Fourteen-Moment Maximum-Entropy-Inspired Closures for Non-Equilibrium Gases and Liquid Sprays

by

Jérémie Laplante

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University of Toronto Institute for Aerospace Studies
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Abstract

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Jérémie Laplante
Master of Applied Science
University of Toronto Institute for Aerospace Studies
University of Toronto
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With the purpose of developing a model able to evaluate transition regime rarefied gas dynamics and disperse liquid spray flows, a novel closed-form bi-Gaussian closure to the 14-moment member of Levermore’s maximum-entropy hierarchy is derived and evaluated. A thorough evaluation of its univariate kinetic equivalent, namely the bi-Maxwellian closure, is first performed in the context of a one-dimensional 5-moment model, where it is shown to possess many modelling advantages over more standard methods. A two-dimensional numerical scheme is then presented for the parallel solution of the 14-moment bi-Gaussian closure. The multi-dimensional bi-Gaussian closure is compared to another maximum-entropy-based (IMEB) closure in rarefied gas dynamics applications, and to the Gaussian closure in a liquid spray application. Though the closure has compared quite well to the IMEB closure and shown a significant modelling advantage over the Gaussian closure, further improvements to the numerical scheme and closure are required.
Résumé

Fermetures à quatorze moments basées sur la maximisation d’entropie: application aux brouillards de gouttes et aux gaz hors-équilibre

Jérémie Laplante
Maîtrise en science appliquée
Département d’études supérieures University of Toronto Institute for Aerospace Studies
University of Toronto
2017

Une nouvelle fermeture bi-Gaussienne à 14 moments de la hiérarchie d’entropie maximale de Levermore est dérivée et évaluée dans le contexte de la dynamique des gaz raréfiés (RGD) et des croisements de particules (PTC) reliés aux brouillards de gouttes. En premier lieu, une évaluation d’un système cinétique unidimensionnel analogue est entreprise. La fermeture bi-Gaussienne est ici comparée avec des méthodes plus conventionnelles et démontre un net avantage de modélisation. Un schéma numérique bidimensionnel est présenté. Lors de prédictions numériques multidimensionnelles, la fermeture bi-Gaussienne est comparée à une fermeture basée sur la maximisation d’entropie (IMEB) pour des problèmes de RGD, ainsi qu’à la fermeture Gaussienne pour des problèmes de PTC. La fermeture bi-Gaussienne se compare très bien à la fermeture IMEB et démontre un net avantage de modélisation sur la fermeture Gaussienne. Malgré les résultats préliminaires encourageants, des améliorations au schéma numérique et à la fermeture sont requises.
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# Contents

Acknowledgements iv  

Contents v  

List of Tables viii  

List of Figures ix  

1 Introduction 1  

1.1 Rarefied Gas Dynamics ........................................ 1  
1.2 Liquid Sprays .................................................. 3  
1.3 Scope of Research .............................................. 5  
1.4 Thesis Outline ................................................. 6  

2 Gaskinetic Theory 7  

2.1 Knudsen Number .................................................. 7  
2.2 Phase-Space Velocity Distribution Function ......................... 8  
  2.2.1 Realizability of Distribution Function ...................... 9  
2.3 Moments of the Distribution Function ............................ 9  
2.4 Boltzmann Equation ............................................. 10  
2.5 Solution Strategies for the Boltzmann Equation ................... 12  
  2.5.1 Discrete Velocity Models. ................................. 13  
  2.5.2 Lagrangian Methods. ...................................... 13  
  2.5.3 Method of Moments. ...................................... 13  

3 Spray Dynamics 15  

3.1 Spray Regimes ................................................... 15  
3.2 Spray Physics: Williams-Boltzmann Equation ....................... 16  
  3.2.1 Solution Strategies for the Williams-Boltzmann Equation .... 18
4 Moment Closure Methods

4.1 Maxwell’s Equation of Change .............................................. 20
4.2 Moment Closures ............................................................... 21
   4.2.1 Grad Moment Closures .................................................. 22
   4.2.2 Quadrature-Based Moment Methods ................................. 23
   4.2.3 Maximum-Entropy Moment Closures ................................. 26
4.3 Maximum Entropy Closure Hierarchy .................................... 27
   4.3.1 Gaussian Closure ......................................................... 29
4.4 Fourteen-Moment Closures .................................................. 31
   4.4.1 Moment Realizability ..................................................... 32
   4.4.2 Interpolative Maximum-Entropy-Based Closure .................. 34
   4.4.3 Bi-Gaussian Closure ..................................................... 37
   4.4.4 Possible Extensions to Multi-Gaussian Closures ................. 43

5 Univariate Kinetic Model ..................................................... 45

5.1 Representative Univariate Kinetic Equation ............................ 45
5.2 Five-Moment System for Univariate Kinetic Model .................... 46
   5.2.1 Grad-Type Moment Closure ............................................ 47
   5.2.2 Interpolative Maximum-Entropy-Based (IMEB) Moment Closure 48
   5.2.3 Quadrature-Based Moment (QMOM) Closure ........................ 49
   5.2.4 EQMOM Bi-Maxwellian Moment Closure ............................ 50
   5.2.5 Closing Moment and Region of Moment Realizability ............ 51
5.3 Numerical Simulation of Stationary Shock Structures ................ 53
   5.3.1 Stationary Shock Structure Results .................................. 55
   5.3.2 Coping with Singularities at the Junk Subspace ................. 57
   5.3.3 Closure Comparisons along Non-Equilibrium Paths .............. 58
   5.3.4 Comparisons to the Maximum-Entropy Distribution ............. 61
5.4 Numerical Simulation of Particle Trajectory Crossings ............... 65
5.5 Conclusions Following from the Univariate Kinetic Model Results .... 67

6 Finite-Volume Numerical Solution Procedure ............................ 69

6.1 HLL Approximate Riemann Solver ....................................... 70
6.2 Kinetic-Based Flux Function ............................................... 71
6.3 Solid-Wall Boundary Conditions ......................................... 72
   6.3.1 Gaussian-Based Perturbative Internal Distribution .............. 73
   6.3.2 Bi-Gaussian Internal Distribution .................................. 74
6.4 Performance Improvements ................................................... 75
7 Numerical Results

7.1 Test Problems for Rarefied Gas Dynamics

7.1.1 Micro-Couette Flow

7.1.2 Heat Transfer Between Parallel Plates

7.2 Test Problems for Sprays

7.2.1 Quasi-2D Simulation of Two Crossing Jets

7.2.2 Fully 2D Simulation of Two Crossing Jets

8 Conclusions and Future Work

Bibliography
## List of Tables

2.1 Gaseous Flow Regimes in Terms of Knudsen Number .......................... 8  
2.2 Total Velocity Moments of the Distribution Function ........................ 10  
2.3 Random Velocity Moments of the Distribution Function ........................ 11  
3.1 Spray Regimes [40] ........................................................................ 16  
4.1 Example of an Optimal Moment Set for a Two-Dimensional Quadrature with Moments up to Fourth-Order ................................................................. 23  
4.2 Variation of the bi-Gaussian distribution’s Parameters for Changes in the Heat Flux Magnitude and Equilibrium Parameter ......................................................... 41  
4.3 Physical Description of the Bi-Gaussian Distribution’s Behaviour for the Moment States of Table 4.2 .............................................................. 41
# List of Figures

3.1 Near-injector atomization regions [56]. ........................................ 16

5.1 Domain of physical realizability for the five-moment system: (a) realizability boundaries [16] and contours of (b) IMEB, (c) QMOM and (d) bi-Maxwellian closing values for $s_*$. ............................................................. 52

5.2 Domain of physical realizability for the five-moment system: (a) realizability boundaries [16] and contours of (b) IMEB, (c) QMOM and (d) bi-Maxwellian closing values for $s_*$. ............................................................. 54

5.3 Predicted normalized density and dimensionless heat transfer through a stationary shock wave for a one-dimensional gas as determined by the IMEB, bi-Maxwellian (bM), Grad and Dirac3 closures: (a)-(b) $M = 1.25$ and (c)-(d) $M = 2$. ............................................................. 55

5.4 Predicted normalized density and dimensionless heat transfer through a stationary shock wave for a one-dimensional gas as determined by the IMEB and bi-Maxwellian (bM) closures: (a)-(b) $M = 4$ and (c)-(d) $M = 8$. ................. 56

5.5 Contours of EQMOM closure parameter, $\sigma_Q$, in physical realizability region and example of a $\sigma_Q^*$ limiting value (white line). ................................. 57

5.6 Predicted dimensionless heat transfer through a $M = 8$ stationary shock wave for a one-dimensional gas as predicted by the bi-Maxwellian closure: (a) effect of changes in the limiting parameter, $\sigma_Q^*$, and (b) closeup of resulting subshocks. 58

5.7 (a) Non-equilibrium shock orbitals as computed from the reference BGK solution for shocks at $M = 1.25$ to $M = 8$ and (b) closeup of the shock orbitals showing near-equilibrium regions. ........................................ 59

5.8 Values of the closing flux, $s_*$, for (a) $M = 1.25$, (b) $M = 2$, (c) $M = 4$ and (d) $M = 8$ orbitals as computed from the moments of the BGK solution along the normalized surface length of each orbital shown in Figure 5.7. ....... 60

5.9 Non-equilibrium path and sample points in realizable moment space for a $M = 8$ shock as predicted by the BGK reference solution. .......................... 61
5.10 Reconstructed maximum-entropy, $F_{\text{MaxEnt}}$, and bi-Maxwellian, $F_{bM}$, non-dimensional distributions for sample points along the $M = 8$ non-equilibrium shock path of Figure 5.9. Asterisks represent non-visible local maxima ($F_{\text{MaxEnt}}$: –*, $F_{bM}$: –*).

5.11 (a) BGK reference solution normalized density profile for a $M = 8$ shock and (b) closing flux prediction compared to the reference for the bi-Maxwellian (bM), maximum-entropy (ME) and interpolative maximum-entropy-based (IMEB) closures as computed from the moments of the reference solution. Reconstructed (c) maximum-entropy ($F_{\text{MaxEnt}}$) and (d) bi-Maxwellian ($F_{bM}$) non-dimensional distributions along the shock profile shown in (a).

5.12 Initial collisionless Riemann problem state for representative monokinetic particle trajectory crossing.

5.13 Non-equilibrium path and sample points in realizable moment space for a representative particle trajectory crossing problem as predicted by the BGK reference solution.

5.14 Reconstructed maximum-entropy, $F_{\text{MaxEnt}}$, and bi-Maxwellian, $F_{bM}$, non-dimensional distributions for sample points along the non-equilibrium particle trajectory crossing path of Figure 5.13.

5.15 (a) BGK reference solution normalized density profile for the representative particle trajectory crossing problem and (b) closing flux prediction compared to the reference for the bi-Maxwellian (bM), maximum-entropy (ME) and interpolative maximum-entropy-based (IMEB) closures as computed from the moments of the reference solution. Reconstructed (c) maximum-entropy ($F_{\text{MaxEnt}}$) and (d) bi-Maxwellian ($F_{bM}$) non-dimensional distributions along the crossing profile shown in (a).

6.1 Two-dimensional quadrilateral computational cells [20].

6.2 Schematic representation of the Knudsen layer [93].

6.3 Example of overlapping ghost cells for a four-block Cartesian grid [25].

7.1 Results for micro-Couette flow: comparison between bi-Gaussian and interpolative maximum-entropy-based 14-moment closures. (a) Velocity profiles in terms of Knudsen number and (b) slip velocity as compared to reference Navier-Stokes and Lees [101] solutions.

7.2 Results for heat transfer between two plates: comparison of temperature profiles for bi-Gaussian and interpolative maximum-entropy-based 14-moment closures for different Knudsen numbers.
<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.3</td>
<td>Comparison of bi-Gaussian and interpolative maximum-entropy-based results for heat transfer between two plates: normalized heat flux at the wall in terms of Knudsen number as compared to reference free-molecular, Navier-Stokes and Navier-Stokes with slip solution.</td>
</tr>
<tr>
<td>7.4</td>
<td>Reference Lagrangian solution for simulation of two jets in a compressive velocity field.</td>
</tr>
<tr>
<td>7.5</td>
<td>Quasi-two dimensional number density results for crossing jets in a compressive velocity field as predicted by the 10-moment Gaussian closure.</td>
</tr>
<tr>
<td>7.6</td>
<td>Quasi-two dimensional number density results for crossing jets in a compressive velocity field as predicted by the 14-moment bi-Gaussian closure.</td>
</tr>
<tr>
<td>7.7</td>
<td>Fully 2D (a) number density results for crossing jets in a compressive velocity field as predicted by the 10-moment Gaussian closure and (b) closeup of particle crossing.</td>
</tr>
<tr>
<td>7.8</td>
<td>Fully 2D (a) number density results for crossing jets in a compressive velocity field as predicted by the 14-moment bi-Gaussian closure and (b) closeup of particle crossing.</td>
</tr>
</tbody>
</table>
Chapter 1

Introduction

Most fluid mechanics models are based on the assumption that flows occur in a continuum or “near-equilibrium” regime [1]. This assumption is in most cases valid when considering gases or liquids near their hydrodynamic limit. Near this limit, collisions or interactions between molecules of a gaseous flow or liquid droplets in a multiphase flow are prevalent and maintain the gas or liquid in an observable continuum state. These categories of flows are traditionally modelled using hydrodynamic models such as the Euler or Navier-Stokes equations. However, it has been shown that the hydrodynamic models break down and are no longer valid for modest-to-moderate departures from continuum flow conditions [2]. Such scenarios often appear in multiphase flow applications such as fuel sprays in internal combustion engines (ICEs) and aeronautical gas turbine combustion chambers [3], as well as fluidized beds and rain droplet formation. Departures from continuum flow conditions can further be observed in rarefied gas dynamics applications [4] such as microscale flows (e.g., micro-electromechanical systems) and high speed aerospace-related flows (e.g., upper atmospheric flight and space vehicle re-entry). Stemming from different motivations in each case, this thesis aims to advance the development of mathematical and computational models valid in both rarefied gas dynamics and multiphase flow applications, such as liquid fuel sprays.

1.1 Rarefied Gas Dynamics

With recent advances in applications involving rarefied and non-equilibrium flows, such as micro-electromechanical systems (MEMS) [5, 6] and high speed aerospace-related flows (e.g. upper atmospheric flight and space vehicle re-entry) [7], it has become more important to consider and take into account issues with the break-down of the Navier-Stokes equations in non-equilibrium regimes [8]. Based on the mean free path between collisions, these high-Knudsen number flows depart from the continuum regime and can approach the transition
Chapter 1. Introduction

and free-molecular regimes, where alternate fluid dynamical descriptions are required. Traditionally, particle-based techniques such as Direct Simulation Monte-Carlo (DSMC) [9] as well as direct discretizations of the Boltzmann equation [10] have been used and shown to be valid for flows ranging from the transition to free-molecular regimes. However, while valid for transition regime flows approaching the continuum limit, these techniques are known to be computationally very expensive. For one, DSMC requires an unreasonably large number of seeded particles to obtain statistical convergence, which can be particularly hindering when seeking converged solutions for practical applications. Additionally, direct discretizations of the Boltzmann equation, or discrete velocity models (DVMs), require a discretization of the velocity distribution into a very large number of space and velocity dimensions, which naturally makes the method very costly for all flow regimes. Thus, to tackle transition regime flows, the idea of using moment closures of the Boltzmann equation arises [4].

Moment closure methods effectively integrate out the velocity dependence of the Boltzmann equation and yield a finite set of space-time dependent partial differential equations (PDEs) for macroscopic quantities that are typically of engineering interest. With respect to the Navier-Stokes equations, moment closure methods have the potential of offering a region of validity that extends beyond the continuum regime into the transition regime while offering comparable computational time. Further, carefully chosen moment systems are known to yield hyperbolic systems of equations that fit very well with today's well-developed parallelized finite-volume [11, 12] and discontinuous Galerkin (DG) schemes. More recently, a family of moment closures based on entropy maximisation principles has been proposed [13–15]. This family of moment closures presents many attractive mathematical and physical properties which make them very well suited for the aforementioned numerical schemes. The 14-moment closure of the maximum-entropy hierarchy stands out as the lowest-order member of this hierarchy allowing to capture significant heat transfer effects [15].

The computational cost of obtaining solutions for the 14-moment maximum-entropy closure has long made this method restrictive. This is due to the absence of closed-form solutions to the assumed particle distribution function [15, 16], thus requiring lengthy and complex iterative procedures. To address this issue, notable alternative “maximum-entropy-based” closures based on interpolative procedures have recently been proposed, which have shown to be affordable and robust [17, 18]. In fact, these alternatives have shown that they can fully encompass the applicability region of the Navier-Stokes equations, and recent applications to micro-scale flows have shown outstanding results [19–22]. Though the results of the interpolative closures are quite promising, the interpolative approach is expected to be quite restrictive when considering more complex physical systems. This research therefore proposes an alternative maximum-entropy-based approach, for which a closed form bi-Gaussian
expression to the distribution function is introduced.

1.2 Liquid Sprays

In other engineering applications with increasingly stringent environmental and societal norms with regards to greenhouse gas emissions, strategies used in hydrocarbon fuel combustion must constantly be improved to lessen their impact on the environment. Of the many processes involved, liquid fuel spray design and atomization have considerable room for improvement, both from performance and emissions standpoints. To exploit advantages, such as ease of transportation and secondary uses such as cooling, liquid fuels are generally preferred to gaseous ones in many land and air transportation applications. This desire for a liquid combustible however requires the fuel to be evaporated prior to combustion. Spray processes are therefore required in order to finely atomized, mix and evaporate the fuel into the surrounding air prior to combustion. Examples of areas where fuel sprays are used include gasoline and diesel internal combustion engines as well as industrial and aerospace gas turbine engines. The complex multiphase flows ensuing from spray combustion require the development of computational models able to capture all the complex interactions between liquid and gas phases and between liquid fuel structures of different scales. Further, practical applications create the additional mandate for implementation of these numerical models on massively parallelized computing architectures, therefore prompting the development of Eulerian droplet descriptions, as will be described below.

In the case of gas turbine engines, fuel atomizers are used to spray and finely distribute fuel droplets in the combustion chamber. Computational fluid dynamics (CFD) methods are often used to model the ensuing sprays and assist in the design of the combustion chamber. Typically, an Euler-Lagrange approach is used, in which the gaseous (or carrier) and liquid (or disperse) phases are modeled using Eulerian and Lagrangian frameworks, respectively. The Lagrangian approach relies on the tracking of individual particles, or representative parcels of particles, using a force balance equation based on Newton’s second law [23].

Though Lagrangian methods can be quite accurate, as they do not introduce any numerical dispersion, they suffer from important drawbacks that suggest the development of new alternative methods to model fuel sprays. Firstly, Lagrangian methods require a large number of seeded particles in order to obtain statistical convergence, especially in the case of polydisperse multiphase flows. Thus, convergence analyses are required for both carrier phase grids and disperse phase droplet count, which can increase both simulation and preparation time substantially. The discrete representation of particles also introduces many challenges. Firstly, it causes a mismatch between the CFD methods used to solve for the gas and dis-
Chapter 1. Introduction

perse phases. In fact, a separate and distinct discretization technique must be employed for the spatial resolution of each phase. The main inconvenience of using Lagrangian particle tracking algorithms however lies in the parallel implementation of the solution methods. Load balancing is an issue, as particles are constantly changing position, thus requiring frequent re-partitioning of the domain (or droplets) between processors in order to minimize communication time. Coupling issues are also known to arise in an Euler-Lagrange approach. For one, particle-cell overlap can occur when the size of a particle is larger than the cell size, and therefore mass and momentum coupling between both phases becomes a challenge. In some cases, increasing the continuous phase grid resolution can decrease the accuracy of the results, as was observed in a commercial implementation of a Lagrangian method [24]. This is especially important and could be quite limiting when seeking grid independent solutions using adaptive mesh refinement (AMR) [25–28]. Finally, Lagrangian methods are quite ineffective in modelling the dense regions of the spray. Phenomena such as flow blockage are in fact quite difficult to capture due to the fact that inter-phase interactions are mainly calculated through a drag term alone [29].

An alternative to the Euler-Lagrange approach described above is a so-called Euler-Euler method, in which both the carrier and disperse phases are modeled in an Eulerian setting, with the possibility of the latter being computed using a moment closure method. Though they are theoretically more complex, Eulerian methods do not suffer from many of the drawbacks stated above. Both phases can be modeled on the same mesh, effectively making phase coupling and code parallelization more efficient and intuitive in a computational sense. The advantage of using a unique computational mesh for both phases is also quite advantageous, as a single convergence analysis is required when seeking grid-independent solutions. They therefore fit very well with finite volume methods using block-based AMR, which have been extensively developed in the CFD and Propulsion Group of the University of Toronto Institute for Aerospace Studies (UTIAS) to model continuous phase gas flow [26–28, 30, 31]. An additional advantage of the Euler-Euler approach is its partial differential equation (PDE)-based treatment of the discrete phase over the entire computational domain. This type of treatment is well-suited for problems such as the implementation of adjoint-based methods for solution error estimation [32, 33] and computational optimization [34, 35].

Though Euler-Euler approaches possess many underlying advantages, they naturally come with some modelling challenges. Firstly, the discretization algorithms used to solve Eulerian disperse phases introduce well-known numerical dissipation. Further, the derivation of transport equations can come less naturally, and result from more tedious and complex derivations. In a more physical sense, it can also be difficult to treat vacuum zones with Euler-Euler schemes, since their PDE-based approach requires a solution over the entire computational do-
main. Finally, the capture of particle trajectory crossings (PTCs), such as occur in moderate-to-high Stokes number sprays, can be difficult, due to the fact that the transported quantities must contain sufficient information to allow for multiple droplet velocities in a single computational cell. Among the others, this last point prompts the development of high-order moment methods.

Recently, the most notable Euler-Euler solution strategies for disperse multiphase flows are extensions of the Quadrature Method of Moments (QMOM) of McGraw [36]. In this approach, quadrature approximations to the droplet velocity distribution can be obtained by assuming a sum of weighted Dirac delta functions in velocity space. For multi-dimensional flows, many variants of the QMOM have been proposed [37–40]. However, few of these approaches seem well-suited for the potential solution of turbulent multiphase flows with PTCs. In these categories of flows, droplets inertial enough to produce PTCs can be present, and turbulence in the gas phase can produce small-scale PTCs, namely velocity dispersion. Purely node-based approaches such as the brute-force QMOM [41], and conditional QMOM (CQMOM) [38] are unable to capture multiple scales of PTCs without making use of an inconveniently large number of delta functions. Extended nodal representations to the distribution have therefore been proposed in the form of extended QMOMs (EQMOMs) [39, 42, 43]. These have the potential of capturing small-scale PTCs through the assumption that a kernel density function lies about each quadrature node. An initial attempt to capture this smaller scale of PTC has shown great promise through the implementation and study of a Gaussian closure [42]. More recently, a multi-Gaussian approach based on the CQMOM has also been studied [43]. This extended CQMOM (ECQMOM) has shown great promise, however it relies on the conditioning of the velocity distribution on a chosen velocity direction. As will be described, this research proposes a fully unconditioned closure which can be derived through concepts arising from the kinetic theory of rarefied gases and maximum-entropy-based closures.

1.3 Scope of Research

The focus of this research is on the development of a 14-moment bi-Gaussian closure for the simulation of both rarefied gases and liquid fuel sprays. In the former case, a comparison to the implementation of the 14-moment interpolative closure by Tensuda et al. [19–22] is of interest, as this closure has been previously validated for benchmark two-dimensional (2D) flows. Comparisons can therefore readily be made using an identical numerical scheme. To isolate the effect of the closure on the solution, models with simplified collision operators are considered.
In the case of liquid fuel sprays, many complex physical phenomena (e.g., transport, drag, evaporation, break-up, coalescence, collisions) are present, which would render the development of a new moment closure quite difficult. Therefore, a simplified model comprising only transport and drag is to be used for the initial development of the bi-Gaussian closure. The field of application will be to disperse multiphase flows with constant-sized particles. The goal will be to compare the 14-moment bi-Gaussian closure to same- \cite{18} and lower-order \cite{42} methods for the simulation of PTC-related flows.

Prior to considering these two physical domains of applicability, the proposed research focuses on the study of a 5-moment bi-Maxwellian based closure for a simplified univariate kinetic system \cite{17, 18, 44} that allow for an in-depth analysis of the closure’s mathematical and physical properties. This analysis further allows for the comparison of the proposed method to reference solutions ranging from the near-equilibrium Navier-Stokes equations to the direct solution of the Boltzmann Equation.

1.4 Thesis Outline

Due to the two areas of applicability of interest, this thesis will cover separate theory and literature as pertains to gaskinetic theory and sprays. Chapter 2 will therefore introduce the gaskinetic approach to the solution of flows of particles ranging from the continuum to the free molecular regime. Chapter 3 will describe similar theory for the modelling of multiphase flows as well as cover some fundamentals of fuel spray physics. Chapter 4 will then describe the chosen solution strategy for the kinetic models presented in Chapters 2 and 3, namely moment closure methods, and present the derivation of the 14-moment bi-Gaussian moment closure. The proposed bi-Gaussian moment closure will then be analyzed for a simplified model in Chapter 5, allowing to understand its behaviour in comparison to others in the literature. The applications of the proposed model rarefied gas dynamics and liquid fuel sprays are finally presented in Chapter 7 using the solution strategy described in Chapter 6.
Chapter 2

Gaskinetic Theory

Classical fluid dynamical descriptions of liquid and gaseous flows rely on a fluid representation based on continuum macroscopic quantities. In relatively dense, collision-dominated flows, such representations are valid, since collisions tend to relax particle velocity distributions towards local thermodynamic equilibrium (LTE), where microscopic fluctuations in particle velocities tend to be averaged out. In such flow regimes, near-equilibrium models such as the Navier-Stokes equations remain valid. However, in cases where the mean free path between inter-particle collisions increases, near-equilibrium models are known to fail. Alternative fluid dynamical descriptions are therefore sought, and gaskinetic theory provides an elaborate framework for describing fluid flow based on microscopic gas particle behaviour.

2.1 Knudsen Number

In terms of the relative scale of inter-particle collisions, flow can be separated into the continuum, transition and free-molecular flow regimes based on the relative importance of particle collisions. To better describe this separation of scales, the Knudsen number, Kn, is introduced, where

\[ \text{Kn} = \frac{\lambda}{D} \]  

represents the ratio between the mean free path between inter-particle collisions, \( \lambda \), and a representative flow dimension, \( D \). The various gaseous flow regimes are summarized in Table 2.1 in terms of the flow Knudsen number. In the continuum regime, the relative mean free path between collisions, and hence the flow Knudsen number, is very small. In this case, the omnipresence of collisions tends to rapidly relax the flow towards LTE, where the effects of microscopic gas fluctuations are rapidly averaged out. In such cases, near-equilibrium models such as the Navier-Stokes and Euler equations present valid assumptions. At the other
end of the Knudsen number spectrum lies the free-molecular regime, where the mean free path between collisions becomes large enough that inter-particle collisions can be neglected altogether. At this level, particles tend to travel directly between surfaces without underlying collisions, and therefore particle-surface interactions tend to dominate flow behaviour.

The transition regime is particular, in that inter-particle collisions in transition regime flows are non-negligible, however the near-LTE assumptions behind continuum-based models no longer hold. This thesis will provide a special focus on improved mathematical descriptions of transition-regime flows, where moment closure methods tend to thrive as they present a good compromise between accuracy and computational cost.

### 2.2 Phase-Space Velocity Distribution Function

Gaskinetic theory relies on a statistical representation of microscopic flow effects through the introduction of a phase-space velocity distribution function, \( F(x_i, v_i, t) \), which is related to the number of gas particles with velocity \( v_i \) at position \( x_i \) and time \( t \). The large number of particles present even in transitional or free-molecular regimes makes this particular representation of gas particle velocities both convenient and complete. In fact, rather than tracking the evolution of individual particles, such a statistical representation is largely preferred. A classical example of a phase-space distribution function is the Maxwell-Boltzmann distribution \([45]\)

given by

\[
M(x_i, v_i, t) = \left( \frac{\rho(x_i, t)}{2\pi\kappa T(x_i, t)} \right)^{\frac{3}{2}} \exp \left( -\frac{mv^2}{2\kappa T(x_i, t)} \right),
\]

which describes the equilibrium behaviour or solution for a gas where \( \rho \) is the gas density, \( T \) is the temperature, \( m \) is the particle mass and \( \kappa = 1.3807 \times 10^{-23} \text{ joule} \cdot \text{K}^{-1} \) is the Boltzmann constant. This representation corresponds to a gas in LTE, where all particles are isotropically distributed about a mean velocity in phase space, with the standard deviation of the distribution depending on the gas temperature.

For non-equilibrium distribution functions and their representations that will be dealt with throughout this thesis, it is often convenient to perform a shift in velocity space such that
Chapter 2. Gaskinetic Theory

$c_i = v_i - u_i$ is random particle velocity, and $u_i$ is the bulk or average velocity. One can therefore consider a random velocity distribution function, $F_i(x_i, c_i, t) = F(v_x - u_x, v_y - u_y, v_z - u_z)$.

It is also convenient at times to perform a normalization of the phase-space distribution function by the fluid density. This normalized distribution, $f$, is written as

$$f(x_i, v_i, t) = \frac{F(x_i, v_i, t)}{\rho(x_i, t)}, \quad (2.3)$$

where the value of $f(x_i, v_i, t)$ represent the probability of finding a fluid particle with velocity $v_i$ at position $x_i$ and time $t$. It therefore follows that integration of $f$ over all velocity space for a given time and position of interest yields

$$\langle f \rangle = \int \int \int f d^3v = 1, \quad (2.4)$$

where the angular brackets denote the integration over all of velocity space.

### 2.2.1 Realizability of Distribution Function

A physically correct description of the phase-space distribution requires that it be realizable throughout all of velocity space. Realizability of the distribution requires that for all physically possible configurations of fluid particles, the distribution function, $f$, must be both real and positive valued. As described in Chapter 4, realizability issues are often encountered in the application of moment closure methods, where certain representative collections of moments do not correspond to a strictly positive definite probability density function.

### 2.3 Moments of the Distribution Function

Insight into the physical significance of the phase-space distribution function can be gained through the values of its velocity moments. The moments of different order represent various macroscopic quantities of the fluid and can often be related to transported variables classically modelled using hydrodynamics. The macroscopic quantities or moments of the distribution function can be defined in terms of the convolution integral of a velocity weight with $F$. In particular, the moment, $M_{\alpha, \beta, \gamma}$, for a velocity weighting $v_x^\alpha v_y^\beta v_z^\gamma$, can be written as

$$M_{\alpha, \beta, \gamma} = \langle mv_x^\alpha v_y^\beta v_z^\gamma F \rangle = \int \int \int mv_x^\alpha v_y^\beta v_z^\gamma F d^3v, \quad (2.5)$$
Table 2.2: Total Velocity Moments of the Distribution Function

<table>
<thead>
<tr>
<th>Order</th>
<th>Weight</th>
<th>Moment</th>
<th>Physical Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>( \rho )</td>
<td>Density</td>
</tr>
<tr>
<td>1</td>
<td>( v_i )</td>
<td>( \rho u_i )</td>
<td>Mass flux or momentum</td>
</tr>
<tr>
<td>2</td>
<td>( v_i v_j )</td>
<td>( \rho u_i u_j + P_{ij} )</td>
<td>Total momentum flux</td>
</tr>
<tr>
<td>3</td>
<td>( v_i v_j v_k )</td>
<td>( \rho u_i u_j u_k + u_j P_{jk} + u_i P_{ik} + u_k P_{ij} + Q_{ijk} )</td>
<td>Third order velocity moment tensor</td>
</tr>
<tr>
<td>4</td>
<td>( v_i v_j v_k v_l )</td>
<td>( \rho u_i u_j u_k u_l + u_j u_k P_{ji} + u_l u_k P_{jl} + u_l u_i P_{jk} + u_l u_j P_{il} + u_k u_l P_{ij} + u_i Q_{jkl} + u_j Q_{ikl} + u_k Q_{jil} + u_l Q_{ijl} + R_{ijkl} )</td>
<td>Fourth order velocity moment tensor</td>
</tr>
</tbody>
</table>

where \( m \) is the gas particle mass. In many cases, this definition of velocity moments corresponds to conserved variables such as the momentum or energy of the gas conventionally used when considering classical hydrodynamics. In a similar fashion, a random, or centered, velocity moment \( C_{\alpha,\beta,\gamma} \) can be defined by the convolution integral of a random velocity weight with \( F' \) such that

\[
C_{\alpha,\beta,\gamma} = \langle m c^\alpha c^\beta c^\gamma F' \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} m c^\alpha c^\beta c^\gamma F' d^3 c. \tag{2.6}
\]

Such random velocity moments describe macroscopic properties of the distribution that are independent of the bulk velocity, such as pressure and heat flux. A summary of the random velocity moments to be considered throughout this thesis are presented in Table 2.3. Total moments of the distribution can be expressed in terms of the random velocity moments and are presented in Table 2.2. Comparing moment expressions in both tables, it can easily be seen that for a bulk or mean velocity of \( \bar{u}_i = 0 \) the expression to the random velocity moments and total velocity moments are identical.

2.4 Boltzmann Equation

The evolution of the phase-space velocity distribution function is described by the Boltzmann equation [1] which is given by

\[
\frac{\partial F}{\partial t} + \left( \mathbf{v}_i \frac{\partial}{\partial x_i} (F) \right) + \left( a_i \frac{\partial}{\partial v_i} (F) \right) = \frac{\delta F}{\delta t}, \tag{2.7}
\]

where

- Advection
- External Forces
- Collisions
which is an integro-differential equation where the time rate of change of $F$ is influenced by the space advection of $F$ and the influence of external acceleration forces as well as inter-particle collisional processes. Examples of these external forces include gravity, the Lorentz force (i.e., in plasmas) and drag forces (i.e., in multiphase flows). For the purpose of this study, external acceleration forces will be neglected, yielding the following governing kinetic equation for gaskinetic theory.

$$\frac{\partial F}{\partial t} + \frac{\partial}{\partial x_i} (v_i F) = \frac{\delta F}{\delta t}$$

The evolution of $F$ is particularly influenced by inter-particle collisions, where $\delta F / \delta t$ represents the Boltzmann collision integral. An accurate and full depiction of inter-particle binary collisions is provided by the Boltzmann collision integral given by

$$\frac{\delta F}{\delta t} = \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{\pi} dv_i^{(2)} d\epsilon d\chi \left[ F_{pc}^{(1)} F_{pc}^{(2)} - F^{(1)} F^{(2)} \right] S(g, \chi) \sin \chi,$$

where the superscripts (1) and (2) correspond to properties of the incident and target particles, respectively, and the subscript ‘pc’ represents post-collision properties of the particles. Furthermore, $S(g, \chi)$ is the differential scattering cross section, which is a function of the relative particle velocity, $g = |v_i^{(1)} - v_i^{(2)}|$, the azimuth angle, $\epsilon$, and the scattering angle, $\chi$. The underlying assumptions behind the derivation of Eq. (2.9) are the presence of molecular chaos, binary collisions, and a spherical symmetric force between particles, which obeys the laws of classical mechanics [1].

Table 2.3: Random Velocity Moments of the Distribution Function

<table>
<thead>
<tr>
<th>Order</th>
<th>Weight</th>
<th>Moment</th>
<th>Physical Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>$\rho$</td>
<td>Density</td>
</tr>
<tr>
<td>1</td>
<td>$c_i$</td>
<td>0</td>
<td>Random velocity momentum</td>
</tr>
<tr>
<td>2</td>
<td>$c_i c_j$</td>
<td>$P_{ij}$</td>
<td>Anisotropic pressure tensor</td>
</tr>
<tr>
<td>3</td>
<td>$c_i c_j c_k$</td>
<td>$Q_{ijk}$</td>
<td>Total heat flux tensor</td>
</tr>
<tr>
<td>3</td>
<td>$c_i c_j c_j$</td>
<td>$Q_{ijj}$</td>
<td>Contracted heat flux tensor</td>
</tr>
<tr>
<td>4</td>
<td>$c_i c_j c_k c_l$</td>
<td>$R_{ijkl}$</td>
<td>Distribution function kurtosis tensor</td>
</tr>
<tr>
<td>4</td>
<td>$c_i c_j c_j c_j$</td>
<td>$R_{ijjj}$</td>
<td>Contracted distribution function kurtosis tensor</td>
</tr>
<tr>
<td>5</td>
<td>$c_i c_j c_k c_m$</td>
<td>$S_{ijklm}$</td>
<td>Fifth-order random velocity moment tensor</td>
</tr>
<tr>
<td>5</td>
<td>$c_i c_j c_k c_k c_k$</td>
<td>$S_{ijjkk}$</td>
<td>Contracted fifth-order random velocity moment tensor</td>
</tr>
</tbody>
</table>
Due its complexity as well as the requirement for adequate knowledge of the distribution function, the challenges, both theoretically and numerically, of evaluating Eq. (2.9) can be prohibitive for practical applications and therefore simplified forms of the collision operator are often introduced. The earliest, simplest and most popular of these simplifications is the relaxation-time, or Bhatnagar-Gross-Krook (BGK), collision operator [46]. This collision models assumes that inter-particle collisions relax the distribution \( F \) to an equilibrium distribution \( M \) with a characteristic relaxation time scale, \( \tau \), such that

\[
\frac{\delta F}{\delta t} = -\frac{F - M}{\tau}.
\] (2.10)

An inconvenient of this simplified representation is that all moments of \( F \) are relaxed towards their equilibrium value over the same time scale, therefore limiting its applicability to gases with a unit Prandtl number, \( Pr \). An extension of the BGK collision operator, namely the ellipsoidal-statistical, or ES-BGK, collision operator has been devised such that it allows for gases with a tunable Prandtl number [47]. In this case, \( F \) relaxes towards a modified Gaussian distribution, \( G_{ES} \) over a relaxation time \( \tau_{ES} = \tau/Pr \) such that

\[
\frac{\delta F}{\delta t} = -\frac{F - G_{ES}}{\tau_{ES}},
\] (2.11)

where \( G_{ES} \) is given by

\[
G_{ES} = \frac{\rho/m}{(2\pi)^{3/2}} \frac{1}{|T_{ij}|^{1/2}} \exp \left( -\frac{1}{2} T_{ij}^{-1} c_i c_j \right)
\] (2.12)

and where

\[
T_{ij} = \frac{P_{ij}}{\rho} - \frac{1}{\rho Pr} (P_{ij} - \rho \delta_{ij}).
\] (2.13)

Throughout this document, Eq. (2.8) with \( \delta F/\delta t \) evaluated using the BGK and ES-BGK collision operators will be referred to as the BGK equation and ES-BGK equation, respectively.

### 2.5 Solution Strategies for the Boltzmann Equation

Different approaches have been developed and are available to numerically solve the full form of the Boltzmann equation as given in Eq. (2.8) for general non-equilibrium gaseous flows, and depending on the flow regime and the nature of the desired solution, several deterministic and probabilistic approaches are available. Deterministic methods of note include discrete velocity models (DVMs) as well as moment methods, and probabilistic solutions are mainly obtained via Lagrangian-based approaches.
2.5.1 Discrete Velocity Models.

DVMs, or discrete ordinates methods, were initially introduced in the context of radiative heat transfer [48] and later in the context of rarefied gas dynamics [49–51]. They rely on the discretization of the phase-space distribution function onto a velocity grid, as is notably performed by Mieussens et al. in more recent applications [10, 52, 53]. These methods are valid for flows ranging from the continuum to the free molecular regimes, however they are known to be computationally very expensive due to the requirement of discretizing Eq. (2.7) into three spatial, three velocity and one time dimensions, as well as numerically evaluating the Boltzmann collision integral. BGK-like simplifications to the collision operator have however been extensively studied to reduce the associated costs [46, 47], and adaptive velocity grid techniques have been studied to reduce the discretization cost of the distribution [53].

2.5.2 Lagrangian Methods.

Lagrangian methods avoid the direct solution of the Boltzmann equation altogether by instead directly modelling inter-particle interactions. The purest Lagrangian approach is the molecular dynamics method [54, 55], which tracks the movement of each individual gas particle as well as inter-particle collisions, therefore resulting in prohibitive computational times for anything but a very dilute gas. Another approach is the direct simulation Monte-Carlo (DSMC) method, initially developed by Bird [9]. The DSMC technique models macro-particles, each representing many individual particles, and instead models collisions statistically using a probabilistic approach. Though DSMC is theoretically valid from the continuum to free-molecular limits, it becomes very expensive for transition regime flows approaching the continuum limit, where the flow becomes more collision-dominated.

2.5.3 Method of Moments.

Moment methods, or moment closure methods, reduce the dimensionality of Eq. (2.7) by instead transporting a finite set of moments representing the non-equilibrium distribution function. Though this approach is known to fail approaching the free-molecular limit, a finite set of moments is often sufficient to predict relevant properties of the distribution function for flows in both the continuum and transition regimes. Furthermore, they can provide a useful bridge to the free-molecular regime and are available at a fraction of the computational cost of DVMs and Lagrangian methods. A known challenge of moment closure methods however arises from the truncated number of transport equations, which yields high-order moments within the advection term of Eq. (2.7) for which the system is unclosed. This is
typically resolved by introducing an assumed form of the phase-space distribution function, as was initially proposed by Grad [4]. Improve descriptions of non-equilibrium flows by moment closure methods are the subject of this thesis and background theory relevant to moment closures is covered more extensively in Chapter 4.
Chapter 3

Spray Dynamics

Liquid spray behavior is highly dependent on the flow conditions. In particular, a spray’s behavior can be represented by both its spray regime and mode of breakup or atomization. The mass and volume ratio of liquid to surrounding air or gas will first determine the spray regime. Next, by considering liquid surface tension and aerodynamic forces, one can predict the breakup mode for the continuous liquid into droplets. As the focus of this thesis is on the mathematical description of post-primary breakup sprays in the disperse regime, break-up modes and models will not be discussed extensively here. Spray regimes will however be introduced in order to define the region of applicability of the proposed model, namely the dispersed phase of a liquid spray.

3.1 Spray Regimes

Faeth et al. [56] have given a general description of fuel spray behavior as it is injected through the nozzle of an engine. It first propagates as a column, referred to as the liquid core, before breaking up into dispersed droplets away from this core. The near-core region is the so-called dense spray region and further away from the core the spray becomes first disperse and then dilute. This behavior is illustrated in the schematic diagram of Figure 3.1.

Marchisio et al. [40] provide a more specific classification of the major spray regimes found in the literature in terms of the droplet volume fraction, $\alpha$, the phase mass ratio $\phi$ and the maximum particle volume fraction for close packing, $\alpha^*$. This classification is summarized in Table 3.1. For the purpose of this thesis, the focus will be on post-primary atomization flows ranging from the onset of the dispersed flow region to the dilute spray region, as moment closure methods are known to be valid within these zones. For more dense sprays however, Eulerian-based representations using techniques such as the volume-of-fluid (VOF) [57] or $\Sigma$-$Y$ [58] spray atomization models are preferred. To encompass the entire spectrum of
spray regimes, a coupling of the Eulerian and disperse spray descriptions is possible leading to Eulerian-Lagrangian Spray Atomization (ELSA) models [29], or the coupling of an Eulerian spray atomization model to the Eulerian description of the disperse phase based on the method of moments as will be considered in this thesis.

3.2 Spray Physics: Williams-Boltzmann Equation

Williams [59] first introduced a kinetic-theory-like statistical formalism for describing spray behavior. Generally, sprays are affected by growth, formation of new droplets (i.e., breakup), collisions and aerodynamic forces. The original assumptions behind Williams’ work allowed the treatment of spherical droplets. By assuming low Weber numbers (i.e., small droplets with low velocity relative to the gas) and disperse sprays, we are able to reduce the spatial description of a droplet to a single radius, \( r \). Under these conditions, a generalized population balance equation (GPBE) for the time rate of change of \( F(r, x_i, v_i, t) \) can be derived.

Table 3.1: Spray Regimes [40]

<table>
<thead>
<tr>
<th>Regime</th>
<th>Characteristics</th>
<th>Considerations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Very dilute</td>
<td>( \alpha \ll 1 ) and ( \phi \ll 1 )</td>
<td>Coupling with carrier phase not required.</td>
</tr>
<tr>
<td>Dilute</td>
<td>( \alpha \ll 1 ) and ( \phi \geq 1 )</td>
<td>Coupling with carrier phase becomes important.</td>
</tr>
<tr>
<td>Moderately Dense</td>
<td>( \alpha &lt; \alpha^* ) and ( \phi \geq 1 )</td>
<td>The binary collision assumption is no longer valid.</td>
</tr>
<tr>
<td>Dense</td>
<td>( \alpha \approx \alpha^* )</td>
<td>The instantaneous collision assumption is no longer valid. Particle-particle contact is sustained.</td>
</tr>
</tbody>
</table>
This governing kinetic equation for spray modeling is commonly referred to as the Williams-Boltzmann equation and is given by

\[
\frac{\partial F}{\partial t} + \frac{\partial}{\partial r}(RF) + \frac{\partial}{\partial x_i}(v_i F) + \frac{\partial}{\partial v_i}(a_i F) = Q + \frac{\delta F}{\delta t}.
\]  

(3.1)

The Williams-Boltzmann equation accounts for the particle growth rate, \( R \equiv \partial r/\partial t \), particle acceleration, \( a_i \equiv \partial v_i/\partial t \), formation of new particles, \( Q \), and collisions between particles, \( \delta F/\delta t \). Particle acceleration is mainly due to drag forces between the liquid drops and the background gas. The acceleration term is thus referred to as the drag term. The Stokes number, \( St \), quantifies the ratio between droplet characteristic time, \( \tau_p \), and carrier phase characteristic time, \( \tau_g \), and is written as

\[
St = \frac{\tau_p}{\tau_g} = \frac{\rho d^2 U}{18 \mu_g L},
\]  

(3.2)

where \( \rho \) and \( d \) are the droplet density and diameter respectively, \( \mu_g \) is the carrier phase kinetic viscosity, and \( U \) and \( L \) are the characteristic flow velocity and length scales respectively. Spray flows with \( St \gg 1 \) indicate very inertial droplets with high relative velocities between the gas and carrier phases, whereas flows with \( St \) well below a critical Stokes number, \( St_c \), indicate non-inertial droplets that instantaneously relax towards the gas phase velocity. A common assumption for low Stokes number sprays is to assume a nearness to the Stokes regime, in the sense that the disperse phase velocity is not far from the carrier phase velocity. In this case, it can be assumed that drag can be evaluated using Stokes’ law [60, 61]:

\[
a_i = \frac{18\pi \mu_g}{\rho_p S} (u_i - u_{gi}) = \frac{u_i - u_{gi}}{\tau_p}
\]  

(3.3)

where \( u_i \) is the droplet velocity, \( u_{gi} \) is the carrier phase velocity, \( \mu_g \) is the carrier phase dynamic viscosity and \( S \) is the droplet surface area, from which the characteristic drag relaxation time, \( \tau_p \), can be obtained. When studying more dense sprays, droplets with greater inertia cause the disperse and carrier phases to have larger differences in velocity. The Stokes drag assumption thus no longer holds and more elaborate formulations of \( a_i \) must be employed.

For the purpose of this study, a simplified Stokes’ drag operator will be adopted for all cases considered, including those with considerably inertial droplets. Although this assumption does not hold in the latter case, it is sufficient when assessing the ability of the proposed moment closure methods to capture PTCs.

The other terms of the Williams-Boltzmann equation of Eq. (3.1) are dependent on several
physical phenomena. Firstly, the growth term is mainly affected by droplet evaporation into
the surrounding carrier phase. The particle source term, $Q$ is dependent on the creation of
new droplets which arises from boundary conditions as well as secondary droplet breakup or
coalescence. Finally, the collision term can be modelled similarly to gaskinetic theory cases,
as was described in Eq. (2.9) and its simplified operators. For the purpose of the multiphase
flow portion of this study, particle sources and growth as well as inter-particle collisions are all
neglected, and constant sized monodisperse particles are considered. This reduced description
of an isolated system of monodisperse particles will allow the of moment closure techniques
for accurate prediction of droplet transport with PTC. In this case, the following simplified
governing kinetic equation is considered

$$\frac{\partial F}{\partial t} + \frac{\partial}{\partial x_i} (v_i F) = \frac{\partial}{\partial v_i} \left( \frac{u_{gi} - u_i}{\tau_p} F \right).$$

(3.4)

Since particle size and gas phase properties are held constant, the flow Stokes number can
easily be tuned through the variation of the characteristic drag relaxation time $\tau_p$ alone.

### 3.2.1 Solution Strategies for the Williams-Boltzmann Equation

For dispersed multiphase flow applications, Lagrangian solution techniques are currently much
more widespread than their Eulerian counterparts, especially when considering commercial
implementations. Dukowicz initially developed the Euler-Lagrange formalism for modeling
fuel sprays in the context of fuel injection in a diesel engine [23]. In this formalism, the gas
phase is typically computed using a hydrodynamic model such as the Navier-Stokes equations
and is coupled to a Lagrangian model for droplet descriptions. A particle motion equation
depending on the gravity, pressure and drag forces acting on a $k^{th}$ particle in a gaseous flow
can be written as

$$\frac{d}{dt} x_i^{(k)} = u_i^{(k)},$$

(3.5)

$$m^{(k)} \frac{d}{dt} u_i^{(k)} = m^{(k)} g_i - \frac{m^{(k)}}{\rho^{(k)}} \frac{\partial p_k}{\partial x_i} + D^{(k)} [u_{gi}] \left( u_{gi} - u_i^{(k)} \right),$$

(3.6)

where the superscript $(k)$ denotes the properties of the $k^{th}$ particle, $x_i$ denotes position, $u_i$
the particle velocity, $m$ the particle mass, $\rho$ the density, $p_k$ the gas phase pressure and $D_k$ the
drag function, which is dependent on the instantaneous gas phase velocity, $u_{gi}$. One challenge
lies in the calculation of this drag function, for which simplified models [62] are required due
to the intractability of fully resolving the flow about each droplet. Lagrangian methods often
rely on the tracking of representative parcels of particles rather than computing the position
of each particle individually.
As discussed in Chapter 1, Lagrangian methods tend to fall short in the areas of computational cost, parallelization and coupling with the carrier phase. More recently, Eulerian solution strategies for resolving dispersed phases have been more widely studied. The most popular methods tend to belong to the quadrature method of moments (QMOM) [40], which has been extensively studied by Fox et al. [38, 39, 63] and Massot et al. [42, 61, 64]. These will be described in greater depth in the following chapter.
Chapter 4

Moment Closure Methods

Moment closure methods offer the possibility of obtaining approximate solutions to the Boltzmann or Williams-Boltzmann equations through the solution of a finite set of PDEs. For the purpose of this thesis and to provide a more straightforward development of the moment equations, a combined system having both drag and collision terms is considered. This is obtained by introducing the source terms of both Eqs. (2.7) and (3.4) to the kinetic equation of interest. The representative kinetic model considered in this section then takes the form

\[
\frac{\partial F}{\partial t} + \frac{\partial}{\partial x_i} \left( v_i F \right) = \frac{\delta F}{\delta t} + \frac{\partial}{\partial v_i} \left( \frac{u_{gi} - u_i}{\tau_p} F \right). \tag{4.1}
\]

The derivation and properties of the resulting moment systems arising from application of the method of moments to Eq. (4.1) is given in the sections to follow.

4.1 Maxwell’s Equation of Change

To properly illustrate a given system of moment transport equations it is convenient to define a vector of velocity weightings corresponding to the transported moments. In particular, the vector

\[
W^{(N)} = m \left[ W_0, W_1, W_2, \ldots, W_N \right] \tag{4.2}
\]

represents a combination of velocity weightings, \( W_k \); \( k = 1, N \), of the form \( v_{\alpha} v_{\beta} v_{\gamma} \) or \( c_{\alpha} c_{\beta} c_{\gamma} \) from which corresponding moments can be integrated. The resulting transport equations for these moments are described by Maxwell’s equation of change, which can be written as

\[
\frac{\partial}{\partial t} \left< mW^{(N)} F \right> + \frac{\partial}{\partial x_i} \left< mW^{(N)} F v_i \right> = \left< mW^{(N)} \frac{\delta F}{\delta t} \right> + \left< m \left( \frac{u_i - u_{gi}}{\tau_p} \right) \frac{\partial W^{(N)}}{\partial v_i} F \right> \tag{4.3}
\]
The first term of Eq. (4.3) represents the time rate of change of the moments, or macroscopic quantities, of $\mathcal{F}$, whereas the second term represents the fluxes of these moments and is known as the flux dyad. The first and second right-hand side (RHS) terms are then source terms representing the respective influences of inter-particle collisions and drag forces on the moments of the distribution, both of which will be considered in this study. Theoretically, transporting an infinite set of these moments is required to fully describe an arbitrary non-equilibrium distribution and therefore fully replicate results from the kinetic equation exactly. This is however practically impossible and certainly not desirable computationally. Instead, a truncated set of moments that can adequately depict the physical phenomena of interest is sought. The desire for a finite set of moments introduces the closure problem: at least one higher order moment will be present in the solution fluxes of the highest moment given in Eq. (4.3) and thus the system of moment transport equations becomes unclosed. An expression for the next higher-order moments is required in terms of the chosen finite set of moments through a moment closure method.

4.2 Moment Closures

Typically, two moment closure approaches are found in the literature. The first involves algebraic-based closures and generally relies on the transport of a limited set of moments, with closures computed using equilibrium assumptions [65], which are generally inspired by RANS turbulence models [66, 67]. This empirical approach is known to suffer from moment realizability issues and furthermore is not applicable to the kinetic descriptions of previous sections. Their domain of applicability has therefore mainly been limited to turbulence applications. The second approach, the kinetics-based moment method (KBMM), relies on the reconstruction of an assumed form of the phase-space distribution function, as was initially described by Grad [4]. An expression for the distribution function can then be obtained in terms of the lower-order moments. This is performed by ensuring the moments of the reconstructed distribution, $\mathcal{F}^{(N)}$, match the given moments of the solution vector such that

$$M^{(N)} = \langle W^{(N)} \mathcal{F}^{(N)} \rangle. \tag{4.4}$$

Other arbitrary moments can then be integrated using this representative distribution function in order to close the system. The calculation of $\mathcal{F}^{(N)}$ is obtained via an inversion procedure known as a moment inversion algorithm.

In order to be valid, a reconstructed distribution function and its corresponding moment inversion algorithm must satisfy certain constraints. Marchisio and Fox define two such
Chapter 4. Moment Closure Methods

constraints (1-2) as well as properties of the inversion algorithm (3-4) that are desirable in the context of its implementation into a numerical solution procedure for the corresponding moment equations [40]. A representative distribution must firstly be (1) positive for all realizable moment values, as a PDF is positive by definition. It must be (2) realizable, and therefore the distribution must be nonzero only for physically realizable values of physical properties. It must also be (3) extensible to arbitrary order. Finally, it must be (4) non-iterative to save on computational cost. In the case that (4) is not achievable, any iterative numerical method must guarantee convergence. This is especially important when applying moment inversion algorithms as part of a numerical solution procedure for the moment equations, since an inversion for $F^{(N)}$ is often performed many times in each computational cell, at every time step. Here, we focus on three main families of moment closures relying on different types of reconstructed distribution functions which satisfy these constraints to different extents, namely the Grad [4], maximum-entropy-based [13–15] and quadrature-based [36, 40] moment closures. Each of these techniques are described now in turn.

4.2.1 Grad Moment Closures

The earliest category of reconstructed distribution functions was introduced by Grad [4]. In his initial work, he assumed a distribution function, $F_{\text{Grad}}^{(N)}$, that is a polynomial expansion about the equilibrium Maxwellian, $M$. The Grad distribution takes the form

$$F_{\text{Grad}}^{(N)} = M \left[ 1 + P^{(N)}(v_i) \right],$$

where $P^{(N)}(v_i)$ is a Hermite polynomial expansion function containing N free parameters. This representation leads to a system of N moment transport equations for which the parameters of $P^{(N)}$ can be determined analytically, therefore allowing for closed-form expressions to the higher order moments. Grad developed a hierarchy of models for which moment systems with $N = \{5, 8, 10, 13, 20\}$ moments are available. A major detractor of the Grad polynomial expansion is that the polynomial $P^{(N)}$ is not guaranteed to be positive for all velocities, therefore resulting in non-positivity of the distribution for certain regions in realizable moment space. Furthermore, the Grad moment closures are known to become non-hyperbolic for moderate departures from LTE, and the closure tends to break down in these cases due to the development of complex wave speeds [68].
4.2.2 Quadrature-Based Moment Methods

An alternative moment closure technique is the quadrature method of moments (QMOM) as originally proposed by McGraw for the treatment of aerosols [36]. In this approach, the reconstructed distribution is based on a summation of weighted Dirac delta functions in velocity space. A quadrature-based distribution, $F_\delta$, can be generally expressed as

$$F_\delta = \sum_{k=1}^{N} w_k \delta(v_i - v_{ki}), \quad (4.6)$$

where an $N$-node quadrature is formed of velocity abscissas positioned at $v_{ki}$ with weights $w_k$. Brute-force approaches for solving for the parameters of $F_\delta$ are available [69]; however, the associated computational cost has prompted the development of different exact and approximate inversion algorithms which will be introduced in the following sections. An advantage of the QMOM is its scalability and adaptability to arbitrary moment sets by simple selection of different moments and an adequate number of nodes, $N$. In practice however, these methods are better suited for “optimal moment sets”, as defined by Fox [70]. The most notable condition for this optimal moment set is the requirement for all linearly independent moments of a certain order to be included before considering higher order moments, therefore producing symmetrical moment combinations, as illustrated in Table 4.1. This is advantageous, in the sense that moments are selected for best correspondence with a given quadrature (and vice-versa), however physical arguments for the selection of these moments (e.g., maximum-entropy considerations) have not been considered or taken into account. Furthermore, efficient quadrature algorithms are not available for solution vectors containing contracted moments such as those given in Table 2.3.

In recent years, many variants of the QMOM have been explored. These are based on different inversion algorithms for the quadrature weights and points $w_k$ and $v_{ki}$, different solution procedures for the moment transport equations, as well as different extended representations of the quadrature-based distribution. These approaches have recently been well catalogued

Table 4.1: Example of an Optimal Moment Set for a Two-Dimensional Quadrature with Moments up to Fourth-Order

<table>
<thead>
<tr>
<th>$M_{0,0}$</th>
<th>$M_{1,0}$</th>
<th>$M_{2,0}$</th>
<th>$M_{3,0}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_{0,1}$</td>
<td>$M_{1,1}$</td>
<td>$M_{2,1}$</td>
<td>$M_{3,1}$</td>
</tr>
<tr>
<td>$M_{0,2}$</td>
<td>$M_{1,2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$M_{0,3}$</td>
<td>$M_{1,3}$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
by Marchiso and Fox in the context of polydisperse multiphase flows [40]. At the core of most QMOMs lies a univariate inversion algorithm for unidirectional or pure moments. The available algorithms that are used are the Partial-Difference (PD) [71] and Wheeler algorithms [72]. The latter contains less restrictions on its applicability to a given moment set and is used in many of today’s moment inversion algorithms [38, 39, 73, 74].

Classical Quadrature Methods of Moments. The original QMOMs obtain expressions for Eq. (4.6) by solving Eq. (4.4) directly. For multivariate systems (i.e., multidimensional moment sets), this is performed by numerically solving a nonlinear system of equations for the moments of the solution vector, where

\[ M_{\alpha, \beta, \gamma} = \sum_{k=1}^{N} w_k v_{k\alpha} v_{k\beta} v_{k\gamma}. \]  

(4.7)

This system has been initially solved by Wright et al. in the context of coalescing and sintering particulate flows using a Newton-Raphson technique [69]. This method can prove difficult to converge due to the requirement for a reasonable initial guess for the distribution’s parameters, and can rapidly fail when in presence of near singular moment sets. Another approach is the Tensor-Product (TP) QMOM, which has been applied in the context of aerosols [73, 74] and gas-solid flows [70, 75]. This approach utilizes knowledge of univariate quadratures of the pure moments, which can be computed using the Wheeler algorithm. Based on these univariate quadratures, a linear system can be constructed and solved for the weights and abscissas of the distribution without an iterative procedure. The TP QMOM is however quite restrictive in possible selections of moment sets and though its solution procedure is non-iterative, the encountered computational remains high.

Direct Quadrature Method of Moments (DQMOM). Rather than constructing transport equations for the moments of the phase-space distribution function, the direct quadrature method of moments relies on an initial quadrature-based distribution, \( F_\delta \). The weights and abscissas of \( F_\delta \) are then transported directly using a modified version of the Williams-Boltzmann kinetic equation [76]. Macroscopic quantities of the distribution of the NDF can then be computed from these transported quantities. The advantage of using the DQMOM is that a moment inversion algorithm can be avoided altogether. However, the nature of the DQMOM transport equations makes dealing with moment realizability problematic, and it has been shown that moment inversion is unavoidable when considering high-order numerical schemes [40]. The study of DQMOM has slowed in recent years due to the development of more efficient moment inversion algorithms such as the extend (EQMOM) and conditional
Chapter 4. Moment Closure Methods

Extended Quadrature Method of Moments (EQMOM). Yuan and Fox were the first to formally introduce extended quadrature methods of moments for population balance equations \[39\]. The idea behind an extended quadrature is to assume that a kernel density function (KDF) associated with or centered about each quadrature node of the reconstructed distribution. KDFs can offer finite, semi-infinite and infinite support and examples considered by Yuan and Fox include the Beta, Gamma and Gaussian distributions respectively. Though they were the first to describe the generalized formalism behind EQMOMs, previously explored moment closure methods such as the Gaussian closure for kinetic theory and multiphase flows \[42, 68, 77–79\] as well as more preliminarily developed multi-gaussian closures \[80, 81\] fit into the EQMOM category. This category of distribution functions has shown some relationship with maximum-entropy-based moment closures \[44\], and even exact correspondence in the case of the Gaussian closure \[42\]. Furthermore, the reconstructed distribution proposed in this thesis is an EQMOM distribution having a number of very interesting properties from a maximum-entropy perspective \[44\]. The proposed moment closure relies on a reconstructed bi-Gaussian distribution, and is introduced in Section 4.4.3 to follow.

Conditional Quadrature Method of Moments (CQMOM). Due to the high computational cost of obtaining exact quadratures satisfying all transported moments, a conditional quadrature method of moments has also been introduced by Yuan and Fox \[38\]. Rather than using the general definition of the quadrature-based distribution, a distribution conditioned in a particular direction in velocity space is used. This is obtained by considering that a distribution in a particular velocity direction can be evaluated assuming a known distribution in other velocity directions. A velocity distribution can therefore be written as a combination of distributions, recursively conditioned on the primary velocity direction. For example, a velocity PDF, $f(v_i)$, conditioned primarily in the $v_x$ direction, and subsequently in the $(v_x, v_y)$ direction, can be written as

$$f(v_i) = f(v_x|v_x, v_y)f(v_x, v_y) = f(v_x|v_x, v_y)f(v_y|v_x)f(v_x),$$  \hspace{1cm} (4.8)

where the notation $f(\xi|\eta)$ denotes the evaluation of a PDF in the $\xi$ direction, conditioned on a fixed PDF in the $\eta$ direction. In this case, the use of the PDF, $f$, rather than the phase-space distribution function, $F$, is required in order to exploit the property of probability multiplication. The value of the nodes of $f$ is obtained by performing a series of nested 1D moment inversions using the Wheeler algorithm, starting with the primary velocity direction ($v_x$ in this case). A purely $v_x$-directional quadrature is therefore initially obtained. The 1D
moment inversion can then subsequently be applied for $v_y$, assuming the $v_x$ quadrature is known. Finally, one can obtain the $v_z$ quadrature for a known quadrature representation of $f(v_x, v_y)$. It is important to note that different quadrature representations of the distribution are obtained for different permutations of the velocity directions, for which two and six permutations are available in bivariate (e.g. 2D) and trivariate (e.g. 3D) kinetic systems respectively. Furthermore, though the pure moments in the primary velocity direction are guaranteed to be satisfied by the CQMOM distribution, the CQMOM algorithm does not guarantee that all the moments of the solution vector will be satisfied, with higher-order moments in non-primary velocity directions suffering from a heightened level of error.

The CQMOM nevertheless remains a powerful moment inversion algorithm, since it is easily scalable to higher-order moment systems and is computationally inexpensive as compared to direct inversion algorithms. Furthermore, recent developments have shown that a combination of the CQMOM and EQMOM approaches (ECQMOM) is possible. Keeping in mind the potential application of turbulent disperse multiphase flows with significant PTC, an ECQMOM utilizing a bi-Maxwellian distribution [80, 81] in place of the Wheeler algorithm for the 1D inversion procedure has shown excellent results for preliminary turbulent multiphase flow applications [43]. This closure should be a strong basis for comparison with future developments of the bi-Gaussian closure proposed herein.

4.2.3 Maximum-Entropy Moment Closures

More recently, a family of reconstructed distribution functions based on thermodynamic entropy maximization has been considered [13–15]. Maximum-entropy moment closures present many attractive mathematical properties. For one, the reconstructed maximum-entropy distribution is the most likely distribution for a given set of moments. It also remains positive for all physically realizable moments. Additionally, since the maximum-entropy distribution is not based on an expansion about the equilibrium Maxwellian, its corresponding moment closures have the potential of offering a region of validity that extends well beyond local equilibrium, unlike conventional Grad closures. Such closures are in fact known to remain hyperbolic for any given set of realizable moments [15], making them very well suited for solution by finite-volume and discontinuous Galerkin (DG) numerical schemes.

The maximum entropy distribution is obtained via an optimization problem, where the Boltzmann entropy (entropy of interest for kinetic equations considered here), defined by $-\kappa [\mathcal{F} \ln \mathcal{F} - \mathcal{F}]$, must be maximized following the constraint

$$\max_{\mathcal{F}} \langle -\kappa [\mathcal{F} \ln \mathcal{F} - \mathcal{F}] \rangle \quad \text{for} \quad \mathcal{F} \geq 0.$$  \hspace{1cm} (4.9)
This problem is solved using the method of Lagrange multipliers, and yields the form

$$F^{(N)}_{\text{MaxEnt}} = \exp(\alpha^T W^{(N)})$$

(4.10)

for the maximum entropy distribution, where the closure coefficients, $\alpha^T$, are the Lagrange multipliers. As described in Section 4.3, different selections of the velocity weights, $W^{(N)}$, yield maximum-entropy distributions which, up to second order, correspond to the well-known Maxwellian and Gaussian distributions. The Gaussian distribution has been notably well-studied for non-equilibrium flows and sprays [42, 68, 77–79], however fails to capture flows with significant heat transfer or PTC. Moment closures with bi-modal distributions and thus velocity weightings higher than second-order are required. Unfortunately, for moment systems with super-quadratic velocity weightings, there exists no closed-form expression to the maximum-entropy distribution function, and the entropy maximization problem must be solved via a complex and computationally expensive iterative procedure, which can often be ill-posed due to singular subspaces in moment space [16]. The associated minimization problem, known as the maximum-entropy problem, has the form

$$\frac{\partial}{\partial \alpha} \left[ \langle \exp(\alpha^T W^{(N)}) \rangle - \alpha^T M^{(N)} \right] = 0,$$

(4.11)

and the computational cost of obtaining iterative solutions to Eq. (4.11) would not seem justifiable for practical simulations of non-equilibrium rarefied flows or polykinetic sprays. An example of a numerical solution procedure for the entropy maximization problem is proposed by Mohammad-Djafari [82], and will be used to perform comparisons with proposed moment closures in Chapter 5.

To circumvent the issues related to solving Eq. (4.11), notable interpolative methods for obtaining moment closures to high-order maximum-entropy systems have recently been proposed [17, 18], and are reviewed briefly in Section 4.4.2.

### 4.3 Maximum Entropy Closure Hierarchy

Though Dreyer [13] and Müller and Ruggeri [14] initially introduced entropy maximization in the context of non-equilibrium flows, Levermore [15] was the first to introduce the maximum entropy closure in a structured, hierarchic form and explore their desirable mathematical properties. He defined a hierarchy of maximum-entropy closures for rarefied gas dynamics satisfying specific requirements on velocity weightings. The first requirement of the maximum-entropy closures is that they must reduce to the Euler closure for equilibrium flow conditions. This
therefore implies that the velocity weighting vector or its contractions must include the Euler weightings $W^{(5)} = m[1, c_i, c_j c_j / 3]$. The maximum entropy hierarchy therefore naturally contains the Euler velocity weighting vector as its most basic member. The next requirement is that the velocity weighting vector be invariant under orthogonal and translational transformations. The ensuing velocity weighting vector, and its resulting moment system, is therefore Galilean invariant. The final condition is that each combination of velocity weightings must lead to a finite distribution function over all of velocity space, including as $v_i \rightarrow \infty$. Following these criteria, Levermore’s hierarchy includes 5-, 10-, 14-, 21-, 26-, and 35-moment closures with

$$N = 5, \quad W^{(5)} = m[1, c_i, c_i c_i / 3], \quad C^{(5)} = [\rho, u_i, p],$$

$$N = 10, \quad W^{(10)} = m[1, c_i, c_i c_j], \quad C^{(10)} = [\rho, u_i, P_{ij}],$$

$$N = 14, \quad W^{(14)} = m[1, c_i, c_i c_j, c_i c_j c_j, c_i c_j c_j c_j], \quad C^{(14)} = [\rho, u_i, P_{ij}, Q_{ij}, R_{ij}],$$

$$N = 21, \quad W^{(21)} = m[1, c_i, c_i c_j, c_i c_j c_k, c_i c_j c_j c_k], \quad C^{(21)} = [\rho, u_i, P_{ij}, Q_{ijk}, R_{ij}],$$

$$N = 26, \quad W^{(26)} = m[1, c_i, c_i c_j, c_i c_j c_k, c_i c_j c_k c_k], \quad C^{(26)} = [\rho, u_i, P_{ij}, Q_{ijk}, R_{ijkl}],$$

$$N = 35, \quad W^{(35)} = m[1, c_i, c_i c_j, c_i c_j c_k, c_i c_j c_k c_k c_k], \quad C^{(35)} = [\rho, u_i, P_{ij}, Q_{ijk}, R_{ijkl}].$$

The 5- and 10-moment members of the maximum entropy hierarchy lead to the equilibrium Maxwellian and anisotropic Gaussian distributions respectively. The Maxwellian distribution corresponds to the well-studied Euler equations for inviscid flow. The 10-moment Gaussian equations are the lowest-order member allowing for the treatment of viscous and non-equilibrium effects through its anisotropic standard deviation tensor. The next member of the hierarchy, the 14-moment closure, is the lowest order closure allowing to capture non-zero heat flux, which are important when considering that significant and unique heat flux effects are present in many non-equilibrium flows [18–22, 44]. The ability to capture non-zero heat flux is due to the fact that 14-moment and above systems allow for multi-modal distributions which permit multiple temperature distributions and therefore heat flux.

Since high-order moment systems tend to produce highly nonlinear systems of equations, it can be difficult to study their physical properties and ensuing eigensystems. It is therefore convenient to consider their corresponding univariate kinetic systems. One can therefore consider a theoretical 1D gas, for which fluid particles are constrained to movement in a single direction. The corresponding univariate kinetic equation is written as

$$\frac{\partial F}{\partial t} + \frac{\partial}{\partial x} \left( v F \right) = \frac{\delta F}{\delta t} + \frac{\partial}{\partial v} \left( \frac{u_g - u}{\tau_p} F \right).$$
Chapter 4. Moment Closure Methods

The resulting monokinetic moment systems satisfying Levermore’s criteria are

\[ N = 3, \quad W^{(3)} = m[1, c, c^2], \quad C^{(3)} = [\rho, u, p], \quad (4.19) \]
\[ N = 5, \quad W^{(5)} = m[1, c, c^2, c^3, c^4], \quad C^{(5)} = [\rho, u, p, q, r]. \quad (4.20) \]

where Eq. (4.19) is a monokinetic contraction of Eqs. (4.12) and (4.13), and Eq. (4.20) is a monokinetic contraction of Eqs. (4.14)-(4.17). The main focus of this study is the application of maximum-entropy-based closures to the 3D 14-moment system and its 5-moment univariate kinetic equivalent. An in-depth analysis of the physical and mathematical properties of the latter is presented in Chapter 5.

4.3.1 Gaussian Closure

In order to compare the performance of the 14-moment closures to be explored, the well-studied Gaussian closure [42, 68, 77–79] will serve as an adequate basis for comparison with a lower-order model capable of capturing non-equilibrium effects. The solution of Eq. (4.9) with the velocity weighting vector \( W^{(10)} = m[1, v_i, v_j] \) yields the random velocity distribution function

\[ \mathcal{F}_{\text{MaxEnt}}^{(10)} = \frac{(\rho_1/m)}{(2\pi)^{3/2} |\Theta_{ij}|^{1/2}} \exp \left[ -\frac{1}{2} \Theta_{ij}^{-1}(v_i - v_{1i})(v_j - v_{1j}) \right], \quad (4.21) \]

where the density weighting \( \rho_1 \), the velocity abscissa \( v_{1i} \) and the anisotropic standard deviation tensor \( \Theta_{ij} \) combine for ten free parameters which can be obtained in terms of the ten transported moments. Through the solution of Eq. (4.4), it can easily be shown that

\[ \rho_1 = \rho, \quad v_{1i} = u_i \quad \text{and} \quad \Theta_{ij} = \frac{P_{ij}}{\rho}. \quad (4.22) \]

The ensuing 10-moment system requires a closure for the 3rd-order random velocity moment, \( Q_{ijk} \), which represents heat flux. Based its unimodal nature, it can be expected that the closure for \( Q_{ijk} \) be zero. This can easily be shown through the fact that the distribution is centered at the mean fluid velocity and therefore that \( \langle mc_i c_j c_k G \rangle = 0 \).

Using the simplified closing relation for \( Q_{ijk} \), the resulting Gaussian transport equations are

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k}(\rho u_k) = C_0 + D_0, \quad (4.23) \]
\[ \frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_k}(\rho u_i u_k + P_{ik}) = C_1 + D_1, \quad (4.24) \]
\[ \frac{\partial}{\partial t}(\rho u_i u_j + P_{ij}) + \frac{\partial}{\partial x_k}(\rho u_i u_j u_k + u_k P_{ij} + u_j P_{ik} + u_i P_{jk} + Q_{ijk}) = C_2 + D_2. \quad (4.25) \]
where the Gaussian closure for the heat flux is $Q_{ijk} = 0$. For colliding particles in rarefied flow applications, the source terms $C_\alpha$, resulting from the BGK (or ES-BGK) collision operator, are written as

$$
\begin{bmatrix}
C_0 \\
C_1 \\
C_2
\end{bmatrix} =
\begin{bmatrix}
0 \\
0 \\
\frac{1}{3\tau} (\delta_{ij} P_{kk} - 3P_{ij})
\end{bmatrix}.
$$

(4.26)

In the case of spray applications with drag-subjected particles, the source terms $D_\alpha$, resulting from the Stokes drag operator, are written as

$$
\begin{bmatrix}
D_0 \\
D_1 \\
D_2
\end{bmatrix} =
\begin{bmatrix}
0 \\
\rho (u_{gi} - u_i) \\
\rho u_i (u_{gi} - u_j) + \rho u_j (u_{gi} - u_i) - 2P_{ij}
\end{bmatrix}.
$$

(4.27)

The Gaussian closure is quite advantageous in the sense that a closed-form expression is available for its distribution function. Furthermore, it has been shown to remain finite for all realizable moments, whereas higher-order closures are known to suffer from singular subspaces within realizable moment space [16–18]. However, its main drawback is the lack of ability to capture heat transfer effects. It therefore is limiting when considering that an important goal of the development of moment closure methods is to capture both Navier-Stokes and non-equilibrium limits, the former allowing for the treatment of heat transfer. The Gaussian closure has however shown applicability for continuum-to-transition regime flows where the effects of heat transfer are negligible. Furthermore, it is possible to consider a regularized Gaussian closure [68, 78], which has shown promise in capturing heat transfer effects using a 10-moment model through the application of a Chapman-Enskog-type expansion [83, 84] about the Gaussian distribution. This however yields the following non-hyperbolic terms for the heat flux

$$
Q_{ijk} = -\frac{\tau}{Pr} \left[ P_{kl} \frac{\partial}{\partial x_l} \left( \frac{P_{ij}}{\rho} \right) + P_{jl} \frac{\partial}{\partial x_l} \left( \frac{P_{ik}}{\rho} \right) + P_{il} \frac{\partial}{\partial x_l} \left( \frac{P_{jk}}{\rho} \right) \right],
$$

(4.28)

where the loss of a strict hyperbolic form is caused by the introduction of additional spatial derivatives within the flux term of Eq. (4.25). The ensuing system of transport equations therefore contains second-order spatial derivatives similar to diffusion terms in the Navier-Stokes equations. The regularized Gaussian closures will therefore not be considered herein.
4.4 Fourteen-Moment Closures

In order to account for appropriate treatment of heat transfer effects, it is necessary to consider higher-order members of Levermore’s maximum-entropy closure hierarchy. Maximum-entropy-based closures of Levermore’s hierarchy above the Gaussian closure have not been extensively studied. It is therefore of interest to consider the next higher-order model, namely the 14-moment closure. The expansion of Maxwell’s equations of change shown in Eq. (4.3) leads to the following system of transport equations for the 14 moments of this system

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_k}{\partial x_k} = \mathbf{C} + \mathbf{D}, \quad (4.29)
\]

where \( \mathbf{U} \) is a vector of moments corresponding to the conserved variables, \( \mathbf{F}_k \) is the flux dyad, and \( \mathbf{C} \) and \( \mathbf{D} \) are source terms representing inter-particle collisions and drag forces respectively. These vectors are given by

\[
\mathbf{U} = \begin{pmatrix} 
\rho \\
\rho u_i \\
\rho u_i u_j + P_{ij} \\
\rho u_i u_j u_k + u_i P_{jk} + u_j P_{ik} + u_k P_{ij} + Q_{ijk} \\
\rho u_i u_j u_k u_l + 2 u_i u_j P_{lk} + 2 u_i u_k P_{lj} + 2 u_j u_k P_{il} + 2 u_i u_j u_l P_{ij} + u_i Q_{ijj} + u_j Q_{ijk} + R_{ijj} \\
\end{pmatrix}, \quad (4.30)
\]

\[
\mathbf{F}_k = \begin{pmatrix} 
\rho u_k \\
\rho u_i u_k + P_{ik} \\
\rho u_i u_j u_k + u_j P_{ik} + u_i P_{jk} + u_k P_{ij} + Q_{ijk} \\
\rho u_i u_k u_j u_l + u_i u_k P_{ij} + 2 u_i u_j P_{lk} + u_j u_k P_{ij} + 2 u_i u_j u_k P_{ij} + u_i Q_{ijj} + u_j Q_{ijk} + R_{ijj} \\
\rho u_k u_i u_j u_l + 2 u_k u_i u_j P_{lk} + 4 u_i u_j P_{lk} + 4 u_i u_k P_{ij} + 2 u_i u_j u_l P_{ij} + 4 u_i u_k Q_{ijj} + 4 u_i u_k Q_{ijj} + 4 u_i u_j Q_{ijk} + 4 u_i u_j R_{ijj} + u_k R_{ijj} + S_{kij} \\
\end{pmatrix}. \quad (4.31)
\]
Chapter 4. Moment Closure Methods

32

\( C = \frac{1}{\tau} \begin{pmatrix} 0 \\ 0 \\ \frac{1}{3} (\delta_{ij}P_{kk} - 3P_{ij}) \\ \frac{1}{3} [2u_i(\delta_{ij}P_{kk} - 3P_{ij}) - 6u_jP_{jk} - 3\Pr Q_{ijj}] \\ \frac{1}{3} \left\{ \frac{1}{\Pr^2} \left[ (3\Pr^2 + 4\Pr - 2) P_{ii}P_{jj} + 6(\Pr - 1)^2 P_{ij}P_{ij} \right] \\ - 3\Pr R_{ijij} - 12\Pr u_{ij}Q_{ijj} + 4u_iu_j(\delta_{ij}P_{kk} - 3P_{ij}) \right\} \end{pmatrix} \) (4.32)

and

\( D = \frac{1}{\tau_p} \begin{pmatrix} 0 \\ \rho (u_{gi} - u_i) \\ \rho u_i (u_{gi} - u_j) + \rho u_j (u_{gi} - u_i) - 2P_{ij} \\ u_{gi} (\rho u^2 + P_{jj}) + 2u_{gi} (\rho u_i u_j + P_{ij}) - 3 [u_i (\rho u^2 + P_{jj}) + 2u_jP_{ij} + Q_{ijj}] \\ -4 (\rho u^4 + 2u^2P_{ij} + 4u_iu_jP_{ij} + 4u_iQ_{ijj} + R_{ijij}) \\ +4u_{gi} (\rho u^2 + u_iP_{jj} + 2u_jP_{ij} + Q_{ijj}) \end{pmatrix} \), (4.33)

Here, the collision term, \( C \), is modelled using the ES-BGK collision operator. The BGK collision operator can simply be recovered by setting the Prandtl number to \( \Pr = 1 \). The drag term is obtained through the expansion of the Stokes drag operator of Eq. (3.3).

A description of all moments contained in Eq. (4.29) can be found in Table 2.3. Here, closures are required for the random velocity moments \( Q_{ijk}, R_{ijjk} \), and \( S_{ijjkk} \), which are not contained in the solution vector, \( U \). Several maximum-entropy-based closures for these high-order moments are to be explored in the following sections. Furthermore, the moment system of Eq. (4.29) is subject to several realizability constraints which are presented below.

4.4.1 Moment Realizability

In the case of the Gaussian closure, moment realizability constraints, such as the requirement for positive definiteness of density and the pressure tensor, are rather intuitive. However, higher-order moment systems such as the 14-moment closure introduce additional realizability constraints on the high-order moments. In the prospect of mathematically determining the physical realizability boundaries of a set of moments, the solution of the Hamburger moment
problem [85] can provide essential conditions on moment realizability. Similar analyses for the 10- and 14-moment systems have been performed by Groth and McDonald [17, 68] and McDonald and Torrilhon [18]. Physical realizability boundaries can be determined by ensuring the matrix \( Y = \langle m \Omega \Omega^T \rangle \) remains positive definite such that \( V^T Y V > 0 \) for any vector \( V \) [85]. The vector \( \Omega \) contains velocity weightings that are selected such that the matrix \( Y \) contains all transported moments. In the case of the 14-moment system, the vector \( \Omega \) is taken to be \( \Omega = [1, c_x, c_y, c_z, c_i c_j] \) and yields the matrix

\[
Y = \begin{pmatrix}
\rho & 0 & 0 & 0 & P_{ij} \\
0 & P_{xx} & P_{xy} & P_{xz} & Q_{xii} \\
0 & P_{xy} & P_{yy} & P_{yz} & Q_{yii} \\
0 & P_{xz} & P_{yz} & P_{zz} & Q_{zii} \\
P_{ii} & Q_{xii} & Q_{yii} & Q_{zii} & R_{ijij}
\end{pmatrix},
\]

leading to the condition for positive-definiteness of

\[
R_{ijij} \geq Q_{kii}(P^{-1})_{kij}Q_{lij} + \frac{P_{ii}P_{jj}}{\rho}.
\]

Additionally, the realizability constraints encompass those of the 10-moment Gaussian model. These are

\[
\rho > 0, \quad P_{ii} > 0 \quad \text{and} \quad P_{ii}P_{jj} > P_{ij}P_{ij} \quad \forall \ i, j.
\]

For univariate kinetic systems, the solution of the Hamburger moment problem provides a necessary and sufficient condition for moment realizability. However, for multivariate kinetic systems such as the 14-moment model, it provides only a necessary condition. McDonald and Torrilhon [18] have nevertheless numerically investigated the 14-moment maximum-entropy distribution within the domain bounded by Eq. (4.35), and it was possible to show that \( \mathcal{F}_{\text{MaxEnt}}^{(14)} \) remains realizable within this space.

Though the Hamburger moment problem can provide constraints for moment realizability based on a general distribution function, additional constraints can arise when considering an assumed form of the distribution. In the case of maximum-entropy distribution functions arising from velocity weighting vectors containing superquadratic entries, it has been demonstrated that there exists a singular region within realizable moment space where the distribution is no longer finite and therefore the closure breaks down. This was shown by Junk in the context of the monokinetic 5-moment system of Eq. (4.20) [16]. This singular region of closure breakdown is therefore known as the Junk subspace. In three dimensions, the Junk
subspace is defined by the line
\[ Q = 0, \quad R_{ijj} > \frac{2P_{ij}P_{ij} + P_{ii}P_{jj}}{\rho}, \quad (4.37) \]
where \( Q = \| Q_{ijj} \| \). As the moment state approaches the Junk line, the distribution itself becomes singular: a peak of the maximum-entropy distribution sees its weight go to zero as its velocity abscissa goes to infinity. In this case, the fourth- and fifth-order velocity moments required to close the system diverge to \( \pm \infty \) on either side of the line. It is interesting to note here that this line coincides with the point where the distribution takes a 10-moment Gaussian form, for which
\[ R_{ijj} = \frac{2P_{ij}P_{ij} + P_{ii}P_{jj}}{\rho}. \quad (4.38) \]
Therefore, for a physical state with zero heat flux, there exists no finite distribution function when the fourth-order moment, \( R_{ijj} \), surpasses its Gaussian-associated value. This is rather troublesome, as the criterion represented by Eq. (4.38) coincides with local thermodynamic equilibrium. One can therefore expect that near-singular regions are often encountered when obtaining closures for moments corresponding to near-equilibrium states. Additionally, practical numerical simulations are often initialized using equilibrium distributions, meaning that for only modest deviations in the initial solution state, singular behaviour is encountered and special treatment must be considered. Strategies for the limitation of this singular behaviour have been previously explored by McDonald and Torrilhon [18] and Chalons et al. [43], and will be described in the following sections.

### 4.4.2 Interpolative Maximum-Entropy-Based Closure

As previously described, a known issue of high-order maximum-entropy-based models is the fact that it is impossible to obtain a generalized closed form expression to the distribution function [16]. Computationally intensive iterative procedures are in this case required in order to obtain solutions to the maximum-entropy problem, and the challenge increases as the singular Junk subspace is approached, as the velocity domain required to numerically obtain the coefficients of the distribution goes to infinity. To avoid this singular behaviour, McDonald and Groth [17] proposed the use of a windowing function, which dampens the distribution as the velocities tend to infinity. This is performed by adding a parameter \( \xi \), such that the distribution takes the form
\[
\mathcal{F}_{\text{MaxEnt}}^{(N)} = \exp \left( \alpha^T \mathbf{W}^{(N)} + \xi \right) = f_w \exp \left( \alpha^T \mathbf{W}^{(N)} \right), \quad (4.39)
\]
where they proposed a solution-dependent windowing function $f_w = e^{\xi}$. This technique was shown to be somewhat encouraging for 1D kinetic theory; however, the addition of the windowing function alters the form of the equilibrium distribution function (a Maxwellian distribution cannot be recovered). Furthermore, the computational costs associated to numerically obtaining the coefficients of the distribution function remain. Therefore, in order to circumvent these issues altogether, McDonald and Groth [17] and McDonald and Torrilhon [18] have considered interpolative alternatives, which avoid the reconstruction of the distribution function altogether, and allow one to obtain closing expressions for $Q_{ijk}$, $R_{ijkk}$ and $S_{ijjkk}$ directly. In both cases, interpolants are constructed based on the numerical evaluation of the closing moments of the maximum-entropy distribution throughout the realizability domain. The interpolants are based on a parabolic mapping between the physical realizability limit and the Junk subspace. In the first case [17], the interpolated closures are obtained through a polynomial curve fit provide, albeit rudimentarily, closed-form expressions for the closing fluxes. The second method [18] offers an approach that is more motivated by the physics and based on knowledge of distribution behaviour at the realizability boundaries. Furthermore, it offers much cleaner closing expressions than the first interpolative approach and has been well validated for stationary shocks [18] and multi-dimensional micro-scale flows [19–22]. It will therefore be used as the reference interpolative closure method for comparison to the proposed multi-Gaussian closures examined in this study.

In order to have a well-defined parameter representing the evolution of a moment state from one realizability boundary to another, McDonald and Torrilhon [18] performed a parabolic surface mapping throughout realizability space. The parabolic surface mapping parameter $\sigma$ is therefore used to represent paraboloids starting from the physical realizability limit of Eq. (4.35) and collapsing towards the Junk space. A fixed value of $\sigma$ represents a distinct paraboloid, and is expressed as

$$
\sigma = \frac{[2P_{ij}P_{ji} + P_{ii}P_{jj} - \rho R_{ijij}] + \sqrt{[2P_{ij}P_{ji} + P_{ii}P_{jj} - \rho R_{ijij}]^2 + 8\rho P_{mn}P_{nm}Q_{kij}(P^{-1})_{kj}Q_{lij}}}{4P_{ij}P_{ji}}, \quad (4.40)
$$

where a value of $\sigma = 0$ represents an infinitely thin paraboloid coinciding with the Junk subspace, and a value of $\sigma = 1$ is a paraboloid coinciding with the physical realizability boundary.

Using the parameter $\sigma$, it is possible to use knowledge of the distribution function behaviour at both realizability limits, and postulate approximate closing expressions for $Q_{ijk}$, $R_{ijkk}$ and $S_{ijjkk}$. The resulting closing expressions required to obtain the closing fluxes are

$$
Q_{ijk} = \frac{\partial Q_{ijk}}{\partial Q_{mnn}} Q_{mnn}, \quad (4.41)
$$
Chapter 4. Moment Closure Methods

\begin{equation}
R_{ijkk} = \frac{1}{\sigma} Q_{ijl}(P^{-1})_{lm} Q_{mkk} + \frac{2(1 - \sigma)P_{ik} P_{kj} + P_{ij} P_{kk}}{\rho} \tag{4.42}
\end{equation}

and

\begin{equation}
S_{ijkk} = \frac{Q_{nnn} Q_{mij} Q_{ikl}}{\sigma^2 P_{kn} P_{lm}} + 2\sigma^{\frac{1}{2}} \frac{P_{ij} Q_{jkk}}{\rho} + (1 - \sigma^{\frac{1}{2}}) W_{in} Q_{mnn}, \tag{4.43}
\end{equation}

where

\begin{equation}
\frac{\partial Q_{ijk}}{\partial Q_{mn}} = \left[ P_{il} (P^2)_{jk} + P_{kl} (P^2)_{ij} + P_{jl} (P^2)_{ik} \right] \left[ P_{lm} (P^2)_{\alpha \alpha} + 2 (P^3)_{lm} \right]^{-1} \tag{4.44}
\end{equation}

and

\begin{equation}
W_{in} = \frac{1}{\rho} \left[ P_{il} (P^2)_{\alpha \alpha}^3 + 6 P_{il} (P^3)_{\alpha \alpha} + 7 (P^2)_{\alpha \alpha} (P^2)_{il} + 10 P_{\alpha \alpha} (P^3)_{il} + 10 (P^4)_{il} \right.
\end{equation}

\[ - (P^2)_{\alpha \alpha} P_{j\beta} P_{il} - 3 (P_{\alpha \alpha})^2 (P^2)_{il} \left[ P_{lm} (P^2)_{\alpha \alpha} + 2 (P^3)_{lm} \right]^{-1}. \tag{4.45} \]

Upon inspection of the closing expressions above, it is possible to observe the singular behaviour arising at the Junk subspace. The first terms of Eqs. (4.42) and (4.43) each contain divisions by \( \sigma \), and as the Junk line is approached, \( \sigma \) tends to zero, and the values of \( R_{ijkk} \) and \( S_{ijkk} \) diverge. This property of the maximum-entropy closures is worrisome in numerical implementations. Firstly, near-singular closures can cause the numerical simulations to rapidly become unstable. Furthermore, moments tending towards infinity produce extremely large wave propagation speeds that can essentially drive the time step to zero and therefore stall simulations. However, this singular property has also proven to be very advantageous. Previous studies on internal shock structures [18, 44] have shown that the high propagation speeds associated with the near-singular closure allow for smooth shock structures without non-physical subshocks that often occur using QMOM or Grad moment closures. In order to numerically deal with values of \( \sigma \) approaching zero, a near-zero but finite threshold for \( \sigma \) is imposed such that propagation speeds are large enough to avoid non-physical subshocks, yet small enough to keep the numerical simulations stable and avoid very small near-zero time steps.

The use of this 14-moment interpolative closure has been well-validated and shown excellent results for the simulation of transition regime micro-scale flows with BGK [19–21] and ES-BGK [22] collision operators. However, though closed-form expressions are available for the closing fluxes, it is known that the absence of a closed-form expression to the distribution function may become inconvenient when considering more complex physical systems. For one, the use of more sophisticated collision operators will warrant the knowledge of an analytical expression to the distribution, as can be seen by inspection of the Boltzmann collision integral of Eq. (2.9). Knowledge of the distribution is furthermore required in the implementation
of adequate boundary conditions. This issue has already arisen in the first multidimensional implementation of the 14-moment interpolative model [19–22], where a Grad-like expansion about a Gaussian distribution was instead used in the rather simple implementation of half-Maxwellian wall boundary conditions [4, 77, 78].

The issues outlined above with the currently available maximum-entropy-based moment closures have motivated us to seek alternative forms of the approximate distribution function that possess the attractive mathematical and physical properties of the maximum-entropy closure, while also resulting in closed form expressions for the coefficients of the distribution function in terms of the transported moments. In a comparative study of several moment closures for the monokinetic 5-moment model of Levermore’s hierarchy [44], it was shown that a bi-Maxwellian closure possesses the same properties and advantages as the interpolative closure of McDonald and Torrilhon [18]. A bi-Gaussian distribution is therefore a natural multidimensional extension to those findings, and is suitable for use with the 14-moment system. The following section presents the assumed form for the bi-Gaussian distribution and the derivation of the closure.

### 4.4.3 Bi-Gaussian Closure

For suitability with the 14-moment system of Eq. (4.29), a bi-Gaussian phase-space distribution function is introduced having the form

\[
\mathcal{F}_{bg}(t, x_i, v_i) = \frac{(\rho_1/m)}{(2\pi)^{3/2} |\Theta_{ij}|^{1/2}} \exp \left[ -\frac{1}{2} \Theta_{ij}^{-1}(v_i - v_{1i})(v_j - v_{1j}) \right] + \frac{(\rho_2/m)}{(2\pi)^{3/2} |\Theta_{ij}|^{1/2}} \exp \left[ -\frac{1}{2} \Theta_{ij}^{-1}(v_i - v_{2i})(v_j - v_{2j}) \right],
\]

(4.46)

where the distribution parameters are the density weights, \(\rho_1\) and \(\rho_2\), the velocity abscissas, \(v_{1i}\) and \(v_{2i}\), and the shared standard deviation tensor \(\Theta_{ij}\). These variables combine and form a set of 14 free parameters which can be obtained in terms of the 14 transported moments. For brevity, the notation \(\mathcal{G}_{\alpha}(t, x_i, v_i; \rho_\alpha, v_{\alpha i}, \Theta_{ij})\) is introduced for a Gaussian distribution with weight \(\rho_\alpha\), velocity abscissa \(v_{\alpha i}\) and standard deviation \(\Theta_{ij}\), such that a bi-Gaussian distribution can be written as

\[
\mathcal{F}_{bg}(t, x_i, v_i) = \mathcal{G}_1(t, x_i, v_i; \rho_1, v_{1i}, \Theta_{ij}) + \mathcal{G}_2(t, x_i, v_i; \rho_2, v_{2i}, \Theta_{ij}).
\]

(4.47)

The relationship of \(\mathcal{F}_{bg}\) to Levermore’s 14-moment model, combined with its extended node-based nature sees it belong to both the maximum-entropy-based moment methods and EQMOM families. This choice of the bi-Gaussian distribution is motivated by: (1) its
potential maximum-entropy properties; (2) the ability to capture non-equilibrium and heat transfer phenomena in rarefied gas dynamics; and (3) the ability to capture two significant scales of PTCs in liquid sprays. The infinite support of each of its Gaussian distributions, combined with its bimodality, suggests the bi-Gaussian distribution is expected to reproduce similar behaviour to the maximum-entropy distribution at the Junk subspace by allowing a peak of $F_{bG}$ to see its velocity go to infinity as its magnitude goes to zero. This would therefore partly satisfy consideration (1) by permitting the large wavespeeds required to obtain smooth internal shock structures. From a rarefied gas dynamics perspective, the bi-Gaussian distribution, which encompasses the 10-moment Gaussian distribution, is expected to capture transition regime non-equilibrium effects quite well, as has been previously demonstrated for the Gaussian closure [77, 78]. Furthermore, the bimodality of $F_{bG}$ allows it to have non-zero third-order random velocity moments, therefore allowing for non-zero heat flux values. In the case of turbulent multiphase flows, two significant scales of PTCs can be observed. The first scale of PTCs is due to large-scale crossings caused by highly inertial droplets. Small-scale crossings, or velocity dispersion, are also known to arise due to gas phase turbulence. The Gaussian support of each peak in $F_{bG}$ has the potential to capture small-scale crossings through a non-zero standard deviation. The two distinct peaks in the approximate form of the distribution should furthermore allow for the capture of large-scale PTCs, as is attainable using purely node-based QMOMs.

**Derivation of the Bi-Gaussian Closure**

The derivation of the closing expressions for the parameters of $F_{bG}$ is performed through an analytical solution of the moment inversion problem stipulated by Eq. (4.4). The corresponding system of moment constraint equations can also be applied to random velocity moments and is in this case represented by

$$C^{(14)} = \langle W^{(14)} F_{bG}(t, x_i, c_i) \rangle, \quad (4.48)$$

where a shift in velocity space is performed to instead consider the random velocity bi-Gaussian distribution, $F_{bG}(t, x_i, c_i)$, which is re-written as

$$F_{bG}(t, x_i, c_i) = G_1(t, x_i, v_i - u_i; \rho_1, v_{1i} - u_i, \Theta_{ij}) + G_2(t, x_i, v_i - u_i; \rho_2, v_{2i} - u_i, \Theta_{ij}) = G_1(t, x_i, c_i; \rho_1, c_{1i}, \Theta_{ij}) + G_2(t, x_i, c_i; \rho_2, c_{2i}, \Theta_{ij}). \quad (4.49)$$

This inversion process requires rather extensive algebraic manipulations, and therefore only the general procedure is presented here, with the complete derivation being available in supple-
Resulting from Eq. (4.48), the system of moment constraints for moments from zeroth- to fourth-order, respectively, can be expressed as

\[ m \langle F \rangle = m \langle G_1 \rangle + m \langle G_2 \rangle \]
\[ = \rho_1 + \rho_2 \]
\[ = \rho \]  \hspace{1cm} (4.50)

\[ m \langle c_i F \rangle = m \langle c_i G_1 \rangle + m \langle c_i G_2 \rangle \]
\[ = \rho_1 c_{1i} + \rho_2 c_{2i} \]
\[ = 0 \]  \hspace{1cm} (4.51)

\[ m \langle c_i c_j F \rangle = m \langle c_i c_j G_1 \rangle + m \langle c_i c_j G_2 \rangle \]
\[ = \rho_1 c_{1i} c_{1j} + \rho_1 \Theta_{ij} + \rho_2 c_{2i} c_{2j} + \rho_2 \Theta_{ij} \]
\[ = P_{ij} \]  \hspace{1cm} (4.52)

\[ m \langle c_i c_j c_j F \rangle = m \langle c_i c_j c_j G_1 \rangle + m \langle c_i c_j c_j G_2 \rangle \]
\[ = \rho_1 c_{1i} c_{1j}^2 + \rho_1 c_{1i} \Theta_{jj} + 2 \rho_1 c_{1j} \Theta_{ij} + \rho_2 c_{2i} c_{2j}^2 + \rho_2 c_{2i} \Theta_{jj} + 2 \rho_2 c_{2j} \Theta_{ij} \]
\[ = Q_{ij} \]  \hspace{1cm} (4.53)

\[ m \langle c_i c_j c_j c_j F \rangle = m \langle c_i c_j c_j c_j G_1 \rangle + m \langle c_i c_j c_j c_j G_2 \rangle \]
\[ = \rho_1 c_{1i}^4 + \rho_2 c_{2i}^4 + 2 \rho_1 c_{1i}^2 \Theta_{ii} + 4 \rho_1 c_{1i} c_{1j} \Theta_{ij} + 2 \rho_2 c_{2i}^2 \Theta_{ii} + 4 \rho_2 c_{2i} c_{2j} \Theta_{ij} + \]
\[ \rho_1 \Theta_{ii} \Theta_{jj} + 2 \rho_1 \Theta_{ij} \Theta_{ij} + \rho_2 \Theta_{ii} \Theta_{jj} + 2 \rho_2 \Theta_{ij} \Theta_{ij} \]
\[ = R_{iiij} \]  \hspace{1cm} (4.54)

Following some rather extensive algebra, the nonlinear system of equations above can be solved analytically to obtain closing expressions to the parameters of the bi-Gaussian distribution. The anisotropic standard deviation tensor can first be expressed as

\[ \Theta_{ij} = \frac{P_{ij}}{\rho} - \frac{Q_{kk} Q_{kk}}{\rho^2} \Sigma, \]  \hspace{1cm} (4.55)

the velocity abscissas as

\[ v_{1i} = u_i + \frac{Q_{ij}}{\rho} \sqrt{\frac{\Sigma}{\alpha}} \quad \text{and} \quad v_{2i} = u_i - \frac{Q_{ij}}{\rho} \sqrt{\frac{\Sigma}{\alpha}}, \]  \hspace{1cm} (4.56)
and the density weights as
\[
\rho_1 = \rho \left( \frac{1}{2} + \gamma \right) \quad \text{and} \quad \rho_2 = \rho \left( \frac{1}{2} - \gamma \right),
\]
where the intermediate parameters \( \alpha \) and \( \gamma \) are written as
\[
\alpha = \frac{1}{2} + \gamma \quad \text{and} \quad \gamma = \frac{1}{2} \left[ 1 + 4 \frac{Q^4 \Sigma^3}{\rho^4} \right]^{-1/2}.
\]

From the fourth-order moment constraint of Eq. (4.54), a third-order polynomial in terms of the intermediate parameter \( \Sigma \) arises. From inspection of Eqs. (4.55) and (4.56), the root \( \Sigma \) is required to be real and positive. The corresponding cubic polynomial can be expressed as
\[
\lambda \Sigma^3 + \mu \Sigma - 1 = 0,
\]
where the density-normalized heat flux parameter, \( \lambda \), and the equilibrium parameter, \( \mu \), are expressed as
\[
\lambda = 2 \left( \frac{Q}{\rho} \right)^4 \quad \text{and} \quad \mu = \frac{1}{\rho} \left[ R_{ijij} - \left( \frac{P_{ii}P_{jj} + 2P_{ij}P_{ij}}{\rho} \right) \right].
\]
A value of \( \mu = 0 \) corresponds to a 10-moment Gaussian distribution function. Upon analysis of the polynomial of Eq. (4.59) for realizable moment values, it can be determined that there exists a single positive real root for \( \Sigma \). Furthermore, Eq. (4.59) is in Cardano’s form, meaning that the coefficient for \( \Sigma^2 \) is zero. Cubic polynomials of this form possess an analytical solution for their real root, which in this case is given by
\[
\Sigma = \begin{cases} 
2 \sqrt{-\frac{\mu}{3\lambda}} \cos \left[ \frac{1}{2} \arccos \left( \frac{1}{2\lambda} \sqrt{-27\lambda^4\mu^3} \right) \right], & \text{if } \Delta < 0, \\
\left( \frac{1+\sqrt{\frac{\Delta}{2\lambda}}}{2\lambda} \right)^{1/3} + \left( \frac{1-\sqrt{\frac{\Delta}{2\lambda}}}{2\lambda} \right)^{1/3}, & \text{otherwise},
\end{cases}
\]
where the discriminant, \( \Delta \), takes the form
\[
\Delta = 4\mu^3 + 27\lambda.
\]
Analysis of the distribution parameters of Eqs. (4.55)-(4.57) allows examination of the behavior of \( \mathcal{F}_{BG} \) as the moment state varies within realizable space. An important observation can be made about the dependence of the standard deviation tensor and velocity abscissas
Table 4.2: Variation of the bi-Gaussian distribution’s Parameters for Changes in the Heat Flux Magnitude and Equilibrium Parameter

<table>
<thead>
<tr>
<th>Case</th>
<th>$Q$</th>
<th>$\mu$</th>
<th>$\Sigma$</th>
<th>$\gamma$</th>
<th>$\alpha$</th>
<th>$\Theta_{ij}$</th>
<th>$\rho_{1}$</th>
<th>$\rho_{2}$</th>
<th>$\rho_{c}$</th>
<th>$c_{1i}$</th>
<th>$c_{2i}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\to 0$</td>
<td>$&gt; 0$</td>
<td>$\to 0$</td>
<td>$\to 1/2$</td>
<td>$\to \infty$</td>
<td>$\to P_{ij}/\rho$</td>
<td>$\to \rho$</td>
<td>$\to 0$</td>
<td>$\to 0$</td>
<td>$\to \infty$</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>$= 0$</td>
<td>$&gt; 0$</td>
<td>$= 1/\mu$</td>
<td>$= 1/2$</td>
<td>$= \infty$</td>
<td>$= P_{ij}/\rho$</td>
<td>$= \rho$</td>
<td>N/A</td>
<td>= 0</td>
<td>N/A</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>$\to 0$</td>
<td>$&lt; 0$</td>
<td>$\to \infty$</td>
<td>$\to 0$</td>
<td>$\to 1$</td>
<td>$&lt; P_{ij}/\rho$</td>
<td>$\to \rho/2$</td>
<td>&gt; 0</td>
<td>$\to \rho/2$</td>
<td>&lt; 0</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$= 0$</td>
<td>$\leq 0$</td>
<td>N/A</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

on both the pressure and heat flux. As the heat flux increases, the two peaks of $\mathcal{F}_{bg}$ become more separated in velocity space. For a given pressure, an increase in the heat flux therefore decreases the standard deviation until the point where the distribution takes the form of two Dirac deltas (in a given velocity direction) when

\[
\frac{P_{ij}}{\rho} = \frac{Q_{iik}Q_{jkk}}{\rho^2}\Sigma \quad \text{for} \quad i = j. \tag{4.63}
\]

Particular attention must also be given to the line $Q = 0$, where physical and mathematical singularities can occur near and away from the Junk subspace respectively. Table 4.2 shows the variation of individual parameters for changes in $Q$ and the equilibrium parameter $\mu$. An explanation of the physical effect on the bi-Gaussian distribution function in each case is provided in Table 4.3.

It can be observed that the singular behaviour approaching the Junk subspace is preserved

Table 4.3: Physical Description of the Bi-Gaussian Distribution’s Behaviour for the Moment States of Table 4.2

<table>
<thead>
<tr>
<th>Case</th>
<th>Physical Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>The moment state approaches the Junk subspace. One Gaussian approaches the 10-moment Gaussian state whereas the second sees its magnitude go to zero as its velocity goes to infinity.</td>
</tr>
<tr>
<td>2</td>
<td>The moment state lies on the Junk space. The velocities abscissas become undetermined and the solution is singular. This space is not attainable.</td>
</tr>
<tr>
<td>3</td>
<td>The solution approaches a purely bimodal state. Each Gaussian peak has equal density and an opposite random velocity component.</td>
</tr>
<tr>
<td>4</td>
<td>The bi-Gaussian distribution takes a purely bimodal form. Eq. (4.59) can no longer be solved and an alternative expression for the closure is required.</td>
</tr>
</tbody>
</table>
by the bi-Gaussian closure, as the near-singular phenomena attributed to the true maximum-entropy distribution occurs in a very similar way. Furthermore, on the Junk line, the resulting bi-Gaussian distribution becomes undetermined, as is the case with the maximum-entropy distribution. The somewhat advantageous property of obtaining high waves speeds near this realizability boundary is therefore conserved when using a bi-Gaussian reconstruction. Below the Junk line, where \( \mu < 0 \), the value of the root \( \Sigma \) goes to infinity as \( Q \to 0 \), and \( \mathcal{F}_{bG} \) tends to a purely bimodal distribution. It should be emphasized that it can be shown that the bi-Gaussian closure remains tractable everywhere within the realizable space of moments except in the singular regions associated with the Junk subspace.

At exactly \( Q = 0 \) and \( \mu < 0 \), the current expressions for the closing parameters no longer hold and an alternate expression to the distribution must be obtained. This is performed by solving the nonlinear system of Eqs. (4.50)–(4.54) by setting the third-order constraint of Eq. (4.53) to zero. The solution of the ensuing nonlinear system is in this case much more straightforward, and the zero heat flux expressions for the parameters of \( \mathcal{F}_{bG} \) are obtained. In the case of \( Q = 0 \) and \( \mu < 0 \), the random velocity abscissas can be expressed as

\[
\begin{align*}
c_{1i}|_{Q=0} &= \sqrt{\frac{P_{ij}}{\rho} \Sigma} \quad \text{and} \quad c_{2i}|_{Q=0} = -\sqrt{\frac{P_{ij}}{\rho} \Sigma} \quad \text{for} \quad i = j, \quad (4.64)
\end{align*}
\]

the anisotropic standard deviation tensor as

\[
\Theta_{ij}|_{Q=0} = \frac{P_{ij}}{\rho} - c_{1i}c_{1j}, \quad (4.65)
\]

and the density weights as

\[
\rho_1|_{Q=0} = \rho_2|_{Q=0} = \frac{\rho}{2}. \quad (4.66)
\]

In this case, the root \( \Sigma \) lies in the interval \( \Sigma \in [0, 1] \) and is simply expressed as

\[
\Sigma|_{Q=0} = \frac{\rho}{P_{ii}} \sqrt{-\frac{\mu}{2}}. \quad (4.67)
\]

As can be observed in Eqs. (4.64) and (4.66), the resulting distribution is purely bimodal, as the values of the velocity abscissas are equal and opposite with identical density weights. In order to alternate between expressions for \( \mathcal{F}_{bG} \) for \( Q = 0 \) and \( Q \neq 0 \), a maximum value of \( \Sigma \), as computed using Eq. (4.61), is chosen such that above this value, the \( Q = 0 \) distribution is used.
Closing Relations for Bi-Gaussian Moment Closure

Once closed-form expressions for the parameters of the bi-Gaussian distribution are obtained, it is possible to integrate the distribution in order to obtain the closing fluxes of Eq. (4.31). For the $Q \neq 0$ bi-Gaussian distribution, the resulting closing expressions for $Q_{ijk}$, $R_{ijkk}$ and $S_{ijjkk}$ are written as

$$Q_{ijk} = m \langle c_i c_j c_k \mathcal{F}_{BG}(t, x_i, c_i) \rangle = \frac{Q_{i\alpha\alpha} Q_{j\alpha\alpha} Q_{k\alpha\alpha}}{Q^2}, \tag{4.68}$$

$$R_{ijkk} = m \langle c_i c_j c_k c_k \mathcal{F}_{BG}(t, x_i, c_i) \rangle$$

$$= \frac{P_{ij} P_{kk}}{\rho} + 2 \frac{P_{ik} P_{jk}}{\rho} - Q_{i\alpha\alpha} Q_{j\alpha\alpha} \left( \frac{\rho}{Q^2 \Sigma} + 2 \frac{Q^2 \Sigma^2}{\rho^3} \right), \tag{4.69}$$

and

$$S_{ijjkk} = m \langle c_i c_j c_j c_k c_k \mathcal{F}_{BG}(t, x_i, c_i) \rangle$$

$$= \frac{2}{\rho} \left( P_{jj} + 2 \frac{P_{jk} Q_{j\alpha\alpha} Q_{k\alpha\alpha}}{Q^2} + 4 \frac{Q^2 \Sigma}{\rho} + \frac{\rho^3}{2 Q^2 \Sigma^2} \right) Q_{i\alpha\alpha} + \frac{4 P_{ij} Q_{j\alpha\alpha}}{\rho}. \tag{4.70}$$

As for the interpolative maximum-entropy-based closure of McDonald and Torrilhon [18], it is possible to observe the divergence of the values of the closing fluxes $R_{ijkk}$ and $S_{ijjkk}$ as the Junk space is approached. Near this singular subspace, the value of $\Sigma$ goes to zero, and therefore at least one term in both corresponding equations goes to infinity. As will be discussed in the Chapter 6, the choice of using these closing expressions directly over using the distribution function parameters depends on the numerical solution scheme used.

### 4.4.4 Possible Extensions to Multi-Gaussian Closures

The concept of using multi-Gaussian closures for members of Levermore’s Maximum-Entropy hierarchy has been described here for the 14-moment closure. Furthermore, lower-order true maximum-entropy closures represent simplifications of multi-Gaussian distributions, such as the 10-moment Gaussian closure and the 5-moment Maxwellian closure. It is therefore of interest to consider if a hierarchy of multi-Gaussian closures is obtainable through the postulation of a Gaussian distribution for each member of Levermore’s hierarchy. A possible formulation for the next higher-order member, namely the 21-moment closure, is potentially
possible through the use of a tri-Gaussian distribution, $\mathcal{F}_{\text{tG}}(t, x_i, c_i)$, which is expressed as

$$\mathcal{F}_{\text{tG}} = \mathcal{G}_0(t, x_i, v_i; \rho_0, c_0; \Theta_{0ij}) + \mathcal{G}_1(t, x_i, c_i; \rho_1, c_1, \Theta_{ij}) + \mathcal{G}_2(t, x_i, c_i; \rho_2, c_2, \Theta_{ij}). \quad (4.71)$$

In this case, the Gaussians $\mathcal{G}_1$ and $\mathcal{G}_2$ share a standard deviation tensor, $\Theta_{ij}$. An additional Gaussian, $\mathcal{G}_0$, is positioned at a random velocity abscissa, $c_0 = 0$. The ensuing distribution counts 21 independent variables, and could potentially be solved using a similar methodology to the one presented herein for $\mathcal{F}_{\text{bG}}$. The study of the multi-dimensional bi-Gaussian distribution being presently in preliminary stages, this study will not focus on these extensions, but rather suggest them as potential future work.
Chapter 5

Univariate Kinetic Model

The current chapter presents an in-depth analysis of the properties of the monokinetic 5-moment maximum-entropy-based model. The focus is on the comparison of different closures as well as their mathematical and physical properties and ability to capture non-equilibrium shocks. The content presented is an extension of the work published by Laplante and Groth [44] within the scope of this thesis.

5.1 Representative Univariate Kinetic Equation

Due to the complexity of the 14-moment system of Eq. (4.29), it can be quite challenging to study its mathematical and physical properties within realizability space. The prediction of the various order moments in the different directions in velocity space adds to this challenge. It is therefore of interest to consider a univariate kinetic model for which fluid particles are limited to movement in a single direction, and for which more simplified and in-depth analyses are possible. The simplification considered herein is represented by the univariate Boltzmann equation, which governs the flow of a theoretical “1D gas”. In this case, we will neglect acceleration forces and consider a simplified BGK collision operator with constant relaxation time, \( \tau \), such that the governing kinetic equation can be written as

\[
\frac{\partial F}{\partial t} + \nu \frac{\partial F}{\partial x} = \frac{F - M}{\tau}.
\]

(5.1)

It can be argued that the use of the BGK collision operator with constant relaxation time oversimplifies the system and misrepresents the physics of the Boltzmann equation. The goal of this 1D study is however to study the isolated effect of modifications in the closing flux on the overall solution properties, and therefore justifies this simplifying assumption.
5.2 Five-Moment System for Univariate Kinetic Model

As stated in Chapter 4, the 5-moment system of Levermore’s maximum-entropy hierarchy equivalent to the 14-moment model for a theoretical 1D gas is

\[ N = 5, \quad W^{(5)} = m[1, c, c^2, c^3, c^4], \quad C^{(5)} = [\rho, u, p, q, r]. \tag{5.2} \]

This 5-moment system has been considered by McDonald and Groth [17] and McDonald and Torrilhon [18] as a prequel to the 14-moment interpolative maximum-entropy-based (IMEB) closure. The study of a univariate model has in these cases provided valuable insight to extensions to three dimensions, and allowed for direct comparisons to the true maximum-entropy closing flux. The 5-moment system of transport equations arising from Eq. (5.2) will therefore also be considered here, and can be written as

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0, \tag{5.3} \]
\[ \frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2 + p) = 0, \tag{5.4} \]
\[ \frac{\partial}{\partial t} (\rho u^2 + p) + \frac{\partial}{\partial x} (\rho u^3 + 3u p + q) = 0, \tag{5.5} \]
\[ \frac{\partial}{\partial t} (\rho u^3 + 3u p + q) + \frac{\partial}{\partial x} (\rho u^4 + 6u^2 p + 4u q + r) = C_3 \tag{5.6} \]
\[ \frac{\partial}{\partial t} (\rho u^4 + 6u^2 p + 4u q + r) + \frac{\partial}{\partial x} (\rho u^5 + 10u^3 p + 10u^2 q + 5u r + s) = C_4, \tag{5.7} \]

where the moments \( \rho, u, p, q, r \) and \( s \) are defined by

\[ \rho = \langle mF \rangle, \quad u = \langle mvF \rangle, \quad p = \langle mc^2F \rangle, \]
\[ q = \langle mc^3F \rangle, \quad r = \langle mc^4F \rangle, \quad s = \langle mc^5F \rangle, \tag{5.8} \]

the third- and fourth-order collision terms \( C_3 \) and \( C_4 \) are

\[ C_3 = -\frac{q}{\tau} \quad \text{and} \quad C_4 = -\frac{1}{\tau} \left( 4uq + r - 3\frac{p^2}{\rho} \right), \tag{5.9} \]

and \( c = v - u \) is the single component of the random velocity. The resulting system is unclosed. A closing expression is required for the fifth random velocity moment, \( s \) in terms of the other known moments. The following subsections will distinguish between four categories of closure methods for \( s \), namely: Grad-type, IMEB, quadrature-based (QMOM) and extended quadrature-based (EQMOM) moment methods.
For the purposes of analysis, it is convenient to define a shift in velocity space such that
\( u = 0 \) and then work with a non-dimensional set of moments defined by

\[
\rho_* = 1, \quad u_* = 0, \quad p_* = 1, \quad q_* = \frac{1}{\rho} \left( \frac{\rho}{\rho} \right)^{3/2} q, \quad r_* = \frac{1}{\rho} \left( \frac{\rho}{\rho} \right)^2 r, \quad s_* = \frac{1}{\rho} \left( \frac{\rho}{\rho} \right)^{5/2} s,
\]

as first performed by Junk [16]. These definitions will allow the study of the properties of the moment closures by considering only the dimensionless values of the heat flux, \( q_* \), and kurtosis, \( r_* \). Using this non-dimensional representation of the moments produces non-dimensionalised forms of the reconstructed distribution functions, which in this case are obtained in terms of a non-dimensional random velocity, \( \xi \).

### 5.2.1 Grad-Type Moment Closure

In the original moment closure of Grad [4], the distribution function is represented as a polynomial expansion about the equilibrium Maxwellian, which for the univariate kinetic equation above can be expressed as

\[
\mathcal{F}_{\text{Grad}} = \mathcal{M} \left[ 1 + \alpha_0 + \alpha_1 \left( \frac{\xi}{a} \right) + \alpha_2 \left( \frac{\xi}{a} \right)^2 + \alpha_3 \left( \frac{\xi}{a} \right)^3 + \alpha_4 \left( \frac{\xi}{a} \right)^4 \right],
\]

where the coefficients, \( \alpha_j \), are determined by ensuring \( \mathcal{F}_{\text{Grad}} \) satisfies the lower order moments. Unfortunately, the distribution above has a limited range in the space of realizable moments for which it is strictly positive. In fact, the usual Grad third-order closures are almost everywhere non-positive. More importantly, it has also been shown that for modest deviations from equilibrium, the hyperbolicity of the associated moment equations is lost and the closure breaks down [86]. The consequences of this form of breakdown will be illustrated in the results to follow.

For the five-moment system considered here, the closure resulting from Grad’s polynomial expansion has been studied previously by McDonald et al. [18] and yields the simple closing relation given by

\[
s_* = 10q_*.
\]
5.2.2 Interpolative Maximum-Entropy-Based (IMEB) Moment Closure

As mentioned previously, Dreyer [13], Müller and Ruggeri [14] and Levermore [15] provided the initial framework for maximum entropy closures as pertains to kinetic theory. This approach assumes a phase-space distribution function that maximizes the thermodynamic entropy of the system, thus producing the most likely distribution while remaining consistent with a set of given moments. For the 1D kinetic equation given above, the form of the maximum-entropy distribution function is

\[ F_{\text{MaxEnt}} = \exp \left( \alpha_0 + \alpha_1 \xi + \alpha_2 \xi^2 + \alpha_3 \xi^3 + \alpha_4 \xi^4 \right) \]

(5.13)

and the coefficients, \( \alpha_i \), are determined via the maximization of the Boltzmann entropy \( m \langle F \ln F \rangle \). Maximum entropy closures have many desirable mathematical properties including global hyperbolicity and a definable entropy [15]. A significant drawback is that, as in the present case, a numerical approach is generally required to determine \( \alpha_i \) in terms of the moments \( \rho, u, p, q \) and \( r \).

Due to the absence of a closed-form expression for this distribution, IMEB moment closures as described in the previous chapter were proposed by McDonald and Torrilhon [18] and subsequently studied by Tensuda et al. [19–22]. For the 5-moment model, the interpolative approximation to the true maximum-entropy closure yields an analytical expression for the random fifth moment, \( s_* \), which closely matches the values of the actual maximum-entropy closure and can be expressed as

\[ s_* = \frac{q_*^3}{\sigma_M^2} + \left( 10 - 8\sigma_M^2 \right) q_* \]

(5.14)

where the parameter \( \sigma_M \) is the result of a parabolic mapping in the \( q_* - r_* \) plane and is given by

\[ \sigma_M = \frac{3 - r_* + \sqrt{(3 - r_*)^2 + 8q_*^2}}{4} \]

(5.15)

Although the IMEB closure presents many modeling and implementation advantages, including strict hyperbolicity of the 5-moment set for virtually all realizable moments [18], it still does not provide a closed-form expression for the distribution function. Arbitrary higher-order moments can therefore not be integrated analytically and this can be viewed as a significant drawback.
5.2.3 Quadrature-Based Moment (QMOM) Closure

Quadrature methods of moments were first described by McGraw in the context of aerosol dynamics [36]. Many variants of the QMOM have since been developed [40], but they have mainly been applied to the prediction of multiphase flows. A simple variant of the QMOM approach is evaluated here. The representation of the distribution function is based on the summation of three weighted Dirac delta functions and can be written as

\[ F_\delta = \sum_{k=1}^{3} w_k \delta (\xi - \xi_k), \]  

with dimensionless velocity weights, \( w_k \), and dimensionless abscissas, \( \xi_k \). In order to produce a five-moment closure, the first abscissa is set to \( \xi_1 = 0 \) here. This choice is made since the second random velocity moment is always null and results in a five-equation system for the parameters of \( F_\delta \) given by

\[ \sum_{k=1}^{3} w_k \xi_k^\alpha = C^\alpha(\alpha), \]  

where \( C^\alpha(\alpha) \) is the \( \alpha \)th element of the dimensionless random velocity moment vector \( C^{\alpha(5)} = \{1, 0, 1, q_*, r_*\} \). The solution to Eq. (5.17) yields an analytic expression for the weights and abscissas. The random fifth moment can then be written as

\[ s_* = \sum_{k=1}^{3} w_k \xi_k^5 = (1 - a^4) (1 + a)^2 \left( \frac{q_*}{1 - a^2} \right)^3, \]  

where the weight ratio, \( a = w_2/w_3 \), is a root of the fourth-order polynomial

\[ (q_*^2 - r_*) a^4 + (q_*^2) a^3 + (2r_*) a^2 + (q_*^2) a + (q_*^2 - r_*) = 0. \]  

While this quadrature approach can be shown to have a strictly positive distribution function for all realizable moments and is expected to be quite flexible in producing solutions for the full range of moment values, it is also expected to have similar issues with closure breakdown as the Grad-type closure, due to the finite extent of the Dirac basis function and hence finite wave propagation velocities represented by the closure. Furthermore, the \( F_\delta \) closure can be expected to be less accurate near local thermodynamic equilibrium, since its node-based structure cannot reduce to an equilibrium Maxwellian for any given combination of moments, in contrast to the \( F_{\text{Grad}}, F_{\text{MaxEnt}} \) and \( F_{bM} \) (to follow) distributions. Recent findings by Patel et al. [87] have however demonstrated that the closure remains hyperbolic throughout realizable moment space in the context of a conditional hyperbolic QMOM (CHyQMOM).
5.2.4 EQMOM Bi-Maxwellian Moment Closure

Univariate multi-Gaussian or multi-Maxwellian closures were previously considered by Chalons et al. [80]. The concept essentially extends the idea of the QMOM closure by replacing the basis function at each quadrature point by a Maxwellian distribution shifted in velocity space, with the influence of the new basis functions now extending over the full range of velocities. Such an approach is also referred to as an extended quadrature method of moments [39, 40]. It is noted that Fan and Li [88] have also recently evaluated bi-Gaussian closures for application to gas kinetic theory and compared various features of the multi-Gaussian approach to that of maximum-entropy closures.

For the 5-moment system, two Maxwellians sharing the same standard deviation, $\sigma$, are used as an ansatz for representing the phase-space distribution function. The bi-Maxwellian form for the distribution function is a simplification of the bi-Gaussian distribution presented in Section 4.4.3 and is written as

$$ F_{bM} = \frac{w_1}{\sigma \sqrt{2\pi}} \exp \left( -\frac{(\xi - \xi_1)^2}{2\sigma^2} \right) + \frac{w_2}{\sigma \sqrt{2\pi}} \exp \left( -\frac{(\xi - \xi_2)^2}{2\sigma^2} \right). \quad (5.20) $$

An analytical solution to the system of equations for $w_k$, $c_k$ and $\sigma$ was previously derived by Chalons et al. [80]. One can also solve the monokinetic system of moment constraints using the dimensionless form of the moments shown by Eq. (5.10). Following the derivation procedure used for the bi-Gaussian closure in Section 4.4.3, the weights of each Maxwellian distribution can be written as

$$ w_1 = \frac{1}{2} + \gamma, \quad w_2 = \frac{1}{2} - \gamma, \quad (5.21) $$

where $\gamma$ is expressed as

$$ \gamma = \frac{\frac{1}{2} q_*}{\sqrt{q_*^2 + 4(1-\sigma^2)^3}}. \quad (5.22) $$

The variance, $\sigma^2$, is found by solving for the real root of a third order polynomial and can be written as

$$ \sigma^2 = 1 - C_2 + \frac{C_1}{C_3}, \quad (5.23) $$

where the constants $C_1$, $C_2$ and $C_3$ are given by

$$ C_1 = \frac{1}{6}(r_* - 3), \quad C_2 = \frac{q_*^2}{4}, \quad C_3 = \left( \sqrt{\frac{C_1^3}{C_2^2 + C_2}} \right)^{1/3}. \quad (5.24) $$
The location of the velocity abscissas may then be written as

\[ \xi_1 = -\sqrt{\frac{w_2}{w_1}} (1 - \sigma^2), \quad \xi_2 = \sqrt{\frac{w_1}{w_2}} (1 - \sigma^2). \]  

(5.25)

Finally, the random fifth moment is expressed as the weighted integral of two Gaussian distributions

\[ s_\star = w_1 \xi_1^3 (10\sigma^2 + \xi_1^2) + w_2 \xi_2^3 (10\sigma^2 + \xi_2^2) + 15\sigma^4 (w_1 \xi_1 + w_2 \xi_2), \]  

(5.26)

which can be re-expressed as

\[ s_\star = \frac{q_\star^3}{\sigma_Q} + (10 - 8\sigma_Q) q_\star, \]  

(5.27)

where \( \sigma_Q = 1 - \sigma^2 \). A similar result was also found by Fan and Li [88]. The form of \( \mathcal{F}_{b\text{M}} \) is such that it will remain positive valued for all realizable moments. An interesting comparison can also be made between the closures of Eqs. (5.14) and (5.27). Both expressions lead to singular behaviour within a portion of realizability space and fixed values of the parameters \( \sigma_M \) and \( \sigma_Q \) both define parabolas in the \( q_\star - r_\star \) plane ranging from the outer physical realizability boundary to the singular region. The strict hyperbolicity of the bi-Maxwellian closure can also be shown [43, 88].

### 5.2.5 Closing Moment and Region of Moment Realizability

As described in Section 4.4.1, the region of moment realizability can be obtained by solving the Hamburger moment problem for the moment set of interest. For the five-moment system of interest corresponding to the univariate kinetic equation, the solution of the Hamburger problem provides a necessary and sufficient condition for the region of moment realizability. In this case, one can chose the velocity weighting vector \( \Omega = [1, c, c^2] \), leading to the dimensional \( \mathbf{Y} \) and non-dimensional \( \mathbf{Y}_\star \) matrices,

\[
\mathbf{Y} = \begin{pmatrix}
\rho & u & p \\
 u & p & q \\
p & q & r
\end{pmatrix}, \quad \mathbf{Y}_\star = \begin{pmatrix}
1 & 0 & 1 \\
0 & 1 & q_\star \\
1 & q_\star & r_\star
\end{pmatrix},
\]

(5.28)

which leads to the positive definiteness condition for \( \mathbf{Y} \) given by

\[ r_\star \geq 1 + q_\star^2 \]  

(5.29)
Any combination of \( q^* \) and \( r^* \) lying above the parabola \( r^* = 1 + q^*^2 \) is therefore said to correspond to a physically realizable solution. Furthermore, Junk [16, 89] has shown that maximum entropy solutions do not exist within this region on the line \( q^* = 0 \), above \( r^* = 3 \) (i.e., for \( r^* > 3 \)). The maximum-entropy distribution function does not remain finite along this line and therefore solutions cannot be found. While strict hyperbolicity and a well-behaved closure is assured everywhere else, the resulting moment equations are also singular on the Junk line. These properties are particularly inconvenient, since the point \((q^* = 0, r^* = 3)\) corresponds to local thermodynamic equilibrium (LTE).

The realizability region and so-called Junk subspace corresponding to the invalid region of the maximum entropy closure are depicted in Figure 5.1. For this theoretical 1D gas, the IMEB closure of McDonald and Torrilhon [18] has been shown to exhibit excellent agreement with the true maximum-entropy closure. It matches the true maximum-entropy distribution exactly at the parabola of the realizability boundary, where \( F_{\text{MaxEnt}} \) reduces to two Dirac deltas. Furthermore, its singular behavior (as evidenced by undefined discontinuous values for \( s^* \)) at the Junk subspace is also reproduced as can be clearly seen in Figure 5.2b. The exact representation of the distribution at the lower realizability boundary is also captured by \( F_\delta \) and \( F_{\text{bM}} \), as both distributions have the capability of reducing to two Dirac delta functions at the lower realizability boundary. The values of \( s^* \) obtained using these two closures therefore exactly replicate the \( F_{\text{MaxEnt}} \) results on this parabola. Refer to Figures 5.2c and 5.2d. Interestingly, the bi-Maxwellian closure has very similar behavior to that of the true maximum entropy solution over the entire realizability region and exhibits the characteristic
singular behaviour along the Junk subspace. This is expected from the similarity between the parameters $\sigma_Q$ and $\sigma_M$, and the similar structure of the resulting expressions for $s_*$. In contrast, the QMOM closure does not replicate the maximum-entropy behavior within the realizability region away from the boundary. Additionally, while a global solution for $s_*$ is obtained, the QMOM closing flux remains finite and non-singular for all possible moments. Although originally a perceived drawback of maximum-entropy-based closures, the singular behaviour along the Junk space is a property that can be coped with numerically and is key to accurate predictions of non-equilibrium shock structures as will be shown in the results to follow. As expected, the more rudimentary Grad-type closure cannot replicate the properties of the maximum-entropy closure at either realizability boundary, as is evidenced in 5.2a. The value of this closure is very far from the reference IMEB closure almost everywhere in the realizability region, except for regions very close to equilibrium and away from the Junk subspace, where a polynomial expansion about the Maxwellian distribution remains a somewhat valid assumption.

5.3 Numerical Simulation of Stationary Shock Structures

To evaluate the capabilities of each moment closure for different degrees of departure from equilibrium, stationary shock structures are studied for upstream Mach numbers of $M = \{1.25, 2, 4, 8\}$, with increasing Mach number representing a larger departure from LTE. The five-moment system of differential equations for each closure was solved using a second-order Godunov-type upwind finite-volume scheme [90] with piece-wise linear reconstruction. An HLL approximate Riemann solver [91] is used with the net flux, $F_{\text{HLL}}$, being expressed as

$$F_{\text{HLL}} = \begin{cases} F_L, & \text{if } \lambda^- > 0 \\ F_R, & \text{if } \lambda^+ < 0 \\ \frac{\lambda^+ F_L - \lambda^- F_R}{\lambda^+ - \lambda^-} + \frac{\lambda^+ \lambda^-}{\lambda^+ - \lambda^-} (U_R - U_L), & \text{otherwise} \end{cases} \quad (5.30)$$

where the wavespeeds $\lambda^-$ and $\lambda^+$ are approximately obtained through a scaling of the local sound speeds by a parameter $\zeta$ such that

$$\lambda^- = u - \zeta \sqrt{\frac{\gamma p}{\rho}}, \quad \lambda^+ = u + \zeta \sqrt{\frac{\gamma p}{\rho}}. \quad (5.31)$$
A minimum value of $\zeta$ is chosen such that simulations remain stable. Slope limitation is performed using a Venkatakrishnan slope limiter [92]. As a reference non-equilibrium solution, Eq. (5.1) was solved directly using the discrete velocity method of Mieussens [10], as was performed in previous comparisons for non-equilibrium shocks [17, 18].

The solution of a three-moment system resulting from a Chapman-Enskog expansion applied to the kinetic equation of Eq. (5.1) is also used as a reference near-equilibrium solution. The latter is the equivalent Navier-Stokes equations for a 1D gas [17, 18], as described by Eqs. (5.32)-(5.34).

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0 \tag{5.32}
\]

\[
\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2 + p) = 0 \tag{5.33}
\]

Figure 5.2: Domain of physical realizability for the five-moment system: (a) realizability boundaries [16] and contours of (b) IMEB, (c) QMOM and (d) bi-Maxwellian closing values for $s_\star$. 
\[
\frac{\partial}{\partial t} \left( \rho u^2 + p \right) + \frac{\partial}{\partial x} \left( \rho u^3 + 3up \right) - \frac{\partial}{\partial x} \left( 3p \tau \frac{\partial}{\partial x} \left( \frac{p}{\rho} \right) \right) = 0
\] (5.34)

The reference non-equilibrium solutions were computed using a phase-space distribution discretization of 1,000 equally spaced points in velocity space ranging from -10,000 to 10,000 m/s. For all reference solutions and five-moment test cases, the spatial mesh consists of 5,000 cells equally spaced between \(-5 \times 10^{-3}\) and \(5 \times 10^{-3}\) m. Convergence studies have been performed for all moment closures, and it has been deemed that this resolution is largely sufficient for all Mach numbers considered.

5.3.1 Stationary Shock Structure Results

Figures 5.3 and 5.4 show shock structure results for the IMEB, Grad-type, QMOM and bi-Maxwellian closures as compared to the reference solutions. The \(M = 1.25\) case represents...
Figure 5.4: Predicted normalized density and dimensionless heat transfer through a stationary shock wave for a one-dimensional gas as determined by the IMEB and bi-Maxwellian (bM) closures: (a)-(b) $M = 4$ and (c)-(d) $M = 8$.

a rather modest departure from equilibrium, and it can be seen that all closure approximations along with the NSF model are in good agreement with the full solution of the kinetic equation. However, the shortcomings of the Grad-type and QMOM can immediately be seen in Figures 5.3c and 5.3d for a $M = 2$ shock, where undesirable and unphysical subshocks are present in both solutions. It is important to note that the Grad-type closure formally becomes non-hyperbolic at this relatively low Mach number; however the approximate numerical flux functions and associated numerical viscosity allowed the computation of solutions for this case. For further departures from LTE, as depicted in Figure 5.4, only first-order solutions of the Grad-type and QMOM moment equations could be obtained and those required an unreasonable number of grid points for grid-independent solutions. Results are therefore not shown for Mach numbers above $M = 2$ for these two closures.

The more interesting comparisons can be made between the IMEB and bi-Maxwellian closures, which provide smooth solutions, with no subshocks, for all Mach numbers, as shown
in Figures 5.3 and 5.4. In fact, the singularity in the closing flux, which presents a slight numerical difficulty, is extremely beneficial in this case since it allows very large wavespeeds which provide upstream influence that prevents the appearance of subshocks in the predicted solutions. Both closures show excellent agreement with the discrete velocity methods for the normalized density in all cases. They however show some increasing discrepancies with the upstream heat transfer profile with the IMEB closure always performing slightly better than the bi-Maxwellian model.

Comparing the moment closure results to the NSF-like model demonstrates their advantage in modeling non-equilibrium phenomena. The near-equilibrium model is clearly unable to accurately capture the density profile for shocks at \( M = 2 \) and up, and completely breaks down in terms of the density and heat transfer profile predictions at \( M = 4 \) and \( M = 8 \).

### 5.3.2 Coping with Singularities at the Junk Subspace

Obtaining reliable simulations requires limitation strategies near the Junk space in the case of the EQMOM and IMEB closures. An effective limitation strategy is to prevent the solution from entering a fixed region around the singular line. The parameters \( \sigma_Q \) and \( \sigma_M \) both represent parabolas emanating from the Junk subspace, and are therefore ideal in defining such a region. The white parabola of Figure 5.5 is an example of a region delimited by a value of \( \sigma_Q = 0.001 \). We can thus define a critical minimum value, \( \sigma_Q^* \) or \( \sigma_M^* \), to which values of \( \sigma_Q \) or \( \sigma_M \) are limited if \( \sigma_Q < \sigma_Q^* \) or \( \sigma_M < \sigma_M^* \) respectively. Though the limitation of these parameters allows to avoid the Junk subspace, it is important to keep in mind that important

![Figure 5.5: Contours of EQMOM closure parameter, \( \sigma_Q \), in physical realizability region and example of a \( \sigma_Q^* \) limiting value (white line).](image)
solution properties arise from the high wave speeds approaching the singularity.

The effect of variations in the critical limiting values was explored by taking the example of the bi-Maxwellian closure and varying the value of $\sigma^*_Q$ between 0.05 and 0.0001. Figure 5.6 shows that an increase in the value of $\sigma^*_Q$ gradually increases the magnitude of aphysical subshocks in the solution. This is attributed to the fact that overly limiting $\sigma_Q$ restricts the maximum allowed wavespeed, and therefore information cannot propagate through the domain rapidly enough to maintain a smooth solution. The solution therefore must undergo a shock in order to recover upstream conditions. A value of $\sigma^*_Q$ is therefore chosen such that subshocks are avoided to the highest extent, while preserving solution stability and preventing the time step from going to zero due to excessively large wave speeds. For shocks up to $M = 8$, values of $\sigma^*_Q = 0.0001$ and $\sigma^*_M = 0.0002$ provided these desired solution properties.

5.3.3 Closure Comparisons along Non-Equilibrium Paths

To more thoroughly assess the validity of each moment closure, it is of interest to compare the closing fluxes for various departures from equilibrium. In this case, reference “non-equilibrium paths” are defined as the solution paths taken through a shock, as represented by the reference BGK solution. The stationary shock solutions can then instead be plotted on the $q_*-r_*$ plane. This representation allows to view the shock path within realizable space, and therefore to truly observe departures from equilibrium that can be difficult to notice on position-dependent plots such as those of Figures 5.3 and 5.4. For shocks ranging from $M = 1.25$ to $M = 8$, the $q_*-r_*$ trajectories take the shape of orbitals emanating from LTE, and traveling upwards
in the counter-clockwise direction as the shock progresses downstream. As can be observed in Figures 5.7a and 5.7b, concentric orbitals with increasingly large departures from LTE are obtained as the Mach number is increased.

It is then possible to plot the closing flux $s_\ast$, as computed by all proposed closures, along the shock orbital’s normalized surface length, where a surface length position of 0 and 1 represent upstream and downstream equilibrium conditions respectively. One can compare the predicted values of $s_\ast$ with the reference BGK solution along this path. The first case considered is the $M = 1.25$ shock, which consists of a very modest departure from equilibrium, as can be observed in Figure 5.7b. In this case, all closures are in relatively good agreement with the reference solution, with the exception of the QMOM closure. The IMEB closure however surprisingly presents a larger discrepancy with the reference solution as compared to the Grad-type and EQMOM closure, as seen in Figure 5.8a. At such a modest departure from LTE, the distribution function remains very close to a Maxwellian. The $\mathcal{F}_\text{Grad}$, $\mathcal{F}_\text{MaxEnt}$ and $\mathcal{F}_{bM}$ distributions each have the ability to reduce to the Maxwellian distribution, which is explicitly contained in their basis functions. It can therefore be argued that they can better perform in conditions closest to equilibrium. The only closure unable to reduce to a Maxwellian is the $\mathcal{F}_\delta$ closure, for which the computed closing flux is quite far from the reference solution. All closures however respect the trend of $s_\ast$ for this low Mach number. As the Mach number is increased to $M = 2$ (Figure 5.8b), it is observed that the Grad-type moment closure begins to depart from the reference solution, and both the QMOM and Grad-type closures fail to
capture the global trend of the closing flux where near-equilibrium assumptions no longer hold. Further increases in Mach number (Figures 5.8c-5.8d) show that the Grad closure falls orders of magnitude under the reference solution. The QMOM closure is however able to remain on the same order of magnitude, and its discrepancies with the reference solution remain comparable to the lower Mach numbers cases.

For all levels of departure from equilibrium, the IMEB and EQMOM closures have shown excellent results in their predictions of $s_\star$. For higher Mach numbers above 1.25, the IMEB closure tends to slightly outperform the bi-Maxwellian closure, however both approximations to $s_\star$ respect the reference trend and present nearly negligible discrepancies with the BGK solution.
5.3.4 Comparisons to the Maximum-Entropy Distribution

It has been shown through the simulation of stationary shock structures that the IMEB and EQMOM closures agree very well with the reference BGK solutions and by far outperform the Grad-type and QMOM closures. The EQMOM closure however has the advantage of presenting a closed-form expression to the distribution function, which can be quite advantageous when considering more complex physical systems. Furthermore, the availability of $F_{bM}$ allows us to perform direct comparisons with the true maximum-entropy distribution, $F_{\text{MaxEnt}}$. In the simplified case of a monokinetic gas, iterative solutions to the maximum-entropy distribution can be obtained relatively quickly. In this study, an algorithm designed by Mohammad-Djafari [82] for geometrical moments of the form $\langle mc^\alpha F \rangle$ is used, which allows to iteratively obtain the Lagrange multipliers, $\alpha_k$, of Eq. (5.13).

To illustrate the similarities between both representative distributions, the non-equilibrium path corresponding to a $M = 8$ shock is used. This case was chosen since it is the solution with the largest departure from LTE. One can take sample points along the shock path, as shown in Figure 5.9, and compute both the bi-Maxwellian and maximum-entropy distributions. At the upstream position of the shock, as the solution state departs the left-state equilibrium conditions, an infinitesimally small distribution peak appears at an infinite velocity abscissa. As we progress downstream in the shock, this peak approaches the mean velocity and its density grows in magnitude until it becomes non-negligible, as can be observed in sample points A through D for both $F_{\text{MaxEnt}}$ and $F_{bM}$. It can also be seen that as the solution leaves the Junk line, the standard deviation of each peak of the distribution decreases. Sample

![Figure 5.9: Non-equilibrium path and sample points in realizable moment space for a $M = 8$ shock as predicted by the BGK reference solution.](image-url)
points D and E in turn show that as downstream equilibrium conditions are approached, the smaller peak of the distribution begins to grow in magnitude, and in the case of $F_{\text{MaxEnt}}$, merges into the main peak of the distribution. A nearly equivalent phenomenon can be seen when observing the behaviour of $F_{\text{bM}}$ from D to E, however the distribution maintains two more distinct peaks than its maximum-entropy counterpart. Approaching the downstream LTE at point E, it can be seen that the two distribution peaks have fully merged and the distribution is now nearly Maxwellian in both cases.

It can encouragingly be observed that for the prediction of shocks very far from equilibrium, the behaviour of the bi-Maxwellian distribution shows excellent qualitative agreement with
Figure 5.11: (a) BGK reference solution normalized density profile for a $M = 8$ shock and (b) closing flux prediction compared to the reference for the bi-Maxwellian (bM), maximum-entropy (ME) and interpolative maximum-entropy-based (IMEB) closures as computed from the moments of the reference solution. Reconstructed (c) maximum-entropy ($F_{\text{MaxEnt}}$) and (d) bi-Maxwellian ($F_{\text{bM}}$) non-dimensional distributions along the shock profile shown in (a).

The maximum-entropy distribution. There are however two main observable discrepancies with $F_{\text{MaxEnt}}$. Firstly, the infinitesimally small peak of the bi-Maxwellian distribution always possesses a smaller velocity abscissa magnitude. Furthermore, $F_{\text{bM}}$ presents a more bi-modal form, whereas $F_{\text{MaxEnt}}$ tends to remain more smeared.

Comparisons between both representative distributions can further be observed in Figure 5.11b, where the value of the closing flux is compared for the bi-Maxwellian, IMEB, and true maximum-entropy closures as computed from the moments of the BGK solution, for which
the density profile is shown in Figure 5.11a. The behaviour of both distributions approaching the Junk space is clearly seen in Figures 5.11c-d, as a peak of each distribution goes to infinite velocity with its magnitude decreasing. Comparisons of the closing flux values away from the Junk space show excellent agreement for all closures. However, as the solution approaches the Junk space, the maximum-entropy distribution becomes singular, and the iterative procedure used failed to accurately converge. Comparisons with the true maximum-entropy distribution are therefore not valid for $x/\lambda < -25$. Reliable solutions to $F_{\text{MaxEnt}}$ were however obtained for moment states away from the Junk space and distributions shown in both Figures 5.11c-d are accurate representations.
Figure 5.14: Reconstructed maximum-entropy, $F_{\text{MaxEnt}}$, and bi-Maxwellian, $F_{\text{bM}}$, non-dimensional distributions for sample points along the non-equilibrium particle trajectory crossing path of Figure 5.13.

5.4 Numerical Simulation of Particle Trajectory Crossings

A similar analysis to that of Section 5.3.4 can be applied to a test case representative of particle trajectory crossings. In this case, a Riemann problem corresponding to two solution states consisting of Maxwellian distributions with equal and opposite velocities is considered, as depicted in Figure 5.12. In this case, the solution is initialized with Maxwellian distributions corresponding to pressures of $p_1 = p_2 = 1/3$, densities of $\rho_1 = \rho_2 = 1$ and mean velocities of $u_1 = -u_2 = 1$. The problem is solved to a time $t = 0.5s$ without collisions, and a high-density
central region with a bi-modal distribution is formed around \( x = 0 \), as seen in Figure 5.15a. Figure 5.13 in turn shows the corresponding non-equilibrium solution path in realizability space. For the sample points labeled in Figure 5.13, the \( F_{\text{bM}} \) distribution can once again be plotted and compared to \( F_{\text{MaxEnt}} \), as depicted in Figure 5.14. Once again, distribution function

Figure 5.15: (a) BGK reference solution normalized density profile for the representative particle trajectory crossing problem and (b) closing flux prediction compared to the reference for the bi-Maxwellian (bM), maximum-entropy (ME) and interpolative maximum-entropy-based (IMEB) closures as computed from the moments of the reference solution. Reconstructed (c) maximum-entropy (\( F_{\text{MaxEnt}} \)) and (d) bi-Maxwellian (\( F_{\text{bM}} \)) non-dimensional distributions along the crossing profile shown in (a).
behaviour is similar, and the more distinct bi-modality of the bi-Maxwellian distribution can be readily seen. It can be argued in this case that the reconstructed bi-Maxwellian distribution is a more accurate representation of pure PTC, as the particles undergo crossings without interactions, and therefore it is expected that two distinct peaks be present.

Figure 5.15 shows the value of the closing flux, as computed by each closure from the moments of the reference BGK solution, and the corresponding reconstructed distribution functions. Similar issues with convergence of the iterative solver for $f_{\text{MaxEnt}}$ near the Junk subspace are encountered here, and reliable predictions are only available for $-0.8 < x < 0.8$. It can readily be seen that the maximum-entropy distribution is everywhere more smeared than the corresponding bi-Maxwellian distribution.

5.5 Conclusions Following from the Univariate Kinetic Model Results

It has been demonstrated that the proposed bi-Gaussian moment closures is able to provide results of an accuracy and quality that are similar to that of true maximum-entropy closures. Furthermore, the multi-Gaussian approach by far outperforms other QMOM and Grad-type moment closures in terms of the ability to predict non-equilibrium phenomena associated with stationary shocks. Due to its singular behaviour, the bi-Gaussian closure, like other maximum-entropy-based closures, provides smooth shock transitions where the more standard closures produce subshocks. The bi-Gaussian and maximum-entropy based closures are furthermore able to capture additional physics, as represented by higher order moments, with considerably more precision than the NSF equations for a 1D gas. Though the IMEB closure always performs slightly better than the bi-Maxwellian in these cases, the fact that the latter provides an analytic expression of the distribution function suggests it as an alternative to both IMEB and true maximum-entropy closures. This could be particularly relevant when considering more realistic collision operators and/or boundary conditions in three-dimensional kinetic descriptions. For both shock- and PTC-related problems, direct comparisons between the bi-Maxwellian and maximum-entropy distributions have furthermore shown excellent qualitative agreement in terms of overall distribution behaviour and excellent quantitative agreement in terms of closing flux predictions.

An additional advantage of multi-Gaussian-type closures is that they may be extended to higher moment systems containing additional non-equilibrium physics by adding more quadrature points (Gaussians) or considering less restrictive ansatzes (e.g., allowing multiple values for $\sigma$). These one-dimensional findings have suggested the extension of the bi-Maxwellian clo-
sure to the 14-moment bi-Gaussian closure of Section 4.4.3. The numerical solution procedure and preliminary 2D results for this extension are presented in the chapters to follow.
Chapter 6

Finite-Volume Numerical Solution Procedure

This chapter of the thesis describes a second-order upwind finite-volume scheme used for obtaining two-dimensional (2D) numerical simulations of the bi-Gaussian moment closure of interest using a parallel finite-volume scheme on multi-block quadrilateral meshes. The scheme has been previously developed by Tensuda et al. [19–22] for the prediction of non-equilibrium gas flows using the 10-moment Gaussian and 14-moment interpolative maximum-entropy-based closures. The following sections briefly present Tensuda et al.’s numerical scheme (refer to [20] for a detailed overview) and propose extensions for multiphase flows as well as new flux functions and boundary conditions.

The finite-volume discretization for the 14-moment system arising from the bi-Gaussian closure must be applied to the system of transport equations of Eq. (4.29). For simplicity, we can group the collision and drag terms into a single source term, \( S = C + D \), such that we now desire a discretized formulation to the governing equations defined by

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_k}{\partial x_k} = \mathbf{S}
\]  

Approaching equilibrium, the characteristic relaxation time associated to interparticle collisions, \( \tau \), can become very small, and therefore the system of equations can become somewhat stiff. Similar stiffness issues are also encountered with the addition of the drag source term when considering multiphase flow simulations, especially when gas-liquid relative velocities are high. To deal with these stiffness, McDonald [93] has initially proposed a two-step semi-implicit time marching scheme for the 10-moment Gaussian closure that treats transport terms explicitly and source terms implicitly through a local time linearization [94]. We consider this time marching scheme here, and the fully discrete form of the evolution of the solution vector...
\( U_{(i,j)} \) in a cell \( (i,j) \) can be written as

\[
\hat{U}_{(i,j)}^{n+1} = U_{(i,j)}^n - \frac{\Delta t}{A_{(i,j)}} \left( \sum_k (F_k \cdot n_k \Delta \ell_{(i,j,k)}^n) \right) + \Delta t \hat{S}_{(i,j)}^{n+1}, \tag{6.2}
\]

\[
U_{(i,j)}^{n+1} = U_{(i,j)}^n - \frac{\Delta t}{2A_{(i,j)}} \left( \sum_k (F_k \cdot n_k \Delta \ell_{(i,j,k)}^n) + \sum_k (\tilde{F}_k \cdot n_k \Delta \ell_{(i,j,k)}^{n+1}) \right) + \Delta t \left( \frac{S_{(i,j)}^n + \hat{S}_{(i,j)}^{n+1}}{2} \right), \tag{6.3}
\]

where \( \Delta t \) is the time step and, for the \( k \)th face of a cell \( (i,j) \), \( A_{(i,j)} \) is the cell area, \( \Delta \ell \) is the cell face surface length and \( n_k \) is the cell face unit normal vector, as depicted in Figure 6.1. The semi-implicit time-marching formulation of Eqs. (6.2)-(6.3) allows to determine the simulation time step via a usual CFL condition based on the global maximum wave speed rather than on the collision relaxation time, \( \tau \), or characteristic drag relaxation time, \( \tau_p \).

In order to determine the solution at each cell interface, a piecewise linear reconstruction is performed via a least-squares approach with either Barth-Jespersen [95] or Venkatakrishnan [92] slope limiters. The value of the flux, \( F_k \), at each interface is then determined via the solution of the HLL approximate Riemann solver [90] or kinetics-based flux function [96] described below.

### 6.1 HLL Approximate Riemann Solver

Similarly to the numerical scheme of Chapter 5 for the one-dimensional case, an HLL approximate Riemann solver is considered for the multi-dimensional implementation of the 14-
moment closure. At the $k^{th}$ interface of a cell $(i,j)$, the flux can be written as

$$
F_{(i,j,k)} = \begin{cases} 
F_{(i,j,k)}^{(L)}, & \text{if } \lambda^- > 0 \\
F_{(i,j,k)}^{(R)}, & \text{if } \lambda^+ < 0 \\
F_{HLL} = \lambda^+ F_{(i,j,k)}^{(L)} - \lambda^- F_{(i,j,k)}^{(R)}, & \text{otherwise}
\end{cases}
$$

(6.4)

where the second term of $F_{HLL}$ introduces wave speed-dependent numerical dissipation and the superscripts $(R)$ and $(L)$ denote the left and right solution states, respectively. Due to the complexity of the eigensystem resulting from the 14-moment closure, approximate wave speeds based on scalings of the local sound speed by a parameter $\zeta$ are used, such that the wave speeds $\lambda^-$ and $\lambda^+$ are expressed as

$$
\lambda^- = \min \left( u_x^{(R)} - \zeta \sqrt{\frac{\gamma P_{xx}^{(R)}}{\rho^{(R)}}}, u_x^{(L)} - \zeta \sqrt{\frac{\gamma P_{xx}^{(L)}}{\rho^{(L)}}} \right),
$$

(6.5)

$$
\lambda^+ = \max \left( u_x^{(R)} + \zeta \sqrt{\frac{\gamma P_{xx}^{(R)}}{\rho^{(R)}}}, u_x^{(L)} + \zeta \sqrt{\frac{\gamma P_{xx}^{(L)}}{\rho^{(L)}}} \right),
$$

(6.6)

in the case of the interpolative maximum-entropy-based closure and

$$
\lambda^- = \min \left( \min \left( v_1^{(R)}, v_2^{(R)} \right) - \zeta \sqrt{3 \Theta_{xx}^{(R)}}, \min \left( v_1^{(L)}, v_2^{(L)} \right) - \zeta \sqrt{3 \Theta_{xx}^{(L)}} \right),
$$

(6.7)

$$
\lambda^+ = \max \left( \max \left( v_1^{(R)}, v_2^{(R)} \right) + \zeta \sqrt{3 \Theta_{xx}^{(R)}}, \max \left( v_1^{(L)}, v_2^{(L)} \right) + \zeta \sqrt{3 \Theta_{xx}^{(L)}} \right),
$$

(6.8)

in the case of the 14-moment bi-Gaussian closure, where the value of the coefficient $\zeta$ is chosen to be large enough to obtain stable solution and small enough to avoid excessive numerical dissipation. The knowledge of the distribution allows for a more insightful approximation of the wave speeds, as seen in Eqs. (6.7)-(6.8), where a scaling based on the maximum wave speeds of the Gaussian closure is preferred [42, 93].

### 6.2 Kinetic-Based Flux Function

The closed-form expression of the distribution function provided by the bi-Gaussian closure allows the exploration of another family of flux functions for numerical solution of the moment equations, namely kinetic-based flux functions, as first considered by Bouchut et al. [96]. The
kinetic-based description separates the distribution function into its positive and negative velocity components to evaluate the advection term of Eq. (4.1) directly. In this case, the convolution integrals of the velocity-weighted bi-Gaussian distribution must be integrated over a semi-infinite domain ranging from zero to $\pm \infty$ in order to recover the moments of the flux dyad. At a cell interface $j + \frac{1}{2}$ rotated into Cartesian coordinates, the net flux corresponding to a moment of order $v_\alpha^x v_\beta^y v_\gamma^z$ across the interface can be expressed as

$$
(F_{\alpha,\beta,\gamma})_{j+\frac{1}{2}} = \int\int_{-\infty}^{+\infty} \left( \int_0^{+\infty} v_\alpha^x v_\beta^y v_\gamma^z F_{BG} \, dv_\alpha \right)_{j} + \left( \int_{-\infty}^{0} v_\alpha^x v_\beta^y v_\gamma^z F_{BG} \, dv_\alpha \right)_{j+1} \, dv_\beta \, dv_\gamma. \tag{6.9}
$$

Though this flux formulation brings forth an additional evaluation cost due to the integration of Gaussian distributions over only a semi-infinite domain, it is highly advantageous due to its preservation of moment realizability at each flux evaluation and natural upwinding of the solution. The upwinding arises from the fact that the direction in which information propagates is implicitly taken into account through the half-integrals of $F_{BG}$ over velocity space. Furthermore, the use of conservative approximate wave speeds do not introduce any additional numerical dissipation in this case.

### 6.3 Solid-Wall Boundary Conditions

The implementation of appropriate solid-wall boundary conditions reproducing desired non-equilibrium phenomena are not intuitive when using moment closure methods, and this can be perceived as a drawback of the method. One method is to employ a half-Maxwellian boundary condition [4, 19–22, 93], for which it is assumed that their exists an infinitesimally thin Knudsen layer adjacent to the solid surface, where the fluid’s distribution function exists as a combination of the internal distribution and a wall-reflected distribution (See Figure 6.2). Assuming a solid-wall parallel to the $y$-axis, the distribution function in the Knudsen layer, $F_{Kn}$, can be separated into two components as follows

$$
F_{Kn} = F_+ + F_- \tag{6.10}
$$

![Figure 6.2: Schematic representation of the Knudsen layer [93].](image)
where $\mathcal{F}_-$ is the portion of the internal flow field distribution, $\mathcal{F}_{\text{int}}$, with negative-valued velocities and is expressed as

$$
\mathcal{F}_- = \begin{cases} 
\mathcal{F}_{\text{int}}(v_x, v_y, v_z) & \text{if } v_x < 0, \\
0 & \text{if } v_x > 0,
\end{cases}
\tag{6.11}
$$

and $\mathcal{F}_+$ is the reflected portion of the internal distribution function. The positive-valued velocity portion of the internal distribution function impacts the wall, and is partially accommodated in terms of an accommodation factor $A$, for which a value of $A = 1$ corresponds to particles being fully accommodated to the wall temperature and a value of $A = 0$ corresponds to particles being specularly reflected off the wall surface. The resulting expression for $\mathcal{F}_+$ is

$$
\mathcal{F}_+ = \begin{cases} 
AM_w(v_x, v_y, v_z) + (1 - A)\mathcal{F}_{\text{int}}(-v_x, v_y, v_z) & \text{if } v_x < 0, \\
0 & \text{if } v_x > 0,
\end{cases}
\tag{6.12}
$$

where $M_w$ is the wall-temperature equilibrium Maxwellian distribution and is expressed as

$$
M_w = n_w \left( \frac{m}{2 \pi k T_w} \right)^{3/2} e^{-\frac{m}{2 k T_w} (v_x^2 + (v_y - u_w v_y)^2 + v_z^2)},
\tag{6.13}
$$

where $T_w$ is the wall temperature. Boundary conditions for individual moments are subsequently obtained through a convolution integral of $\mathcal{F}_{Kn}$ over velocity space. The distribution $\mathcal{F}_{Kn}$ is only defined for negative $x$-velocity abscissas, and therefore the boundary condition, or Knudsen layer moment, $(M_{\alpha,\beta,\gamma})_{Kn}$, of order $u^\alpha v^\beta w^\gamma$ is expressed as

$$
(M_{\alpha,\beta,\gamma})_{Kn} = \int_0^\infty \left( \int_{-\infty}^\infty \int_{-\infty}^\infty v_x^\alpha v_y^\beta v_z^\gamma \mathcal{F}_{Kn} dv_x ight) dv_y dv_z.
\tag{6.14}
$$

6.3.1 Gaussian-Based Perturbative Internal Distribution

A known drawback of the interpolative 14-moment closure of McDonald and Torrilhon [18] and a motivation behind the development of the bi-Gaussian closure is the absence of a closed-form expression for the distribution function. This drawback can readily be seen in the implementation of the half-Maxwellian boundary condition, where an expression for the internal distribution, $\mathcal{F}_{\text{int}}$ is required. In initial implementations of the 14-moment closure, Tensuda et al. [19–22] have used a Grad-like expansion about a Gaussian distribution [97–99] containing 14 free parameters, which is compatible with the 14-moment closure and can be
expressed as

$$F_{\text{int}} = F^{(14)} = G \left[ 1 + \frac{D_{\beta}}{5} \left[ \Theta_{\alpha\beta}^{-1} \left( c_{\alpha} c^2 - \frac{P_{\gamma\gamma}}{\rho} c_{\alpha} \right) - 2c_{\beta} \right] 
+ 3E \left( c^4 - 2\frac{P_{\alpha\alpha}}{\rho} c^2 - 4\frac{P_{\alpha\beta}}{\rho} c_{\alpha} c_{\beta} + \frac{P_{\alpha\alpha} P_{\beta\beta}}{\rho^2} + 2\frac{P_{\alpha\beta}^2}{\rho^2} \right) \right].$$  \hspace{1cm} (6.15)

where the closure coefficients can be obtained in terms of the moments of \( U \). The resulting boundary conditions for individual moments are obtained through Eq. (6.14) and are developed by Tensuda et al. [20].

### 6.3.2 Bi-Gaussian Internal Distribution

A benefit of the 14-moment bi-Gaussian closure over the interpolative closure can be readily seen in this first implementation of boundary conditions. The 14-moment perturbative distribution above does not possess desired maximum-entropy properties, and initial work has already shown that its use is problematic [19–22]. The bi-Gaussian distribution, \( F_{\text{bG}} \), obtained through the closing expressions of Eqs. (4.55)-(4.57), can be substituted for \( F_{\text{int}} \), and boundary condition moments can subsequently be obtained from Eq. (6.14).

![Figure 6.3: Example of overlapping ghost cells for a four-block Cartesian grid [25].](image)
6.4 Performance Improvements

As the focus of this thesis was not the development of the numerical scheme, the current chapter will not go into details on the various code capabilities for improvements in computational time. Tensuda et al. focused on the parallel implementation of a Newton-Krylov-Schwarz (NKS) algorithm with adaptive mesh refinement (AMR) [19–22]. These capabilities are available in the current implementation of the 14-moment interpolative and bi-Gaussian closures, however they have not been extensively studied in the scope of this thesis.

The finite-volume scheme for the 14-moment closure has also been implemented within a framework allowing for block-based AMR, which has been developed by Groth and co-workers [25–28]. Using physics-based criteria, the AMR technique seeks to refine an initial multi-block mesh in areas that will lead to the highest increase in solution accuracy. The current implementation allows for isotropic mesh refinement, meaning that each block flagged for refinement is subdivided into four blocks of identical resolution. This subdivision technique allows for a light and efficient data structure that can be stored on each processor, therefore reducing computational time. For simple and efficient parallel implementation, computations are performed independently on each solution block, around which a layer of ghost cells is stored. The storage of ghost cells allows for the linear reconstruction of the solution as well as adequate formulation of boundary conditions at the block edges. An example of a ghost cell layer for a simple four-block Cartesian mesh is schematically shown in Figure 6.3 [25].

The current implementation also allows for fully implicit time advancement through an NKS algorithm [25, 100]. Fully implicit schemes are quite advantageous in finding solutions to computationally stiff systems of equations such as the 14-moment system, since they are unconditionally stable and therefore allow for very large time steps. In cases where the transient solution is not important, convergence through a Newton’s method is possible, as is performed within the NKS algorithm. A more complete description of the implementation of the NKS algorithm is provided by Tensuda [20].
Chapter 7

Numerical Results

The current chapter presents some preliminary numerical results for rarefied gas dynamics and liquid spray problems in two dimensions using the numerical scheme presented in Chapter 6. Results for the bi-Gaussian closure are first compared to the interpolative maximum-entropy-based closure for several problems in rarefied gas dynamics. Preliminary comparisons for a PTC-related problem are then made between the 14-moment bi-Gaussian and 10-moment Gaussian closures. Although the preliminary test cases have been performed using the kinetics-based flux function (Section 6.2), numerical results are shown here using only the HLL flux function.

7.1 Test Problems for Rarefied Gas Dynamics

The focus of the rarefied gas dynamics simulations here is to verify the asymptotic limits of the bi-Gaussian closure for simplified 2D test cases. The two test cases considered herein allow to do so while comparing with reference analytic solutions, as well as continuum and free-molecular models. Namely, a micro-Couette flow and the heat transfer between two stationary plates is considered. In both cases, the Grad-like perturbative Gaussian solid-wall boundary conditions with an accommodation factor of $A = 1$ are used along with periodic boundary conditions in the wall-parallel direction. Computations were performed so as to achieve to steady-state solutions using the NKS solution method outlined in the previous chapter.

7.1.1 Micro-Couette Flow

The Couette flow problem is a good initial test case to assess the ability of a moment closure to capture non-equilibrium phenomena which are independent of heat transfer. The case of two parallel plates moving in opposite direction with equal velocity has been previously considered
by McDonald and Groth [17] using the 10-moment Gaussian closure and subsequently by Tensuda et al. [19–22] for the interpolative 14-moment closure. Both of these alternate closures show excellent agreement with reference solutions, and results were very comparable in both cases, as heat transfer effects are negligible. The interpolative 14-moment closure will therefore be used as a reference 14-moment solution.

Assuming a hard sphere collision model [9], the mean free path between inter-particle collisions, \( \lambda \) can be written as

\[
\lambda = \frac{16\mu}{5\sqrt{2\pi}\rho}.
\]  

(7.1)

The Knudsen number, \( \text{Kn} = \lambda/D \), can in this case simply be modified by changing the distance between the plates, \( D \). As \( D \) is decreased and the free-molecular regime is approached, it is anticipated slip flow effects become more prominent, as inter-particle collisions become less frequent and the flow becomes dominated by interactions between the wall and the gas particles.

The Couette flow features a monatomic gas, argon, between two parallel plates moving in opposite directions, each at a velocity of \( U_w = 30 \text{ m/s} \). The gas between the plates is initialized with a density of \( \rho = 1.225 \text{ kg/m}^3 \), a pressure of \( p = 101.325 \text{ kPa} \) and a Prandtl number of \( \text{Pr} = 0.7 \). The temperature of both the gas and plates is 397.37 K to ensure minimal heat transfer between them. Computations are performed to steady-state on a mesh with 10 cells in the \( x \)-direction and 100 cells in the \( y \)-direction.

![Figure 7.1: Results for micro-Couette flow: comparison between bi-Gaussian and interpolative maximum-entropy-based 14-moment closures. (a) Velocity profiles in terms of Knudsen number and (b) slip velocity as compared to reference Navier-Stokes and Lees [101] solutions.](image)
Figure 7.1a shows the wall-normalized velocity profile between both plates in terms of the Knudsen number as predicted by both 14-moment closures considered. It can be observed that as the distance between the plates is decreased, the velocity profile becomes steeper, and important slip effects occur. At \( \text{Kn} = 0.01 \), the continuum solution is nearly recovered, as the slip velocity is negligible. However, as the Knudsen number is increased to \( \text{Kn} = 10 \), the flow regime approaches the free-molecular limit, and the mean gas velocity is almost everywhere near zero. Both closures agree very well in all cases. A plot of the normalized wall velocity on a logarithmic scale allows a comparison of the 14-moment interpolative and bi-Gaussian closure predictions with the reference Lees solution [101], as well as the conventional continuum limit Navier-Stokes result, as shown in Figure 7.1b. It can be seen that both the Bi-Gaussian and IME fourteen-moment closures agree very well with the Lees solution, with the maximum-entropy solution matching the reference slightly better approaching free-molecular Knudsen number values.

### 7.1.2 Heat Transfer Between Parallel Plates

The next test case considers the heat transfer between two fixed parallel plates as a function of the Knudsen number. Since the gas particles are fully accommodated to the wall temperature, a linear temperature profile matching the wall temperatures at the boundaries is expected to form between both plates in the continuum limit. Similarly to the velocity boundary condition for the Couette flow case, a temperature slip is expected which increases with Knudsen number. This case is a good benchmark to measure the ability of each 14-moment closure to capture non-equilibrium heat transfer effects, where lower-order closures are known to fail.

The gas between the heated plates is once again argon at a temperature of \( T_0 = 397.37 \) K, density of \( \rho = 1.225 \) kg/m\(^3\), pressure of \( p = 101.325 \) kPa and Prandtl number of \( \text{Pr} = 0.7 \). The upper and lower plate temperatures are set to \( T_U = 407.37 \) K and \( T_L = 387.37 \) K, respectively. Computations are performed on an identical \( 10 \times 100 \) mesh.

Figure 7.2 shows the predicted temperature profiles between both plates for increasing Knudsen number. For lower Knudsen numbers, both closures agree quite well, however a convergence issue for \( \text{Kn} = 0.1 \) was encountered for the bi-Gaussian closure approaching the top surface. As the Knudsen number is increased, the interpolative closure shows an offset with the mean plate temperature at the plate midpoint, which does not occur in the case of the bi-Gaussian closure. This offset was previously associated to improper boundary conditions [19–22]. The use of identical boundary conditions in this case however suggests a cause related to the interpolative closure itself which requires further investigation.

Figure 7.3 depicts the resulting wall heat flux, normalized with respect to its free-molecular
Figure 7.2: Results for heat transfer between two plates: comparison of temperature profiles for bi-Gaussian and interpolative maximum-entropy-based 14-moment closures for different Knudsen numbers.

Figure 7.3: Comparison of bi-Gaussian and interpolative maximum-entropy-based results for heat transfer between two plates: normalized heat flux at the wall in terms of Knudsen number as compared to reference free-molecular, Navier-Stokes and Navier-Stokes with slip solution.
value \([102]\), \(q_x\), which is expressed as
\[
q_x = \rho_m \sqrt{\frac{RT_m}{2\pi}} \left( c_v + \frac{1}{2} R \right) (T_U - T_L),
\] (7.2)
and where \(\rho_m\) is the density midway between the plates, \(R\) is the specific gas constant and \(c_v\) is the heat capacity at constant volume. In this case, both the bi-Gaussian and IME closures agree very well with a reference Navier-Stokes solution with slip boundary conditions, and both converge from the Navier-Stokes to the free-molecular limit with increasing Knudsen number.

### 7.2 Test Problems for Sprays

An evaluation of the bi-Gaussian closure’s ability to capture pure PTC representative of monodisperse spray flows has also been considered here. For these purposes, the test case designed by Vié et al. [42] is reconsidered here. As illustrated in Figure 7.4, the spray flow test case consists of two liquid jets of particles in a compressive gas flow field undergoing several crossings without collisions. The \(y\)-direction gas phase velocity varies linearly with \(y\) following
\[
u_{gy} = -\epsilon y,
\] (7.3)

![Figure 7.4: Reference Lagrangian solution for simulation of two jets in a compressive velocity field.](image-url)
Chapter 7. Numerical Results

where the slope, $\epsilon$, is set to $-1 \, \text{s}^{-1}$ in this case. The $x$-direction gas phase velocity is set to $u_{gx} = 0.2 \, \text{m/s}$. Liquid droplets of constant size are injected into a vacuum with a velocity $u_x = u_{gx}$ and $u_y = 0$ between $-0.6 < y < 0.4$ and $0.4 < y < 0.6$ with a number density of $n = 1 \, \text{m}^{-3}$. There exists an analytical Lagrangian solution to the jet trajectories, which are bounded between the streamlines shown in Figure 7.4. The following sections present both quasi-2D and 2D solutions to the crossing jets problem. In both cases, the HLL flux function is used along with the semi-implicit time marching scheme of Chapter 6.

7.2.1 Quasi-2D Simulation of Two Crossing Jets

Numerically dealing with particles injected into a vacuum can be quite challenging. Furthermore, singular pressure tensors can arise at crossing locations. This is due to the fact that the pressure in vacuum zones is very low compared to the high density crossing regions, where the standard deviation relatively large due to the presence of a bimodal distribution. These issues make it very difficult to solve this problem in multiple dimensions. We therefore chose to initially solve an equivalent quasi-2D problem, in which a reference frame moving at $u_{gx}$ is considered. This essentially allows us to solve a time-dependent 1D problem, for which it

![Figure 7.5: Quasi-two dimensional number density results for crossing jets in a compressive velocity field as predicted by the 10-moment Gaussian closure.](image)
is only required to maintain the positivity of the diagonal pressure terms: \( P_{xx} \) and \( P_{yy} \). To undoubtedly ensure solution stability, a basic first-order scheme is used in this case with a very high resolution of 10,000 cells in the \( y \)-direction and a single cell in \( x \)-direction, which nevertheless did not allow for full spatial convergence of the results.

Figure 7.5 shows results obtained using the 10-moment Gaussian closure. The unimodal Gaussian distribution does not allow for large-scale PTCs, and therefore after the first crossing, droplets diffuse into a single region. Figure 7.5 also shows that the average droplet trajectories are somewhat well-predicted, as the majority of the droplets remain within the external Lagrangian trajectories.

Results obtained using the 14-moment bi-Gaussian closure are in turn shown in Figure 7.6, where the distinct modelling advantage of the bi-Gaussian closure can immediately be seen. At the location of the first crossing, the moment state contains sufficient information to reproduce a bimodal distribution, and particles can successfully undergo a crossing. Furthermore, the number density is largely contained within the internal and external Lagrangian trajectories. The number density contained outside these trajectories can be attributed to the excessive numerical diffusion caused by the first-order scheme.
7.2.2 Fully 2D Simulation of Two Crossing Jets

The capabilities of each closure have been assessed in a simple manner through the quasi-2D results above. However, fully two-dimensional results are also desired and examined here. We therefore present preliminary results using the fully second-order scheme presented in Chapter 6 for both the Gaussian and bi-Gaussian closures. Results are computed on the computational domain of Figure 7.4 on a mesh of \(2000 \times 1000\) cells. Using the Gaussian closure, it was possible to obtain satisfactory 2D results which replicate the findings of Vé et al. [42] quite well. Refer to Figure 7.7a. A similar velocity diffusion can be observed following the first crossing, as is evidenced in Figure 7.7b. The use of the second-order scheme is however readily seen, as significantly less numerical diffusion occurs outside of the Lagrangian trajectories.

The extension to the second-order fully two-dimensional scheme has however shown to be problematic in the case of the proposed bi-Gaussian closure, as shown by the number density contours of Figure 7.8a. The solution remains smooth until the first crossing, however as random velocity abscissas become more important following the first crossing, the solution rapidly becomes unstable. This is readily seen as the particle jets interact with the vacuum zones and oscillations begin to form. The crossing is however very well captured by this 14-moment closure (refer to Figure 7.8b), and initial observations are encouraging, as the number density is well-contained within the reference Lagrangian trajectories. The observed unstable, oscillatory behaviour warrants further study of the proposed numerical solution methods and its treatment of vacuum conditions, which is required to ensure robust and accurate solutions of the PTC spray problem with the bi-Gaussian closure.
Figure 7.7: Fully 2D (a) number density results for crossing jets in a compressive velocity field as predicted by the 10-moment Gaussian closure and (b) closeup of particle crossing.
Figure 7.8: Fully 2D (a) number density results for crossing jets in a compressive velocity field as predicted by the 14-moment bi-Gaussian closure and (b) closeup of particle crossing.
Chapter 8

Conclusions and Future Work

A 14-moment bi-Gaussian closure has been proposed and developed for potential application to rarefied gas dynamics and liquid sprays. The thesis research can be separated into two main parts, namely (1) the study of a univariate kinetic system and (2) the extension of univariate findings to multiple space and velocity dimensions.

In order to better understand the properties of multi-Gaussian closures, a univariate kinetic model has been thoroughly analysed through descriptions of closing flux behaviour in realizable moment space and applications related to non-equilibrium shocks and PTCs. In 1D, the associated bi-Maxwellian closure has shown great promise when compared to a competing model, namely the IMEB closure, as well more conventional Grad-like and QMOM closures. These comparisons have undoubtedly demonstrated the advantage of maximum-entropy-based closures over more conventional closures. Furthermore, both the IMEB and bi-Maxwellian closures have outperformed near-equilibrium Navier-Stokes solutions in all cases considered, and quantitative and qualitative agreement with a reference DVM solution was observed for a large range of departures from LTE. The consideration of a bi-Gaussian closure for use within Levermore’s maximum-entropy hierarchy also warranted direct comparisons of the bi-Maxwellian and maximum-entropy distributions. These comparisons have demonstrated good qualitative agreement for the most part, however a consistent observation was a more modular bi-Maxwellian distribution. This can nonetheless be seen as an advantage when considering PTC-related applications, where obtaining multi-modal distributions is essential.

The multi-dimensional extension of the bi-Maxwellian closure was performed through the derivation of a 3D bi-Gaussian closure and its implementation within a multi-block parallel finite-volume code allowing for inter-particle collisions and Stokes drag. A kinetics-based flux function and bi-Gaussian half-Maxwellian boundary conditions have also been derived and implemented without however being formally tested. Preliminary 2D results for non-equilibrium gaseous flows have allowed initial comparisons with the interpolative 14-moment
closure, and the asymptotic limits of the bi-Gaussian closure have been verified, while showing that it is very comparable to its interpolative counterpart for cases with and without important heat transfer effects.

Preliminary results for liquid sprays have however shown to be more challenging. The ability to capture PTC has nevertheless been adequately demonstrated in the case of a quasi-2D solution strategy for the crossing jets problem considered, where the clear advantage of using a 14-moment closure over a lower 10-moment closure is readily observed. In the testing of the fully two-dimensional second-order scheme, the inadequate treatment of vacuum zones and post-crossing regions has been attributed to the unstable solutions obtained. Results are however quite encouraging, as the general behaviour of the crossing problem was well captured by the bi-Gaussian closure.

Though a thorough and complete validation of the bi-Gaussian closure has not yet been performed, success in doing so would be highly desirable, as many anticipated advantages are associated with the availability of a maximum-entropy-inspired closure with a closed-form for the approximate distribution function. The BGK and Stokes models studied herein are not ideal to fully showcase these advantages, since they do not require additional information on the distribution. Benefits are to be expected when considering such systems, with the main advantages being expected in the consideration of more physically accurate collision operators as well as boundary conditions.

Future follow-on research will aim to perfect the practical implementation of the bi-Gaussian closure and the 2D numerical scheme, especially in its adaptation to multi-phase flows. In particular, a second-order scheme able to preserve moment realizability is required in interactions with vacuum zones and in regions where the pressure tensor becomes nearly singular, as is observed in pure PTC. The development and testing of the kinetics-based flux function is also of interest, as it possesses many potential benefits that are only achievable when relying on a closed-form expression to the distribution function. The bi-Gaussian closure has shown good agreement with the 14-moment interpolative closure, however the advantages related to its closed-form distribution function have not yet been exploited. Future studies with bi-Gaussian-based boundary conditions will allow to fully assess its benefits, as compared to other maximum-entropy-based methods. Finally, a thorough comparison of the bi-Gaussian and interpolative 14-moment models with the 10-moment Gaussian model will be a good exercise in determining the ideal closures for rarefied gas and spray applications.
Bibliography


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