability leads one to question whether entropy minimization is equivalent to extended thermodynamics (see Appendix 1). The problem is that the extended thermodynamic approach assumes the existence of an entropy minimizing distribution explicitly provided by the minimizer of \mathcal{H} , which is not always the case.

The issue of existence of the minimizing entropy distribution (or equivalently, the corresponding Lagrange multipliers) was studied by Hauck *et. al.* [17], Schneider [31] and Pavan [29]. In what follows, their results [17, 29, 31] are merely presented. Their proofs are not discussed since that is well beyond the scope of this work.

An important result concerning the existence of a minimizer for (2.3) is summarized as follows. Recalling the set \mathcal{F} in (1.7), let \mathcal{R}_ϑ denote the set of realizable densities expressed as

$$\mathcal{R}_\vartheta := \{\boldsymbol{\rho} \in \mathbb{R}^\theta : \boldsymbol{\rho} = \langle g, \vartheta \rangle, g \in \mathcal{F}_\vartheta\} \quad (2.25)$$

Denote the set of degenerate densities

$$\mathcal{D}_\vartheta := \{\boldsymbol{\rho} \in \mathcal{R}_\vartheta : \text{the minimizer in (2.3) does not exist}\} \quad (2.26)$$

and recall the definition of the set \mathcal{I}_ϑ in (2.8)

THEOREM 2.3 (Hauck *et. al.* [17]). *The set \mathcal{D}_ϑ is empty if and only if \mathcal{I}_ϑ is open.*

This means that if \mathcal{I}_ϑ is open, then for any realizable moment $\boldsymbol{\rho} \in \mathcal{R}_\vartheta(\Omega)$ the full constraints problem (2.3) admits a unique minimizer which reads

$$\exists \zeta \in \mathcal{I}_\vartheta : \mathbf{F} = e^{\zeta \cdot \vartheta} \quad (2.27)$$

Such a result is also obtained by Pavan ([29], Theorem 1). Hauck *et. al.* continue to explain that \mathcal{I}_ϑ is only open when the moment closure equation (2.9) includes velocity moments of polynomials of, at most, second degree. Otherwise, for velocity moments of super-quadratic polynomials, \mathcal{I}_ϑ is not open. This can be seen in light of the aforementioned example in (2.20)–(2.23), one need only realize that for cases in which velocity moments of super-quadratic polynomials are included, the vector $\zeta \in \mathcal{I}_\vartheta$ corresponding to any Maxwellian \mathcal{M} lying on the boundary $\partial\mathcal{I}_\vartheta$.

4. Modified Minimization Problem

In degenerate situations, the entropy-based closure will not be well defined. Consider two suggestions to address this issue [17]:

1. Ensure that values corresponding to degenerate densities will never be attained by the moment system generated by the entropy closure. One can either
 - (a) show that the set of densities for which (2.3) does have a solution is invariant under the dynamics of the moment system, or,
 - (b) impose this condition in a way that is physically reasonable and mathematically justifiable.
2. Develop a modified approach that
 - (a) agrees with the minimum entropy approach for well-posed cases of (2.3)
 - (b) produces closures that generate symmetric hyperbolic systems that dissipate a physically meaningful entropy.

Previous studies of (2.3) can be found in [17–19, 31], where the entropy minimization problem is altered in an attempt to handle the ill-posed cases. In [19] the problem is redefined by replacing the minimum in (2.3) with an infimum,

$$\arg \inf_g \{\mathcal{H}(g) : \langle g, \vartheta \rangle = \rho\} \quad (2.28)$$

This was done to include cases where the minimizer in (2.3) does not exist. While in [31], the problem is rewritten as

$$\arg \inf_g \{\mathcal{H}(g) : \langle g, \vartheta \rangle \preceq^* \rho\} \quad (2.29)$$

where \preceq^* roughly means that inequalities between certain components are allowed. To further elaborate the latter problem, first recall that condition (iii) for admissible subspaces implies that Θ contains polynomials of even maximal degree to ensure the decay necessary for integrability. Hence, for an even $\theta = 2p$, where p is some integer, one has that $\vartheta_\theta(\mathbf{v}) = \mathbf{v}^{2p}$. Moreover, let $\rho := (\rho_1, \rho_2, \dots, \rho_\theta)$. Define the set

$$\mathcal{F}_\vartheta^{\text{relax}} := \{g \in \mathcal{F} : \forall j < \theta = 2p, \langle g, \vartheta_j \rangle = \rho_j, \langle g, \mathbf{v}^{2p} \rangle \leq \rho_{2p}\} \quad (2.30)$$

The relaxed problem in (2.29) can be rewritten as

$$\arg \inf_{g(\zeta) \in \mathcal{F}_\vartheta^{\text{relax}}} \mathcal{H}(g) \quad (2.31)$$

Hauck *et al.* [17] analyzed the relationship between problems in (2.28) and (2.29) in detail by applying a dual formulation to (2.29) based on the theory of convex optimization. He has shown that (2.28) and (2.29) are equivalent, i.e., that the respective infima are equal. Schneider [31] and Pavan [29] show that the relaxed minimization problem exhibits a unique solution, corresponding to the exponential distribution. Such a result is summarized as follows

THEOREM 2.4 (Pavan [29], Schneider [31]). *The relaxed problem (2.31) admits a unique solution that reads*

$$\exists \zeta \in \mathcal{I}_\vartheta : \quad \mathbf{F} = e^{\zeta \cdot \vartheta} \quad (2.32)$$

It can be shown [17, 29, 31] that the minimizer of (2.28) is also the unique minimizer of (2.3) whenever (2.3) has a minimum. This was summarized by Hauck [16] in the following result. Recalling the set \mathcal{I}_ϑ in (2.8), denote by $\mathcal{R}_\vartheta^{\text{exp}}$ the set of exponentially realizable densities,

$$\mathcal{R}_\vartheta^{\text{exp}} := \{\rho \in \mathbb{R}^\theta : \rho = \langle e^{\zeta \cdot \vartheta}, \vartheta \rangle, \zeta \in \mathcal{I}_\vartheta\} \quad (2.33)$$

It is clear that $\mathcal{R}_\vartheta^{\text{exp}} \subset \mathcal{R}_\vartheta$.

COROLLARY 2.5 (Hauck [16]). *The infimum in (2.28) is a minimum if and only if $\rho \in \mathcal{R}_\vartheta^{\text{exp}}$. Thus (2.3) has a solution if and only if $\rho \in \mathcal{R}_\vartheta^{\text{exp}}$.*

In summary, the exponential closure is retained when the closure procedure is modified in such a way that the constraints of the minimization problem are relaxed. Pavan [29] employs these results to construct a moment closure system that, as opposed to Levermore's system [23], restricts the problem to a hierarchy in the basis such that a minimizer always exists for the entropy minimization problem. This can be done by checking the condition in theorem 2.3 for each moment system in the hierarchy and assigning the corresponding minimization problem to it such that a minimizer always exists for each member of the hierarchy. Finally, Pavan [29] checks that all properties of Levermore's moment closure system [23] are recovered.

Chapter 3

Analytical Approximation of the Moment Closure System

Any numerical approximation to the moment closure system (2.9) would require the evaluation of the density, flux and collision terms which, in turn, involve evaluating moments of exponentials of polynomials of, in principle, arbitrary order. It is generally accepted that the derivation of closed-form expressions for such moments is intractable, and accurate approximation of the moments is a notoriously difficult problem [22]. The problem can be circumvented by numerical integration. However, in that case, the hyperbolic systems engendered by the moment closure approximation are not explicitly available, which impedes both their analysis, and the development of advanced numerical techniques. Moreover, within the context of numerical schemes, numerical integration is generally computationally intensive. This chapter investigates the novelty of this work: a tractable system approximating the moment closure system (2.9) constructed by an approximation of the minimum entropy distribution.

1. Approximation of Collision Operator

So far the collision operator was dealt with in abstract terms using properties described in section 1.1, that is, no explicit expression was used. Following Levermore [23], this section develops a generalized B.G.K. operator \mathcal{C} to approximate the collision operator \mathcal{C} .

Recall the definition, given in section 1.2.1, characterizing an admissible subspace Θ with basis vectors $\{\vartheta^i\}_{i=1}^\theta \in \mathcal{V}$ and let, for convenience, $\Theta_0 := \mathcal{C} \equiv \text{span}\{1, \mathbf{v}, |\mathbf{v}|^2\}$. Consider any finite sequence of subspaces $\{\Theta_k\}_{k=0}^K$ ordered by strict inclusion and strictly contained within Θ , i.e.

$$\Theta_0 \subsetneq \Theta_1 \subsetneq \dots \subsetneq \Theta_K \subsetneq \Theta \quad (3.1)$$

For each k , let $\{\vartheta_{(k)}^i\}_{i=0}^\theta \in \mathcal{V}_{(k)}$ form a basis for Θ_k and let $\boldsymbol{\rho}_{(k)} := \langle f, \boldsymbol{\vartheta}_{(k)} \rangle$. The entropic projection of f with respect to \mathcal{V} is defined by the entropy minimizing distribution, denoted by $\mathbf{F}_f := \mathbf{F}(f; \mathcal{V})$. Furthermore, let $\mathbf{F}_f^k := \mathbf{F}(f; \mathcal{V}_{(k)})$ be the entropic projection of f with respect to $\mathcal{V}_{(k)}$ defined as the solution of

$$\arg \min_{g(\zeta_{(k)})} \{ \mathcal{H}(g) : \langle g, \boldsymbol{\vartheta}_{(k)} \rangle = \boldsymbol{\rho}_{(k)} \} \quad (3.2)$$

where $\zeta_{(k)} \in \mathbb{R}^\theta$ is uniquely determined by the constraints. Assuming the solution exists, it would be given by $e^{\zeta_{(k)} \cdot \boldsymbol{\vartheta}_{(k)}}$ where $\zeta_{(k)} \cdot \boldsymbol{\vartheta}_{(k)} \in \Theta_k$. Using the sequence of entropic projections $\{\mathbf{F}_f^k\}_{k=0}^K$, a

multistage relaxation operator $\tilde{\mathcal{E}}$ approximating the collision operator \mathcal{E} is defined as

$$\tilde{\mathcal{E}}(f) = -\nu_K(f - \mathbf{F}_f^K) - \sum_{k=0}^{K-1} \nu_k(\mathbf{F}_f^{k+1} - \mathbf{F}_f^k) \quad (3.3)$$

where $\{\nu_k\}_{k=0}^K$ is an increasing sequence of positive relaxation rates depending on $\boldsymbol{\rho}_{(k)}$. Note that ν_k is the rate at which \mathbf{F}_f^{k+1} relaxes to \mathbf{F}_f^k and ν_K is the rate at which f relaxes to \mathbf{F}_f^K . Moreover, (3.3) can be re-written as

$$\tilde{\mathcal{E}}(f) = - \sum_{k=0}^K \eta_k (f - \mathbf{F}_f^k), \quad (3.4)$$

where $\eta_k = \nu_k - \nu_{k-1}$ and setting $\nu_{-1} = 0$.

1.1 Note on Realizability

In order to circumvent the realizability problem it is important to ensure that an entropy minimizer is attained for every member of the hierarchy. Following Pavan [29], this can be done by considering the following cases

- If $\boldsymbol{\vartheta}_{(k)}$ is such that the corresponding $\mathcal{I}_{\boldsymbol{\vartheta}}$ is open, then consider the full minimization problem;
- If $\boldsymbol{\vartheta}_{(k)}$ is such that the corresponding $\mathcal{I}_{\boldsymbol{\vartheta}}$ is not open, then consider the relaxed minimization problem given by

$$\arg \inf_{g(\boldsymbol{\zeta}_{(k)}) \in \mathcal{F}_{\boldsymbol{\vartheta}_{(k)}}^{\text{relax}}} \mathcal{H}(g) \quad (3.5)$$

This guarantees that for every member of the hierarchy a solution to the corresponding optimization problem exists such that exponential closure is attained.

1.2 Properties of the Generalized B.G.K. Operator

It remains to check whether the approximate generalized B.G.K. operator $\tilde{\mathcal{E}}$ satisfies the properties assumed for the full collision operator \mathcal{E} in section 1.1:

1. Entropy Dissipation: H-Theorem

Note that from the constrains of (3.2) it follows that $\forall \boldsymbol{\vartheta}_{(k)} \in \boldsymbol{\Theta}_k$, $\langle \mathbf{F}_f^k - f, \boldsymbol{\vartheta}_{(k)} \rangle = 0$. It follows that since $\ln \mathbf{F}_f^k \in \boldsymbol{\Theta}_k$, $\langle \tilde{\mathcal{E}}(f), \ln \mathbf{F}_f^k \rangle = 0$. Consider the relation

$$\begin{aligned} \langle \tilde{\mathcal{E}}(f), \ln f \rangle &= \sum_{k=1}^K \eta_k \langle \mathbf{F}_f^k - f, \ln f \rangle \\ &= \sum_{k=1}^K \eta_k \left\langle \mathbf{F}_f^k - f, \ln \frac{f}{\mathbf{F}_f^k} \right\rangle \leq 0 \end{aligned} \quad (3.6)$$

where, in the last step, the fact that $\forall y, z \in \mathbb{R}$, $(z - y) \ln \frac{z}{y} \geq 0$ was used, where equality is attained if and only if $z = y$. If one would consider the relaxed minimization problem (3.5), the conditions imposed by the set $\mathcal{F}_{\boldsymbol{\vartheta}}^{\text{relax}}$ would change the argument slightly: $\forall \boldsymbol{\vartheta}_{(k)} \in \boldsymbol{\Theta}_k$, $\langle \mathbf{F}_f^k - f, \boldsymbol{\vartheta}_{(k)} \rangle \geq 0$, it follows that since $\ln \mathbf{F}_f^k \in \boldsymbol{\Theta}_k$, $\langle \tilde{\mathcal{E}}(f), \ln \mathbf{F}_f^k \rangle \geq 0$. Consequently,

$$\begin{aligned} \langle \tilde{\mathcal{E}}(f), \ln f \rangle &= \sum_{k=1}^K \eta_k \langle \mathbf{F}_f^k - f, \ln f \rangle \\ &\leq \sum_{k=1}^K \eta_k \left\langle \mathbf{F}_f^k - f, \ln \frac{f}{\mathbf{F}_f^k} \right\rangle \leq 0 \end{aligned} \quad (3.7)$$

and a similar result is obtained. Thus, $\tilde{\mathcal{E}}(f)$ satisfies the H -Theorem. In addition, from (3.7) it follows that for any entropic projection \mathbf{F}_f^k

$$\left\langle \tilde{\mathcal{E}}(f), \ln \frac{f}{\mathbf{F}_f^k} \right\rangle \leq 0 \quad (3.8)$$

2. Conservation: Mass, Momentum and Energy

From the constrains of (3.2) or the conditions imposed by (3.5) for problems involving super-quadratic moments of velocity, it can be seen that each term in the sum in (3.4) employs $\gamma \in \{1, \mathbf{v}, |\mathbf{v}|^2\}$ as locally conserved quantities. Thus, $\tilde{\mathcal{E}}(f)$ satisfies the local conservation law

$$\langle \tilde{\mathcal{E}}(f), \gamma \rangle = 0 \quad (3.9)$$

As each term of the sum in (3.6) or (3.7) is non-positive, the only way the sum can vanish is if each term vanishes. This will happen if and only if the $k = 1$ term vanishes because in that case one must have $f = \mathcal{M}$, which would imply all the other terms would also vanish. This implies that the only locally conserved quantities are those in the collection of collision invariants $\mathcal{C} \equiv \text{span}\{1, \mathbf{v}, |\mathbf{v}|^2\}$, thereby establishing the equivalence between the following statements

- (a) $\langle \tilde{\mathcal{E}}(f), g \rangle = 0$
- (b) $g \in \mathcal{C} \equiv \text{span}\{1, \mathbf{v}, |\mathbf{v}|^2\}$

3. Galilean Invariance

Finally, the translational and rotational symmetries follow for each term in the sum (3.6) from the fact that, being admissible, each $\Theta_{(k)}$ is Galilean invariant.

2. Modified Kinetic System

This section introduces a novel tractable system that approximates Levermore's moment closure system in (2.9) by applying an approximation to the entropy minimizing distribution. The resulting approximate system is checked for the structural properties of Levermore's moment closure system, more specifically, properties pertaining to well-posedness and entropy dissipation.

Recalling the entropy minimizing distribution given by (2.6), an entropic projection \mathcal{E} of the same exponential form can be factorized such that the entropy minimizing distribution can be rewritten as

$$\mathbf{F} = \mathcal{E}(\zeta_0) e^{(\zeta - \zeta_0) \cdot \vartheta} \quad (3.10)$$

More specifically, \mathcal{E} could be an entropic projection corresponding to the global equilibrium distribution \mathcal{E}_g or the local equilibrium distribution \mathcal{E}_l (for example, the equilibrium solutions of the 5-moment or the 10-moment system) and ζ_0 the corresponding vector of (known) Lagrange multipliers.

2.1 Approximation of Moment Closure

In this section the minimum entropy system is linearized in an attempt to approximate the integrals with closed form expressions. For ease of exposition consider 1-dimensional exponential densities of the form

$$\tilde{f}(\boldsymbol{\eta}) = e^{\boldsymbol{\eta}^\top \cdot \mathbf{x}} = e^{\eta_0 + \eta_1 x^1 + \dots + \eta_{2k} x^{2k}} \quad (3.11)$$

where for $k \in \mathbb{N}$

$$\boldsymbol{\eta} = [\eta_0, \eta_1, \dots, \eta_{2k}]^\top \quad (3.12)$$

$$\mathbf{x} = [x^0, x^1, \dots, x^{2k}]^\top \quad (3.13)$$

Define moments of order i of the exponential density in (3.11) by

$$M_i(\boldsymbol{\eta}) := \int_{-\infty}^{\infty} x^i e^{\boldsymbol{\eta}^\top \cdot \boldsymbol{x}} dx \quad (3.14)$$

Furthermore, let the known $\boldsymbol{\eta}_0$ correspond to some special case for which the moment $M_i(\boldsymbol{\eta}_0)$ is known. Inserting the power series definition of the exponential into $\tilde{f}(\boldsymbol{\eta})$, there holds

$$\tilde{f}(\boldsymbol{\eta}) = e^{\boldsymbol{\eta}_0^\top \cdot \boldsymbol{x}} \sum_{n=0}^{\infty} \frac{1}{n!} [\boldsymbol{x} \cdot (\boldsymbol{\eta} - \boldsymbol{\eta}_0)]^n \quad (3.15)$$

Furthermore, from (3.15) it follows that an unknown moment corresponding to some $\boldsymbol{\eta}_1$ can be expressed as

$$M_i(\boldsymbol{\eta}_1) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} x^i e^{\boldsymbol{\eta}_0^\top \cdot \boldsymbol{x}} [\boldsymbol{x} \cdot (\boldsymbol{\eta}_1 - \boldsymbol{\eta}_0)]^n dx \quad (3.16)$$

Note that the integrations involved in (3.16) are just higher order moments of the exponential density corresponding to $\boldsymbol{\eta}_0$. More specifically, if Gaussian densities are considered to correspond to $\boldsymbol{\eta}_0$, these integrals can be seen as higher order moments of Gaussian integrals. Such moments are computable (see Appendix II).

Applying the expansion in (3.15) to the minimum entropy (3.10) and denoting the approximation to the minimum entropy corresponding to the truncated series expansion by $\tilde{\mathbf{F}}$, gives

$$\begin{aligned} \tilde{\mathbf{F}}(\boldsymbol{\zeta}_1) &= e^{\boldsymbol{\zeta}_0^\top \cdot \boldsymbol{\vartheta}} \sum_{n=0}^N \frac{1}{n!} [\boldsymbol{\vartheta} \cdot (\boldsymbol{\zeta} - \boldsymbol{\zeta}_0)]^n \\ &=: \mathcal{E}[1 + \tilde{F}(\boldsymbol{\zeta}_1)] \end{aligned} \quad (3.17)$$

where $\boldsymbol{\zeta}_1$ represents the unknown Lagrange multipliers and $\boldsymbol{\zeta}_0$ are those of the corresponding equilibrium distribution. Applying the approximation in (3.16) to the minimum entropy system in (2.9) yields an approximation of the closed minimum entropy system :

$$\partial_t \langle \mathcal{E}(1 + \tilde{F}), \boldsymbol{\vartheta} \rangle + \partial_{x_j} \langle \mathcal{E}(1 + \tilde{F}), v_j \boldsymbol{\vartheta} \rangle = \langle \mathcal{L}(\mathcal{E}[1 + \tilde{F}]), \boldsymbol{\vartheta} \rangle \quad (3.18)$$

Introducing the generalized B.G.K. operator in (3.3) to the approximated system (3.18)

$$\partial_t \langle \mathcal{E}(1 + \tilde{F}), \boldsymbol{\vartheta} \rangle + \partial_{x_j} \langle \mathcal{E}(1 + \tilde{F}), v_j \boldsymbol{\vartheta} \rangle = \langle \tilde{\mathcal{L}}(\mathcal{E}[1 + \tilde{F}]), \boldsymbol{\vartheta} \rangle \quad (3.19)$$

It still remains to check whether the approximated moment closure system (3.19) exhibits entropy dissipation and hyperbolicity, as did Levermore's moment closure system. In section 2.2 the entropy dissipation property of (3.19) is considered. Section 2.3 is concerned with the symmetric hyperbolic structure of (3.19).

2.2 Entropy Dissipation

This section investigates the entropy dissipation of the approximate moment closure system resulting from linearization about some equilibrium distribution. Recall the entropy minimizing distribution given by \mathbf{F} in (2.7) and note that $\ln \mathbf{F} = \boldsymbol{\zeta} \cdot \boldsymbol{\vartheta}$, similarly $\ln \mathcal{E} = \boldsymbol{\zeta}_0 \cdot \boldsymbol{\vartheta}$. Truncating the series in (3.17) at $N = 2$ yields

$$\begin{aligned} \tilde{F}(\boldsymbol{\zeta}) &= (\boldsymbol{\zeta} - \boldsymbol{\zeta}_0) \cdot \boldsymbol{\vartheta} + \frac{1}{2} [(\boldsymbol{\zeta} - \boldsymbol{\zeta}_0) \cdot \boldsymbol{\vartheta}]^2 \\ &= \ln \frac{\mathbf{F}}{\mathcal{E}} + \frac{1}{2} \left[\ln \frac{\mathbf{F}}{\mathcal{E}} \right]^2 \end{aligned} \quad (3.20)$$

This implies that

$$(\zeta - \zeta_0) \cdot \vartheta = \ln \frac{F}{\mathcal{E}} = \sqrt{2\tilde{F} + 1} - 1 \quad (3.21)$$

Noting the inverse relationship between $\ln x$ and e^x , the motivation behind the choice of this solution and ignoring $-\sqrt{2\tilde{F} + 1}$, is that the former captures an approximation of that inverse property while the latter solution does not. The entropy density for the linearized moment closure system can be rewritten as

$$\tilde{\mathcal{H}}(\tilde{F}) := \left\langle \mathcal{E}(1 + \tilde{F}), \ln \frac{F}{\mathcal{E}} \right\rangle = \left\langle \mathcal{E}(1 + \tilde{F}), \sqrt{2\tilde{F} + 1} - 1 \right\rangle \quad (3.22)$$

Note that $\min_{(\zeta - \zeta_0) \cdot \vartheta} \tilde{F} = -\frac{1}{2}$ and that the second (functional) derivative

$$\left. \frac{d^2}{d\epsilon^2} \tilde{\mathcal{H}}(\tilde{F} + \epsilon\psi) \right|_{\epsilon=0} = \left\langle -\frac{\mathcal{E}\psi^2(1 + \tilde{F})}{(1 + 2\tilde{F})^{3/2}} + \frac{2\mathcal{E}\psi^2}{\sqrt{1 + 2\tilde{F}}} \right\rangle > 0 \quad (3.23)$$

for all functions ϕ , thus, $\tilde{\mathcal{H}}$ is strictly convex. Using the inequality in (3.8) and in light of the Galerkin projection description in (2.11) of the moment closure system, noting that $\ln \frac{F}{\mathcal{E}} = (\zeta - \zeta_0) \cdot \vartheta \in \mathcal{W}(\Omega; \Theta)$, the space of (polynomial) test functions, one has that

$$\partial_t \langle \mathcal{E}(1 + \tilde{F}), (\zeta - \zeta_0) \cdot \vartheta \rangle + \partial_{x_j} \langle \mathcal{E}(1 + \tilde{F}), v_j (\zeta - \zeta_0) \cdot \vartheta \rangle = \langle \tilde{\mathcal{E}}(\mathcal{E}[1 + \tilde{F}]), (\zeta - \zeta_0) \cdot \vartheta \rangle \leq 0 \quad (3.24)$$

Thus, (3.22) provides an auxiliary convex entropy density to the moment system (3.19) that dissipates locally as in (3.24). Note that no distinction was made in this section between global and local equilibrium because showing entropy dissipation for a moment system linearized about either of them follows in a fashion similar to what was previously shown. In other words, the moment system (3.19) written in terms of a global or local equilibrium solution also posses (3.24) as a convex entropy extension that is locally dissipated.

2.3 Symmetry and Hyperbolicity

This section investigates the symmetric hyperbolicity of the approximate moment closure system resulting from linearization about either a global or local equilibrium distribution. With regard to showing symmetric hyperbolicity, distinction will be made between local and global equilibrium since the procedure differs slightly. In section 2.3.1 a moment closure system resulting from linearization about a global equilibrium distribution is considered. Section 2.3.2 is concerned with a moment closure system resulting from linearization about a local equilibrium distribution.

2.3.1 Linearization about Global Equilibrium

This section investigates symmetric hyperbolicity of a moment closure system resulting from linearization about a global equilibrium distribution. Rewriting equation (3.19) in terms of a global equilibrium solution gives

$$\partial_t \langle \mathcal{E}_g(1 + \tilde{F}), \vartheta \rangle + \partial_{x_j} \langle \mathcal{E}_g(1 + \tilde{F}), v_j \vartheta \rangle = \langle \tilde{\mathcal{E}}(\mathcal{E}_g[1 + \tilde{F}]), \vartheta \rangle \quad (3.25)$$

The approximated moment system (3.25) can be recast (using the chain rule) into the form of (2.12) by rewriting it such that

$$\langle \mathcal{E}_g \partial_\zeta \tilde{F}, \vartheta \rangle \partial_t \zeta + \langle \mathcal{E}_g \partial_\zeta \tilde{F}, v_j \vartheta \rangle \partial_{x_j} \zeta = \langle \tilde{\mathcal{E}}(\mathcal{E}_g[1 + \tilde{F}]), \vartheta \rangle \quad (3.26)$$

where from (3.20) one has that

$$\partial_\zeta \tilde{F} = [1 + (\zeta - \zeta_0) \cdot \vartheta] \vartheta^\top \quad (3.27)$$

Thus,

$$\langle \mathcal{E}_g[1 + (\zeta - \zeta_0) \cdot \vartheta], \vartheta \vartheta^\top \rangle \partial_t \zeta + \langle \mathcal{E}_g[1 + (\zeta - \zeta_0) \cdot \vartheta], v_j \vartheta \vartheta^\top \rangle \partial_{x_j} \zeta = \langle \tilde{\mathcal{E}}(\mathcal{E}_g[1 + \tilde{F}]), \vartheta \rangle \quad (3.28)$$

The symmetry of system (3.28) is clear.

Remark. Note that the term $[1 + (\zeta - \zeta_0) \cdot \vartheta]$ appearing in the coefficient matrices of the derivatives of ζ is always non-negative. This can be seen from the fact that solutions of the moment system (3.25) should satisfy (3.21) (and hence, the local dissipation relation (3.24)). In other words, given an initial condition in which ζ satisfies (3.21), the evolution of ζ should satisfy (3.21). In contrast to solutions of Levermore's system, the fact that the solutions of the linearized system should satisfy (3.21) can be conceived of as a restriction of the solution space to some ζ such that (3.24) is satisfied.

It remains to investigate the second requirement in definition 2.2. For any $\gamma \in \mathbb{R}^\theta$ one has that

$$\gamma^\top \langle \mathcal{E}_g[1 + (\zeta - \zeta_0) \cdot \vartheta], \vartheta \vartheta^\top \rangle \gamma = \langle \mathcal{E}_g[1 + (\zeta - \zeta_0) \cdot \vartheta], (\gamma \cdot \vartheta)^2 \rangle \geq 0 \quad (3.29)$$

where equality is attained if and only if $\gamma = \mathbf{0}$ or $\zeta \cdot \vartheta = \zeta_0 \cdot \vartheta - 1$. In the latter case, ζ follows from the known ζ_0 corresponding to global equilibrium, thus, the system becomes trivial. Therefore, the approximate moment closure system (3.28) is symmetric hyperbolic.

2.3.2 Linearization about Local Equilibrium

This section investigates symmetric hyperbolicity of a moment closure system resulting from linearization about a local equilibrium distribution. Rewriting equation (3.19) in terms of a local equilibrium solution gives

$$\partial_t \langle \mathcal{E}_l(1 + \tilde{F}), \vartheta \rangle + \partial_{x_j} \langle \mathcal{E}_l(1 + \tilde{F}), v_j \vartheta \rangle = \langle \tilde{\mathcal{E}}(\mathcal{E}_l[1 + \tilde{F}]), \vartheta \rangle \quad (3.30)$$

The approximated moment system (3.30) can be recast (using the chain rule) into the form of (2.12):

$$\begin{aligned} & \langle \mathcal{E}_l \partial_\zeta \tilde{F}, \vartheta \rangle \partial_t \zeta + \langle \mathcal{E}_l \partial_\zeta \tilde{F}, v_j \vartheta \rangle \partial_{x_j} \zeta \\ &= \langle \tilde{\mathcal{E}}(\mathcal{E}_l[1 + \tilde{F}]), \vartheta \rangle - \langle (1 + F) \partial_{\zeta_0} \mathcal{E}_l, \vartheta \rangle \partial_t \zeta_0 - \langle (1 + F) \partial_{\zeta_0} \mathcal{E}_l, v_j \vartheta \rangle \partial_{x_j} \zeta_0 \end{aligned} \quad (3.31)$$

where from (3.20) one has that

$$\partial_\zeta \tilde{F} = [1 + (\zeta - \zeta_0) \cdot \vartheta] \vartheta^\top \quad (3.32)$$

Thus,

$$\begin{aligned} & \langle \mathcal{E}_l[1 + (\zeta - \zeta_0) \cdot \vartheta], \vartheta \vartheta^\top \rangle \partial_t \zeta + \langle \mathcal{E}_l[1 + (\zeta - \zeta_0) \cdot \vartheta], v_j \vartheta \vartheta^\top \rangle \partial_{x_j} \zeta \\ &+ \langle (1 + F) \partial_{\zeta_0} \mathcal{E}_l, \vartheta \rangle \partial_t \zeta_0 + \langle (1 + F) \partial_{\zeta_0} \mathcal{E}_l, v_j \vartheta \rangle \partial_{x_j} \zeta_0 \\ &= \langle \tilde{\mathcal{E}}(\mathcal{E}_l[1 + \tilde{F}]), \vartheta \rangle \end{aligned} \quad (3.33)$$

The symmetry of system (3.33) is clear.

Remark. Note that the term $[1 + (\zeta - \zeta_0) \cdot \vartheta]$ appearing in the coefficient matrices of the derivatives of ζ is always non-negative. This can be seen from the fact that solutions of the moment system (3.30) should satisfy (3.21) (and hence, satisfying the local dissipation relation (3.24)). In other words, given an initial condition in which ζ satisfies (3.21), the evolution of ζ should satisfy (3.21). In contrast to solutions of Levermore's system, the fact that the solutions of the linearized system should satisfy (3.21) can be conceived of as a restriction of the solution space to some ζ such that (3.24) is satisfied.

It remains to investigate the second requirement in definition 2.2. For any $\gamma \in \mathbb{R}^\theta$ one has that

$$\gamma^\top \langle \mathcal{E}_l [1 + (\zeta - \zeta_0) \cdot \vartheta], \vartheta \vartheta^\top \rangle \gamma = \langle \mathcal{E}_l [1 + (\zeta - \zeta_0) \cdot \vartheta], (\gamma \cdot \vartheta)^2 \rangle \geq 0 \quad (3.34)$$

where equality is attained if and only if $\gamma = \mathbf{0}$ or $\zeta \cdot \vartheta = \zeta_0 \cdot \vartheta - 1$. In the latter case ζ is no longer an unknown since it follows from the known Lagrange multipliers ζ_0 corresponding to equilibrium, thus, the system becomes trivial. Therefore, the approximate moment closure system (3.33) is symmetric hyperbolic.

Remark. An interesting observation about (3.33) relates to the derivatives of ζ_0 that appear. The contribution of these terms can be perceived as source/sink terms. Since it is not known whether these terms act as sources or sinks, it maybe that the solutions blow up in the limit $t \rightarrow \infty$. Hence, any claim about well-posedness may only make sense in finite time.

2.4 Linearization about a Gaussian Distribution

More generally, \mathcal{E} in (3.19) could also correspond to a general Gaussian distribution form, denoted by \mathcal{G} , such that the vector of Lagrange multipliers ζ_0 remain unknown. Moreover, the definition of \tilde{F} changes slightly. This section investigates the properties of the approximate moment closure system resulting from linearization about a Gaussian distribution \mathcal{G} where the corresponding vector of Lagrange multipliers ζ_0 remains as part of the approximation. More specifically, properties pertaining to entropy dissipation and hyperbolicity are studied. It has been noted that Grad's moment closure can be perceived as a first order linearization of the Levermore's exponential closure [32].

2.4.1 Approximation of Minimum Entropy

For ease of exposition consider 1-dimensional exponential densities of the form

$$\tilde{f}(\boldsymbol{\eta}) = e^{\boldsymbol{\eta} \cdot \mathbf{x}} = e^{\eta_0 + \eta_1 x^1 + \dots + \eta_{2k} x^{2k}} \quad (3.35)$$

where for $k \in \mathbb{N}$

$$\boldsymbol{\eta} = [\eta_0, \eta_1, \dots, \eta_{2k}]^\top \quad (3.36)$$

$$\mathbf{x} = [x^0, x^1, \dots, x^{2k}]^\top \quad (3.37)$$

Let $\boldsymbol{\eta}_0$, \mathbf{x}_0 and $\boldsymbol{\eta}_1$, \mathbf{x}_1 be defined such that for $l \in \mathbb{N}$ and $l < k$

$$\begin{aligned} \boldsymbol{\eta}_0 &= [\eta_0, \eta_1, \dots, \eta_{2l}]^\top \\ \mathbf{x}_0 &= [x^0, x^1, \dots, x^{2l}]^\top \\ \boldsymbol{\eta}_1 &= [\eta_{2l+1}, \eta_{2l+2}, \dots, \eta_{2k}]^\top \\ \mathbf{x}_1 &= [x^{2l+1}, x^{2l+2}, \dots, x^{2k}]^\top \end{aligned} \quad (3.38)$$

This implies that $\boldsymbol{\eta} = [\boldsymbol{\eta}_0, \boldsymbol{\eta}_1]$ and $\mathbf{x} = [\mathbf{x}_0, \mathbf{x}_1]$. Thus, (3.35) can be rewritten as

$$\tilde{f}(\boldsymbol{\eta}) = e^{\boldsymbol{\eta}_0 \cdot \mathbf{x}_0} e^{\boldsymbol{\eta}_1 \cdot \mathbf{x}_1} \quad (3.39)$$

Define moments of order i of the exponential density in (3.36) by

$$M_i(\boldsymbol{\eta}) = \int_{-\infty}^{\infty} x^i e^{\boldsymbol{\eta} \cdot \mathbf{x}} dx \quad (3.40)$$

Furthermore, let $\boldsymbol{\eta}_0$ correspond to some special case for which the moment $M_i(\boldsymbol{\eta}_0)$ is known, more specifically it could correspond to some Gaussian distribution \mathcal{G} . Invoking the power series definition

of the exponential onto the second term in $\tilde{f}(\boldsymbol{\eta})$ in (3.39), gives

$$\tilde{f}(\boldsymbol{\eta}) = e^{\boldsymbol{\eta}_0 \cdot \mathbf{x}} \sum_{n=0}^{\infty} \frac{1}{n!} (\mathbf{x} \cdot \boldsymbol{\eta}_1)^n \quad (3.41)$$

Furthermore, from (3.41) it follows that an unknown moment corresponding to some $\boldsymbol{\eta}_1$ can be expressed

$$\begin{aligned} M_i(\boldsymbol{\eta}) &= \int_{-\infty}^{\infty} x^i e^{\boldsymbol{\eta}_0 \cdot \mathbf{x}} \sum_{n=0}^{\infty} \frac{1}{n!} x^n \boldsymbol{\eta}_1^n dx \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \left[\int_{-\infty}^{\infty} x^i x^n e^{\boldsymbol{\eta}_0^\top \cdot \mathbf{x}} dx \right]^\top \boldsymbol{\eta}_1^n \end{aligned} \quad (3.42)$$

Note that the integrations involved in (3.42) are just higher order moments of the exponential density corresponding to $\boldsymbol{\eta}_0$. More specifically, if the Gaussian densities are considered to correspond to $\boldsymbol{\eta}_0$, these integrals can be seen as higher order moments of Gaussian integrals. Such moments are computable (see Appendix II).

Applying the expansion in (3.41) to the minimum entropy (2.7) and denoting the approximation to the minimum entropy corresponding to the truncated series expansion by $\tilde{\mathbf{F}}$, gives

$$\begin{aligned} \tilde{\mathbf{F}}(\boldsymbol{\zeta}) &= e^{\boldsymbol{\zeta}_0 \cdot \boldsymbol{\vartheta}_0} \sum_{n=0}^N \frac{1}{n!} (\boldsymbol{\vartheta}_1 \cdot \boldsymbol{\zeta}_1)^n \\ &=: \mathcal{G}(\boldsymbol{\zeta}_0)[1 + \tilde{F}(\boldsymbol{\zeta}_1)] \end{aligned} \quad (3.43)$$

where $\boldsymbol{\zeta} = [\boldsymbol{\zeta}_0, \boldsymbol{\zeta}_1]^\top$. Note that $\boldsymbol{\zeta}$ represents all the unknown Lagrange multipliers and $\boldsymbol{\zeta}_0$ are those unknown Lagrange multipliers corresponding to some Gaussian distribution \mathcal{G} . Applying the expansion in (3.43) to the minimum entropy system in (2.9) yields the approximated moment closure system

$$\partial_t \langle \mathcal{G}(1 + \tilde{F}), \boldsymbol{\vartheta} \rangle + \partial_{x_j} \langle \mathcal{G}(1 + \tilde{F}), \mathbf{v}_j \boldsymbol{\vartheta} \rangle = \langle \mathcal{C}(\mathcal{G}[1 + F]), \boldsymbol{\vartheta} \rangle \quad (3.44)$$

Introducing the generalized B.G.K. operator in (3.3) to the approximated system yields

$$\partial_t \langle \mathcal{G}(1 + \tilde{F}), \boldsymbol{\vartheta} \rangle + \partial_{x_j} \langle \mathcal{G}(1 + \tilde{F}), \mathbf{v}_j \boldsymbol{\vartheta} \rangle = \langle \tilde{\mathcal{C}}(\mathcal{G}[1 + F]), \boldsymbol{\vartheta} \rangle \quad (3.45)$$

2.4.2 Entropy Dissipation

Recall the entropy minimizing distribution given by \mathbf{F} in (2.7) and note that $\ln \mathbf{F} = \boldsymbol{\zeta} \cdot \boldsymbol{\vartheta} = \boldsymbol{\zeta}_0 \cdot \boldsymbol{\vartheta}_0 + \boldsymbol{\zeta}_1 \cdot \boldsymbol{\vartheta}_1$, similarly $\ln \mathcal{G} = \boldsymbol{\zeta}_0 \cdot \boldsymbol{\vartheta}_0$. Truncating the series in (3.17) at $N = 2$ yields

$$\begin{aligned} \tilde{F}(\boldsymbol{\zeta}_1) &= \boldsymbol{\zeta}_1 \cdot \boldsymbol{\vartheta}_1 + \frac{1}{2} (\boldsymbol{\zeta}_1 \cdot \boldsymbol{\vartheta}_1)^2 \\ &= \ln \frac{\mathbf{F}}{\mathcal{G}} + \frac{1}{2} \left[\ln \frac{\mathbf{F}}{\mathcal{G}} \right]^2 \end{aligned} \quad (3.46)$$

This implies that

$$\ln \frac{\mathbf{F}}{\mathcal{G}} = \sqrt{2\tilde{F} + 1} - 1 \quad (3.47)$$

The entropy density for the approximate moment closure system can be rewritten as

$$\tilde{\mathcal{H}}(\tilde{F}) := \left\langle \mathcal{G}(1 + \tilde{F}), \ln \frac{\mathbf{F}}{\mathcal{G}} \right\rangle = \left\langle \mathcal{G}(1 + \tilde{F}), \sqrt{2\tilde{F} + 1} - 1 \right\rangle \quad (3.48)$$

Note that the $\min_{\zeta_1 \cdot \vartheta_1} \tilde{F} = -\frac{1}{2}$ and that the second (functional) derivative

$$\frac{d^2}{d\epsilon^2} \tilde{\mathcal{H}}(\tilde{F} + \epsilon\psi) \Big|_{\epsilon=0} = \left\langle -\frac{\mathcal{G}\psi^2(1 + \tilde{F})}{(1 + 2\tilde{F})^{3/2}} + \frac{2\mathcal{G}\psi^2}{\sqrt{1 + 2\tilde{F}}} \right\rangle > 0 \quad (3.49)$$

Thus, $\tilde{\mathcal{H}}$ is strictly convex. Using the inequality in (3.8) and in light of the Galerkin projection description in (2.11) of the moment closure system, noting that $\ln \frac{F}{\mathcal{G}} = \zeta_1 \cdot \vartheta_1 \in \mathcal{W}(\Omega; \Theta)$, the space of (polynomial) test functions, one has that

$$\partial_t \langle \mathcal{G}(1 + \tilde{F}), \zeta_1 \cdot \vartheta_1 \rangle + \partial_{x_j} \langle \mathcal{G}(1 + \tilde{F}), v_j \zeta_1 \cdot \vartheta_1 \rangle = \langle \tilde{\mathcal{C}}(\mathcal{G}[1 + \tilde{F}]), \zeta_1 \cdot \vartheta_1 \rangle \leq 0 \quad (3.50)$$

Thus, there exists an auxiliary entropy to the moment system (3.45) that is locally dissipated.

2.4.3 Symmetry and Hyperbolicity

The approximated moment system (3.45) can be recast (using the chain rule) into the form of (2.12) by rewriting it such that

$$\mathcal{A}_0 \partial_t \zeta + \mathcal{A}_j \partial_{x_j} \zeta = \langle \tilde{\mathcal{C}}(\mathcal{G}[1 + \tilde{F}]), \vartheta \rangle \quad (3.51)$$

where

$$\begin{aligned} \mathcal{A}_0 &= \begin{pmatrix} \langle \mathcal{G}(1 + \tilde{F}), \vartheta_0 \vartheta_0^\top \rangle & \langle \mathcal{G}(1 + \zeta_1 \cdot \vartheta_1), \vartheta_0 \vartheta_1^\top \rangle \\ \langle \mathcal{G}(1 + \tilde{F}), \vartheta_1 \vartheta_0^\top \rangle & \langle \mathcal{G}(1 + \zeta_1 \cdot \vartheta_1), \vartheta_1 \vartheta_1^\top \rangle \end{pmatrix} \\ \mathcal{A}_j &= \begin{pmatrix} \langle \mathcal{G}(1 + \tilde{F}), v_j \vartheta_0 \vartheta_0^\top \rangle & \langle \mathcal{G}(1 + \zeta_1 \cdot \vartheta_1), v_j \vartheta_0 \vartheta_1^\top \rangle \\ \langle \mathcal{G}(1 + \tilde{F}), v_j \vartheta_1 \vartheta_0^\top \rangle & \langle \mathcal{G}(1 + \zeta_1 \cdot \vartheta_1), v_j \vartheta_1 \vartheta_1^\top \rangle \end{pmatrix} \end{aligned} \quad (3.52)$$

The symmetry of system (3.51) is lost. Note that at equilibrium i.e. $\zeta_1 = \mathbf{0}$ and thus $\tilde{F} = 0$, symmetry is retained, but is no longer guaranteed at any deviation from equilibrium.

With regard to the positive definiteness of \mathcal{A}_0 , a similar result is obtained. For any $\gamma \in \mathbb{R}^\theta$, rewritten such that $\gamma = \{\gamma_0, \gamma_1\}$, consider

$$\begin{aligned} & \begin{pmatrix} \gamma_0^\top & \gamma_1^\top \end{pmatrix} \begin{pmatrix} \langle \mathcal{G}(1 + \tilde{F}), \vartheta_0 \vartheta_0^\top \rangle & \langle \mathcal{G}(1 + \zeta_1 \cdot \vartheta_1), \vartheta_0 \vartheta_1^\top \rangle \\ \langle \mathcal{G}(1 + \tilde{F}), \vartheta_1 \vartheta_0^\top \rangle & \langle \mathcal{G}(1 + \zeta_1 \cdot \vartheta_1), \vartheta_1 \vartheta_1^\top \rangle \end{pmatrix} \begin{pmatrix} \gamma_0 \\ \gamma_1 \end{pmatrix} \\ & \equiv \langle (\gamma_0^\top \vartheta_0)^2 \mathcal{G}(1 + \tilde{F}) \rangle + \langle (\gamma_1^\top \vartheta_1)^2 \mathcal{G} \rangle + \gamma_1^\top \langle (1 + \vartheta_1^\top \zeta_1) \vartheta_1 \vartheta_0^\top \mathcal{G} \rangle \gamma_0 + \gamma_0^\top \langle \mathcal{G} \vartheta_0 \vartheta_1^\top (1 + \vartheta_1^\top \zeta_1) \rangle \gamma_1 \end{aligned} \quad (3.53)$$

The positive definiteness of system (3.51) is lost. Note that at equilibrium i.e. $\zeta_1 = \mathbf{0}$ and thus $\tilde{F} = 0$, positive definiteness is retained, but is no longer guaranteed at any deviation from equilibrium.

2.4.4 Concluding Remarks

Consequently, it can be shown that at equilibrium a symmetric hyperbolicity is recovered, but it is not guaranteed at any deviation from equilibrium. It is worthy to note at this point that well-posedness of Cauchy's initial value problem is not only implied for symmetric hyperbolic systems, but also for all hyperbolic systems, i.e. systems with real and distinct characteristics. However, investigating the requirement of distinctness of the characteristics can be difficult task [14] and requires further investigation beyond the scope of this work. Brown [8] performed an eigensystem analysis for the Levermore's 10-moment system and showed that the system is hyperbolic. Note that the approximate system (3.45) could be conceived as a perturbative expansion about the Gaussian distribution which, in fact, corresponds to the entropy minimizing distribution of the 10-moment system. Thus, heuristically, one might expect (3.45) to be hyperbolic for, at least, some finite region in phase-space. However, this hypothesis is subject to criticism and needs further investigation.

Chapter 4

Numerical Approximation: Discontinuous Galerkin

The previous chapters conveyed that the relaxed minimization problem (2.31) yields an exponential closure that retains the structural features of Levermore's moment closure system without suffering from the realizability problem. Moreover, it was shown that the resulting moment closure system is symmetric hyperbolic, which implies well posedness of Cauchy's initial value problem (at least, for finite time). Furthermore, for moment closure systems that consider super-quadratic velocity polynomials, approximate systems were derived to obtain a tractable system with closed form expressions of the integrals. It was seen that these derived approximate systems retain the structural features of Levermore's moment closure pertaining to well-posedness and entropy dissipation. This chapter aims at developing a numerical approximation to Cauchy's initial value problem corresponding to the aforementioned moment closure systems using the discontinuous Galerkin method. This chapter is an extension to the work of Barth [1] aimed at developing a numerical approximation to the developed tractable moment system (3.18).

Any of the aforementioned moment closure systems, (Levermore's system in (2.9) or linearized approximations to it about an equilibrium solution (3.19)), can be recast into the form

$$\partial_t \boldsymbol{\rho} + \partial_{x_j} \mathcal{J}_j(\boldsymbol{\rho}) - \mathcal{Q}(\boldsymbol{\rho}) = 0 \quad (4.1)$$

where $\boldsymbol{\rho}$ is the corresponding density, \mathcal{J}_j corresponds to flux and $\mathcal{Q}(\boldsymbol{\rho})$ corresponds to the collision term. For example, for Levermore's system,

$$\boldsymbol{\rho} := \langle \mathbf{F}(\boldsymbol{\rho}, \mathbf{v}), \boldsymbol{\vartheta}(\mathbf{v}) \rangle, \quad \mathcal{J}_j := \langle \mathbf{F}(\boldsymbol{\rho}, \mathbf{v}), v_j \boldsymbol{\vartheta}(\mathbf{v}) \rangle, \quad \mathcal{Q} := \langle \mathcal{C}(\mathbf{F}(\boldsymbol{\rho}, \mathbf{v})), \boldsymbol{\vartheta}(\mathbf{v}) \rangle \quad (4.2)$$

Moreover, any of the corresponding convex entropy extensions can be recast into the form given by equation (2.2). Following Barth [1], it is assumed that the considered spatial domain is either periodic in all space dimensions or non-periodic with compactly supported initial data. This is done in order to deliberately avoid complications arising from analysis of the boundary conditions.

1. Finite Element Approximation

This section develops finite element meshes, i.e. substructures of an approximation space, and the consequent finite element approximation that will be used in order to apply the discontinuous Galerkin method.

Consider a family of finite element meshes denoted by $\{\tau_h\}_{h>0}$, parametrized by the strictly positive mesh parameter h , each consisting of n simplices of maximum diameter h covering the spatial domain Ω . In other words, $\{\tau_h\}_{h>0}$ partitions the space domain Ω into elemental domains denoted by κ . Denote the diameter of a simplex $\kappa \in \tau_h$ by h_κ and the diameter of the largest inscribed hypersphere by r_κ . That is,

$$\forall \kappa \in \tau_h, h_\kappa = \text{diam}(\kappa) = \max_{x_1, x_2 \in \kappa} \|x_1 - x_2\|_D \quad (4.3)$$

where $\|\cdot\|_D$ is the Euclidean norm in \mathbb{R}^D . The parameter h is given by

$$h = \max_{\kappa \in \tau_h} h_\kappa \quad (4.4)$$

DEFINITION 4.1 (Shape-regularity). *A family of meshes $\{\tau_h\}_{h>0}$ is said to be regular if there exists a constant \bar{c} such that for all h*

$$\forall \kappa \in \tau_h \quad \bar{c}_\kappa := \frac{h_\kappa}{r_\kappa} \leq \bar{c} \quad (4.5)$$

Remark. [13] The motivation behind imposing the regularity condition can be understood within the context of a 2-dimensional example as follows: let κ be a triangle and denote by θ_κ the smallest of its angles. It can be shown that

$$\frac{h_\kappa}{r_\kappa} \leq \frac{2}{\sin \theta_\kappa} \quad (4.6)$$

Therefore, for a shape-regular family of triangulations, the triangles are restricted from becoming too flat as $h \rightarrow 0$.

In addition, let $\{\tau_h\}_{h>0}$ be a shape-regular family of meshes of the spatial domain Ω . Assume (for simplicity) that Ω is composed of stationary non-overlapping elements κ :

- $\bar{\Omega} \equiv \bigcup_{\kappa \in \tau_h} \kappa$.
- $\kappa_i \cap \kappa_j = \emptyset, \quad i \neq j$
- $\partial \mathcal{K}_h \equiv \bigcup_{\kappa \in \tau_h} \partial \kappa$.

Let $\mathcal{P}^k(Q)$ denote the set of polynomials of degree at most $k \geq 0$ in a domain $Q \subset \mathbb{R}^D$. Employing the discontinuous Galerkin method, the following finite element space is introduced

$$\mathcal{V}_h = \{ \mathbf{w} : \forall \kappa \in \tau_h, \mathbf{w}|_\kappa \in [\mathcal{P}^k]^\theta \} \quad (4.7)$$

Thus, the approximating functions are polynomials from \mathcal{V}^h . Note that \mathcal{V}^h contains piecewise discontinuous polynomials (with no continuity requirement across inter-element boundaries).

2. Space-Time Discontinuous Galerkin

This section describes the the space-time discontinuous Galerkin formulation of Cauchy's initial value problem corresponding to (4.1) in the context of the aforementioned finite element approximation. The space-time discontinuous Galerkin method considers a setting that does not distinguish between

space and time variables [13]. Consider an element κ and let $\bar{\mathbf{n}}$ denote the exterior unit normal to its boundary. Introduce the following notation: for some $\mathbf{g} = \mathbf{g}(\mathbf{y})$, let $\mathbf{g}_\pm := \lim_{\varepsilon \rightarrow 0} \mathbf{g}(\mathbf{y} \pm \varepsilon \bar{\mathbf{n}})$.

DEFINITION 4.2 (Quasi-uniformity). *A family of meshes $\{\tau_h\}_{h>0}$ is said to be quasi-uniform if and only if it is shape-regular and there exists a \underline{c} such that for all h*

$$\forall \kappa \in \tau_h, \quad h_\kappa \geq \underline{c}h \quad (4.8)$$

Consider the partitioning of the time interval $[t^0, t^N]$ by an ordered series of $(N + 1)$ time levels $t^0 < t^1 < \dots < t^N$ and let

- the time interval $I^n := [t_+^n, t_-^{n+1}]$
- $\mathcal{I} = \{I^n\}_{0 \leq n \leq N-1}$ be a quasi-uniform mesh of $]t^0, t^N[$

Remark. [13] The motivation for assuming quasi-uniformity can be seen as follows: let

$$\Delta t_{\min} := \min_{0 \leq n < N} |t^{n+1} - t^n|, \quad \Delta t_{\max} := \max_{0 \leq n \leq N-1} (t^{n+1} - t^n) \quad (4.9)$$

The quasi-uniformity of \mathcal{I} implies that there is a c such that

$$\Delta t_{\max} \leq \frac{\Delta t_{\min}}{c} \quad (4.10)$$

Relation (4.10) can be conceived as a CFL condition.

Employing a space-time discontinuous Galerkin formulation, define $\mathcal{V}_{h,I^n}^k = [\mathcal{P}^k(I^n; \mathcal{V}_h)]^\theta$ and introduce the following finite element space

$$\mathcal{V}_{h,\mathcal{I}}^k = \{\mathbf{w} : \forall I^n \in \mathcal{I}, \mathbf{w}|_{I^n} \in \mathcal{V}_{h,I^n}^k\} \quad (4.11)$$

Complementing equation (4.1) with an initial condition to set up Cauchy's initial value problem

$$\mathcal{P} \begin{cases} \partial_t \boldsymbol{\rho} + \partial_{x_j} \mathcal{J}_j(\boldsymbol{\rho}) = \mathcal{Q}(\boldsymbol{\rho}), & \Omega \times]t^0, t^N[\\ \boldsymbol{\rho}(\zeta(\mathbf{x}, t_-^0)) = \boldsymbol{\rho}_0(\mathbf{x}) \end{cases} \quad (4.12)$$

supplemented with the convex entropy extension of the form given by equation (2.2). The problem statement for the strong form of the differential equations (4.12):

$$\text{Find } \zeta(\mathbf{x}, t) \text{ such that (4.12) is satisfied } \forall \mathbf{x} \in \Omega \text{ and } \forall t \in [t_+^n, t_-^{n+1}] \quad (4.13)$$

In order to obtain the weak formulation, the following consecutive consistent reformulations of (4.12) are considered:

1. multiplication by a test function $\mathbf{w}_h \in \mathcal{V}_{h,\mathcal{I}}^k$
2. integrate over space and time
3. replace integrals over space and time with summation over space-time slabs $\kappa \times I^n$
4. perform integration by parts
5. weakly enforce continuity of the density across the time interface
6. substitute \mathcal{J}_j with a numerical flux $\tilde{\mathcal{J}}_j$ that posses the following properties:

- (a) **Discrete cell conservation:** This property ensures that fluxes from adjacent cells sharing a mutual interface exactly cancel when summed. This is achieved if the numerical flux satisfies

$$\tilde{\mathcal{J}}(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) = -\tilde{\mathcal{J}}(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); -\mathbf{n}) \quad (4.14)$$

- (b) **Consistency:** Consistency is obtained if the numerical flux with identical state arguments reduces to the true total flux passing through an element interface of that same state, i.e.

$$\tilde{\mathcal{J}}(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) = \mathcal{J}(\zeta) \cdot \mathbf{n} \quad (4.15)$$

Consider the bilinear form

$$\begin{aligned} a_h(\mathbf{u}, \mathbf{w}) &= \sum_{n=0}^{N-1} \sum_{\kappa \in \tau_h} \int_{I^n} \int_{\kappa} -[\boldsymbol{\rho}(\mathbf{u}) \cdot \partial_t \mathbf{w} + \mathcal{J}_j(\mathbf{u}) \cdot \partial_{x_j} \mathbf{w}] \quad dx \, dt \\ &+ \sum_{n=0}^{N-1} \sum_{\kappa \in \tau_h} \int_{I^n} \int_{\partial \kappa} \mathbf{w}(\mathbf{x}_-) \cdot \tilde{\mathcal{J}}(\mathbf{u}(\mathbf{x}_-), \mathbf{u}(\mathbf{x}_+); \mathbf{n}) \quad ds \, dt \\ &+ \sum_{n=0}^{N-1} \sum_{\kappa \in \tau_h} \int_{I^n} \int_{\kappa} [\mathbf{w}(t_-^{n+1}) \cdot \boldsymbol{\rho}(\mathbf{u}(t_-^{n+1})) - \mathbf{w}(t_+^n) \cdot \boldsymbol{\rho}(\mathbf{u}(t_+^n))] \quad dx \\ &- \sum_{n=0}^{N-1} \sum_{\kappa \in \tau_h} \int_{I^n} \int_{\kappa} \mathcal{Q}(\boldsymbol{\rho}) \cdot \mathbf{w} \end{aligned} \quad (4.16)$$

The weak formulation of (4.12):

$$\text{Find } \zeta_h(\mathbf{x}, t) \in \mathcal{V}_{h,\mathcal{I}}^k \text{ such that : } \quad a_h(\zeta_h, \mathbf{w}) = 0 \quad \forall \mathbf{w} \in \mathcal{V}_{h,\mathcal{I}}^k \quad (4.17)$$

Remark. Note that a solution along the element edge can not be uniquely determined because continuity restriction along an edge is not enforced in a discontinuous Galerkin method. As a consequence of the independence of local spaces, the solution along edges can not be uniquely determined because it may be discontinuous. Thus, the flux across an inter-element edge depends on $\boldsymbol{\rho}$ across the interface. Furthermore, wave interaction takes place at the discontinuity along an element edge, this situation can be conceived as a Riemann problem. This suggests that $\tilde{\mathcal{J}}(\zeta_h(\mathbf{x}_-), \zeta_h(\mathbf{x}_+); \mathbf{n})$ can be perceived as an approximate Riemann solver that numerically approximates the interface-flux along an element edge

3. Nonlinear Stability: Entropy and Energy Analysis

The entropy inequality (2.2) is necessary in order to single out a unique, physically relevant solution among the possibly many weak solutions of (4.12). Weak solutions of (4.12), which in addition satisfy the inequality (2.2) for all entropy pairs (\mathcal{H}, ϕ) connected with that system, are called entropy solutions. In fact, the notion of nonlinear stability is strongly related to entropy dissipation. Physically, such a relation stems from the minimum entropy postulate at which the system in consideration attains equilibrium, i.e. is most stable. Mathematically, the basic idea behind this relation can be understood by first showing that the total entropy in the domain is bounded. This can be done by showing that it steadily increases and that it cannot increase above a certain level. The next step is to show that if the entropy is bounded, the solution is bounded in a certain norm (see Merriam [26] and Dutt [11]).

An energy analysis for discontinuous Galerkin method by Barth [2] gives sufficient conditions that when imposed on the numerical flux yield discrete entropy inequalities and total entropy bounds obtained for the discretization of Cauchy's initial value problem:

- Assuming a semi-discrete approximation for $\zeta_h \in \mathcal{V}_{h,\mathcal{I}}^k$ and that the entropy flux flows out through the boundary, integrating the inequality (2.2) over an element κ yields a local cell entropy inequality given by

$$\frac{d}{dt} \int_{\kappa} \mathcal{H}(\zeta_h) d\mathbf{x} + \int_{\partial\kappa} \tilde{\phi}(\zeta_h(\mathbf{x}_-), \zeta_h(\mathbf{x}_+); \mathbf{n}) d\mathbf{x} \leq 0, \quad \forall \kappa \in \tau_h \quad (4.18)$$

where $\tilde{\phi}(\zeta_h(\mathbf{x}_-), \zeta_h(\mathbf{x}_+); \mathbf{n})$ denotes a consistent and conservative numerical entropy flux. Summing over all elements then yields the global inequality

$$\frac{d}{dt} \int_{\Omega_h} \mathcal{H}(\zeta_h) d\mathbf{x} \leq 0 \quad (4.19)$$

- The total entropy bound, written for a full space-time approximation as

$$\int_{\Omega} \mathcal{H}(\rho^*(t^0)) d\mathbf{x} \leq \int_{\Omega_h} \mathcal{H}(\rho(\zeta_h(\mathbf{x}, t^N))) d\mathbf{x} \leq \int_{\Omega_h} \mathcal{H}(\rho(\zeta_h(\mathbf{x}, t^0))) d\mathbf{x} \quad (4.20)$$

where $\rho^*(t^0)$ denotes the minimum total entropy state of the projected initial data

$$\rho^*(t^0) := \frac{1}{|\Omega|} \int_{\Omega_h} \rho(\zeta_h(\mathbf{x}, t^0)) d\mathbf{x} \quad (4.21)$$

which is the usual \mathbb{L}^2 -stability statement familiar from the linear theory of symmetric hyperbolic systems. Thus, entropy stability could be viewed as a nonlinear extension of the \mathbb{L}^2 linear stability set-up to general, non-symmetric $N \times N$ systems.

3.1 E-Flux Schemes and the E-flux Condition

E-flux schemes are a class of monotone numerical fluxes introduced by Osher [28]. They are called E-fluxes due to their relationship to Oleinick's well-known E-condition which characterizes entropy satisfying discontinuities. Letting $[q]_{\pm}^{\pm} := q|_{+} - q|_{-}$, E-fluxes denoted by $\tilde{\mathcal{J}}^E$ satisfy the inequality

$$[\zeta]_{\pm}^{\pm} \cdot \left(\tilde{\mathcal{J}}^E(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) - \tilde{\mathcal{J}}(\rho(\zeta)) \right) \leq 0, \quad \forall \zeta \in [\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+)] \quad (4.22)$$

Note that any numerical flux can be written in the form

$$\tilde{\mathcal{J}}(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) = \frac{1}{2} [\mathcal{J}_+ \cdot \mathbf{n} + \mathcal{J}_- \cdot \mathbf{n}] - \frac{1}{2} {}^v \tilde{\mathcal{J}}(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) \quad (4.23)$$

where ${}^v \tilde{\mathcal{J}}(\cdot)$ denotes a viscosity for the numerical scheme. Approximate solutions satisfying (4.20) are obtained by entropy stable schemes satisfying the cell entropy inequality (4.18). Barth [1] has shown that if $\tilde{\mathcal{J}}(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n})$ satisfies the system E-flux condition given by (4.22)

$$[\zeta]_{\pm}^{\pm} \cdot \left[\tilde{\mathcal{J}}(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) - \mathcal{J}(\zeta(\chi)) \cdot \mathbf{n} \right] \leq 0, \quad \forall \chi \in [0, 1] \quad (4.24)$$

where ζ is parameterized by χ such that $\zeta(\chi) = \zeta(\mathbf{x}_-) + \chi[\zeta]_{\pm}^{\pm} \forall \chi \in [0, 1]$, then the cell entropy inequality (4.18) and the total entropy bound (4.20) are satisfied, hence implying (entropy/nonlinear) stability. Consider the following numerical fluxes:

- Barth [1] introduced an approximation to the the interface-flux given by the mean value Kinetic Boltzmann moment system E-flux, $\tilde{\mathcal{J}}^{LKMV}$, for Levermore's moment closure system (2.20) written in the form (4.23), where

$${}^v \tilde{\mathcal{J}} := {}^v \tilde{\mathcal{J}}^{LKMV}(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) = \int_0^1 \langle e^{\zeta(\chi) \cdot \boldsymbol{\vartheta}}, |\mathbf{v} \cdot \mathbf{n}| \boldsymbol{\vartheta} \otimes \boldsymbol{\vartheta} \rangle [\zeta]_{\pm}^{\pm} d\chi \quad (4.25)$$

Note that the integration in (4.25) is path dependant. Following the results by Dumbser *et. al.* [10] and Barth [1], the linear path connecting the states ζ_+ and ζ_- is chosen. This approximate flux can be conceived off as an Osher-Solomon flux with a linear integration path.

- A kinetic Boltzmann moment system E-flux for the linearized Levermore's moment closure system (about an equilibrium solution \mathcal{E}) (3.19), $\tilde{\mathcal{J}}^{eKMV}$, written in the form (4.23), where

$${}^v \tilde{\mathcal{J}} := {}^v \tilde{\mathcal{J}}^{eKMV}(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) = \int_0^1 \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], |\mathbf{v} \cdot \mathbf{n}| \vartheta \otimes \vartheta [\zeta]_{\pm}^{\pm} d\chi \quad (4.26)$$

In what follows it will be shown that the numerical fluxes corresponding to (4.25) and (4.26) satisfy the E-flux condition given by (4.24).

3.2 E-flux condition for $\tilde{\mathcal{J}}^{LKMV}$

Barth [1] has stated that $\tilde{\mathcal{J}}^{LKMV}$ satisfies the system E-flux condition (4.22). However, the proof is incorrect (this can be seen in the first identity of Barth's proof of his Lemma 3). An alternate proof is provided as follows; first note that

$$\begin{aligned} \frac{1}{2}[\mathcal{J}_+ - \mathcal{J}(\zeta(\xi))] \cdot \mathbf{n} &= \frac{1}{2}(\langle e^{\zeta_+ \cdot \vartheta}, (v \cdot \mathbf{n})\vartheta \rangle - \langle e^{\zeta(\xi) \cdot \vartheta}, (v \cdot \mathbf{n})\vartheta \rangle = \frac{1}{2} \langle e^{\zeta(x) \cdot \vartheta}, (v \cdot \mathbf{n})\vartheta \rangle \Big|_{\xi}^1 \\ &= \frac{1}{2} \int_{\xi}^1 \langle e^{\zeta(x) \cdot \vartheta}, (v \cdot \mathbf{n})\vartheta \otimes \vartheta [\zeta]_{\pm}^{\pm} d\chi \end{aligned} \quad (4.27)$$

$$\begin{aligned} \frac{1}{2}[\mathcal{J}_- - \mathcal{J}(\zeta(\xi))] \cdot \mathbf{n} &= -\frac{1}{2}(\langle e^{\zeta_- \cdot \vartheta}, (v \cdot \mathbf{n})\vartheta \rangle - \langle e^{\zeta(\xi) \cdot \vartheta}, (v \cdot \mathbf{n})\vartheta \rangle = -\frac{1}{2} \langle e^{\zeta(x) \cdot \vartheta}, (v \cdot \mathbf{n})\vartheta \rangle \Big|_0^{\xi} \\ &= -\frac{1}{2} \int_0^{\xi} \langle e^{\zeta(x) \cdot \vartheta}, (v \cdot \mathbf{n})\vartheta \otimes \vartheta [\zeta]_{\pm}^{\pm} d\chi \end{aligned} \quad (4.28)$$

It can be seen that $\tilde{\mathcal{J}}^{KMV}$ satisfies the E-flux condition since

$$[\zeta]_{\pm}^{\pm} \cdot [\tilde{\mathcal{J}}^{KMV} - \mathcal{J}(\zeta(x)) \cdot \mathbf{n}] \quad (4.29)$$

$$= \frac{1}{2}[\zeta]_{\pm}^{\pm} \left([\mathcal{J}_+ - \mathcal{J}(\zeta(\xi))] \cdot \mathbf{n} + [\mathcal{J}_- - \mathcal{J}(\zeta(\xi))] \cdot \mathbf{n} - {}^v \tilde{\mathcal{J}}^{KMV} \right) \quad (4.30)$$

$$\begin{aligned} &= \frac{1}{2} \int_{\xi}^1 \langle e^{\zeta(x) \cdot \vartheta}, (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi - \frac{1}{2} \int_0^{\xi} \langle e^{\zeta(x) \cdot \vartheta}, (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \\ &\quad - \frac{1}{2} \int_0^1 \langle e^{\zeta(x) \cdot \vartheta}, |\mathbf{v} \cdot \mathbf{n}| (\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \end{aligned} \quad (4.31)$$

$$\begin{aligned} &= \frac{1}{2} \int_0^1 \langle e^{\zeta(x) \cdot \vartheta}, (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi - \frac{1}{2} \int_0^{\xi} \langle e^{\zeta(x) \cdot \vartheta}, (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \\ &\quad - \frac{1}{2} \int_0^{\xi} \langle e^{\zeta(x) \cdot \vartheta}, (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi - \frac{1}{2} \int_0^1 \langle e^{\zeta(x) \cdot \vartheta}, |\mathbf{v} \cdot \mathbf{n}| (\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \end{aligned} \quad (4.32)$$

$$= \frac{1}{2} \int_0^1 \langle e^{\zeta(x) \cdot \vartheta}, [(v \cdot \mathbf{n}) - |\mathbf{v} \cdot \mathbf{n}|] (\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi - \int_0^{\xi} \langle e^{\zeta(x) \cdot \vartheta}, (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \leq 0 \quad (4.33)$$

3.3 E-flux condition for $\tilde{\mathcal{J}}^{eKMV}$

In this section it is shown that $\tilde{\mathcal{J}}^{eKMV}$ satisfies the system E-flux condition (4.22). To show this, first note that

$$\begin{aligned} \frac{1}{2}[\mathcal{J}_+ - \mathcal{J}(\zeta(\xi))] \cdot \mathbf{n} &= \frac{1}{2}(\langle \mathcal{E}(1 + \tilde{F}_+), (v \cdot \mathbf{n})\vartheta \rangle - \langle \mathcal{E}[1 + \tilde{F}(\zeta(\xi))], (v \cdot \mathbf{n})\vartheta \rangle) \\ &= \frac{1}{2} \langle \mathcal{E}[1 + \tilde{F}(\zeta(\chi))], (v \cdot \mathbf{n})\vartheta \rangle \Big|_{\xi}^1 \end{aligned} \quad (4.34)$$

$$\begin{aligned} &= \frac{1}{2} \int_{\xi}^1 \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], (v \cdot \mathbf{n})\vartheta \otimes \vartheta \rangle [\zeta]_{\pm}^{\pm} d\chi \\ \frac{1}{2}[\mathcal{J}_- - \mathcal{J}(\zeta(\xi))] \cdot \mathbf{n} &= \frac{1}{2}(\langle \mathcal{E}(1 + \tilde{F}_-), (v \cdot \mathbf{n})\vartheta \rangle - \langle \mathcal{E}[1 + \tilde{F}(\zeta(\xi))], (v \cdot \mathbf{n})\vartheta \rangle) \\ &= -\frac{1}{2} \langle \mathcal{E}[1 + \tilde{F}(\zeta(\chi))], (v \cdot \mathbf{n})\vartheta \rangle \Big|_0^{\xi} \\ &= -\frac{1}{2} \int_0^{\xi} \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], (v \cdot \mathbf{n})\vartheta \otimes \vartheta \rangle [\zeta]_{\pm}^{\pm} d\chi \end{aligned} \quad (4.35)$$

It can be seen that $\tilde{\mathcal{J}}^{eKMV}$ satisfies the E-flux condition since

$$[\zeta]_{\pm}^{\pm} \cdot [\tilde{\mathcal{J}}^{eKMV} - \mathcal{J}(\zeta(\chi)) \cdot \mathbf{n}] \quad (4.36)$$

$$= \frac{1}{2} [\zeta]_{\pm}^{\pm} \left([\mathcal{J}_+ - \mathcal{J}(\zeta(\xi))] \cdot \mathbf{n} + [\mathcal{J}_- - \mathcal{J}(\zeta(\xi))] \cdot \mathbf{n} - v \tilde{\mathcal{J}}^{eKMV} \right) \quad (4.37)$$

$$\begin{aligned} &= \frac{1}{2} \int_{\xi}^1 \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \\ &\quad - \frac{1}{2} \int_0^{\xi} \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \end{aligned} \quad (4.38)$$

$$\begin{aligned} &\quad - \frac{1}{2} \int_0^1 \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], |\mathbf{v} \cdot \mathbf{n}| (\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \\ &= \frac{1}{2} \int_0^1 \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \\ &\quad - \frac{1}{2} \int_{\xi}^1 \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \end{aligned} \quad (4.39)$$

$$\begin{aligned} &\quad - \frac{1}{2} \int_0^{\xi} \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \\ &\quad - \frac{1}{2} \int_0^1 \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], |\mathbf{v} \cdot \mathbf{n}| (\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \\ &= \frac{1}{2} \int_0^1 \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], ((v \cdot \mathbf{n}) - |\mathbf{v} \cdot \mathbf{n}|)(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \\ &\quad - \int_0^{\xi} \langle \mathcal{E}[1 + (\zeta(\chi) - \zeta_0) \cdot \vartheta], (v \cdot \mathbf{n})(\vartheta \cdot [\zeta]_{\pm}^{\pm})^2 \rangle d\chi \leq 0 \end{aligned} \quad (4.40)$$

3.4 Discrete Numerical Flux

Consider Levermore's kinetic Boltzmann moment system E-flux (4.25), evaluation of the state space integrations can be very difficult. It follows from the E-flux condition (4.24) that the entropy stability results derived for a numerical flux $\tilde{\mathcal{J}}^E$ are retained using another numerical fluxes, $\tilde{\mathcal{J}}^D$, satisfying

$$[\zeta]_{\pm}^{\pm} \cdot \tilde{\mathcal{J}}^D(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) \leq [\zeta]_{\pm}^{\pm} \cdot \tilde{\mathcal{J}}^E(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) \quad (4.41)$$

Barth [1] has shown that a discrete kinetic Boltzmann moment E-flux which replaces exact path integration in state space with q -point Gauss-Lobatto quadrature satisfies the system E-flux comparison principle. More specifically, letting $\omega_i \in \mathbb{R}^+$ and $\chi_i \in [0, 1]$ denote q -point Gauss-Lobatto quadrature weights and locations. The discrete kinetic Boltzmann moment numerical flux, $\tilde{\mathcal{J}}^{DLMKV(q)}$, of the form (4.23) where

$${}^v \tilde{\mathcal{J}} = {}^v \tilde{\mathcal{J}}^{DLKMV(q)}(\zeta, \zeta; \mathbf{n}) := \sum_{i=1}^q \omega_i \langle e^{\zeta(\chi) \cdot \vartheta}, |\mathbf{v} \cdot \mathbf{n}| \vartheta \otimes \vartheta \rangle [\zeta]_{\pm}^+ \quad (4.42)$$

satisfies the system E-flux comparison principle

$$[\zeta]_{\pm}^+ \cdot \tilde{\mathcal{J}}^{DLKMV(q)}(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) \leq [\zeta]_{\pm}^+ \cdot \tilde{\mathcal{J}}^{KMV}(\zeta(\mathbf{x}_-), \zeta(\mathbf{x}_+); \mathbf{n}) \quad (4.43)$$

for $q \geq 2$. Note that this issue is not raised for the E-flux given by (4.26) since the integrations involved are computable with closed form expressions. Therefore, the E-flux given by (4.26) does not need a discrete approximation.

4. Concluding Remarks

In order to solve Cauchy's initial value problem posed in (4.12), one seeks weak solutions of (4.17) yielding an expression for ρ_h . The remaining task is then to obtain the Lagrange multipliers ζ_h from $\rho_h(\zeta_h)$. Considering Levermore's moment closure system, the issue would be that for cases involving moments of super-quadratic polynomials there is no explicit expression for ζ_h as a function of ρ_h since the moment integrals are incomputable. Moreover, the Legendre duality relationship between the entropy density and the exponential distribution is not guaranteed (see, Appendix I). Hence, it is unclear how the vector of Lagrange multipliers, ζ_h , is obtained. The developed approximate moment closure (3.19) system overcomes this issue, since the explicit expressions in question are available, thus providing means to compute the Lagrange multipliers ζ_h for moment systems involving moments of super-quadratic polynomials. This issue was not raised in the work of Barth [1] since only moment closure systems involving, at most, quadratic polynomials (5-moment and 10-moment systems) were considered.

Chapter 5

Conclusions

1. Summary

In this study, moments of the Boltzmann equation with exponential closure [23] (2.20) were introduced. More specifically, applying the moment method to approximate the Boltzmann equation, the consequent moment closure problem and the entropy minimization technique used to attain closure were discussed. Moreover, an analysis of the properties resulting moment closure system is presented, it was shown that the entropy based closure retained the existence of a convex entropy extension (entropy dissipation) as well as exhibiting well-posedness. However, it was noted that such an analysis is based on the assumption that a minimizer to entropy minimization problem (2.3) exists.

Attention was given to the realizability issue that was first raised by Junk [18], i.e. that the set containing realizable densities for which the minimum entropy solution is undefined is non-void. Recent results addressing this issue [17, 29, 31] which suggest a modified closure procedure by relaxing the constraints of the entropy minimization problem, were presented. This relaxed entropy minimization technique retains the exponential closure.

It was noted that any numerical approximation of the Levermore's entropy-based moment closure system requires the evaluation of moments of exponentials of polynomials of, in principle, arbitrary orders. For that, an analytical approximation of the moment closure system based on a series expansion procedure that results in a mathematically tractable system, was studied. It was shown that the properties of this approximate moment system recover the properties of the Levermore's full moment closure system and, thus, properties of the Boltzmann equation. More specifically, they retain well-posedness and entropy dissipation.

Finally, a numerical approximation of the approximate moment closure system (3.19) is considered within a discontinuous Galerkin finite element framework. The work of Barth [1] is extended to devise a numerical approximation for the resulting moment system. Energy analysis is employed to show stability of an energy stable numerical flux function which is used for the discontinuous Galerkin finite element discretization. The use of the kinetic mean value numerical flux introduced by Barth [1] is extended to approximate a numerical flux corresponding to the linearized moment system (3.19). In contrast to the work of Barth [1], the numerical flux function suggested for the tractable system does not require a simplified construction since it is computable, in addition, higher order (approximated) moment systems can be considered.

2. Future Outlook

This study can be perceived as a first milestone towards the development and analysis of a finite-element methodology using a suitable hierarchy of moment-closure systems, which facilitates implementation in a finite element method, while retaining the fundamental properties of the underlying Boltzmann equation. Though there may be many ways to carry forward this research, from the author's perspective, future prospects would involve implementation of the finite-element method and eventual development of an adaptive refinement strategy for the developed hierarchy.

In the context of developing a suitable hierarchy, open questions still remain about the suggested approximation in equation (3.45) with regard to well-posedness. From an approximation perspective this form of linearization is interesting because it does not impose restrictions on the term the approximation is taken about. Though symmetric hyperbolicity can't be guaranteed for (3.45), it may be worthwhile to investigate general hyperbolicity of this approximation. This can be done by studying the eigen-structure of (3.45). If the eigenvalues of the flux coefficient matrix are real and the corresponding eigenvectors distinct, the system is considered to be hyperbolic (see Definition 5.1). Brown [8] performed an eigensystem analysis for the Levermore's 10-moment system and showed that the system is hyperbolic. Note that the approximate system (3.45) could be conceived as a perturbative expansion about the Gaussian distribution which, in fact, corresponds to the entropy minimizing distribution of the 10-moment system. Thus, heuristically, one might expect (3.45) to be hyperbolic for, at least, some finite region in phase-space. However, this hypothesis is subject to criticism and needs further investigation. Another open question pertains to an error analysis that would estimate how well the solution of any of the moment system presented in this work (both Levermore's system and the developed approximation to it) approximate solution(s) of the Boltzmann equation.

In the context of numerical approximations, an analysis incorporating boundary conditions still remains open. In addition, implementation of the approximate moment systems devised in this work into a discontinuous Galerkin finite element algorithm is needed in order to apply the developed theory.

Appendix I

Extended Thermodynamics and Levermore's Entropy Minimization: The Correlation

For the moments system (1.9) closure based on the principles of extended thermodynamics [27] impose an entropy structure at the continuum level. In extended thermodynamics moments $\langle f, \mathbf{v}\boldsymbol{\vartheta} \rangle$ and $\langle \mathcal{L}(f), \boldsymbol{\vartheta} \rangle$ can be expressed in terms of the densities $\boldsymbol{\rho} := \langle f, \boldsymbol{\vartheta} \rangle$ through constitutive relations that are local in space-time¹ to provide a closure of the form (2.9). Thus, if the constitutive functions are known explicitly, the moments $\langle f, \mathbf{v}\boldsymbol{\vartheta} \rangle$ and $\langle \mathcal{L}(f), \boldsymbol{\vartheta} \rangle$ could be eliminated between the equations of balance and the constitutive relations to yield explicit field equations for the densities $\boldsymbol{\rho}$. They form a quasi-linear system of partial differential equations of first order. Every solution of this system is called a thermodynamic process. For an arbitrary vector $\boldsymbol{\vartheta}$, the formulation of constitutive relations is based on the following postulates [27]:

1. *Entropy principal*: It is assumed that there exists an entropy density $\mathcal{H} = \mathcal{H}(\mathbf{F}(\boldsymbol{\rho}, \mathbf{v}))$ and entropy flux $\phi = \phi(\mathbf{F}(\boldsymbol{\rho}, \mathbf{v}))$ and a dissipation term $\sigma = \sigma(\mathbf{F}(\boldsymbol{\rho}, \mathbf{v}))$ such that (2.2) is satisfied for all thermodynamic processes. Note that is also assumed that \mathcal{H} , ϕ and σ are constitutive quantities that can be expressed in terms of the densities $\boldsymbol{\rho} := \langle f, \boldsymbol{\vartheta} \rangle$.
2. *The requirement of convexity and causality*: This imposes that \mathcal{H} is a convex function of the densities so that the matrix of second derivatives is positive definite. Mathematically, it is to ensure well-posedness of Cauchy problems for the field equations and physically it guarantees finite speed of propagation and thermodynamic stability.
3. *Principal of relativity (material frame indifference)*: The field equations are assumed to be independent of an observer, i.e. assuming material frame indifference or Galilean invariance. This means that the field equations and the entropy inequality have the same forms in all Galilee frames.

It has been observed that entropy-based closures resulting from entropy minimization are formally equivalent to the systems derived from extended thermodynamics [27]. Recall the minimization problem (2.3); if the minimizer exists, and if \mathcal{H} is differentiable at the solution, the standard Lagrange multiplier theory yields relation (2.7). Furthermore, it is clear from (2.3) that $\boldsymbol{\zeta} \in \mathbb{R}^\theta$ is related to $\boldsymbol{\rho}$

¹Thus no gradients or time derivatives occur among the variables in the constitutive equations.

through the constraints

$$\langle e^{\zeta \cdot \vartheta}, \vartheta \rangle = \rho \quad (\text{I.1})$$

Following [23], one can identify explicitly the density and flux potentials

$$\begin{aligned} \mathcal{H}^*(\zeta) &\equiv \langle e^{\zeta \cdot \vartheta}, 1 \rangle \\ \phi^*(\zeta) &\equiv \langle e^{\zeta \cdot \vartheta}, \mathbf{v} \rangle \end{aligned} \quad (\text{I.2})$$

Differentiating \mathcal{H}^* with respect to ζ recovers the constraint relations in (2.7). Note that the equality in the constraints relation (I.1) implies that

$$\mathcal{H}(\rho) + \mathcal{H}^*(\zeta) = \zeta^\top \rho \quad (\text{I.3})$$

which means that \mathcal{H}^* is the Legendre dual of \mathcal{H} . Moreover, because

$$\partial_\zeta^2 \mathcal{H}^*(\zeta) = \langle e^{\zeta \cdot \vartheta}, \vartheta \vartheta^\top \rangle \quad (\text{I.4})$$

is positive definite, the relation is invertible for ζ as a function of ρ . Consequently, the closure in (2.9) possesses an auxiliary entropy equation of the form (2.2).

Remark. However, the function relating the density ρ to the vector of Lagrange multipliers ζ may not be explicitly available since the left hand side of (I.1) is not computable for moments of super-quadratic polynomials of velocity. Therefore, it remains unclear how to obtain ζ

Furthermore, differentiating (I.3) with respect to ρ shows that

$$\zeta = [\partial_\rho \mathcal{H}(\rho)]^\top \quad (\text{I.5})$$

moreover, it shows that

$$\partial_\rho^2 \mathcal{H} = [\partial_\alpha^2 \mathcal{H}^*]^{-1} \quad (\text{I.6})$$

is positive definite and, thus, \mathcal{H} is convex. Within the context of an extended thermodynamics framework, one must also show that \mathcal{H} is dissipated by solution of (2.9). This can be done by the same procedure as in (2.17)-(2.19).

Remark. In the degenerate cases, however, \mathcal{H} is not always dissipated by solutions of (1.1). Thus, there is no guarantee that $\sigma(\rho) < 0$. This issue can be circumvented by considering the relaxed minimization problem (2.29) instead which retains the exponential entropy minimizing distribution (2.7) and, thus, the exponential closure.

In addition to a kinetic-based formulation and an entropy-based closure, the minimum entropy method also provides an algorithm for computing ζ that is not readily available in the extended thermodynamics theory. This can be observed in light of the Legendre duality in (I.3). Differentiating (I.3) results in the gradient

$$\partial_\zeta \mathcal{H} = \rho - \partial_\zeta \mathcal{H}^* \quad (\text{I.7})$$

Recall from (I.4) \mathcal{H} is strictly convex. From the constrains in (I.1)

$$\partial_\zeta \mathcal{H} = 0 \quad (\text{I.8})$$

This suggests that the vector of Lagrange multipliers ζ can be obtained by solving (I.8), or equivalently, the minimization problem

$$\min_{\zeta \in \mathbb{R}^n} \{\zeta^\top \rho - \mathcal{H}(\rho)\} \quad (\text{I.9})$$

Note that (I.9) is the Legendre dual problem for (2.3)

Remark. However, in the degenerate cases, the Legendre duality relationship in (I.3) does not hold. Note that considering the relaxed minimization problem (2.29) does not overcome this issue since the equality in (I.1) of the constraints of the full minimization problem (2.3) is no longer guaranteed. The constraints of the relaxed minimization problem (2.29) allows for inequalities between certain components instead. Therefore an algorithm based on (I.9) is remains lacking.

Appendix II

Generalized Gaussian Integral

Consider an integral of the form

$$J_0 = \int_{-\infty}^{\infty} e^{-(\alpha x^2 + \beta x)} dx \quad (\text{II.1})$$

where $\alpha > 0$. Using the fact that

$$(ax + b)^2 = a^2 x^2 + 2abx + b^2 \quad (\text{II.2})$$

the exponent in (II.1) is rewritten as a squared term such that

$$\alpha x^2 + \beta x = \left(\sqrt{\alpha} x + \frac{\beta}{2\sqrt{\alpha}} \right)^2 - \left(\frac{\beta}{2\sqrt{\alpha}} \right)^2 \quad (\text{II.3})$$

$$= \alpha \left(x + \frac{\beta}{2\alpha} \right)^2 - \frac{\beta^2}{4\alpha} \quad (\text{II.4})$$

Letting

$$y := x + \frac{\beta}{2\alpha} \quad (\text{II.5})$$

the integral can be written in the form

$$J_0 = e^{\frac{\beta^2}{4\alpha}} \int_{-\infty}^{\infty} e^{-\alpha y^2} dy = \sqrt{\frac{\pi}{\alpha}} e^{\frac{\beta^2}{4\alpha}} \quad (\text{II.6})$$

Proceeding to evaluate moments of this integral, the first moment is given by

$$J_1 = \int_{-\infty}^{\infty} x e^{-\alpha y^2} dy \quad (\text{II.7})$$

$$= \int_{-\infty}^{\infty} -\frac{\partial}{\partial \beta} \left[e^{-\alpha x^2 - \beta x} \right] dx \quad (\text{II.8})$$

$$= -\frac{\partial}{\partial \beta} J_0 \quad (\text{II.9})$$

The second moment is given by

$$J_2 = \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2 - \beta x - \gamma} dx \quad (\text{II.10})$$

$$= \int_{-\infty}^{\infty} \frac{\partial}{\partial \alpha} [e^{-\alpha x^2 - \beta x}] dx \quad (\text{II.11})$$

$$= -\frac{\partial}{\partial \alpha} J_0 \quad (\text{II.12})$$

Subsequent moments of can be evaluated by similar techniques resulting int he following general expressions

$$J_{2m+1} = (-1)^{2m+1} \frac{\partial^{2m+1} J_0}{\partial \beta^{2m+1}} \quad (\text{II.13})$$

$$= (-1)^{2m+1} \frac{\partial^{2m+1}}{\partial \beta^{2m+1}} \left[\sqrt{\frac{\pi}{\alpha}} e^{\frac{\beta^2}{4\alpha}} \right] \quad (\text{II.14})$$

and

$$J_{2m} = (-1)^m \frac{\partial^m J_0}{\partial \beta^m} \quad (\text{II.15})$$

$$= (-1)^m \frac{\partial^m}{\partial \beta^m} \left[\sqrt{\frac{\pi}{\alpha}} e^{\frac{\beta^2}{4\alpha}} \right] \quad (\text{II.16})$$

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