INTERPOLATIVE HYPERBOLIC REALIZABLE MOMENT CLOSURES FOR NON-EQUILIBRIUM FLOWS WITH HEAT TRANSFER

by

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A thesis submitted in conformity with the requirements for the degree of Master of Applied Science Graduate Department of Aerospace Engineering University of Toronto

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Abstract

Interpolative Hyperbolic Realizable Moment Closures for Non-Equilibrium Flows with Heat Transfer

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The predictive capabilities of a novel, 14-moment, maximum-entropy-based, interpolative closure are explored for multi-dimensional non-equilibrium flows of a monatomic gas with heat transfer. Unlike the maximum-entropy closure on which it is based, the interpolative closure provides closed-form expressions for the closing fluxes while retaining a large region of hyperbolicity. Properties of the moment system are explored via a dispersion analysis and an implicit finite-volume solution procedure is proposed. Multi-dimensional applications of the closure are then examined for several canonical non-equilibrium flow problems in order to provide an assessment of its capabilities. The predictive capabilities of the closure were found to surpass those of the 10-moment Gaussian closure. It was also found to predict interesting non-equilibrium phenomena, such as counter-gradient heat flux. The proposed implicit solver showed improved computational performance compared to the previously studied semi-implicit technique.
Acknowledgements

My experience at the University of Toronto Institute for Aerospace Studies (UTIAS) has been very enjoyable and rewarding, and this is for the most part thanks to the wonderful community present. I would like to thank all the faculty, staff, and students at UTIAS for providing such a positive environment for study, research, and leisure. I especially thank my thesis supervisors, Prof. Clinton Groth and Prof. James McDonald, for their support, guidance, and contagious passion for research. I am gracious also of the opportunities which I have been provided to participate in the aerospace research community. Furthermore, I am thankful to my research committee, Professors J.J. Gottlieb, Ö.L. Gülder, P.S. Sampath, and A.M. Steinberg, for their questions and guidance during my research assessment committee meetings.

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Boone Tensuda
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Chapter 1

Introduction

1.1 Motivation

The prediction of transition-regime non-equilibrium flows has proven to be a challenging branch of study in computational fluid dynamics (CFD). Transition-regime flows are encountered in a variety of engineering scenarios including: upper atmosphere flight and orbital reentry \cite{1}, flows in micro-electromechanical systems (MEMS) \cite{2,3}, chemical vapour deposition in semi-conductor manufacturing, and the study of internal shock structure \cite{4,5}. These high-Knudsen-number flows cannot be modelled using typical continuum approaches, such as the Euler and Navier-Stokes-Fourier (NSF) equations. Traditional methods for modelling non-equilibrium flows, such as direct simulation Monte Carlo (DSMC) methods \cite{6} and techniques involving direct discretization of the Boltzmann equation \cite{7}, are limited by their high computational cost, especially when applied in the transition regime \(0.01 \lesssim \text{Kn} \lesssim 10\) or at low Mach numbers. The DSMC technique models a large number of representative particles, and therefore will suffer from slow convergence when many particles are needed. The downfall of solving the discretized Boltzmann equation is the high dimensionality, which leads to high computational cost and storage; especially for physically realistic three-dimensional cases. The discretized Boltzmann approach also becomes intractable when a wide range of fluid velocities are considered, since the discretized region of velocity space must be very large.

The method of moment closures offers an alternative technique for accurately treating transition-regime flows with the potential of greater robustness and a significantly reduced computational cost. The moment-closure method considers an assumed form of the particle distribution function to avoid modelling individual particles. It yields
an approximation to the Boltzmann equation that consists of a finite set of partial differential equations (PDEs). These equations are of lower dimensionality as compared with the Boltzmann equation, and thus computational cost is reduced. Furthermore, the purely hyperbolic and first-order quasilinear nature of some moment closures also presents several numerical advantages which extend into both the transition and continuum regimes \[8\]. These hyperbolic systems are less sensitive to grid irregularities, making them well suited to adaptive mesh refinement (AMR) and complex geometries. They also only require evaluating first derivatives, which means that an extra order of spatial accuracy, relative to a mixed hyperbolic-parabolic system, can often be gained using the same stencil.

However, moment closures do have weaknesses, which historically have prevented them from being a mainstream non-equilibrium simulation method. The traditional Grad \[9\] closures assume the distribution function is a Hermite expansion function about the equilibrium Maxwellian. Unfortunately, it is possible for this assumed distribution to become negative, which is nonphysical. Also, as the distribution strays further from equilibrium, there is a loss of hyperbolicity of the resulting moment equations, and a closure breakdown \[8\]. Furthermore, when modelling internal shock structure the closures are also prone to developing unphysical sub-shocks for moderate Mach numbers.

The Chapman-Enskog closure is another popular moment-closure technique. This closure assumes that the distribution is in the form of a small perturbation about the equilibrium Maxwell-Boltzmann distribution \[10, 11\]. Unfortunately, closures resulting from Chapman-Enskog expansions contain both hyperbolic and elliptic terms, which is less desirable for numeric applications. Similar to the Grad closures, they are based on expansions about the equilibrium distribution, and thus also break down for moderate departures from equilibrium.

Recently, new moment closures have been proposed which are no longer limited by the issues which have hindered the traditional Grad and Chapman-Enskog closures. In particular, a hierarchy of moment closures having a number of desirable properties has been derived based on the maximization of thermodynamic entropy \[12, 13\]. These so-called maximum-entropy moment closures do not rely on an expansion about the Maxwellian, and therefore avoid many of the issues associated with the traditional Grad and Chapman-Enskog closures. Unfortunately, complications encountered when considering closures with a treatment for higher-order moments, such as heat transfer, have severely limited the use of these maximum-entropy closures for general non-equilibrium
flows. Nevertheless, new, interpolative-type, maximum-entropy-based, 5-moment (one-dimensional gas) and 14-moment (three-dimensional gas) closures, initially investigated by McDonald and Groth [8], and expanded upon by McDonald and Torrilhon [14], have been proposed that successfully navigate the aforementioned problems. These closures also have high wave speeds, which allows them to model internal shock structure without developing sub-shocks, even at high Mach numbers.

1.2 Scope of the Current Study

This study presents a further numerical and mathematical investigation of these new interpolative, maximum-entropy-based, 5- and 14-moment closures. The goal being to assess the performance of this novel closure technique for simulating multi-dimensional non-equilibrium flows, particularly those with heat transfer, as well as to further develop the numeric algorithm with which the closure is solved. A mathematical dispersion analysis of the governing moment transport equations has also been performed in order to gain insight into the system’s wave speeds, stiffness, and stability. The applicability of the 14-moment interpolative closure to multidimensional flows was examined by solving several two-dimensional canonical flow problems, including Couette flow, conduction between heated flat plates, subsonic flow past a circular cylinder, and lid-driven cavity flow. As such, this study represents the first application of this novel closure to multi-dimensional flows.

These results are compared to analytic solutions; continuum-regime solutions found using the Navier-Stokes-Fourier equations; other moment closures, such as the Gaussian and regularized Gaussian closures; DSMC results; and experiment. Based on these comparisons the performance of this new solution technique is appraised. By comparing to the Gaussian closure, which is a 10-moment maximum-entropy closure that does not consider heat transfer, the effect of the addition of heat-transfer moments in the 14-moment interpolative closure can be observed. The regularized Gaussian closure is a closure that seeks to approximately model heat transfer, through the addition of elliptic terms found through a regularization technique [15], and insight into the validity of this approximation is also gained through these comparisons.

In order to obtain solutions to this new equation system, the finite-volume numeric solver, which has previously been used to solve maximum-entropy type closures [14,16], has been further developed. In particular, an implicit time-marching method has been
integrated, which is compared to a previously used semi-implicit method. A novel set of boundary conditions, based on the solid-wall half-Maxwellian method, were also derived.

1.3 Overview

The thesis begins with an overview of relevant gas kinetic theory (Chapter 2) and the moment-closure technique with emphasis on the maximum-entropy type closures (Chapter 3). The 5- and 14-moment, maximum-entropy-based, interpolative-type closures are then presented in Chapter 4. The finite-volume procedure and time marching schemes utilized to solve the 14-moment interpolative closure on two-dimensional computational domains, and the associated boundary condition technique, are discussed in Chapter 5. Various results are presented in Chapter 6, including the description and results of dispersion analyses in Section 6.1 and the multi-dimensional flow cases of Couette flow, conduction between heated flat plates, subsonic flow past a circular cylinder, and lid-driven cavity flow in Sections 6.2, 6.3, 6.4 and 6.5 respectively. Finally, in Chapter 7, conclusions are made based on the results of the dispersion analyses and multi-dimensional flow simulations, and possible future work is suggested.
Chapter 2

Gaskinetic Theory

2.1 Gaseous Flow Regimes

A useful non-dimensional parameter when discussing non-equilibrium gases is the Knudsen number, Kn. The Knudsen number is a non-dimensional value which expresses the ratio between the mean free path of gas particles, Λ, and some characteristic length scale, L: \( \text{Kn} = \frac{\Lambda}{L} \). The value of the Knudsen number is inversely proportional to the frequency of collisions in the gas, and therefore also represents the distance of the gas from local equilibrium. Gases with small Knudsen numbers experience many collisions, and thus will be near equilibrium, this is the so-called continuum regime. In this regime the fluid can be considered continuous and in local thermodynamic equilibrium (LTE). Traditional methods, which make use of macroscopic mathematical models such as the Euler and Navier-Stokes equations, can be accurately applied in this regime. Conversely, gases with very large Knudsen numbers will have a negligible number of collisions; this is known as the free-molecular regime. In this regime the molecular interactions at solid surfaces dominate, and it’s assumed that particles travel in straight lines between these surface interactions.

The transition regime lies between the continuum and free-molecular regimes, and presents the largest challenges in modelling. In this regime the LTE assumption is no longer well founded, and thus the macroscopic mathematical models are inaccurate. However, the gas is still relatively dense compared to the free-molecular regime, meaning that particle-based methods are expensive. It is in this regime that moment closures show the most promise, since they model non-equilibrium physics, but are not particle based. Although definitions of the flow regimes vary, typically the continuum regime exists for
Kn \lesssim 0.01, the transition regime for 0.01 \lesssim Kn \lesssim 10, and the free-molecular regime for Kn \gtrsim 10.

2.2 The Phase-Space Distribution Function

On a molecular level, a gas is an extraordinarily complex system. At even relatively low densities, gases consist of a very large number of particles. These particles are moving in all directions, with speeds that are quickly changing (as a result of collisions). To analyze a gas at this level would take a considerable effort. This analysis is simplified by treating the gas in statistical terms. Instead of hoping to track the velocity of the particles individually, a statistical distribution is used. In general, this distribution is a function of physical space, \(x_i\), a space of particle velocities, \(v_i\), and time, \(t\); the combination of physical and velocity space is referred to as phase-space. The expected fraction of particles within a small volume in phase-space confined by, \(x_i\) to \(x_i + d^3x_i\), and \(v_i\) to \(v_i + d^3v_i\), is \(f(x_i,v_i,t)d^3x_i d^3v_i\), where \(f(x_i,v_i,t)\) is the normalized phase-space distribution function.

To add more physical significance to this distribution function it is convenient to multiply by the number density, \(n(x_i,t)\), this allows a formulation of the general phase-space distribution function,

\[
\mathcal{F}(x_i,v_i,t) = n(x_i,t)f(x_i,v_i,t).
\] (2.1)

In this document non-normalized phase-space distribution functions are always denoted by capital calligraphic letters. Multiplying the general phase-space distribution function by small volumes in phase-space now reveals the expected number of particles inside that volume, as opposed to the fraction of the total.

An important distribution function is the equilibrium Maxwell-Boltzmann distribution [17], which for a monatomic gas is given as

\[
\mathcal{M}(x_i,v_i,t) = \left(\frac{\rho}{2\pi \kappa T(x_i,t)}\right)^{\frac{3}{2}} \exp\left(-\frac{mv_i^2}{2\kappa T(x_i,t)}\right),
\] (2.2)

where \(m\) is the particle mass, \(\rho\) is the density, \(\kappa\) is the Boltzmann constant, and \(T\) is the temperature of the gas. This distribution is valid for a gas under a set of assumptions known as Maxwell’s assumptions [18]. It has been proven that a monatomic gas will be
in thermodynamic equilibrium, i.e. the total time derivative of the distribution function caused by inter-particle collisions is zero, if and only if its phase-space distribution function is Maxwellian [19].

### 2.3 Moments of the Distribution Function

The phase-space distribution function contains a huge amount of information about the state of the gas. However, practically, it is usually only a handful of macroscopic properties that are desired. Moments help to bridge the gap between the information dense microscopic description and a more practical macroscopic description of a gas. These macroscopic properties can be found by multiplying the phase-space distribution function by a velocity-dependant weight, $W$, and integrating over all velocity space; this is know as taking a moment of the distribution function. The resulting expression is

$$M(x_i, t) = \iiint_{-\infty}^{\infty} mW F \, d^3v_i = \langle mW F \rangle, \quad (2.3)$$

where $M(x_i, t)$ is the value of the considered macroscopic property. The weight, $W$, is a function of the velocity vector, $v_i$, or the random velocity, $c_i = v_i - u_i$, where $u_i$ is the bulk velocity. The angle bracket notation is used to denote integration over the entire velocity space. When using the random velocity weights, fundamental properties of the gas, which are independent of its bulk motion, can be found. Examples of such moments are presented in Table 2.1. The results of moments using the full particle-velocity weighting can be interpreted as fluxes of molecular quantities, several examples are found in Table 2.2.
<table>
<thead>
<tr>
<th>Order</th>
<th>( W(c_i) )</th>
<th>Moment</th>
<th>Description</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>Zero by definition of the random velocity.</td>
</tr>
<tr>
<td>2</td>
<td>( \frac{1}{3} c_i c_i )</td>
<td>( p )</td>
<td>Contracted second-order moment, the hydrostatic pressure.</td>
</tr>
<tr>
<td>2</td>
<td>( c_i c_j )</td>
<td>( P_{ij} )</td>
<td>Anisotropic pressure tensor. Note that ( P_{ij} = \delta_{ij} p - \tau_{ij} ), where ( \tau_{ij} ) is the deviatoric stress tensor.</td>
</tr>
<tr>
<td>3</td>
<td>( \frac{1}{2} c_i c_j c_j )</td>
<td>( q_i )</td>
<td>Contracted third-order moment, the heat-flux vector.</td>
</tr>
<tr>
<td>3</td>
<td>( c_i c_j c_k )</td>
<td>( Q_{ijk} )</td>
<td>Heat-flux tensor.</td>
</tr>
<tr>
<td>4</td>
<td>( \frac{1}{15} c_i c_j c_j c_j )</td>
<td>( r )</td>
<td>Contracted fourth-order moment, related to the kurtosis of the distribution function.</td>
</tr>
<tr>
<td>4</td>
<td>( c_i c_j c_k c_l )</td>
<td>( R_{ijkl} )</td>
<td>Fourth-order moment, related to the kurtosis of the distribution function.</td>
</tr>
<tr>
<td>5</td>
<td>( c_i c_j c_k c_l c_m )</td>
<td>( S_{ijklm} )</td>
<td>Fifth-order moment, related to the hyperskewness of the distribution function.</td>
</tr>
</tbody>
</table>

Table 2.1: Moments found using random velocity weightings, \( W = W(c_i) \).

<table>
<thead>
<tr>
<th>Order</th>
<th>( W(v_i) )</th>
<th>Moment</th>
<th>Description</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>The 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>The 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_i P_{jk} + u_j P_{ik} + u_k P_{ij} + Q_{ijk} )</td>
<td>The third velocity moment.</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_i u_j P_{lk} + u_j u_k P_{il} + u_k u_l P_{ij} + u_l Q_{ijk} + u_i Q_{jkl} + u_j Q_{ikl} + u_k Q_{ijl} + R_{ijkl} )</td>
<td>The fourth velocity moment.</td>
</tr>
</tbody>
</table>

Table 2.2: Moments found using standard velocity weightings, \( W = W(v_i) \).

### 2.4 The Boltzmann Equation

For a monatomic gas, the evolution of the general phase-space distribution function in time and space is fully described by the Boltzmann equation [18][20],

\[
\frac{\partial F}{\partial t} + v_i \frac{\partial F}{\partial x_i} + \frac{\partial (a_i F)}{\partial v_i} = \frac{\delta F}{\delta t},
\]  

(2.4)

where \( F(x_i, v_i, t) \) has been written as \( F \) for brevity, and \( a_i \) is the particle acceleration due to external forces, such as gravity or the Lorentz force. This equation is accurate for both equilibrium and non-equilibrium gases. The rightmost term of Equation (2.4) is known
as the collision term, and represents the rate of change of the distribution function as a result of interparticle collisions. It is difficult to derive an analytical formulation for the collision term, and many assumptions are made to obtain a practical form. The original form is the Boltzmann collision integral as given by

$$\frac{\delta F}{\delta t} = \int_{-\infty}^{\infty} \int_{0}^{2\pi} \int_{0}^{\pi} \left[ F_{\text{pc}}^{(1)} F_{\text{pc}}^{(2)} - F^{(1)} F^{(2)} \right] gS(g, \chi) \sin \chi,$$

where the superscripts (1) and (2) correspond to properties of the incident and target particles, respectively, and the subscript ‘pc’ represents post-collision properties. Furthermore, $S(g, \chi)$ is the differential scattering cross section, which is a function of the relative velocity, $g = |v_{i}^{(1)} - v_{i}^{(2)}|$, the azimuth angle, $\epsilon$, and the scattering angle, $\chi$. The primary assumptions of Equation (2.5) are that of molecular chaos, exclusively binary collisions, and a spherical symmetric force between particles, which obeys classical mechanics. A detailed derivation of this equation can be found in any standard kinetic-theory text [18,21,22].

The Boltzmann equation has several important features worth mentioning. Firstly, from Boltzmann’s H-theorem, it has been proven that the evolution of the distribution function leads to monotonically increasing total entropy of the gas, thus the Boltzmann equation is in agreement with the second law of thermodynamics [18]. As such the evolution is also irreversible, which is a direct result of the assumption of molecular chaos. Furthermore, it can be shown that the distribution function will evolve towards the equilibrium Maxwellian distribution over time.

Due to its mathematical complexity, in most cases it is impossible to obtain a closed form analytical solution to the Boltzmann collision integral. In order to make the solution of the Boltzmann equation tractable, the collision integral is either simplified using approximations, or solved numerically. However numerical methods, such as the Monte Carlo solvers suggested by Nordsieck and Hicks [23] or quadrature-based integration approaches, are very expensive. Various simplified collision operators have been proposed such as the Fokker-Planck approximation [24], BGK and BGK-based collision operators [25,26], the ellipsoidal-statistical (ES)-BGK model [27], and the Shakhov model [28]. Since the goal of this study is to provide initial validation of new closure systems themselves, the simple BGK approximation has been used, and this operator is described in detail in the following section.
2.5 The BGK Collision Operator

A very simple approximation to the Boltzmann collision integral (Equation (2.5)), which retains several of its important features, has been proposed by Bhatnagar, Gross, and Krook [25] and is known as the BGK collision operator. This operator assumes that particles described by the distribution, $F$, are removed exponentially and replaced with particles following the Maxwellian distribution, $M$, on a characteristic time scale, $\tau$. Mathematically this is expressed as

$$\frac{\delta F}{\delta t} = -\frac{F - M}{\tau}. \quad (2.6)$$

In the present work the relaxation time is approximated as, $\tau = \mu/p$, where $\mu$ is the dynamic viscosity of the gas. The BGK collision operator maintains conservation of mass, momentum, and energy if the Maxwellian distribution is defined such that

$$\langle \begin{bmatrix} 1 & v_i \\ \frac{1}{2}v_i v_j \end{bmatrix} \frac{F - M}{\tau} \rangle = 0 \quad \text{for} \quad F \geq 0. \quad (2.7)$$

Equation (2.4) is commonly referred to as the BGK equation when the BGK operator is used to model the collision source term. It can be concluded from inspection that the BGK operator will cause the distribution to evolve to the Maxwellian, which is consistent with the laws of thermodynamics and the H-theorem. It is also apparent that the BGK operator is much simpler than the Boltzmann collision integral of Equation (2.5) which leads to computational advantages. However, there are a greater number of assumptions made. One such assumption is that the relaxation times associated with viscosity and heat-transfer are equivalent. This leads to a Prandtl number of unity for monotonic gases, which is inconsistent with the physically expected value of about 2/3. An alternative collision operator, which extends from the BGK operator but allows for a tunable Prandtl number, is the ellipsoidal statistical model originally proposed by Holway [27]. However, as mentioned, for the objectives of this study the BGK model is sufficient.

2.6 Solution Techniques for the Boltzmann Equation

As mentioned previously, solution of the seven dimension, non-linear, integro-differential Boltzmann equation in a general sense is a formidable task. Of course the equilib-
rium solution is well known as the Maxwellian distribution and corresponds to the Euler equations. However, methods of finding more general solutions, valid both in the equilibrium and non-equilibrium regimes, are not so clear. Potential solution strategies include the discretized velocity methods, Lagrangian direct-simulation techniques, and moment-closure methods.

Discretized velocity methods (DVM), such as those proposed by Mieussens [7] and Buet [29], solve the Boltzmann equation using numerical methods by discretizing the spatial, temporal, and velocity domains. The collision integral is calculated using quadrature summation or Monte Carlo sampling techniques. These methods are typically expensive due to the high dimensionality of the problem, and the large domain required in velocity space to capture a sufficient fraction of the distribution function. This has limited its application mostly to problems with reduced dimensionality, such as assuming axial symmetry in velocity space, or to problems considering a narrow range of fluid velocities.

Lagrangian direct-simulation techniques have also been a popular approach. These techniques avoid direct solution of the Boltzmann equation altogether, and instead simulate the gas molecules and their interactions directly. Two subsets of this approach are the molecular-dynamics method and the direct-simulation Monte Carlo technique (DSMC). The molecular-dynamics method was pioneered by Alder and Wainwright [30]. This method tracks individual particles and determines when collisions will occur based on the inter-particle distances. There are two main stages, evaluation of the interactions between particles, and movement of the particles based on these interactions. These steps are decoupled, which places a strict limit on the time step. Since the distance between each set of particles must be calculated at each time step to determine if a collision occurs, the technique scales as the square of the number of particles, and is therefore very expensive for anything but a very dilute gas. The direct-simulation Monte Carlo technique of Bird [6, 31] is similar to the molecular-dynamics approach, however the collisions are determined in a probabilist manner as opposed to deterministically. This decreases the computational intensity significantly, however the limit on the time-step and the need to simulate individual particles (or macroparticles), means the technique begins to struggle for relatively dense gases and/or low speed flows. DSMC also uses macroparticles that each represent many real particles. The number of needed particles is therefore reduced as compared to molecular dynamics.

Finally, the moment-closure method [8, 18], which is the focus of this study, seeks to approximate the Boltzmann equation as finite set of partial-differential equations (PDEs).
These equations consider moments of the distribution function that are independent of the particle velocities, thus reducing the dimensionality. The technique does not consider the particles individually, thus avoiding the costs associated with the DSMC and molecular-dynamics methods. The Knudsen number range is limited by how many moments, and corresponding transport equations, are considered. However, it is possible for the technique to remain valid into the transition regime. The resulting transport equations will also reduce to the Navier-Stokes-Fourier solution in the continuum regime. The moment closure method will be described extensively in the following chapter.
Chapter 3

Moment Closures and the Maximum-Entropy Closure

3.1 Maxwell’s Equations of Change

As mentioned, the moment-closure method seeks to find approximate solutions to the Boltzmann equation by solving a finite set of PDEs. This set of transport equations for macroscopic properties is found by taking the appropriate moments of the Boltzmann equation. In general, a set of \( N \) transport equations can be found by defining a vector of \( N \) velocity weights,

\[
W^{(N)} = m[W_0, W_1, W_2, \ldots, W_N]^T.
\]  (3.1)

The resulting transport equations, known as Maxwell’s equations of change, are

\[
\frac{\partial}{\partial t} \langle W^{(N)} F \rangle + \frac{\partial}{\partial x_i} \langle v_i W^{(N)} F \rangle = \left\langle W^{(N)} \frac{\delta F}{\delta t} \right\rangle.
\]  (3.2)

The first term, \( \frac{\partial}{\partial t} \langle W^{(N)} F \rangle / \partial t \), is the rate of change of the solution vector, the second term, \( \frac{\partial}{\partial x_i} \langle v_i W^{(N)} F \rangle / \partial x_i \), is the divergence of the flux of the solution vector, the so-called flux dyad, and the final term, \( \langle W^{(N)} \frac{\delta F}{\delta t} \rangle \), is the source of the considered macroscopic property resulting from interparticle collisions. It should be noted that the flux dyad always contains moments of one higher order than the solution vector, and thus the equation system is not closed. This implies that in order to solve the Boltzmann equation for an arbitrary phase-space distribution an infinite number of moments must be
taken. This is obviously impossible and approximate methods, which yield a finite set of transport equations, must be used. This technique of approximating the Boltzmann equation using a finite set of transport equations is called a moment closure.

### 3.2 Moment Closures

In order to close a given set of $N$ transport equations the phase-space distribution function must be restricted to an assumed form. The assumed distribution function must have the same number of degrees of freedom as there are moments available in the solution vector. This technique was pioneered by Grad [9], who suggested a distribution of the following form [8]

$$F = \mathcal{M}[1 + \mathcal{P}^{(N)}(c_i)],$$  \hspace{1cm} (3.3)

where $\mathcal{P}^{(N)}(c_i)$ is a Hermite expansion function about the equilibrium Maxwellian. This closure has been applied with success when considering near equilibrium distributions. However, it is possible for the assumed distribution function to become negative, which is nonphysical. Also, as the assumed distribution strays further from equilibrium, there is a loss of hyperbolicity of the resulting moment equations, and a closure breakdown [8].

The Chapman-Enskog closure is an alternative technique which assumes that the distribution is in the form of a small perturbation about the equilibrium Maxwell-Boltzmann distribution [10,11,32]. Depending on the order of the perturbation this technique can be used to form the Euler, Navier-Stokes, Burnett, and Super-Burnett equation systems. A Chapman-Enskog like expansion has been applied to the Grad closure hierarchy to obtain the regularized Grad closures [33]. Unfortunately, closures resulting from Chapman-Enskog expansions contain hyperbolic and elliptic terms, which is less desirable for numeric applications. Also, higher-order Chapman-Enskog expansions seem to yield models that are linearly unstable.

### 3.3 Maximum-Entropy Closure

The closures discussed thus far have all arrived at an assumed distribution function through an expansion about the equilibrium Maxwellian distribution. As mentioned, this limits the closures applicability to gases with only moderate departures from equilibrium.
More recently, an alternative moment-closure technique, known as the maximum-entropy closure, has been proposed \[12\], \[13\]. This closure technique is not based on an expansion about equilibrium, and thus avoids some of the issues associated with the Grad and Chapman-Enskog closures. It assumes a phase-space distribution function which maximizes thermodynamic entropy, and is therefore the most likely distribution, while remaining consistent with a given set of moments.

To derive this distribution, two constraints are considered. Firstly, the distribution function must be consistent with the moments in the solution vector of Equation (3.2), referred to as $M^{(N)}$, mathematically this is written as

$$ M^{(N)} = \langle W^{(N)} F \rangle. \quad (3.4) $$

Secondly, the entropy must be maximized, leading to the constraint that

$$ \max_{\mathcal{F}} \left( -\kappa \left[ \mathcal{F} \ln(\mathcal{F}) - \mathcal{F} \right] \right) \quad \text{for} \quad \mathcal{F} \geq 0. \quad (3.5) $$

This optimization problem is solved using the method of Lagrange multipliers which leads to the condition that

$$ \langle \ln(\mathcal{F}) - \alpha^T W^{(N)} \rangle = 0 \quad (3.6) $$

where $\alpha = [\alpha_1, \alpha_2, ..., \alpha_N]$ are the closure coefficients, which are the Lagrange multipliers. By inspection of Equation (3.6) it is clear that the distribution function must have the form

$$ \mathcal{F} = e^{\alpha^T W^{(N)}}. \quad (3.7) $$

Note that the Maxwellian distribution is a subset of this distribution function, which is expected since it is the entropy-maximizing distribution for a gas at equilibrium conditions. The values of the coefficients, $\alpha$, are chosen such that Equation (3.4) is satisfied. For higher-order closures, when $W$ contains super-quadratic velocity weights, the moment integrals cannot be expressed in closed form. In this case, the coefficients must be found through a minimization problem in which moments are integrated numerically. The associated so-called maximum-entropy problem is

$$ \frac{\partial}{\partial \alpha} \left[ \langle e^{\alpha^T W^{(N)}} \rangle - \alpha^T M^{(N)} \right] = 0. \quad (3.8) $$
The highest-order non-zero coefficient, $\alpha_i$, in the set $\alpha$ must be negative in order to obtain a finite distribution for all velocity space. The solution is unique due to the convexity of Equation (3.8). When the iterative numeric procedure is required to generate the distribution function and closing fluxes significant numerical expense is in encountered; this is often prohibitive. However, a new interpolation technique has been proposed to avoid this issue \[14,34\], and will be discussed in Chapter 4. Since these closures are not based on an expansion about the Maxwellian they can potentially be applied to gases far from equilibrium. Not only is the maximum-entropy closure attractive from a physical viewpoint, it also has many desirable mathematical features, such as being hyperbolic whenever the maximum-entropy problem can be solved. Section 3.3.2 presents more details on the hyperbolicity of the closure.

### 3.3.1 Hierarchy of Levermore Closures

The maximum-entropy closure idea has been presented in a clean form by Levermore \[35\], and he has suggested a hierarchy of closures which utilize the theory. In general, Levermore proposes three requirements when defining the velocity weighting vector used in Maxwell’s equations of change to derive the moment transport equations. Firstly, the system must reduce to the Euler description in the continuum regime, therefore the space of weighting monomials must contain, $W = m[1, v_i, v_i v_i]$. The weighting space must also be invariant under translational and orthogonal transformations, therefore it is Galilean invariant. This leads to the requirement that the weightings are velocity polynomials. Finally, the weightings must correspond to a finite distribution function. Valid examples of such weightings and their corresponding moments for a three-dimensional gas are:

\begin{align*}
N = 5, & \quad W^{(5)} = m[1, c_i, c_i^2/3], \quad M^{(5)} = [\rho, u_i, p] \quad (3.9) \\
N = 10, & \quad W^{(10)} = m[1, c_i, c_i c_j], \quad M^{(10)} = [\rho, u_i, P_{ij}] \quad (3.10) \\
N = 14, & \quad W^{(14)} = m[1, c_i, c_i c_j, c_i^2/2, c_i^4/15], \quad M^{(14)} = [\rho, u_i, P_{ij}, q_i, r] \quad (3.11) \\
N = 21, & \quad W^{(21)} = m[1, c_i, c_i c_j, c_i c_j c_k, c_i^2/15], \quad M^{(21)} = [\rho, u_i, P_{ij}, Q_{ijk}, r_{ij}] \quad (3.12) \\
N = 26, & \quad W^{(26)} = m[1, c_i, c_i c_j, c_i c_j c_k, c_i^2 c_k^2], \quad M^{(26)} = [\rho, u_i, P_{ij}, Q_{ijk}, R_{ijkl}] \quad (3.13) \\
N = 35, & \quad W^{(35)} = m[1, c_i, c_i c_j, c_i c_j c_k, c_i^2 c_j c_k c_l], \quad M^{(35)} = [\rho, u_i, P_{ij}, Q_{ijk}, R_{ijkl}] \quad (3.14)
\end{align*}
and the corresponding systems for a one-dimensional gas, meaning that gas molecules are confined to move in only one direction, are:

\[
N = 3, \quad \mathbf{W}^{(3)} = m[1, c, c^2], \quad \mathbf{M}^{(3)} = [\rho, u, p] \tag{3.15}
\]

\[
N = 5, \quad \mathbf{W}^{(5)} = m[1, c, c^2, c^3, c^4], \quad \mathbf{M}^{(5)} = [\rho, u, p, q, r] \tag{3.16}
\]

The lower-order, three-dimensional, 5- and 10-moment closures (Equation (3.9) and (3.11)) correspond to the Euler and Gaussian equations, respectively. The Euler system is well studied and is the standard technique for modelling inviscid flows in the continuum regime. The Gaussian closure system takes into consideration different temperatures in each physical direction, which is possible in non-equilibrium regimes, and deviatoric fluid stresses \[14, 16, 34, 36–43\]. The Gaussian closure is further discussed in Section 3.3.4. The 14-moment system (Equation (3.11)) is the lowest-order, three-dimensional, maximum-entropy system that considers a non-zero heat flux, the corresponding closure for a one-dimensional gas is the 5-moment system (Equation (3.16)). The 5- and 14-moment interpolative closures, which are the main subject of this study, are based on these maximum-entropy closures, and are described in Chapter 4.

### 3.3.2 Hyperbolicity

As mentioned, the maximum-entropy closures are hyperbolic whenever the maximum-entropy problem can be solved. This can be proven by first defining a density potential,

\[
h(\alpha^{(N)}) = \langle e^{\alpha^T \mathbf{W}^{(N)}} \rangle, \tag{3.17}
\]

and flux potential,

\[
f_i(\alpha^{(N)}) = \langle v_i e^{\alpha^T \mathbf{W}^{(N)}} \rangle. \tag{3.18}
\]

Derivatives of the density and flux potentials with respect to the \( \alpha \) coefficients are expressed as,

\[
h_{\alpha^{(N)}} = \frac{\partial h(\alpha^{(N)})}{\partial \alpha^{(N)}} = \langle \mathbf{W}^{(N)} e^{\alpha^T \mathbf{W}^{(N)}} \rangle, \tag{3.19}
\]

and

\[
f_{i, \alpha^{(N)}} = \frac{\partial f_i(\alpha^{(N)})}{\partial \alpha^{(N)}} = \langle v_i \mathbf{W}^{(N)} e^{\alpha^T \mathbf{W}^{(N)}} \rangle, \tag{3.20}
\]
respectively, and the source term is,

\[ R(\alpha) = \left\langle mW \frac{\delta F}{\delta t} \right\rangle. \]  

(3.21)

The moment transport system can now be rewritten in the potential form,

\[ \frac{\partial}{\partial t} h_\alpha(N) + \nabla_i \cdot f_i,\alpha(N) = R(\alpha) \]  

(3.22)

By evaluating the second derivatives of the flux and density potentials with respect to the \(\alpha\) coefficients,

\[ h_\alpha(N)\alpha(N) = \frac{\partial h_\alpha(N)}{\partial \alpha(N)} = \left\langle W^{(N)} [W(N)]^T e^{T} w^{(N)} \right\rangle, \]  

(3.23)

and

\[ f_{i,\alpha(N)}\alpha(N) = \frac{\partial f_{i,\alpha(N)}}{\partial \alpha(N)} = \left\langle v_i W^{(N)} [W(N)]^T e^{T} w^{(N)} \right\rangle, \]  

(3.24)

Equation (3.22) can now be manipulated to form a transport equation for the \(\alpha\) coefficients,

\[ h_\alpha(N)\alpha(N) \frac{\partial}{\partial t} \alpha + f_{i,\alpha(N)}\alpha(N) \cdot \nabla_i \alpha = R(\alpha). \]  

(3.25)

The hessian matrix, \(h_\alpha(N)\alpha(N)\), is positive-definite since,

\[ w^T h_\alpha(N)\alpha(N) w = \left\langle w^T W^{(N)} [W(N)]^T w e^{T} w^{(N)} \right\rangle = \left\langle (w^T W^{(N)})^2 F \right\rangle \geq 0, \]  

(3.26)

for any coefficient vector \(w\). Furthermore, both \(h_\alpha(N)\alpha(N)\) and \(f_{i,\alpha(N)}\alpha(N)\) are symmetric. This leads to a Godunov form of a symmetric hyperbolic system for the transport of \(\alpha\), and thus the system is hyperbolic as long as the maximum-entropy problem can be solved [44].

It can be argued that this hyperbolicity is more physically realistic than an elliptic or parabolic description, such as that found in the Navier-Stokes-Fourier equations, since it ensures that information is propagated at finite speeds. Furthermore, it proves to have many computational advantages. Numerical methods such as the Godunov-type finite-volumes schemes and discontinuous-Galerkin technique are more well suited to solve hyperbolic conservation laws, as opposed to mixed systems such as the Navier-Stokes-Fourier equations. The fact that the hyperbolic system requires only the evaluation of first-derivatives leads to a possible increased order of accuracy for a given stencil size.
relative to the solution of a system requiring second-derivative calculations. Evaluation of the first-derivative is also less sensitive to grid-irregularities, which leads to potentially better performance of hyperbolic systems in problems with cut-cells, embedded boundaries, or adaptive grids \[34\]. The application of a 10-moment maximum-entropy closure to problems with embedded boundaries has been investigated by McDonald \[34\] and was found to outperform the Navier-Stokes-Fourier equations.

### 3.3.3 Realizability

When solving the maximum-entropy problem, it must be ensured that the phase-space distribution function remains realizable. To ensure moment realizability the given set of moments should, as a minimum, correspond to a set that could arise from a bounded and strictly positive distribution. Physical realizability can be maintained by ensuring that a matrix \( Y = \langle m \Omega \Omega^T F \rangle \) is positive definite \[8, 41, 45\], this is known as the Hamburger moment problem \[45\]. The velocity weighting \( \Omega \) in \( Y \) is chosen such that all considered moments are contained in \( Y \), and is not necessarily equivalent to \( W \). For example, considering a one-dimensional 5-moment system (Equation (3.16)) which is stationary, i.e. \( u = 0 \), and with moments normalized such that the density and pressure are unity \((\rho = p = 1)\), the velocity weighting required is, \( \Omega = m[1, v, v^2] \), leading to the \( Y \) matrix,

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

where the \( * \) subscript denotes non-dimensionalized values. This leads to the following condition necessary to ensure positive definiteness of \( Y \) and thus physical realizability,

\[
r_* \geq q_*^2 + 1.
\]

In general, the theory discussed is only valid for a one-dimensional gas, however, as will be seen in Section 4.1 in the case of the 14-moment closure it can be extended to three-dimensions.

It has been shown by Junk that unrealizable regions are encountered within physically realizable moment space for maximum-entropy moment systems which contain superquadratic velocity weightings (necessary to provide a treatment for heat transfer) \[46\].
Chapter 3. Moment Closures and the Maximum-Entropy Closure

Examples of which are the three-dimensional 14-, 21-, 26-, and 35-moment systems seen in Equations (3.11)-(3.14) and the one-dimensional 5-moment system seen in Equation (3.16). In this so-called Junk region bounded solutions to the maximum-entropy problem do not exist, and a singularity in the closing flux(s) develops.

For example, again returning to the simplified one-dimensional 5-moment system discussed above, Junk has shown that in order to obtain a bounded distribution, where $a_4$ is negative, the following condition on the closing flux must be satisfied \[ q_* s_* > (r_* - 3)(r_* - 1) + 4q_*^2. \] (3.29)

It is clear that this inequality is no longer satisfied on the half-line where, $q_* = 0$ and $r_* \geq 3$. Also note that $q_* = 0$ and $r_* = 3$ is the equilibrium state, therefore the non-realizable half line includes the equilibrium state. The region of realizability, including both the physically realizable region, and the Junk region, is shown in Figure 3.1 (a).

The behaviour of the closing flux, $s_*$, as it approaches this Junk region, is considered by introducing the variable $\epsilon$, which is greater than 0, and assuming $r_* \geq 3 + \epsilon$, therefore Equation (3.29) becomes

\[ s^* \geq \lim_{q^* \to 0^+} \frac{\epsilon(2 + \epsilon)}{q^*} + 4q^* = +\infty, \] (3.30)
\[ s^* \leq \lim_{q^* \to 0^-} \frac{\epsilon(2 + \epsilon)}{q^*} + 4q^* = -\infty. \] (3.31)

The singularity in the closing flux can be clearly observed. It can also be seen in Figure 3.1 (b) which displays numerical solutions to the maximum-entropy problem. Obviously this singular nature is an undesirable feature of the closure, however past research has found that it can be advantageous in practical implementation [14]. The effect of the Junk region and closing flux singularity is further discussed in Chapter 3.3.4 The Gaussian Closure

At this point, it is worthwhile to present a summary of the 10-moment maximum-entropy closure, known as the Gaussian closure, since it will be used in this study as a benchmark for comparisons. As mentioned earlier, the Gaussian closure is the lowest-order three-dimensional closure of the Levermore hierarchy that considers non-equilibrium physics and its solutions have now been studied quite extensively [14, 16, 34–43]. The Gaussian equation system extends from the Maxwellian by including a non-zero deviatoric stress, thus viscous effects in non-equilibrium are accounted for. It also takes into consideration the possibility of different temperatures in each physical direction.

Apart from the usual advantages of the maximum-entropy closures, namely their hyperbolicity and robustness, this closure also has the advantage of not containing super-quadratic velocity terms in the weighting vector, therefore the unrealizable Junk region does not appear. Furthermore, it is possible to derive a closed-form expression for the distribution function, thus the expensive resynchronization procedure of Equation (3.8) need not be used; this is not possible for the systems which consider heat transfer (Equations (3.11)-(3.14)). The largest disadvantage of the closure is its lack of heat transfer modelling, making it only applicable to flows where heat transfer is not important, regardless of the flow regime. This has limited the closure to modelling only certain flow cases at moderate Knudsen numbers.

The velocity weighting vector used to generate the moment transport equation system is, \( \mathbf{W} = m[1, v_i, v_i v_j] \), leading to the following general transport equations:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k} (\rho u_k) = 0, \] (3.32)

\[ \frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_k} (\rho u_i u_k + P_{ik}) = 0, \] (3.33)
The maximum-entropy problem can be solved analytically resulting in the following form of the phase-space distribution function, which is a Gaussian distribution,

$$
F^{(10)}(t, x_i, v_i) = G(t, x_i, v_i) = \frac{\rho}{m(2\pi)^{\frac{3}{2}}(\det\Theta)^{\frac{1}{2}}} \exp\left(-\frac{1}{2} \frac{1}{\Theta_{ij}} c_i c_j\right),
$$

where $\Theta_{ij} = \frac{P_{ij}}{\rho}$. The closing flux, $Q_{ijk}$, is zero since, $\langle m c_i c_j c_k G \rangle = 0$. Numerical solutions to the Gaussian closure using Godunov-type finite-volume methods have been studied by Brown et al. [47] and McDonald and Groth [8,36], and generate reliable results in both the continuum and transition regimes when heat transfer is not important. The Gaussian closure system presented in Equations (3.32) - (3.34) is valid for monatomic gases, however it can be modified to account for the energy of the rotational and vibrational modes needed for diatomic molecules [48].

An extension to the Gaussian closure which considers heat transfer has also been found [8,39]. This so-called regularized Gaussian closure uses a perturbative Chapman-Enskog-like expansion of the moment equations to find an approximate expression for the heat-flux moments, $Q_{ijk}$. The resulting expression is given by

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

It should be noted that since the approximation to $Q_{ijk}$ includes spatial derivatives, the equation system is no longer hyperbolic. Thus, the price for the inclusion of this heat transfer approximation in this manner is the loss of the attractive numerical features associated with the fully hyperbolic equations of the original maximum-entropy closure.
Chapter 4

Maximum-Entropy Based Interpolative Closures

A new interpolative-type closure technique has recently been proposed which seeks to resolve the issues associated with the maximum-entropy closure when super-quadratic velocity weightings are considered [14,41]. In particular, the lack of closed form expressions for the closing fluxes is addressed. This chapter describes a 14-moment interpolative closure valid for a three-dimensional gas with heat transfer (Section 4.1), as well as a 5-moment interpolative closure valid for a one-dimensional gas with heat transfer (Section 4.2). These closures are based on the corresponding maximum-entropy closures, however their closing fluxes are approximated to avoid the expensive maximum-entropy problem described in Section 3.3.

4.1 The 14-Moment Interpolative Closure

The velocity weighting vector used to generate the 14-moment interpolative closure is, \( W = m[1, v_i, v_i v_j, v_i v^2, v_i v^4] \), where \( v^2 = v_i v_i \). Therefore, the closure system considers transport of the density, momentum, the anisotropic pressure tensor, heat-flux vector, and contracted fourth-order moment. This velocity weighting vector is substituted into Maxwell’s equations of change. For a three-dimensional monatomic gas, this leads to a set of 14-moment equations, which include a non-zero heat-flux vector, in the form

\[
\frac{\partial U}{\partial t} + \frac{\partial F_k}{\partial x_k} = S, \tag{4.1}
\]
where \( \mathbf{U} \) is the vector of conserved variables, \( \mathbf{F}_k \) is the flux dyad, and \( \mathbf{S} \) is the source vector resulting from inter-particle collisions modelled using the BGK operator. These vectors are

\[
\mathbf{U} = \begin{pmatrix}
\rho \\
\rho u_i \\
\rho u_i u_j + P_{ij} \\
\rho u_i u_j u_j + u_i P_{jj} + 2u_j P_{ij} + Q_{ijj} \\
\rho u_i u_j u_j + 2u_i u_j P_{jj} + 4u_i u_j P_{ij} + 4u_i Q_{ijj} + R_{iijj}
\end{pmatrix},
\]

(4.2)

\[
\mathbf{F}_k = \begin{pmatrix}
\rho u_k \\
\rho u_i u_k + P_{ik} \\
\rho u_i u_k u_j + u_i u_k P_{jk} + u_j P_{ik} + u_k P_{ij} + Q_{ijk} \\
\rho u_i u_k u_j u_j + u_i u_k P_{jj} + 2u_i u_j P_{jk} + 2u_j u_k P_{ij} + u_j u_j P_{ik} + u_i Q_{kjj} + u_k Q_{ijj} + 2u_j Q_{ijk} + R_{ikjj} \\
\rho u_k u_i u_j u_j + 2u_k u_i u_j P_{jj} + 4u_i u_j u_k P_{jk} + 4u_i u_j u_k P_{ij} + 2u_i u_j Q_{kjj} + 4u_i u_k Q_{ijj} + 4u_i u_j Q_{ijk} + 4u_i R_{ikjj} + u_k R_{iijj} + S_{kijj}
\end{pmatrix},
\]

(4.3)

\[
\mathbf{S} = \begin{pmatrix}
0 \\
0 \\
\frac{\delta_{ij} P_{kk} - 3P_{ij}}{3\tau} \\
\frac{2u_i (\delta_{ij} P_{kk} - 3P_{ij}) - 6u_i P_{ik} - 3Q_{ijj}}{3\tau} \\
\frac{1}{3\tau} \left( -3R_{iijj} + \frac{5P_{ik} P_{jj}}{\rho} - 12u_i Q_{ijj} + 4u_i u_j (\delta_{ij} P_{kk} - 3P_{ij}) \right)
\end{pmatrix}.
\]

(4.4)

It should be noted that the 14-moment system as presented above is not closed; to close the system the moments \( Q_{ijk}, R_{ijkk}, \) and \( S_{ijjkk} \) in the flux vector must be approximated. In order to circumvent the problems associated with higher-order maximum-entropy closures, the interpolative closure of McDonald and Torrilhon [14] approximates these closing fluxes using closed-form expressions, as opposed to numerically solving the maximum-entropy problem. These closed-form expressions are found in three steps. Firstly, the region of realizability between the physical realizability boundary and Junk...
region is determined, and a suitable remapping of moments is employed. The region of realizability, including the Junk region, is determined by following the procedure outlined in Section 3.3.3. For this case the $Y$ matrix is:

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

leading to the condition for positive-definiteness of

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

This defines the physically realizable region in moment space. The Junk region, which contains physically realizable states that cannot be realized by a bounded maximum-entropy distribution, is

\[
Q_{ijij} = 0, \quad R_{ijij} > \frac{2P_{ji}P_{ij} + P_{ii}P_{jj}}{\rho}.
\]

These two realizability conditions define a realizable space, similar to the example for the one-dimensional gas shown in Figure 3.1 of Section 3.3.3.

It is convenient when forming the closing fluxes to define a parabolic surface mapping using an additional variable, $\sigma$, where $\sigma$ is constant on paraboloids in the realizable moment space, with $\sigma = 1$ corresponding to the physically realizable boundary, and $\sigma = 0$ corresponding to the Junk region. In this case, $\sigma$ is related to the known moments such that the following equality is satisfied, and given by

\[
\sigma = \left[2P_{ij}P_{ji} + P_{ii}P_{jj} - \rho R_{ijij}\right] + \sqrt{\left[2P_{ij}P_{ji} + P_{ii}P_{jj} - \rho R_{ijij}\right]^2 + 8\rho P_{im}P_{nm}Q_{kii}(P^{-1})_{kl}Q_{ljj}}.
\]

Information about the behaviour of the closing flux is then found at equilibrium and on the realizability boundaries. Finally, a closing flux is postulated which is consistent with the constraints at the boundaries and also transitions between them with values that approximate those found by solving the maximum-entropy problem numerically. The reader should refer to the paper by McDonald and Torrilhon for a full and complete description of the derivation of the 14-moment system and the closing fluxes.
The resulting closing fluxes are

\[ Q_{ijk} = \frac{\partial Q_{ijk}}{\partial Q_{mnn}} Q_{mnn}, \tag{4.9} \]

where

\[ \frac{\partial Q_{ijk}}{\partial Q_{mnn}} = \left[ P_{il}(P^2)_{jk} + P_{kl}(P^2)_{ij} + P_{jl}(P^2)_{ik} \right] \left[ P_{lm}(P^2)_{\alpha\alpha} + 2(P^3)_{lm} \right]^{-1}, \tag{4.10} \]

\[ R_{ijkk} = \frac{1}{\sigma} Q_{ijl}(P^{-1})_{lm} Q_{mkk} + \frac{2(1 - \sigma)P_{ik}P_{kj} + P_{ij}P_{kk}}{\rho}, \tag{4.11} \]

\[ S_{ijjkk} = \frac{Q_{npp}Q_{mi\bar{j}}Q_{kl}}{\sigma^2 P_{kn} P_{lm}} + 2\sigma^2 \frac{P_{ij}Q_{ikk}}{\rho} + (1 - \sigma^2)W_{im} Q_{mnn}, \tag{4.12} \]

with

\[ W_{im} = \frac{1}{\rho} \left[ P_{il}(P_{\alpha\alpha})^3 + 6P_{il}(P^3)_{\alpha\alpha} + 7(P^2)_{\alpha\alpha}(P^2)_{il} + 10P_{\alpha\alpha}(P^3)_{il} + 10(P^4)_{il} ight. \]

\[ - (P^2)_{\alpha\alpha} P_{\beta\beta} O_{il} - 3(P_{\alpha\alpha})^2 (P^2)_{il} \left[ P_{lm}(P^2)_{\alpha\alpha} + 2(P^3)_{lm} \right]^{-1}. \tag{4.13} \]

By inspection of Equation (4.11) or (4.12), it is clear that a singularity in the closing flux continues to be encountered in the Junk region (when \( \sigma = 0 \)), as was also the case in the original maximum-entropy closure. However, past research has found that this singular nature is advantageous in practical implementation \[14\]. It produces very large propagation speeds and was found to yield accurate solutions of stationary, one-dimensional, shock structure having smooth transitions, without undesirable non-physical sub-shocks, even for high Mach numbers \[14\]. The effect of the singularity on wave propagation speed is further explored in Section 6.1. The singularity also motivates the use of the fully implicit solver proposed in Section 5.3 for the solution of the 14-moment closure.

### 4.2 The 5-Moment Interpolative Closure

The analogous closure system for a one-dimensional gas, in which particle movement is confined to a single direction, is:
\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0, \]  
(4.14)

\[ \frac{\partial (\rho u)}{\partial t} + \frac{\partial}{\partial x} (\rho u^2 + p) = 0, \]  
(4.15)

\[ \frac{\partial (\rho u^2 + p)}{\partial t} + \frac{\partial}{\partial x} (\rho u^3 + 3up + q) = 0, \]  
(4.16)

\[ \frac{\partial (\rho u^3 + 3up + q)}{\partial t} + \frac{\partial}{\partial x} (\rho u^4 + 6u^2p + 4uq + r) = -\frac{q}{\tau}, \]  
(4.17)

\[ \frac{\partial (\rho u^4 + 6u^2p + 4uq + r)}{\partial t} \frac{\partial}{\partial x} (\rho u^5 + 10u^3p + 10u^2q + 5ur + s) = -\frac{1}{\tau} \left( 4uq + r - 3 \frac{p^2}{\rho} \right). \]  
(4.18)

The closing flux in this case is given by

\[ s = \frac{q^2}{\sigma^2 p^2} + \left( 10 - 8\sigma^2 \right) \frac{pq}{\rho}, \]  
(4.19)

with

\[ \sigma = \frac{3p^2 - \rho r + \sqrt{(3p^2 - \rho r)^2 + 8\rho p^2}}{4p^2}. \]  
(4.20)

Similar to the three-dimensional closure, this system also continues to contain a singularity in the closing flux at the Junk region (see Section 3.3.3). Application of this 5-moment interpolative closure for the prediction of internal shock structure has been studied previously by McDonald, Torrilhon and Schärer [14,49].
Chapter 5

Numerical Solution of the 14-Moment Interpolative Closure

This chapter describes details of both the semi-implicit and fully-implicit Newton-Krylov-Schwarz (NKS) finite-volume schemes which are proposed to find steady-state solutions to the 14-moment interpolative closure herein. The semi-implicit scheme has been used extensively in previous studies of the Gaussian, regularized Gaussian, and 5- and 14-moment interpolative closures [14, 39, 40, 50]. A NKS solver for the Gaussian and regularized Gaussian closures has also been developed in recent studies by Lam and Groth, and was found to significantly reduce computational cost [16]. A similar NKS solution procedure is applied here to the solution of the 14-moment interpolative closure. This represents the first study of the solution of this novel closure using an NKS method. The computational performance of the two methods is compared in Chapter 6.

The chapter begins with a general description of the finite-volume scheme, Section 5.1. Specifics of the numeric solver’s application to the 14-moment interpolative closure are discussed in Section 5.1.2. The semi-implicit and fully-implicit time-marching schemes are discussed in Sections 5.2 and 5.3, respectively. Section 5.3.1 discusses an alternative Jacobian calculation method. Finally, the boundary conditions are described in Section 5.4.

5.1 Upwind Finite-Volume Scheme

The moment transport equation system of the 14-moment interpolative closure for two-dimensional planar flows on multi-block quadrilateral meshes have been solved herein
using a parallel higher-order Godunov-type finite-volume scheme. The general conservation form of the PDE system is

$$\frac{\partial U}{\partial t} + \vec{\nabla} \cdot \vec{F} = S,$$

(5.1)

where $U$ is the solution vector, $\vec{F}$ is a hyperbolic flux dyad, and $S$ is the source vector. Note that this equation has the same form as the 14-moment system presented in Equations (4.1) - (4.4), however to avoid confusion with the indices associated with the spatial and temporal discretizations, vector notation is used in this chapter, as opposed to tensor notation. Equation (5.1) can be rewritten in integral form by applying the divergence theorem,

$$\frac{d}{dt} \int_{A(t)} U dA + \oint_{C(t)} \vec{F} \cdot \hat{n} dl = \int_{A(t)} S dA,$$

(5.2)

where $A(t)$ is the area of the control surface, which can be time dependant, $C(t)$ is a closed curve around the control surface, and $\hat{n}$ is the unit outward vector normal to $C(t)$.

Godunov’s finite-volume method [51] is a numerical technique for solving the integral form of transport equations on a discretized domain of computational cells. An example of two quadrilateral computational cells can be found in Figure 5.1. The spatial domain of interest is divided into a large number of such cells, and each cell is given unique indices $(i, j)$, roughly corresponding to perpendicular directions. The integral form of the conservation law seen in Equation (5.2) is applied to each of the computational cells. Cell averaged solution and source vectors can now be defined as
\[ U_{(i,j)} \equiv \frac{1}{A_{(i,j)}} \int_{A_{(i,j)}} \mathbf{U} \, dA, \quad (5.3) \]

\[ S_{(i,j)} \equiv \frac{1}{A_{(i,j)}} \int_{A_{(i,j)}} S \, dA, \quad (5.4) \]

where \( A_{(i,j)} \) is the area of cell \((i, j)\), which is assumed to be constant. After discretizing in space the integral equation (Equation \((5.2)\)) is rewritten in the semi-discrete form, resulting in a coupled set of non-linear ordinary differential equations given by

\[
\frac{dU_{(i,j)}}{dt} = -\frac{1}{A_{(i,j)}} \left( \sum_k (\mathbf{F} \cdot \mathbf{n} \Delta l)_{(i,j,k)} \right) + S_{(i,j)} = -R(U_{(i,j)}),
\]

where \( \Delta l \) is the length of the cell face, \( \mathbf{n}_{i,j,k} \) is the unit vector normal to the \( k^{th} \) face of cell \((i, j)\), and \( R(U_{(i,j)}) \) is the residual vector. The term, \((\mathbf{F} \cdot \mathbf{n} \Delta l)_{(i,j,k)}\), is the numerical flux at the \( k \)th cell face, which is found by approximately solving Riemann problems at the corresponding cell interfaces. For this two-dimensional quadrilateral example the fluxes will need to be calculated at four faces. These fluxes are found by solving the Riemann problem presented by the discontinuity between the solution states directly to the left, \( U_L \), and right, \( U_R \), of the cell interface. For example, the flux at the interface \((i + 1/2, j)\) is found as

\[
\mathbf{F}_{(i+\frac{1}{2},j,k)} \cdot \mathbf{n}_{(i,j,k)} = \mathbf{F}(\mathcal{R}\mathcal{P}(U_L, U_R, \mathbf{n}_{(i,j,k)})),
\]

where \( \mathcal{R}\mathcal{P}() \) is the solution to the Riemann problem in the direction of the unit normal, \( \mathbf{n}_{(i,j,k)} \).

The Riemann problem can be solved exactly for some PDEs using the Riemann invariants and Rankine-Hugoniot conditions \([52, 53]\), however it is found that in most situations approximate solutions are adequate. Popular approximate Riemann solvers make use of the Roe \([54]\), HLLE (Harten, Van Leer, Lax, and Einfeldt) \([55]\), and HLLL (Harten, Van Leer, Lax, and Linde) \([56]\) flux functions.

Regardless of whether the Riemann problem is being solved exactly or approximately, the solution states immediately to the left and right of the cell interface, \( U_L \) and \( U_R \), are required. In order to generate the left and right solution states using the cell-averaged values a reconstruction process is required. The most straightforward reconstruction method is to assume that the solution is constant over the entire cell, this is known as
piece-wise constant reconstruction and results in a first-order scheme. To form higher-order schemes more advanced reconstruction techniques are required, such as piece-wise linear or quadratic reconstruction. The solver employed for this study uses a least-squares piece-wise linear solution reconstruction method.

As shown by Godunov’s theorem [51], linear, monotonicity preserving schemes can have at most first-order global accuracy, thus linear schemes resulting from higher-order reconstruction are not monotonic. This leads to undesirable numerical oscillations in the solutions, particularly in the area of discontinuities, which can lead to intangible values such as negative densities. A method of retaining monotonicity, while remaining higher-order everywhere except near discontinuities, is to limit the slope used in the reconstruction such that no new extrema are formed. In the case of a piece-wise linear reconstruction of the conserved variables the limited left and right solution states at the interface \((i + 1/2, j)\) are

\[
U_L = U_{(i,j)} + \Phi_{(i,j)} \vec{\nabla}U_{(i,j)} \cdot \Delta \vec{x}_L, \tag{5.7}
\]

\[
U_R = U_{(i+1,j)} + \Phi_{(i+1,j)} \vec{\nabla}U_{(i+1,j)} \cdot \Delta \vec{x}_R, \tag{5.8}
\]

where \(\Phi\) is the corresponding slope limiter, which could have different values for different components of \(\vec{\nabla}U\), and \(\Delta \vec{x}_L\) and \(\Delta \vec{x}_R\) are the distances between the centre of the cell and the left and right cell interfaces, respectively.

A multitude of limiter types have been proposed, including the Van Leer [57], Van Albada [58], Barth-Jespersen [59], and Venkatakrishnan [60] limiters. The Venkatakrishnan limiter, which is a modification to the Barth-Jespersen limiter that reduces the likelihood of convergence stall, has been used in the present work. It is expressed as,

\[
\Phi_{(i,j)} = \min_k (\Phi_{(i,j,k)}) \tag{5.9}
\]

\[
\Phi_{(i,j,k)} = \begin{cases} 
\phi \left( \frac{U_{\text{max}} - U_{(i,j,k)}}{U_{(i,j,k)} - U_{(i,j)}} \right) & \text{for } U_{(i,j,k)} - U_{(i,j)} > 0 \\
\phi \left( \frac{U_{\text{min}} - U_{(i,j,k)}}{U_{(i,j,k)} - U_{(i,j)}} \right) & \text{for } U_{(i,j,k)} - U_{(i,j)} < 0 \\
1 & \text{otherwise}
\end{cases} \tag{5.10}
\]
where \( \phi(y) \) is a smooth function given by

\[
\phi(y) = \frac{y^2 + 2y}{y^2 + y + 2},
\]

\( U_{\text{max}} = \max(U_{(i,j)}, U_{\text{neighbours}}), \)

\( U_{\text{min}} = \min(U_{(i,j)}, U_{\text{neighbours}}), \)

\( \text{and } U_{(i,j,k)} \) is the unlimited reconstructed solution value at the \( k \)th flux quadrature point. The above description has assumed reconstruction and limiting of the conserved variables, \( U \), however other sets of variables, such as the primitive variables can be used. The gradient required in the reconstruction can be calculated using a Green-Gauss or least-squares approach \cite{61}. The last step required to formulate the higher-order finite-volume scheme is to implement a higher-order time-marching scheme. In the present work both a semi-implicit and fully-implicit time-marching scheme are used, these schemes are described in Sections \ref{5.2} and \ref{5.3} respectively.

### 5.1.1 Block-Based Mesh Refinement and Parallelization

The upwind finite-volume procedure described above is implemented within a framework that enables block-based adaptive mesh refinement (AMR), which has been developed by...
Groth and co-workers [62–67]. The AMR technique seeks to refine an initial multi-block mesh in areas which will lead to the most substantial increase in solution accuracy, these regions are determined using physics-based criteria. Coarsening of blocks is also possible for areas with unnecessarily fine meshes. The blocks marked for refinement are divided into four identical blocks which have the same number of cells as the original block. This block-based approach allows for straightforward organization of block location and inter-connectivity using a hierarchical quadtree data structure (see Figure 5.2). The data structure is light weight and efficient, and thus can be stored on each processor, reducing communication time. Furthermore, the block-based approach simplifies load balancing when parallelizing, since every block is identical. Each block contains ghost cells that: admit the passing of solution information between blocks, allow second-order reconstruction at all locations within the domain, and apply the boundary conditions. An example of such overlapping ghost cells for a simple four-block Cartesian grid is shown in Figure 5.3.

The parallelization procedure on multi-processor distributed-memory computing systems is straightforward thanks to the similarity of the blocks. The blocks are distributed, as equally as possible, among the available processors via domain decomposition. This couples naturally with the Schwarz type preconditioner used in the NKS solver that is discussed in Section 5.3. The message passing interface (MPI) library for the C++ programming language has been used for the parallel implementation. Computations for this study were performed on desktop machines containing Intel Core i7-980X processors, which have 6 cores (12 with hyper-threading) at a base frequency of 3.33 GHz, and 24 GB of RAM, as well as on a cluster of Intel Xeon E5540 (2.53 GHz) nodes connected with DDR Infiniband interconnect. This cluster was provided by the SciNet High Performance Computing Consortium at the University of Toronto and Compute/Calcul Canada through funding from the Canada Foundation for Innovation (CFI) and the Province of Ontario, Canada. The studies were performed using between 2 and 128 cores, depending on the case.

At this early stage of research of the 14-moment closure system only simple uniform refinements have been used, however these refinements and associated parallelization, are performed in the general framework of the block-based AMR technique discussed. Past studies by McDonald and Groth have considered the application of AMR to the Gaussian closure, a 10-moment maximum-entropy closure, and have demonstrated the resilience of such hyperbolic equation systems to the grid irregularities that can arise.
5.1.2 Application to the 14-Moment Interpolative Closure

Due to the system’s hyperbolicity, the Godunov finite-volume scheme described in Section 5.1 is readily applied to solve the 14-moment interpolative closure. The HLL-type approximate Riemann solver [68] is used to find an approximate solution to the Riemann problem. Using the HLL technique the intermediate flux at the cell interface, $F_{\text{HLL}}$, is found as

$$F_{\text{HLL}} = \frac{\lambda^+ F_L - \lambda^- F_R}{\lambda^+ - \lambda^-} + \frac{\lambda^+ \lambda^-}{\lambda^+ - \lambda^-} (U_R - U_L),$$  \hspace{1cm} (5.12)$$

where $F_R$ and $F_L$ are the right and left fluxes, and $\lambda^+$ and $\lambda^-$ are the maximum and minimum solution wave propagation speeds, respectively. Typically, the maximum and minimum wave speeds are found using the eigenvalues of the flux Jacobian. However, due to the complexity of the 14-moment system, at this stage in development the maximum and minimum wave speeds are approximated based on the acoustic wave speeds in a monatomic gas which obeys a Gaussian distribution. The approximate wave speeds at a
cell interface with a normal in the $x$-direction are taken to be

$$
\lambda^- = \min \left( u_x^{(R)} - \xi \sqrt{\frac{\gamma \rho^{(R)}}{\rho^{(R)}}}, u_x^{(L)} - \xi \sqrt{\frac{\gamma \rho^{(L)}}{\rho^{(L)}}} \right), \tag{5.13}
$$

$$
\lambda^+ = \max \left( u_x^{(R)} + \xi \sqrt{\frac{\gamma \rho^{(R)}}{\rho^{(R)}}}, u_x^{(L)} + \xi \sqrt{\frac{\gamma \rho^{(L)}}{\rho^{(L)}}} \right), \tag{5.14}
$$

where the superscripts (R) and (L) denote properties at the right and left states, respectively, $\gamma$ is the ratio of specific heats and equal to $5/3$ for a monatomic gas, and $\xi$ is a tuning coefficient which is set large enough that the scheme is stable, while remaining small enough to ensure there is not excess numerical dissipation or excessively small time steps. Due to the singular nature of the closing flux and numerical restrictions, the values of $\sigma$ must be limited, a lower limit of $\tilde{\sigma} = 2.0 \times 10^{-4}$ is found to be sufficient. If $\sigma$ becomes less than this value, it is then replaced with $\sigma = \tilde{\sigma}$.

### 5.2 Semi-Implicit Time-Marching Scheme

After discretizing the spatial domain using the Godunov finite-volume method described in Section 5.1, the resulting system of ODEs (Equation (5.5)) must be discretized temporally. As the continuum regime is approached the values of the relaxation time, $\tau$, can become very small, leading to excessive numerical stiffness of the system. Furthermore, the stiffness is exacerbated by the high wave speeds caused by the singularity in the closing flux near the Junk region. This has motivated the consideration of both semi- and fully-implicit time-marching schemes.

The semi-implicit scheme was proposed previously by McDonald and Groth [36]. It uses a point-implicit treatment, which integrates the hyperbolic flux explicitly and the source term implicitly. The resulting fully-discrete solution scheme applied to cell $(i,j)$ is,

$$
\tilde{U}^{n+1}_{(i,j)} = U^n_{(i,j)} - \frac{\Delta t}{A_{(i,j)}} \left( \sum_k (\mathbf{F} \cdot \hat{n} \Delta l)_{(i,j,k)}^n \right) + \Delta t S^{n+1}_{(i,j)}, \tag{5.15}
$$

$$
U^{n+1}_{(i,j)} = U^n_{(i,j)} - \frac{\Delta t}{2A_{(i,j)}} \left( \sum_k (\mathbf{F} \cdot \hat{n} \Delta l)_{(i,j,k)}^n + \sum_k (\mathbf{F} \cdot \hat{n} \Delta l)_{(i,j,k)}^{n+1} \right) + \Delta t \left( \frac{S^n_{(i,j)} + S^{n+1}_{(i,j)}}{2} \right), \tag{5.16}
$$
where $n$ is the temporal index and $\Delta t$ is the time step.

### 5.3 Newton-Krylov-Schwarz Algorithm

Due to the limit on the time step by the Courant-Friedrichs-Lewy condition [69], explicit and semi-implicit methods, such as the algorithm described in Section 5.2, tend to have slow convergence for very numerically stiff systems. Implicit methods however are unconditionally stable, and thus a much higher time step can be used, leading to a lower number of iterations needed to reach a steady-state solution. The trade-off is that each iteration now requires solving a linear system, which has large computational cost and memory requirements. However, various techniques have been developed to minimize the cost of solving this system, and for many problems the gain in time step size is sufficient to offset the added computational cost and memory requirement at each iteration [69].

Due to the stiffness of the proposed 14-moment system, especially near the Junk region, it is expected that an implicit solver will lead to improved computational performance.

An implicit scheme which has proven to be effective at solving a variety of transport equation systems is the Newton-Krylov-Schwarz (NKS) algorithm [62, 70]. It has been found in past studies that the implementation of this method to solve maximum-entropy type closures has significantly reduced computational cost [16]. This algorithm is based on the well established Newton’s method, however the resulting linear system of equations is solved inexactly using a Krylov subspace iterative method, GMRES (Generalized Minimal RESidual) [71], with a Schwarz-type preconditioner [72].

When considering steady-state solutions, Equation (5.5) is simplified by setting the residual to zero. The resulting nonlinear algebraic system can be solved iteratively using Newton’s method. Based on an initial estimate at step $n = 0$, an improved solution at the next step, $n + 1$, is found as $U^{n+1} = U^n + \Delta U^n$, where $\Delta U^n$ is the solution update. This update value is found by solving the linear system,

$$J(U^n)\Delta U^n = -R(U^n),$$  

(5.17)

where $J(U^n)$ is the residual Jacobian, $(\partial R(U)/\partial U)^n$. This procedure is iterated to generate improved steady state solutions until the solution residual is sufficiently small, i.e.,
\[ \| R(U^{n+1}) \|_2 < \epsilon \| R(U^0) \|_2, \quad (5.18) \]

where \( \epsilon \) is the convergence tolerance, typically \( 10^{-6} - 10^{-11} \).

The matrices considered are large, and thus direct solution of the linear system presented in Equation (5.17) is not feasible. For this reason approximate iterative methods are typically used. In particular the GMRES technique [71] has proven to be a robust and fast method for the solution of the large, sparse, and non-symmetric matrix associated with the linear system [73,74]. Equation (5.17) can be rewritten in the more general form, \( Ax = b \), where \( A = J(U^n) \), \( x = \Delta U \), and \( b = -R(U^n) \). The GMRES technique is an iterative projection method where solution updates are chosen from an orthogonalized Krylov subspace such that the \( L_2 \)-norm of the residual, \( r = b - Ax \), is minimized. This results in a two-tiered scheme containing an inner iterative GMRES linear solver and an outer iterative Newton’s method non-linear solver (see Figure 5.4).

In order to speed up the solver the requirements on the convergence of the GMRES solver are relaxed, such that the inner iterations are carried out only until

\[ \| R + J\Delta U \|_2 \leq \zeta \| R \|_2, \quad (5.19) \]

where the convergence tolerance, \( \zeta \), is set to a modest value between 0.01 and 0.5. This results in what is known as an inexact Newton’s method. Previous studies of such methods have found that it is not necessary to perform the inner linear solve exactly in order to obtain rapid convergence of the outer Newton solver [75].

The effectiveness of the GMRES algorithm for solving the system, \( Ax = b \), can be increased using preconditioning. The preconditioned system is

\[ (AP^{-1})(Px) = b, \quad (5.20) \]

where \( P \) is the preconditioning matrix. A good preconditioning matrix will approximate \( A^{-1} \), while being less expensive to invert than \( A \). In this study the additive Schwarz preconditioner has been used [71,76,77]. This is a domain-decomposition method, whereby the domain is separated into smaller blocks, and the solutions on these block boundaries are passed amongst each other and used as Dirichlet boundary conditions. Furthermore, a local block preconditioner is applied to each of these subdomains. This preconditioner is formed via incomplete lower-upper (LU) factorization on the approximate Jacobian.
of the solution residual for the considered block. In order to maintain a fast solver, the accuracy of the LU factorization is limited by a level of fill, $f$, of 2 or 3. This method of preconditioning couples well with the block-based parallelization and adaptive mesh refinement of the solver [66, 78].

The implementation of the NKS solver is based on that of Groth and Northrup [62, 79]. This solver has already been successful for a number of equation systems, such as non-equilibrium flows evaluated with the Gaussian closure [16], and reacting flows [62]. When applying this solver to the 14-moment interpolative closure the Jacobians which are required to obtain the local preconditioner have been approximated using finite differences, as opposed to exact algebraic expressions which are traditionally used. This is because of the complexity of the closing fluxes for this particular moment closure. This approximation is expected to have some detriment on the performance of the NKS scheme, however it is a good first step.

5.3.1 Extension to Analytic Jacobians

As mentioned in Section 5.3, a finite-differencing technique has been used to find the Jacobians required for the local preconditioner used in the NKS solver. Finite differencing was used due to the complexity of the equation system being considered. However, the use
of an analytically determined Jacobian is ideal, and is expected to reduce computational cost. As a first-step and proof-of-concept, an analytic source term Jacobian and flux-Jacobian are found which are valid in the continuum regime. When formulating the flux-Jacobian it was assumed that the closing fluxes, $R_{ijkk}$ and $S_{ijjkk}$, stay constant. Since these are high-order moments it is expected that they will not have a significant influence in the continuum regime, and thus this assumption is justified. No simplifications were necessary when forming the source term Jacobian as it remains manageable in its most general form.

These analytic Jacobians are then used to solve three different continuum-regime flow cases: Couette flow, heat transfer between flat plates, and sub-sonic flow past a circular cylinder. The parameters are the same as the equivalent cases considered in Sections 6.2, 6.3, and 6.4.1. Each of the comparisons use identical parameters, such as initial conditions, grid, and NKS parameters. The validity of the formulated analytic Jacobians is confirmed by comparing to the finite-difference approximations. Both the steady-state solutions and individual Jacobian matrix terms are compared, and are found to be consistent. A comparison of the $L_2$-norm convergence histories with respect to CPU time are presented in Figure 5.5. It can be concluded that the analytic Jacobians perform far better than the finite-difference approximations, reaching the desired residual reductions in a third of the amount of CPU time for the Couette flow case, and about half the amount of CPU time for the cylinder and heat transfer between flat plates cases. The improved performance of the analytic Jacobian relative to the finite-difference approximation was also found to increase as the mesh density increased. Furthermore, the analytic Jacobian was found to be more robust to parameter choices and converged further before stalling for some cases.

5.4 Boundary Conditions

Appropriate solid-wall boundary conditions for moment-closure methods, which produce the correct non-equilibrium phenomena, are not obvious. Determining the boundary conditions at a solid wall is simplified by assuming that a Knudsen layer of infinitesimal thickness forms adjacent to the wall [9]. In this Knudsen layer, the particle distribution function is a combination of the distribution function of particles from the interior flow field and particles reflected from the solid wall. It is also assumed that particle reflection is either specular or diffusive. The probability of a diffusive interaction occurring is
defined using an accommodation coefficient, $A$, which can have values between 0 and 1, inclusively. When $A = 0$ the interactions are exclusively specular, and particles will experience an elastic collision with the wall. When $A = 1$ the interactions will be exclusively diffusive, and particles will be fully accommodated by the wall before being reintroduced into the Knudsen layer with velocities described by a Maxwellian distribution, which depends on the wall’s temperature and velocity. This so-called half-Maxwellian solid-wall boundary condition technique has been utilized previously for studies of the Gaussian moment closure [37,40].

Using these assumptions, a distribution function for the particles at the solid-wall boundary can be defined as

$$ F_{Kn} = F_+ + F_- , $$

(5.21)

where $F_{Kn}$ is the distribution of particles in the Knudsen layer, $F_-$ is the distribution of the particles entering the Knudsen layer from the interior flow field, and $F_+$ is the distribution of the reflected particles. Assuming that the wall lies parallel to the $y$-axis (see Figure [5.6]), these distribution functions are

$$ F_- = \begin{cases} 
F_{int}(v_x, v_y, v_z) & \text{if } v_x > 0, \\
0 & \text{if } v_x < 0 
\end{cases} $$

(5.22)
\[ F_+ = \begin{cases} \mathcal{M}_W(v_x, v_y, v_z) + (1 - A)F_{\text{int}}(-v_x, v_y, v_z) & \text{if } v_x < 0, \\ 0 & \text{if } v_x > 0 \end{cases} \] (5.23)

where \( F_{\text{int}} \) is the distribution function of particles in the interior flow, and \( \mathcal{M}_W \) is the Maxwellian distribution of the particles accommodated by the wall,

\[ \mathcal{M}_w = n_w \left( \frac{m}{2\pi k T_w} \right)^{3/2} e^{-\frac{m}{2kT_w} (v_x^2 + (v_y - u_{wy})^2 + v_z^2)} , \] (5.24)

where \( T_w \) is the temperature of the wall, \( u_{wy} \) is the wall velocity, and \( n_w \) is the number density of the reflected Maxwellian. These distributions are used in conjunction with known properties at the wall, such as zero normal net flux, to find expressions for the moments in the Knudsen layer, which are then used to determine boundary conditions.

Since the 14-moment interpolative closure is formulated by postulating relations between the closing fluxes and known moments directly, as opposed to assuming a certain distribution function, it is not obvious what interior flow distribution, \( F_{\text{int}} \), should be used. However, since the closure is based on the maximum-entropy closure, it would be expected that the interior distribution would be near a maximum-entropy distribution. In this study a Grad-like perturbative expansion applied to the Gaussian distribution function, a 10-moment maximum-entropy closure, has been used as the interior distribution [80–82]. This distribution has 14 free parameters and permits the direct evaluation of moments of all orders by analytical means. Thus, it is a natural choice to use with the present 14-moment interpolative closure.

The 14-moment Gaussian-based perturbative distribution is expressed as [80–82]

\[ F^{(14)} = G \left[ 1 + \frac{D_\alpha}{5} \left( \Theta^{-1} \left( c_\alpha c^2 - \frac{P_{\gamma\gamma}}{\rho} c_\alpha \right) - 2 c_\beta \right) \\ + 3E \left( c^4 - 2 \frac{P_{\alpha\alpha}}{\rho} c^2 - 4 \frac{P_{\alpha\beta}}{\rho} c_\alpha c_\beta + \frac{P_{\alpha\alpha} P_{\beta\beta}}{\rho^2} + 2 \frac{P_{\alpha\beta}^2}{\rho^2} \right) \right] \] (5.25)

The coefficients, \( D_\alpha \) and \( E \), are required to satisfy the following relations:

\[ q_i = \frac{1}{5\rho} \left[ P_{j\alpha}^2 D_i + 2 P_{i\alpha} P_{j\alpha} D_j \right] , \] (5.26)
Figure 5.6: Representation of the Knudsen layer.

\[ E = \frac{5\rho^3}{8} \frac{\mathcal{K}}{P_{\alpha\gamma} P_{\beta\delta}^2 + 2P_{\alpha\gamma} P_{\alpha\delta} P_{\beta\gamma} P_{\beta\delta}} \] \quad (5.27)

where

\[ \mathcal{K} = r - \left( P_{\alpha\alpha} P_{\beta\beta} + 2P_{\alpha\beta}^2 \right) / 15\rho. \] \quad (5.28)

The 14-moment Gaussian-based perturbative distribution of Equation (5.25) is now used as the interior distribution, \( F_{\text{int}} \), in Equations (5.22) and (5.23) to obtain values for the moments in the Knudsen layer. The resulting expressions are:

\[ n_{Kn} = \frac{(2 - A)}{2\sqrt{\pi} P_{xx}^{3/2} m} \left\{ \sqrt{\pi} \rho P_{xx}^{3/2} - \frac{\sqrt{2}}{5} D_x \sqrt{\bar{\rho}} \left( P_{xy}^2 + P_{xx}^2 \right) \right\} + \frac{\mathcal{A} n_w}{2}, \] \quad (5.29)

\[ u_{xKn} = 0, \] \quad (5.30)

\[ u_{yKn} = -\frac{3(2 - A) n}{2\sqrt{\pi} P_{xx}^{5/2} \rho^3 n_{Kn}} \left\{ \frac{\sqrt{2}}{15} \rho^{5/2} P_{xx} \left( D_x P_{xx}^2 u_y - 5P_{xx} P_{xy} + D_x P_{xy}^2 u_y \right) - \frac{\sqrt{\pi}}{3} \rho^3 P_{xx}^{5/2} u_y \right\} + \frac{\mathcal{A} n_w}{2n_{Kn}} u_{wy}, \] \quad (5.31)
\[ P_{xyKn} = \frac{(2 - A)}{2\sqrt{\pi}\rho P^{3/2}_{xx}} \left\{ \sqrt{\frac{2}{5}} \rho^{3/2} \left[ D_y P^3_{xx} + D_x P^2_{xx} P_{xy} + P_{xx} P_{xy} \left( D_y P_{xy} + 2D_x P_{yy} \right) - D_x P^3_{xy} \right] \right\} \]
\[ \quad - \sqrt{\frac{2}{9}} \rho^{5/2} P^2_{xx} \left( u_{yKn} - u_y \right) + \sqrt{\frac{2}{9}} \rho P^{3/2}_{xx} P_{xy} + 3\sqrt{2}E\sqrt{\rho} \left( P^2_{xx} + P^2_{xy} \right)^2 \left( u_{yKn} - u_y \right) \}
\[ \quad - A \sqrt{\frac{n_w\rho_k T_{w}}{2\pi}} \left( u_{wy} - u_{yKn} \right), \]
\[ (5.32) \]

\[ Q_{xiiKn} = \frac{9(2 - A)\rho}{2\sqrt{\pi}\rho P^{5/2}_{xx}} \left\{ \frac{2\sqrt{2}}{45} \rho^{5/2} P_{xx} \left[ - P_{xx} P_{xy} \left( P_{xy} \left( D_y u_{yKn} - D_y u_y - \frac{5}{2} \right) \right) \right] + 2D_x P_{yy} \left( u_{yKn} - u_y \right) + P^3_{xx} \left( 5 + D_y(u_y - u_{yKn}) \right) + P^3_{xy} D_x(u_{yKn} - u_y) \right\} \]
\[ \quad + P^2_{xx} \left( - D_x P_{xy} \left( u_{yKn} - u_y \right) + \frac{5}{2} P_{yy} \right) \left[ + \frac{4\sqrt{\pi}}{45} D_y \rho^2 P^{7/2}_{xx} P_{xy} \right] \]
\[ \quad - \frac{\sqrt{2}}{3} E\rho^{3/2} P_{xx} \left( P^2_{xy} + P^2_{xx} \right)^2 \left( u_{yKn} - u_y \right) + \frac{\sqrt{2}}{9} \rho \rho^{7/2} P^3_{xx} \left( u_{yKn} - u_y \right)^2 \]
\[ \quad + \frac{2\sqrt{\pi}}{15} D_x \rho^2 P^{9/2}_{xx} - \frac{1}{3} P^5_{xx} \left( P_{yy} + \frac{8\sqrt{\pi}}{45} \rho^2 P^{5/2}_{xx} \left( \frac{1}{4} D_x \left( P^2_{zz} + P^2_{yy} \right) \right) \right) \]
\[ \quad + P_{yy} \left( - \frac{5}{4} \rho u_{yKn} + \frac{5}{4} \rho u_y + \frac{1}{2} D_y P_{yy} \right) + D_x P^2_{xy} \right) + \sqrt{2}\rho \left( 2P^6_{xx} + P^6_{xy} \right) \]
\[ \quad + \frac{1}{3} P^4_{xx} \left( 19P^2_{xy} + 4P^2_{zz} + 4P^2_{yy} \right) + \frac{8}{3} P^2_{xx} P^2_{xy} \left( \frac{1}{2} P^2_{zz} + \frac{3}{2} P^2_{yy} + P^2_{xy} \right) \]
\[ \quad + 2P^3_{xx} P^2_{xy} \left( P_{yy} + \frac{1}{3} P_{zz} \right) - 3P_{xx} P^4_{xy} \left( P_{yy} + \frac{1}{9} P_{zz} \right) \right\} \]
\[ - \frac{A\rho^2 m^3}{\sqrt{2\pi} m^{3/2}} \left\{ m(u_{yKn} - u_{yw})^2 + 4kT_w \right\}. \]
\[ (5.33) \]

An interesting result of the formulated boundary conditions is the coupling between the shear stress, \( P_{xy} \), and heat flux, \( Q_{xii} \) and \( Q_{yi} \). The influence of the heat flux and shear stress in the interior fluid on the shear stress and heat flux in the Knudsen layer is explored in Figure 5.7. Figure 5.7(a) depicts how the \( x \)-direction heat flux in the Knudsen layer changes as the shear stress of the interior fluid increases. In the equilibrium regime this shear stress is expected to be zero, however as the Knudsen number is increased the
stress will also increase (this effect is seen in Figure 6.4 (b) of Section 6.2). It is clear that in the equilibrium and near-equilibrium regimes, when the shear stress is small, the resulting heat flux in the Knudsen layer is also small. However, as the Knudsen number, and thus shear stress, is increased the heat flux in the Knudsen layer also increases rapidly. Additionally, as the heat flux parallel to the boundary increases, the shear stress in the Knudsen layer also increases as seen in Figure 5.7 (b). However, in this case the relationship is linear. In conclusion, it is quite evident that at high Knudsen numbers the boundary conditions become tightly coupled.
Chapter 6

Numerical Results

In this chapter numerical results are presented for the interpolative moment closures corresponding to a monatomic gas. Section 6.1 outlines the results of the dispersion analyses and maximum wave speed study of the 5- and 14-moment interpolative closures. Sections 6.2, 6.3, 6.4, and 6.5 explore the application of the 14-moment interpolative closure to solve the canonical multi-dimensional flow problems of Couette flow, heat transfer between flat plates, subsonic flow past a circular cylinder, and lid driven cavity flow, respectively.

6.1 Dispersion Analyses and Maximum Wave Speeds

The solutions of hyperbolic relaxation systems of PDEs are in the form of waves. Therefore, when studying systems of such equations, understanding the properties of these waves is of great importance. Two such properties are the wave speed and damping rate. The PDE systems considered in moment closures, and similar types of generalized transport equations, exhibit dispersive wave behaviours, meaning that their wave speeds and damping are a function of the wavenumber of the propagating solution wave. In order to gain insight into what these wave speeds and damping rates are, and how they vary with wavenumber, a dispersion analysis is performed. In general, a dispersion analysis describes how a certain linear operator acts on Fourier modes of perturbations with different wave numbers \[48\]. In the case of a system of PDEs in weakly conservative form this linear operator is \( \partial/\partial t + A\partial/\partial x - Q \), where \( A \) is the flux-Jacobian, and \( Q \) is the source-term Jacobian. For this analysis the Jacobians are evaluated at the reference
state of interest, and then held fixed. The perturbative solutions are assumed to be of
the form
\[ u(x,t) = \text{Re} \left[ v(t)e^{-ikx} \right], \] (6.1)
where, \(v(t)\) is the amplitude of the solution wave, \(k\) is the wavenumber, and \(i\) is \(\sqrt{-1}\). The linearized differential operator applied to Equation (6.1) yields a set of ordinary
differential equations (ODEs) given by
\[ \frac{dv}{dt} = (ikA + Q)v, \] (6.2)
which has the non-trivial solution
\[ v(t) = e^{i(kA+iQ)t}u_0, \] (6.3)
where \(u_0\) is the initial amplitude of the solution. The wave speed and decay constants of
this solution are proportional to the real and imaginary components of the eigenvalues
of \((kA - iQ)\), respectively. The wavenumber \(k\) can be related to the Knudsen number
by \(Kn = \frac{2\pi k}{47}\), and therefore the properties of the solution waves can be determined
for the entire range of Knudsen numbers.

Dispersion analyses were applied to the 5- and 14-moment interpolative closure for a
monatomic gas. Recall the 5-moment interpolative closure is applicable to gases for which
particle movement is confined to a single direction, and is summarized in Section 4.2.
The 14-moment analysis assumed only variations in the \(x\)-direction and an axi-symmetric
distribution function about the \(v_x\) axis, leading to moment relations: \(u_y = u_z = 0,\)
\(P_{xy} = P_{xz} = P_{yz} = 0\), and \(Q_{yii} = Q_{zii} = 0\). The particle distribution function is
transformed such that \(u_x = 0\), and the moments are non-dimensionalized such that
\(\rho = P_{xx} = P_{yy} = P_{zz} = 1\). Since the distribution function remains axi-symmetric
about the \(v_x\) axis, a radial pressure can be introduced as, \(P_{rr} = P_{yy} + P_{zz}\). Under these
assumptions, the 14-moment equation system simplifies to
\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u_x) = 0 \] (6.4)
\[ \frac{\partial}{\partial t} (\rho u_x) + \frac{\partial}{\partial x} (\rho u_x^2 + P_{xx}) = 0 \] (6.5)
\[ \frac{\partial}{\partial t} (\rho u_x^2 + P_{xx}) + \frac{\partial}{\partial x} (\rho u_x^2 + 3u_x P_{xx} + Q_{xxx}) = \frac{P_{rr} - 2P_{xx}}{3\tau} \] (6.6)
\[ \frac{\partial}{\partial t} (P_{rr}) + \frac{\partial}{\partial x} (u_x P_{rr} + Q_{xrr}) = \frac{2P_{xx} - P_{rr}}{3\tau} \]  
(6.7)

\[ \frac{\partial}{\partial t} \left( \rho u_x^3 + u_x(3P_{xx} + P_{rr}) + Q_{xii} \right) + \frac{\partial}{\partial x} \left( \rho u_x^4 + u_x^2(6P_{xx} + P_{rr}) + 2u_x(Q_{xii} + Q_{xxx}) + R_{xii} \right) = \frac{2u_x(P_{rr} - 2P_{xx}) - 3Q_{xii}}{3\tau} \]  
(6.8)

\[ \frac{\partial}{\partial t} \left( \rho u_x^4 + u_x^2(6P_{xx} + 2P_{rr}) + 4u_xQ_{xii} + R_{iiij} \right) + \frac{\partial}{\partial x} \left( \rho u_x^5 + u_x^3(10P_{xx} + 2P_{rr}) + u_x^2(6Q_{xii} + 4Q_{xxx}) + u_x(R_{iiij} + 4R_{xii} + S_{xiiij}) \right) = \frac{1}{3\tau} \left( 4u_x^2(P_{rr} - 2P_{xx}) - 12u_xQ_{xii} + 5 \left( \frac{P_{xx} + P_{rr}}{\rho} \right)^2 - 3R_{iiij} \right). \]  
(6.9)

The corresponding closing fluxes are:

\[ Q_{xxx} = A Q_{xii}, \quad Q_{xrr} = (1 - A)Q_{xii}, \]  
(6.10)

\[ R_{xii} = \frac{A Q_{xii}^2}{\sigma P_{xx}} + \frac{2(1 - \sigma)P_{xx}^2 + (P_{xx} + P_{rr})P_{xx}}{\rho}, \]  
(6.11)

\[ S_{xiiij} = \frac{A Q_{xii}^3}{\sigma^2 P_{xx}^2} + \frac{2}{\rho} \left( P_{xx} + P_{rr} + (1 - \sigma^{1/2}) \frac{P_{rr}^3 + 2P_{rr}^2 P_{xx} + 24P_{xx}^3}{P_{xx}^2 + 6P_{xx}^2} \right) Q_{xii}, \]  
(6.12)

with

\[ A = \frac{6P_{xx}^2}{P_{rr}^2 + 6P_{xx}^2}, \]  
(6.13)

and

\[ \sigma = \frac{1}{2(2P_{xx}^2 + P_{rr}^2)} \left\{ 2P_{xx}^2 + P_{rr}^2 + (P_{xx} + P_{rr})^2 - \rho R_{iiij} \right. \]

\[ + \left. \sqrt{[(2P_{xx}^2 + P_{rr}^2) + (P_{xx} + P_{rr})^2 - \rho R_{iiij}]^2 + 4\rho(2P_{xx}^2 + P_{rr}^2)Q_{xii}^2/P_{xx}} \right\}. \]  
(6.14)

The dispersion analysis has been performed on this simplified one-dimensional system, but the conclusions are expected to extend to multidimensional systems.

Of particular interest are the maximum frozen wave speeds, which are the maximum wave speeds as \( \kappa \to \infty \), since these values will limit the Mach numbers for which internal shock structures can be resolved without generating unphysical sub-shocks. They will also influence the stiffness of the system. For the Grad-13 and Gaussian closure the
maximum frozen wave speeds at equilibrium have been found to be Mach 1.65 and Mach 3/\sqrt{5}, respectively \cite{13, 47}. The 5- and 14-moment closures however has been found to provide smooth shock structure even up to Mach numbers of 8 \cite{14}. It is expected that the singularity in the closing flux encountered at the Junk region results in arbitrarily large frozen wave speeds as the subspace is approached, leading to smooth shock structures. This is confirmed by the dispersion analysis of the moment systems as shown in Figure 6.1, which display the maximum frozen wave speeds on constant $\sigma$ contours for both the 5-moment (a) and 14-moment (b) closures. Recall that $\sigma$ is equal to zero at the Junk region, therefore the maximum wave speed is expected to increase as $\sigma$ approaches zero. This behaviour is seen in Figure 6.1 although it is observed that the wave speeds reduce rapidly at points below equilibrium. These large wave speeds, especially near equilibrium, suggest that a fully implicit solution scheme may be ideal, due to the resulting stiffness of the equation system.

The dispersion analysis is also performed at a reference state very close to equilibrium, $q_* = 0$ and $r_* = 2.99$ for the 5-moment closure and $Q_{xii} = 0$ and $R_{ijjj} = 14.99$ for the 14-moment closure, since the presence of the Junk region prevents analysis exactly at equilibrium. The attenuation rate results are shown in Figure 6.2 (a) and 6.3 (a) for the 5- and 14-moment interpolative closures, respectively. It is clear that these attenuation values remain between zero and one for all wavenumbers and thus the system is stable at all Knudsen numbers. The wave speed results are shown in Figure 6.2 (b) and 6.3 (b), for the 5- and 14-moment closure respectively. The wave speeds approach the speed of sound in the continuum regime, i.e., as $\kappa \to 0$, which is expected.
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Figure 6.1: Maximum wave speed on constant $\sigma$ contours for the (a) 5-moment and (b) 14-moment interpolative closures.

Figure 6.2: 5-moment interpolative closure dispersion analysis results for the (a) attenuation rate and (b) wave speed.
Figure 6.3: 14-moment interpolative closure dispersion analysis results for the (a) attenuation rate and (b) wave speed.

6.2 Couette Flow

A good initial test case for non-equilibrium models is that of planar subsonic Couette flow between two oppositely moving plates, as studied previously by McDonald and Groth [8, 36] and McDonald et al. [34]. The Knudsen number for this case is found as $\text{Kn} = \frac{\Lambda}{d}$ where $d$ is the distance between the plates, and the mean free path is given by

\begin{equation}
\Lambda = \frac{16\mu}{5\sqrt{2\pi\rho p}}.
\end{equation}

This model of the mean free path assumes that the gas molecules interact as hard spheres [6]. For this case, the Knudsen number can be adjusted by simply changing the distance between the plates. It is expected that as the Knudsen number is raised, and the free-molecular regime is approached, the appearance of slip flow at the plates will become more pronounced, since fewer interactions between the gas and plate particles are occurring. The ability to recreate this slip flow accurately is a good benchmark for both the moment-closure method and the boundary conditions considered.

The Couette flow case which has been studied consists of two parallel plates moving in opposite directions at a velocity, $U_w$, of 30 m/s in the $x$-direction. The gas between the plates is argon with standard atmospheric free stream density of 1.225 kg/m$^3$ and pressure
of 101.325 kPa, and therefore a temperature of 397.37 K. The temperature of the plates, \( T_w \), is 397.37 K to ensure minimal heat transfer between the plates and internal gas. The transport equations of the 14-moment interpolative closure, summarized in Section 4.1, were solved using both the semi-implicit and NKS numeric algorithms described in Chapter 5, on a mesh containing 10 cells in the \( x \)-direction, and 100 cells in the \( y \)-direction, for a total of 1000 computational cells. Periodic boundaries were specified in the \( x \)-direction and the solid-wall half-Maxwellian boundary conditions, Equations (5.29)-(5.33), were specified at the plate surfaces. An accommodation coefficient of \( A = 1 \) was used. The results for the normalized flow velocity \( u_x/U_w \), and normalized shear stress,

\[
P_{xy}^* = \frac{-P_{xy}}{\rho U \sqrt{\frac{2kT}{\pi m}}},
\]

for a wide range of Knudsen numbers are shown in Figure 6.4. These computed values are compared with results found using the Gaussian closure [8], and an analytical solution developed by Lees [83]. It is evident that the predicted values of the 14-moment closure are in very good agreement with those of the Gaussian and Lees solution throughout the continuum, transition, and free-molecular regimes. The figures also illustrate the failure of both the NSF equations and free-molecular solution in the transition regime, emphasizing the importance of moment closures and their ability to model gases throughout this regime.

A comparison between convergence histories for the semi-implicit and NKS solvers is presented in Figure 6.5. The L2-norm values are with respect to the density component of the residual and are normalized by the residual value of the first iteration. The semi-implicit solver uses a CFL number of 0.5. The NKS solver shows improved performance over the semi-implicit scheme, with a factor of CPU time savings of between 3 and 11 times, for each of the Knudsen numbers considered. As discussed in Section 6.1 the wave speeds become higher as the continuum regime is approached, i.e., the Knudsen number is lowered, and based on this finding it was hypothesized that the performance of the NKS solver would be most pronounced in the continuum regime. Furthermore, in the continuum regime the relaxation time scales become very small, leading to additional stiffness of the system. As a result the \( \text{Kn}=0.01 \) case shows an improved NKS performance relative to the semi-implicit scheme when compared to the \( \text{Kn}=0.1 \) and \( \text{Kn}=1 \) cases.
Figure 6.4: (a) Normalized flow velocity at the plate as a function of Knudsen number. (b) Normalized shear stress between the plates with respect to Knudsen number.

Figure 6.5: Comparison of convergence of the solution residuals for the NKS and semi-implicit solvers when applied to a Couette flow case with a Knudsen number of (a) 0.01, (b) 0.1, and (c) 1.
6.3 Heat Conduction Between Flat Plates

The case of heat conduction between two infinite flat plates oriented parallel to the $x$-axis has also been considered. In this case it is expected that in the continuum regime the temperature of the interior fluid adjacent to the wall will be equivalent to the wall temperature. However, as the Knudsen number is increased a temperature jump between the wall and internal fluid will develop, due to the reduced number of interactions between the internal gas particles and particles reflected from the plate. Accurately predicting this phenomena is a good benchmark for the 14-moment closure and heat-flux boundary conditions.

The gas between the heated plates is argon at a temperature of 397.37 K, density of 1.225 kg/m$^3$ and pressure of 101.325 kPa. The upper plate temperature, $T_U$, has been set to 407.37 K, and the lower plate temperature, $T_L$, has been set to 387.37 K; resulting in a temperature difference of 20 K between the plates. The computational domain consisted of 4 cells in the $x$-direction and 100 cells in the $y$-direction, for a total of 400 computational cells. The solid-wall half-Maxwellian boundary conditions, with $A = 1$, were specified at the plate surfaces, and periodic boundaries were used in the $x$-direction. The values of normalized wall temperature, $T^*$, and normalized heat flux between the plates were found for a large range of Knudsen numbers.

The numerical results for heat transfer between the two plates are presented in Figure 6.6. In the figure, the wall temperature has been normalized as

$$T^* = \frac{T - T_m}{T_w - T_m}, \tag{6.17}$$

where $T$ is the temperature of the gas adjacent to the wall, $T_m$ is the gas temperature midway between the plates, and $T_w$ is the temperature of the plate. The normalized temperature is found with respect to the lower plate. Ideally it should not matter whether the upper or lower plate is used, however it was found that at large Knudsen numbers there was a small discrepancy. The suspected mechanism leading to this discrepancy will be further discussed below. The heat flux between the plates has been normalized with respect to the free-molecular heat flux given by

$$q_x = \rho_m \sqrt{\frac{RT_m}{2\pi}} \left( c_v + \frac{1}{2} \right) (T_U - T_L), \tag{6.18}$$
where $\rho_m$ is the density of the gas midway between the plates, $R$ is the specific gas constant, and $c_v$ is the heat capacity at constant volume. The results are compared to the free-molecular solution, the continuum NSF solution, and the NSF solution with temperature jump boundary conditions. The temperature jump distance, $g$, is found as

$$g = \frac{2 - A}{A} \frac{K}{(\gamma + 1) c_v p}, \quad (6.19)$$

where $K$ is the thermal conductivity. In order to stay consistent with the BGK approximation the thermal conductivity is taken to be $K = c_p \mu$, where $c_p$ is the heat capacity at constant pressure, thus ensuring a Prandtl number of unity. The temperature directly adjacent to the wall is then found as,

$$T = g \frac{\partial T}{\partial y} + T_w, \quad (6.20)$$

which is used as the temperature boundary condition in the NSF equations. Overall the results from the 14-moment interpolative closure are in very good agreement with the analytic Navier-Stokes-Fourier solution with slip boundary conditions. Since this is a very simple flow problem this analytic solution is expected to be valid.
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The performance of the NKS and semi-implicit schemes are compared in Figure 6.7. The $L_2$-norm values of the residual of density and are normalized by the residual value of the first iteration. The semi-implicit solver uses a CFL number of 0.5. The NKS solver continues to outperform the semi-implicit scheme, in fact even more so than in the Couette flow case. Savings in CPU time of between 8 and 15 times were found for the cases considered. This improved performance is expected since it was found that the maximum wave speed of the system increases as the heat flux increases, see Figure 6.1. It is also found that the convergence stalls earlier for the $Kn=0.1$ and $Kn=1$ cases when solved using the semi-implicit scheme.

Although promising results have been found for temperature slip and heat flux between the plates there are still some issues with this case. It was found that the temperature in the middle of the plates drifted from the expected value of 397.37 K. This phenomena can be observed in Figure 6.8 (a) which displays the temperature distributions between the plates at several Knudsen numbers. The heat flux between the plates has also been considered in Figure 6.8 (b). Steep changes in the heat flux are observed adjacent to either wall, which is in contrast to the expected constant heat flux. This implies an inaccuracy of the boundary condition, and also lead to the discrepancy between the top and bottom plate temperatures which was mentioned above. Similar inaccuracies have also been observed in previous studies of moment closures applied to heat transfer problems using a solid-wall half-Maxwellian boundary condition [85].

In conclusion, the results found show potential for the 14-moment closure’s ability to model heat transfer. The normalized temperature results, Figure 6.6(a), display the

![Figure 6.7: Comparison of convergence of the solution residuals for the NKS and semi-implicit solvers when applied to a heated flat plates case with a Knudsen number of (a) 0.01, (b) 0.1, and (c) 1.](image)
expected temperature jump, beginning in the transition region, and the values are in close agreement with those predicted by the NSF solution with slip-temperature boundary conditions. The results for normalized heat flux, Figure 6.6(b), are also consistent with the NSF solution with slip-temperature boundary conditions. Some intangible results are found for the heat flux and temperature distributions. However, it is suspected that these can be mitigated by implementing a more carefully formulated boundary condition, such as the modification to the solid-wall half-Maxwellian boundary conditions considered by Struchtrup [86].

### 6.4 Subsonic Flow Past a Circular Cylinder

Subsonic flow past a circular cylinder is considered for several Knudsen numbers spanning the continuum and transition regimes. For comparison, simulations were also executed using the Gaussian [8, 36] and regularized Gaussian [8, 39] closures. Recall that the Gaussian closure is a 10-moment maximum-entropy closure. The regularized Gaussian closure is an extension of the Gaussian closure which incorporates anisotropic thermal-diffusion effects using added elliptic terms. For all cases the gas considered is argon at standard atmospheric density and pressure of 1.225 kg/m$^3$ and 101.325 kPa, respectively, and a temperature of 397.37 K. Solutions were found using each closure technique on a quadrilateral, body fitted, computational mesh of between 16 640 and 32 000 cells. The
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Figure 6.9: Mesh refinement study for subsonic flow around a circular cylinder at Kn=0.1 and S=0.027. N is the total number of computational cells.

Mesh was stretched resulting in a much greater concentration of cells near the cylinder surface. These mesh sizes were chosen based on past studies by McDonald [40] and Lam [16] and a mesh refinement study, the results of which are summarized in Figure 6.9. The figure shows the drag coefficient, \( c_d \), for a circular cylinder at Kn=0.1 and S=0.027 when calculated at several mesh densities. Three uniform mesh refinements were performed, each quadrupling the mesh density. It is clear that refinement after about 30 000 cells doesn’t significantly change the drag coefficient. An example mesh is presented in Figure 6.10. The outer boundary is set far from the cylinder surface since the boundary layers are large, relative to the cylinder radius, for non-equilibrium flows.

The speed ratios, \( S \), considered for the subsonic cylinder flows were 0.027 and 0.107, corresponding to Mach numbers of 0.030 and 0.117, respectively. The speed ratio is defined as the ratio between the free stream gas speed and the most probable “random” particle speed,

\[
S = \frac{u_\infty}{\sqrt{\frac{2kT}{m}}}
\]

(6.21)

The temperature of the cylinder was set equivalent to the free-stream gas temperature of 397.37 K. The solid-wall half-Maxwellian boundary conditions, with an accommodation coefficient of \( A = 1 \), were used at the cylinder edge.
This section begins with comparisons of various gas property contours for flows with \( Kn = 0.002 \) and \( Kn = 1 \), found using the 14-moment, Gaussian, and regularized Gaussian closures (Sections 6.4.1 and 6.4.2). Various important non-equilibrium flow features and discrepancies amongst the models are noted. A more quantitative investigation is then presented in Section 6.4.3 by considering the coefficient of drag of the cylinder. Finally, the solution convergence of the NKS and semi-implicit solvers are compared for several cases (Section 6.4.4).

### 6.4.1 Results for \( Kn=0.002 \) and \( S=0.027 \)

Solutions found for this continuum case, \( Kn = 0.002 \), are presented in Figures 6.11 and 6.12. For this case the Reynolds number is 24.3728. It can be seen that the Mach number contours are very similar for each of the solution methods, as is expected, since each closure should recover the NSF solution. Since this case is in the continuum regime, negligible velocity slip is observed at the surface of the cylinder. The velocity streamlines show the formation of a recirculation region downstream of the cylinder. This is a well established phenomena at the Reynolds number considered. The gas is close to local thermodynamic equilibrium for this low Knudsen number case, and therefore the variations in temperature are small, however the Gaussian solution shows slightly higher temperatures near the cylinder, signifying that, even for this continuum-regime case, heat transfer is starting to have an effect. The regularized Gaussian and 14-moment closure solutions are in good agreement. The temperature field for both solution methods is
overall uniform, with very slight increases in front and downstream of the cylinder. This case is a good verification of the 14-moment closure’s predictive ability for continuum-regime flows in two-dimensions.
Figure 6.11: Mach number contours and velocity streamlines for subsonic flow past a circular cylinder at Kn=0.002 found by solving the (a) Gaussian, (b) regularized Gaussian, and (c) 14-moment closures.
Figure 6.12: Temperature contours for subsonic flow past a circular cylinder at $Kn=0.002$ found by solving the (a) Gaussian, (b) regularized Gaussian, and (c) 14-moment closures.
6.4.2 Results for Kn=1 and S=0.027

Solutions found for the transition-regime case, Kn = 1, are presented in Figures 6.13, 6.14, and 6.15. For this case the Reynolds number is 0.0487. It can be observed that the Mach number contours now show discrepancy between the closure techniques, although all show significant slip, as expected. The recirculation region observed in the continuum regime has disappeared, as would be anticipated for this much lower Reynolds number. The boundary layer thickness relative to the cylinder diameter has also increased, which is expected from kinetic theory. The Gaussian solution shows very significant localized temperature rises, which are caused by a combination of flow compression and viscous dissipation, when compared with the regularized Gaussian and 14-moment closures. This is anticipated as the Gaussian solution does not consider heat transfer, which is significant in this regime. The heat-flux streamlines (Figure 6.15) are similar for the regularized Gaussian and 14-moment solutions, however the temperature contours differ. The regularized Gaussian shows a decrease in temperature in front of the cylinder and increased temperature behind, whereas the opposite is true for the 14-moment closure. Therefore, the heat flux in the 14-moment solution is oriented in the opposite direction to that expected by modelling based on the temperature gradient. This so-called temperature polarization and non-gradient transport effect have been previously observed when considering flows in the transition regime, such as in analytical solutions for flow around a sphere by Torrilhon [87]. The 14-moment closure’s ability to predict this non-equilibrium phenomena is very promising.
Figure 6.13: Mach number contours and velocity streamlines for subsonic flow past a circular cylinder at Kn=1 found by solving the (a) Gaussian, (b) regularized Gaussian, and (c) 14-moment closures.
Figure 6.14: Temperature contours for subsonic flow past a circular cylinder at Kn=1 found by solving the (a) Gaussian, (b) regularized Gaussian, and (c) 14-moment closures.
Figure 6.15: Temperature contours and heat-flux streamlines for subsonic flow past a circular cylinder at Kn=1 found by solving the (a) regularized Gaussian and (b) 14-moment closures. Note that the temperature contours have been rescaled to show more detail.
6.4.3 Drag Prediction

The predicted values of the drag coefficient, $c_d$, are also considered for the 14-moment and Gaussian closures. These results are compared with experimental values found by Coudeville et al. [88] (Figure 6.16). Although these experimental values were found for air, they are expected to be very similar to those of argon due to their similar viscosity, and are therefore still used for comparison, particularly to get an idea of the trends of the drag coefficient into the free-molecular regime. Furthermore, when these cases were run for both air and argon using the Gaussian closure the drag value was found not to change significantly. The 14-moment closure has not been solved using air in this case because the solver currently only has the capacity to treat monatomic gases. The values of drag coefficient are in excellent agreement with those of the Gaussian closure for the lower Knudsen number cases of Kn=0.01, Kn=0.03, and Kn=0.1. This is expected since the heat transfer contributions are small. As the free-molecular regime is approached the predicted drag coefficients for the closure methods begin to diverge. However, the 14-moment closure seems to follow the trends of the experimental solution more closely than the Gaussian closure. This is expected since the 14-moment closure considers a higher number of moments, and thus should capture more of the non-equilibrium physics, allowing it to remain valid to a higher Knudsen number. These results are significant as

![Figure 6.16: Comparison of predicted drag coefficients found using the 14-moment and Gaussian closures and experimental values for air found by Coudeville et al. [88].](image)
they not only validate the 14-moment closure at the beginning of the transition regime, but also show its improved predictive capabilities at higher Knudsen numbers.

6.4.4 Solver Performance

Finally, a comparison of solution convergence histories are considered for the semi-implicit and NKS solvers for the circular-cylinder calculations (Figures 6.17 and 6.18). The semi-implicit solver uses a CFL number of 0.15-0.3 depending on the Knudsen number (higher Knudsen number cases require lower CFL numbers). The NKS solver is found to continue to offer significant gains in computation speed, with a factor of at least 2.5 times saving

![Figure 6.17](image1.png)

(a) Comparison of solution convergence using the NKS and semi-implicit schemes for the circular cylinder case with a Knudsen number of (a) 0.01, (b) 0.1, and (c) 1 and a speed ratio of $S=0.027$.

![Figure 6.18](image2.png)

(a) Comparison of solution convergence using the NKS and semi-implicit schemes for the circular cylinder case with a Knudsen number of (a) 0.01, (b) 0.1, and (c) 1 and a speed ratio of $S=0.107$. 
in CPU time. Furthermore, the NKS solver is less prone to convergence stall than the semi-implicit scheme.

### 6.5 Lid-Driven Cavity Flow

The final case considered is lid-driven cavity flow. A square computational domain of 150 x 150 Cartesian cells, for a total of 22,500 cells, with three stationary solid walls and one moving wall with a tangential $x$-direction velocity, $U = 50 \text{ m/s}$, is utilized (see Figure 6.19). The square cavity contains argon with an initial pressure of 101.325 kPa and temperature of 273 K. The wall temperatures, $T_w$, are set equivalent to the internal gas, i.e. $T_w = 273 \text{ K}$. The residuals for this case are reduced by at least four orders of magnitude.

Solutions are found at $Kn=0.001$, $Kn=0.05$ and $Kn=0.1$. These results are compared to results found using the regularized Gaussian closure [16], as well as solutions found using the NSF equations for the continuum case, and a DSMC solution found by John, Gu, and Emerson [89, 90] for the transition-regime cases. The DSMC method is considered to be accurate in the transition regime, however due to its particle nature is very computationally intensive. In the DSMC study a variable hard sphere collision model is used, this leads to some discrepancy with the 14-moment results since they employed the BGK collision model. The Knudsen number in the DSMC study is adjusted by varying the reference pressure, however for the 14-moment closure, regularized Gaussian, and NSF solutions the geometry of the cavity was adjusted instead, leading to a Knudsen

![Figure 6.19: Schematic of the lid-driven cavity geometry.](image)
number defined as: \( \text{Kn} = \Lambda / L \). To remain consistent with the DSMC study the mean free path, \( \Lambda \), is now found as

\[
\Lambda = \frac{\mu}{p} \sqrt{\frac{\pi R T}{2}}.
\]

(6.22)

6.5.1 Results for \( \text{Kn}=0.001 \)

The resulting Mach number and temperature profiles for this case can be seen in Figures 6.20 and 6.21. The solutions found using the regularized Gaussian closure, 14-moment closure, and NSF equations are compared. The Mach number contours and velocity streamlines show good agreement for all three methods, as expected. The temperature profiles are also in fair agreement for each solution technique, showing an overall uniform temperature distribution as expected in this regime. However, the regularized Gaussian and 14-moment closures result in slightly higher temperatures overall. This is again good validation of the 14-moment closure’s ability to reproduce the NSF solution in the continuum regime.
Figure 6.20: Mach number contours for lid-driven cavity flow at $Kn = 0.001$ found using the (a) regularized Gaussian closure, (b) 14-moment closure, and (c) NSF equations.
Figure 6.21: Temperature contours for lid-driven cavity flow at Kn = 0.001 found using the (a) regularized Gaussian closure, (b) 14-moment closure, and (c) NSF equations.
6.5.2 Results for Kn=0.05

Results at Kn=0.05 are now considered. Plots comparing Mach number, shear stress, and temperature contours can be found in Figures 6.22, 6.23, and 6.24, respectively. Since heat flux is no longer negligible at this Knudsen number, the heat-flux streamlines are now overlaid on the temperature contours. The Mach number contours all display velocity slip at the lid as anticipated, however the slip seems to be slightly overpredicted in the regularized Gaussian solution. Furthermore, the regularized Gaussian overpredicts the slip at the top of the left and right walls when compared to the DSMC solution. It is clear that the 14-moment solution is in better agreement with the DSMC result’s Mach number contours. The shear stress contours are now also presented in Figure 6.23. All three solution techniques show fair agreement, but the 14-moment solution is closer to the DSMC result than the regularized Gaussian. Both the 14-moment closure and DSMC method predict a high temperature region in the top right corner, and a low temperature region in the top left corner, however the absolute temperature values are much larger for the 14-moment results. This low temperature region is a consequence of gas cooling by expansion and the high temperature region results from viscous dissipation [89,90]. The regularized Gaussian closure predicts both high temperature and low temperature areas in each corner, which is inconsistent with the DSMC results. The heat-flux streamlines show discrepancies between all three methods, especially in the lower half of the cavity. However, in the top half of the cavity, where heat transfer is most significant, the heat-flux lines for each method show a similar left to right trend. Interestingly, both the 14-moment closure technique and DSMC method predict a counter-gradient heat flux, whereas the regularized Gaussian closure does not. A similar result was observed for the circular cylinder case (see Figure 6.15).
Figure 6.22: Mach number contours for lid-driven cavity flow at Kn=0.05 found using the (a) regularized Gaussian closure, (b) 14-moment closure, and (c) DSMC technique [89,90].
Figure 6.23: Shear stress contours for lid-driven cavity flow at $Kn=0.05$ found using the (a) regularized Gaussian closure, (b) 14-moment closure, and (c) DSMC technique [89, 90].
Figure 6.24: Temperature contours and heat-flux streamlines for lid-driven cavity flow at $Kn=0.05$ found using the (a) regularized Gaussian closure, (b) 14-moment closure, and (c) DSMC technique [89, 90].
6.5.3 Results for $Kn=0.1$

Finally, a transition-regime case with $Kn=0.1$ is considered (Figures 6.25, 6.26, and 6.27). The conclusions drawn from the $Kn=0.05$ case continue to apply. The regularized Gaussian closure continues to slightly overpredict slip in the top corners, as seen in Figure 6.25. The 14-moment closure’s prediction of shear stress continues to be in closer agreement with the DSMC results than the regularized Gaussian, however its prediction is now considerably worse than at $Kn=0.05$. At this higher Knudsen number the high and low temperature regions have increased in size in the 14-moment and DSMC solutions. The 14-moment closure continues to overpredict the absolute temperatures in the top corners, and the counter-gradient heat flux is present in the both 14-moment and DSMC results, but completely absent from the regularized Gaussian results.
Figure 6.25: Mach number contours for lid-driven cavity flow at $Kn=0.1$ found using the (a) regularized Gaussian closure, (b) 14-moment closure, and (c) DSMC technique \cite{89, 90}. 
Figure 6.26: Shear stress contours for lid-driven cavity flow at $Kn=0.1$ found using the (a) regularized Gaussian closure, (b) 14-moment closure, and (c) DSMC technique [89, 90].
Figure 6.27: Temperature contours and heat-flux streamlines for lid-driven cavity flow at Kn=0.1 found using the (a) regularized Gaussian closure, (b) 14-moment closure, and (c) DSMC technique [89, 90].
Chapter 7

Conclusions and Future Work

7.1 Conclusion

A novel, 14-moment, maximum-entropy-based, interpolative closure for a monatomic gas has been investigated and employed to solve a variety of canonical two-dimensional flow problems. Dispersion analyses of the 5- and 14-moment interpolative closure systems have been presented, which verify the systems’ stability as well as demonstrate their potential to be applied to high Mach number flows. Smooth solutions at high Mach numbers are possible due to their high frozen wave speeds near the Junk region. This analysis also motivated the exploration of an implicit solver, due to its prediction of large wave speeds for near-equilibrium flows.

This thesis describes the first two-dimensional solutions to this new 14-moment interpolative closure. Specific cases studied were planar Couette flow, conduction between heated flat plates, subsonic flow past a circular cylinder, and lid-driven cavity flow. In order to consider these cases, valid boundary conditions, which reproduce non-equilibrium phenomena, were developed based on the solid-wall half-Maxwellian boundary condition. The Couette-flow results for normalized velocity and shear stress were found to be in excellent agreement with both the well established Gaussian closure and the analytical solution of Lees [83]. The case of conduction between two heated plates was also found to be in good agreement with the expected result found using the NSF equations with temperature jump boundary conditions. The results for subsonic flow around a circular cylinder showed expected behaviours such as velocity slip and an increase in boundary-layer thickness with increasing Knudsen number. The solutions found in the continuum regime were in good agreement with the well established regularized Gaussian closure,
and the results found in the transition regime displayed temperature polarization and counter-gradient heat flux. These results also showed an improved prediction of drag for high Knudsen number flows, relative to the 10-moment Gaussian closure.

The lid-driven cavity flow results were compared to those of the NSF equations, regularized Gaussian closure, and DSMC technique. The 14-moment interpolative closure was found to be in better agreement with the DSMC technique in the transition regime than the regularized Gaussian closure. It was successful in predicting the presence of regions of expansion cooling and viscous heating, as well as a counter-gradient heat flux, which is also seen in the DSMC results. In conclusion, the 14-moment interpolative closure showed improvements over the 10-moment Gaussian closure, as would be expected since more moments are considered. Furthermore, it was able to predict a counter-gradient heat flux, which was not possible using the regularized Gaussian closure.

Finally, compared to the semi-implicit approach, the use of an implicit NKS solver was found to significantly decrease the computational cost of obtaining solutions to the 14-moment interpolative closure. The savings ranged between 2 and 15 times in terms of CPU time, depending on the problem. Additionally, based on the preliminary results found using a simplified analytic Jacobian, which were described in Section 5.3.1, it is expected that an additional savings of 2-3 times could be achieved by implementing a general non-finite-difference procedure for finding the Jacobians. This would lead to a factor of savings on the order of 30 times compared to the semi-implicit approach. The NKS solver was also found to be more robust; it was able to obtain converged solutions for cases where the semi-implicit method stalled. The effectiveness of the solver was consistent with the conclusions about the maximum wave speeds and stiffness of the system predicted by the dispersion and wave speed analyses.

### 7.2 Future Work

Although the study presented has been successful in many respects, there is still further development potential for this novel 14-moment interpolative closure. The equation system and numerical solver should be extended to be suitable for three-dimensional flows of both monatomic and polyatomic gases. Furthermore, improved collision models, such as the ellipsoidal-statistical or Shakhov model [27,28], which are discussed in Section 2.4, should be implemented. It is clear that the chosen boundary condition technique has some issues, such as those seen in the heat transfer between flat plates cases. This
boundary condition should be reconsidered and possible modifications, which mitigate these issues, should be explored. The 14-moment interpolative closure’s application to flows which contain external acceleration fields, such as the Lorentz force in the case of plasmas, could also be explored.

The computational cost of the NKS method could be further reduced by implementing a more accurate method of calculating the required Jacobians, such as algebraic formulations. Based on findings for a simplified analytic flux-Jacobian in the continuum regime, it is expected that a general analytic form of the flux-Jacobian will greatly improve the computational time required to find solutions. However, due to the complexity of the system a feasible form of this Jacobian will not be trivial, and clever algebraic and physical simplifications or assumptions may be necessary. Alternatively, automatic differentiation could be investigated.
Bibliography


