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Verification of the Radiation Package in ALEGRA

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Verification of the Radiation Package in ALEGRA

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Abstract

The ALEGRA radiation transport package implements diffusion, flux-limited diffusion, and SP_n radiation transport for both gray and multigroup photon spectra. Comparisons of ALEGRA calculations with known solutions for a selection of benchmark problems for these transport theories are presented. ALEGRA returns accurate solutions in each case. This verifies that each transport theory has been implemented correctly, though it does not prove that the transport theories are valid for problems of interest at Sandia. A validation study will be presented in a future report.

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Summary

ALEGRA has a robust radiation transport package that provides diffusion, flux-limited diffusion, and SPn transport formulations for both gray and multigroup calculations. This package has been verified by comparing calculations for a set of benchmark problems against their known solutions for various transport theories. ALEGRA calculates solutions that are very close to the expected result for each transport theory tested.

1. Introduction

ALEGRA is an arbitrary Lagrangian-Eulerian shock physics code based on a flexible C++ framework architecture [6]. This framework architecture supports the addition of new physics packages to ALEGRA using an operator-splitting formalism. This makes ALEGRA a powerful tool for the simulation of high-energy phenomena in which various forms of transport are strongly coupled.

This document presents a verification study of the radiation transport capability that has been added to ALEGRA in support of Sandia's Z-pinch program and related programs. The ALEGRA radiation package provides radiation transport in the form of diffusion, flux-limited diffusion, or SPn transport with either gray or multigroup photon spectra. A number of benchmark problems exist for which the exact solution is known for one or more of these transport theories. Each transport option in ALEGRA has been verified by comparing the ALEGRA calculation for the appropriate benchmark with the exact solution.

1.1 Radiation Transport Approximations

This section describes the radiation transport equations and the transport approximations employed by ALEGRA and verified in this study.

1.1.1 The Radiation Transport Equations

The transport of radiation is described by the equation

$$\frac{1}{c} \frac{\partial I}{\partial t} + \hat{n} \cdot \nabla I = \eta - \chi I \quad (1)$$

where I is the specific intensity, a function of position, time, energy, and direction having dimensions of energy per area per second per solid angle. The emission η is in general a function of the same variables as I and has dimensions of energy per volume per second per solid angle. The total opacity χ is also in general a function of the same variables as I and has dimensions of inverse length. The unit vector $\hat{n}$ is the direction towards which the photons are propagating and c is the velocity of light.

The formal solution of this equation is

$$I(\vec{x}, \hat{n}, t, \nu) = c \int_{-\infty}^t \eta(\vec{x} + \hat{n}c(t' - t), \hat{n}, t', \nu) e^{-\int_t^{t'} \chi(\vec{x} + \hat{n}c(t'' - t), t'', \nu) c dt''} dt' \quad (2)$$

for an infinite domain. (We ignore the matter of boundary conditions for now.) The formal solution is awkward to work with, but it does allow us to see some of the properties of the intensity. For example, it is clear that the intensity will be nonnegative everywhere if the

emissivity η and extinction χ are nonnegative everywhere. For real physical situations, this will always be the case.

In general, the emissivity at a given point will depend on the density and temperature of the medium *and* the intensity of the radiation at that point. The latter contribution arises from the scattering of radiation. The temperature and density evolution of the medium is also coupled to the radiation intensity, because absorption or emission of radiation heats or cools the medium. Both these phenomena greatly complicates the solution of the transfer equation, since they cause I to appear within the integral on the right side of Equation (2). Thus Equation (2) is an implicit integral equation with a complicated kernel.

The time domain can be truncated by splitting the integral and replacing the early portions with initial conditions:

$$I(\hat{x}, \hat{n}, t, \nu) = c \int_{t_0}^t \eta(\hat{x} + \hat{n}c(t' - t), \hat{n}, t', \nu) e^{-\int_t^{t'} \chi(\hat{x} + \hat{n}c(t'' - t), t'', \nu) c dt''} dt' + I(\hat{x} + \hat{n}c(t_0 - t), \hat{n}, t_0, \nu) e^{-\int_{t_0}^t \chi(\hat{x} + \hat{n}c(t' - t), t', \nu) c dt'} \quad (3)$$

The formal solution of Equation (2) for the static case is

$$I(\hat{x}, \hat{n}, \nu) = \int_{-\infty}^0 \eta(\hat{x} + \hat{n}s', \hat{n}, \nu) e^{-\int_s^0 \chi(\hat{x} + \hat{n}s'', \nu) ds''} ds' \quad (4)$$

For the static case, it is customary to define the *optical depth*

$$\tau(\hat{x}, \hat{n}, s, \nu) = \int_s^0 \chi(\hat{x} + \hat{n}s', \nu) ds' \quad (5)$$

One can also speak of an optical depth for the case of slightly time-dependent opacity. If the opacity is strongly time-dependent, the concept of optical depth loses much of its meaning. For the static case, we substitute Equation (5) into Equation (4) to obtain

$$I = \int_{-\infty}^0 \frac{\eta}{\chi} e^{-\tau} d\tau \quad (6)$$

showing that the intensity is equal to the Laplace transform over optical depth of the *source function*

$$S = \frac{\eta}{\chi} \quad (7)$$

The time-dependent case is more complicated because one must use retarded values for the emissivity and extinction, just as in electrodynamics, and for similar reasons.

We see that the intensity is dependent on the history of the source function on those points of the past light cone that intersect the ordinate direction. However, the dependence decays

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very quickly with optical depth, so only those points on the light cone within about an optical depth or so of the point of interest contribute greatly to the intensity.

To illustrate, suppose the source function is everywhere zero until time $t = 0$, when a uniform source is turned on simultaneously at all points. Then the formal solution yields

$$I(\mathbf{\hat{x}}, \mathbf{\hat{n}}, t, \nu) = \frac{\eta}{\chi} (1 - e^{-\chi c t}) \quad (8)$$

showing that the intensity quickly equilibrates to the source function as the past light cone is filled in with the nonzero source function. This illustrates the tendency of the radiation intensity in thick media (where the source function changes slowly with optical depth) to equilibrate to the source function.

We have seen that the intensity is positive and causal (since it is determined by the source function on the past light cone.) In addition, the transport equation conserves energy, since

$$\frac{1}{c} \frac{\partial I}{\partial t} + \mathbf{\hat{n}} \cdot \nabla I \quad (9)$$

is a conservative operator, while

$$\eta - \chi I \quad (10)$$

correctly represents the net energy gained (or lost) by the medium through absorption (or emission) of radiation.

Another property of the intensity is that it satisfies the inequality:

$$J \geq |\mathbf{\hat{F}}| \quad (11)$$

where

$$J = \frac{1}{4\pi} \int_{4\pi} I d\mathbf{\hat{n}} = \frac{c}{4\pi} E_R \quad (12)$$

is the mean intensity, which is related to the total radiative energy density E_R , and

$$F = \frac{1}{4\pi} \int_{4\pi} I \mathbf{\hat{n}} d\mathbf{\hat{n}} = \frac{\mathcal{F}}{4\pi} \quad (13)$$

is the astrophysical flux, which is related to the physical flux $\mathcal{F}$ as shown. The inequality (11) follows directly from these definitions and the triangle theorem, since $|\mathbf{\hat{n}}| = 1$. The physical interpretation of Equation (11) is that the ratio of flux to energy density can be no greater than that of a perfectly collimated beam, in which all the photons are travelling in the same direction at the speed of light, c . Equation (11) is called the flux limit.

A highly accurate time-dependent solution of I for an arbitrary problem geometry and set of initial conditions would require detailed knowledge of its variation in a 7-dimensional phase space (three space coordinates, two direction coordinates, the time coordinate, and

the energy coordinate), which taxes the capability of current computing resources. A solution on a rather coarse grid of ten points in each variable would require a million words of storage per time step. And ten points per variable falls far short of useful resolution for the vast majority of interesting problems. We usually have little choice but to make simplifying approximations that retain as much of the original physical behavior as possible. Ideally, these approximation should be positive, causal, conservative, and should not violate the flux limit, in addition to providing a realistic approximation of the flow of energy as radiation.

It should be noted that crude approximations are not necessary on restricted geometries, especially if a static solution is all that is desired. Highly accurate solutions to the radiation transport problem have been calculated for stellar atmospheres, where one can usually assume the intensity is a function of a single spatial variable (due to the high degree of spherical symmetry of most stars) and where a static solution is often sufficient. However, the current ALEGRA radiation package is not designed to address such restricted (though interesting) problems.

1.1.2 The P1 Approximation

The first approximation to the transport equation that we will consider is the *P1 approximation*, which is that

$$I(\hat{r}, \hat{n}, t, E) = J(\hat{r}, t, E) + 3\hat{n} \cdot \hat{F}(\hat{r}, t, E) \quad (14)$$

That is, one expands the intensity in a Taylor series in the direction vector and retains only terms up to first order. The reason for introducing a factor 3 to the linear term will be evident shortly.

One also assumes that the opacity is *isotropic*, which is very nearly true so long as the material velocities are nonrelativistic. The emission generally consists of a thermal component, which is nearly isotropic for nonrelativistic material velocities, and a scattering component, which can usually be approximated by a dipole scattering function. Then

$$\chi = \chi(\hat{r}, t, E) \quad (15)$$

$$\eta = \eta_0(\hat{r}, t, E) + \frac{3}{4}\sigma_0(\hat{r}, t, E) \int I(\hat{r}, \hat{n}', t, E)(1 + (\hat{n} \cdot \hat{n}')^2) \frac{d\Omega'}{4\pi} \quad (16)$$

Plugging Equation (14) into Equation (16), we obtain the perhaps surprising result

$$\eta = \eta_0 + \sigma_0 J \quad (17)$$

indicating that the emissivity is also isotropic if the radiation field is accurately represented by the P1 approximation. Thus, we obtain

$$\frac{1}{c} \frac{\partial J}{\partial t} + \frac{3}{c} \hat{n} \cdot \frac{\partial}{\partial t} \hat{F} + \hat{n} \cdot \nabla J + 3\hat{n} \cdot \nabla(\hat{n} \cdot \hat{F}) = \eta - \chi J - 3\chi \hat{n} \cdot \hat{F} \quad (18)$$

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This is a single equation in two variables, which would seem to make us worse off than before; we solve this difficulty by taking zeroth and first angular moments of the equation, which yields the system

$$\frac{1}{c} \frac{\partial J}{\partial t} + \nabla \cdot \mathbf{\hat{r}} = \eta - \chi J \quad (19)$$

$$\frac{1}{c} \frac{\partial \mathbf{\hat{r}}}{\partial t} + \frac{1}{3} \nabla J = -\chi \mathbf{\hat{r}} \quad (20)$$

where J and $\mathbf{\hat{r}}$ are identical to the quantities defined in Equation (12) and Equation (13), respectively. We now have a fully determined system of equations in terms of these two quantities. These can be solved to give an approximate solution to the radiation field.

The P1 equations are obviously most accurate when the intensity varies only slowly with angle. This is true whenever the source function varies slowly with optical depth. The P1 equations are approximately causal and are conservative for reasonable spatial discretizations of the operators appearing in the equations. However, it can be shown that the P1 equations are not positive for reasonable spatial discretizations on a nonuniform mesh.

Consider a very simple 1-D mesh in spherical geometry consisting of two elements, whose nodes are located at $r = 0, 1, 2$. Let the intensities be element-centered and the fluxes be node-centered, and assume that no material is present. Assume the inner and outer boundaries are both reflecting boundaries, so that the flux is zero. One quite reasonable spatial discretization of the P1 equations on this mesh is

$$\frac{1}{c} \frac{\partial J_1}{\partial t} + 3F_1 = 0 \quad (21)$$

$$\frac{1}{c} \frac{\partial J_2}{\partial t} - \frac{3F_1}{7} = 0 \quad (22)$$

$$\frac{1}{c} \frac{\partial F_1}{\partial t} + \frac{1}{3}(J_2 - J_1) = 0 \quad (23)$$

This has the solutions

$$\begin{aligned} J_1 &= 1 \\ J_2 &= 1 \\ F_1 &= 0 \end{aligned} \quad (24)$$

$$\begin{aligned} J_1 &= \cos \sqrt{\frac{8}{7}} ct \\ J_2 &= -\frac{1}{7} \cos \sqrt{\frac{8}{7}} ct \\ F_1 &= \frac{1}{3c} \sqrt{\frac{8}{7}} c \sin \sqrt{\frac{8}{7}} ct \end{aligned} \quad (25)$$

We can combine these to form the solution

$$\begin{aligned} J_1 &= \frac{1}{7} + \cos \sqrt{\frac{8}{7}} ct \\ J_2 &= \frac{1}{7} - \frac{1}{7} \cos \sqrt{\frac{8}{7}} ct \\ F_1 &= \frac{1}{3c} \sqrt{\frac{8}{7}} c \sin \sqrt{\frac{8}{7}} ct \end{aligned} \quad (26)$$

which satisfies the quite reasonable initial conditions

$$\begin{aligned} J_1 &= \frac{8}{7} \\ J_2 &= 0 \\ F_1 &= 0 \end{aligned} \quad (27)$$

but which eventually evolves to

$$\begin{aligned} J_1 &= -\frac{6}{7} \\ J_2 &= \frac{2}{7} \\ F_1 &= 0 \end{aligned} \quad (28)$$

at time $t = \sqrt{\frac{7}{8}} \frac{\pi}{c}$. Clearly these very reasonable initial values evolve to a nonpositive solution.

Another weakness of the P1 equations is that they can exceed the flux limit. Consider a point source in a vacuum. In the static limit the radiation field has the exact solution

$$J = \frac{F_0(v)}{r^2} \quad (29)$$

$$\vec{F} = \frac{F_0(v)}{r^3} \vec{r} \quad (30)$$

satisfying the flux equality characteristic of streaming radiation. However, the P1 solution is

$$F_r = \frac{F_0(v)}{r^3} \vec{r} \quad (31)$$

$$J = J_0 \quad (32)$$

where J_0 is indeterminate. In other words, although P1 gives the correct flux for this situation, it returns the wrong mean intensity. Clearly there will be some r within which the flux inequality is violated.

Finally, P1 has a tendency to “turn corners.” Although we do not present a formal solution to the P1 equation, we note that the mean intensity J contains contributions from all past points to which the point of interest can be connected by an arbitrary path of length $c(t-t')$. This path need not be a straight line. This implies that collimated beams will not remain collimated even in the vacuum.

In spite of these weaknesses, P1 is a popular transport theory for certain problem domains. The P1 equations are fairly easy to solve and capture the exact solution in the diffusion limit. They remain soluble (if highly inaccurate) in vacuum regions.

1.1.3 The Diffusion Approximation

The most obnoxious failing of the P1 approximation is the lack of positivity. One way to solve the positivity problem is to neglect the time derivative term in Equation (20). This is equivalent to assuming that the flux approaches a steady value on a time scale much shorter than that required for the intensity to reach a steady value. This will be the case if the transport process is essentially *diffusive*; that is, if the mean free path, defined as

$$l \approx \frac{1}{3\chi}, \quad (33)$$

is much shorter than any other length scale of interest. Hence, the diffusion approximation takes the form

$$\frac{1}{c} \frac{\partial J}{\partial t} + \nabla \cdot \hat{F} = \eta - \chi J \quad (34)$$

$$\hat{F} = -\frac{1}{3\chi} \nabla J \quad (35)$$

or

$$\frac{1}{c} \frac{\partial J}{\partial t} - \nabla \cdot \frac{1}{3\chi} \nabla J = \eta - \chi J \quad (36)$$

This approximation changes the basic character of the equations from hyperbolic to parabolic. The solution is no longer causal; the mean intensity is dependent on the source function at points outside the past light cone. On the other hand, the equations are now positive definite, so J will never go to negative values. Like the P1 equations, the diffusion equations can violate the flux limit (the diffusion and P1 equations are identical in the static limit.)

Another problem with the diffusion equations is that they are usually solved in the form given by Equation (36). This causes difficulties in vacuum regions, where χ goes to zero. One can arbitrarily assign a very small opacity to the vacuum, but the equations remain ill-conditioned unless the opacity is large enough to affect the physics. This is not the case for

P1, in which the flux time derivative term acts like an artificial opacity that keeps the equations well-conditioned in the vacuum so long as the time step is not too large.

ALEGRA does not actually provide a distinct P1 option. P1 is identical to SP1, which is the lowest order SP_n approximation (see section 1.1.5 on page 16.)

1.1.4 Flux Limited Diffusion

Although the diffusion equations are robust and easily solved, we have seen that they break down whenever important regions of the problem are optically thin. The problem is that the diffusion approximation imposes the constraint that the mean intensity must be constant within transparent regions. This is in fact almost never the correct solution for the radiation field in such regions. In transparent regions, a better approximation is the streaming approximation, which is that

$$\vec{F} = J \frac{\nabla J}{|\nabla J|} \quad (37)$$

that is, the flux is equal in magnitude to the mean intensity and is directed parallel to the intensity gradient. Of course, this approximation is of no use in opaque regions.

A widely accepted refinement to the diffusion approximation is to apply a *flux limiter*. This is a reduction factor applied to the flux to improve the quality of the solution. In regions where the material is optically thick, this limiter approaches unity, so the diffusion approximation is recovered where it is most applicable. In regions where the material is optically thin, the limiter becomes small and reduces the flux to the value given by the streaming approximation. In fact, the flux is never permitted to exceed the streaming value, which is dictated by the flux limit, Equation (11).

There are many formulations for the flux limiter, all showing the same behavior in either limit but differing in the details of the transition between the limits. For ALEGRA, we chose the form [3]

$$\lambda = \frac{6 + 3R}{6 + 3R + R^2} \quad (38)$$

where

$$R = \frac{|\nabla J|}{\chi \omega J} \quad (39)$$

and

$$\omega = \frac{\sigma_a B + \sigma_s J}{\sigma J} \quad (40)$$

is the albedo. Its inclusion allegedly improves the solution for certain problems dominated by scattering. The flux equation then becomes

$$\hat{F} = -\frac{\lambda}{3\omega\chi} \nabla J \quad (41)$$

In optically thick regions,

$$R \rightarrow 0 \quad (42)$$

$$\lambda \rightarrow 1 \quad (43)$$

$$\omega \rightarrow 1 \quad (44)$$

$$\hat{F} \rightarrow -\frac{1}{3\chi} \nabla J \quad (45)$$

so the diffusion limit is recovered, while in optically thin regions

$$R \rightarrow \infty \quad (46)$$

$$\lambda \rightarrow \frac{3}{R} = \frac{3\chi\omega J}{|\nabla J|} \quad (47)$$

$$\hat{F} \rightarrow -J \frac{\nabla J}{|\nabla J|} \quad (48)$$

so the streaming limit is also recovered.

The flux limiter does introduce the complication that the radiation equations are no longer linear. ALEGRA ignores this by using the value of the flux limiter calculated at the beginning of the time step in its solution algorithm for the radiation equations.

1.1.5 The SPn Approximation

The most sophisticated approximation available in the ALEGRA radiation package is the simplified Pn approximation, or SPn. This approximation can be derived via an asymptotic analysis of the transport equations [2]. We do not reproduce the derivation here, but only the final result:

$$\frac{1}{c} \frac{\partial u_m}{\partial t} + \nabla \cdot \mathfrak{F}_m + \chi u_m = \eta \quad (49)$$

$$\frac{1}{c} \frac{\partial \mathfrak{F}_m}{\partial t} + \mu_m^2 \nabla u_m + \chi \mathfrak{F}_m = 0 \quad (50)$$

Here u_m are pseudo-intensities and $\mathfrak{F}_m$ are pseudo-fluxes. The mean intensity and flux are given by

$$J = \sum w_m u_m \quad (51)$$

$$\hat{F} = \sum w_m \mu_m \mathfrak{F}_m \quad (52)$$

and the weights w_m and direction factors μ_m are identical in value to the weights and sampling points for Gauss-Legendre integration.

It can be shown that the SP_n equations converge to the exact solution of the transport equation if the medium is homogeneous or the geometry is 1-D. For multidimensional, inhomogeneous problems, the SP_n equations do not converge to the exact solution, but they do seem to provide a better approximation to the solution than either flux-limited diffusion or P1.

One can think of the SP_n equations as being the result of discretizing the transport equation in only one angle coordinate rather than two. They are much less expensive than a full discretization in angle, but also less accurate. We note also that SP1 is identical to P1.

1.2 Coupling the Radiation to the Material

The radiation is coupled to the material through the emissivity and opacity. Both of these quantities are functions of the detailed microscopic state of the material, which evolves under the influence of the radiation field and heating from mechanical work or electromagnetic or nuclear energy sources.

1.2.1 The Approximation of Local Thermodynamic Equilibrium

ALEGRA greatly simplifies the material couplings by assuming the material is in a state of *local thermodynamic equilibrium*. The microscopic state of the material is assumed to be completely determined by its temperature, density, and composition. It can be shown that the only form for the opacity and emissivity consistent with this assumption are

$$\chi = \sigma(\rho, T, \nu) + \kappa(\rho, T, \nu) \quad (53)$$

$$\eta = \sigma(\rho, T, \nu)J + \kappa(\rho, T, \nu)B_\nu(T) \quad (54)$$

that is, radiation is either completely absorbed and its energy instantaneously thermalized, or it is completely scattered without changing the state of the material. Here $B_\nu(T)$ is the Planck black-body function. The transport equation then becomes

$$\frac{1}{c} \frac{\partial I}{\partial t} + \hat{n} \cdot \nabla I + \chi I = \sigma J + \kappa B \quad (55)$$

The zeroth moment of this equation, which describes the radiation energy density, is

$$\frac{1}{c} \frac{\partial J}{\partial t} + \nabla \cdot \mathbf{F} = \kappa(B - J) \quad (56)$$

This makes explicit an important physical behavior: the radiation field tends to equilibrate to the black body function at the temperature of the material. That is, the source function

tends towards the black body function. In strict thermodynamic equilibrium, the source function is equal to the black body function.

1.2.2 The Transfer Equation in the Lagrangian Frame

It is convenient to solve radiation transfer in the presence of a moving medium by using the Lagrangian frame. In this frame, to lowest order, the transfer equation takes the form [1]

$$\frac{1}{c} \frac{DI}{Dt} + n_i \frac{\partial I}{\partial x_i} + \frac{1}{c} I (\delta_{ij} + n_i n_j) \frac{\partial v_j}{\partial x_i} = \eta - \chi I \quad (57)$$

where

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + v_i \frac{\partial}{\partial x_i} \quad (58)$$

is the material or Lagrangian time derivative. We have neglected all terms which will prove to be of order v/c or greater in the zeroth and first moment equations (energy and momentum equations) [7].

All material and radiation quantities in this equation are measured in the Lagrangian frame. However, coordinates and time are in the laboratory frame.

1.2.3 Energy Conservation

We obtain an energy conservation equation by taking the zeroth angular moment of (57) and integrating over frequency:

$$\rho \frac{D}{Dt} \left(\frac{E_R}{\rho} \right) + \frac{\partial F_i}{\partial x_i} + P_{ij} \frac{\partial v_j}{\partial x_i} = \int_0^\infty (4\pi\eta - \chi c E_R(v)) dv \quad (59)$$

It is clear that the most significant energy coupling is through direct absorption and emission of energy as photons by the medium. This is represented by the term

$$\int_0^\infty (4\pi\eta - \chi c E_R(v)) dv \quad (60)$$

Another significant energy coupling comes through radiation work, represented by the term

$$P_{ij} \frac{\partial v_j}{\partial x_i} \quad (61)$$

This cannot be neglected, since it is of order 1 in the dynamic diffusion limit.

1.2.4 Momentum Conservation

We obtain a momentum conservation equation by taking the first angular moment of (57):

$$\frac{\rho}{c^2} \frac{D}{Dt} \left(\frac{F_i}{\rho} \right) + \frac{\partial P_{ij}}{\partial x_j} = -\frac{1}{c} \int_0^\infty \chi F_R(v) dv \quad (62)$$

Radiation exerts a pressure on opaque material through the term

$$-\frac{1}{c} \int_0^\infty \chi F_i(v) dv \quad (63)$$

which represents the radiation forces on the material.

In the case of diffusion, we find that

$$F_i(v) = -\frac{1}{3\chi} \nabla J(v) = -\frac{1}{\chi} \nabla P_R(v) \quad (64)$$

so that

$$-\frac{1}{c} \int_0^\infty \chi F_i(v) dv = \frac{1}{c} \int_0^\infty \nabla P_R(v) dv = \frac{1}{c} \nabla P_R \quad (65)$$

Thus, for diffusion only, the radiative pressure acts exactly like a thermodynamic pressure. For SPn, one cannot make such a simplification, since the flux is not a function solely of the radiation pressure. Under the diffusion approximation, momentum transferred to the radiation field at one point in the material is instantaneously deposited at other points. Under SPn this is not the case, and momentum transferred to the radiation field may not be deposited into the material again for some time.

1.2.5 The Radiation/Hydrodynamics Operator Split

Based on the results in the previous sections, a conservative set of equations for the evolution of a hydrodynamic material subject to radiation transport is

Radiation transport:
$$\frac{1}{c} \frac{DI}{Dt} + n_i \frac{\partial I}{\partial x_i} + \frac{1}{c} I (\delta_{ij} + n_i n_j) \frac{\partial v_j}{\partial x_i} + \chi I = \eta \quad (66)$$

Mass conservation:
$$\frac{D\rho}{Dt} = -\rho \frac{\partial v_i}{\partial x_i} \quad (67)$$

Momentum conservation:
$$\rho \left(\frac{Dv_i}{Dt} - g_i \right) = -\frac{\partial p}{\partial x_i} + \frac{1}{c} \int_0^\infty \chi F_i(v) dv \quad (68)$$

Compliance:
$$\frac{Dx_i}{Dt} = v_i \quad (69)$$

Energy conservation:
$$\rho \frac{DU}{Dt} = \frac{p D\rho}{\rho Dt} + c \chi E_R - 4\pi \eta + \rho \epsilon \quad (70)$$

The quantities appearing in these equations are:

Introduction

- ρ Material density (mass per unit volume).
- I Specific intensity, with dimensions of power per area per solid angle per unit frequency. This is a measure of the number of photons per unit volume at a point in space x_i that are headed in the direction n_i and have frequency ν .
- v_i Material velocity (length per unit time).
- χ Extinction, with units of inverse length. It's a measure of the mean free path of photons. It includes the effects of both scattering and absorption.
- η Emissivity, with units of power per solid angle per volume per unit frequency. It's a measure of the rate at which photons of a particular frequency travelling in a particular direction are introduced to a volume of space. Such photons have either been newly created by various thermal mechanisms or have been scattered into the new direction from their previous direction.
- g_i External body forces, such as gravitation (units of acceleration).
- p Material pressure (force per unit area)
- $\mathcal{F}_i$ Radiation energy flux (power per unit area per unit frequency), defined by the auxiliary equation

$$\mathcal{F}_i = \oint n_i d\omega \quad (71)$$

- U Material specific internal energy (energy per gram). This is primarily thermal energy.
- E_R Radiation energy density (energy per volume), defined by the auxiliary equation

$$E_R = \frac{1}{c} \oint I d\omega d\nu \quad (72)$$

Note that this is an integral over frequency as well as direction.

- ϵ Specific energy deposition rate (power per gram). This can be anything from energy released by chemical or nuclear reactions to energy deposited by Ohmic heating to energy stolen by evil spirits. It's a hook for all the other physics in your code.

ALEGRA handles the material couplings through an operator split. The hydrodynamic equations are first solved assuming a static radiation field and including a force term due to radiation:

$$m_n \left(\frac{v_{in}^{t+1/2} - v_{in}^{t-1/2}}{\Delta t^t} - g_{in}^t \right) = - \sum_e \text{Div}_{ine}^t p_e^t + \frac{1}{c} \sum_{ge} \chi_{gne}^t F_{igne}^t \quad (73)$$

$$\frac{x_{in}^{t+1} - x_{in}^t}{\Delta t^{t+\frac{1}{2}}} = v_{in}^{t+1/2} \quad (74)$$

$$\rho_e^{t+1} = \rho_e^t \frac{V_e^t}{V_e^{t+1}} \quad (75)$$

$$Q_e^{t+1/2} = -\frac{1}{2} \sum_{in} \text{Grad}_{ine}^t p_e^t (v_{in}^{t+1/2} + v_{in}^{t-1/2}) + \rho_e^t \epsilon_e^t \quad (76)$$

The quantities appearing in these equations are:

m_n	Lumped mass at node n
$v_{in}^{t+1/2}$	Velocity at node n at staggered time $t + 1/2$
x_{in}^t	Coordinate of node n at centered time t
Δt^t	t th staggered time step
$\Delta t^{t+1/2}$	t th centered time step
g_{in}^t	Body forces at node n at time t
Grad_{ine}^t	Discretized gradient operator, which maps quantities at element e to quantities at node n at time t
χ_{gne}^t	Total opacity of element e where it connects to node n at time t for energy group g
F_{igne}^t	Radiation flux at element e where it connects to node n at time t for energy group g .
ρ_e^t	Density of element e at time t
V_e^t	Volume of element e at time t
$Q_e^{t+1/2}$	Nonradiative material heating rate at element e at time $t + 1/2$
ϵ_e^t	Chemical/nuclear/prescribed energy deposition rate in cell e at time t

For diffusion, the momentum equation takes the form

$$m_n \left(\frac{v_{in}^{t+1/2} - v_{in}^{t-1/2}}{\Delta t^t} - g_{in}^t \right) = - \sum_e \text{Grad}_{ine}^t (p_e^t + P_{Re}^t) \quad (77)$$

where P_{Re}^t is the radiation pressure.

Now the transfer equations are solved:

$$\begin{aligned} \frac{J_{gme}^{*(t+1)} - J_{gme}^t}{c \Delta t^{t+1/2}} + \sum_f \text{Div}_{fe}^t F_{gmf}^{t+1} + \chi_{ge}^t J_{gme}^{*(t+1)} = \\ \kappa_{ge}^t \left(B_{ge}^t + (T_e^{*(t+1)} - T_e^t) \frac{\partial}{\partial T} B_{ge}^t \right) + \sigma_{ge}^t \sum_m w_m J_{gme}^{*(t+1)} \end{aligned} \quad (78)$$

$$(\text{diffusion}) \quad F_{gmf}^{t+1} = -\mu_m^2 \sum_f \left[\frac{\lambda}{\omega \chi} \text{Grad} \right]_{fe}^t J_{gme}^{*(t+1)} \quad (79)$$

$$(\text{SPn}) \quad F_{gmf}^{t+1} = -\mu_m^2 \sum_f \left[\frac{1}{\chi + \frac{1}{c \Delta t}} \text{Grad} \right]_{fe}^t J_{gme}^{*(t+1)} + \frac{F_{gmf}^t}{1 + c \chi_{gmf}^t \Delta t^{t+1/2}} \quad (80)$$

$$C_{Ve}^t \frac{T_e^{*(t+1)} - T_e^t}{\Delta t^{t+1/2}} = Q_e^{t+1/2} + \sum_g \kappa_{ge}^t \left(\sum_m w_m J_{gme}^{*(t+1)} - \left(B_{ge}^t + (T_e^{*(t+1)} - T_e^t) \frac{\partial}{\partial T} B_{ge}^t \right) \right) \quad (81)$$

Here

J_{gme}^{*t} is the static estimate of the intensity integrated over energy group g in angle group m in cell e at time t

J_{gme}^t is the intensity integrated over energy group g in angle group m in cell e at time t

Div_{fe}^t is the discretized divergence operator which maps a quantity in element e to face f at time t

F_{gmf}^t is the flux across face f at time t in angle group m integrated over energy group g

χ_{ge}^t is the total opacity in element e at time t averaged over group g

κ_{ge}^t is the absorption in element e at time t averaged over group g

B_{ge}^t is the Planck function in element e at time t averaged over group g

T_e^{*t} is the linearized estimate of the temperature in element e at time t

T_e^t is the temperature in element e at time t

σ_{ge}^t is the scattering in element e at time t averaged over group g

w_m are the angle integration weights

μ_m are the angle integration ordinates

$[D\text{Grad}]_{fe}$ is the D -weighted gradient operator which maps quantities at elements e to quantities on faces f . The weight D depends on the transport theory used, but always behaves like a diffusion coefficient.

C_{Ve}^t is the volumetric heat capacity at constant volume in element e at time t .

Note that the flux equation can take one of two forms, depending on whether flux-limited diffusion or SPn is being used. For flux-limited diffusion, there is only one angle group m .

Finally, the reaction of the radiation field to the motion of the mesh is calculated:

$$J_{mge}^{t+1} = \frac{V_e^t}{V_e^{t+1}} \left(J_{mge}^{*(t+1)} - \frac{(V_e^{t+1} - V_e^t) J_{mge}^t}{3} \right) \quad (82)$$

This includes radiation work as well as radiation sweeping.

1.2.6 Gray Approximation

If the diffusion approximation is accurate, then the radiation field will satisfy the condition

$$J_\nu \approx B_\nu \quad (83)$$

where J_ν denotes the mean intensity at a particular energy ν . If we integrate the diffusion equations over the energy spectrum, we obtain

$$\frac{1}{c} \frac{\partial J}{\partial t} + \nabla \cdot \vec{F} = \int \sigma_{a,\nu} (B_\nu - J_\nu) d\nu \quad (84)$$

$$\vec{F} = - \int \frac{1}{3\chi_\nu} (\nabla J_\nu) d\nu \quad (85)$$

where J is now the total mean intensity and $\vec{F}$ the total flux. We can write these equations as

$$\frac{1}{c} \frac{\partial J}{\partial t} + \nabla \cdot \vec{F} = \sigma_a (B - J) \quad (86)$$

$$\vec{F} = - \frac{1}{3\chi} \nabla J \quad (87)$$

if we define

$$\sigma_a = \frac{\int \sigma_{a,\nu} (B_\nu - J_\nu) d\nu}{B - J} \quad (88)$$

$$\frac{1}{\chi} = \frac{\int \frac{1}{\chi_v} (\nabla J_v) dv}{\nabla J} \quad (89)$$

Of course, this buys us nothing. However, if we can find reasonable, inexpensive approximations to (88) and (89), we will have reduced the radiation transport problem to that of solving a single diffusion equation.

We can approximate (89) by applying condition (83). Then

$$\frac{1}{\chi} = \frac{\int \frac{1}{\chi_v} (\nabla B_v) dv}{\nabla B} = \frac{\int \frac{1}{\chi_v} \frac{\partial B_v}{\partial T} (\nabla T) dv}{\frac{\partial B}{\partial T} \nabla T} = \frac{\int \frac{1}{\chi_v} \frac{\partial B_v}{\partial T} dv}{\frac{\partial B}{\partial T}} \quad (90)$$

This is the *Rosseland mean opacity*, which, because it is a function only of the material state, can be tabulated or otherwise made cheaply available as required. Extensive tables of Rosseland mean opacities have been published, particularly in the astrophysical literature.

We have no such convenient approximation for (88). Some researchers have argued for the *Planck mean*, defined as

$$\sigma_a = \frac{\int \sigma_{a,v} B_v dv}{B} \quad (91)$$

but this is unsatisfactory because it puts the greatest weight on energies where the least radiative transfer is taking place. Since one choice is as good (or bad) as another, ALEGRA uses a Rosseland mean here as well:

$$\frac{1}{\sigma_a} = \frac{\int \frac{1}{\sigma_{a,v}} \frac{\partial B_v}{\partial T} dv}{\frac{\partial B}{\partial T}} \quad (92)$$

Though not rigorous, this choice at least emphasizes those energies at which the most radiative transfer is occurring.

The gray approximation implies radiation diffusion. However, flux-limited diffusion and SPn also support a gray option, which is primarily useful for benchmarking and scoping calculations. They are also applicable in those rare instances where the opacity is largely independent of frequency.

2. Benchmark Results

This section describes the benchmark problems against which ALEGRA has been tested and a comparison of ALEGRA calculations with the exact solutions.

2.1 The Pomraning Benchmark

Pomraning [5] first proposed this benchmark, and complete solutions for nonequilibrium diffusion have been given by Su and Olsen [8]. A semi-infinite slab of cold material is subject to a radiation source of temperature T_0 on its surface at $z = 0$. The opacity is independent of temperature but the heat capacity goes as αT^3 . The opacity is assumed to be purely absorbing. Hydrodynamic motions and thermal conduction are ignored. This test is a strong verification problem for nonequilibrium diffusion and a weak verification problem for other transport theories.¹ The exact solution is given as a function of dimensionless distance x and time τ for various values of a single parameter, ϵ , characterizing the ratio of material to radiation heat capacities.

2.1.1 Nonequilibrium Diffusion

Figure 1 compares the exact nonequilibrium diffusion solution of the Pomraning benchmark (circles) with the solution calculated by ALEGRA (lines). The parameter ϵ was set to 0.1 for this calculation.

To obtain a solution to this high level of accuracy, it was necessary to start with a time step of $10^{-9}\tau$ and a grid interval of $0.2x$. The time step was permitted to grow by a factor of 1.2 on each step. The computation required 160 time steps and took 5 seconds to complete for 100 elements on a Sun Ultra-2 workstation running with a single processor.

Figure 2 is for the case $\epsilon = 1$. This solution required a similar starting time step, but a finer grid interval of $0.1x$ and a maximum temperature change limit of 0.2. The computation required 542 time steps and took 35 seconds to complete for 200 elements.

Figure 3 is the same case, but at time $\tau = 10$. The solution is rapidly approaching the equilibrium diffusion limit.

The solutions are fully converged, so the slight remaining discrepancies are real. Nevertheless, our excellent solutions to this benchmark verify the ALEGRA nonequilibrium ra-

1. I define a *strong verification problem* to be a problem for which an exact solution is known to which the code being tested should converge. A *weak verification problem* is a problem for which only approximate solutions are known or for which known exact solutions are based on slightly different equations than are solved in the code being tested. A code need not necessarily converge to the benchmark solution of a weak verification problem, but should be "in the ball park." Thus, the Pomraning benchmark is a strong verification problem for nonequilibrium diffusion, for which the exact solution has been worked out, but it is only a weak verification problem for other transport theories, for which no such solution exists.

diation diffusion package for strongly varying heat capacity and weakly varying absorption opacity with no scattering.

2.1.2 Flux-Limited Nonequilibrium Diffusion

Figure 4 is the same calculation as in Figure 1, except that now the flux limiter has been turned on. To achieve convergence, the mesh interval must be reduced to $0.1x$ and the maximum temperature change must be limited to 0.1 . The computation requires 2190 time steps and took 252 seconds to complete for 200 elements.

Figure 5 is the same calculation as in Figure 3, except that now the flux limiter has been turned on. To achieve convergence, the mesh interval must be $0.1x$ and the maximum temperature change must be limited to 0.2 . The computation requires 751 time steps and took 88 seconds to complete for 200 elements.

This is only a weak verification benchmark for flux limited diffusion, since for this theory the exact solution is unknown. The comparison is with the exact solution without a limiter, and one naturally sees significant differences. It is reassuring that the case $\epsilon = 1$ at late times approaches the diffusion value, since the flux limiter should have a rapidly decreasing effect as the equilibrium diffusion limit is approached. Much less reassuring is the fact that the discrepancy is in the direction of *increased* propagation rather than more limited propagation. This seems to confirm a criticism by Olson that "the Livermore flux limiter doesn't." [4]

2.1.3 P1 Transport

Figure 6 is the same calculation as in Figure 1, except that now the P1 package is being used. To achieve convergence, the mesh interval must be reduced to $0.1x$ and the maximum temperature change must be limited to 0.05 for really thorough convergence. The computation requires 2663 time steps and took 184 seconds to complete for 200 elements.

This is only a weak verification benchmark for P1 transport, since an exact solution is not available for P1. The comparison is with the nonequilibrium diffusion solution, and it is no surprise that there are significant differences. Note the abrupt drop in temperatures at $x = 9.5$. This drop propagates from the left boundary in a steady and quite striking manner and represents the P1 approximation to the speed of light of $\sqrt{3}c$. Likewise, the reduced propagation relative to the diffusion solution is as expected. These results are satisfactory.

2.2 The Su-Olsen Picket Fence Benchmark

Su and Olson have modified the Pomraning benchmark to produce an analytically tractable non-grey problem [9]. A semi-infinite slab of cold material is subject to a radiation source of temperature T_0 in the region $[0, z_0]$ over the time interval $[0, t_0]$. A reflection boundary condition is imposed at $z = 0$. The opacity is independent of temperature but the heat capacity goes as αT^3 . Hydrodynamic motions and thermal conduction are ignored. The opacity is assumed to vary with frequency as a "picket fence"; that is, the opacity takes one of two values with equal probability in each interval of the spectrum. Analytic solutions are avail-

able for nonequilibrium diffusion and for full transport. This benchmark is therefore a strong verification problem for nonequilibrium diffusion and transport and a weak verification problem for flux-limited diffusion and P1.

2.2.1 Nonequilibrium Diffusion

Figure 7 shows the ALEGRA results for the multigroup nonequilibrium diffusion package. The source term was treated using the method of partial temperatures. The computation required a grid interval of $0.05x$, a maximum temperature change limit of 0.2, and 40 groups to converge. The computation required 570 time steps and took 1910 seconds. The agreement is very good.

This benchmark verifies multigroup diffusion for strongly varying heat capacity and weakly varying absorption opacity with no scattering.

2.2.2 Flux-Limited Diffusion

Figure 8 shows the ALEGRA results for the multigroup nonequilibrium flux-limited diffusion package. The source term was treated using the method of partial temperatures. The computation required a grid interval of $0.0125x$, a maximum temperature change limit of 0.2, and 40 groups to converge. The computation required 912 time steps and took 3834 seconds for 200 elements.

No exact solutions are available for flux-limited diffusion for this benchmark. The figure shows both the exact diffusion (circles) and transport (crosses) solutions. Note that flux-limited diffusion lies between the two solutions, but closer to the transport solution. This suggests that the flux limiter really does buy us something, though it's hard to quantify just how much better it does than non-flux-limited diffusion.

2.2.3 SPn Transport

Figure 9 shows the ALEGRA results for the multigroup SPn transport package. The source term was treated using the method of partial temperatures. For P1, the computation required a grid interval of $0.05x$, a maximum temperature change limit of 0.2, and 40 groups to converge. The computation required 314 time steps and took 1366 seconds. Results are shown for P1, SP3, and SP5. (Note that P1 is identical to SP1.) It is clear that the solution has converged in angle at the SP3 level to the exact transport solution, which is expected in this case, because the problem is 1-D and SPn is an exact theory for 1-D problems and problems on homogeneous media.

2.3 The Marshak Benchmark

This benchmark is similar to the Pomraning problem, but because it is a nonlinear problem, it is analytically intractable. A semi-infinite slab of material with constant heat capacity but strongly temperature-dependent opacity is irradiated by a constant source on its boundary. A very sharp wave front propagates into the material. This benchmark is less satisfactory

that the others in that exact solutions are available only for the wave front position and a few other parameters describing the wave, and only in the equilibrium diffusion approximation. It is therefore only a weak verification benchmark. However, it's the best we have for strongly varying opacity, and it is of great significance, since it models behavior that is seen in a wide variety of applications.

Table 1 shows the comparison of the radiation front arrival times with the analytic value. Note that the agreement is only moderately good. However, as noted previously, the only known solution is for equilibrium diffusion. These results are satisfactory.

2.4 The RADSHOCK Problem

This is similar to the Marshak problem, except that hydrodynamics are turned on. Because a Marshak wave slows down as it propagates, a point is reached at which a hydrodynamic shock wave separates from the Marshak front. Table 1 shows the comparison of radiation front arrival times and the shock separation time with the analytic values. The latter results are better than they appear; judging the moment of shock separation from temperature profiles is uncertain at best. These results are satisfactory.

3. Conclusions

These benchmarks indicate that both the gray and multigroup diffusion packages are very close to their theoretical accuracy. Flux limited diffusion is harder to assess, but it appears to preserve the diffusion limit and introduce some transport-like character to the solutions. There are indications that Olson's criticism of the Livermore limiter has some basis. Grey and multigroup SP_n are also close to their theoretical accuracy.

It seems clear that my efforts should now be directed towards improving the flux limiter. I also plan to implement Olson's P1/3 method, which is a slight variation on the P1 method, and benchmark it.

An effort is now underway to implement S_n as an option in ALEGRA. This option will be exercised using the benchmarks listed in this memo as well as additional benchmarks not discussed here.

I have not yet attempted to quantify the convergence *rates* for these various methods, but only the fact of convergence (or nonconvergence.) I will examine convergence rates and other efficiency metrics in a future report.

Conclusions

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Conclusions

Figure 1. Pomraning benchmark for grey nonequilibrium diffusion for $\epsilon=0.1$ at $\tau=1$

Mesh for radiation pressure test problem

Figure 2. Pomraning benchmark for grey nonequilibrium diffusion for $\epsilon=1$ at $\tau=1$

Mesh for radiation pressure test problem

Figure 3. Pomraning benchmark for grey nonequilibrium diffusion for $\epsilon=1$ at $\tau=10$

Mesh for radiation pressure test problem

Figure 4. Pomraning benchmark for flux-limited grey nonequilibrium diffusion for $\epsilon=0.1$ at $\tau=1$

Mesh for radiation pressure test problem

Figure 5. Pomraning benchmark for flux-limited grey nonequilibrium diffusion for $\epsilon=1$ at $\tau=10$

Mesh for radiation pressure test problem

Figure 6. Pomraning benchmark for grey nonequilibrium diffusion for $\epsilon=0.1$ at $\tau=1$

Mesh for radiation pressure test problem

Figure 7. Su-Olsen picket fence benchmark using multigroup diffusion

Mesh for radiation pressure test problem

Figure 8. Su-Olsen picket fence benchmark using multigroup flux-limited diffusion

Mesh for radiation pressure test problem

Figure 9. Su-Olsen picket fence benchmark using multigroup P1
Mesh for radiation pressure test problem

Table 1. Analysis of Radiation Options

Benchmark	Gray diffusion	Gray flux-limited diffusion	Gray P1	Multigroup Diffusion	Multigroup flux-limited diffusion	Multigroup P1
Marshak front at 0.1E-9 seconds	-14.1%	-20.3%	-14.1%	-14.1%	-20.3%	-12.0%
Marshak front at 0.4E-9 seconds	+8.6%	+2%	+8.6%	+5.2%	+0.9%	+16.5%
Marshak front total time	17	30	17	573	832	5150
RADSHOCK front at 0.1E-9 seconds	-1.5%	-14.1%	-1.5%	+1.0%	-4.2%	+3.7%
RADSHOCK front at 0.2E-9 seconds	+4.4%	+4.3%	+4.4%	+6.1%	+4.4%	+6.1%
RADSHOCK shock separation time	-20%	-18%	-12%	-18%	-18%	-18%
RADSHOCK total time	38	51	49	1030	1472	3721

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