EVALUATION OF MAXIMUM ENTROPY MOMENT CLOSURES FOR PREDICTING RADIATIVE HEAT TRANSFER PHENOMENA

by

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A thesis submitted in conformity with the requirements for the degree of Master of Applied Science
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Abstract

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2017

This study considers an evaluation of moment closures based on the principle of maximization of entropy ($M_N$, where $N$ refers to the order of the closure) for providing approximate solutions to the radiative heat transfer equation (RTE). Several representative test cases in both one- and two-dimensions are considered whereby the predictions of the $M_N$ models are compared to those of the discrete ordinates method (DOM) as well as the more commonly used spherical harmonics solutions ($P_N$, where $N$ refers to the order of the approximation) in terms of accuracy. More specifically, the present analysis is concerned with the lower-order approximations of the hierarchy of the $M_N$ closures, namely $M_1$ and $M_2$ and, for comparison purposes, the $P_1$ and $P_3$ spherical-harmonic closures are also considered. The potential of the $M_1$ and $M_2$ closures is explored and discussed for a range of problems involving radiative heat transfer in gray media.
Acknowledgements

I would like to express my greatest gratitude to the people who have helped and supported me throughout my thesis and made my two years of study at the University of Toronto’s Institute for Aerospace Studies very memorable. I am foremost grateful to my supervisor, Professor C.P.T. Groth, for his continuous guidance and insight into the field of CFD, which has helped to shape my future academic pursuits in the same field.

I wish to thank my parents for their constant support and care over all of these years. Their unwavering encouragement and belief in the choices I make are what allow me to be here today. And last, but not least, I want to thank all of my friends here at UTIAS, who have made my journey through my Masters very enjoyable and memorable. I will never forget all of the experiences we have shared together.

Computational resources for performing all of the calculations reported herein were 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. Part of this thesis funding was provided by the Fonds de Recherche du Quebec - Nature et Technologie (FRQNT).

Toronto, 2017

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Chapter 1

Introduction

1.1 Background And Motivation

Fully understanding soot formation in flames is of crucial importance in the development of efficient and environmentally friendly combustion devices for transportation systems as well as industrial energy production [1]. Such particulate matter is generally formed from the incomplete combustion of hydrocarbons and is known for its negative effects on human health as well as its contribution to global warming and air pollution [2]. Despite the tremendous efforts directed towards proper characterization of soot formation, there is still a large number of unanswered questions, which require investigation. Numerical combustion modeling is an attractive way to achieve this goal and has received a widespread attention in the past few decades. Furthermore, the development of improved and more accurate numerical combustion models should allow the future design of more efficient and greener combustion systems.

Combustion of hydrocarbons can produce highly radiating flames, especially at high pressures, due to the presence of carbon dioxide (CO$_2$) and water (H$_2$O) molecules [3]. The radiant losses become even more significant in the presence of soot. Such heat losses can greatly affect the temperature distribution in combustion chambers, which heavily affects the prediction of pollutant species. In fact, the chemical kinetics governing the formation of combustion-generated particles are highly dependent on temperature. It therefore follows that detailed radiation modeling is essential in numerical simulations of combustion [3].

Radiative transfer describes the physical process in which molecular energy, in the form
of electromagnetic waves, is transferred to a background medium. The transfer of such energy is described by three processes, namely absorption, emission and scattering, which are mathematically contained and described by the radiative transfer equation (RTE) \[3\]. The RTE is a complex integro-differential equation which describes the distribution of the radiative intensity as a function of time, space and velocity space. Due to its high dimensionality, exact analytical solutions only exist for some idealized cases. Stochastic models such as the Monte Carlo method \[4\] have been reported to yield realistic solutions of the RTE. The zonal method \[5\] has also been used widely for engineering radiative heat transfer calculations in multidimensional enclosures. Its implementation is however limited to non-scattering media as it cannot be readily adapted for a scattering medium. Both of those methods are limited in the sense that they are not compatible with the usual numerical methods used for solving the appropriate variants of the partial differential equations (PDEs) governing the flow and temperature fields arising from the Navier-Stokes equations for a reactive mixture.

When the underlying flow field must also be considered, it is preferable to calculate radiative quantities by making use of approximate radiation models that are compatible with conventional schemes reserved for coupled systems of PDEs. Such techniques include the spherical harmonics (P\(_N\)) approximation \[6–9\], the discrete ordinates method (DOM) \[10\], the finite volume method (FVM) \[11,12\], and moment closures. The DOM is one of the most widely used approximate numerical techniques to solve the RTE. It provides a good balance between accuracy and computational costs for problems with relatively simple geometry and simplified physics (no scattering), for which the space marching solution techniques can be extremely efficient. However, when scattering effects are important, space marching methods lose their effectiveness since the intensities in different directions become tightly coupled. Additionally, arriving at efficient and effective space marching algorithms for complex, three dimensional geometries and for parallel implementation on multi-processors distributed memory computer architectures can be problematic.

The method of moments provides a hierarchy of models allowing a possible reduction in the numerical costs associated with solving the RTE \[13\]. This approach, initially introduced by Grad \[14\] in the context of rarefied gases, replaces the representation of the angular dependence of the radiative distribution by a finite set of angular integrals or moments of the latter. However, closure is required for moment models since there are more unknowns than equations in the resulting moment equations. The spherical harmonics approximation (P\(_N\), where \(N\) refers to the order of the approximation) has been
extensively used to model radiation heat transfer in combustion systems. This approach consists of approximating the distribution of the radiative intensity by a Fourier series expansion, which is generally truncated to a finite order $N$ for the sake of simplifying the study of radiative transfer problems. Such an approximation does not always guarantee the positivity of the solution, and can therefore lead to unphysical results. Moreover, low order approximations of this hierarchy are generally only accurate in the optically thick limit, where the radiative intensity is close to the radiative equilibrium.

More recently, moment closure techniques based on the principle of maximization of entropy [15–17] have gained lots of attention in the radiative transfer community. The approximation of the radiative distribution by an entropy-maximizing distribution yields a system of moment equations which has many desirable properties and always guarantees the positivity of the intensity distribution. This hierarchy of models also generally yields accurate predictions for both equilibrium and non-equilibrium radiative transfer, as well as the regime that lies between those two limits.

1.2 Objectives

The focus of the present study is to evaluate moment closures based on the principle of maximization of entropy [15–17] (so called $M_N$ models where here $N$ refers to the order of the closure) by comparing their solutions to those obtained using the DOM. More specifically, the accuracy of the first- and second-order maximum entropy closures ($M_1$ and $M_2$, respectively) will be compared to those of DOM for a range of radiative transfer problems in both one- and two-dimensions. The predictions of the first- and third-order spherical harmonics approximations ($P_1$ and $P_3$, respectively) are also examined here and used for comparison. The general theoretic framework for the $M_N$ models was laid out by Dubroca and Feugeas [17]; however, the computational results were limited to the $M_1$ model. In fact, for higher order $M_N$ models ($N \geq 2$), there is exist no analytical expression to the closure for any choice of entropy, and the optimization problem is especially hard to solve for highly anisotropic distribution. The $M_1$ model was then subsequently examined by Fan et al. [18,19], Berthon et al. [20], among others. Despite some limitations, especially in cases where radiation travels in more than one important direction at a time, this model has shown promising results, which have encouraged the examination of higher order maximum entropy moment closures for the sake of further improvements. In this respect, the $M_2$ model in one dimension has been previously analyzed by Monreal and Frank [21] and Hauck [22]. While this previous research demonstrated the considerable
promise of these closures, there has been no significant further development of this model in higher space dimensions until recently, with the approximate $M_2$ closure developed by Pichard et al. [13,23]. This closure is however based on the Boltzmann entropy, which is particularly used in applications such as radiation therapy. In this study, an extension of the newly developed approximate $M_2$ model is proposed for the case of the Bose-Einstein entropy, which is of interest for radiation modeling in combustion systems.

1.3 Scope

The organization of the remainder of this thesis is as follows. In Chapter 2 and 3, various approximate numerical methods for solving the RTE, including both direction-discretization methods (DOM and FVM) and spherical harmonics approximations ($P_N$), are introduced and mathematical derivations of $M_1$ and $M_2$ models are presented. Chapter 4 will then describe the finite-volume numerical solution procedure used for solving the discrete governing equations. Finally, a discussion of the numerical results for several one- and two-dimensional test cases will be presented in Chapter 5, and suggestions for future research will conclude the thesis.
Chapter 2

Brief Review of Radiation Transport Theory

In this chapter, radiation transport theory is briefly reviewed along with two approximate radiation models for solving the RTE, based on direction discretization.

2.1 Radiation Transport Theory

The interaction of thermal radiation with a “radiatively participating medium” is described by three processes: absorption (absorption or gain of radiative energy by the medium), emission (emission or loss of radiative energy by the medium) and scattering (deviation of radiative particles in a direction that is different from the initial direction of travel) [3], as depicted in Fig. 2.1. More specifically, the radiative particles traveling in a given directions $\vec{s}$ will be attenuated by absorption as well as scattering in another direction $\vec{s}'$ (out-scattering). While traveling in the medium, the incident radiant energy will also be augmented by emission from the medium and scattering from other directions $\vec{s}'$ into the direction of travel $\vec{s}$ (in-scattering). For a Cartesian coordinate system, the direction of travel of radiant energy is represented by the vector $\vec{s}$, also called the direction cosine vector, which can be expressed in terms of the polar and azimuthal angles, $\theta$ and $\psi$, as

$$\vec{s} = (\sin \theta \cos \psi)\vec{i} + (\sin \theta \sin \psi)\vec{j} + (\cos \theta)\vec{k} = \Omega_1\vec{i} + \Omega_2\vec{j} + \Omega_3\vec{k}. \quad (2.1)$$
Figure 2.1: Processes resulting from the interaction of incident radiation (arrows) with matter (circles).

In the above expression, \( \vec{i}, \vec{j} \) and \( \vec{k} \) are unit normal vectors in the direction of the \( x, y \) and \( z \) axes respectively, and \( \Omega_1 = \sin \theta \cos \psi, \Omega_2 = \sin \theta \sin \psi \) and \( \Omega_3 = \cos \theta \) are the corresponding direction cosines.

The equation governing the transport radiative energy, commonly called the radiative transfer equation, determines the radiative intensity distribution as a function of time \( t \), location \( \vec{r} \), direction \( \vec{s} \), and spectral variable \( \nu \), i.e., \( I_{\nu} = I_{\nu}(t, \vec{r}, \Omega, \nu) \). Assuming a homogeneous, non-polarizing medium at rest (as compared to the speed of light) and at local thermodynamic equilibrium (LTE), with constant index of refraction (electromagnetic waves travel along straight lines), the RTE can be formulated as follows [3]:

\[
\frac{1}{c} \frac{\partial I_{\nu}}{\partial t} + \vec{s} \cdot \nabla I_{\nu} = \kappa_{\nu} I_{b\nu} - (\kappa_{\nu} + \sigma_{s\nu}) I_{\nu} + \frac{\sigma_{s\nu}}{4\pi} \int 4\pi I_{\nu}(\vec{s}^{'}) \Phi_{\nu}(\vec{s}^{'}, \vec{s}) d\Omega^{'},
\]  

(2.2)

where \( c \) is the speed of light in a vacuum, \( \vec{s} \) represents the direction in which radiation travels, \( I_{\nu} \) is the specific intensity at frequency \( \nu \), \( I_{b\nu} \) is the blackbody specific intensity, \( \Omega \) is the solid angle, \( \kappa_{\nu} \) and \( \sigma_{s\nu} \) are the spectral absorption and scattering coefficients, respectively, and \( \Phi_{\nu}(\vec{s}^{'}, \vec{s}) \) is the scattering phase function. The latter describes the probability that a ray traveling in direction \( \vec{s}' \) will be scattered into direction \( \vec{s} \). All the radiative quantities in the RTE depend on location in space, time and frequency while the intensity and the phase function also vary with direction.

Equation (2.2) is a first-order integro-differential equation with seven independent vari-
ables: frequency, $\nu$, three space coordinates, $x, y$ and $z$, two angular coordinates describing the direction of travel of radiant energy, $\theta$ and $\psi$, and time, $t$. A treatment of both space and directional variables as well as frequency dependence is therefore required to solve this equation for the distribution of radiative intensity. However, in this work, the spectral dependence of the radiative quantities is neglected. Adopting this so-called gray-gas approximation \[3\], the RTE can be rewritten in the following form

$$\frac{1}{c} \frac{\partial I}{\partial t} + \vec{s} \cdot \vec{\nabla} I = \kappa I - (\kappa + \sigma_s) I + \frac{\sigma_s}{4\pi} \int_{4\pi} I(\vec{s}') \Phi(\vec{s}', \vec{s}) d\Omega',$$  \tag{2.3}

where $I = \int_0^\infty I_\nu d\nu$ now represents the total radiative intensity.

### 2.2 Treatment for the Angular Dependence of the RTE

#### 2.2.1 Discrete Ordinates Methods

The discrete ordinates method is used to transform the equation of radiative transfer into a set of PDEs with only spatial and temporal dependence. This angular discretization technique makes use of the assumption that the radiation is transported only along a finite set of discrete directions, instead of the effectively infinite number of directions allowed in Eq. (2.3) by a continuous representation of the solid angle. In other words, the solid angle is divided into a finite number, $M$, of discrete directions (or ordinates) $\vec{s}_m$. In this way, the RTE is transformed into a system of $M$ coupled equations given by

$$\frac{1}{c} \frac{\partial I_m}{\partial t} + \vec{s}_m \cdot \vec{\nabla} I_m = \kappa I_b - (\kappa + \sigma_s) I_m + \frac{\sigma_s}{4\pi} \sum_{n=1}^M w_n I_n \Phi(\vec{s}_n, \vec{s}_m),$$  \tag{2.4}

where the subscript $m$ denotes the discrete ordinate direction, $I_m$ is the intensity in the $m^{th}$ direction and $w_m$ is the quadrature weight associated with the direction $\vec{s}_m$.

The DOM has been used extensively to solve the RTE in laminar flames test cases \[1, 24\] due its good balance between accuracy and computational requirements. It can be applied to non-isothermal, non-homogeneous, anisotropically scattering, and non-gray media in complex geometries. However, this direct discretization technique for the RTE is associated with two major limitations \[25\]: false scattering and ray effects. The former is due to the spatial discretization of the RTE whereas the latter is related to the
discretization of the angular distribution of the radiative intensity. The error associated with false scattering can be reduced by refining the spatial grid or by making use of more accurate differencing schemes [26, 27]. For the sake of reducing ray effects, several quadratures have been proposed [28, 29], and the modified discrete ordinates method (MDOM) was also proposed [30, 31].

### 2.2.2 Finite Volume Method

The FVM equations for describing radiation transport are obtained by discretizing the solid angle into \( M \) control-angle elements and integrating the RTE over each element to give [11]

\[
\frac{1}{c} \frac{\partial I_m}{\partial t} + \vec{s} \cdot \vec{\nabla} I_m = -(\kappa + \sigma_s)I_m + \kappa I_b + \frac{\sigma_s}{4\pi} \sum_{n=1}^{M} I_n \Phi_{mn} \Delta \Omega_n, \tag{2.5}
\]

where the phase function, \( \Phi_{mn} \), is defined as

\[
\Phi_{mn} = \frac{1}{\Delta \Omega_m \Delta \Omega_n} \int_{\Delta \Omega_m} \int_{\Delta \Omega_n} \Phi(\vec{s}', \vec{s}) d\Omega' d\Omega. \tag{2.6}
\]

Equation (2.5) is obtained by assuming piecewise-constant intensity over each control angle. This approximation limits the overall order of the solution in both spatial and temporal discretization methods.
3.1 Macroscopic Moments and Closure Problem

As mentioned previously, the radiative transfer equation, Eq. (2.3), is a statistically-based microscopic description requiring the solution of a single scalar integro-differential equation, which can be computationally very expensive to solve by numerical methods in the general case. Furthermore, considering the applications of interest, where radiation must be coupled with phenomena such as the fluid flow, chemical kinetics, and particulate transport, one is generally more interested in macroscopic radiative quantities such as the mean energy or mean flux that directly affect the other macroscopic multi-physics processes, rather than the photon distribution, $I$. Such macroscopic quantities are merely moments of the intensity distribution. The $n^{th}$ order moment of the radiative intensity is obtained by pre-multiplying the latter by the $n^{th}$ order tensor of the vector representing the direction of travel, i.e., $\vec{s}^n = \vec{s} \otimes \vec{s} \otimes \ldots \otimes \vec{s}$, and performing component-wise angular integration over the solid angle $4\pi$, resulting in the following expression

$$I^{(n)} = \langle \vec{s}^n I \rangle,$$

$$= \int_{4\pi} \vec{s}^n I \, d\Omega,$$

$$= \int_0^{2\pi} \int_0^{\pi} \vec{s}^n I \sin \theta d\theta d\psi.$$  \hspace{1cm} (3.1)

The corresponding normalized $n^{th}$ order moment is defined as

$$N^n = \frac{I^{(n)}}{I^{(0)}}.$$  \hspace{1cm} (3.2)
The first two angular moments of the radiative intensity distribution, the zeroth- and first-order moments, correspond to the radiative energy density and the radiative flux vector, which are respectively defined as follows:

\[ E = \langle I \rangle = \int_0^{2\pi} \int_0^\pi I \sin \theta d\theta d\psi, \quad (3.3) \]

\[ F_i = \langle s_i I \rangle = \int_0^{2\pi} \int_0^\pi s_i I \sin \theta d\theta d\psi. \quad (3.4) \]

Equations describing the transport of the macroscopic quantities up to a given order \( N \) can be derived by multiplying the RTE by each element of \( \vec{s} \), \( n \in 0, 1, 2, ..., N \), and performing component-wise integration over all directions spanning the whole range of solid angles \( 4\pi \). This yields a system of moment equations of order \( N \), which reads as

\[
\frac{1}{c} \frac{\partial \langle \vec{m}(\vec{s}) I \rangle}{\partial t} + \vec{\nabla}.\langle \vec{s} \vec{m}(\vec{s}) I \rangle = \kappa \langle \vec{m}(\vec{s}) I_b \rangle - (\kappa + \sigma) \langle \vec{m}(\vec{s}) I \rangle \\
+ \frac{\sigma_s}{4\pi} \left\langle \vec{m}(\vec{s}) \int_{4\pi} I(\vec{s}') \Phi(\vec{s}', \vec{s}) d\Omega' \right\rangle, \quad (3.5)
\]

where \( \vec{m}(\vec{s}) \) is the basis of the space of polynomials of up to order \( N \) over the unit sphere, which has the following form

\[
\vec{m}(\vec{s}) = (1, \Omega_1, \Omega_2, \Omega_3, \Omega_1^2, \Omega_2^2, \Omega_3^2, \Omega_1\Omega_2, \Omega_1\Omega_3, \Omega_2\Omega_3, ...), \quad (3.6)
\]

and \( \vec{E}(\vec{s}) \) is a vector containing the moments of the intensity distribution associated with \( m(\vec{s}) \), which reads as follows

\[
\vec{E}(\vec{s}) = \langle \vec{m}(\vec{s}) I \rangle = (I^{(0)}, I_1^{(1)}, I_2^{(1)}, I_3^{(1)}, I_{11}^{(2)}, I_{22}^{(2)}, I_{33}^{(2)}, I_{12}^{(2)}, I_{13}^{(2)}, I_{23}^{(2)}, ...). \quad (3.7)
\]

The vector \( \vec{m}(\vec{s}) \) defined by Eq. (3.6) above contains the various linearly independent entries of all \( \vec{s} \), for \( i = 0 \ldots N \). The tensors \( \vec{s} \), \( i \geq 2 \) are indeed symmetric. As such, taking the entries of \( \vec{E}(\vec{s}) \) as a representative set of dependent variables would allow a simplification of the analysis by avoiding repeated direct solution of the RTE in high-dimensional phase space.

In practice, an infinite set of moments \( (N \to \infty) \) is required in order to reproduce the exact form of the arbitrary solution for the distribution of the radiative intensity. However, the approximation of the intensity distribution by an infinite number of moments would
not be feasible for implementation in a computer code. Moreover, the resulting coupled system of moment equations given by Eq. (3.5) cannot readily be solved as it contains more unknowns than equations. In particular, the $N^{th}$ order moment system always involves the divergence of the $(N+1)^{th}$ order moment of the radiative distribution. Solving a system of moment equations of this type therefore presents two challenges: the identification of the appropriate moments of interests and the choice of an appropriate closure in order to obtain a closed and solvable system. The closing expression is generally obtained by expressing the highest order moments of the system of equations Eq. (3.5) in terms of the lower order moments and often involves an approximation for the form the distribution, which is obviously not known a priori. The choice of the closure is crucial as it directly affects the mathematical properties of the resulting closed moment system and their solutions such as moment realizability [32], strict hyperbolicity [17], and well posedness [17], as well as consistency with the physics of the problem under consideration such as positivity of the distribution, flux limitation, and accuracy of the approximation. For combustion modeling, where radiation heat transfer must be coupled to the flow solver via the total energy balance equation, only the radiative energy density (zeroth moment of the radiative intensity distribution) and the radiative heat flux (first-order moment of the radiative intensity distribution) are needed. Those two quantities can be readily obtained by solving the first-order moment system ($N = 1$) after providing suitable closure conditions. The closing relations for the first-order moment system are obtained by reconstructing the form of the approximate distribution using the zeroth and first-order moments, the latter moment corresponding to the lowest angular information available. Considering higher order moments would provide greater resolution of the angular distribution and would result in more accurate solutions.

Moment closures based on spherical harmonics expansion of the intensity distribution have been widely used to solve the RTE, due to their simplicity and relatively straightforward implementation [3], and have been first proposed by Jeans [33] in his work on radiative transfer in stars. However, spherical harmonics representation of the radiative intensity distribution do not guarantee positivity of the latter. More recently, closures based on the principle of maximization of entropy [15] have gained particular attention in the field of radiative heat transfer modeling. The entropy maximizing distribution has the desirable feature that it corresponds to the most likely form of the radiative intensity distribution, as described by Jaynes [34]. Furthermore, maximum entropy closures are attractive since they possess many desirable properties [35]: each member of the hierarchy is a flux-limited, hyperbolic system which dissipates mathematical entropy. This therefore motivates the study and comparison of low order moment closures based on
the principle of maximization of entropy to the most commonly used spherical harmonics approximations.

3.2 Spherical Harmonics $P_N$ Approximations

At a given location in space, $\vec{r}$, the radiative intensity distribution can be regarded as a scalar function on the surface of a unit sphere, surrounding the point $\vec{r}$. Any function of such type can be expanded in terms of a set of orthogonal basis functions also defined on the unit sphere which themselves satisfy Laplace’s equation. Such functions are usually defined using a spherical coordinate system and are commonly called spherical harmonics functions. The spherical harmonic expansion technique is one of the oldest and most well known approximate method used in the radiation modeling community and can also be viewed as a moment closure technique. In the spherical harmonics approximation as first proposed by Jeans [33], the radiative intensity is expressed in terms of a series of spherical harmonic functions given by [3]

$$I(\vec{r}, \theta, \psi) = \sum_{n=1}^{N} \sum_{m=-n}^{n} I_n^m(\vec{r}) Y_n^m(\theta, \psi),$$

where $I_n^m(\vec{r})$ are location-dependent coefficients and are determined such that the elements of $E(\hat{s})$ correspond to the moments of the distribution Eq. (3.8). Each of these coefficients is associated with a given spherical harmonic, $Y_n^m(\theta, \psi)$, which is related to the corresponding Legendre polynomial, $P_n^m(\cos \theta)$, as follows

$$Y_n^m(\theta, \psi) = \begin{cases} 
\cos(m\psi)P_n^m(\cos \theta), & \text{for } m \geq 0, \\
\sin(m\psi)P_n^m(\cos \theta), & \text{for } m < 0.
\end{cases}$$

(3.9)

This method has the advantage of resulting in relatively simple closing relations for the moment equations governing radiative transfer. The closed system of PDEs is obtained by integrating the RTE over all directions after premultiplying it by the appropriate spherical harmonic function, $Y_n^m(\theta, \psi)$, i.e.,

$$\int_0^{2\pi} \int_0^\pi [\text{Eq. (2.3)}] Y_n^m(\theta, \psi) \sin \theta \, d\theta \, d\phi,$$

(3.10)

for $n = 0, 1, ..., N$ and $m = -n, -n + 1, ..., n$.

Experience has shown that low-order $P_N$ approximations are usually only accurate in
media with near-isotropic radiative intensity. More anisotropy can be captured using higher-order approximations, however, for higher-order $P_N$ closures, accuracy improves only slowly while mathematical complexity increases rapidly. While even order spherical harmonic closures are generally not considered as they are less accurate than the lower-order odd approximations of the same hierarchy, odd-order closures are commonly considered. The $P_1$ and $P_3$ odd-order spherical harmonic moment closures are commonly used approximations and are examined as part of this thesis. Figure 3.1 shows a visual representation of the spherical harmonic basis functions, $Y_{nm}(\theta, \psi)$, of order up to 3.

![Figure 3.1: Visual representation of the first few spherical harmonics.](image)

### 3.3 Maximum-Entropy $M_N$ Moment Closures

Maximum-entropy moment closures have been considered by number of researchers [36, 37] in the field of gas kinetic theory because of their ability to predict with reasonable accuracy non-equilibrium behaviour of gaseous flows using a relatively small number of moments. Radiative transfer displays some analogies with non-equilibrium gaseous
flows, since it involves a transition between two extremes: the diffusion (equilibrium) limit where the distribution of radiative intensity is near-isotropic and the free-streaming limit in which the intensity distribution is highly anisotropic and where non-equilibrium transport effects are significant. In this respect, inspired by previous studies by Levermore [38] for gas kinetic theory, Dubroca and Feugeas [17] extended the application of this form of closure method to the solution of the RTE. The resulting hierarchy of moments models (here referred to as $M_N$ models) is attractive since it ensures the nonnegativity of the distribution of the radiative intensity. Furthermore, the $M_N$ moment closures have many desirable mathematical properties [39]: the flux is limited (any signal is propagated at a velocity below the speed of light), the system is hyperbolic (moments are physically realizable) and locally dissipates entropy. For problems related to combustion, the radiative entropy of interest has the following form

$$H_R(I_\nu) = \langle h_R \rangle = \int_{4\pi} h_R(I_\nu) d\Omega,$$

(3.11)

where the radiative entropy density, which corresponds to the entropy for Bose-Einstein statistics in this case, is given by

$$h_R(I_\nu) = \frac{2k\nu^2}{c^3} [(n+1)\ln(n+1) - n\ln(n)] , \ n = \left( \frac{c^2}{2h\nu^3} \right) I_\nu ,$$

(3.12)

and where $n$ is the occupation number, $h$ and $k$ are the Planck and Boltzmann constants, respectively. The maximum entropy closure involves the determination of the radiative intensity distribution that maximizes the radiative entropy Eq. (3.11) subject to the constraints that the finite set of moments, $E$, are exactly reproduced by this approximate form of the distribution. Such an optimization problem can be formulated as

$$I_\nu = \arg \max_{I_\nu} H_R(I_\nu)$$

s.t. \ $\langle m(\vec{s})I_\nu \rangle = E$

(3.13)

The Lagrangian of this optimization problem is

$$\mathcal{L}(I_\nu, \alpha) = H_R(I_\nu) - \alpha^T (\langle m(\vec{s})I_\nu \rangle - E)$$

(3.14)

where $\alpha$ is the vector of Lagrange multipliers associated with the moment constraints. The entropy maximizing distribution, which satisfies $\partial \mathcal{L}(I_\nu, \lambda)/\partial I_\nu = 0$, then takes the
In the case of the gray gas model for radiation transport, the distribution function Eq. (3.15) can be integrated over the full spectrum of frequencies \((\nu \in [0, \infty])\), yielding

\[
I(\alpha, m) = \frac{\sigma_{stef}}{\pi} \left[ \alpha^T m(\vec{s}) \right]^{-4}, \quad (3.16)
\]

where \(\sigma_{stef} = \frac{2\pi^5 k^4}{15 c^2 h^3}\) is the Stephan Boltzmann constant. In Eq. (3.16), the radiative intensity distribution is not given explicitly but is rather expressed in terms of the Lagrange multipliers, \(\alpha\), which have to be determined from the set of nonlinear coupled algebraic equations \(\langle m(\vec{s})I \rangle = E\). A closed form expression for the closure only exists for the first-order approximation of this hierarchy, i.e., the M\(_1\) model; beyond the M\(_1\) model, exact analytical expressions for the closure are not possible and one must rely only on numerical solution of the entropy maximization problem. In such cases, the Lagrange multipliers are determined by solving the dual problem

\[
\max_{\alpha} \{ \mathcal{L}^*(\alpha) \}, \quad (3.17)
\]

where \(\mathcal{L}^*(\alpha)\) is the Legendre transform of \(\mathcal{L}(I_\nu, \alpha)\) and has the form

\[
\mathcal{L}^*(\alpha) = -\frac{\sigma_{stef}}{3\pi} \left[ \alpha^T m(\vec{s}) \right]^{-3} - \alpha^T E. \quad (3.18)
\]

The corresponding first-order optimality conditions for Eq. (3.17) satisfy the consistency relation on the moments of the distribution

\[
\langle m(\vec{s})I \rangle = E. \quad (3.19)
\]

### 3.4 First-Order Moment Closure Techniques

As discussed earlier in this chapter, the radiative energy density and the radiative heat flux are the only radiative quantities that enter in the equation of conservation of energy. The transport equations for those two quantities can be obtained by taking angular moment of the RTE with respect to the vector of Legendre polynomial
\[ \mathbf{m}(\mathbf{s}) = (1, \Omega_1, \Omega_2, \Omega_3), \] yielding the following system of moment equations

\[ \begin{align*}
\frac{1}{c} \frac{\partial I^{(0)}}{\partial t} + \vec{\nabla} I^{(1)} & = \kappa (4\sigma T^4 - I^{(0)}) \\
\frac{1}{c} \frac{\partial I^{(1)}}{\partial t} + \vec{\nabla} I^{(2)} & = -(\kappa + \sigma_s) I^{(1)}
\end{align*} \] \tag{3.20}

In Eq. (3.20), which has been obtained by assuming isotropic scattering \((\Phi(\mathbf{s}', \mathbf{s}) = 1)\), \(I^{(0)}\) is a scalar, \(I^{(1)}\) is a 3-component vector and \(I^{(2)}\) is a second-order tensor with six independent entries. This system of moment equations, which is of order one (because it describes the transport equations for moment of order up to one), cannot be readily solved as it involves the elements of the second-order moment tensor \(I^{(2)}\). An additional equation, which expresses the second-order moment \(I^{(2)}\) in terms of the lower-order moments \(I^{(0)}\) and \(I^{(1)}\), must be provided in order to make the system solvable. This so-called first-order closure condition (the order of the closure corresponds to the order of the system of moment equations it closes), is generally written in the following form:

\[ I^{(2)} = D I^{(0)} \] \tag{3.21}

where \(D = D(N^1)\) is the so-called Eddington tensor.

### 3.4.1 First Order Spherical Harmonics P\(_1\) Approximation

In the spherical harmonics approximation, an approximate radiative intensity distribution of the form given in Eq. (3.8) is used in order to close the system of moment equations given by Eq. (3.20). The reconstruction of the approximate distribution in terms of the finite set of moment \(E = (I^{(0)}, I^{(1)}_1, I^{(1)}_2, I^{(1)}_3)\) yields the following expression

\[ I(\vec{r}, \theta, \psi) = \frac{1}{4\pi} \left[ I^{(0)} + 3 \left( I^{(1)}_1 \Omega_1 + I^{(1)}_2 \Omega_2 + I^{(1)}_3 \Omega_3 \right) \right]. \] \tag{3.22}

This form of the distribution can be used to express \(I^{(2)}\) in terms of \(I^{(0)}\) and \(I^{(1)}\), which yields the following form for the Eddington tensor

\[ D = \frac{1}{3} I_d, \] \tag{3.23}

where \(I_d\) is the second-order identity tensor or dyad. This is the so-called P\(_1\) approximation, which is generally only accurate for optically thick media since it is associated with a nearly-isotropic distribution of the radiative intensity.
3.4.2 First Order Maximum-Entropy $M_1$ Moment Closure

The maximum entropy closure procedure provides a means for solving the system of equation given by Eq. (3.20) using an entropy-maximizing distribution of the form of Eq. (3.16) as an approximation of the radiative intensity distribution. In the case of a gray gas, the Lagrange multipliers of the approximate intensity distribution can be expressed in term of the finite set of moments $E = (I^{(0)}, I^{(1)}_1, I^{(1)}_2, I^{(1)}_3)$ by enforcing the conditions $\langle m(s)I_\nu \rangle = E$. The resulting distribution has the form

$$I(\alpha, m) = \frac{2\pi^4 k^4 T^4}{15 e^2 h^3} \left( 1 - \frac{2 - \sqrt{4 - 3 \|\vec{f}\|^2}}{\|\vec{f}\|^2} \vec{f} \cdot \vec{s} \right)^{-4}$$

The approximate distribution of radiative intensity given in Eq. (3.24) is a function of its zeroth and first moments only, the latter moment containing the lowest order angular information available. This implies that all the anisotropy lies in the direction of the flux, and the intensity distribution is therefore symmetric about that direction. Using this property of first-order moment closures, Levermore [16] derived an expression for the Eddington tensor, $D$, having the form

$$D = \frac{1 - \chi}{2} \vec{s} + \frac{3\chi - 1}{2} \vec{n} \otimes \vec{n},$$

where $\chi$ is the Eddington factor, which reads as follows

$$\chi = \frac{3 + 4\|N^1\|^2}{5 + 2\xi}, \quad \xi = \sqrt{4 - 3\|N^1\|^2},$$

and $\vec{n} = N^1/\|N^1\|$ is the unit vector in the direction of the flux vector. This is the so-called $M_1$ closure. Several different approaches have been used to derive the expression for the Eddington factor given in Eq. (3.26) and are highlighted in the review by [40]. Other expressions for the Eddington factor have also been proposed in the literature [16, 41]. It has been observed [42] that solutions derived using the $M_1$ model may exhibit non-physical discontinuities, especially when more than one direction of propagation for the radiation is significant. In regions where fluxes occur in more than one direction, the assumption that the intensity is symmetric about the direction of the flux is indeed no longer valid and the $M_1$ produces unphysical solutions with shocks. Several modifications of the $M_1$ model have then been proposed to overcome this difficulty. Dubroca and Klar [43] have developed an analytical formulation of the half-space first-order maximum...
entropy moment closure, which consists of taking moments of the underlying distribution in the positive and the negative sides separately, instead of the full moment (as in $M_1$). However, there exist no analytical formulation of the closure of such method for multidimensional radiative transfer problems. Frank et al [44] proposed an extension of this concept to multidimensional cases, which is based on a tabulation of the closing fluxes in the different quarters of the unit circle.

It is also worth mentioning that the expression for the Eddington factor given in Eq. (3.26) is only valid when dealing with spectrally integrated quantities. However, in the case of non-gray radiation transport, where the rather strong spectral dependence of the radiative properties must also be taken into account, there exist no analytical expression for $\chi$, and one must generally rely on solving the optimization problem. In this case, Turpault [45] proposed a multigroup $M_1$ model. This approach was later extended to the half-space $M_1$ closure by Turpault et al. [46].

### 3.5 Higher-Order Moment Closure Techniques

The moment closure techniques described in the previous section for solving the first-order system of moment equations are based on the reconstruction of the corresponding approximate form of the distribution of radiative intensity in terms of its zeroth and first-order moment only. In this case, the angular dependence of the resulting distribution is solely dictated by its first-order moment. Considering the limitations of the $P_1$ and $M_1$ closures discussed previously, improved solutions could be obtained with the inclusion of higher-order moments, as this would provide greater resolution of the angular variations in the distribution of radiative intensity.

#### 3.5.1 Second Order Maximum-Entropy $M_2$ Moment Closure

The next higher-order system of moment equations can be obtained by taking angular moment of the RTE with respect to the vector of Legendre polynomial $m(s) = (1, \Omega_1, \Omega_2, \Omega_3, \Omega_1^2, \Omega_2^2, \Omega_3^2, \Omega_1\Omega_2, \Omega_1\Omega_3, \Omega_2\Omega_3)$, yielding the following second-order system
of moment equations

\[
\frac{1}{c} \frac{\partial I^{(0)}}{\partial t} + \vec{\nabla} I^{(1)} = \kappa (4\sigma T^4 - I^{(0)}) \\
\frac{1}{c} \frac{\partial I^{(1)}}{\partial t} + \vec{\nabla} I^{(2)} = -(\kappa + \sigma_s) I^{(1)} \\
\frac{1}{c} \frac{\partial I^{(2)}}{\partial t} + \vec{\nabla} I^{(3)} = \frac{1}{3} (\kappa T^4 + \sigma_s I^{(0)}) \delta_{ij} - (\kappa + \sigma_s) I^{(2)}
\]

In Eq. (3.27), where again the assumption of isotropic scattering has been made, \(I^{(0)}\) is a scalar, \(I^{(1)}\) is a 3-component vector, \(I^{(2)}\) is a second-order tensor with six independent entries, and \(I^{(3)}\) is a third-order tensor with ten independent entries. In order to solve this system of equations, an additional relation expressing the third-order moment tensor \(I^{(3)}\) in terms of \(I^{(0)}, I^{(1)}\) and \(I^{(2)}\) is required.

As mentioned previously, there exist no analytical expression for higher-order maximum entropy closures (i.e., \(N \geq 2\)), even in one dimension. Hauck [22] compared several higher-order maximum entropy moment closures for problems involving radiative transfer in one space dimension. His approach was however based on the repeated calculations of the Lagrange multipliers by solving the optimization problem Eq. (3.13) numerically and then evaluating the distribution from Eq. (3.16). This purely numerical approach tends to be very expensive, especially for problems involving multidimensional radiative heat transfer. The computational costs would significantly decrease if one could obtain an analytical approximation of the closure, rather than repeatedly solving by numerical means the maximization problem. However, the challenge of such an approach is that one must ensure that the approximated closure preserves the desired properties of the original model, such as realizability and hyperbolicity. Similarly to the closure developed by Kershaw [47], Monreal and Frank [21] developed an analytical approximation of the \(M_2\) closure in 1D and showed that this extended model is able to overcome the inability of the \(M_1\) model to properly distinguish between radiative equilibrium and two identical beams traveling in opposite directions. While previous research described above shows the promise of higher-order maximum entropy closures, the application of the \(M_2\) model to multi-dimensional problems has not received much attention. Recently, Pichard et al. [13,23] have proposed an approximation to the \(M_2\) closure for the case of the Boltzmann entropy, which is of particular use in applications such as radiation therapy. The proposed approximate \(M_2\) model, which is based on an interpolative closure, appears very promising and would seem readily extendable to the case of Bose-Einstein entropy, as given by Eq. (3.12) and which is of
interest for radiation modeling for combustion systems. The remainder of this section presents the details of the derivation of the approximate interpolative closure used to solve the system of moment equations given by Eq. (3.27) for the Bose-Einstein entropy. The basis of the space of polynomials of up to order two over the unit sphere, used in the $M_2$ closure, can be defined as follows:

$$m(\vec{s}) = (\Omega_1, \Omega_2, \Omega_3, \Omega_1^2, \Omega_2^2, \Omega_3^2, \Omega_1\Omega_2, \Omega_1\Omega_3, \Omega_2\Omega_3),$$

(3.28)

and the form of the radiation distribution for the gray version of the $M_2$ model reads as in Eq. (3.16), where $\alpha \in \mathbb{R}^9$. Unlike the $M_1$ model, an exact analytical expression cannot be obtained for the $M_2$ closure. Moreover, repeatedly solving the maximization problem of Eq. (3.13) for each evaluation of the closure would result in large computational costs. The approximation described in this section takes advantage of the hierarchical nature of the $M_N$ models, i.e., the fact that $M_{N-1}$ is a subcase of $M_N$. More specifically, the closure for the $M_2$ model is obtained as follows: an approximation for the closure is first obtained for the $M_1$ distribution, the latter is then extended progressively until obtaining an approximation for the full three-dimensional $M_2$ distribution. For this purpose, the following hierarchy of subdomains for the Lagrange multipliers in the maximization problem is considered:

$$\mathcal{L}_0 = \mathbb{R}^9$$

(3.29a)

$$\mathcal{L}_1 = \{(\alpha_1, 0, 0, \alpha_4, \alpha_5, \alpha_6, 0, 0, 0), \quad \text{s.t.} \quad (\alpha_1, \alpha_4, \alpha_5, \alpha_6) \in \mathbb{R}^4 \} \subset \mathcal{L}_0$$

(3.29b)

$$\mathcal{L}_2 = \{(\alpha_1, 0, 0, \alpha_4, \alpha_5, 0, 0, 0), \quad \text{s.t.} \quad (\alpha_1, \alpha_4, \alpha_5) \in \mathbb{R}^3 \} \subset \mathcal{L}_1$$

(3.29c)

$$\mathcal{L}_3 = \{(\alpha_1, 0, 0, \alpha_4, 0, 0, 0), \quad \text{s.t.} \quad (\alpha_1, \alpha_4) \in \mathbb{R}^2 \} \subset \mathcal{L}_2$$

(3.29d)

Choosing the vector of Lagrange multipliers, $\alpha$, in one of the sets in Eq. (3.29) leads to the corresponding following forms for the distribution function:

$$\mathcal{E}_0 = \left\{ \frac{\sigma_{\text{step}} T^4}{\pi} (\alpha.m(\vec{s}))^{-4}, \quad \alpha \in \mathcal{L}_0 \right\}$$

(3.30a)

$$\mathcal{E}_1 = \left\{ \frac{\sigma_{\text{step}} T^4}{\pi} (\alpha_1\Omega_1 + \alpha_4\Omega_1^2 + \alpha_5\Omega_2^2 + \alpha_6\Omega_3^2)^{-4} \quad \text{s.t.} \quad (\alpha_1, \alpha_4, \alpha_5, \alpha_6) \in \mathbb{R}^4 \} \subset \mathcal{E}_0$$

(3.30b)

$$\mathcal{E}_2 = \left\{ \frac{\sigma_{\text{step}} T^4}{\pi} (\alpha_5 + \alpha_1\Omega_1 + (\alpha_4 - \alpha_5)\Omega_1^2)^{-4} \quad \text{s.t.} \quad (\alpha_1, \alpha_4, \alpha_5) \in \mathbb{R}^3 \} \subset \mathcal{E}_1$$

(3.30c)

$$\mathcal{E}_3 = \left\{ \frac{\sigma_{\text{step}} T^4}{\pi} (\alpha_4 + \alpha_1\Omega_1)^{-4} \quad \text{s.t.} \quad (\alpha_1, \alpha_4) \in \mathbb{R}^2 \} \subset \mathcal{E}_2$$

(3.30d)
A closer look at Eq. (3.29) shows that

- distributions of the form of Eq. (3.30d) correspond to the $M_1$ distribution in one-dimension;
- distributions of the form of Eq. (3.30c) are 1D distributions, since they only depend on one variable $\Omega_1$; and
- computations show that the moments $I^{(1)}$ and $I^{(2)}$ of distributions of the form of Eq. (3.30b) are such that $I^{(1)}$ is an eigenvector of $I^{(2)}$.

Taking the moments up to order two of the distribution functions in Eq. (3.30) leads to define the following hierarchy of moment sets

\[
\mathcal{R}_0 = \{\langle mI \rangle, \text{ s.t. } I \in E_0\} \quad (3.31a)
\]

\[
\mathcal{R}_1 = \{\langle mI \rangle, \text{ s.t. } I \in E_1 \} \subset \mathcal{R}_0 \quad (3.31b)
\]

\[
\mathcal{R}_2 = \{\langle mI \rangle, \text{ s.t. } I \in E_2 \} \subset \mathcal{R}_1 \quad (3.31c)
\]

\[
\mathcal{R}_3 = \{\langle mI \rangle, \text{ s.t. } I \in E_3 \} \subset \mathcal{R}_2 \quad (3.31d)
\]

The full realizability domain $\mathcal{R}$ for moments of order up to two is characterized as follows

\[
\mathcal{R} = \{(I^{(0)}, I^{(1)}, I^{(2)}) \in \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}^{3\times3}, \text{ s.t. } tr(I^{(2)}) = I^{(0)} > 0 \text{ and } I^{(0)}I^{(2)} - I^{(1)} \otimes I^{(1)} \text{ is symmetric positive definite}\}
\]

In order to simplify the analysis for the approximate interpolative closure, the development of Pichard et al. [13] makes use of a transformation of the realizability domain consisting of a normalization and rotation of the moments. We denote by $R$ the rotation matrix that diagonalizes $I^{(0)}I^{(2)} - I^{(1)} \otimes I^{(1)}$. This also diagonalizes $N^2 - N^1 \otimes N^1$. The realizability domain $\mathcal{R}_T$ resulting from these transformations (rotation and normalization) of $\mathcal{R}$ is defined as

\[
\mathcal{R}_T = \{(N^1, N^2) \in \mathbb{R}^3 \times \mathbb{R}^{3\times3}, \text{ s.t. } tr(N^2) = 1 \text{ and } N^2 - N^1 \otimes N^1 \text{ is diagonal positive}\}
\]

In the rotated frame, one can write

\[
N^2 = N^1 \otimes N^1 + (1 - \|N^1\|^2)\text{diag}(\gamma_1, \gamma_2, 1 - \gamma_1 - \gamma_2)
\]

Computing the moments of order up to two of the distribution functions Eq. (3.30) and...
applying the preceding transformations (normalization by \( I^{(0)} \) followed by rotation by \( R \)) yields

\[
I \in \mathcal{E}_0 \implies \begin{cases}
N^1 = N_1^1 e_1 \\
N^2 = N_1^1 \otimes N_1^1 + (1 - \|N_1^1\|^2) \text{diag}(\gamma_1, \gamma_2, 1 - \gamma_1 - \gamma_2)
\end{cases} \quad (3.32a)
\]

\[
I \in \mathcal{E}_1 \implies \begin{cases}
N^1 = N_1^1 e_1 \\
N^2 = (N_1^1)^2 e_1 \otimes e_1 + (1 - \|N_1^1\|^2) \text{diag}(\gamma_1, \gamma_2, 1 - \gamma_1 - \gamma_2)
\end{cases} \quad (3.32b)
\]

\[
I \in \mathcal{E}_2 \implies \begin{cases}
N^1 = N_1^1 e_1 \\
N^2 = (N_1^1)^2 e_1 \otimes e_1 + (1 - \|N_1^1\|^2) \text{diag}(\gamma_1, \frac{1-\gamma_1}{2}, \frac{1-\gamma_2}{2})
\end{cases} \quad (3.32c)
\]

\[
I \in \mathcal{E}_3 \implies \begin{cases}
N^1 = N_1^1 e_1 \\
N^2 = \frac{3\chi_2(N_1^1)-1}{2} e_1 \otimes e_1 + \frac{1-\chi_2(N_1^1)}{2} \Id
\end{cases} \quad (3.32d)
\]

where \( \chi_2 \) is the Eddington factor for the \( M_1 \) model (see Eq. (3.26)) and \( e_i \) is a 3-component vector for which all elements are zero except for the \( i \)th entry which has a value of unity. Similarly, computing the normalized third-order moment of the distribution functions given in Eq. (3.30) in the transformed realizability domain \( \mathcal{R}_T \) leads to the following closure expressions for \( N^3 \):  

\[
I \in \mathcal{E}_1 \implies N^3 = \kappa_2 1_{111} + \kappa_3 T_{222} + (N_1^1 - \kappa_2 - \kappa_3) T_{333} \quad (3.33a)
\]

\[
I \in \mathcal{E}_2 \implies N^3 = \kappa_1 1_{111} + \frac{N_1^1 - \kappa_1}{2} (T_{222} + T_{333}) \quad (3.33b)
\]

\[
I \in \mathcal{E}_3 \implies N^3 = \chi_3 1_{111} + \frac{N_1^1 - \chi_3}{2} (T_{222} + T_{333}) \quad (3.33c)
\]

\[
T_{iij} = 1_{iij} + 1_{jij} + 1_{jji}, \quad 1_{ijk} = e_i \otimes e_j \otimes e_k \quad (3.33d)
\]

where \( \chi_3, \kappa_1, \kappa_2 \) and \( \kappa_3 \) are scalar coefficients such that, \( \chi_3 \) is a function of \( N^1 \in [0, 1[, \kappa_1 \) of \( N^1 \in [0, 1[ \) and \( \gamma_1 \in ]0, 1[ \) and \( \kappa_2 \) and \( \kappa_3 \) of \( N^1 \in [0, 1[, \gamma_1 \in ]0, 1[ \) and \( \gamma_2 \in ]0, 1 - \gamma_1[ \).

**Strategy for the Interpolative Approximation**

The first step in the approximation of \( N^3 \) consists of constructing a realizable and hyperbolic approximation to the closure of functions of the form Eq. (3.30d). The closure is then extended progressively to the sets \( \mathcal{E}_2, \mathcal{E}_1 \) and finally \( \mathcal{E}_0 \). At each step of the extension, the closure is defined such that it is exact on the boundaries of the realizability domain and approximates the entropy-maximizing closure, obtained by solving numerically the optimization problem, Eq (3.13), inside the realizability domain of the corresponding subset.
Approximation of the Closure in $\mathcal{R}_3$

The realizability domain given by $\mathcal{R}_3$ corresponds to that of the $M_1$ model with a one-dimensional intensity distribution. In this subset of $\mathcal{R}_T$, a given set of moments $(I^{(0)}, I^{(1)}, I^{(2)}, I^{(3)})$ in 1D corresponds to the moments of a positive distribution function if and only if [47]

$$b_-(N^1_1, N^2_1) < N^3_{111} < b_+(N^1_1, N^2_1)$$

$$b_-(N^1_1, N^2_1) = -N^2_{11} + \frac{(N^1_1 + N^2_1)^2}{(1 + N^1_1)}, \quad b_+(N^1_1, N^2_1) = N^2_{11} - \frac{(N^1_1 - N^2_1)^2}{(1 - N^1_1)}$$  \hspace{1cm} (3.34a)

(3.34b)

For any set of moments in $\mathcal{R}_3$ satisfying the realizability conditions Eq. (3.34) as given above and due to Kershaw [47], the corresponding closure, $\chi_3 = N^3_{111}$, can be approximated as a convex combination of $b_-$ and $b_+$ of the form

$$\chi_3(x) = b_-(x, \chi_2(x))\theta_2(x) + b_+(x, \chi_2(x))(1 - \theta_2(x))$$  \hspace{1cm} (3.35)

where the coefficient $\theta_2$, which must be in $[0, 1]$, is chosen such that $\chi_3$ is an odd function and the values of $\chi_3$ and its corresponding derivatives are satisfied on the boundary of the realizability domain (i.e., at $x = 1$) as well as for the isotropic case (i.e., for $x = 0$). This leads to the following constraints on $\chi_3$:

$$\chi_3(1) = 1, \quad \chi_3(0) = 0, \quad \chi'_3(1) = 3, \quad \chi'_3(0) = \frac{1}{2}$$

and the following form for the expression for $\theta_2$ is then used

$$\theta_2(x) = \frac{1}{2} + x \left( -\frac{1}{2} + (1 - x^2)(d_0 + d_1x^2 + d_2x^4) \right)$$  \hspace{1cm} (3.36)

which satisfies these constraints. The coefficients $d_i$ are fitted to approximate the exact values of $\chi_3$ for 1,000 values of $x$ equally distributed in $[0, 1]$. Using the least squares fitting (lsfit) toolbox of C++, the following values for the coefficients were obtained $d_0 = 0.41343577$, $d_1 = 0.12635689$, $d_2 = 0.96674234$. It can be shown that in this case $\theta_2(x) \in [0, 1]$ for all $x \in [-1, 1]$. Figure (3.2) shows comparison between the approximated and exact closures for values of the normalized flux $N^1_1$ ranging from the isotropic case ($N^1_1 = 0$) to the free-streaming limit ($N^1_1 = 1$).
Extension of the Closure to $\mathcal{R}_2$

For any given set of moment in $\mathcal{R}_2$, the realizability conditions given by Eq. (3.34) still hold and the closure $N^3$ can be defined such that it is exact on the boundaries of $\mathcal{R}_2$ and approximates the entropy maximizing closure within the realizability domain as well as the closure $\chi_3$ in the case where we fall within the subset $\mathcal{R}_3$. As such, the parameter $\kappa_1 = N^3_{111}$ is approximated as follows

$$\kappa_1(x, y) = b_-(x, y)\theta_3(x, y) + b_+(x, y)(1 - \theta_3(x, y))$$  \hspace{1cm} (3.37)

where the form of the coefficient $\theta_3$ in Eq. (3.37) is selected such that $N^3$ is an odd function of $N^1$. It is also chosen such that the exact values of $N^3$ at the boundary of the realizability domain ($\gamma_1 = 0$ or $\gamma_1 = 1$), as well as the previous approximation in the $M_1$ case are exactly reproduced. This leads to the following approximation for $\theta_3$ given by

$$\theta_3(N^1_1, \gamma_1) = E((A_1, a_1), (A_2, a_2), (A_3, a_3))\gamma_1) + Z(a_1, a_2, a_3)\gamma_1)Q_1(N^1_1, \gamma_1)$$  \hspace{1cm} (3.38)
where

\begin{align}
a_1 &= 0, & \kappa_1(N_1^1, a_1) &= (N_1^1)^3, & A_1 &= \frac{b_+ - \kappa_1}{b_+ - b_-}(N_1^1, a_1) \quad (3.39a) \\
a_2 &= \chi_2(N_1^1) - |N_1^1|^2, & \kappa_1(N_1^1, a_2) &= \chi_3(N_1^1), & A_2 &= \frac{b_+ - \kappa_1}{b_+ - b_-}(N_1^1, a_2) \quad (3.39b) \\
a_3 &= 1, & \kappa_1(N_1^1, a_3) &= N_1^1, & A_3 &= \frac{b_+ - \kappa_1}{b_+ - b_-}(N_1^1, a_3) \quad (3.39c)
\end{align}

and $Q_1$ is a polynomial in $N_1^1$ and $\gamma_1$ of degree sixteen. The coefficients of $Q_1$ were computed such that the $L^2$-norm of the error in the approximated and exact values for $\kappa_1$, the latter computed by solving Eq. (3.13), for 10,000 values of $(N_1^1, \gamma_1) \in [0, 1] \times [0, 1]$, was minimized. Those values are chosen from 100 values of $N_1^1$ equally distributed in $[0, 1]$ and 100 of $\gamma_1$ equally distributed in $[0, 1]$. For those values of the coefficients for $Q_1$, the $L^\infty$-norm of the error in the fit compared to the solution of the maximization problem for those 10,000 values of $(N_1^1, N_2^1) \in \mathcal{R}_2$ was found to be $1.896 \times 10^{-3}$. For the form given in Eq. (3.38), the polynomial $\theta_3(x, y) \in [0, 1]$ for all $x \in [-1, 1]$ and $y \in [0, 1]$. In Eq. (3.38), $E((A, a), (B, b), (C, c))(x)$ is Lagrange polynomial of degree two, returning the values $A$, $B$ and $C$ at the points $a$, $b$, and $c$, and is defined as follows

$$E((A, a), (B, b), (C, c))(x) = A \frac{x - b}{a - b} \frac{x - c}{a - c} + B \frac{x - a}{b - a} \frac{x - c}{b - c} + C \frac{x - a}{c - a} \frac{x - b}{c - b} \quad (3.40)$$

**Figure 3.3:** Approximated variation of $\kappa_1$
and $Z(a, b, c)(x)$ is a polynomial of degree three, which has a value of zero at $a$, $b$ and $c$, and is therefore taken to have the form

$$Z(a, b, c)(x) = (x - a)(x - b)(x - c) \quad (3.41)$$

Figures 3.3 and 3.4 show the approximated closure $\kappa_1$ and the error between the approximated closure and the exact values obtained by solving the optimization problem, respectively, for a range of values of $(N_1^1, \gamma_1)$.

**Extension of the Closure to $\mathcal{R}_1$**

A similar approach to the one used for the approximation of $N^3$ in $\mathcal{R}_2$ can be used to approximate the latter in $\mathcal{R}_1$, i.e., approximate $N^3$ such that the fit returns the exact values of $N^3$ on the boundaries of $\mathcal{R}_1$ ($\gamma_2 = 0$ or $\gamma_2 = 1 - \gamma_1$), and exactly reproduces the approximate closure within $\mathcal{R}_2$. However, unlike for $\mathcal{R}_2$, there are no sufficient conditions for moment realizability in $\mathcal{R}_1$, and the closure is approximated such that $\kappa_2 = N^3_{111}$ and $\kappa_3 = N^3_{122}$ are defined as follows

$$\kappa_2(N_1^1, \gamma_1, \gamma_2) = E((B_1, b_1), (B_2, b_2), (B_3, b_3))(\gamma_2) + Z(b_1, b_2, b_3)(\gamma_2)Q_2(N_1^1, \gamma_1, \gamma_2) \quad (3.42)$$
\[ \kappa_3(N_1^1, \gamma_1, \gamma_2) = E((C_1, b_1), (C_2, b_2), (C_3, b_3)) (\gamma_2) + Z(b_1, b_2, b_3) (\gamma_2) Q_3(N_1^1, \gamma_1, \gamma_2) \]  
(3.43)

and where
\[ b_1 = 0, \quad b_2 = \frac{1 - \gamma_1}{2}, \quad b_3 = 1 - \gamma_1 \]

\[ B_1 = \kappa_2(N_1^1, \gamma_1, b_1) = \kappa_1(N_1^1, \gamma_1), \quad C_1 = \kappa_3(N_1^1, \gamma_1, b_1) = 0, \]
\[ B_2 = \kappa_2(N_1^1, \gamma_1, b_2) = \kappa_1(N_1^1, \gamma_1), \quad C_2 = \kappa_3(N_1^1, \gamma_1, b_2) = \frac{1}{2} (N_1^1 - \kappa_1(N_1^1, \gamma_1)), \]
\[ B_3 = \kappa_2(N_1^1, \gamma_1, b_3) = \kappa_1(N_1^1, \gamma_1), \quad C_3 = \kappa_3(N_1^1, \gamma_1, b_3) = N_1^1 - \kappa_1(N_1^1, \gamma_1) \]

In Eqs. (3.42) and (3.43), \( Q_2 \) and \( Q_3 \) are polynomials dependent on \( N_1^1, \gamma_1 \) and \( \gamma_2 \) and in this case having degree eight. The coefficients of those polynomials were computed such that the \( L^2 \)-norm of the error in the fit between the approximated and exact values of \( \kappa_2 \) and \( \kappa_3 \) computed by solving Eq. (3.13) for 8,000 values of \( (N_1^1, \gamma_1, \gamma_2) \in [0, 1] \times [0, 1] \times [0, 1 - \gamma_1] \) was minimized. The 8,000 values were chosen from 20 values of \( N_1^1 \) equally distributed in [0, 1], 20 of \( \gamma_1 \) equally distributed in [0, 1] and 20 of \( \gamma_2 \) equally distributed in [0, 1 - \( \gamma_1 \)]. The \( L^\infty \)-norm errors compared to the solution of the maximization problem for those 8,000 values of \( (N^1, N^2) \in \mathcal{R}_1 \) were found to be \( 1.778 \times 10^{-3} \) for \( \kappa_2 \) and \( 1.111 \times 10^{-3} \) for \( \kappa_3 \), respectively.

**Extension to \( \mathcal{R}_T \)**

The expressions presented in Eqs. (3.42) and (3.43) yield an approximation to the closing expressions for \( N^3 \) in \( \mathcal{R}_1 \), which is a subset of \( \mathcal{R}_T \). This section proposes an approximation of the closure in \( \mathcal{R}_T \), which will then provide an approximation of \( I^{(3)} \) for any set of moments \( (I^{(0)}, I^{(1)}, I^{(2)}) \in \mathcal{R} \) using the inverse transformation from \( \mathcal{R} \) to \( \mathcal{R}_T \).

Consider a point \( P = (N^1, N^2) \) in \( \mathcal{R}_T \) parametrized by \( P = (N_1^1, \gamma_1, \gamma_2) \). The projections of \( P \) onto the each Cartesian axes at fixed \( \gamma_1 \) and \( \gamma_2 \) are respectively defined as (please refer to Fig. 3.5)

\[ P_1 = (N_1^1 e_1, \gamma_1, \gamma_2), \quad P_2 = (N_2^1 e_2, \gamma_1, \gamma_2), \quad P_3 = (N_3^1 e_3, \gamma_1, \gamma_2) \]

(3.45)

Those points belong to \( \mathcal{R}_1 \) since \( N^1 \) is along one of the Cartesian axes, and Eqs. (3.42) and (3.43) can be used to approximate the closure at each of those points. Now let us define the lines \( L_i, i \in \{1, 2, 3\} \) as follows

\[ L_1 = (P_1, P), \quad L_2 = (P_2, P), \quad L_3 = (P_3, P) \]
The intersection points of each of those lines with the surface of the unit sphere are denoted $P_{i+3}$ and can then be defined as follows

$$P_4 = L_1 \cap S^2 = (N_1^1 e_1 + a_1 N_2^1 e_2 + a_1 N_3^1 e_3, \gamma_1, \gamma_2), \quad a_1 = \sqrt{\frac{1 - (N_1^1)^2}{(N_1^1)^2 + (N_2^1)^2}}$$

$$P_5 = L_2 \cap S^2 = (a_2 N_1^1 e_1 + N_2^1 e_2 + a_2 N_3^1 e_3, \gamma_1, \gamma_2), \quad a_2 = \sqrt{\frac{1 - (N_2^1)^2}{(N_1^1)^2 + (N_2^1)^2}}$$

$$P_6 = L_3 \cap S^2 = (a_3 N_1^1 e_1 + a_3 N_2^1 e_2 + N_3^1 e_3, \gamma_1, \gamma_2), \quad a_3 = \sqrt{\frac{1 - (N_3^1)^2}{(N_1^1)^2 + (N_2^1)^2}}$$

The points $P_4$, $P_5$, and $P_6$ lie on one of the boundaries of the realizability domain since $\|N^1\| = 1$, which corresponds to the free-streaming limit. On this boundary there exist an exact analytical expression for the closure $N^3$, which, for each of those points, is given by the expressions

$$N^3(P_4) = (N_1^1 e_1 + a_1 N_2^1 e_2 + a_1 N_3^1 e_3)^\otimes 3,$$

$$N^3(P_5) = (a_2 N_1^1 e_1 + N_2^1 e_2 + a_2 N_3^1 e_3)^\otimes 3,$$

$$N^3(P_6) = (a_3 N_1^1 e_1 + a_3 N_2^1 e_2 + N_3^1 e_3)^\otimes 3$$

respectively. The procedure for obtaining the closure at point $P$ then consists of an approximation of the entry $N^3_{i,j}$ by an interpolation between the approximated closure at $P_i$ and the exact closure at $P_{i+3}$ (surface of the unit sphere). Accordingly, the following relations can be formulated

$$N_{111}^3(P) \approx (1 - \alpha_1)N_{111}^3(P_1) + \alpha_1 N_{111}^3(P_4) \quad (3.46a)$$

$$N_{122}^3(P) \approx (1 - \alpha_1)N_{122}^3(P_1) + \alpha_1 N_{122}^3(P_4) \quad (3.46b)$$

$$N_{133}^3(P) \approx (1 - \alpha_1)N_{133}^3(P_1) + \alpha_1 N_{133}^3(P_4) \quad (3.46c)$$

$$N_{112}^3(P) \approx (1 - \alpha_2)N_{112}^3(P_2) + \alpha_2 N_{112}^3(P_5) \quad (3.46d)$$

$$N_{222}^3(P) \approx (1 - \alpha_2)N_{222}^3(P_2) + \alpha_2 N_{222}^3(P_5) \quad (3.46e)$$

$$N_{233}^3(P) \approx (1 - \alpha_2)N_{233}^3(P_2) + \alpha_2 N_{233}^3(P_5) \quad (3.46f)$$

$$N_{113}^3(P) \approx (1 - \alpha_3)N_{113}^3(P_3) + \alpha_3 N_{113}^3(P_6) \quad (3.46g)$$

$$N_{223}^3(P) \approx (1 - \alpha_3)N_{223}^3(P_3) + \alpha_3 N_{223}^3(P_6) \quad (3.46h)$$

$$N_{333}^3(P) \approx (1 - \alpha_3)N_{333}^3(P_3) + \alpha_3 N_{333}^3(P_6) \quad (3.46i)$$
Figure 3.5: Configuration at fixed $\gamma_1$ and $\gamma_2$

\[ N_{123}^3(P) \approx (1 - \alpha_4)N_{123}^3(P_0) + \alpha_4 N_{123}^3(P_7) \] (3.46j)

Figure 3.6: Configuration at fixed $N_1^1$, $\gamma_1$ and $\gamma_2$
\[
\alpha_1 = \frac{|N_2|^2 + |N_1|^2}{1 - |N_1|^2}, \quad \alpha_2 = \frac{|N_1|^2 + |N_3|^2}{1 - |N_2|^2}, \\
\alpha_3 = \frac{|N_1|^2 + |N_2|^2}{1 - |N_3|^2}, \quad \alpha_4 = \|N^1\|
\]

In order to assess the accuracy of the resulting closure represented by Eq. (3.46), the latter was compared to the solution of the maximization problem for 3.2 million values of \((N_1, N_2) \in \mathcal{R}_T\). Those values are obtained from 20 values of \(N_1^1\) equally distributed in \([0, 1]\), 20 of \(N_2^1\) in \([0, \sqrt{1 - (N_1^1)^2}]\), 20 of \(N_3^1\) in \([0, \sqrt{1 - (N_1^1)^2} - (N_2^1)^2]\), 20 of \(\gamma_1\) in \([0, 1]\) and 20 of \(\gamma_2\) in \([0, 1 - \gamma_1]\). The corresponding \(L^\infty\)-error in the approximation was found to be \(1.65 \times 10^{-2}\).

**Solution of the Maximization Problem**

The numerical solution of the maximization or optimization problem defined by Eq. (3.13), and used in determining the coefficients for the proposed M_2 interpolative closure, was obtained using NLOPT [48, 49], a C++ open source optimization toolbox allowing to solve a constrained nonlinear optimization problem, with user-supplied objective function and gradient. Numerical integration of the intensity distribution over the solid angle was performed by means of DCUHRE [50], an open source Fortran subroutine which performs adaptive quadrature for functions of multiple variables.

### 3.5.2 Third Order Spherical Harmonics \(P_3\) Approximation

For comparison to the proposed M_2 interpolative closure, the \(P_3\) moment closure is also considered. The \(P_3\) approximation is used to solve the system of moment equations of order up to three, which, under the assumption of isotropic scattering, reads as follows

\[
\begin{align*}
\frac{1}{c} \frac{\partial I^{(0)}}{\partial t} + \vec{\nabla} I^{(1)} &= \kappa (4\sigma T^4 - I^{(0)}) \\
\frac{1}{c} \frac{\partial I^{(1)}}{\partial t} + \vec{\nabla} I^{(2)} &= -(\kappa + \sigma_s) I^{(1)} \\
\frac{1}{c} \frac{\partial I^{(2)}}{\partial t} + \vec{\nabla} I^{(3)} &= \frac{1}{3} (\kappa T^4 + \sigma_s I^{(0)}) \delta_{ij} - (\kappa + \sigma_s) I^{(2)} \\
\frac{1}{c} \frac{\partial I^{(3)}}{\partial t} + \vec{\nabla} I^{(4)} &= -(\kappa + \sigma_s) I^{(3)}
\end{align*}
\]  

(3.47)
In Eq. (3.47), $I^{(4)}$ is a fourth-order symmetric tensor with fifteen independent variables, which must be expressed in terms of the lower-order moments $I^{(0)}$, $I^{(1)}$, $I^{(2)}$ and $I^{(3)}$ in order to obtain a solvable. Following a similar procedure as the one for the determination of the $P_1$ distribution, the approximate form of the distribution of the radiative intensity given by Eq. (3.8) (with $N = 3$) can be expressed in terms of the known set of moments $E = (I^{(0)}, I^{(1)}, I^{(2)}, I^{(3)})$ as follows

$$I(\vec{r}, \theta, \psi) = \frac{1}{4\pi} \left[ M_0 + M_1 \Omega_1 + M_2 \Omega_2 + M_3 \Omega_3 + M_4 \Omega_4 + M_5 \Omega_5 + M_6 \Omega_6 \right.$$ 

$$+ M_7 \Omega_1 \Omega_2 + M_8 \Omega_1 \Omega_3 + M_9 \Omega_2 \Omega_3 + M_{10} \Omega_4 + M_{11} \Omega_5 + M_{12} \Omega_6$$ 

$$+ M_{13} \Omega_1 \Omega_2 \Omega_3 + M_{14} \Omega_1^2 \Omega_3 + M_{15} \Omega_2^2 \Omega_3 + M_{16} \Omega_1 \Omega_2 \Omega_3 + M_{17} \Omega_2 \Omega_3^2 \right],$$

(3.48)

where the $M_k$ are given by

$$M_0 = \left[ \frac{(9/4)I^{(0)} - (15/4)I^{(3)}_{333}}{8} \right],$$

$$M_1 = \left[ -\frac{(15/2)I^{(1)}_1 + (105/2)I^{(3)}_{122}}{8} \right],$$

$$M_2 = \left[ -\frac{(15/2)I^{(1)}_2 + (105/2)I^{(3)}_{112}}{8} \right],$$

$$M_3 = \left[ -\frac{(75/4)I^{(1)}_3 - (105/4)I^{(3)}_{333}}{8} \right],$$

$$M_4 = \left[ -\frac{(15/4)(I^{(2)}_{111} - I^{(2)}_{222})}{8} \right],$$

$$M_5 = -M_4,$$

$$M_6 = \left[ -\frac{(45/4)I^{(2)}_{333} - (15/4)I^{(0)}}{8} \right],$$

$$M_7 = \left[ 15I^{(2)}_{12} \right],$$

$$M_8 = \left[ 15I^{(2)}_{13} \right],$$

$$M_9 = \left[ 15I^{(2)}_{23} \right],$$

$$M_{10} = \left[ -\frac{(35/2)(I^{(3)}_{111} - 3I^{(3)}_{122})}{8} \right],$$

$$M_{11} = \left[ -\frac{(35/2)(I^{(3)}_{222} - 3I^{(3)}_{111})}{8} \right],$$

$$M_{12} = \left[ -\frac{(175/4)I^{(3)}_{333} - (105/4)I^{(3)}_{333}}{8} \right],$$

$$M_{13} = \left[ 105I^{(3)}_{222} \right],$$

$$M_{14} = \left[ -\frac{(105/4)(I^{(3)}_{111} - I^{(3)}_{222})}{8} \right],$$

$$M_{15} = -M_{14},$$

$$M_{16} = \left[ -\frac{(105/2)(I^{(3)}_{133} - I^{(3)}_{122})}{8} \right],$$

$$M_{17} = \left[ -\frac{(105/2)(I^{(3)}_{233} - I^{(3)}_{122})}{8} \right].$$

(3.49)

This higher-order approximation for the form of the intensity distribution, Eq. (3.48), yields the following closure conditions for $I^{(4)}$, appearing in the $P_3$ moment equations:

$$I^{(4)}_{iii} = -(3/35)I^{(0)} + (6/7)I^{(2)}_{ii},$$

$$I^{(4)}_{ijij} = (4/35)I^{(0)} - (1/7)I^{(2)}_{jk},$$

$$I^{(4)}_{iiij} = (3/7)I^{(2)}_{ij},$$

$$I^{(4)}_{iijk} = (1/7)I^{(2)}_{jk}.$$  

(3.50)

It has been shown previously that the third-order spherical harmonics or so-called $P_3$ approximation yields much better predictions than $P_1$ for radiative transfer in two-dimensional geometries [51]. Moreover, it is worth mentioning that higher-order ap-
proximations \((N \geq 5)\) result in a significant increase in the computational effort while the accuracy improvements are somewhat more modest \([52, 53]\). For these reasons, it is felt that the \(P_3\) approximation provides a reasonable balance between accuracy and computational costs as compared to \(P_5\) and higher-order models.

### 3.6 Eigenstructure for System of Moment Equations in 2D

For problems involving radiation transport in a gray medium, the conservation form for the system of equations for moments of order up to three in two dimensions can be expressed in the following form

\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = S
\]

where \(U\) is the vector of conserved moments, \(F\) and \(G\) are the flux vectors (in the \(x\)- and \(y\)-directions, respectively) and \(S\) is the source term such that

\[
U = \begin{bmatrix}
I^{(0)} \\
I_x^{(1)} \\
I_y^{(1)} \\
I_{xx}^{(2)} \\
I_{xy}^{(2)} \\
I_{yy}^{(2)} \\
I_{xxx}^{(3)} \\
I_{xyy}^{(3)} \\
I_{yyy}^{(3)}
\end{bmatrix}, \quad F = c \begin{bmatrix}
I_x^{(1)} \\
I_x^{(2)} \\
I_y^{(2)} \\
I_{xx}^{(3)} \\
I_{xy}^{(3)} \\
I_{yy}^{(3)} \\
I_{xxx}^{(4)} \\
I_{xyy}^{(4)} \\
I_{yyy}^{(4)}
\end{bmatrix}, \quad G = c \begin{bmatrix}
I_y^{(1)} \\
I_x^{(2)} \\
I_y^{(2)} \\
I_{yy}^{(3)} \\
I_{xxx}^{(3)} \\
I_{xyy}^{(3)} \\
I_{yyy}^{(3)} \\
I_{xxx}^{(4)} \\
I_{xyy}^{(4)} \\
I_{yyy}^{(4)}
\end{bmatrix}
\]
and the source term \( \mathbf{S} \) has the form

\[
\mathbf{S} = c \begin{bmatrix}
\kappa(aT^4 - I^{(0)}) \\
-(\kappa + \sigma_s)I_x^{(1)} \\
-(\kappa + \sigma_s)I_y^{(1)} \\
\frac{1}{3}(\kappa a T^4 + \sigma_s I^{(0)}) - (\kappa + \sigma)I_{xx}^{(2)} \\
-(\kappa + \sigma)I_{xy}^{(2)} \\
\frac{1}{3}(\kappa a T^4 + \sigma_s I^{(0)}) - (\kappa + \sigma)I_{yy}^{(2)} \\
-(\kappa + \sigma)I_{xx}^{(3)} \\
-(\kappa + \sigma)I_{xy}^{(3)} \\
-(\kappa + \sigma)I_{yy}^{(3)} \\
-(\kappa + \sigma)I_{xxx}^{(3)} \\
-(\kappa + \sigma)I_{xxy}^{(3)} \\
-(\kappa + \sigma)I_{xyy}^{(3)} \\
-(\kappa + \sigma)I_{yyy}^{(3)}
\end{bmatrix}
\] (3.53)

For the first-order moment closures (\( M_1 \) and \( P_1 \)), only the transport equations for moments of order up to one are considered and the corresponding closing fluxes can be expressed in terms of the lower order moments using either Eq. (3.23) for \( P_1 \), or Eq. (3.25) for \( M_1 \). Similarly, for the \( M_2 \) closure, the moments of order up to two are considered and the closure conditions of Eq. (3.46) can be used to approximate the closing fluxes (third-order moments of the distribution) in terms of the lower order moments. Finally, the \( P_3 \) approximation describes the transport of moments up to order three, and the closing expression for the fourth moments is given in Eq. (3.50).

Equation (3.51) can be re-expressed in a weak conservation form as follows

\[
\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{U}}{\partial x} + \mathbf{B} \frac{\partial \mathbf{U}}{\partial y} = \mathbf{S}
\] (3.54)

where \( \mathbf{A} = \frac{\partial \mathbf{F}}{\partial \mathbf{U}} \) and \( \mathbf{B} = \frac{\partial \mathbf{G}}{\partial \mathbf{U}} \) are the flux Jacobians in the \( x \)- and \( y \)-directions, respectively.

For the \( P_1 \) approximation, the \( x \)-direction flux Jacobian reads as

\[
\frac{\partial \mathbf{F}}{\partial \mathbf{U}} = \begin{bmatrix}
0 & c & 0 \\
\frac{c}{3} & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\] (3.55)

and the corresponding vector of eigenvalues is

\[
\lambda_x = \begin{bmatrix} 0, \ -\frac{\sqrt{3}}{3}c, \ \frac{\sqrt{3}}{3}c \end{bmatrix}
\] (3.56)
For the P₃ approximation, the x-direction flux Jacobian is given by:

\[
\frac{\partial F}{\partial U} = \begin{bmatrix}
0 & c & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & c & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & c & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & c & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & c & 0 & 0 \\
-\frac{3}{35}c & 0 & 0 & \frac{6}{7}c & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{3}{7}c & 0 & 0 & 0 & 0 \\
-\frac{c}{35} & 0 & 0 & \frac{c}{7} & 0 & \frac{c}{7} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{3}{7}c & 0 & 0 & 0 & 0
\end{bmatrix}
\]

(3.57)

and the corresponding eigenvalues are

\[
\lambda_x = [0, \ 0, \ -\frac{\sqrt{525} - 70\sqrt{30}}{35}c, \ -\frac{\sqrt{525} + 70\sqrt{30}}{35}c, \ \frac{\sqrt{525} - 70\sqrt{30}}{35}c, \ \frac{\sqrt{525} + 70\sqrt{30}}{35}c, \ -\frac{\sqrt{7}}{7}c, \ \frac{\sqrt{7}}{7}c, \ -\frac{\sqrt{21}}{7}c, \ \frac{\sqrt{21}}{7}c]
\]

(3.58)

In the case of the M₁ model, the flux Jacobian is

\[
\frac{\partial F}{\partial U} = \begin{bmatrix}
0 & c & 0 & (3f_x+2+\xi)(3f_x-2-\xi) \\
-\frac{\xi^2-2\xi+18f_x^2-8}{6\xi f_x f_y} & \frac{c f_x (3\xi^2+8\xi-4+9f_x^2)}{\xi (\xi+2)^3} & -\frac{(3f_x+2+\xi)(3f_x-2-\xi)}{3\xi (\xi+2)^4} & 0 \\
-\frac{6c f_x f_y}{\xi (\xi+2)} & \frac{c f_y (\xi^2+2\xi+3f_x^2)}{\xi (\xi+2)^4} & -\frac{3c f_x (2\xi-3f_x^2+4)}{\xi (\xi+2)^3} & 0
\end{bmatrix}
\]

(3.59)

where the variable ξ has been defined in Eq. (3.26). The corresponding eigenvalues have been previously derived by Berthon et al. [20] and are as follows

\[
\lambda_{x,1,2} = c \left(\frac{f_x}{\xi} \pm \frac{\sqrt{2(\xi-1)(\xi+2)(2\xi-1)(\xi+2)+3f_x^2}}{3\xi (\xi+2)}\right)
\]

\[
\lambda_{x,3} = c \frac{f_x (2-\xi)}{f_x^2}
\]

(3.60)
Finally, for the $M_2$ closure, the flux Jacobian read as follows

$$\frac{\partial F}{\partial U} = c \begin{bmatrix}
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
\partial I^{(3)}_{xx} & \partial I^{(3)}_{xy} & \partial I^{(3)}_{xz} & \partial I^{(3)}_{xw} & \partial I^{(3)}_{xv} & \partial I^{(3)}_{xu} \\
\partial I^{(0)}_{xx} & \partial I^{(0)}_{xy} & \partial I^{(0)}_{xz} & \partial I^{(0)}_{xw} & \partial I^{(0)}_{xv} & \partial I^{(0)}_{xu} \\
\partial I^{(3)}_{yx} & \partial I^{(3)}_{yy} & \partial I^{(3)}_{yz} & \partial I^{(3)}_{yw} & \partial I^{(3)}_{yw} & \partial I^{(3)}_{u} \\
\partial I^{(0)}_{yx} & \partial I^{(0)}_{yy} & \partial I^{(0)}_{yz} & \partial I^{(0)}_{yw} & \partial I^{(0)}_{yw} & \partial I^{(0)}_{v} \\
\partial I^{(3)}_{zx} & \partial I^{(3)}_{zy} & \partial I^{(3)}_{zw} & \partial I^{(3)}_{zx} & \partial I^{(3)}_{yz} & \partial I^{(3)}_{zw} \\
\partial I^{(0)}_{zx} & \partial I^{(0)}_{zy} & \partial I^{(0)}_{zw} & \partial I^{(0)}_{zx} & \partial I^{(0)}_{yz} & \partial I^{(0)}_{zw}
\end{bmatrix} (3.61)$$

The evaluation of the derivatives appearing in Eq. (3.61) from the approximate interpolated closure represented by Eq. (3.46) yields very lengthy expressions requiring extensive derivation. For the sake of simplification, the flux derivative terms in the flux Jacobian Eq. (3.61) are approximated by standard second-order accurate numerical differentiation of the form

$$\frac{\partial f}{\partial x} = \lim_{\epsilon \to 0} \frac{f(x + \epsilon) - f(x - \epsilon)}{2\epsilon} (3.62)$$

where $\epsilon$ is a parameter which is generally chosen to be small ($\epsilon = 1 \times 10^{-5}$ in the present analysis). In this way, it is possible to verify by at least numerical means that the interpolative $M_2$ closure is hyperbolic, i.e., the eigenvalues of the flux Jacobian given by Eq. (3.61) are real. This is a very important property as it impacts the compatibility of the resulting model with the proposed upwind finite-volume technique used to solve the resulting moment equations as described in Chapter 4 to follow. By means of “eispack” [54], the eigenvalues of Eq. (3.61) were numerically evaluated for a finite number of points in $\mathcal{R}_T$. The analysis showed that the closure was found to be hyperbolic at each of the points, which where obtained from 10 values of $N_1^1$ equally distributed in $[0, 1]$, 10 of $N_2^1$ in $[0, \sqrt{1 - (N_1^1)^2}]$, 10 of $N_3^1$ in $[0, \sqrt{1 - (N_1^1)^2 - (N_2^1)^2}]$, 10 of $\gamma_1$ in $[0, 1]$ and 10 of $\gamma_2$ in $[0, 1 - \gamma_1]$. It should be pointed out that, at this stage of the closure development, no closed form analytical expression have been found for the eigenvalues. Fortunately, the flux function evaluation (HLLE flux function) used in the approximate Riemann solver described in Section 4.1.1 of Chapter 4 only requires knowledge of the largest and lowest wavespeeds of the system. Since no information can travel faster than the speed of light, it therefore follows that the values $c$ and $-c$ represent a good choice for the largest and smallest wavespeeds, respectively.
3.7 Boundary Conditions

One of the main challenges of solving the moments equations is the proper implementation of the boundary conditions. In fact, at a boundary, only the outgoing partial moments are known. In order to prescribe values for the full moments, the partial incoming moments must also be known, and can be obtained by integrating the approximate form of the distribution of the radiative intensity over the appropriate domain. In most practical combustion systems, the wall surfaces can generally be assumed to be diffusively reflecting and emitting [55]. In such situations, the outgoing radiation intensity at the boundary is isotropic and can be expressed as follows

\[
I_w = \epsilon_w I_b(T_w) + \frac{(1 - \epsilon_w)}{\pi} \int_{\Omega = \frac{2\pi}{\pi}} s(i)Id\Omega
\]  

The outgoing partial moments can be derived from Eq. (3.63) by integration over the appropriate hemisphere. The derivation of such partial moments is straightforward for black walls ($\epsilon_w = 1$). However, if the walls also reflect a portion of the incoming radiation, the derivation of the outgoing partial moments can be quite challenging, especially for entropy-maximizing distributions for which analytical integrals of the underlying intensity distribution cannot be obtained. For the $P_N$ approximations, the partial moments can directly be expressed in terms of the moments of the distribution.

The Marshak boundary condition [55] is the most widely used approach for solving the $P_N$ approximations, where the full moments at the boundaries are fully determined based on the incoming and outgoing partial odd order moments. Unlike the $P_N$ closures, analytical expression for the partial moments of the entropy-maximizing distribution do not exist, which makes the implementation of such type of boundary conditions for the $M_N$ a very challenging task. In this work, we make use of the partial moments boundary conditions, where the incoming partial moments are obtained by directly integrating the corresponding form of the distribution in the appropriate half space.
3.7.1 Partial Moments for the P₁ Approximation

The partial moments for the P₁ approximation, obtained by integrating the corresponding distribution Eq. (3.22), are given by

\[ (I^{(0)})^+ = \frac{I^{(0)}}{2} + \frac{3I^{(1)}}{4} \]  \hspace{1cm} (3.64a)

\[ (I^{(1)})^+ = \frac{I^{(0)}}{4} + \frac{I^{(1)}}{2} \]  \hspace{1cm} (3.64b)

\[ (I^{(1)})^+ = \frac{I^{(1)}}{2} \]  \hspace{1cm} (3.64c)

Note that all of the partial moments can be readily expressed in terms of the known full moments.

3.7.2 Partial Moments for the P₃ Approximation

For the P₃ Approximation, taking the angular integrals of the underlying distribution Eq. (3.48) for moments of order up to three in the appropriate hemisphere yields the
following expressions for the partial moments

\[
I^{(0)}_1 = \frac{I^{(0)}}{2} + \frac{45I^{(1)}_1}{32} - \frac{35I^{(3)}_{111}}{32} \\
I^{(1)}_1 = \frac{3I^{(0)}}{32} + \frac{I^{(1)}_1}{2} + \frac{15I^{(2)}_{11}}{32} \\
I^{(1)}_2 = \frac{I^{(1)}_2}{2} + \frac{15I^{(2)}_{11}}{16} \\
I^{(2)}_1 = \frac{5I^{(1)}_1}{32} + \frac{I^{(2)}_{11}}{2} + \frac{35I^{(3)}_{111}}{96} \\
I^{(2)}_2 = \frac{5I^{(1)}_2}{64} + \frac{I^{(2)}_{12}}{2} + \frac{35I^{(3)}_{112}}{64} \\
I^{(2)}_3 = \frac{5I^{(1)}_1}{64} + \frac{I^{(2)}_{12}}{2} - \frac{35I^{(3)}_{111}}{192} + \frac{35I^{(3)}_{112}}{32} \\
I^{(3)}_1 = \frac{15I^{(1)}_{11}}{32} - \frac{I^{(0)}_{11}}{32} + \frac{I^{(3)}_{111}}{2} \\
I^{(3)}_2 = \frac{I^{(3)}_{112}}{2} + \frac{75\pi I^{(2)}_{12}}{512} \\
I^{(3)}_3 = \frac{5I^{(1)}_{12}}{64} - \frac{I^{(0)}_{12}}{64} + \frac{5I^{(2)}_{12}}{32} + \frac{I^{(3)}_{122}}{2} \\
I^{(3)}_4 = \frac{15I^{(2)}_{12}}{32} + \frac{I^{(3)}_{122}}{2}
\]

Again, here, the partial moments can be expressed directly in terms of the known full moments.

### 3.7.3 Partial Moments for the M\textsubscript{N} Closures

For the M\textsubscript{N} models, analytical expressions for the partial moments cannot be obtained. In order to avoid the computational costs associated with the repeated solution of the maximization problem for evaluating the partial moments, analytical approximations of the latter for the M\textsubscript{1} distribution in two dimensions have been proposed and are summarized below. Unfortunately, no accurate approximation of the partial moments could be obtained for the multi-dimensional M\textsubscript{2} distribution. This difficulty can be partially associated with the increased number of dependent variables compared to M\textsubscript{1}. As a result, the partial moments for the M\textsubscript{2} model are evaluated by repeatedly solving the maximization problem Eq. (3.17) using the optimization toolbox NLOPT described previously in Section 3.5.1. For a given set of moments, the corresponding Lagrange multipliers...
are determined from the solver. The entropy-maximizing distribution of Eq. (3.16) can then be integrated over the appropriate hemisphere to obtain the corresponding values of the partial moments. Despite the fact that this is the most accurate approach for determining the partial moments, the repeated numerical solution of the maximization problem obviously significantly increases the computational efforts required for solving the governing equations of the M2 model. In the future, approximate boundary treatment would therefore be highly desirable.

3.7.4 Approximation of the Partial Moments for the M1 Closure

This section proposes to approximate the partial moments for the M1 distribution in two dimensions using an interpolative fitting procedure, thereby avoiding the computationally costly numerical evaluation of the partial moments during a computation. The idea consists of approximating the partial moments for the case of a one-dimensional distribution, and then extend it to multi-dimensional distributions. Figures 3.7, 3.8 and 3.9 show the variation of the partial radiative energy and the partial radiative fluxes in the x- and y-directions respectively for different values of the normalized flux. For the one-dimensional case, the partial moments can be approximated with the following expression

\[ \langle . \rangle_{1D}^+ = E_1((A_1, a_1), (A_2, a_2))(N_1^1) + Z_2(a_1, a_2)(N_1^1)Q_1(N_1^1) \] (3.66)

Figure 3.7: Partial Radiative Energy for the M1 Distribution in a) One Dimension and b) Two Dimensions.
Figure 3.8: Partial $x$-direction Radiative Flux for the $M_1$ Distribution in a) One Dimension and b) Two Dimensions.

\[ a_1 = -1, \quad a_2 = 1 \]
\[ A_1 = 0, \quad A_2 = \begin{cases} 1 & \text{for } E^+ \\ 1 & \text{for } F^{x+} \\ 0 & \text{for } F^{y+} \end{cases} \]

where $Q_1$ is a polynomial of degree 8 in $N_1^1$ for which the coefficients are determined such that the $L^2$ norm between the approximated and exact values (obtained by solving the

Figure 3.9: Partial $y$-direction Radiative Flux for the $M_1$ Distribution in a) One Dimension and b) Two Dimensions.
corresponding optimization problem) of the corresponding partial moments is minimized. The $L^\infty$ - norm of the error of the approximation for 1000 values of $N_1$ equally distributed between $[-1, 1]$ was found to be $6.4 \times 10^{-5}$ for $E^+$, $9 \times 10^{-6}$ for $F^+$ and $1.408 \times 10^{-2}$ for $F^y$.

In Eq. (3.66), $E_1((A, a), (B, b))(x)$ is a Lagrange polynomial of degree one, interpolating the values of $A$ and $B$ at the points $a$ and $b$, and is given by

$$E_1((A, a), (B, b))(x) = A \frac{x - b}{a - b} + B \frac{x - a}{b - a}$$

(3.67)

and $Z_2$ is a polynomial of degree two, which is zero in $a$ and $b$ and has the form

$$Z_2(a, b)(x) = (x - a)(x - b)$$

(3.68)

The previous approximation of the partial moments in one dimension can now be extended to two-dimensional problems. More specifically, the partial moments in two dimensions are approximated such that they are exact on the boundaries of the realizability domain, i.e., $N_2 = \pm \sqrt{1 - N_1^2}$, and approximate the corresponding values of the partial moments away from the boundaries. Moreover, the approximation is defined such that it reproduces Eq. (3.66) in the one-dimensional case, i.e., $N_2 = 0$. Hence, the following approximation is made

$$\langle \rangle_{2D}^+ = E((A_1, a_1), (A_2, a_2), (A_3, a_3))(N_2) + Z(a_1, a_2, a_3)(N_2)Q_2(N_1, N_2)$$

(3.69)

$$a_1 = -\sqrt{1 - (N_1^2)}, \quad A_1 = \begin{cases} 0 & \text{if } f_x < 0 \text{ and } 1 & \text{if } f_x > 0 \text{ for } E^+ \\ 0 & \text{if } f_x < 0 \text{ and } f_x & \text{if } f_x > 0 \text{ for } F^+_x \\ 0 & \text{if } f_x < 0 \text{ and } f_y & \text{if } f_x > 0 \text{ for } F^+_y \end{cases}$$

$$a_2 = 0, \quad A_2 = \begin{cases} E_{1D} & \text{for } E^+ \\ F_{x, 1D} & \text{for } F^+_x \\ F_{y, 1D} & \text{for } F^+_y \end{cases}$$

$$a_3 = \sqrt{1 - (N_1^2)}, \quad A_3 = \begin{cases} 0 & \text{if } f_x < 0 \text{ and } 1 & \text{if } f_x > 0 \text{ for } E^+ \\ 0 & \text{if } f_x < 0 \text{ and } f_x & \text{if } f_x > 0 \text{ for } F^+_x \\ 0 & \text{if } f_x < 0 \text{ and } f_x & \text{if } f_x > 0 \text{ for } F^+_x \end{cases}$$

where $Q_2$ is a polynomial of degree 16 in $N_1$ and $N_2$ for which the coefficients were determined such that the $L^2$ - norm of the error between the approximated and exact values of the corresponding partial moments for 10,000 values of $(N_1, N_2) \in [-1, 1] \times [-\sqrt{1 - (N_1^2)}, \sqrt{1 - (N_1^2)}]$ is minimized. These values were chosen from 100 values of
$N_1^1$ equally distributed in $[-1, 1]$ and 100 of $N_2^1$ equally distributed in $[-\sqrt{1 - (N_1^1)^2}, \sqrt{1 - (N_1^1)^2}]$. The $L^\infty$– norm of the error of the resulting fits were found to be $3.472 \times 10^{-2}$ for $E^+$, $1.493 \times 10^{-3}$ for $F_x^+$, and $5.076 \times 10^{-2}$ for $F_y^+$. 
Chapter 4

Finite-Volume Solution Method

In this chapter, the main elements of the proposed upwind finite-volume scheme and the time marching and iterative techniques used to solve the discrete form of the governing equations of the $M_N$ and $P_N$ models described previously are presented. The key elements of the finite-volume spatial discretization scheme as well as the details on the numerical flux evaluations are summarized in Section 4.1. Section 4.2 of the chapter describes the iterative technique based on Newton’s method used to obtain steady state solutions of the semi-discrete form of the governing equations. Finally, the incorporation of the finite-volume scheme within a block-based anisotropic adaptive mesh refinement (AMR) is discussed in Section 4.3.

4.1 Finite-Volume Spatial Discretization Method

The hyperbolicity of the systems of moment equations for the $M_1$, $M_2$, $P_1$ and $P_3$ closures makes them very well suited for solution by the now standard family of upwind finite-volume techniques originally developed by Godunov [56] for hyperbolic systems of conservation laws. More specifically, in this study, the systems of moment equations are solved using an upwind Godunov-type finite-volume method (FVM) with block-based anisotropic AMR. The proposed scheme is similar to that described by Groth and co-workers [57–61] for a range of physically-complex flows including laminar and turbulent reactive flows, where the moment equations are integrated over quadrilateral cells of a two-dimensional body-fitted, multi-block mesh.

The finite-volume method used in this work is based on the integral form of the gov-
erning conservation equations. Applying the divergence theorem for a two-dimensional coordinate frame to the differential form of the governing equations given in Eq. (3.51) yields the following integral form

$$\frac{d}{dt} \int_A U \, dA + \oint_C \vec{n} \cdot \vec{F} \, dl = \int_A S \, dA, \quad (4.1)$$

where $\vec{F} = (F, G)$ is the flux dyad, $A$ is the control volume, $C$ is the closed contour of the control volume and $\vec{n}$ is the unit outward vector normal to the closed contour. In the finite-volume method, the integral form of the governing equations is enforced discretely in each of many small contiguous control volumes making up a computational mesh. Using Eq. (4.1), the net rate of change of any radiative quantity, for example radiative energy density, radiative heat flux, within each finite control volume can be expressed as a balance between the net solution fluxes through the surface containing the volume of interest and volumetric sources tending to increase or decrease its value.

The averaged values of $U$ and $S$ in each cell or control volume can be defined by an integrated average applied each control volume as follows

$$\bar{U} = \frac{1}{A} \int_A U \, dA, \quad (4.2)$$

$$\bar{S} = \frac{1}{A} \int_A S \, dA, \quad (4.3)$$

where $A$ is the cell area. Substituting these expressions into Eq. (4.1) results in the following final form of equation (4.1)

$$\frac{d\bar{U}}{dt} + \frac{1}{A} \oint_C \vec{n} \cdot \vec{F} \, dl = \bar{S}(\bar{U}), \quad (4.4)$$

where $dl$ is an element of the closed contour containing the control volume of interest. Under the assumption that the control volume $(i, j)$ is a polygon defined by $N_f$ cell faces ($N_f = 4$ in this case since the FVM method makes use of a quadrilateral mesh), a semi-discrete form of Eq. (4.4) can be written as

$$\frac{d\bar{U}_{ij}}{dt} = -\frac{1}{A_{ij}} \sum_{m=1}^{N_f} \vec{F}_{ij,m} \cdot \vec{n}_{ij,m} \, \Delta l_{ij,m} + \bar{S}_{ij}(\bar{U}_{ij}), \quad (4.5)$$

or

$$\frac{d\bar{U}_{ij}}{dt} = -\bar{R}_{ij}(\bar{U}), \quad (4.6)$$
where $\Delta l_{i,j,m}$ and $\vec{n}_{i,j,m}$ are the length and unit outward normal vector of the $m^{th}$ face of cell $(i,j)$, respectively, and $R_{i,j}(\mathbf{U})$ is the residual operator for computational cell $(i,j)$.

The solution procedure for solving the coupled non-linear ordinary differential equations of Eq. (4.6) involves three steps: reconstruction, flux function evaluation and evolution or time marching. In the first step, for given values of $\mathbf{U}$ in each cell, an approximation of $\mathbf{U}(\vec{x})$ throughout each cell is constructed and used to find $\mathbf{U}$ at the boundaries of the corresponding cell. The accuracy of this so-called solution reconstruction procedure dictates the accuracy of the evaluation of cell-averaged solution and its derivatives for the cell-normal flux evaluation. In this work, a piecewise linear limited reconstruction is used, as presented in Section 4.1.1. Next, the flux, $\mathbf{F}(\mathbf{U})$ at the cell boundaries is evaluated as a function of the discontinuous states on either side of the interface, where the discontinuities arise due to the piecewise approximations of $\mathbf{U}$ within each control volume. In this work, the numerical flux at each cell face is evaluated as the solution of the approximate Riemann problem based on either the Harten-Lax-van-Leer-Einfeldt (HLLE) flux function [62] or Roe flux function [63]. Finally, steady-state solutions are obtained using an implicit Newton-Krylov Schwarz (NKS) iterative algorithm with General Minimal Residual (GMRES) method for the associated linear system. Details of the NKS method adopted and developed in this work can be found in Section 4.2.

### 4.1.1 Hyperbolic Flux Evaluation

Godunov-type finite-volume methods make use of the solution of locally one-dimensional Riemann problem in order to evaluate the numerical flux at the cell boundaries. The original Godunov method is however based on a piecewise constant reconstruction of the solution within each cell of the computational domain, which reduces the accuracy of the overall scheme to first order. The accuracy of the scheme can be further improved with high-resolution schemes. As such, a second order formulation of the original Godunov method, based on approximate Riemann solvers and least-squares piece-wise limited linear solution reconstruction procedure is used in this work in order to solve the systems of moments equations for $M_1$, $M_2$, $P_1$ and $P_3$. The emergence of high-resolution Godunov-type methods motivated the design of effective limiters for use in one-dimensional higher-order reconstructions [64–66].
Piecewise Limited Linear Reconstruction

The solution reconstruction used in this work can be summarized as follows. For higher-order accuracy (second-order in smooth regions), a limited linear spatial reconstruction of the solution in each computational cell is required. The values of the left and right solution states at a cell interface are determined by means of a least-squares piecewise limited linear solution reconstruction. More specifically, for a given cell \((i, j)\), at the cell interface \((i + \frac{1}{2}, j)\), the flux is computed as follows

\[
\mathbf{F}_{(i,j,m)} \cdot \mathbf{n}_{(i,j,m)} = \mathbf{F} \left( \mathcal{R} \left( \mathbf{W}_L, \mathbf{W}_R, \mathbf{n}_{(i,j,m)} \right) \right)
\]

(4.7)

where \(\mathbf{n}_{(i,j,m)}\) corresponds to the unit outward unit vector normal to the cell interface \(m\), \(\mathcal{R}\) represents the solution of the Riemann problem, and \(\mathbf{W}_L\) and \(\mathbf{W}_R\) are the left and right primitive solution vectors from the piecewise limited linear reconstruction procedure at the cell interface \((i + \frac{1}{2}, j)\), which are respectively given by

\[
\begin{align*}
\mathbf{W}_L &= \mathbf{W}_{i,j} + \Phi_{i,j} \mathbf{\nabla} \mathbf{W}_{i,j} \cdot d\mathbf{x}_L \\
\mathbf{W}_R &= \mathbf{W}_{i+1,j} + \Phi_{i+1,j} \mathbf{\nabla} \mathbf{W}_{i+1,j} \cdot d\mathbf{x}_R
\end{align*}
\]

(4.8)

In Eq. (4.8), \(\Phi\) is the slope limiter, \(d\mathbf{x}_L = \mathbf{x} - \mathbf{x}_{i,j}\) and \(d\mathbf{x}_R = \mathbf{x} - \mathbf{x}_{i+1,j}\) (where \(\mathbf{x}\) is the location of the cell interface and \(\mathbf{x}_{i,j}\) and \(\mathbf{x}_{i+1,j}\) represent the position vectors at the centers of the left and right cells, respectively), and \(\mathbf{W}_{i,j}\) and \(\mathbf{W}_{i+1,j}\) are cell-averaged primitive solution vectors.

The slope limiter, \(\Phi\), is used to limit the solution gradient in order to ensure solution monotonicity. Various slope limiters are available, with the Barth-Jespersen [67] and the Venkatakrishnan [68] slope limiters studied here. The two slope limiters behave similarly, with the only difference lying in the way they vary when encountering nearly smooth regions of the solution. The Barth-Jespersen limiter is evaluated using

\[
\phi_{ik} = \begin{cases} 
\min(1, \frac{u_{\text{max}} - \bar{u}_i}{u_{\text{ik}} - \bar{u}_i}) & \text{if } u_{\text{ik}} - \bar{u}_i > 0 \\
\min(1, \frac{u_{\text{min}} - \bar{u}_i}{u_{\text{ik}} - \bar{u}_i}) & \text{if } u_{\text{ik}} - \bar{u}_i < 0 \\
1 & \text{otherwise}
\end{cases}
\]

(4.9)

where \(\bar{u}_i\) is the mean value in cell \(i\), \(u_{\text{ik}} = u_i(x = x_{ik})\) is the original unlimited cell values at each of the quadrature locations \(x_{ik}\) used in the flux evaluations at the faces of cell \(i\), and \(u_{\text{max}}\) and \(u_{\text{min}}\) are the maximum and minimum cell averaged values of cell \(i\) and its
neighboring cells used in the reconstruction procedure, respectively. Finally, the slope limiter $\phi_i$ is determined as the overall minimum value from the set of $\phi_{ik}$. The Barth-Jespersen limiter is known to have convergence issues as it is active in the near-constant regions and responds to oscillations at the noise level, as stated by Venkatakrishnan [68]. The latter then proposed a limiter, which is a modification of the Barth-Jespersen approach that helps suppress oscillations in the near-constant regions of the solution in a smooth manner, and is expected to overcome these convergence issues. The limiter of Venkatakrishnan is evaluated using

$$\phi_{ik} = \begin{cases} 
\phi\left(\frac{u_{\text{max}} - \bar{u}_i}{u_{ik} - \bar{u}_i}\right) & \text{if } u_{ik} - \bar{u}_i > 0 \\
\phi\left(\frac{u_{\text{min}} - \bar{u}_i}{u_{ik} - \bar{u}_i}\right) & \text{if } u_{ik} - \bar{u}_i < 0 \\
1 & \text{otherwise}
\end{cases}$$

(4.10)

where $\phi(y)$ is a smooth function given by

$$\phi(y) = \frac{y^2 + 2y}{y^2 + y + 2}$$

(4.11)

The gradients of the primitive variables, $\vec{\nabla} W$, are determined by applying a least squares approach [69], a suitable technique which relies on a stencil formed by the nearest and possibly next to nearest neighboring cells. For the boundary stencil, a layer of ghost cells containing boundary condition informations is used to generalize the procedure without reducing the reconstruction stencil. For a cell-centered discretization in two-dimensions, the stencil is formed by joining the nearest eight neighboring cell centroids. The approximate gradients using the least-squares gradient construction procedure are obtained by minimizing the error defined by

$$\sum_{k=1}^{k=N} \epsilon_{ik}^2 = \sum_{k=1}^{k=N} (\Delta W_{ik} - \vec{\nabla} W_i \cdot d\vec{x}_{ik})^2$$

(4.12)

where $\Delta W_{ik} = W_i - W_k$, $d\vec{x}_{ik} = \vec{x}_i - \vec{x}_k$, $N = 8$ in two dimensions. The $2 \times 2$ system of linear algebraic equations resulting from the minimization problem can be expressed as

$$\begin{bmatrix}
(\Delta x)^2 & \Delta x \Delta y \\
\Delta x \Delta y & (\Delta y)^2
\end{bmatrix}
\begin{bmatrix}
\frac{\partial W}{\partial x} \\
\frac{\partial W}{\partial y}
\end{bmatrix}
= \begin{bmatrix}
W \Delta x \\
W \Delta y
\end{bmatrix}$$

(4.13)
where

\[ \Delta x^2 = \frac{1}{N} \sum_{k=1}^{N} \Delta x_{ki}^2 \]  

(4.14)

\[ \Delta x \Delta y = \frac{1}{N} \sum_{k=1}^{N} \Delta x_{ki} \Delta y_{ki} \]  

(4.15)

and

\[ \Delta W \Delta x = \frac{1}{N} \sum_{k=1}^{N} \Delta W_{ki} \Delta x_{ki} \]  

(4.16)

The other terms in Eq. (4.13) can be formulated similarly. The above expressions only depend on grid geometry and can therefore be precomputed and stored. Solutions of the 2 × 2 linear system represented by Eq. (4.13) can be readily obtained using Cramer’s rule.

**Approximate Riemann Solvers**

The Riemann problem is a special form of an initial value problem (IVP) with discontinuous initial states and self-similar solutions. It is posed at the interface between adjacent cells, and provides a means for evaluating the numerical flux functions at cell boundaries. For a one-dimensional system of conservation laws given by

\[ \frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0, \]  

(4.17)

the corresponding initial conditions for the Riemann problem can be expressed as

\[ U(x,0) = \begin{cases} U_L & \text{if } x < 0 \\ U_R & \text{if } x > 0 \end{cases}, \]  

(4.18)

where \( U_L \) and \( U_R \) are the left and right initial states on either side of the discontinuity (cell interface) at \( x = 0 \) respectively. The discontinuous initial states and the subsequent time evolution of the discontinuities that develop are representative of conditions present between neighbouring cells in finite-volume methods. Figure 4.1 shows an illustration of the Riemann problem for a one-dimensional system of conservative equations with two wavespeeds. The state variables in the intermediate region, represented by \( U_* \), are the conservative unknowns in this problem, and can be solved for using Rankine-Hugoniot relations to calculate the overall flux between \( U_L \) and \( U_R \).
Solving the Riemann problem by making use of a very efficient exact solution procedure, such as the one described by Gottlied and Groth [70] for the conservation equations governing a compressible polytropic gas, is not generally possible for other systems of conservation equations as considered here. Often, an approximation is sufficient for use in finite-volume schemes. The Roe solver [63], which is based on a local linearization of the flow equations, is one of the most detailed approximations for the wave system associated with the Riemann problem. The family of solvers presented by Harten, Lax, and van Leer (HLL) [62] is also widely used for providing approximate solutions of the Riemann problem due to their simplicity.

**Approximate Roe Riemann-Solver-Based Flux Function**

Roe’s approximate Riemann solver is based on the fact that for a strictly linear system of equations, the Riemann problem can be solved exactly by using the eigenstructure of the system. For nonlinear hyperbolic equations, locally linearized characteristic variables are used to provide approximation to the solution. In order to understand Roe’s approximation, let us consider the nonlinear system of conservation equations in one-space dimension of the form

\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = \frac{\partial U}{\partial t} + \mathbf{A} \frac{\partial U}{\partial x} = 0
\]  

(4.19)

with the Jacobian matrix \( \mathbf{A} = \frac{\partial F}{\partial U} \). This Jacobian can be replaced in an approximate manner with a Roe matrix, \( \bar{\mathbf{A}} \), dependent on some intermediate state \( U^* \), which in turn

\[
\begin{aligned}
\frac{\partial U}{\partial t} + \mathbf{A} \frac{\partial U}{\partial x} &= \mathbf{0} \\
\frac{\partial \mathbf{U}}{\partial t} + \bar{\mathbf{A}} \frac{\partial \mathbf{U}}{\partial x} &= \mathbf{0}
\end{aligned}
\]  

Figure 4.1: Illustration of the one-dimensional Riemann problem.
is a function generally depending non-linearly on the initial states $U_L$ and $U_R$.

The creation of this replacement matrix for the flux Jacobian is subject to a number of stipulations, which are outlined below, in order to accurately mimic the behaviour of the original Jacobian. The conditions on $\bar{A}$ making up Roe’s so-called property $U$ are [71,72]:

1. In the limit that $U_L = U_R = U$, $\bar{A}$ should be able to recover the same system as the original Jacobian such that

$$\bar{A}(U_L, U_R) = \bar{A}(U, U) = A(U) = \frac{\partial F}{\partial U} \quad (4.20)$$

2. An exact solution exists for an isolated discontinuity between $U_L$ and $U_R$, such that

$$\Delta F = \bar{A}(U_L, U_R) \Delta U \quad (4.21)$$

3. The Roe matrix $\bar{A}$ has real, distinct eigenvalues and a complete set of linearly independent eigenvectors to retain the hyperbolic nature of the original system of equations.

The first and second properties are necessary to obtain the correct net change of density and flux in each cell from one time step to the next. The third property is used in the transformation of conserved variables into characteristic variables.

The final form of the flux function can be written as

$$F = \frac{1}{2} \bar{A}(U_L + U_R) - \frac{1}{2} \sum_{k=1}^{n} |\lambda_k| (W_{c,k}^R - W_{c,k}^L) \bar{r}_k \quad (4.22)$$

where $n$ is the number of conserved variables, $W_{c,k}^L$ and $W_{c,k}^R$ are characteristic variables of the left and right states of the cell interface, and $\lambda_{*,k}$ and $\bar{r}_{*,k}$ are the eigenvalues and the right eigenvectors associated with each conserved variable. Using property 2 (Eq. (4.21)), the above equation can be simplified even further to obtain

$$F = \frac{1}{2} (\bar{F}_L + \bar{F}_R) - \frac{1}{2} \sum_{k=1}^{n} \bar{r}_k |\lambda_k| (l_k \cdot \Delta U) \quad (4.23)$$

where $\bar{F}_L$, $\bar{F}_R$ are the left and right states of the interface, and $l_k$ are the left eigenvectors associated with each conserved variable. The complete eigenstructure of the $M_1$, $P_1$ and $P_3$ closures can be derived from their corresponding flux Jacobians, i.e., Eqs. (3.59),
(3.55) and (3.57), respectively, and the Roe flux can then be evaluated using Eq. (4.23).

**HLL Riemann-Solver-Based Flux Function**

The HLL approximate Riemann solver [62] is based on a two-wave solution or 3-state approximate solution to the Riemann problem. In this approach, the corresponding flux function is given by

\[
\mathcal{F} = \begin{cases} 
\bar{F}_L, & \text{if } \lambda^- \geq 0 \\
\bar{F}_*, & \text{if } \lambda^- < 0 < \lambda^+ \\
\bar{F}_R, & \text{if } \lambda^+ \leq 0 
\end{cases}
\]

where \(\lambda^-\) and \(\lambda^+\) are the left and right signal velocities, respectively. The flux function \(\bar{F}_*\) in the intermediate region is a function of the state vector \(U_*\) in that region, which can be expressed in terms of the known quantities on the left and right states using Rankine-Hugoniot conditions [73]. Applying such conditions across each of the wavespeeds \(\lambda^-\) and \(\lambda^+\) yields,

\[
\bar{F}_* - \bar{F}_L = \lambda^- (U_* - U_L), \tag{4.24}
\]

\[
\bar{F}_* - \bar{F}_R = \lambda^+ (U_* - U_R). \tag{4.25}
\]

Solving the system of equations formed by Eqs. (4.26) and (4.27) for the solution vector in the intermediate state as well as its corresponding flux results in the following expressions

\[
U_* = \frac{\lambda^+ U_R - \lambda^- U_L}{\lambda^+ - \lambda^-} - \frac{\bar{F}_R - \bar{F}_L}{\lambda^+ - \lambda^-} \tag{4.26}
\]

\[
\bar{F}_* = \frac{\lambda^+ \bar{F}_L - \lambda^- \bar{F}_R}{\lambda^+ - \lambda^-} + \frac{\lambda^+ \lambda^-}{\lambda^+ - \lambda^-} (U_R - U_L) \tag{4.27}
\]

One primary defect of this scheme is exposed by contact discontinuities, shear waves and material interfaces due to the missing intermediate waves.

Einfeldt [74] proposed the following estimates for \(\lambda^-\) and \(\lambda^+\)

\[
\lambda^- = \min(\lambda_L^{\min}, \bar{\lambda}^{\min} (U_L, U_R)) \tag{4.28}
\]

\[
\lambda^+ = \max(\lambda_R^{\max}, \bar{\lambda}^{\max} (U_L, U_R)) \tag{4.29}
\]

where \(\bar{\lambda}\) represents Roe’s averaged eigenvalue. Einfeldt’s contribution yields a more effective and robust scheme, which is referred to in this work as the HLLE approximate Riemann solver.
An advantage of the HLLE flux function is that estimates of the fastest and slowest wavespeeds are all that are required when evaluating the flux. For the moments closures of interest here (M₁, M₂, P₁ and P₃), the fastest and slowest eigenvalues can be obtained directly from the eigenstructure of the corresponding system of moment equations (see Eq. (3.60), (3.56) and (3.58) for M₁, P₁ and P₃ respectively), or estimated as the maximum and minimum allowable wavespeeds c and −c, as was done for the approximate M₂ closure in this work since no analytical expression could be obtained for the corresponding eigenvalues.

4.1.2 Frame Rotation

In order to deal with the two-dimensional features of the quadrilateral computational grids considered herein, the evaluation of the hyperbolic numerical fluxes at each cell face is performed by solving a Riemann problem in a rotated frame, for which the x-axis is aligned and in the same direction as the outward vector normal to the cell face. The boundary conditions discussed in Section 3.7 also make use of such transformation in order to evaluate the partial outgoing moments. This greatly simplifies the implementation of the moment closure methods in a computer code. In fact, instead of deriving the expressions for the numerical fluxes or boundary conditions for each coordinate direction, the only expressions that are needed are those in the x-direction, and those in the other directions can be obtained by an appropriate transformation of the frame. In

![Frame rotation in two dimensions.](image)

**Figure 4.2:** Frame rotation in two dimensions.

two dimensions, the rotation matrix Σ describing the transformation from the original
frame, \( X \), to the new frame, \( x \), such that \( X = \sum x \), has the following form

\[
R = \begin{bmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{bmatrix}
\]

(4.30)

where \( \theta \) is the angle between the rotated coordinate system \( x \) and the unrotated one \( X \). This transformation can be reexpressed in tensor notation as follows:

\[
x_i = R_{ij}x'_j, \quad x'_i = R_{ji}x_j
\]

(4.31)

The expressions of the moments of order up to three in the rotated frame then read as follows

\[
I^{(1)}_i = R_{ij}I^{(1)'}_j, \quad I^{(1)'}_i = R_{ji}I^{(1)}_j
\]

(4.32)

\[
I^{(2)}_{ij} = R_{ip}R_{jq}I^{(2)'}_{pq}, \quad I^{(2)'}_{ij} = R_{pi}R_{qj}I^{(2)}_{pq}
\]

(4.33)

\[
I^{(3)}_{ijk} = R_{ip}R_{jq}R_{rk}I^{(3)'}_{pqr}, \quad I^{(3)'}_{ijk} = R_{ipi}R_{qji}R_{kr}I^{(3)}_{pqr}
\]

(4.34)

4.2 Newton Krylov Schwarz (NKS) Method

Numerical simulations of combustion generally require modeling of many different and relevant phenomena, such as heat transfer (via conduction, convection and/or radiation), chemical kinetics, turbulence, and multi-phase flows. Compared to the other phenomena involved in such multidisciplinary field, radiative transport occurs at much faster rates. As a result of the relatively small time scales associated with radiative heat transfer, we are generally only interested in the steady state solution of the RTE. Moreover, for most practical engineering applications, the problem of interest may involve very complex geometries and realistic physics (anisotropic scattering, non-gray medium), therefore requiring the determination of a large number of unknowns to compute the solution. In such situations, the use of an explicit method, for which stability issues would limit the maximum allowable time step, would require excessive iterations. Such problems can be effectively addressed by application of Newton’s method to the resulting system of algebraic equations, and subsequently a Krylov subspace method, such as the generalized minimal residual (GMRES) algorithm proposed by Saad [75–78], in combination with an additive Schwarz preconditioning technique to solve the large, sparse system of linear equations at each Newton step.

Newton’s method is applied herein to obtain steady-state solutions for the system of
linear/non-linear moment equations given in Eq. (3.51) by relaxing the semi-discrete form of the latter to a steady-state such that

\[ R(U) = \frac{dU}{dt} = 0 \]  

(4.35)

The particular implementation of the Newton method used here has been developed previously by Groth and Northrup [79] as well as Charest et al. [1,24] for computations on large multi-processor parallel clusters. It consists of a Jacobian-free inexact Newton method coupled with an iterative Krylov subspace linear solver. Given an initial estimate \( U^0 \), Newton’s method seeks a solution to Eq. (4.35) by iteratively solving a sequence of linear systems until a desired reduction of the residual is achieved, i.e., \( \| R(U^k) \| < \epsilon \| R(U^0) \| \), where the parameter \( \epsilon \) is the tolerance and is given a value of \( 10^{-10} \) in this work. At the \( k^{th} \) Newton step iteration, the linear system to be solved has the form

\[ \left( \frac{\partial R}{\partial U} \right)_k \Delta U^k = J(U_k) \Delta U^k = -R(U^k) \]  

(4.36)

where \( J = \frac{\partial R}{\partial U} \) is the residual Jacobian, and the improved solution at the \( k^{th} \) step is determined from

\[ U^{k+1} = U^k + \Delta U^k \]  

(4.37)

The linear system of equations (4.36) tends to be large, sparse, and non-symmetric. One effective approach that is widely used for solving systems of such type is the generalized minimal residual (GMRES) technique, developed by Saad and co-workers [75–78]. The GMRES is an Arnoldi-based solution technique which generates orthogonal bases of the Krylov subspace to construct the solution. The technique is particularly attractive because the matrix \( J \) is not explicitly formed and instead only matrix-vector products are required at each iteration to create new trial vectors, hence reducing the required storage. Termination also generally only requires solving the linear system to some specified tolerance, \( \| R(U^k) + J(U^k) \Delta U^k \| < \zeta \| R(U^k) \| \), where \( \zeta \) is typically in the range \( 0.1 - 0.5 \) [80].

To guarantee effectiveness of the GMRES method, right preconditioning of the matrix \( J \) is performed, which helps facilitate the solution of Eq. (4.36) without affecting the solution residual vector \( b = -R(U^k) \). The preconditioning is performed as follows

\[ (JM^{-1})(Mx) = b \]  

(4.38)
where $M$ is the preconditioning matrix and $x = \Delta U^k$. A combination of and additive Schwarz preconditioner and a block incomplete lower-upper (BILU) local preconditioner is used which is easily implemented in the block-based anisotropic AMR scheme. The additive Schwarz preconditioner updates the solution in each block simultaneously whereas shared boundary data is not updated until a full cycle of updates has been performed on all domains. The preconditioner is defined as follows

$$M^{-1} = \sum_{k=1}^{N_B} B_k^T M_k^{-1} B_k$$

where $N_B$ is the number of blocks and $B_k$ is the gather matrix for the $k^{th}$ domain. The local preconditioner $M_k^{-1}$ is based on block ILU(p) factorization [78] of the Jacobian for the first-order approximation of each domain. In this work, the level of fill, $p$, was maintained at 4 in order to minimize storage requirements.

The application of Newton’s method to the system of moment equations does not yield an unconditionally stable scheme, and failure can occur, especially when the initial solution estimates fall outside the radius of convergence. To ensure global convergence of the algorithm, the implicit Euler startup procedure with switched evolution/relaxation (SER) that was proposed by Mulder and Van Leer [81] was used. Application of this startup procedure to the semi-discrete form of the governing equations gives

$$\left[-\frac{\Gamma}{\Delta t^n} + \left(\frac{\partial R}{\partial U}\right)^n\right] \Delta U^n = -R^n$$

where $\Delta t^n$ is the time step. In the SER approach, the time step is varied from some small finite value and gradually increased as the steady state solution is approached. As $\Delta t^n \to \infty$, Newton’s method is recovered. In the quasi-Newton and SER methods, the time step size was determined by considering the inviscid Courant-Friedrichs-Lewy (CFL) conditions, which read as follows

$$\Delta t^n = \text{CFL} \times \min \left[ \frac{\Delta x}{\lambda_i} \right]$$

where CFL is a constant greater than zero, which determines the time step size, and $\lambda_i$ are the eigenvalues of the system of moment equations under consideration. A value for CFL between $10 - 100$ is typically used during the startup phase of the Newton calculation.
4.3 Anisotropic Adaptive Mesh Refinement

Typical computational fluid dynamics (CFD) problems are usually hard to solve due to numerical stiffness associated with disparate spatial and temporal scales. More specifically, certain areas of the computational domain may require more resolution than others due to the existence of particular features (shock, steep gradients, discontinuities) that must be captured accurately. A block-based hierarchical data structure is used in conjunction with the finite-volume scheme described above to facilitate automatic solution-directed mesh adaptation on multi-block mesh according to physics-based criteria. By changing the mesh based on the physics-based criteria as the computation is performed, areas of interest are resolved with high mesh densities, while areas with smaller solution changes are evaluated with larger cells. When used in conjunction with the finite-volume scheme described above, the entire technique can be used to treat problems with steep radiation gradients and small length scales accurately with reduced computational costs.

A flexible block-based AMR scheme has been proposed by Groth and co-workers [60, 61, 82–84], which is suitable for implementation on large-scale distributed-memory computing clusters and has been successfully used for a range of physically-complex flows. The scheme borrows aspects from previous work by Berger and co-workers [85–88], Quirk [89], and De Zeeuw and Powell [90] for Cartesian grids. In the AMR scheme, the system of moment equations are first integrated forward in time on an initial structured, multi-block mesh in order to obtain volume-averaged solution quantities. The mesh is then adapted
Figure 4.4: Adaptive mesh refinement binary-tree data structure and associated solution blocks for a quadrilateral mesh.

by coarsening or refining the block designated by the refinement criteria. A hierarchical tree-like data structure, shown in Fig. 4.3, is used to retain connectivity between solution blocks and track their refinement history. The blocks requiring refinement are termed “parents” and are divided into four new block called “children”. Each child is a new block with the same number of cells as its parent, doubling the mesh resolution in the region. Coarsening flagged blocks is carried out by reversing this process and combining four children into one single parent.

The AMR scheme described above refines the mesh equally in all directions based on the refinement criteria. However, in problems with anisotropic features, refinement of the mesh may only be needed in a specific direction. In such situations, an anisotropic variant of the AMR techniques would offer greater flexibility and further computational savings by adding directionality to the refinement process. Following the work by Groth et al. [91,92] for computational magnetohydrodynamics, Zhang and Groth [93] proposed an anisotropic AMR technique for computations in two dimensional problems. The procedure is somewhat similar to that of the isotropic AMR, the main distinction lying in the way blocks are divided. For a 2D Cartesian mesh, isotropic AMR divides each parent block into four children, which is equivalent to doubling the mesh resolution in both directions. In comparison, the anisotropic AMR technique allows each parent block to be divided into two children by splitting the parent blocks in either one of the directions of interest, as shown in Fig. 4.5. As a result, cell resolution doubles in the direction of interest, but remains the same in the other directions. Fig. 4.4 illustrates the hierarchical tree-like data structure used to retain connectivity between blocks and
Figure 4.5: Illustration of refinement and coarsening of an 8 x 8 block, during (i) anisotropic AMR in $\xi$, (ii) anisotropic AMR in $\zeta$ and (iii) isotropic AMR cell division. Their geometrical relationships are also represented.

track their refinement history.

In this study, both isotropic and anisotropic versions of the block-based AMR scheme were implemented. Comparisons of the two refinement techniques is presented in Section 5.4 of Chapter 5. The refinement criteria are based on the gradient of the radiative energy $E$ determined numerically from neighboring cells, which is defined by

$$\epsilon_1 \propto \frac{\left| \nabla E \right|}{E}$$  \hspace{1cm} (4.42)

for the isotropic mesh refinement and

$$\epsilon_{1x} \propto \frac{\left| \nabla_x E \right|}{E}$$  \hspace{1cm} (4.43)

$$\epsilon_{1y} \propto \frac{\left| \nabla_y E \right|}{E}$$  \hspace{1cm} (4.44)

for the anisotropic AMR. In the case of the isotropic AMR, the mesh is refined equally in both directions and blocks are added wherever $\epsilon_1$ is large. For the anisotropic AMR, mesh refinement is performed in the $x$-direction when $\epsilon_{1x}$ is large and the refinement in the $y$-direction is dictated by values of $\epsilon_{1y}$. 
To further decrease the overall computational time of the AMR schemes, integration of the governing equations is performed in parallel. This is achieved by distributing the computational blocks among available processors and simultaneously computing the solutions for each block on each processor. Both AMR schemes (isotropic and anisotropic) were implemented using the message passing interface (MPI) library of the C++ programming language [94].

Ghost cells which surround the solution block and overlap cells on neighboring blocks, as shown in Fig. 4.6, are used to share solution content through inter-block communication. The conservation properties of the finite-volume discretization are retained across blocks with resolution changes by using the fine-grid interface flux to correct the flux computed on neighboring coarse blocks. Passing these flux corrections and the overlapping cell solution content between processors at each stage of the integration scheme accounts for the main source of inter-processor communication.
Chapter 5

Numerical Results

In this section, the predictive capabilities and accuracy of the $M_1$ and $M_2$ maximum-entropy closures are compared to and evaluated against the $P_1$ and $P_3$ spherical harmonics closure approximations as well as the DOM for several canonical test cases in both one and two space dimensions. For all the cases studied, a gray medium with isotropic scattering ($\Phi(\hat{s}', \hat{s}) = 1$) is assumed. Numerical results for all cases have been obtained for each of the moment models studied herein using the finite-volume method presented in Chapter 4. For the DOM, the finite-volume method used to obtain numerical results is described by Charest et al. [57]. Unless specified otherwise, the DOM is used with quadrature rules based on the $S_8$ scheme of Lathrop and Carlson [95]. Whenever available, the exact analytical solution is also used as a reference for comparisons. Otherwise, the solutions of a high resolution finite volume method (FVM) [57], which consists of 36 and 72 control angles in the polar and azimuthal directions, respectively, is used as an approximation to the exact solution. The choice of the FVM as an approximation to the exact solution is justified by the fact the one can chose as many control angles as needed for computations of radiative quantities.

The first set of test cases consists of radiative transfer between two parallel plates of infinite length. Different scenarios are considered whereby the properties of the medium (radiative properties and temperature) between those two plates, as well as the distance between the plates, are varied in order to assess their impact on the predictive capabilities of the $M_1$ and $M_2$ models. The next test case consists of evaluating the accuracy of the solutions of the $M_N$ closures in predicting radiative heat transfer throughout a cold medium contained within square enclosure for which all walls are cold except the bottom one. The radiative transfer within the enclosure is studied for a range of radiative
properties (absorption and scattering coefficients), allowing to assess the effect of optical thickness and scattering Albedo on the predictions of the $M_N$ closures. The ability of the maximum-entropy closures to properly predict radiative heat transfer in geometries involving sharp convex corners is then assessed by means of a test case consisting of a square enclosure with a centered obstruction. Finally, a test case with a discontinuous absorbing-emitting medium confined between two concentric circular enclosures as previously examined by Charette et al. [57] is studied in order to assess the efficiency of the anisotropic AMR. Finally, a comparison of the computational costs of the different methods is presented and a systematic comparison between accuracy and computational costs is conducted in order to determine the approximate radiation model that provides best balance between those two criteria. It should be pointed out that numerical results for the $M_2$ closure are presented only for the one-dimensional test cases, as consistent boundary conditions for the closure in multiple space dimensions could not be found.

5.1 Parallel Plates

Radiative transfer between two hot parallel plates of infinite length compared to their separation distance is studied. In the first variant of this test case, the medium between the plates is assumed to be cold (non-emitting) non-scattering, and the predictions of the different radiation models are compared for different plate separation distances. The second test case considers the effect of the temperature of the medium on the accuracy of the $M_N$ models. Finally, the last variant of this test case the effect of scattering on the predicting capabilities of the $M_N$ closures is investigated.

5.1.1 Exact Solution

For a non-scattering medium confined between two black, parallel plates, there exist an exact analytical expression to the radiative transfer equation as given by [96]. The distribution of the radiative intensity emitted from the lower and upper plates are given by

\begin{align}
I^+(\tau l, \mu) &= I_{w1}e^{-\tau /\mu} + \frac{1}{\mu} \int_0^{\tau l} I_b(\tau l)e^{-(\tau - \tau l)/\mu} d\tau l \\
&= I_b + (I_{w1} - I_b) e^{-\tau /\mu} \quad 0 < \mu < 1 \\
I^-(\tau l, \mu) &= I_{w2}e^{\tau l - \tau /\mu} - \frac{1}{\mu} \int_0^{\tau l} I_b(\tau l)e^{(\tau l - \tau)/\mu} d\tau l \\
&= I_b + (I_{w2} - I_b) e^{(\tau l - \tau)/\mu} \quad -1 < \mu < 0
\end{align} (5.1)
respectively, where \( \tau_L = \int_0^L \beta(s)ds \) is the optical thickness (or optical depth), \( L \) is the distance between the two plates, \( I_{w1} \) and \( I_{w2} \) are the intensities leaving the lower and upper plates respectively, \( I_b(\tau t) = I_b \) is the constant blackbody radiative intensity distribution of the medium, and the substitution \( \mu = \cos \theta \) is made to simplify the analysis.

Very accurate zeroth and first moments of the above exact solutions of the radiative intensities can be achieved by using a 20-point Gauss-Legendre quadrature rule such that

\[
E^\pm = \pm 2\pi \int_0^{\pm 1} I^\pm(\tau, \mu) d\mu = 2\pi \sum_{n=1}^{20} w_n I^\pm(\tau, \mu_n) \quad (5.3)
\]

\[
F^\pm = \pm 2\pi \int_0^{\pm 1} \mu I^\pm(\tau, \mu) d\mu = 2\pi \sum_{n=1}^{20} w_n \mu_n I^\pm(\tau, \mu_n) \quad (5.4)
\]

where points \( \mu_n \) and weights \( w_n \) are determined by the Gauss-Legendre quadrature in the appropriate domains (i.e. \( \mu_n \in [0, 1] \) for lower plate and \( \mu_n \in [-1, 0] \) upper plate). The overall radiative energy at any optical distance, \( \tau \), between the two plates is the sum of the radiative energy arising from both the lower and upper plates. This sum also holds true for the overall radiative heat flux.

### 5.1.2 Cold Medium

As a first test case, radiative transfer throughout a cold \((T = 0 \text{ K})\) non scattering medium with an absorption coefficient \( \kappa = 2 \text{ m}^{-1} \) between two parallel plates was studied. Each of the plates was taken to have a radiative intensity of \( 0.5 \text{ W m}^{-2} \text{ sr}^{-1} \). The predictions for the radiative energy density and the radiative heat flux, obtained using the DOM, and \( M_1, M_2, P_1 \) and \( P_3 \) moment closures are compared for two plate separation distances: 1 and 10 m, respectively, as shown in Figs. 5.1 and 5.2. The results presented have been computed using 100 uniformly-spaced computational cells to discretize the space between the plates. The analytical solution derived in Eqs. (5.3) and (5.4), is used as a reference for the comparisons. In both cases, the discrete ordinates method is observed to be very close to the exact solution.

For the small plate separation, it is readily apparent that the \( P_N \) approximations (\( P_1 \) and \( P_3 \)) yield more accurate predictions than the \( M_N \) models (\( M_1 \) and \( M_2 \)). It is also observed that the \( M_1 \) model produces an unphysical discontinuity in the radiative energy. Previous analysis [97] have shown that this jump is due to its inability to handle radiative flux occurring in opposite directions. In fact, the closure conditions for \( M_1 \) are derived under
the assumption that the intensity is symmetric about the direction of the flux. Such an

**Figure 5.1:** Numerical predictions of (a) the radiative energy, $E$, (left panel) and (b) $y$-direction flux, $F_y$, (right panel) obtained using the $M_1$ and $M_2$ maximum-entropy closures, $P_1$ and $P_3$ spherical harmonics approximations and DOM for radiative emission between two infinitely long parallel plates with a separation distance of 1 m and a cold ($T = 0 \text{K}$) non-scattering medium, showing comparisons to exact analytical solution.

**Figure 5.2:** Numerical predictions of (a) the radiative energy, $E$, (left panel) and (b) $y$-direction flux, $F_y$, (right panel) obtained using the $M_1$ and $M_2$ maximum-entropy closures, $P_1$ and $P_3$ spherical harmonics approximations and DOM for radiative emission between two infinitely long parallel plates with a separation distance of 10 m and a cold ($T = 0 \text{K}$) non-scattering medium, showing comparisons to exact analytical solution.
assumption is however violated in this test case. Nevertheless, for the larger plate separation, the discontinuity in the $M_1$ solution is less important and the predictions of the $M_2$ closure are closer to the exact solution than the $P_N$ approximations. In both cases, the higher-order $M_2$ model overcomes the inability of the $M_1$ model to adequately represent radiative transport in more than one important direction by producing a solution that is qualitatively in good agreement with the exact solution.

5.1.3 Absorbing-Emitting Medium

The next set of one-dimensional radiation problems are similar to the previous cases, the primary differences being that the temperature of the non-scattering medium was varied to evaluate the ability of the $M_1$ and $M_2$ models to predict radiative emission from the medium. Temperatures of $T = 20, 40$ and $60 \text{ K}$ were considered with the distance between the plates maintained at $1.0 \text{ m}$. The comparisons of both the radiative energy density and radiative flux again, computed with 100 computational cells in the direction normal to the plates, are presented in Fig. 5.3, 5.4 and 5.5 for medium temperatures of $20, 40$ and $60 \text{ K}$, respectively.

It can be observed from the figures that the $M_1$ model still possesses a discontinuity in the

![Figure 5.3](image)

**Figure 5.3:** Numerical predictions of (a) the radiative energy, $E$, (left panel) and (b) y-direction flux, $F_y$, (right panel) obtained using the $M_1$, $M_2$, $P_1$, $P_3$ and DOM for radiative emission between two infinitely long parallel plates with a separation distance of $1 \text{ m}$ and a non-scattering medium with a temperature of $T = 20 \text{ K}$, showing comparisons to exact analytical solution.
Figure 5.4: Numerical predictions of (a) the radiative energy, $E$, (left panel) and (b) $y$-direction flux, $F_y$, (right panel) obtained using the $M_1$, $M_2$, $P_1$, $P_3$ and DOM for radiative emission between two infinitely long parallel plates with a separation distance of 1 m and a non-scattering medium with a temperature of $T = 40\text{ K}$, showing comparisons to exact analytical solution.

predictions of the radiative energy density, and this is especially evident at small medium temperatures. The discontinuity however becomes less important as the temperature of

Figure 5.5: Numerical predictions of (a) the radiative energy, $E$, (left panel) and (b) $y$-direction flux, $F_y$, (right panel) obtained using the $M_1$, $M_2$, $P_1$, $P_3$ and DOM for radiative emission between two infinitely long parallel plates with a separation distance of 1 m and a non-scattering medium with a temperature of $T = 60\text{ K}$, showing comparisons to exact analytical solution.
the medium increases and the predictions of the M$_1$ closure then agree both qualitatively and quantitatively with the exact solution. It is also observed that the M$_2$ model yields better predictions with increasing temperature, which are in better agreement overall with the exact solution than the M$_1$ model especially near the center of the medium.

### 5.1.4 Scattering Medium

The final one-dimensional test problem that was considered evaluated the impact of scattering on the M$_N$ closure solutions. In this case, the first one-dimensional problem was reconsidered with a cold medium for which there is also isotropic scattering with $\sigma_s = 2.0 \text{ m}^{-1}$. An exact solution does not exist for this case and instead the numerical solution obtained by the high-resolution FVM is used as an approximation to the exact solution. Again, 100 computational cells were used for all computations.

The numerical results for the one-dimensional scattering problem are depicted in Fig. 5.6. The results shown in the figure indicate that the M$_1$ solution now no longer contains an unphysical jump and. It also observed that the M$_2$ and P$_3$ closures lie very close to the exact solution.
5.2 Square Enclosure

The first two-dimensional test case considers a square enclosure with a cold (non-emitting), absorbing and isotropically scattering medium. All of the walls are cold at $T = 0$ K except for the bottom one which is maintained at $T = 1000$ K. Fig. 5.8 illustrates the predictions of both the radiative energy and radiative flux for the high-resolution FVM, computed using a cartesian computational domain consisting of $100 \times 100$ uniformly-spaced cells as shown in Fig. 5.7. The predictions of both the radiative energy density and the heat flux on the wall opposite to the hot wall (top wall) are now compared for $M_1$, $P_1$ and $P_3$, as well as DOM and FVM. The results, displayed in Fig. 5.9 show that the DOM $S_8$ method exhibits rather strong ray effects as illustrated by the oscillatory nature of the solutions. By using a directional-discretization method with more discrete directions, as with the high resolution FVM method, the ray effects become less important, but are not entirely removed and are still present. This difficulty of the directional-discretization methods to provide smooth solution without oscillations in such cases is due the fact that the distribution of radiative intensity is assumed to be transported in a finite numbers of discrete directions. A smoother solution could be obtained as the number of discrete discrete direction increases; however, computational costs considerations would limit the resolution of the angular discretization.

The predicted radiative heat flux incident to the wall opposite to the hot wall (top wall)
Figure 5.8: Contours of (a) radiative energy density and (b) radiative flux using the FVM method for a cold medium with an absorption coefficient $\kappa = 1 \text{ m}^{-1}$ and scattering coefficient $\sigma = 1 \text{ m}^{-1}$.

for the square enclosure problem is now used to further assess the accuracy of the $M_1$, $P_1$ and $P_3$ closures for different values of optical thicknesses ($\beta = \kappa + \sigma$) and scattering albedo ($\omega = \sigma/\beta$). In order to illustrate the effect of these parameters on the performance of the moments methods compared to the DOM, a relative error with respect to the high-resolution FVM is used as an indicator of accuracy, which is calculated in the $L_2$ norm.

Figure 5.9: Comparisons of the predictions of a) the radiative energy density and b) the radiative heat flux at the top wall using $M_1$, $P_1$, $P_3$, DOM and FVM.
The results of Fig. 5.10 show that, for all five methods, the error is minimized for optically thick ($\beta > 1$), purely scattering media ($\omega = 1$), which corresponds to the purely diffusive regime, where the distribution is close to isotropic. For optical thicknesses close to unity, the $M_1$ model is less accurate than the $P_1$ approximation. However, for optically thick ($\beta > 1$) cases with moderate to highly scattering media, the $M_1$ closure yields better predictions than $P_1$. The $P_3$ closure yields an increased accuracy compared to the $P_1$
approximation. It is also observed that for optically thick cases ($\beta \to 10$) with small to moderate scattering Albedo, where the distribution is indeed highly anisotropic, the accuracy of the $M_1$ closure is comparable to that of $P_3$.

### 5.3 Square Enclosure with a Centered Obstruction

A square enclosure with a centered obstruction, as shown in Fig. 5.12, is now considered in order to assess the ability of the moment methods to adequately predict radiative heat transfer around sharp edges. The medium within the enclosure is cold (non-emitting), non-absorbing, with a scattering coefficient of $\sigma_s = 1.0 \text{ m}^{-2}$. All walls are assumed to be black ($\epsilon_w = 1$) and maintained at a temperature $T = 500 \text{ K}$, with the exception of the bottom one (wall 1) which has a temperature of $T = 1000 \text{ K}$. This problem, having a more realistic and complex geometry, is often used as a test case to demonstrate the drawbacks of the DOM concerning ray effects and false scattering [31]. Numerical solutions for all the approximate radiation models used here for comparisons were obtain using a computational domain consisting of a uniform body-fitted mesh with eight unequal blocks and a total of 7500 cells as illustrated in Fig. 5.11.

The predicted distributions of both the radiative energy density and radiative heat flux for the square enclosure with obstruction problem obtained using the FVM method are

![Figure 5.11: Mesh distribution for the square enclosure.](image-url)
Figure 5.12: Geometry of the square enclosure with a centered obstruction.

shown in Fig. 5.13 for the entire two-dimensional computation domain. Even for this high angular resolution method, ray effects are observed, especially near the upper wall (wall 3). Fig. 5.14 compares the radiative energy and radiative heat flux distributions along wall 3 obtained using $M_1$, $P_1$, and $P_3$ closures as well as the DOM and FVM. The moment closure methods provide smoother solutions compared to the directional-discretization methods (DOM and FVM), which display rather strong ray effects, especially near the

Figure 5.13: Numerical predictions of the distribution of a) the radiative energy, $E$ and b) the radiative heat flux, $F$, for a cold isotropic scattering medium inside a square enclosure with a centered obstruction using the FVM method.
ends of wall 3. However, the amplitude of the oscillations in the solutions predicted by
the DOM is more important than that of the FVM, which is justified by the fact that
the latter provides a larger number of discrete directions than the former. Near the
center of the wall, the $M_1$ closure is observed to over-predict the radiative heat flux by
a factor of at least 10, whereas its spherical harmonics counterpart ($P_1$ approximation)
overestimates the radiative flux by a factor of about 4. The higher-order $P_3$ closure
provides more accurate solutions near the center of the upper plate, as its predictions
lie close to those of the high resolution FVM. It is also observed that there exist a
big discrepancy between the results of the moment closure methods and those of the
directional-discretization methods near either end of the wall, which correspond to the
uppermost corners of the geometry studied in this test case. This is an indication that
some issues may still exist in prescribing accurate boundary conditions for the moment
 closures in problems with more complex geometries, and this issue may contribute to the
under-prediction of both the radiative energy density and radiative heat flux seen in Fig.
5.14.

5.4 Circular Enclosure with AMR

A circular enclosure is now considered in order to assess the accuracy and efficiency of
the anisotropic AMR described in Section 4.3. The enclosure consists of two circulars
cylinders with radii of 0.1 and 2.0 m for the inner and outer cylinders, respectively. The inner wall temperature is 100 K and the outer wall is maintained at $T = 1$ K. The absorbing-emitting medium inside the enclosure is taken to be discontinuous at a radius of 0.5 m with inner absorption coefficient of $\kappa_1 = 10 \text{ m}^{-1}$ and outer absorption coefficient of $\kappa_2 = 100 \text{ m}^{-1}$. The corresponding inner and outer temperatures of the medium are $T_1 = 100$ K and $T_2 = 1$ K, respectively.

The initial computational domain consists of a non-uniform body-fitted mesh with two equally-sized blocks and a total of 256 cells (refer to Charest et al. [98] for full description of problem and solution parameters for the DOM). Numerical solutions for $P_1$ were then obtained on the initial mesh and then the proposed anisotropic AMR algorithm was applied to obtain numerical solutions on a sequence of computational mesh with up to four levels of refinement. Similar computations were also performed using the isotropic mesh refinement in order to illustrate the advantages of its anisotropic counterpart. As shown in Fig. 5.15, which depicts the block boundaries as well as the mesh distribution at the fourth mesh refinement level and computed solutions for the radiative energy using $P_1$ models, the anisotropic AMR algorithm correctly identifies the rapid variation in the medium properties at $r = 0.5$ m and correspondingly refines the mesh in the appropriate direction.

![Figure 5.15](image)

**Figure 5.15:** Numerical predictions of the radiative energy, $E$, for the circular enclosure with: a) the block boundaries and b) the mesh distribution throughout the computational domain using the $P_1$ closure with anisotropic AMR.
Fig. 5.16 then compares the predictions of the $P_1$ closure using both isotropic and anisotropic AMR at different levels of refinement. It is observed that, with increasing level of refinement, comparable levels of accuracy are obtained by using either of the AMR algorithms. However the anisotropic mesh refinement only required a total of 26 blocks and 3328 cells after fourth refinement level, whereas its isotropic counterpart used 224 blocks and a total of 28672 cells. Comparisons of computational time also revealed that using the anisotropic AMR resulted in a reduction of the CPU time by a factor
of about 15 compared to the isotropic AMR. Similar comparisons were also performed using the M_1 model. The results, presented in Fig. 5.17, show similar trends as for the P_1 closure, with reductions in CPU time by a factor of 16 when using the anisotropic AMR.

This test cases clearly illustrates the advantages of refining the grid independently in each direction rather making use of a uniform AMR.

Figure 5.18: Comparison of the computational costs of: (a) DOM, (b) M_1, (c) P_1 and (d) P_3 for a range of optical thicknesses and scattering Albedo in the case of radiative transfer throughout a cold isotropic scattering medium inside a square enclosure.
5.5 Comparison of Computational Cost

In addition to comparing the accuracy of the solutions obtained by the $M_1$, $P_1$ and $P_3$ moment closures to those of the DOM, it is also necessary to analyze their computational time for problems with various degrees of geometric complexities or different radiative properties. Among all the cases presented in this work, the square enclosure problem presented in Section 5.2 represents the best choice for comparing the efficiency of the different approximate radiation models for a range radiative properties. Such comparisons can be somewhat biased in favour of the DOM by the fact that the space marching scheme used in the latter method is very efficient in cases with low scattering Albedo, especially when the parameters for the Newton-Krylov solver used to solve the moment equations are not carefully optimized.

Fig. 5.18 shows comparisons of the required CPU times of the various solution methods for the square enclosure problem, where the results were obtained using a uniform Cartesian computational grid with $100 \times 100$ cells. It can be seen that for low to moderate values of the scattering coefficients, as well as for small to moderate values of the optical thickness, the DOM greatly outperforms the other models in terms of CPU time, due to the efficiency of the space marching algorithm in such regimes. However, for highly scattering cases with large optical thicknesses, the difference of CPU time between DOM and the other numerical methods decreases rapidly by a factor of more than 10. It is also observed that the $P_1$ model is cheaper than all the other models, including DOM, in this region. Despite the fact that both $M_1$ and $P_1$ models only require to solve for 3 angular moments of the distribution in two dimensions; it is observed that $P_1$ solutions are less costly than $M_1$ solutions due to the nonlinearity of the latter model. The $P_3$ approximation is more expensive than both $P_1$ and $M_1$ as it results in a system of 10 moments equations in 2D. For radiation transport in complex three-dimensional domains with scattering media, the benefits of a moment closure approach are expected to be even more substantial compared to the DOM, as space marching techniques generally lose their high efficiency in such cases.

It is also worth mentioning that the $M_2$ model was not considered in this analysis. In fact, the repeated solution of the minimization problem for evaluating the partial outgoing moments at the boundaries significantly increases the computational efforts and hence would clearly disadvantage the $M_2$ closure as far as the computational costs are concerned. If an analytical approximation of the partial moments could be found, it is anticipated that the computational costs associated with the solutions of the nonlinear $M_2$ closure
would be comparable, or even higher, to those of $P_3$, even though the former only requires
to solve for 6 moments in 2D. Note that due to the non-linearity of the maximum-entropy
closures, the initial CFL number used for the NKS calculations was set to 1 in order to
guarantee convergence. The same initial CFL number was also used for the spherical
harmonics closures for a fair comparison. However, larger initial CFL could have been
used for the $P_N$ approximations, since they transform the RTE into a linear system of
moment equations, in which case the stability region is much larger than that of the $M_N$
closures. However, the linearity of the $P_N$ closures would allow the use of much larger
initial CFL number without affecting the stability of the resulting scheme. As such
computational savings relatively to the DOM results could be obtained by increasing
the initial CFL for both $P_1$ and $P_3$. For the $M_N$ methods, the nonlinearity of the
corresponding closures however limits the maximum allowable initial CFL and hence
somewhat increases the overall computational costs.

5.6 Systematic Comparison of Accuracy and Computational Costs

In practical CFD applications, it is generally desirable to have a model that describes a
given phenomena very accurately. However, high accuracy generally comes at a price:
the one of increased computational costs, which can sometimes be undesirable. In this
section, the results from Sections 5.2 and 5.5 are used in order to perform a systematic
comparison between accuracy and computational costs for the moments models studied
herein. The objective function used for these comparisons was defined as follows

$$ F = w \times \text{Err} + (1 - w) \times \text{CPU}_T, \quad (5.6) $$

where $\text{Err}$ is the relative error defined in Eq. (5.5), $\text{CPU}_T$ corresponds to the associated
computational time (normalized by that of the $P_3$ approximation), and $w$ represents the
weight associated with the accuracy of the method, or, in other words, the importance
of accuracy in the evaluation of the objective function Eq. (5.6). In this analysis,
we arbitrarily set $w = 0.6$ such that the accuracy is slightly more important than the
computation costs. The best candidate would be the one that gives the smallest value of
the objective function for a given set of radiative properties.

Fig. 5.19 shows the different regions where each of the moment methods studied herein
Figure 5.19: Systematic comparison between accuracy and computational costs for $M_1$, $P_1$ and $P_3$ for a range of optical thicknesses and scattering Albedo in the case of radiative transfer throughout a cold isotropic scattering medium inside a square enclosure.

is advantageous compared to the other methods. The red area corresponds to the $M_1$ closure, the green region to the $P_1$ approximation and the blue domain to the $P_3$ approximation. It is observed that, for this particular problem and the specific criteria considered, the $M_1$ model provides best balance between accuracy and computational costs for large optical thicknesses ($\beta \geq 2$), whereas the $P_1$ approximation outperforms the other models for small to moderate optical thicknesses ($\beta < 1$). Despite the advantages of the $P_3$ approximation in terms of accuracy, its relatively large computational costs limit the region in which it outperforms the other closure methods considered in this analysis.
Chapter 6

Conclusions and Future Research

6.1 Conclusions

The potential of the $M_1$ and $M_2$ maximum-entropy closures for describing radiative transport phenomena has been evaluated through direct comparisons of their predictions to those of the DOM, as well as the $P_1$ and $P_3$ spherical harmonics closures for several representative problems in both one and two spatial dimensions. Inaccuracies of the $M_1$ model were identified for problems where radiative energy emanating from multiple sources meet, in which cases a discontinuity in the radiative energy is observed in the predictions of the first-order approximation of the hierarchy of maximum entropy closures. The proposed approximate interpolative $M_2$ closure was shown to provide promising results, as it corrects the inability of the $M_1$ closure to properly predict emission of radiative energy from more than one source. Comparisons of the maximum entropy closure to the spherical harmonics closures for a range of optical thicknesses and scattering Albedos revealed that $P_N$ approximations provide more accurate solutions than the $M_N$ closures for optical thicknesses approaching unity, and that the opposite holds in the optically thick regime ($\beta > 1$). It has also been observed that even the $M_1$ model is able to properly capture a rather important range of anisotropic situations, sometimes yielding solutions even more accurate than those of the $P_3$ approximation in such cases. Comparisons of computational costs have shown that the $P_1$ solutions are faster to generate than the $M_1$ closure results, which in turn are much cheaper than solutions of the $P_3$ approximation which are roughly three times slower to generate than those of the $P_1$ closure. Despite the important computational savings associated with the approximation of the $M_2$ closure, accurate prescription of the boundary conditions still requires solving
the optimization problem, therefore resulting in considerably large CPU times compared to those of $M_1$, $P_1$ and $P_3$ for which analytical expressions/approximations to the partial incoming moments could be found.

Anisotropic AMR was successfully achieved on a two-dimensional domain with curved boundaries using both the $P_1$ approximation and the $M_1$ closure. Comparisons of the predictions of the anisotropic AMR to those of its isotropic variant using both the $P_1$ and $M_1$ closures showed that refining the mesh independently in each direction greatly reduces the computational efforts compared to the isotropic refinement while maintaining comparable level of accuracy.

6.2 Future Research

The predictive capabilities of the first and second order maximum entropy moment closure in the case of gray media are rather promising. Further computational savings for the $M_2$ model can be achieved by avoiding to repeatedly solve the minimization problem for the prescription of the boundary conditions. This can be done by tabulating the corresponding partial moments for sets of moments spanning the whole realizability domain of this second order closure. Furthermore, the analysis carried out in this work is a first step towards the evaluation of maximum entropy closures for predicting radiative heat transfer in non-gray media, where the spectral dependence of the radiative intensity distribution must also be taken into account (see Eq. (3.15)). For such distribution, there exist no exact analytical expression for the closure, even for $M_1$ model (unlike in the gray case). Determination of the Lagrange multipliers must therefore be performed by solving the optimization problem, which can be an arduous task, especially when the occupation number density $n$ (see Eq. (3.12)) is very large or very small. In the former regime, which corresponds to the logarithmic limit, Fu [99] showed that the term $\alpha(E_R).m(\vec{s})$ is small and the exponential expression in the distribution function Eq. (3.15) can be expanded into a Taylor series expansion. In the latter regime, which corresponds to the hyperbolic limit, the distribution maximizing the Bose-Einstein entropy approaches the Maxwell-Boltzmann limit. For the treatment of the spectral dependence of radiative properties, such as the absorption coefficient, which vary rather strongly with frequency, efficient and accurate techniques such as the statistical narrow-band correlated-k (SNBCK) [100] and the full spectrum correlated-k (FSCK) [101] have been developed and successfully used with both DOM and $P_1$ approximation. Coupling of such techniques with the non-gray maximum entropy closures will be subject of future work. The resulting non-gray...
maximum entropy closures will be evaluated in laminar flames simulation. An extension of the analysis to turbulent flames simulations will then be performed, after developing suitable Reynolds averaged Naviers-Stokes (RANS) models for each of the radiation models considered.
Appendix A

Form of the Distribution on the Boundaries of the Realizability Domain

The realizability condition for moments of order up to two are defined as follows

\[ 0 \leq \| N \|_1^1 \leq 1 \]  \hspace{1cm} (A.1)

\[ N_{ij}^2 - N_i^1 N_j^1 \geq 0 \]  \hspace{1cm} (A.2)

The boundaries of such realizability domain correspond to the case where \( \| N \|_1^1 = 1 \) or \( N_{ij}^2 - N_i^1 N_j^1 = 0 \). In the case where \( \| N \|_1^1 = 1 \), which corresponds to the free streaming limit, the distribution is zero everywhere except on the line \( \vec{s} = N_i^1 \), i.e.,

\[ I = I^{(0)} \delta(\vec{s} - N_i^1) \]  \hspace{1cm} (A.3)

The form of the distribution in Eq. (A.3) can be integrated directly to obtain analytical expression for \( N^3 \)

\[ N_{ijk}^3 = N_i^1 N_j^1 N_k^1 \]  \hspace{1cm} (A.4)

Let us now consider a frame that diagonalizes \( N_{ij}^2 - N_i^1 N_j^1 \). In this rotated frame, one can write

\[ N_{ij}^2 - N_i^1 N_j^1 = \lambda_i \delta_{ij} \]  \hspace{1cm} (A.5)
If at least one of the values of \( \lambda_i (i \in 1, 2, 3) \) is equal to zero, then \( N_{ij}^2 \) attains one of its boundary values and one can write

\[
\int (\Omega_i - N_{i}^1)^2 Id\Omega = N_{ii}^2 - (N_{i}^1)^2 = 0 \quad (A.6)
\]

which means that the distribution is zero everywhere except on the line \( \Omega_i = N_{i}^1 \), and all higher order moments are constrained by the theory of moments for probability measures on the unit circle.
References


