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APPROXIMATE MODELS FOR RADIATIVE TRANSFER

BY

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Abstract

In this paper we give a summary of the partial moment approach for radiative transfer, combined with a minimum entropy closure. This approach is a generalization of the moment approach. We review some well-established models, like the method of Spherical Harmonics, Discrete Ordinates, diffusion, higher-order diffusion and flux-limited diffusion. We present numerical examples, where different methods are compared.

1. Introduction

Radiative transfer plays a prominent role in many applications in physics and engineering. Especially when high temperatures are involved the effect of radiation becomes very important. Applications include astrophysics [39] (stellar atmospheres), reentry of space vehicles [61], combustion in gas turbine combustion chambers [17], industrial glass cooling [31], and external photon beam radiotherapy [20], among others.

Assuming coherent scattering and stationary matter, the radiative transfer equations read [39, 41, 46]; For all $\Omega \in \mathcal{S}$

$$\frac{1}{c}\partial_t I(x,t,\Omega,\nu) + \Omega\nabla I(x,t,\Omega,\nu) = \kappa(B(x,t,\nu) - I(x,t,\Omega,\nu))$$
$$+\sigma(\int_{\mathcal{S}} g(\Omega\cdot\Omega')I(x,t,\Omega',\nu)d\Omega' - I(x,t,\Omega,\nu)). \tag{1.1}$$

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Here, $I(x,t,\Omega,\nu)\cos\theta dA d\Omega d\nu$ is the radiative energy flow at point x and time t through the area dA with a frequency in the interval $[\nu,\nu+d\nu]$, into a surface element $d\Omega$ around Ω, where θ is the angle between the outer normal of dA and Ω. The directions are elements of the unit sphere $\mathcal{S}$ in three dimensions. The speed of light is c, κ is the absorption coefficient, σ is the scattering coefficient. The black body intensity is denoted by B and $g(\Omega\cdot\Omega')$ is the scattering kernel. Without loss of generality, we will neglect the frequency dependence in the following (i.e. we consider all quantities to be grey or frequency-averaged) and consider only isotropic scattering ($g\equiv\frac{1}{4\pi}$). All the ideas presented in this paper can be generalized. Note however, that additional difficulties can occur. For frequency-dependent coefficients, further approximations have to be introduced. One approach is to take moments in frequency, cf. for example [56]. In the multigroup approach [62], one uses a piecewise constant approximation of the intensity in frequency space. Advantages and drawbacks of both approaches will be briefly discussed in Section 5.

We supplement this system with the following boundary conditions. For the radiative intensity we prescribe the ingoing radiation,

$$I(\Omega)|_{n\cdot\Omega<0}=I_{\text{out}}(\Omega), \tag{1.2}$$

where n denotes the outward normal. These boundary conditions can be extended to semi-transparent boundaries. As initial data we prescribe the radiative intensity I inside the domain.

Analytical results concerning the existence and uniqueness of solutions to the transfer equation itself and to the radiative heat transfer equations, where also energy conservation and additionally heat conduction are considered, have been obtained by many authors. A rather recent review on methods for transport equations can be found in [2], cf. also [1]. The transfer equation together with energy conservation is considered in [19, 38]. The issue of heat conduction is addressed in [24, 28, 29]. Convection, conduction and radiation is treated in [33, 48].

We will also consider the special case of a one-dimensional slab geometry. In slab geometry, the equations simplify to: For all $\mu\in[-1,1]$

$$\begin{aligned}\frac{1}{c}\partial_t I(x,t,\mu)+\mu\partial_x I(x,t,\mu) &= \kappa(B(x,t)-I(x,t,\mu))\\ &\quad+\sigma(\frac{1}{2}\int_{-1}^{1} I(x,t,\mu')d\mu'-I(x,t,\mu)).\end{aligned} \tag{1.3}$$

Here, μ is the cosine of the angle between direction and x-axis. At the left boundary I has to be prescribed for $\mu > 0$, at the right boundary for $\mu < 0$.

The purpose of this paper is to give a sumary of the partial moment approach, combined with a minimum entropy closure. This approach is a generalization of the moment approach and was developed in [12, 13, 16, 63]. In Section 2 we give a review of the moment method and examine different closures, which, in this form, cannot be found in standard textbooks. Furthermore, we discuss the connections between the moment method and other widely used approximate methods, e.g. the method of Discrete Ordinates, Diffusion approximation and Flux-Limited Diffusion. The partial moment idea is explained in Section 3. Mathematical and physical properties of this approximation are discussed. Again, different closures are considered. In Section 4 we present several numerical examples, where the methods presented before are compared.

2. Moment Models

First we briefly review the basics of the moment approach. Consider again the transport equation (1.1) for the radiation. This equation is in fact a system of infinitely many coupled integro-differential equations that describes the distribution I of all photons in time, space and velocity space. On the one hand this system is computationally very expensive and on the other hand we are not interested in the photon distribution itself but in macroscopic quantities like the mean energy or mean flux of the radiation field. For instance, only the gradient of the radiative flux enters into the energy balance. The macroscopic quantities are moments of the distribution function. Let

$$\langle \cdot \rangle := \int_{\mathcal{S}} \cdot \, d\Omega \tag{2.1}$$

denote the average over all directions. The energy, flux vector and pressure tensor of the radiation field are defined, respectively, as

$$E := \langle I \rangle, \quad F := \langle \Omega I \rangle, \quad P := \langle (\Omega \otimes \Omega) I \rangle. \tag{2.2}$$

To derive equations for the macroscopic quantities we multiply the transport equation by 1 and Ω and average over all directions. We obtain the conservation laws

$$\frac{1}{c}\partial_t E + \nabla F = \kappa(\langle B\rangle - E) \tag{2.3}$$
$$\frac{1}{c}\partial_t F + \nabla P = -(\kappa+\sigma)F. \tag{2.4}$$

These are four equations (the first is a scalar equation, the second has three components) for 10 unknowns (E scalar, F 3-component vector, P symmetric 3×3-matrix). Hence we have to pose an additional condition. Usually this condition is a constitutive equation for the highest moment P, expressed in terms of the lower moments E and F. This is referred to as the closure problem. The simplest approximation, the so-called P_1 approximation, is obtained if we assume that the underlying distribution is isotropic. Thus, we obtain $P = \frac{1}{3}E$ and therefore

$$\frac{1}{c}\partial_t E + \nabla F = \kappa(\langle B\rangle - E) \tag{2.5}$$
$$\frac{1}{c}\partial_t F + \nabla \frac{1}{3} E = -(\kappa+\sigma)F. \tag{2.6}$$

The general P_N closure is usually derived in a different way.

2.1. Spherical harmonics

The Spherical Harmonics approach is one of the oldest approximate methods for radiative transfer [14, 21]. For the sake simplicity, we restrict our explanation to the case of slab geometry. The derivation for three-dimensional case can be found for example in [7] and also in standard text-books [9, 26, 43]. The idea of the spherical harmonics approach is to express the angular dependence of the distribution function in terms of a Fourier series,

$$I(\mu) = \sum_{l=0}^{\infty} I_l^{SH} \frac{2l+1}{2} P_l(\mu), \tag{2.7}$$

where P_l are the Legendre polynomials. These form an orthogonal basis of the space of polynomials with respect to the standard scalar product on $[-1,1]$,

$$\int_{-1}^{1} P_l(\mu)P_k(\mu)d\mu = \frac{2}{2l+1}\delta_{lk}. \tag{2.8}$$

In more space dimensions, one uses spherical harmonics, which are an orthogonal system on the unit sphere.

If we truncate the Fourier series at $l = N$ we have

$$I^{SH}(\mu) = \sum_{l=0}^{N} I_l^{SH} \frac{2l+1}{2} P_l(\mu). \tag{2.9}$$

One can obtain equations for the Fourier coefficients

$$I_l^{SH} = \int_{-1}^{1} I^{SH}(\mu) P_l(\mu) d\mu \tag{2.10}$$

by testing (1.1) with $P_l(\mu)$ and then integrating. Thus we get

$$\frac{1}{c}\partial_t I_l^{SH} + \nabla \int_{-1}^{1} \mu P_l(\mu) I^{SH}(\mu) d\mu = \kappa(2\langle B\rangle \delta_{l0} - I_l^{SH}) + \sigma(I_0 \delta_{l0} - I_l^{SH}) \tag{2.11}$$

for the moments I_l^{SH} of the distribution function. Using the recursion relation

$$(l+1)P_{l+1}(\mu) + lP_{l-1}(\mu) = (2l+1)\mu P_l(\mu) \tag{2.12}$$

we obtain

$$\frac{1}{c}\partial_t I_l^{SH} + \nabla\left(\frac{l+1}{2l+1} I_{l+1}^{SH} + \frac{l}{2l+1} I_{l-1}^{SH}\right) = \kappa(2\langle B\rangle \delta_{l0} - I_l^{SH}) + \sigma(I_0 \delta_{l0} - I_l^{SH}). \tag{2.13}$$

This is a linear system of first order partial differential equations. For a criterion on how many moments are sufficient for a given problem see [57].

The two most widely used boundary conditions are Mark [34, 35] and Marshak [36] boundary conditions. The idea of the Mark boundary conditions is to assign the values of the distribution at certain directions μ_i which are the zeros of the Legendre polynomial of order $N+1$. That this is in fact a natural boundary condition becomes clear in the next section.

Marshak's boundary conditions, on the other hand, demand that the ingoing half moments of the distribution are prescribed, i.e. for the left boundary

$$\int_0^1 P_l(\mu) I(\mu) d\mu. \tag{2.14}$$

This, in some sense, reflects the boundary conditions (1.2) for the full equations.

2.2. Discrete ordinates and spherical harmonics

The idea of the discrete ordinates (S_N) approach [6] is to choose a certain set of directions (Ω_i) and to replace the angular integration by a numerical quadrature. Let I_i^{DO} be an approximation to $I(\Omega_i)$. Then the S_N approximation to (1.1) reads for all $i = 1, \ldots, N$

$$\frac{1}{c}\partial_t I_i^{DO} + \Omega_i \nabla I_i^{DO} = \kappa(\langle B\rangle - I_i^{DO}) + \sigma(\frac{1}{4\pi}\sum_{j=0}^{N} w_j I_j^{DO} - I_i^{DO}). \qquad (2.15)$$

The w_j are the weights of a quadrature rule on the unit sphere. This is again a system of linear partial differential equations. Depending on the number of directions, this system can become quite large [25].

The formulation of boundary conditions is straight-forward. We simply prescribe the value of the distribution function for the ingoing directions.

It is well-known [5] that the Discrete Ordinates and the Spherical Harmonics approach are equivalent. If we choose Gauss quadrature as the quadrature rule then the P_N and S_N solutions have the same value at the nodes μ_i. This can be seen by multiplying the equation for the coefficients of the Spherical Harmonics, Eq. (2.13), with

$$\frac{2l+1}{2} P_l(\mu_i) \qquad (2.16)$$

and summing over l.

At this point it becomes clear that Mark's boundary conditions are in fact a natural choice. Indeed they are just a translation of the simple boundary conditions for the Discrete Ordinates method.

2.3. Diffusion approximation and spherical harmonics

Consider the equation for the Fourier coefficient corresponding to the zeroth order Legendre polynomial (or spherical harmonic) and recall that the radiative energy density E and the energy flux F satisfy

$$\frac{1}{c}\partial_t E + \nabla F = \kappa(\langle B\rangle - E). \qquad (2.17)$$

The diffusion approximation now consists of expressing F as a function of E and ∇E and other known quantities. The classical diffusion approximation uses Fick's law [41],

$$F = -\frac{1}{3(\sigma+\kappa)}\nabla E, \tag{2.18}$$

and hence

$$\frac{1}{c}\partial_t E - \nabla\frac{1}{3(\sigma+\kappa)}\nabla E = \kappa(\langle B\rangle - E). \tag{2.19}$$

By $\nabla\frac{1}{3(\sigma+\kappa)}\nabla E$ we actually mean $\nabla(\frac{1}{3(\sigma+\kappa)}\nabla E)$, but we will skip the brackets in the following. This equation is called diffusion approximation because of its similarity to Fourier's law of heat diffusion. It has been derived in [51] in the field of radiative transfer and in [30] in the field of neutron transport. The classical diffusion approximation can be obtained, in an ad hoc manner, from the P_1 equations,

$$\frac{1}{c}\partial_t E + \nabla F = \kappa(\langle B\rangle - E) \tag{2.20}$$

$$\frac{1}{c}\partial_t F + \nabla\frac{1}{3}E = -(\sigma+\kappa)F, \tag{2.21}$$

by dropping the time derivative of the flux, $\partial_t F$, then solving the second equation for F, and plugging the result into the first equation.

The most simple boundary conditions would be Dirichlet boundary conditions, i.e. we prescribe the value of E at both boundaries. More accurate conditions can be derived by employing Marshak's approach. This leads to

$$\frac{2}{3\kappa}n\cdot\nabla E = \langle B\rangle - E. \tag{2.22}$$

These boundary conditions are of Robin type.

2.4. Simplified P_N approximations

In the same ad-hoc manner, one can derive diffusion-type equations of higher order, the so-called Simplified P_N (SP_N) equations, from any P_N approximation of odd order. This can be done in the following way [18]: First, neglect the time derivatives of the higher order moments. Then, algebraically solve every second equation for the odd order moment. Insert this into the equation above to obtain a system of second-order partial differential equations.

This ad-hoc-manner can be made more rigorous by a diffusive scaling of the equations and an asymptotic expansion of the differential operator [31, 47]. To that end we neglect the time-derivative and assume that the interaction coefficients are large. Mathematically, we introduce a small parameter ε and scale the equations,

$$\Omega\nabla I = \frac{\kappa}{\varepsilon}(B-I) + \frac{\sigma}{\varepsilon}(\frac{1}{4\pi}\int I - I). \tag{2.23}$$

The parameter

$$\varepsilon = \frac{1}{(\sigma_{\text{ref}} + \kappa_{\text{ref}})x_{\text{ref}}},$$

where x_{ref} is the typical size of the medium and σ_{ref}, κ_{ref} are reference values for the scattering and absorption coefficients, is the inverse optical depth of the medium. For the diffusion and SP_N approximations to be valid one should have $\varepsilon \ll 1$.

Equation 2.23 is equivalent to

$$(1+\varepsilon\frac{\Omega}{\sigma+\kappa}\nabla)I = \frac{\kappa}{\sigma+\kappa}B + \frac{\sigma}{\sigma+\kappa}\frac{1}{4\pi}\int I. \tag{2.24}$$

Inverting the operator using Neumann's series yields

$$I = (1-\varepsilon\frac{\Omega}{\sigma+\kappa}\nabla + \varepsilon^2\frac{\Omega^2}{(\sigma+\kappa)^2}\nabla^2 - \cdots)(\frac{\kappa}{\sigma+\kappa}B + \frac{\sigma}{\sigma+\kappa}\frac{1}{4\pi}\int I). \tag{2.25}$$

Now we integrate both sides with respect to Ω over the unit sphere and get

$$E = (1+\frac{\varepsilon^2}{3(\sigma+\kappa)^2}\nabla^2 + \frac{\varepsilon^4}{5(\sigma+\kappa)^4}\nabla^4 + \cdots)(\frac{\kappa}{\sigma+\kappa}\langle B\rangle + \frac{\sigma}{\sigma+\kappa}E). \tag{2.26}$$

Using Neumann's series again, we arrive at

$$(1-\frac{\varepsilon^2}{3(\sigma+\kappa)^2}\nabla^2 - \frac{4\varepsilon^4}{45(\sigma+\kappa)^4}\nabla^4 + \cdots)E = (\frac{\kappa}{\sigma+\kappa}\langle B\rangle + \frac{\sigma}{\sigma+\kappa}E). \tag{2.27}$$

Multiplication by $\sigma+\kappa$ yields

$$(-\frac{\varepsilon^2}{3(\sigma+\kappa)}\nabla^2 - \frac{4\varepsilon^4}{45(\sigma+\kappa)^3}\nabla^4 + \cdots)E = \kappa(\langle B\rangle - E). \tag{2.28}$$

If we neglect terms of the order ε^4, ε^6, ε^8 and perform substitutions to obtain only second derivatives, we arrive at the SP_1, SP_2, SP_3 equations, respectively.

For example, the SP_3 equations finally read

$$-\nabla\frac{\mu_1^2}{\sigma+\kappa}\nabla\psi_1=\kappa(\langle B\rangle-\psi_1) \tag{2.29}$$

$$-\nabla\frac{\mu_2^2}{\sigma+\kappa}\nabla\psi_2=\kappa(\langle B\rangle-\psi_2), \tag{2.30}$$

where ψ_n are related to

$$E \quad \text{and} \quad \phi=\left(1-\frac{11\varepsilon^2}{21\,(\sigma+\kappa)^2}\nabla^2\right)^{-1}\left(\frac{2\varepsilon^2}{15\,(\sigma+\kappa)^2}\nabla^2E\right) \tag{2.31}$$

via a linear transformation

$$\psi_n=E+\gamma_n\phi, \quad \gamma_n=\frac{5}{7}\left(1+(-1)^n\sqrt{\frac{54}{5}}\right). \tag{2.32}$$

Furthermore,

$$\mu_1^2=\frac{3}{7}-\frac{2}{7}\sqrt{\frac{6}{5}} \quad \text{and} \quad \mu_2^2=\frac{3}{7}+\frac{2}{7}\sqrt{\frac{6}{5}}. \tag{2.33}$$

Boundary conditions can again be derived by Marshak's idea. For the SP_3 equations they are a linear system of equations involving the values of ψ_1 and ψ_2 and their normal derivatives, cf. [31].

We want to remark that in this derivation we actually apply Neumann's series to an unbounded operator, which is mathematically not rigorous. The SP_N approximation is based on the suitable asymptotic expansion of the differential operator, not of the solution itself. However, the SP_1 or classical diffusion approximation can also be derived by a Chapman-Enskog expansion, i.e. an expansion of the solution I in terms of ε,

$$I=I_0+\varepsilon I_1+\cdots. \tag{2.34}$$

If we collect orders of ε and note that up to higher order terms,

$$E=\langle I_0\rangle \quad \text{and} \quad F=\langle\varepsilon\Omega I_1\rangle, \tag{2.35}$$

we obtain Fick's law (2.18).

2.5. Minimum entropy closure

The approximations based on the expansion of the distribution function into a polynomial or the equivalent diffusion approximations suffer from serious drawbacks. First, anisotropic situations are not correctly described. This becomes apparent most drastically for a ray of light, where $|P| = E$. Also, the distribution function can become negative and thus the moments computed from the distribution can become unphysical. Second, boundary conditions cannot be incorporated exactly. At a boundary we usually prescribe the ingoing flux only. Here we have to prescribe values for the full moments. These moments contain the unknown outgoing radiation. Moreover, a polynomial expansion cannot capture discontinuities in the angular photon distribution. Krook [27] remarks that at the boundary there is usually a discontinuity in the distribution between in- and outgoing particles.

In this section, we want to describe one idea which resolves the first problem The idea is to use an Entropy Minimization Principle to obtain the constitutive equation for P. This principle has become the main concept of Rational Extended Thermodynamics [42].

We want to explain the Entropy Minimization Principle and its practical application by means of our simple moment system (2.3-2.4). To close the system we determine a distribution function $\mathcal{J}$ that minimizes the radiative entropy

$$H_R^*(I) = \int_{\mathcal{S}^2} \int_0^\infty h_R^*(I) d\nu d\Omega \tag{2.36}$$

with

$$h_R^*(I) = \frac{2k\nu^2}{c^3}(n \log n - (n+1)\log(n+1)) \quad \text{where} \quad n = \frac{c^2}{2h\nu^3} I \tag{2.37}$$

under the constraint that it reproduces the lower order moments,

$$\langle \mathcal{J} \rangle = E \quad \text{and} \quad \langle \Omega \mathcal{J} \rangle = F. \tag{2.38}$$

The entropy is the the well-known entropy for bosons adapted to radiation fields [44, 50]. At first sight, it is not clear why the distribution should minimize the entropy when all that is known for non-equilibrium processes is that there exists an entropy inequality. But it can be shown [10] that the minimization of the entropy for given moments and the entropy inequality are equivalent.

The above minimization problem can be solved explicitly and the pressure can be written as [11]

$$P = D(f)E. \tag{2.39}$$

Here, $f = \frac{F}{E}$ is the relative flux,

$$D(f) = \frac{1-\chi(f)}{2}I + \frac{3\chi(f)-1}{2}\frac{f\otimes f}{|f|^2} \tag{2.40}$$

is the Eddington tensor and

$$\chi(f) = \frac{5-2\sqrt{4-3|f|^2}}{3} \tag{2.41}$$

is the Eddington factor. The Eddington tensor can always be written in the form (2.40) under the assumption that the intensity is symmetric about a preferred direction [32]. The minimum entropy Eddington factor satisfies the natural constraints

$$\mathrm{tr}(D) = 1 \tag{2.42}$$

$$D(f) - f\otimes f \geq 0 \tag{2.43}$$

$$f^2 \leq \chi(f) \leq 1 \tag{2.44}$$

In the literature, the Eddington factor (2.41) has been derived based on many, apparently not connected, ideas. Levermore [32] assumed that there existed a reference frame in which the distribution was exactly isotropic and used the covariance of the radiation stress tensor. Anile et al. [3] derived it by collecting physical constraints on the Eddington factor and supposing the existence of an additional conservation law, where the conserved quantity behaves like the physical entropy near radiative equilibrium. The minimum entropy system was thoroughly investigated in [11, 62]. Further variable Eddington factors have been proposed, cf. [32, 40] and references therein.

The closed system has several desirable properties. The flux is limited in a natural way, i.e. $|f| < 1$. Physically, this corresponds to the fact that information cannot travel faster than the speed of light. Furthermore, the underlying distribution function is always positive. Also, the system can be transformed to a symmetric hyperbolic system [3], which makes it accessible to a general mathematical theory [15]. Again, Marshak type boundary conditions can be derived.

2.6. Flux-limited diffusion and entropy minimization

The classical diffusion approximation is a linear parabolic partial differential equation. In this equation, information is propagated at infinite speed. This can also be seen from the fact that the flux $|F|$ is not bounded by the energy E (relative flux $f < 1$). But this should hold, due to the definition of the moments. Thus the classical diffusion approximation contradicts fundamental physical concepts.

Therefore the concept of flux-limited diffusion has been introduced. A diffusion equation is called flux-limited if

$$|F| \leq E. \tag{2.45}$$

The following is a summary of [32]. We begin by writing the moment equations in the form

$$\frac{1}{c}\partial_t E + \nabla F = \kappa(\langle B\rangle - E) \tag{2.46}$$

$$\frac{1}{c}\partial_t F + \nabla(DE) = -(\sigma+\kappa)F, \tag{2.47}$$

with the Eddington tensor D. Two assumptions in the derivation of the classical diffusion equation will be modified. First, the Eddington tensor is only identically equal to $\frac{1}{3}$ for isotropic radiation. For a ray of light ("free-streaming"), on the other hand, we should have $|DE| = E$. Second, one should not neglect $\partial_t F$. Instead, we note that in the diffusive as well as in the free-streaming regime, the spatial and temporal derivatives of the relative flux $f = \frac{F}{E}$ and the Eddington tensor D can be neglected.

Rewriting the equations in terms of f and E we get

$$\frac{1}{c}\partial_t E + \nabla(fE) = \kappa(\langle B\rangle - E) \tag{2.48}$$

$$\frac{1}{c}\partial_t(fE) + \nabla(DE) = -(\sigma+\kappa)fE. \tag{2.49}$$

The second equation becomes

$$\frac{1}{c}E\partial_t f + \frac{1}{c}f\partial_t E + \nabla(DE) = -(\sigma+\kappa)fE. \tag{2.50}$$

Inserting (2.48) into (2.50), we obtain

$$\Big(\frac{1}{c}\partial_t f + f\nabla f\Big)E + \nabla\left((D - f\otimes f)E\right) + \bar\sigma f E = 0 \tag{2.51}$$

with $\bar\sigma = \frac{\kappa\langle B\rangle + \sigma E}{E}$. If we drop the derivatives of f and D, we arrive at

$$(D - f\otimes f)\nabla E + \bar\sigma f E = 0, \tag{2.52}$$

or

$$(D - f\otimes f)R = f \quad \text{with} \quad R = -\frac{1}{\bar\sigma}\frac{\nabla E}{E}. \tag{2.53}$$

The idea is now to

1. choose D as a function of f,
2. solve $(D - f\otimes f)R = f$ for f,
3. insert $f(R)$ into the first moment equation to obtain a diffusion approximation.

The first step shows how the concept of flux-limited diffusion is related to a (nonlinear) moment closure. If

$$D = \frac{1-\chi}{2}I + \frac{3\chi - 1}{2}\frac{f\otimes f}{|f|} \tag{2.54}$$

then f is an eigenvector of D and also of $(D - f\otimes f)$ with

$$(D - f\otimes f)f = (\chi - |f|^2)f. \tag{2.55}$$

Hence the equation $(D - f\otimes f)R = f$ has the solution

$$R = \frac{f}{\chi - f^2}. \tag{2.56}$$

Solving this equation for f and writing the result as

$$f = \lambda(R)R \tag{2.57}$$

we arrive at the closure

$$F = -\frac{1}{\bar\sigma}\lambda\left(\frac{1}{\bar\sigma}\frac{\nabla E}{E}\right)\nabla E. \tag{2.58}$$

If one chooses for D the minimum entropy Eddington factor then [32]

$$\lambda = \frac{3(1-\beta^2)^2}{(3+\beta^2)^2} \tag{2.59}$$

where β is implicitly given by

$$R = \frac{4\beta(3+\beta^2)}{(1-\beta^2)^2}. \tag{2.60}$$

The same boundary conditions as for the diffusion approximation can be used.

3. Partial Moments

In spite of its advantages the minimum entropy system still suffers from a major drawback. In Figure 3.1 we show a numerical test case [4] with two colliding beams. The parameters are $\kappa = 2.5$, $\sigma = 0$. The temperature inside the medium is zero. At both sides, beams with a radiative temperature $T_R := \left(\frac{E}{\sigma_{SB}}\right)^{1/4}$, where σ_{SB} is Stefan-Boltzmann's constant, of 1000 and relative fluxes of $f = \pm 0.99$, respectively, enter. Figure 3.1 shows the radiative energy. The full moment model has a qualitatively wrong solution with two shocks. This is not surprising since this Eddington factor, as stated above, is related to radiation which is isotropic in a certain frame [32]. This assumption is violated in the test case above. The unphysical behavior can be remedied by combining Minimum Entropy with the partial moment idea described in the following.

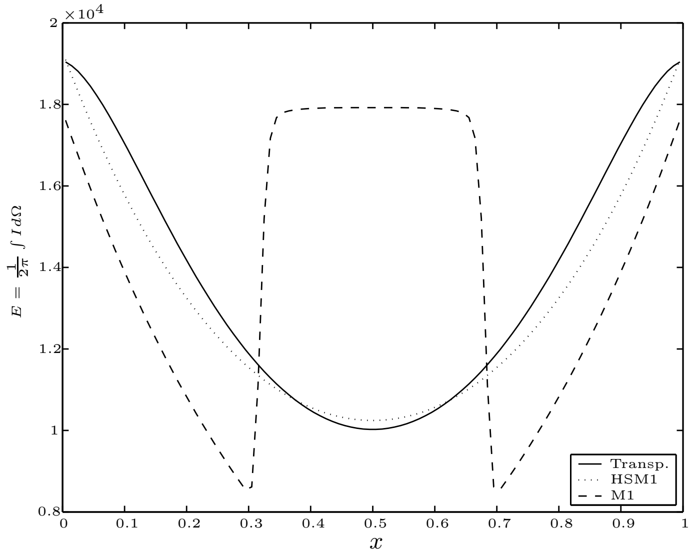

Figure 3.1. Radiative energy. Artificial radiative shock wave in the full moment entropy (M_1) model.

The partial moment idea is somehow intermediate between the Discrete Ordinates approach and Moment Models. In Discrete Ordinates models the integral over all directions is discretized with a numerical quadrature rule. This yields a coupled system of finitely many transport equations, each describing transport into one direction.

Let $\mathcal{A}$ be a partition of the unit sphere $\mathcal{S}$, where $A \in \mathcal{A}$ denotes the set of the angular integration. Instead of integrating over all directions we average over each $A \in \mathcal{A}$ separately. Thus we define the average

$$\langle \cdot \rangle_A := \int_A \cdot \, d\Omega. \tag{3.1}$$

Again, we multiply the transport equation by 1 and Ω and average over each $A \in \mathcal{A}$ to obtain

$$\frac{1}{c}\partial_t E_A + \nabla F_A = \langle S \rangle_A \tag{3.2}$$

$$\frac{1}{c}\partial_t F_A + \nabla P_A = \langle \Omega S \rangle_A. \tag{3.3}$$

We define the corresponding partial moments by

$$E_A = \langle I \rangle_A \tag{3.4}$$

$$F_A = \langle \Omega I \rangle_A \tag{3.5}$$

$$P_A = \langle (\Omega \otimes \Omega) I \rangle_A. \tag{3.6}$$

To close this system we have to find an equation for the partial pressures P_A as functions of the partial energies E_A and partial fluxes F_A.

Examples for the choice of $\mathcal{A}$, which are used later, are

- For the full moment model we have $A = \mathcal{S}$, i.e. the integral is over the full sphere.
- For the half moment model we have $A \in \{\mathcal{S}_+, \mathcal{S}_-\}$. Here, $\mathcal{S}_+ = \{\Omega \in \mathcal{S} : \Omega_x > 0\}$ is the positive half sphere, where the x-component of Ω is positive, and $\mathcal{S}_- = \{\Omega \in \mathcal{S} : \Omega_x < 0\}$ analogously is the negative half sphere.
- For the quarter moment model we have $A \in \{\mathcal{S}_{++}, \mathcal{S}_{+-}, \mathcal{S}_{--}, \mathcal{S}_{-+}\}$. Here, $\mathcal{S}_{++} = \{\Omega \in \mathcal{S} : \Omega_x > 0, \Omega_y > 0\}$ is the quarter sphere in the first quadrant. Analogously, $\mathcal{S}_{+-} = \{\Omega \in \mathcal{S} : \Omega_x > 0, \Omega_y < 0\}$ etc.

One could also choose other sets for the angular integration.

3.1. Partial moment P_N closure

The basic idea of the P_N closure is to expand the photon distribution into a polynomial. Here we use the same idea, but separately for both half ranges. This approach has been investigated in the literature in different forms and contexts and mostly in connection with boundary conditions, for example recently in [4]. Schuster and Schwarzschild [53, 54] introduce two constant distributions for left- and rightgoing photons (P_0 approximation). Krook [27], based on ideas of Sykes [58], considers half moment in one space dimension with a P_N closure. Sherman [55] compares full-P_N and half-P_N numerically in 1D. Özisik et al. [45] derive a half moment P_1 closure in spherical geometry. Further references can be found in [37], where also an octuple P_1 closure in cylindrical geometry is introduced. Similar ideas appear in related subjects, like gas dynamics, cf. [8] and references therein.

For the half moment P_1 system in one space-dimension, for instance, we assume that in each half range the distribution can be represented by a polynomial of degree one. The coefficients of the polynomial are determined by the constraint that the lower order half moments should be reproduced. The half moment P_1 system reads,

$$\frac{1}{c}\partial_t E_+ + \partial_x F_+ = \kappa(\frac{1}{2}\langle B\rangle - E_+) + \sigma(\frac{1}{2}(E_+ + E_+) - E_+) \quad (3.7)$$

$$\frac{1}{c}\partial_t F_+ + \partial_x(\chi_+(f_+)E_+) = \kappa(\frac{1}{4}\langle B\rangle - F_+) + \sigma(\frac{1}{4}(E_+ + E_+) - F_+) \quad (3.8)$$

$$\frac{1}{c}\partial_t E_- + \partial_x F_- = \kappa(\frac{1}{2}\langle B\rangle - E_-) + \sigma(\frac{1}{2}(E_+ + E_+) - E_+) \quad (3.9)$$

$$\frac{1}{c}\partial_t F_- + \partial_x(\chi_-(f_-)E_-) = \kappa(-\frac{1}{4}\langle B\rangle - F_-) + \sigma(-\frac{1}{4}(E_+ + E_+) - F_-). \quad (3.10)$$

The partial Eddington factors are

$$\chi_\pm(f_\pm) = -\frac{1}{6} \pm f_\pm \quad \text{with} \quad f_\pm = \frac{F_\pm}{E_\pm}. \quad (3.11)$$

We note that this is a hyperbolic system. The eigenvalues associated to the "+" moments are positive, while the eigenvalues associated to the "-" moments are negative, in accordance with physical intuition. This structure makes the formulation of accurate boundary conditions easy. We simply prescribe the ingoing half moments, in accordance with the conditions (1.2) for the full equations. For more discussions, including existence and uniqueness results, and the explicit quarter moment P_1 closure in two space-dimensions we refer the reader to [52].

3.2. Partial moment entropy closure

The partial moment entropy closure was introduced for radiative heat transfer in [13] and developed in [12, 16, 63]. For the sake of completeness we recall the procedure explained earlier. We have to find a distribution function $\mathcal{J}$ that minimizes the radiative entropy H_R^* given by (2.36-2.37), under the constraint that it reproduces the lower order partial moments,

$$\langle \mathcal{J} \rangle_A = E_A \quad \text{and} \quad \langle \Omega \mathcal{J} \rangle_A = F_A \tag{3.12}$$

for all $A \in \mathcal{A}$. The minimizer is given by

$$\mathcal{J} = \sum_{A \in \mathcal{A}} \frac{1}{\alpha_A^4 (1 + \beta_A \cdot \Omega)^4} \mathbf{1}_A, \tag{3.13}$$

where α_A and β_A are Lagrange multipliers corresponding to the constraints. This formula differs from the one given in [13] since we consider frequency-averaged quantities here. It can be obtained from the minimizer in [13] by integration over ν.

In the case of $\mathcal{A} = \{\mathcal{S}_+, \mathcal{S}_-\}$, the half moments over this distribution can be computed explicitly and the half Eddington factors are [13],

$$\chi_\pm = \frac{8 f_\pm^2}{1 \pm 6 f_\pm + \sqrt{1 \pm 12 f_\pm - 12 f_\pm^2}}. \tag{3.14}$$

For the full moment and the half moment model an explicit closure is possible only if we take the two lowest order moments. If we were to test with $\Omega \otimes \Omega$ and to obtain an equation for the pressure P an explicit closure would be impossible. In the case of quarter moments in 2D even the integrals over the distribution function cannot be computed explicitly. However, the system can be closed numerically by tabulating the pressure tensor as a function of energy and flux, for more details see [16].

The Partial Moment Entropy approximation has a lot of desirable physical and mathematical properties. The underlying distribution function is always positive. Hence the relative flux and the speed of propagation are limited. The system is symmetriziable hyperbolic. This makes it accessible to a powerful mathematical theory guaranteeing well-posedness locally in time. Like the full moment entropy approximation [11], the system correctly approaches the diffusive limit and the free-streaming limit. The eigenvalues of the half moment and quarter moment entropy aproximation have a special structure. For the half moment case, the eigenvalues of the "+" direction are always positive, the eigenvalues of the "−" direction are always negative. Both are bounded in modulus by the speed of light c. This property makes very simple and accurate numerical schemes possible, for example kinetic schemes or upwind schemes. The formulation of accurate boundary conditions is again straight-forward.

4. Comparison of the Models

The approximations presented above have different mathematical structures. The Discrete Ordinates, Spherical Harmonics and partial P_N equations are linear first order partial differential equations. The minimum entropy and the partial moment entropy system are nonlinear hyperbolic first order partial differential equations. On the other hand the diffusion and flux-limited diffusion equations are parabolic equations, whereas the SP_N equations are elliptic/parabolic. We remark that, although they are closely related, the minimum entropy moment model and flux-limited diffusion with the same Eddington factor are not completely equivalent, but can in fact have very different solutions. For example, the solutions for the minimum entropy system can have shocks whereas this is impossible for flux-limited diffusion.

In Figures 4.1 and 4.2 we show some numerical comparisons of the different models. The abbreviations in the legends mean

- *S40/Transport*: Discrete Ordinates Solution with 40 directions
- *P1*: P_1 approximation with Marshak boundary conditions
- *SP1*: SP_1/Diffusion approximation with Marshak boundary condition
- *FLD*: flux-limited diffusion with minimum entropy Eddington factor and Marshak boundary conditions
- *HSP1*: half P_1 approximation
- *HSM1*: half moment entropy approximation
- *Quarter Space*: quarter moment entropy approximation.

The *transport* solution has been obtained with a source iteration method [59]. The parabolic equations *SP1* and *FLD* have been discretized with a standard finite difference scheme. For the balance laws *P1*, *HSP1*, *HSM1* and

Quarter Space we used kinetic schemes based on the distribution function from the moment closure. All of the latter systems have eigenvalues in modulus less than the speed of light. Thus, similar CFL conditions hold. To be valid in the diffusive limit, the kinetic schemes can be modified to become asymptotic preserving, cf. [13] for a simple analysis in 1D.

In Figure 4.1 we consider a given temperature profile in the unit interval $[0,1]$, $T(x) = 1000 + 800x$. This temperature enters into the Planck source term $\langle B\rangle$ via Stefan-Boltzmann's law

$$\langle B\rangle(T) = \sigma_{SB}T^4. \tag{4.1}$$

At the boundary we prescribe black body radiation at the corresponding temperature as ingoing radiation. In Figure 4.1 we see that the high order Discrete Ordinates solution (considered as benchmark result) and the half moment approximations agree very well, whereas P_1, SP_1 and flux-limited diffusion differ significantly.

This becomes more striking in the 2D example in Figure 4.2. The P_1 and SP_1 approximations are unable to capture the simple anisotropy in this test case, whereas the quarter moment model and the solution of the full equations agree very well.

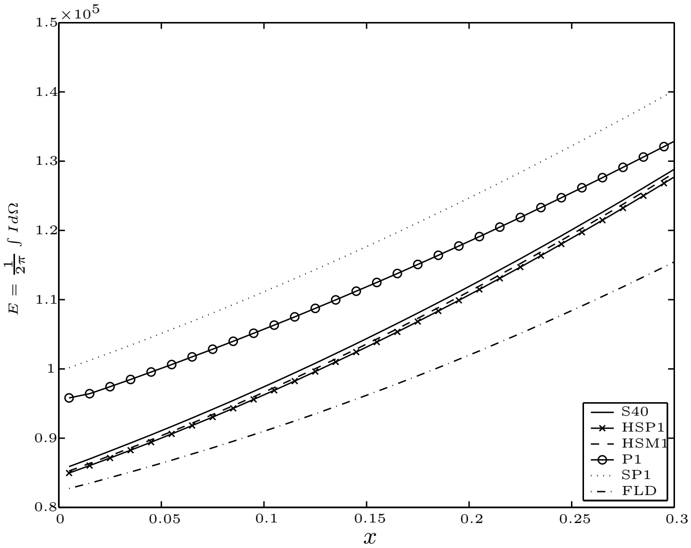

Figure 4.1. Steady radiative energy for a fixed temperature profile $T(x) = 1000 + 800x$ in the interval $[0,1]$, $\kappa = 1$, $\sigma = 0.1$.

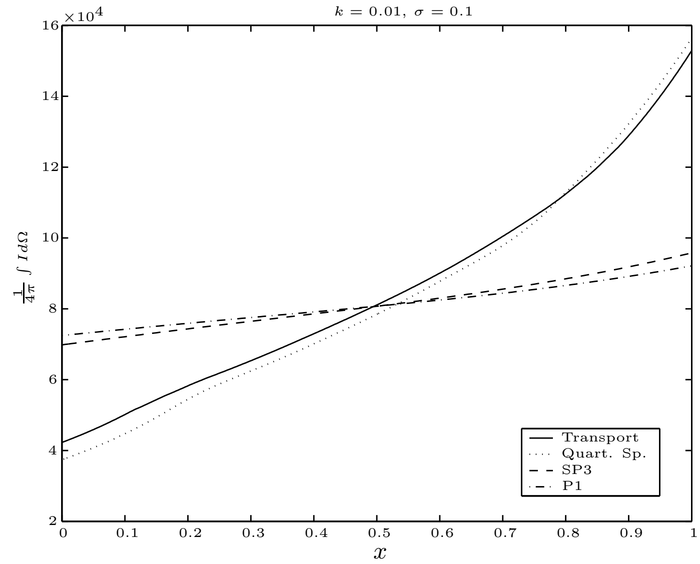

Figure 4.2. Steady radiative energy for a fixed temperature profile $T(x) = 1000 + 400(x+y)$ in $[0,1]^2$, $\kappa = 0.01$, $\sigma = 0.1$. Cut along the diagonal.

5. Conclusion

Of course, the diffusion approximation has the smallest computational effort. Due to the nonlinearity, flux-limited diffusion has roughly twice to three times the computational effort. For P_1 the factor is about 2, for half P_1 4, for half moment entropy 7, for the full solution up to 300 depending on the number of directions.

Partial Moment models generalize the method of moments. Combined with the P_N closure, this class of models can be seen as intermediate between the method of Spherical Harmonics and the method of Discrete Ordinates. The partial moment entropy model removes the major drawback from the minimum entropy closure, namely the possibility of unphysical shocks.

The minimum entropy method leads to problems in the field of rarefied gas dynamics if moments of higher order are used [22, 23]. This is related to the unbounded velocity space. Hence it is not an issue here if we take only angular moments. If one wants to treat also frequency-dependent coefficients, one could use moments of the distribution in terms of frequency, cf. [56]. But then the existence of a minimum entropy solution cannot be guaranteed. This is the reason why the minimum entropy as well as the partial moment minimum entropy model have been generalized [60, 62, 63] to frequency-dependent coefficients using a multigroup approach.

The partial moment entropy model has been further developed to an adaptive half moment model in [49].

In conclusion, the partial moment entropy model has many mathematical and physical advantages compared to the established models. Its computational effort is slightly higher but its accuracy is comparable to high order direct methods.

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