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CHARTB MULTIGROUP TRANSPORT
PACKAGE

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CHARTP MULTIGROUP TRANSPORT PACKAGE

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Abstract

We discuss the physics and numerical implementation of the radiation transport routine used in the CHARTP MID code. It is a one-dimensional (Cartesian, cylindrical, and spherical symmetry), multigroup, diffusion approximation. Tests and applications will be discussed as well.

NOTES
1. The purpose of this report is to describe the radiation transport routine used in the CHARTP MID code. It is a one-dimensional (Cartesian, cylindrical, and spherical symmetry), multigroup, diffusion approximation. Tests and applications will be discussed as well.

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CHARTB MULTIGROUP TRANSPORT PACKAGE

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Introduction and Overview

We document the transport scheme developed for use in the CHARTB MHD code. This should provide users of that code, or those who wish to adopt the subroutine package to other codes, with a basis for doing so and understanding what they are doing. The first section reviews basic transfer theory and presents the basic equations and approximations employed in the multigroup radiation transport scheme. In the next section, we discuss the finite difference form used to treat these equations and discuss the actual implementation in the code. Finally, we give a specific example of the usage of the package on a specific problem, that of the formation of an ionized channel in air by an exploding wire. This problem had been treated previously with the CHARTB code, using a phenomenological heat conduction coefficient in a diffusion equation. Here we discuss the effect of using a five and eight band multigroup scheme.

I. Discussion of the Basic Equations and Approximations

A. The Equations of Transport

The radiation field is completely described by specifying the intensity function $I(t, \vec{r}, \vec{\mu}, \nu)$, where t is the time, $\vec{r}$ the location, $\vec{\mu}$ the direction of photon flight (i.e., $-\vec{\mu}$ is the direction in which we are looking and asking the question: "What photon flux do I see?") and ν is the frequency. The equation of radiative transfer is simply a conservation equation for I , taking account of the sources and sinks of photons, and has the form:

$$\left(\frac{\partial}{\partial t} + c\vec{\mu} \cdot \nabla \right) I = S - \text{Sinks} \quad (1)$$

Here, S is the source term and c the speed of light. We can view the left-hand side as the "substantial" or comoving derivative of fluid mechanics, for a "gas" of photons, all of which move at the speed c . One may also view it as a Boltzmann equation with I taking the role of the distribution function f , with the following special properties of the radiation field noted:

- (1) photons can be absorbed and created, hence the source and sink terms,
- (2) as Maxwell's equations are linear, there cannot be collisions between photons and hence no collision operator--this is an approximation neglecting vacuum polarization effects,
- (3) the $F \cdot \partial/\partial \nu$ term of the Boltzmann equation is absent from the left-hand side, since we neglect the gravitational force on photons, and that is the only force the photon is subject to

(caveat--again this is an approximation--quantum-electrodynamic effects are neglected)⁴ as noted above, all photons move with the same speed, c .

All of the approximations employed here are valid for the situations we will consider; highly energetic, relativistic situations that engage astrophysicists, with matter moving relativistically, etc., would require more careful treatment (see, e.g., Pomraning¹).

B. The Source and Sink Terms

Before going into details about the approximation used, it is useful to discuss the specific forms assumed for the source and sink terms. For the sink or "loss-of-photons" term, we use "Beer's law," $\text{sink} = kI$. Here k may be thought of as a probability per unit length for a photon to be lost, that is, absorbed or scattered. If it is scattered, it becomes a photon travelling in a different direction; such photons become a source term. We may write $k = k_{\text{abs}} + k_{\text{scat}} = k_{\text{line}} + k_{\text{cont}} + k_{\text{scat}}$. The absorption coefficient k_{abs} has been broken up into line and continuum contributions, as is useful either in treating line transport or in discussing "line blanketing" effects upon continuum transport. The absorption term is usually defined so as to include the effects of stimulated emission, $k_{\text{abs}} = k_{\text{uncorrected}} (1 - \exp(-E/kT))$, where E is the photon energy and $k_{\text{uncorrected}}$ is the absorption uncorrected for such stimulated emission as computed from atomic physics.

The source term S , we will write as $S = k_{\text{abs}} B(T) + S_{\text{scat}}$. Here, S_{scat} is the effective source due to photons scattered into the beam. Such scattering is usually approximated as isotropic, and we will use

this ansatz as it is a great simplification: $\beta_{\text{scat}} = k_{\text{scat}} \int I \, d\omega/h\nu$. Strictly speaking, we should assume k_{scat} is a function of incident and emitted photon energies, which may not be equal. This is very important in the treatment of resonance line transport, since the change in frequency allows energy to diffuse in frequency space away from the line center and escape more readily. For our purposes, the assumption of coherent or elastic photon scattering without a change in photon energy is sufficient, since we do not propose to treat lines in detail and therefore assume the frequency range of any frequency band used is much larger than any frequency shift upon scattering. The treatment of transport of resonance line radiation is a subject in itself and requires additional approximations to be tractable. We will assume that either such lines are not treated or are included in a phenomenological manner by changes to the absorption and scattering coefficients.

The other term in the source function S is proportional to $B(T)$, the blackbody temperature at the local (electron) temperature T . This is an expression of Kirchhoff's law and can be derived for local thermodynamic equilibrium conditions in which emission and absorption must balance. Deviations from this condition do not necessarily invalidate it, and the scattering term included in S has the effect of "patching things up" when Kirchhoff's law fails, since the failure is usually in the form of resonance radiation or other externally imposed radiation "input" into a system with little emission of itself, and in this situation scattering will appropriately model the source function. Such an approximation should work well for a collisionally-dominated (i.e., sufficiently dense) plasma; for a tenuous plasma, one would have to use a non-LTE equation of state package to solve for the various level

populations, in conjunction with the transport code. Such complexities are beyond the scope of this code.

C. Approximate Treatment of the Equation of Transfer

As it stands, (1) must be solved at every timestep t , at each frequency or energy E , for all angles (a two-dimensional manifold) and all positions. We can and will discretize the energy space, solving for a few "bands" with average values of I , B , and k . The angular coordinate space (the various S_n or DS_n methods) can be treated by Monte Carlo methods or by expansion methods (the P_n methods). Here we use the simplest of the P_n methods, the P_1 method, also known variously as the Eddington or diffusion approximation. We sacrifice detailed knowledge of the angular distribution of I at each point for simplicity.

The method is to take moments of (1), multiplying it by 1 , $\vec{\mu}$, in much the same way moments of the Boltzman equation, multiplied by powers of v , are used to obtain the usual equations of fluid mechanics (e.g., Ref. 2). First, we define the first three moments as follows:
 $E = \frac{1}{c} \int I \, d\omega/4\pi$, the 0th moment, the energy density; $F = \int I \, \vec{\mu} \, d\omega/4\pi$, the 1st moment, the energy flux; and $K = \int I \, \vec{\mu} \vec{\mu} \, d\omega/4\pi$, the 2nd moment, the radiation pressure. Note that the radiation pressure, as is the usual stress tensor, is a second order tensor or dyad; as in fluid mechanics, we will treat K as the diagonal element, or $1/3$ of the trace of that tensor. This is perfectly consistent with the Eddington approximation, which assumes the radiation field is approximately isotropic (see, e.g., Ref. 3). Then upon integrating (1) over all angles

$$\left(\frac{1}{c} \frac{\partial}{\partial t} + k\right) E + \nabla \cdot F = \frac{1}{4\pi} k_{\text{abs}} B + k_{\text{scat}} E \quad (2)$$

and upon multiplying by $\vec{\mu}$ and integrating:

$$(\partial_t/c + k) F + \nabla \cdot K = 0 \quad (3)$$

We close the system of moments by relating K to E , by assuming that we may represent I as $I = I_0 + 3(\vec{j} \cdot \vec{\mu})$, neglecting any higher powers of $\vec{\mu}$ in an expansion of the angular dependence of I . Then j is equivalent to F and I_0 , the isotropic part of I to E . K is then found to be equal to $F/3$. One may also obtain this result (in plane or spherical geometry, at least) if one assumes that I has one constant value in the hemisphere corresponding to "outward" flow and another constant value in the "inward direction." Calling these values I_1 and I_2 , $E = \frac{1}{2}(I_1 + I_2)$, $|\vec{F}| = \frac{1}{4}(I_1 - I_2)$, and $K = E/3$. Then (3) becomes

$$(\partial_t/c + k) \vec{F} + \nabla E/3 = 0 \quad (4)$$

One can solve the system of (2), (4) for E and F (see, e.g., Ref. 4). However, we obtain considerable simplification (from a bi-tridiagonal system to a simple tridiagonal system) if we neglect the time derivative in (4). This is very often done (e.g., Ref. 5 and 6) and can be justified when $\Delta t \gg (ck)^{-1} = L(c\tau)^{-1}$, where Δt , L , τ are characteristic system, time and length scales, and optical depth, respectively. It is therefore a good approximation for quasi-steady or optically thick systems, among others.

In place of (4) we will therefore use

$$F = -\nabla E / (3k) . \quad (5)$$

This is of the same form as Fick's law for diffusive flux or Fourier's law of heat conduction, and should make clear the diffusive nature of the approximate system of equations.

To evaluate the accuracy of the Eddington approximation, one generally needs to consider the boundary conditions and other aspects of the problem. However, it has been shown¹¹ that for both optically thick and thin systems, the correct heating rate (flux divergence) is obtained. Hence the energy transport calculated should not be significantly in error, whatever the system optical depth--assuming, of course, all else (opacities, band structure, zoning, etc.) is well done.

We have to specify boundary conditions. For the complete equations, we might specify the incident flux. In the context of moments, we use the Marshak approximation to relate the moments and their derivatives to the incident flux (which is usually zero in most problems of interest). We have,^{1,4}

$$\frac{1}{4}E - \frac{1}{2}n \cdot I_{\text{inc}} = F \quad (6a)$$

at the ends of a plane slab, or the outside of a sphere or cylinder. At the center of a sphere or cylinder, symmetry requires

$$\partial_x E = 0 . \quad (6b)$$

If we have an external boundary with reflectivity ρ and emitting at blackbody temperature T , then (6a) becomes, through the Eddington approximation

$$(1 + \rho) \frac{2}{3\lambda} \frac{\partial E}{\partial r} + (1 - \rho) E = 137 T_w^4 n^2 FB,$$

where

λ = mean free path in outermost mesh zone of band

ρ = reflectivity of wall

n = refractive index (taken as 1)

FB = fraction of blackbody energy emitted into band by blackbody
emitted at temperature T

The variables ρ and T_w (called REFL and TWALL in the computer code) are set internally in the transport code's main routine, MGXPA.

II. Finite Difference Implementation

We must solve (2),(5), subject to the boundary conditions (6j). This may be done as a tridiagonal system, upon substituting for F, using (5) in (2). One has only the variable E in (2) and (6) after this replacement.

As CHARTB is a Lagrangian code, we must modify (2) slightly; ρ_t in the Eulerian frame becomes $d/dt - u \cdot \nabla$, where d/dt is the Lagrangian or comoving derivative; for any moving Lagrangian material element, the change in the radiation energy density E is given by dE/dt .

For stability, we use fully implicit equations, although this can easily be altered.

We divide frequency space into m bands and calculate using source functions B, energy densities E, and absorption coefficients k integrated (or averaged in the case of k) over each band. We will use a mean free path L rather than an absorption coefficient k; $L(\text{cm}) = 1/k$.

Let E_{jk}^i denote the energy density at the i th timestep at the j th grid point for the k th band. We will suppress the k index, as we neglect scattering between bands, and therefore all the k indices within one equation are the same. We define the following auxiliary variables:

$w_k(t)$ = fraction of energy emitted by a blackbody at temperature T into energy bank k

$f_{ik} = L_{ik}c/3$ = diffusion coefficient

$f_{l_{ik}} = c \Delta t / L_{ik}$ = cell thickness parameter (dimensionless)

$DX2 = \Delta t / x_{i+1} - x_{i-1}$

$GFP = \frac{x_{i+1} + x_i}{2x_i}$

$GFM = \frac{x_{i-1} + x_i}{2x_i}$

$GMA = \begin{cases} 1 & \text{plane} & \text{geometry (IGM = 1 in CHARTE)} \\ GFP & \text{cylindrical} & \text{geometry (IGM = 2 in CHARTE)} \\ GFP^2 & \text{spherical} & \text{geometry (IGM = 3 in CHARTE)} \end{cases}$

$GMB = \begin{cases} 1 & \text{plane} & \text{geometry (IGM = 1 in CHARTE)} \\ GFM & \text{cylindrical} & \text{geometry (IGM = 2 in CHARTE)} \\ GFM^2 & \text{spherical} & \text{geometry (IGM = 3 in CHARTE)} \end{cases}$

$A = \frac{F_{i,k} + F_{i+1,k}}{2(x_{i+1} - x_i)} \quad GMA \quad DX2$

$B = \frac{F_i F_1 + F_{i-1}}{2(x_i - x_{i-1})} \quad GMB \quad DX2$

$B = aT^4 \quad a = 137 \text{ erg/(eV)}^4/\text{sec}$

Then the tridiagonal system to be solved possesses a typical row of the form:

$$E_{i+1}^{n+1} (-A - U_1 DX2) + E_i^{n+1} (1 + F_{1ik} + A + B) + E_{i-1}^{n+1} (-B + U_1 DX2) =$$

$$F_i^n + F_{1ik} (137 w_{ik} T_b^h)$$

The outer boundary condition, imposed on the 1st zone in the CHARTS code, is (6a)

$$E_1 (1 - \text{REFL} + \text{AUX1}) - E_2 \text{AUX1} = \text{AUX2}$$

where

$$\text{AUX1} = \frac{\rho^2}{3(X(1) - X(2)) L_{1k}} (1 + \text{REFL})$$

$$\text{AUX2} = \begin{cases} 0 & \text{No incident flux.} \\ w_k(T_b) 137 T_b^h & \text{For fixed incident flux} \\ & \text{due to nearby wall at} \\ & \text{temperature } T_b \text{ (eV).} \end{cases}$$

The inner boundary condition currently in use is $E(r=0) = E(r=r)$, appropriate for cylindrical or spherical geometry.

The tridiagonal system is solved by standard means.

The flux is then tested to see if it exceeds the freestreaming limit, i.e.,

$$\text{if } \left| \frac{(F_1 + F_{i-1})}{2} \frac{E_1 - E_{i-1}}{X_1 - X_{i-1}} \right| > c(E_1 + E_{i-1})/2$$

If this ratio exceeds 1, call it AUX2. Then F_1 , F_{i+1} , F_{i-1} are divided by AUX2 and the calculation repeated. This is done up to a fixed number of times, MAXIT, currently 1.

The code computes the source term in the energy equation, ZJ_1

$$= \sum_k \frac{c}{L_{1k}} (E_{1k} - B_{1k})/\rho_1 \quad \text{ergs/sec/gm}$$

$$= \sum_k \frac{c}{L_{ik}} (E_{ik} - 137. w_k T^4) / \rho$$

For diagnostic purposes, we compute a radiation temperature:

$$T_{\text{rad}}^4 = \sum_k E_k / 137.$$

The auxiliary routine FFBB(X) computes the fraction of blackbody radiation emitted between $X = 0$ and $X = X$, where $X = h\nu/kT$. $W_{ik} = \text{FFBB}(X_2) - \text{FFBB}(X_1)$, where $X_2 = E_{i+1}/T_i$, $X_1 = E_k/T_i$. These values of W_{ik} are stored in an array since W is used more than once in the code. E_k is the lower energy bound of the k th band, E_{k+1} the upper bound--we assume the energy bands are contiguous. $\text{FFBB}(X)$ is computed

$X < 1$. by series expansion.

$X > 7$. by asymptotic expansion.

$1 < X < 7$. by logarithmic interpolation in a table.

Subroutine OPAC returns $1/L_{ik}$, from a logarithmic tabular interpolation.

We attempted to use the definition of diffusion coefficient f_{ik} of Alme and Wilson,⁵

$$f = \frac{Lc}{3 + L \left| \frac{1}{E} \frac{\partial E}{\partial r} \right| \left(1 + 3 \exp - \frac{L}{2} \left| \frac{1}{E} \frac{\partial E}{\partial r} \right| \right)}$$

which for thin systems gives a flux limiting effect. Tests on homogeneous cylindrical emitters at uniform temperature, however, showed that the simpler form is superior, at least for steady state problems (see below).

III. Verification of the Eddington Approximation and the Basic Transport Algorithm

A number of test cases were run to verify the algorithms described above. First, we tested the validity of the Eddington approximation itself, as well as the tridiagonal numerical algorithm used to implement it. Kesten⁷ gives an exact, analytic solution for a radiating cylinder, but we found that computation with his formula is numerically ill-conditioned. Henslet and Warming⁸ give an exact analytic solution for the surface flux from a homogeneous infinite cylinder; their result may easily be generalized for the flux at arbitrary radial depth in the cylinder. This formula was used for comparison with computed results (we should note that the paper by Henslet and Warming also includes some results obtained with the Eddington approximation, but we emphasize that our comparisons were with the exact formula). Table 1 presents the computed surface fluxes for various cylinder optical depths (measured along a radius) for the exact answer, and the Eddington approximation computed with and without the Alme and Wilson flux-limiting procedure; 101 mesh points were used. In general, the accuracy of the surface flux gives a good estimate of the accuracy of the fluxes at smaller radii. We conclude that for such problems (radiating cylinders) the Eddington approximation is valid and the code correctly implements it.

IV. Typical Run: Verification of Multigroup Package

To verify and illustrate the use of the multigroup routine, we repeated the calculation, reported by Miller et al.,⁹ of the evolution of a plasma channel in air. Both five and eight band models were used.

TABLE I

Surface flux from homogeneus radiating cylinder.

<u>Optical Depth along Radius</u>	<u>Numerically Computed Eddington Approx.</u>		<u>Exact</u>
	<u>Simple</u>	<u>Alme/Wilson Limiting</u>	
.1	.56	.52	.556
1.	2.67	1.68	2.56
10.	3.186	2.03	3.135

For the five band simulation, the energy boundaries were 0., 4., 7., 9., 12., 30. eV. For the eight band, the boundaries were 0., 1., 3., 5., 7., 9., 12., 50., and 500. The 9-12 eV band was chosen to model as a unit the Schuman-Runge band of the oxygen molecule. The opacity data was taken from the SAI calculations supplied by R. Johnston.¹⁰ The mean free path for each band was found by averaging over the values within that band in the SAI tables. Photon energies below .5 eV were not included in computing the opacity in the lowest energy band, as the SAI tables did not include detailed treatment of molecular band structure and are unreliable here. Previous CHARTB calculations employed a phenomenological mean free path (see Ref. 9 for a complete discussion) with the one-temperature diffusion transport algorithm of CHARTB. This resulted in a channel of the correct dimensions, but one that was too cold to explain holographic data.

We are interested not only in the comparison with experiment but in the sensitivity of the results to:

- (1) the choice of band structure: five vs. eight band models
- (2) sensitivity of results to initial channel properties
(radius, temperature)
- (3) sensitivity to ambient density (assumed uniform)

We will again compare to experiment (and between varying initial conditions) at one and six microseconds after the start of the discharge. In forming our group opacities, we had to average the more detailed opacity table of Ref. 10 over frequency within the bands. For the five band results, we tried taking both harmonic and arithmetic means.

The former are, of course, consistently smaller. We found it made little difference to the results and used the arithmetic mean of the eight band opacities (the reciprocal mean data of Ref. 10 was employed). We stored the logarithm of the opacity internally and interpolated linearly (in the logarithm) in density and temperature to find the inverse mean free path used in the calculations. The data of Ref. 10 applies for 13 temperatures between 2000 K and 20 eV, and eight densities from 10 times normal ($1.293 \times 10^{-3} \text{ gm/cm}^3$) down by factors of 10 each step. Table II summarizes the results of the parameter variations, showing the results are reasonably insensitive to initial conditions. The most influential parameter seems to be the initial channel radius. Figure 1 gives the expected holographic fringe shift (double exposure holographic interferograms taken with He-Ne laser). This may be compared with Fig. 2 of Ref. 9. Note that agreement has improved over the one-temperature model in that the channel temperature is calculated to be somewhat higher. These results suggest to us the value of the multigroup transport routine for use in such channel studies and the ability of such a routine to provide valuable data for designing plasma channel beam transport systems.

Conclusions

We have documented here in some detail the MGXPA transport package. It is our hope that in this way a prospective user of CHARTD or CHARTB will have little trouble understanding and using it. It should also be easily adoptable to similar codes if desired. We have

TABLE II

Sensitivity of results to model.
 (8 band, $\rho = 1.E-3$, $r_c = .06$, $T_o = 1$. unless noted)

<u>Case</u>	<u>t = 2 μs</u>		<u>t = 6 μs</u>	
	<u>r</u>	<u>T</u>	<u>r</u>	<u>T</u>
5 band harm	.26	2.6	.7	2.6
5 band arith	.26	2.4	.7	2.7
8 band	.26	2.4	.78	2.8
$r_o = .03$	.22	4.0	.73	3.0
$\rho = 1.293-3$	.24	1.8	.7	2.9
$\rho = 1.293-3$ $T_o = .75$	.25	2.3	.73	2.9

FIGURE 1

FRINGE
SHIFT

FIGURE 2

FRINGE
SHIFT

FIGURE 3

discussed the test's run to show that it does indeed correctly model transport of radiation in cylindrical systems and have shown with a comparison of calculated and experimental results that CHARTB with the MGXPA multigroup package can be a formidable tool for use in MHD problems of interest.

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