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A multigroup diffusion solver using pseudo transient continuation for a radiation-hydrodynamic code with patch-based AMR*

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Abstract

We present a scheme to solve the nonlinear multigroup radiation diffusion (MGD) equations. The method is incorporated into a massively parallel, multidimensional, Eulerian radiation-hydrodynamic code with adaptive mesh refinement (AMR). The patch-based AMR algorithm refines in both space and time creating a hierarchy of levels, coarsest to finest. The physics modules are time-advanced using operator splitting. On each level, separate “level-solve” packages advance the modules. Our multigroup level-solve adapts an implicit procedure which leads to a two-step iterative scheme that alternates between elliptic solves for each group with intra-cell group coupling. For robustness, we introduce pseudo transient continuation (Ψtc). We analyze the magnitude of the Ψtc parameter to ensure positivity of the resulting linear system, diagonal dominance and convergence of the two-step scheme. For AMR, a level defines a subdomain for refinement. For diffusive processes such as MGD, the refined level uses Dirichet boundary data at the coarse-fine interface and the data is derived from the coarse level solution. After advancing on the fine level, an additional procedure, the sync-solve (SS), is required in order to enforce conservation. The MGD SS reduces to an elliptic solve on a combined grid for a system of G equations, where G is the number of groups. We adapt the “partial temperature” scheme for the SS; hence, we reuse the infrastructure developed for scalar equations. Results are presented. We consider a multigroup test problem with a known analytic solution. We demonstrate utility of Ψtc by running with increasingly larger timesteps. Lastly, we simulate the sudden release of energy Y inside an Al sphere

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($r = 15$ cm) suspended in air at STP. For $Y = 11$ kT, we find that gray radiation diffusion and MGD produce similar results. However, if $Y = 1$ MT, the two packages yield different results. Our large Y simulation contradicts a long-standing theory and demonstrates the inadequacy of gray diffusion.

1 Introduction

This paper describes a numerical method to solve the radiation multigroup diffusion (MGD) equations. Two themes are presented. One is the scheme itself. We add Pseudo Transient Continuation (Ψ tc) to the familiar “fully implicit” method of Axelrod et al [2]. The second theme is code-specific. Our MGD solver is embedded in a multidimensional, massively parallel, Eulerian radiation-hydrodynamic code, which has patch-based, time-and-space Adaptive Mesh Refinement (AMR) capability. Our code’s AMR framework stems from the Berger and Olinger idea [3] developed for hyperbolic, compressible hydrodynamic schemes. The idea was expanded by Almgren et al [1] and applied to the type of elliptic solvers required for the incompressible equations of Navier-Stokes. Howell and Greenough [7] applied the Almgren et al framework to the scalar, parabolic “gray” radiation diffusion equation, thereby creating the start of our radiation-hydrodynamic code.

The AMR framework works as follows. A domain, referred to as the “coarse” or L0 level, is discretized using a uniform, coarse spatial mesh size h_c .¹ After advancing with a timestep Δt_c , the result is scanned for possible improvement. One may refine subregions containing a chosen material, at material interface(s), or at shocks, etc. Whatever refinement criteria are used, after the subdomains are identified, specific routines define a collection of “patches,” which cover the subdomains. In two dimensions, the patches are unions of rectangles; in 3D, they are unions of hexahedra. The patches need not be connected, but they must be contained within the coarse level. The patches denote the “fine” or L1 level and are discretized with a uniform, spatial mesh size h_f . A typical refinement ratio h_c/h_f equals two, but higher multiples of two are also allowed.

Because the original framework was designed for temporally explicit hyperbolic schemes, Δt_c is restricted by a CFL condition. This implies a similar restriction for the L1 level timestep Δt_f . For the case, $h_c/h_f = 2$, level L1 time-advances twice using $\Delta t_f = \Delta t_c/2$. Boundary conditions for level L1 are supplied as follows. Wherever level L1 extends to the physical boundary, the level uses the conditions prescribed by the problem. Portions of level L1’s boundary which lie inside the physical domain have conditions prescribed by time and space interpolated data obtained from the L0 solution. For diffusion equations, these conditions are of Dirichlet type. The numerical solution consists of both coarse and fine grid results. Unfortunately, as it stands, the composite solution does not guarantee conservative fluxes across the level boundaries. To maintain

¹In multiple dimensions, coordinates have their own mesh spacing.

conservation, a separate procedure, dubbed a sync-solve (SS) is required. The SS reduces to an elliptic unstructured grid solve on the composite grid of L0 and L1 levels. The AMR procedure may be recursive. That is, a level L1 grid may generate its own subdomain for refinement, i.e., a level L2. In that case, one SS couples results from levels L1 and L2. Once the levels advance to the L0 level time, a SS coupling all three levels ensues. For the multigroup equations, the SS requires an unstructured grid solve for a coupled system of reaction-diffusion equations. Our scheme for a multigroup SS is an important theme of this paper.

The MGD equations stem from a discretization of the multifrequency radiation diffusion equations. The latter is an approximation to the equations of radiation transfer, obtained by assuming the matter to be optically thick, which suppresses the directional dependence of the radiation intensity. Details of the derivation may be found in various sources: Mihalas and Mihalas [10], Zel'dovich and Raizer [19], Pomraning [12].

The gray radiation diffusion equation is a simplification of the MGD equations. It is essentially a one-group equation and is derived by integrating over all frequencies. Surprisingly, it gives very good results in many cases. However, it clearly cannot display frequency-dependent effects. When those are important, it gives incorrect results. Unfortunately, unless one solves a problem with both gray and MGD, one never knows when the former is adequate.

We now summarize the paper. Our MGD scheme consists of two parts. Sections 2 and 3 develop the level-solve algorithm, which is applied on each level. Section 2 develops the equations, the discretization, and our Ψ tc scheme. Section 3 proves three lemmas which determine the magnitude of the Ψ tc parameter, σ . Our philosophy for setting the magnitude is as follows. The result of the level solve is the time-advanced radiation group energy density, which physics dictates to be nonnegative. Zeroing anomalously negative values is not an option since they are the correct conservative solution to the linear system that stems from the discretization of the system. Thus, the unphysical result nonetheless conserves energy. The difficulty is avoided if in the original formulation of the linear system $Ax = b$, A is an M-matrix and the right-hand-side (RS) is nonnegative. Since we solve $Ax = b$ using an iterative scheme, the magnitude of σ is determined to ensure $b \geq 0$, a diagonally dominant A , and that the iterations converge. Section 4 describes the second part of our solver, viz., the sync-solve. Section 5 contains results. Three problems are presented. The first, in Sec. 5.1, displays the accuracy of the method and its convergence properties: first order in time and second order in space. Section 5.2 demonstrates the utility afforded by Ψ tc. For hard problems, it accelerates convergence; for very hard problems, Ψ tc is indispensable. Section 5.3 models the explosive expansion of a hot metal sphere suspended in cold air. The simulation couples all of the code's physics modules. The problem is an ideal candidate for AMR since effects propagate a large distance away from the source, yet in early times, resolution is needed only near the sphere. The problem also demonstrates the necessity of multigroup diffusion. We find that if the sphere's energy is very high, gray diffusion gives the wrong answer. For a 1 MT energy source, our MGD simulation contradicts results of Brode [5], who used gray diffusion. Section 6 contains

concluding remarks. Tabular data, used for comparing the results of Sec. 5.1, is listed in the Appendix.

2 Level Solve

Ignoring velocity terms and Compton scattering, the multifrequency radiation equations (CGS units) (Mihalas and Mihalas [10]) are:

$$\partial_t u_\nu = \nabla \cdot D_\nu \nabla u_\nu + c \rho \kappa_\nu (B_\nu - u_\nu), \quad (1)$$

$$\rho \partial_t e = -c \rho \int_0^\infty d\nu \kappa_\nu (B_\nu - u_\nu), \quad (2)$$

In (1)–(2), u_ν and e represent the spectral radiation energy density and matter specific energy, respectively. The former is a function of position x , time t and frequency ν , while e is a function of the mass density ρ and material temperature T , quantities which themselves depend on x and t . Evolution of ρ is governed by hydrodynamics. Hence, in our context, ρ is a known function. Introducing the specific heat $c_\nu = \partial e / \partial T$ turns (2) into an evolutionary equation for T ; hence, the left-hand-side (LS) becomes $\rho c_\nu \partial_t T$. The subscript ν designates that the term varies with frequency. In (1)–(2), c denotes the speed of light, κ_ν the absorption opacity, and B_ν the Planck function,

$$B_\nu = (8\pi h/c^3) \nu^3 / [\exp(h\nu/kT) - 1] \quad (\text{erg sec cm}^{-3}),$$

where h and k are the Planck and Boltzmann constants, respectively. The diffusion coefficient D_ν depends on the total inverse mean free path $\chi_\nu = \rho\kappa_\nu + \rho\kappa_{\nu,s}$, where κ_ν and $\kappa_{\nu,s}$ are the absorption and scattering opacities, respectively. (The opacities are also functions of material composition, ρ and T .) In (1), the term $-D_\nu \nabla u$ denotes the spectral radiation energy flux. To limit energy streaming faster than c , a flux limiter is introduced, e.g.,

$$D_\nu = c / (3\chi_\nu + |\nabla(u_\nu)|/u_\nu).$$

The multigroup equations are derived as follows. The frequency domain is discretized into G groups with boundaries $\{\nu_g\}_{g=0}^G$ satisfying

$$0 \leq \nu_0 < \nu_1 < \dots < \nu_G < \infty.$$

The equations are integrated over groups. We define

$$u_g(x, t) = \int_g u_\nu = \int_{\nu_{g-1}}^{\nu_g} d\nu u_\nu.$$

Time derivatives are replaced by differences and the system is multiplied by the timestep Δt . Integration of the transport and absorption terms requires defining group-averaged opacities. Linearizing the Planck function about a known temperature T^* , the absorption term is expressed as

$$\int_g \kappa_\nu (B_\nu - u_\nu) = \kappa_g [B_g + B'_g(T - T^*) - u_g],$$

where κ_g is the group-averaged absorption opacity, $B_g = \int_g B_\nu|_{T=T^*}$, and $B'_g = \int_g (\partial B_\nu / \partial T)|_{T=T^*}$. In a semi-implicit scheme, $T^* = T^0$, where T^0 is the temperature at the start of the time cycle. For fully implicit differencing, we must iterate until T^* converges to T . For the transport term, we define

$$\Delta t \int_g \nabla \cdot D_\nu \nabla u = \nabla \cdot D_g \nabla u_g,$$

where D_g depends on a group-averaged inverse mean free path χ_g . Note that Δt has been absorbed into D_g .

The above definitions yield the multigroup equations,

$$0 = u_g^0 - u_g + \nabla \cdot D_g \nabla u_g + K_g(u, T), \quad g = 1, \dots, G \quad (3)$$

$$0 = \rho c_v (T^0 - T) - \sum_{\ell=1}^G K_\ell(u, T), \quad (4)$$

where u_g^0 and T^0 denote values at the start of the time-advance,

$$\begin{aligned} K_g(u, T) &= a_g [B_g + B'_g (T - T^*) - u_g], \\ a_g &= \Delta t c \rho \kappa_g. \end{aligned}$$

Equations (3)–(4) comprise a nonlinear system with the strongest nonlinearity due to the emission term B . To a lesser extent, opacities also have a temperature dependence and for nonideal gases, so does c_v . However, for ease of solution, we may choose to view (3)–(4) as a linear system in which case all coefficients are evaluated at the old temperature T^0 . For simulations in which matter and radiation are tightly coupled, i.e., where we expect to have $u_\nu = B_\nu$, the solution to the semi-implicit difference equations is $u_g = B_g + B'_g (T - T^0)$, with B_g and B'_g evaluated at $T = T^0$. For high frequencies, $\lim_{\nu \rightarrow \infty} (B_\nu / B'_\nu) \sim 1/\nu$; hence, $B_g \ll B'_g$ for large g . Unfortunately, if the temperature is decreasing, i.e., if $(T - T^0) < 0$, the linearized emission term is negative for large g , leading to the unphysical result: $u_g < 0$. On the other hand, if we are able to iterate on T^* so that it converges to T , then in tightly coupled simulations, we obtain the desired solution $u_g = B_g$ with B_g evaluated at the advanced temperature.

In our code we provide both options, i.e., solving a linear system, or converging on the implicit source.² In either case, solving (3)–(4) on a large domain with many groups presents a formidable task. To facilitate the task, we introduce pseudo transient continuation (Ψ tc) and replace the zeros on the LS of (3)–(4) with the Ψ tc derivatives,

$$\tau (u_g - u_g^*) \quad \text{and} \quad \rho c_v \tau (T - T^*),$$

where $\tau \geq 0$, the inverse of the pseudo-timestep, is the Ψ tc parameter whose magnitude is at our disposal.

²At the time of this writing, opacities and c_v were time-lagged.

The variables u_g^* and T^* represent advances in pseudo time; they always appear on the LS of (3)–(4). As mentioned above, we provide the option of running in either semi-implicit (SI) or fully-implicit (FI) mode. With SI, since B_g is linearized about $T = T^0$, in the definition of the coupling term K_g , we substitute T^0 for T^* . However for FI, K_g is defined as above; B_g is linearized about the pseudo time temperature T^* . The two modes lead to subtle differences in the scheme, as shown below.

For the FI scheme, if the matter equation is solved for the temperature change, we obtain

$$\delta^{-1} (T - T^*) = \rho c_v (T^0 - T^*) - \sum_{\ell=1}^G a_\ell (B_\ell - u_\ell), \quad (5)$$

where

$$\delta^{-1} = \rho c_v \sigma + \sum_{\ell=1}^G a_\ell B'_\ell \quad \text{and} \quad \sigma \doteq 1 + \tau. \quad (6)$$

The domain of relevance $\tau \geq 0$ corresponds to $\sigma \geq 1$.

For the SI scheme, the temperature change is,

$$\delta^{-1} (T - T^0) = \rho c_v (\sigma - 1) (T^* - T^0) - \sum_{\ell=1}^G a_\ell (B_\ell - u_\ell). \quad (7)$$

The term δ is defined as above, but B_g and B'_g are evaluated at $T = T^0$.

For the FI scheme, if (5) is substituted into the equation for u_g , we obtain

$$\begin{aligned} -\nabla \cdot D_g \nabla u_g + (\sigma + a_g) u_g - f_g \sum_{\ell=1}^G a_\ell u_\ell = \\ u_g^0 + (\sigma - 1) u_g^* + a_g B_g + f_g \left(\rho c_v (T^0 - T^*) - \sum_{\ell=1}^G a_\ell B_\ell \right), \end{aligned} \quad (8)$$

where $f_g \doteq \delta a_g B'_g$. Equation (6) implies $f_g < 1$, for all g . For the SI scheme, the RS of (8) changes: $\rho c_v (T^0 - T^*)$ is replaced with $\rho c_v (\sigma - 1) (T^* - T^0)$.

Equation (8) corresponds to a linear system

$$\mathcal{A} u = w$$

of order $(N \times G)$, where N is the number of mesh cells and G the number of groups. The first term on the LS of (8) consists of second order, central differences over space. We write this term as

$$-\nabla \cdot D_g \nabla u_g = +\mathcal{D}_{d,g} u_g - \mathcal{D}_{o,g} u_g.$$

The first part represents multiplication of the vector u_g by a *diagonal* matrix; the second term denotes multiplication by the off-diagonal part. The coefficients of \mathcal{D}_d and \mathcal{D}_o are nonnegative.

On the LS of (8), the term $-f_g \sum_{\ell=1}^G a_\ell u_\ell$ is referred to as the “re-emission source” [11], since it represents radiation energy absorbed by matter and re-emitted. If we define the *column* vectors f and a with components f_g and a_g , respectively, the re-emission term is expressed as the matrix-vector product

$$- (f a^T) u , \quad (9)$$

where $a^T = \text{transpose}(a)$, and u is the column vector of unknowns. Since the re-emission term does not couple cells, (9) corresponds to separate products: one per cell, with each product of order G .

These observations allow expressing the matrix as

$$\mathcal{A} = \Lambda - M_1 - M_2, \quad (10)$$

where Λ is diagonal, M_1 contains the offdiagonal terms due to the (spatial) diffusion term, and M_2 contains the offdiagonal terms due to interfrequency coupling. The corresponding elements are

$$\begin{aligned} \Lambda_g &= \mathcal{D}_{d,g} + \sigma + a_g - f_g a_g , \\ (M_1 u)_g &= \mathcal{D}_{o,g} u_g , \\ (M_2 u)_g &= f_g \sum_{\ell \neq g}^G a_\ell u_\ell . \end{aligned}$$

The decomposition (10) leads to the iterative scheme proposed by Axelrod et al [2], which improves a guess $u^{(i)}$ by successively solving

$$(\Lambda - M_2) u^{(i+1/2)} = w + M_1 u^{(i)} \quad (11)$$

$$(\Lambda - M_1) u^{(i+1)} = w + M_2 u^{(i+1/2)} . \quad (12)$$

We solve (11)–(12) until $u^{(i)}$ converges. Convergence is gauged by evaluating the 1-norms of w and the residual $r = w - \mathcal{A} u$; the latter defined as,

$$r = w - \mathcal{A} u^{(i+1)} = M_2 (u^{(i+1)} - u^{(i+1/2)}) .$$

The procedure is fast since multiplication by M_2 is local to each cell, which is very convenient if the spatial domain is decomposed on multiple processors.

We now review the derivation of the system $\mathcal{A} u = w$. First, we assume that Ψ_{tc} is not used, i.e., that $\sigma = 1$ in (6)–(8). For the SI scheme, the terms B_ℓ and B'_ℓ are evaluated at $T = T^0$. For FI differencing, we require two types of iterations. Equations (11) and (12) comprise the *inner* iteration. It is initialized with $u^{(0)}$ equal to u^0 . Once the inner iteration has converged to sufficient accuracy, (5) yields the new temperature. The SI scheme essentially ends after the inner iteration converges (see below). For FI differencing, after T is computed, the *outer* iteration sets $T^* = T$, recomputes B_ℓ and B'_ℓ at $T = T^*$ and returns to the inner iteration. The outer iteration halts when T^* converges.

If Ψ_{tc} is invoked, more care is required because when $\sigma > 1$, the system $\mathcal{A} u = w$ is not a true discretization of the multigroup equations. Despite this

complication, Ψtc brings robustness to the scheme. The Ψtc parameter τ plays the role of an inverse timestep in pseudo-time. In principle, we could set τ to a large value and solve a succession of linear systems. The solution of each system represents an advance in pseudo-time. We continue advancing until we reach the pseudo-time steady-state. This is easily seen by letting $u_g^* = u_g$ on the RS of (8) and moving the term to the LS. However, making τ large is not practical as it involves many pseudo-time advances. Furthermore, the intermediate pseudo-time results are of no interest. Consequently, we adopt the strategy of making τ as small as possible. We discuss the strategy in section 3.

Ψtc may be used with either SI or FI differencing. In the former, once (11) and (12) are converged, (7) yields the new temperature T . We then compute the 1-norm of the “nonlinear” residual of the linearized equation for the matter energy,

$$r_{nl} = V \left(\rho c_v (T - T^0) - \sum_{\ell=1}^G a_\ell [B_\ell + B'_\ell (T - T^0) - u_\ell] \right), \quad (13)$$

where V is the cell volume. The residual is compared with the 1-norm of the matter “energy” $V \rho c_v T$, and in order to monitor stagnation, it is also compared with the energy change over the pseudo-timestep $V \rho c_v (T - T^*)$. With FI, the temperature T , obtained from (5), is used to compute the emission B_ℓ . The residual r_{nl} is defined as in (13), except without the $B'_\ell (T - T^0)$ term.

Unfortunately, unless the iterations converge to round-off accuracy, energy may not be conserved. Lack of conservation stems from values of user-set parameters that control stopping criteria for the iterations. For example, it may be efficient to halt once $\|r_{nl}\|_1 < 10^{-6}$, and the norm of the iterates $\|(\Delta T)/T\|_\infty < 10^{-2}$ since continuing brings little noticeable (visual) improvement to the solution. However, if one were to stop at that point, energy may not be conserved to desired accuracy. To restore conservation, we provide the option of an additional step. After the iterations stop, we assume that the last computed temperature T is “frozen” and use it to compute emission. In the SI scheme, emission into the g th group is defined as $S_g = B_g + B'_g (T - T^0)$, where B_g and B'_g are evaluated using T^0 . (To prevent unphysical behavior, S_g is not allowed to be negative.) In the FI scheme, we evaluate B_g using T and set $S_g = B_g$. Having a known emission allows us to compute the energy-conserving radiation field. The groups decouple. For $g = 1, \dots, G$, we solve

$$-\nabla \cdot D_g \nabla u_g + (1 + a_g) u_g = u_g^0 + a_g S_g.$$

After computing u_g , the matter energy density change is

$$\Delta \mathcal{E} = - \sum_{\ell=1}^G a_\ell (B_g - u_g),$$

where, if using the SI scheme, B_g is linearized about $T = T^0$, or with FI, is evaluated at T . The quantity $V \Delta \mathcal{E}$ represents the average energy change of

the matter. In cells with more than one material, we adapt a suggestion of Zimmerman [21], which simulates intra-cell gray diffusion. The scheme assumes each material resides in its own sub-volume. We solve for separate, frequency-averaged radiation energy densities and matter temperatures in the sub-volumes. The energy change of the materials depends on the individual, frequency-averaged opacities as well as on $\Delta\mathcal{E}$.

This concludes the description of the algorithm used to advance the multi-group equations on an AMR level. In the following section, we analyze the convergence of (11)-(12), and we focus on how the Ψ tc parameter σ ensures stable, robust iterations, to yield a physical, i.e., nonnegative result.

3 Analysis of Ψ tc

Recalling that $\sigma = 1 + \tau$, in this section we develop lemmas that set the *initial* magnitude of τ , where by initial we mean the following. A new value of τ is determined at each time advance for each AMR level. The level advance consists of nested loops. For the “inner” iterations, τ is fixed. After convergence, τ is reset to $\tau \rightarrow \alpha_\tau \tau$, where α_τ is a user-set input whose default value is $1/2$. Section 5.2 describes an experiment with another setting of α_τ . Our strategy for the initial τ is to ensure a nonnegative w , diagonal dominance, and a convergent inner iteration. For the derivation, it is convenient to define

$$\mathcal{B} \doteq \sum_{\ell=1}^G a_\ell B_\ell \quad , \quad \mathcal{B}' \doteq \sum_{\ell=1}^G a_\ell B'_\ell \quad , \quad (14)$$

$$\mathcal{C}'_g \doteq a_g B'_g / \rho c_v \quad , \quad \mathcal{C} \doteq \mathcal{B} / \rho c_v \quad , \quad \mathcal{C}' \doteq \mathcal{B}' / \rho c_v \quad . \quad (15)$$

3.1 Positivity of w

Before analyzing the effect of Ψ tc, we examine the scheme’s behavior without it. If $\sigma = 1$, the term u_g^* disappears from (8). In the following discussion, we ignore the $T^0 - T^*$ term since for the SI scheme, or for the first FI inner iteration, $T^* = T^0$. Since $u_g^0 \sim B_g$, if either Δt is large or the coupling is strong, $a_g B_g \gg u_g^0$. Hence, in this case, the RS of the system, $w \approx a_g B_g - f_g \mathcal{B}$, where \mathcal{B} is defined in (14). If $\sigma = 1$, $f_g = a_g B'_g / (\rho c_v + \mathcal{B}') = \mathcal{C}'_g / (1 + \mathcal{C}')$. Hence,

$$w \approx a_g (B_g + B_g \mathcal{C}' - B'_g \mathcal{C}) / (1 + \mathcal{C}') \quad .$$

Since \mathcal{C} and \mathcal{C}' are proportional to Δt times the opacity, the sole B_g term in the numerator is swamped by the other two terms when Δt is large or the matter is optically thick. In this limit, the sign of w equals the sign of $(B_g \mathcal{C}' - B'_g \mathcal{C})$, which may be negative.

However, with Ψ tc, nonnegativity of w is equivalent to the inequality

$$0 \leq p(\sigma) = u_g^* \sigma^2 + 2\tilde{b} \sigma + \tilde{c} \quad ,$$

where

$$\begin{aligned} 2\tilde{b} &= u_g^0 - u_g^* + a_g B_g + \mathcal{C}' u_g^*, \\ \tilde{c} &= \mathcal{C}' (u_g^0 - u_g^* + a_g B_g) + a_g B_g' [T^0 - T^* - \mathcal{C}], \end{aligned}$$

for the fully-implicit (FI) scheme. The SI scheme, adds the term $a_g B_g' (T^* - T^0)$ to the definition of $2\tilde{b}$. If $\sigma = 1$, we recover the non- Ψ tc scheme, which as shown, may have indeterminate $\text{sign}(w)$. At the end of the section we show that the SI scheme is less robust. We first analyze the FI scheme.

For large σ , p is positive—even if $u_g^* = 0$. The derivative $dp/d\sigma$ increases monotonically and is positive for $\sigma = 1$. If $u_j^* = 0$, p increases linearly with σ and has slope $u_g^0 + a_g B_g > 0$. Hence, we have proved:

Lemma 1 *If $p|_{\sigma=1} \geq 0$, the RS of (8) is nonnegative for all $\sigma \geq 1$. Otherwise, (1) If $u_j^* > 0$, the RS of (8) is nonnegative if*

$$\sigma \geq \sigma_{\min} = \max \left[\left(\sqrt{\tilde{b}^2 - u_g^* \tilde{c} - \tilde{b}} \right) / u_g^* \right].$$

(2) *If $u_j^* = 0$, the RS of (8) is nonnegative if $\sigma \geq \sigma_{\min} = -\max(\tilde{c}/2\tilde{b})$.* ■

The lemma's limit is very restrictive for large Δt , as we now show. As $\Delta t \rightarrow \infty$, the terms a_g , \mathcal{C} and \mathcal{C}' dominate the definitions of \tilde{b} and \tilde{c} . Hence,

$$\begin{aligned} \lim_{\Delta t \rightarrow \infty} 2\tilde{b} &= a_g B_g + \mathcal{C}' u_g^*, \\ \lim_{\Delta t \rightarrow \infty} \tilde{c} &= a_g B_g \mathcal{C}' - a_g B_g' \mathcal{C}. \end{aligned}$$

Substituting into the expression for the root and factoring out $a_g u_g^*$ yields

$$\lim_{\Delta t \rightarrow \infty} \sigma_{\min} = \max \frac{a_g}{2} \left(\sqrt{(\alpha - \beta)^2 + 4\gamma} - (\alpha + \beta) \right),$$

where $\alpha = B_g/u_g^*$, $\beta = \sum_{\ell} \kappa_{\ell,g} B_{\ell}' / \rho c_v$, $\gamma = (B_g'/u_g^*) \sum_{\ell} \kappa_{\ell,g} B_{\ell}' / \rho c_v$ and $\kappa_{\ell,g} = \kappa_{\ell} / \kappa_g$. The term $a_g = c \Delta t \rho \kappa_g$ equals ℓ_c / ℓ_g , where ℓ_c is the maximum distance a photon can travel in time Δt and ℓ_g is the absorption mean free path for the g th group. We now show the remaining expression is of order one. If the radiation field is at equilibrium, $\alpha = 1$. The term B_{ℓ}' is of order B_{ℓ}/T . If it is exactly equal to B_{ℓ}/T , the expression multiplying $a_g/2$ vanishes.

If $u_g^* = u_g^0 = 0$ and $p|_{\sigma=1} < 0$, then for large Δt , $\sigma_{\min} \rightarrow (B_g' \mathcal{C} - B_g \mathcal{C}') / B_g$, which equals $c \Delta t$ times a term of order one.

We now consider the SI scheme. As noted above, SI adds the expression $a_g B_g' (T^* - T^0)$ to the definition of $2\tilde{b}$. Effectively, the extra term means that rather than having $2\tilde{b}$ depend on the emission source B_g (which is evaluated at T^*), the coefficient depends on the linearization $B_g + B_g' (T^* - T^0)$, with B_g and B_g' evaluated at T^0 . If the temperature is decreasing the expression may be negative. As a consequence, we are not assured that $dp/d\sigma$ is positive. If u_g^* is nonzero, we can find a suitable σ . However, if $u_g^* = 0$, $p(\sigma)$ is a linear function with possibly a negative derivative. If that case arises as we query the cells, we set $\sigma = 1$ for the cell in question. Because of these uncertainties, by default, we run with the FI scheme.

3.2 Diagonal dominance

To prove diagonal dominance, we compute row sums. The diffusion terms sum to zero, since the matrix composed of just these terms must annihilate the vector $(1, 1, \dots)$.³ Thus, for diagonal dominance,

$$\sigma + a_g - f_g \sum_{\ell=1}^G a_\ell > d \geq 0.$$

Recalling the definition of f_g , the relation is equivalent to

$$0 \leq q(\sigma) = \sigma^2 + 2\tilde{b}\sigma + \tilde{c},$$

where

$$\begin{aligned} 2\tilde{b} &= a_g + C' - d, \\ \tilde{c} &= a_g C' - C'_g \sum_{\ell=1}^G a_\ell - C' d, \end{aligned}$$

and C' , C'_g are defined in (15). As before, $\sigma \geq 1$ is the domain of interest. The quadratic $q(\sigma)$ is nonnegative for sufficiently large σ . However,

$$q|_{\sigma=1} = (1 + C') (1 + a_g - d) - C'_g \sum_{\ell=1}^G a_\ell.$$

The a_g and C' terms are proportional to Δt . Hence, as $\Delta t \rightarrow \infty$, the sign of the expression is dominated by $\text{sign}(C' - C'_g \sum_{\ell=1}^G a_\ell)$. Since the expression varies as $\sum_{\ell=1}^G a_\ell (B'_\ell - B'_g)$, the sign is indeterminate. However, $(dq/d\sigma)|_{\sigma=1}$ is positive for $d < 2$. We have proved:

Lemma 2 *If $q|_{\sigma=1} \geq 0$ and $d > 0$, \mathcal{A} is strictly diagonally dominant for all $\sigma \geq 1$. Otherwise, \mathcal{A} is strictly diagonally dominant if*

$$\sigma \geq \sigma_{\min} = \sqrt{\tilde{b}^2 - \tilde{c}} - \tilde{b}. \blacksquare$$

Remark For large Δt ,

$$\lim_{\Delta t \rightarrow \infty} \sigma_{\min} = \max \frac{a_g}{2} \left(\sqrt{(1 - \beta)^2 + 4\delta} - (1 + \beta) \right),$$

where $\delta = (B'_g/\rho c_v) \sum_{\ell} \kappa_{\ell,g}$ and, as before, $\beta = \sum_{\ell} \kappa_{\ell,g} B'_\ell / \rho c_v$, and $\kappa_{\ell,g} = \kappa_\ell / \kappa_g$. As in Lemma 1, when Δt is large, $\sigma_{\min} = \ell_c / \ell_g$ times a term which should be of order one.

³In extreme cases, because of finite precision, the diffusion terms may swamp the other terms. We discuss the possibility in Appendix B.

3.3 Two-step iterative scheme

We've shown that for sufficiently large σ , \mathcal{A} is an M-matrix. Hence, $(\Lambda - M_1) - M_2$ and $(\Lambda - M_2) - M_1$ are regular splittings, and each half of the two-step scheme (11)–(12) is a convergent iteration [18], Thm. 3.13, p. 89. Here we analyze how the scheme reduces the error. Of particular interest is that for large Δt , the scheme (11)–(12) may *not* converge unless the Ψ tc parameter σ is sufficiently large.

It is convenient to change variables,

$$v_j \doteq a_j u_j .$$

The system of interest is then $\mathcal{A}'v = w$, where

$$\mathcal{A}' = \Lambda - M_1 - M_2$$

and Λ is diagonal,

$$\begin{aligned} \Lambda_g &= (\mathcal{D}_{a,g}/a_g) - f_g + 1 + \sigma/a_g \\ (M_1 v)_g &= \mathcal{D}_{o,g} v_g / a_g \\ (M_2 v)_g &= f_g \sum_{\ell \neq g}^G v_\ell . \end{aligned}$$

If $e^{(i)} = v - v^{(i)}$ defines the error for (11)–(12), the error satisfies

$$\begin{aligned} (\Lambda - M_1) e^{(i+1/2)} &= M_2 e^{(i)} \\ (\Lambda - M_2) e^{(i+1)} &= M_1 e^{(i+1/2)} . \end{aligned} \quad (16)$$

We express the error as a product of spatial and frequency components. For a 2D spatial domain,

$$e_{k,m,g}^{(i)} = \epsilon_g^{(i)} e^{\sqrt{-1}(k\theta_k + m\theta_m)} , \quad (17)$$

where the indices k and m refer to distinct spatial axes. We now analyze the iteration error

$$e^{(i+1)} = (\Lambda - M_2)^{-1} M_1 (\Lambda - M_1)^{-1} M_2 e^{(i)} .$$

Consider the unit vector \hat{e}_ℓ consisting of N components, with unity in the ℓ th position and zeros for the rest. Since the initial error $e^{(i)}$ is a linear combination of such vectors, it suffices to analyze the case when the frequency component of $e^{(i)}$ equals \hat{e}_ℓ . We will prove that for a properly chosen $\sigma \geq 1$,

$$\|e^{(i+1)}\|_1 \leq \zeta < 1 .$$

In other words, if σ is sufficiently large, one iteration of the two-step scheme reduces the error, which we will show occurs for $\zeta' < \zeta$, $\sigma(\zeta') > \sigma(\zeta)$. However, larger σ denote a smaller Ψ tc time step, resulting in a longer pseudo-time to reach the desired steady-state.

Assuming that the diffusion coefficient does not vary in space⁴ and that we use a uniform 2D spatial mesh with mesh size h , the error after the first half step is

$$\epsilon_g^{(i+1/2)} = f_g / [1 - f_g + (\sigma/a_g) + 2\eta_g (2 - \cos \theta_k - \cos \theta_m)], \quad (18)$$

where

$$\eta_g = D_g/a_g h^2 = l_{g,D} l_{g,a} / 3h^2,$$

$l_{g,a} = 1/\rho\kappa_g$ is the absorption mean free path, and $l_{g,D}$ is the diffusion mean free path; the latter is the sum of the absorption and scattering opacities. In (18), the expression multiplying η_g is nonnegative.⁵ Since $f_g < 1$, $\epsilon_g^{(i+1/2)}$ is nonnegative. Assuming the worst case $\theta = 0$ yields,

$$0 < \epsilon_g^{(i+1/2)} \leq f_g / (1 - f_g + \sigma/a_g), \quad (19)$$

a result which also holds in 1 and 3 dimensions. The bound is *sharp*; i.e., $\epsilon^{(i+1/2)}$ equals the bound if the original error $e^{(i)}$ has no spatially varying component.

Since (17) holds for i , $i + 1/2$, and $i + 1$, we now analyze the second half step. In 2 dimensions,

$$M_1 e^{(i+1/2)} = (\cos \theta_k + \cos \theta_m) 2 \eta_g e^{(i+1/2)}.$$

In $n = 1, 2$ or 3 dimensions, the parenthetical expression contains 1, 2 or 3 cosine terms. If we again assume $\theta = 0$, the expression is bounded by n .

To determine $e^{(i+1)}$ from (16) we invert $(\Lambda - M_2)$ using the Sherman-Morrison formula by noting that

$$\Lambda - M_2 = \Lambda' - \mathbf{f} \mathbf{e}^T,$$

where \mathbf{e} is the vector consisting of all ones, the components of \mathbf{f} are the previously defined f_g , and Λ' is diagonal with

$$\Lambda'_g = \eta'_g + 1 + \sigma/a_g, \quad \eta'_g \doteq 2n\eta_g. \quad (20)$$

In (20), we generalized by allowing for $n = 1, 2$, or 3 spatial dimensions. After some algebra, we obtain

$$|\epsilon_g^{(i+1)}| \leq \frac{1}{\Lambda'_g} \left[\eta'_g \epsilon_g^{(i+1/2)} + \left(\frac{f_g}{1 - \mathbf{e}^T (\Lambda')^{-1} \mathbf{f}} \right) \sum_{\ell=1}^G \frac{\eta'_\ell \epsilon_\ell^{(i+1/2)}}{\Lambda'_\ell} \right],$$

where

$$1 - \mathbf{e}^T (\Lambda')^{-1} \mathbf{f} = 1 - \sum_{\ell=1}^G f_\ell / \Lambda'_\ell. \quad (21)$$

⁴Since, as we show, the worst error arises for spatially constant error, we are free to ignore the diffusion flux limiter in the analysis.

⁵The corresponding expression in 1 and 3 spatial dimensions is also nonnegative and bounded by 1.0 and 3.0, respectively.

Summing yields the 1-norm,

$$\|\epsilon^{(i+1)}\|_1 \leq [1 - \mathbf{e}^T (\Lambda')^{-1} \mathbf{f}]^{-1} \sum_{\ell=1}^G \frac{\eta'_\ell \epsilon_\ell^{(i+1/2)}}{\Lambda'_\ell}.$$

Our task is done if we can show that the RS is bounded by ζ . Using (21) this entails showing that

$$\sum_{\ell=1}^G \frac{\eta'_\ell \epsilon_\ell^{(i+1/2)}}{\Lambda'_\ell} \leq \zeta \left(1 - \sum_{\ell=1}^G \frac{f_\ell}{\Lambda'_\ell} \right).$$

After substituting the bound (19) and simplifying, the inequality becomes

$$\sum_{g=1}^G \left(\frac{C'_g}{\Lambda'_g} \right) \left(\frac{\eta'_g}{1 - f_g + \sigma/a_g} \right) \leq \zeta \left[\sigma + \sum_{g=1}^G \left(\frac{C'_g}{\Lambda'_g} \right) (\Lambda'_g - 1) \right]. \quad (22)$$

To summarize, if (22) is satisfied the two-step scheme (11)–(12) converges and each iteration reduces the error by a factor ζ .

We now show that if Ψ tc is not used, i.e., if $\sigma = 1$, and Δt is large, the scheme may not converge. If $\sigma = 1$, since $a_g \propto \Delta t$, $\lim_{\Delta t \rightarrow \infty} \Lambda'_g = \eta'_g + 1$ and $\lim_{\Delta t \rightarrow \infty} f_g = p_g$, where $p_g > 0$ and $\sum_g p_g = 1$. Also, if $\sigma = 1$, since $C'_g \propto \Delta t$, for large Δt , the lone σ on the RS of (22) is swamped by the sum. Dividing both sides of (22) by $c \Delta t$, the LS becomes

$$\sum_{g=1}^G \left(\frac{\rho \kappa_g B'_G \eta'_g}{\rho c_v (1 + \eta'_g)} \right) (1 - p_g)^{-1}.$$

On the other hand, if $\zeta = 1$, the RS tends to the same sum, but without the term $(1 - p_g)^{-1}$. This makes the LS larger than the RS, giving the desired contradiction. We have proved:

Lemma 3 *If $\sigma = 1$ and Δt is large, (11)–(12) may not converge. ■*

We now estimate how large to make σ in order to satisfy (22). The terms a_g and C'_g are proportional to Δt ; also, $\sigma \geq 1$ and $\Lambda'_g > 1$. Hence, (22) holds for small Δt . To obtain a tractable expression, we derive a relation that stems from a more stringent inequality. Equation (22) holds if we derive a σ that satisfies a relation insensitive to the lone σ on the RS and is obtained by requiring that the individual terms in the sum satisfy the inequality. This allows canceling the common term C'_g/Λ'_g . Hence, we seek σ satisfying

$$\eta'_g / (1 - f_g + \sigma/a_g) \leq \zeta (\Lambda'_g - 1).$$

Recalling that $f_g = C'_g / (\sigma + C')$ and using (20) leads to

$$0 \leq s(\sigma) \doteq \sigma^3 + \alpha_s \sigma^2 + \beta_s \sigma + \gamma_s,$$

where

$$\begin{aligned}\alpha_s &= a_g (1 + \eta'_g) + C', \\ \beta_s &= a_g [(1 + \eta'_g) C' - C'_g + a_g \eta'_g (1 - \zeta^{-1})], \\ \gamma_s &= a_g^2 \eta'_g [(1 - \zeta^{-1}) C' - C'_g].\end{aligned}$$

As before, $\sigma \geq 1$ is the domain of interest.

To simplify the analysis, we assume $\zeta = 1$, i.e., we seek a σ that guarantees marginal convergence. To this end, we define

$$\begin{aligned}\tilde{\beta}_s &= a_g [(1 + \eta'_g) C' - C'_g], \\ \tilde{\gamma}_s &= -a_g^2 \eta'_g C'_g.\end{aligned}$$

Consider the cubic

$$s(\sigma) = \sigma^3 + \alpha_s \sigma^2 + \tilde{\beta}_s \sigma + \tilde{\gamma}_s.$$

For $\sigma \geq 1$, all derivatives of s are positive. If

$$s(1) = 1 + \alpha_s + \tilde{\beta}_s + \tilde{\gamma}_s \geq 0,$$

then the scheme (11)–(12) converges. However, if $s(1) < 0$, we need a $\sigma > 1$ that renders $s \geq 0$. To avoid computing cubic roots, we approximate s by a quadratic $w(\sigma)$,

$$w(\sigma) = (3 + \alpha_s) \sigma^2 + (\tilde{\beta}_s - 3) \sigma + \tilde{\gamma}_s + 1,$$

and determine the root of w . The polynomials w and s and their first two derivatives agree at $\sigma = 1$. The difference $s(\sigma) - w(\sigma) = (\sigma - 1)^3$, i.e., $w(\sigma) < s(\sigma)$ for $\sigma > 1$. Hence, the positive root of $w(\sigma)$ overestimates the σ needed for marginal stability. We have proved:

Lemma 4 *If $w|_{\sigma=1} \geq 0$, the scheme (11)–(12) converges. If $w|_{\sigma=1} < 0$, the scheme converges if*

$$1 + \tau = \sigma \geq \sigma_{\min} = \frac{\sqrt{(\tilde{\beta}_s - 3)^2 - 4(3 + \alpha_s)(\tilde{\gamma}_s + 1)} + 3 - \tilde{\beta}_s}{6 + 2\alpha_s}. \quad \blacksquare$$

4 Multigroup AMR scheme

In this section, we describe our implementation of AMR for the multigroup diffusion (MGD) system. The scheme necessarily adheres to the code's general architecture. That is, on each grid level each physics module (hydrodynamics, radiation) is called in order. These comprise the *level solves*. If AMR is used, the code refines in both space and time, as described by Howell and Greenough [7]. After a refined level is time-advanced to the next coarse level time, a synchronization is required in order to maintain conservation. For a scalar diffusion equation and only two levels, coarse and fine, the “sync-solve” is difficult

enough since it reduces to effectively an unstructured grid solve over the combined coarse and fine grids. For MGD, the difficulty is compounded by having to sync-solve a coupled system of diffusion equations.

We begin by recalling the equations,

$$\partial_t u_g = \nabla \cdot D_g \nabla u_g + \kappa_g (B_g - u_g), \quad g = 1, \dots, G \quad (23)$$

$$c_v \partial_t T = - \sum_{g=1}^G \kappa_g (B_g - u_g), \quad (24)$$

where c_v is now the heat capacity, while D_g and κ_g are the diffusion and coupling coefficients. For ease of exposition, it is convenient to consider the one-dimensional case. The level solve module computes the solution to

$$u_{g,i} - u_{g,i}^0 = (F_{g,i+1/2} - F_{g,i-1/2})/h_i + \gamma_{g,i} [B_g(T_i) - u_{g,i}], \quad (25)$$

$$c_{v,i}(T_i - T_i^0) = - \sum_{g=1}^G \gamma_{g,i} [B_g(T_i) - u_{g,i}], \quad (26)$$

where i is the cell index, $\gamma_{g,i} = \Delta t \kappa_{g,i}$, and $F_{g,i+1/2}$ is the fluence on the right edge of the i th cell,

$$F_{g,i+1/2} = \Delta t D_{g,i+1/2} (u_{g,i+1} - u_{g,i})/h_i.$$

For simplicity, assume there are only two levels, coarse and fine. Since (23)-(24) are reaction-diffusion equations, advanced with backward Euler temporal differencing, the discretization is unconditionally stable. Hence, in the following, in order to simplify the derivation, we assume that both levels are advanced with the *same* timestep. However, in the code we also time-cycle. If $i = 1, \dots, N$ define the indices of all coarse-level cells, let $j = 1, \dots, J$ define the indices of the refined cells and $i = I, \dots, N$ define the indices of those coarse cells which are not refined. Coarse cells indexed with $i = 1, \dots, I - 1$ are defined as the “covered” cells. We first update the entire coarse level, then the fine level. Both levels require boundary conditions (BC). The coarse level uses the user-specified BC. In the following example, the refined domain abuts the left side boundary and consists of J cells. Hence, the fine level uses the same BC on the left edge. The fine cell indexed with $j = J$ lies in the interior of the domain. We reuse the Howell and Greenough [7] infrastructure to provide a Dirichlet condition for the cell. The datum is obtained by interpolating coarse grid data. Let k_j and h_i define the mesh widths of the fine and coarse cells, respectively. After multiplying by the mesh widths and summing over all cells and groups,

we obtain

$$\begin{aligned}
& \sum_{j=1}^J k_j \left[c_{v,j}(T_j - T_j^0) + \sum_{g=1}^G (u_{g,j} - u_{g,j}^0) \right] + \\
& \sum_{i=I}^N h_i \left[c_{v,i}(T_i - T_i^0) + \sum_{g=1}^G (u_{g,i} - u_{g,i}^0) \right] \\
& = \sum_{g=1}^G (F_{g,N+1/2} - F_{g,1/2} - \delta F_{g,cf}) , \tag{27}
\end{aligned}$$

where the last term is the fluence miss-match of the g th group at the coarse-fine interface,

$$\delta F_{g,cf} = F_{g,J+1/2} - F_{g,I-1/2}.$$

The AMR scheme assumes that the system is linear. Hence, the emission is expressed as

$$B_g(T_i) = B_{g,i}^\bullet + \dot{B}_{g,i}^\bullet(T_i - T_i^\bullet),$$

where $B_{g,i}^\bullet$ and its derivative with respect to T , i.e., $\dot{B}_{g,i}^\bullet$, are evaluated at a temperature T_i^\bullet , e.g., $B_{g,i}^\bullet = B_g(T_i^\bullet)$. For semi-implicit Euler differencing, $T_i^\bullet = T_i^0$; if fully implicit, $T_i^\bullet = T_i$. Either way, because $\delta F_{g,cf}$ need not be zero, (27) shows that energy may not be conserved after the two level advances. To restore conservation, we introduce the system for the corrections

$$u'_{g,i} = (F'_{g,i+1/2} - F'_{g,i-1/2})/h_i + \gamma_{g,i} [\dot{B}_{g,i}^\bullet T'_i - u'_{g,i}] + \delta F_{g,cf}/h_i, \tag{28}$$

$$c_{v,i} T'_i = - \sum_{g=1}^G \gamma_{g,i} [\dot{B}_{g,i}^\bullet T'_i - u'_{g,i}], \tag{29}$$

where $F'_{g,i\pm 1/2}$ denote the implicit fluxes; they are functions of u'_g .

Equation (28) holds for all groups $g = 1, \dots, G$. In (28)–(29), the mesh index i varies over the coarse cells not marked for refinement ($i = I, \dots, N$) as well as the fine cells ($j = 1, \dots, J$). Following the methodology of [7], we put the fluence mis-match $\delta F_{g,cf}$ into the coarse cell(s) abutting the interface of the coarse and fine domains.

Summing the level-advance and correction solutions yields conservation. If $u_{g,i}^* = u_{g,i} + u'_{g,i}$ and $T_i^* = T_i + T'_i$, combining (28)–(29) with (25)–(26), multiplying by the mesh widths, and summing over cells and groups, yields the desired conservation relation,

$$\begin{aligned}
& \sum_{j=1}^J k_j \left[c_{v,j}(T_j^* - T_j^0) + \sum_{g=1}^G (u_{g,j}^* - u_{g,j}^0) \right] + \\
& \sum_{i=I}^N h_i \left[c_{v,i}(T_i^* - T_i^0) + \sum_{g=1}^G (u_{g,i}^* - u_{g,i}^0) \right] = \sum_{g=1}^G (F_{g,N+1/2}^* - F_{g,1/2}^*).
\end{aligned}$$

Equations (28)–(29) present a formidable task as it requires solving a simultaneous system of equations for $(G + 1)\bar{N}$ unknowns, where \bar{N} denotes the number of refined cells plus the number of coarse cells not marked for refinement. The grid is effectively unstructured since it combines coarse and fine discretizations of the domain. We attack the problem by applying a variant of the “Partial Temperature” scheme [9], [13]. In this scheme, groups are assigned a random order. As we cycle through the groups, each group computes a correction u'_g and a partial temperature T_g . Note the group index g for the temperature. Although the scheme decouples the groups from each other, the partial temperature T_g changes as we cycle through the groups. To be precise, for each group, we solve the system

$$u'_{g,i} = (F'_{g,i+1/2} - F'_{g,i-1/2})/h_i + \gamma_{g,i} [\dot{B}_{g,i} T_{g,i} - u'_{g,i}] + \delta F_{g,cf}/h_i, \quad (30)$$

$$c_{v,i} (T_{g,i} - T_{g-1,i}) = -\gamma_{g,i} [\dot{B}_{g,i} T_{g,i} - u'_{g,i}], \quad (31)$$

where, as above, the mesh index i ranges over all refined cells and all coarse cells not covered by the fine grid. For the group index g_1 that we first pick, $T_{g-1,i} = 0$ on the LS of (31). Solving (30)–(31) for $g = g_1$ yields the first partial temperature T_{g_1} . This temperature replaces $T_{g-1,i}$ on the LS of (31) for the second randomly picked group g_2 . After cycling through the groups, the last one, g_G , gives the desired corrected temperature, i.e., $T'_i = T'_{g_G,i}$.

If (31) is summed over all g , the LS telescopes and we obtain,

$$c_{v,i} T'_i = - \sum_{g=1}^G \gamma_{g,i} [\dot{B}_{g,i} T_{g,i} - u'_{g,i}].$$

Because we have $T_{g,i}$ on the RS instead of T'_i , this is not exactly (29). However, if $T_{g,i}$ doesn't vary too much as we cycle through the groups, the result is no worse than one obtained with the (commonly-used) partial temperature (PT) scheme since we apply PT to only corrections of the level-solve solution. Cycling through the groups in random order avoids biasing the deviation since the coupling in (30)–(31) may lower T for one group while raising it for another. In any case, the combined solution (u_g^*, T^*) is still conservative.

Equations (30)–(31) are solved using a Schur complement. Since (31) does not involve spatial derivatives, we can easily solve for $T_{g,i}$. After substituting the result into (30), we obtain a single scalar equation for $u'_{g,i}$, albeit now, on the unstructured grid composed of coarse and fine cells, viz.,

$$u'_{g,i} = (F'_{g,i+1/2} - F'_{g,i-1/2})/h_i + \gamma_{g,i} \eta_{g,i} [\dot{B}_{g,i} T_{g-1,i} - u'_{g,i}] + \delta F_{g,cf}/h_i,$$

where, $\eta_{g,i} = c_{v,i} / (c_{v,i} + \gamma_{g,i} \dot{B}_{g,i})$. After solving for $u'_{g,i}$, equation (30) yields $T_{g,i}$. The fluence miss-match $\delta F_{g,cf}$ acts as a source to the corrections. For groups with long mean free paths (mfp) and weak coupling, $\delta F_{g,cf}$ diffuses over the mesh. For groups with short mfp and strong coupling, $\delta F_{g,cf}$ is spread locally over the group energy $u'_{g,i}$ and “absorbed” into the matter.

Before closing this section, we note an inconsistency in the above *multilevel* scheme, indeed in any scheme embedded in a multi-physics code like ours, which advances several modules (hydrodynamics, heat conduction, radiation) using operator splitting. With splitting, on each level, the modules are advanced in order. For simulations using hydrodynamics and radiation diffusion and running with coarse L0 and fine L1 levels, the order of operations is as follows. Level L0 first advances hydrodynamics, then radiation. Next, if refining by a factor of two, L1 advances in the order: hydrodynamics, radiation, hydrodynamics, radiation. The multilevel solve advances in the same order: hydrodynamics, then radiation. This implies that the radiation multilevel solve uses coefficients, e.g., ρ , that are not the same as those used by the radiation level solve modules. In principle, one cannot simply add the correction equations to the level solve equations and claim that the sum satisfies a consistent set of equations. Nonetheless, the solution remains conservative.

5 Simulations

This section presents results using the multigroup scheme. We consider three problems. In Section 5.1, we present a test problem with a known analytic solution. We compare numerical results with tabular data, previously published by Shestakov and Bolstad [15]. Using Richardson extrapolation, we show that our Ψ tc scheme, i.e., what we apply on a level, is second (first) order correct in space (time). When running with AMR, the temporal accuracy is first order. Accuracy of the spatial order depends on the norm used to measure convergence. In the most stringent ∞ -norm, the order degrades to first, or worse, as shown at the end of section 5.1. Section 5.2 develops a variation of the Section 5.1 test problem in order to demonstrate the benefits brought by Ψ tc. We do this by running with and without Ψ tc. We make several runs, each for only one timestep. Runs are made with successively larger Δt . Because of fully implicit differencing, as $\Delta t \rightarrow \infty$, the numerical solution should approach the time-independent, steady-state. The problem in Section 5.3 brings everything together. We simulate the explosive expansion of a metal sphere suspended in air. The expansion is due to sourcing a large amount of energy in a short time into the sphere. Simulations are done with the code's full functionality, i.e., we couple all of the physics modules and also use AMR.

5.1 Linear MGD test problem

In this section we present results for a MGD problem with a known solution. Due to the nonlinearity of the equations, there are no test problems with analytic solutions. Thus, to validate and verify our algorithm, we consider the linearized multigroup equations developed by Shestakov and Bolstad (S&B) [15] and compare with tabular data.

The S&B tables present results for a 64-group discretization of the linearized, nondimensional, multifrequency diffusion equations derived by Hald and Shes-

takov (H&S) [6]. In the following, we briefly derive the nondimensional system, describe the test problem, explain how to set up the problem in a radiation-hydrodynamic code, demonstrate the problem's relevance to typical applications of multigroup diffusion, compare results with an improved-accuracy table [4] (supplied in the Appendix), and conclude by proving that our multigroup scheme's convergence is first order in time and second order in space.

The nonlinear multifrequency H&S system is derived by assuming slab symmetry, constant density, an ideal gas EOS, and an opacity characteristic of free-free transitions. One advantage of the H&S system is its nondimensional form, which enables comparing results from codes using different dimensional units. The equations are obtained by choosing characteristic values for density ρ_0 , temperature T_0 , and inverse mean free path (mfp) $\kappa = \kappa_0/\nu^3$ with $\kappa_0 = \text{const}$ and ν the frequency variable. Radiation emission is given by a Wien distribution⁶, i.e., $B_W = B_0 \nu^3 \exp(-h\nu/kT)$, where $B_0 \doteq 8\pi h/c^3$ is the same constant defining the Planck function. The inverse mfp appears in both the diffusion, $D = c/3\kappa$, and the radiation-matter coupling terms, $c\kappa$. (The diffusion is *not* flux-limited.) The normalization proceeds as follows. The values ρ_0 , κ_0 , and T_0 define the other normalization constants,

$$\begin{aligned} \nu_0 &\doteq kT_0/h, & \ell_0 &\doteq \nu_0^3/\kappa_0, & x_0 &\doteq \ell_0/\sqrt{3}, \\ t_0 &\doteq \ell_0/c, & u_0 &\doteq B_0\nu_0^3, & E_0 &\doteq u_0\nu_0. \end{aligned}$$

By defining nondimensional variables, $x' = x/x_0$, $t' = t/t_0$, $u' = u/u_0$, $\nu' = \nu/\nu_0$, etc., (and dropping the primes) we obtain the normalized system,⁷

$$\partial_t u = \nabla \cdot \nu^3 \nabla u + (\nu^3 e^{-\nu/T} - u) / \nu^3, \quad (32)$$

$$R\partial_t T = -T + \int_0^\infty (u/\nu^3) d\nu, \quad (33)$$

where the constant

$$R = (h/k) (\rho_0 c_v / u_0)$$

and c_v is the specific heat. Henceforth, unless stated otherwise, we use nondimensional variables.

The H&S system yields a precise definition of the multigroup equations since the group integrals can be computed exactly, an impossible task for definite integrals of the Planck function. Given a group structure $\{\nu_g\}_{g=0}^G$, after integrating

⁶It is noteworthy that H&S's choice of opacity and Wien spectrum for B gives the same emission source κB_W as would be obtained by including stimulated emission (SE) effects [19] and using the Planck function, since SE multiplies κ by the factor $(1 - e^{-h\nu/kT})$. Also note that without SE, the resulting Planck-averaged gray opacity does not exist; the integral diverges.

⁷If instead of B_W , H&S had used the Planck function, the factor $e^{-\nu/T}$ in Eq. (32) would be replaced by $(e^{\nu/T} - 1)^{-1}$. However, H&S would then be unable to form Eq. (33), since the integral over all ν (the total emission) diverges—see prior footnote.

over groups,

$$\partial_t u_g = \bar{\nu}_g^3 \partial_{xx} u_g + p_g T - u_g / \bar{\nu}_g^3, \quad g = 1, \dots, G \quad (34)$$

$$R \partial_t T = -T + \sum_{g=1}^G u_g / \bar{\nu}_g^3 \quad (35)$$

where $u_g = \int_g u d\nu$ and $\bar{\nu}_g$ is a group's representative frequency. S&B define $\bar{\nu}_g$ as $\sqrt{\nu_g \nu_{g-1}}$ and $\bar{\nu}_1$ as $\nu_1/2$ since the lowest group boundary is zero. The emission coefficients are

$$p_g \doteq \exp(-\nu_{g-1}/T) - \exp(-\nu_g/T). \quad (36)$$

If the group structure is broad enough, $\sum_g p_g = 1$.

Equations (34)–(35) are *nonlinear* because of the product $p_g T$. To derive an analytic solution, S&B follow the approach of Su and Olson [16], [17], which requires a *linear* system since it uses Fourier and Laplace transforms. S&B linearize by defining a *fixed* temperature T_f and substituting T_f for T in (36).

Except for one item, it is easy to assemble the S&B linearized MGD system in a conventional radiation-hydrodynamic code. Such codes usually allow an ideal gas EOS and a desired analytic form for the opacity. One chooses arbitrary values for ρ_0 , κ_0 , T_0 , and picks a specific heat c_v to set R . In our simulations, $\rho_0 = 1.8212111 \cdot 10^{-5} \text{ g cm}^{-3}$, $T_0 = 0.1 \text{ keV}$, and $\kappa_0 = 4.0628337 \cdot 10^{43} \text{ cm}^{-1} \text{ s}^{-3}$. To comply with S&B, we chose c_v to obtain $R = 1$. Our ρ_0 , T_0 , and κ_0 choices were dictated purely by reasons of convenience. Since we compare with a nondimensional result, other constants may be used instead.

The subtle item is how to force a code's spectral emission rate to equal $p_g(T_f) T$. We accomplish the task as follows. The g th group's emission is $a_g [B_g + B'_g (T - T^*)]$, where $a_g = \Delta t c \rho \kappa_g$ and κ_g is the group-averaged opacity. The terms B_g and B'_g are integrals over the g th group, at temperature T^* , of the Planck function and its derivative w.r.t. T . The integrals are computed by a FORTRAN subroutine, which takes T^* as an input variable. For the test problem, we use a different subroutine, which when called, first defines

$$B'_g = (\bar{\nu}_g \nu_0)^3 (8\pi k/c^3) [\exp(-y_{g-1}) - \exp(-y_g)],$$

where $y_g = h\nu_g \nu_0 / k T_f T_0$. After computing B'_g , the routine sets $B_g = B'_g T^*$. In the y_g definition, ν_g and T_f are nondimensional, while ν_0 and T_0 are the normalization constants. The $(\bar{\nu}_g \nu_0)^3$ term cancels the $1/\nu^3$ dependence of the opacity.

For the test, we consider S&B's problem 1. The nondimensional domain is $0 < x < X$, where we set $X = 4$. The initial condition is $T = 1(0)$ for $x < (>) 0.5$ and $u = 0$ everywhere. We use symmetry boundary conditions at $x = 0$ and homogeneous Milne at $x = X$. We use the same group structure as S&B: 64 groups, starting at zero, with widths increasing geometrically by the factor 1.1. We set $\nu_1 = 5 \cdot 10^{-4}$ as the width of the first group.⁸ The

⁸A misprint in [15] erroneously has $\nu_1 = 10^{-4}$.

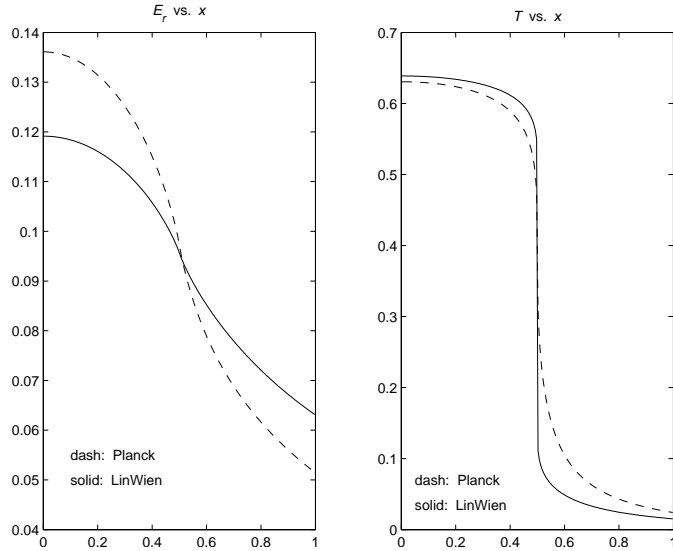


Figure 1: Linear MGD test. Comparison of the linear solution ($T_f = 1.0$) with the solution of the nonlinear MGD system with Planckian emission; $t = 1$.

test simulates an initially hot slab of material encased by cold matter. Since u is initially zero throughout, the solution evolves by first coupling in the hot subdomain. As radiation diffuses out, it couples to cold matter thereby heating it. Because of the opacity’s $1/\nu^3$ dependence, the group’s diffusion and coupling rates differ.

Although the problem appears contrived, it represents effects of radiation diffusion. We prove the assertion in Fig. 1 where we display the temperature T and the total radiation energy density E_r ($= \sum_g u_g$) for two simulations ending at $t = 1$. Solid lines pertain to the linearized system, where $T_f = 1.0$. Dashed lines are solutions of the “physical” nonlinear MGD system using Planckian emission. The similarity of the solutions validates the relevance of the test problem. We used $T_f = 1.0$ (instead of S&B’s $T_f = 0.1$) because over the short duration of the simulation, the emission temperature in the hot subdomain is of order 1.0 rather than 0.1.

We now present our MGD result using S&B’s parameter $T_f = 0.1$. Table 1 displays the relative errors of T and E_r for various x , at $t = 1.0$. For a variable f , we define the error $\varepsilon(f) = |(f_x - f_k)/f_x|$, where f_k are our numerical results and f_x are the S&B table values, listed in the Appendix. Table 1 shows that we obtain better than 0.5% accuracy over the domain $0 \leq x \leq 1$. The worst error 0.48% occurs for T at $x = 0.51$. At that point, according to the table in the Appendix, T undergoes more than a 20-fold drop from its value at $x = 0.49$. We focus attention at the domain near $x = 0.5$ since that is where the variables undergo the sharpest change. At these points, we obtain better than 0.1% errors,

x	$\varepsilon(T) \cdot 10^3$	$\varepsilon(E_r) \cdot 10^3$	x	$\varepsilon(T) \cdot 10^3$	$\varepsilon(E_r) \cdot 10^3$
0.00	0.0016	0.3012	0.51	4.8468	0.2785
0.20	0.0015	0.3028	0.52	1.8220	0.0031
0.40	0.0005	0.3268	0.53	1.0528	0.1293
0.46	0.0081	0.3903	0.54	0.7320	0.2128
0.47	0.0174	0.4252	0.60	0.3316	0.5263
0.48	0.0467	0.4945	0.80	0.6099	1.3841
0.49	0.2205	0.6979	1.00	1.4253	2.2138
0.50	0.0019	0.3518			

Table 1: Linear MGD test. Relative errors times 1000. Numerical result obtained with $T_f = 0.1$, $h = 1/400$, $\Delta t = 1/200$.

except for T at $x = 0.52$ and 0.53 . Errors near $x = 1.0$ are less important for two reasons. First, the S&B domain extends to infinity while ours extends to only $X = 4$. Hence, our results near the RS may be polluted by the boundary condition. Second, our code requires having a positive $\min(T)$. Hence, we cannot initialize with $T = 0$ in the cold region. At the end of the run, at $x = 1$, our temperature has risen by only a factor of 10^4 , which precludes reaching much better than 0.1% accuracy there.

We were unable to use the S&B tables for a convergence study to verify our scheme's convergence properties w.r.t. timestep Δt and mesh size h . We speculate that the reason is that the truncation is a mix of errors due to finite Δt and h . Hence, a refinement study of one may be polluted by an overly coarse value for the other. However, we can use Richardson extrapolation to prove that our scheme is correct to first order in time and second order in space. Let v_k denote a numerical solution to an equation discretized by a constant parameter k . For an initial value ODE, k represents the timestep; for a time independent equation, k is the mesh width. If v is the analytic solution,

$$v_k = v + \alpha k^a + \mathcal{O}(k^b),$$

where $0 < a < b$, and where α is independent of k . In the asymptotic regime, the k^a term dominates the error, which allows ignoring the $\mathcal{O}(k^b)$ term. Assuming we have three solutions v_k, v_{2k}, v_{4k} , a ratio of differences yields

$$\frac{v_{2k} - v_{4k}}{v_k - v_{2k}} = 2^a.$$

The order of convergence a is found by taking logarithms.

We apply this procedure to estimate the orders of convergence. First, for the Δt study, we fix $h = 0.01$ and obtain three results using $k = 0.5 \cdot 10^{-8}$ s, $2k$ and $4k$. For the Δx study, we fix $\Delta t = 0.5 \cdot 10^{-8}$ s and use $k = 0.0025$. In both studies, runs are halted when $t = t_0$. We compute a at 15 points across the domain $[0, 1]$ for both E_r and T and focus attention at $x = 0.5$, where the fields undergo the sharpest change. Results are presented in Fig. 2. The left plot

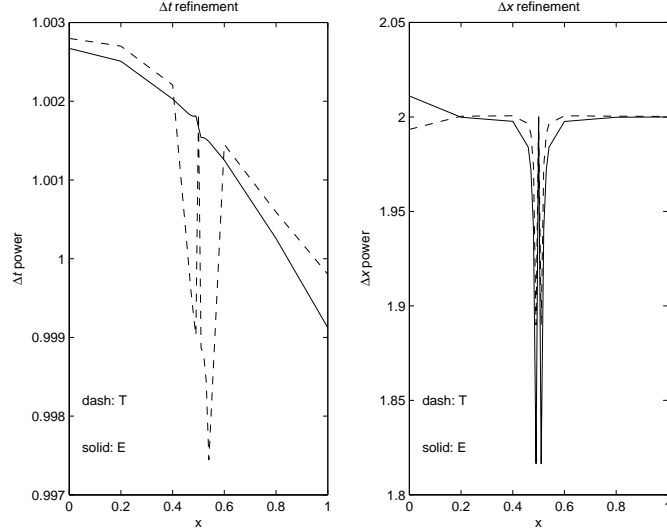


Figure 2: Timestep and meshsize orders of convergence; Δt (Δx) on left (right) sides; $t = 1.0$; see text.

clearly displays first order temporal convergence since $a \approx 1$ across the domain. The right plot supports our contention of second order spatial convergence. The low $a \approx 1.82$ (1.89) values for E_r (T) arise only at the two points $x = 0.49, 0.51$. We claim that at these points, we are not yet in the asymptotic regime.

The results of Fig. 2 pertain to a solution obtained on a single level, i.e., without using AMR. We now analyze how AMR affects the order of spatial and temporal convergence. For each study, Δx and Δt , we make three simulations (as before, we halt at $t = 1.0$) in order to apply our Richardson extrapolation technique. In each study, the composite grid consists of a “base” level L0 mesh over the entire domain and two AMR levels. Each level refines by a factor of two. Both L1 and L2 levels refine around $x = 0.5$. We examine convergence at points x in *all levels*.

For the Δt study, all three runs use the same composite spatial mesh. We make three runs; each with fixed timesteps Δt_0 , $2\Delta t_0$ and $4\Delta t_0$, where $\Delta t_0 = 1/400$. The composite mesh uses $\Delta x = 1/100$ on level L0. The L1 mesh extends over $0.36 \leq x \leq 0.64$, and the L2 mesh extends over $0.42 \leq x \leq 0.58$. We obtain nearly the same temporal order as for the level solve. Figure 3 displays a for the 128 cells on $0 < x < 1$. The lowest order, $a \approx 0.94$, occurs at $x = 0.38$ (0.62) for E_r (T) near the L0 and L1 coarse-fine interface.

The Δx study requires more care. For each run, the L1 mesh extends over $0.25 \leq x \leq 0.75$, and the L2 mesh extends over $0.375 \leq x \leq 0.625$. We refer to the three runs as R1, R2 and R4, where R1 and R4 use the “coarsest” and “finest” composite grids, respectively. For the three runs, the level L0 mesh

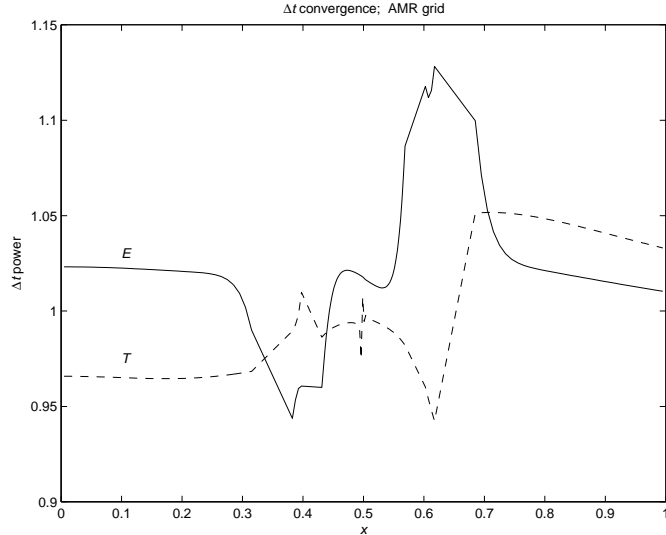


Figure 3: Timestep order of convergence on composite AMR mesh; see text.

sizes are $1/40$, $1/80$ and $1/160$, respectively. Because each AMR level refines by a factor of two, for R1, the L0, L1 and L2 mesh sizes are also $1/40$, $1/80$ and $1/160$. The R2 mesh widths are $1/80$, $1/160$, and $1/320$; R4's are $1/160$, $1/320$ and $1/640$. The composite grids are constructed so that within each level, the R1 cell boundaries are also cell boundaries of runs R2 and R4. Hence, by arithmetic averaging adjoining cell-centered data, we obtain numerical results at the same points for each run. These (averaged) values are used for Richardson extrapolation. Figure 4 displays the ratio $(f_{R2} - f_{R1}) / (f_{R4} - f_{R2})$ for the 79 faces on $0 < x < 1$. The ratio is approximately 4 over most of the domain, which indicates second order convergence. However at the coarse-fine interfaces, the order drops significantly; especially for T at $x = 0.25$ and 0.375 .

The loss of accuracy at the coarse-fine (C-F) interfaces is due to the discretization of the diffusion operator. We use the infrastructure developed by Howell and Greenough [7] to assemble the linear systems. Unfortunately, the difference stencils—which are not discussed in detail in [7]—have a shortcoming near the interface. A more accurate discretization would yield an asymmetric matrix; for reasons of efficiency, symmetric linear solvers were preferred.

The inaccuracy can be analyzed by considering a derivative such as u_{xx} near the C-F interface. Assume that level L0 lies to the left of L1. For $i = 0, 1, 2$, let x_i denote the first three cell centers on L1 and let h define the L1 mesh size. Let x_c denote the center of the coarse cell next to the C-F interface. On L1 interior points, e.g., on x_1 , u_{xx} is approximated by the difference: $(u_0 - 2u_1 + u_2)/h^2$. Hence, $1/h^2$ is the off-diagonal matrix coefficient corresponding to u_0 on the x_1 row. For the matrix to remain symmetric, the u_1 coefficient on the x_0 row

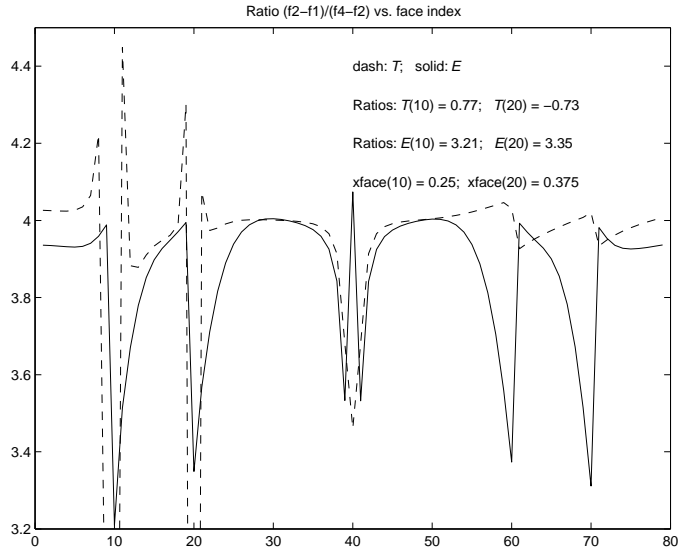


Figure 4: Meshsize order of convergence on composite AMR mesh; see text.

must equal $1/h^2$. At x_0 , u_{xx} is written as a difference of the right and left fluxes divided by the cell width h . The right flux is $(u_1 - u_0)/h$. The left flux is expressed as the difference $(u_0 - u_c)$ divided by the distance between the cell centers. If L1 refines by a factor of two, the distance $x_0 - x_c = 3h/2$. Thus, at x_0 , to maintain symmetry, u_{xx} is approximated by

$$\left(\frac{u_1 - u_0}{h} - \frac{u_0 - u_c}{3h/2} \right) / h.$$

Unfortunately, the left flux is not centered on L1's left-most face (at $x = x_0 - h/2$). A Taylor expansion shows that the difference is inconsistent; it equals $(5/4)u_{xx} + \mathcal{O}(h)$ and this is the source of the error. However, the error is localized. In a global sense, it is $\mathcal{O}(h)$, when computed by integrating over the entire domain: $\int u_{xx} dV$. This concludes the refinement study on an AMR mesh.

To summarize, in this section we have shown: (a) With a proper choice of T_f , the test problem mimics MGD physics. (b) We obtain excellent agreement with the S&B tables. (c) Our scheme is correct to first order in time and second order in space. (d) On an AMR mesh, the scheme incurs the same loss of accuracy as the one presented by Howell and Greenough [7] since we use the same discretization at coarse-fine interfaces.

5.2 Benefits of Ψ tc

We now present results that illustrate the benefits obtained by using Ψ tc. We show that for sufficiently large Δt , the conventional (ADR) scheme of Axelrod et al [2] i.e., where $\sigma = 1$, fails to converge. Furthermore, if Δt is only moderately large, so that the ADR scheme does converge, introducing Ψ tc accelerates convergence.

We begin by considering a variation of the problem introduced in Section 5.1. In this section, unless stated otherwise, we use normalized variables. First, we replace the Wien distribution with the Planck function. After normalizing, we obtain an equation similar to (32) except that $e^{-\nu/T}$ is replaced by $(e^{\nu/T} - 1)^{-1}$. Without stimulated emission effects, the *multifrequency* system is ill posed since the RS of the temperature equation integrates the coupling term over all ν . (The integral of B_ν/ν^3 diverges.) Since this is only a test, we ignore this complication. We use seven geometrically spaced groups, whose widths double with increasing frequency. The leftmost group boundary is zero; the first group width $\nu_1 = 0.5$; the last boundary $\nu_7 = 63.5$. As in Section 5.1, the first group's opacity is evaluated at $\nu_1/2$ and the rest are evaluated at the square root average. The spatial domain is $0 < x < 2$. The initial conditions are as before, viz., $T = 1$ (0) for $x < (>) 0.5$ and u is initially zero. We impose symmetry boundary conditions on both left and right endpoints. Hence, at all times, the total energy should equal the initial amount $\int_0^{1/2} R T dx = 1/2$.

Our test consists of several runs, each for only one timestep. All runs use $h = 0.01$. We run in fully implicit mode; hence, upon convergence, the temperature T and emission source $B_\nu(T)$ are consistent. For infinitely large Δt , a single time advance yields the steady-state with $T = T_r$, where the radiation energy $E_r = aT_r^4$. In the nondimensional system, since B_ν is the Planck function, $a = \pi^4/15$. Hence, the equilibrium temperature is the solution to,

$$2(T_e + aT_e^4) = 1/2, \text{ i.e., } T_e = 0.2314.$$

The Ψ tc result, where $\Delta t = 1000$, is displayed in Fig. 5. The figure shows that the two fields are nearly in equilibrium and almost spatially constant; T_r and T vary less than 1% and 2.4% respectively. The initially high T in $x < 0.5$ has decayed more than fourfold. The radiation field, as it coupled in the initially hot region, diffused outwards thereby heating the cold region.

The simulations were run with and without Ψ tc. Both runs consist of nested “inner” and “outer” loops. The inner iterations (11)–(12) progress until the residual and the iterate difference $\|u^{(i+1/2)} - u^{(i)}\|$ fall below specified tolerances (which may not happen). At that point, the outer iteration computes a revised temperature T using (5). We then reset $T^* = T$ and use it to recompute the B_ℓ and B'_ℓ coefficients. For the first outer iteration, $T^* = T^0$. The iterations conclude when the temperature change and the nonlinear residual fall below their specified tolerances.

The problem's difficulty increases with Δt . Without Ψ tc, it becomes impossible to solve if Δt is very large because of the computer's finite precision. For large Δt , the time derivatives, e.g., $(u - u^0)/\Delta t$, are dominated by the

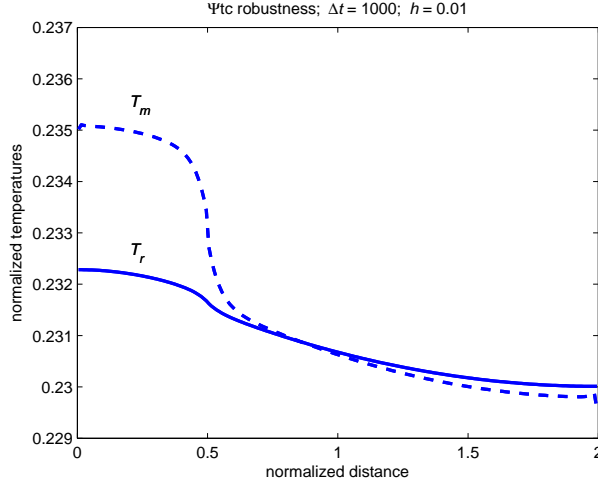


Figure 5: Ψ tc robustness test; solution after one time advance; $h = 0.01$, $\Delta t = 1000$.

other terms. Hence, the initial condition (u^0, T^0) becomes less relevant. Unfortunately, energy conservation depends on “remembering” the initial condition. The boundary conditions enhance the difficulty. If the initial condition is indeed “forgotten,” the solution is not unique. Any equilibrium temperature $T_e = T = T_r$ is a steady-state.

For runs without Ψ tc, we impose $\sigma = 1$ and determine for which magnitude Δt the iterations fail to converge. Runs using Ψ tc proceed as follows. We first compute the three different σ required to have (1) a nonnegative RS, (2) diagonal dominance, and (3) convergence of inner iterations. That is, the σ must satisfy the lemmas of Sections 3.1, 3.2 and 3.3. The iterations commence using the largest σ . The parameter σ is fixed for each outer iteration. Experience has shown that the lemmas give an overly large σ . Hence, we use the lemmas to set σ for only the first outer iteration. Subsequent outer iterations decrease σ as follows. Recall $\sigma = 1 + \tau$ and that only when $\tau = 0$ do we solve the correct discretization of the equations. Successive outer iterations multiply τ by a constant factor, i.e., $\tau \rightarrow \alpha_\tau \tau$. The factor may be changed by the user. For small α_τ , τ decreases quickly, but the resulting linear system is harder to solve. For the hardest test, where $\Delta t = 1000$ (see below), we experimented and found better results with $\alpha_\tau = 0.5$ than with $\alpha_\tau = 0.25$.

Our tests begin with $\Delta t = 20$, a magnitude at which both modes, with and without Ψ tc, converge and give nearly identical results. For this moderately large Δt , Ψ tc brings the benefit of faster convergence: 37 vs. 50 CPU sec, i.e., nearly 33% faster. For $\Delta t = 100$, the two modes still converge and give very similar results, but they are now at the limit of convergence. The Ψ tc run is

significantly faster: 56 vs. 205 sec, an almost fourfold improvement. For $\Delta t = 200$, the non Ψ tc run does not converge. However, its final iterate temperatures still look physical; T_r is 0.5% uniformly higher than the corresponding converged Ψ tc profile. Our Ψ tc implementation has its own limit. The Fig. 5 result, where $\Delta t = 1000$, also fails to converge. Nonetheless, the result is physical and conserves energy to nearly 11 decimal digits. Non-convergence is evidenced by small dips in the matter temperature T_m at the cells abutting the left and right boundaries. At the end points, T_m changes very slowly from one iteration to the next. The iterations effectively stall. Although the residuals continue to decrease, they have such a slow decay that the run halts when it reaches the iteration limit. The run without Ψ tc and $\Delta t = 1000$ diverges due to negative internal energies. To summarize, Ψ tc not only decreases the runtime but also brings an extra degree of robustness.

5.3 Expansion of a hot aluminum sphere

In our opinion, the hardest aspect of code development is integrating a module into a multi-physics code and running “real” problems. For us, this implies simulations of multiple materials, whose properties are listed in tables, using hydrodynamics, heat conduction, radiation modules, and, naturally, AMR.

For the final test we consider the following problem. An Aluminum (Al) sphere of radius 15.5 cm is suspended in air. The initial densities are $\rho = 2.68118198$ and 0.00129 g/cm³ for Al and air, respectively. Both materials are initially at $T = 375.936$ K.⁹ There is initially no radiation energy: $E_r|_{t=0} = 0$. At $t = 0$, we inject energy into the radiation field, but only into the domain containing Al. The energy is added over 0.1 ns, at which point we have loaded a yield Y (erg) into the problem. Energy is added with a Planckian spectrum. Unless stated otherwise, the simulations presented in this section use two AMR levels; $h = 2, 4$ cm, and a base grid with $h = 8$ cm.

We compare simulations in which radiation transport is modeled by a single diffusion equation for the radiation energy density (gray diffusion) to runs where the transport is modeled with multigroup diffusion (MGD). We describe results where $Y \approx 11$ kT and $Y \approx 1$ MT.¹⁰

The problem simulates a strong explosion in air; the parameter choice corresponds to a nuclear source. The effects are well-known: Zel’dovich and Raizer [19] Ch. IX, Brode [5], Landshoff [8]. Initially, radiation dominates the dynamics: a fast thermal wave propagates through the surrounding air. When the wave slows to sonic speeds (of the hot air), the steep pressure gradient gives rise to a strong shock. Finally, hydrodynamics dominates. Salient effects are similar to the simulation of a point explosion using hydrodynamics and nonlinear heat conduction (Shestakov [14], “Non-Self-Similar-Problem” section).

Before presenting our results, we summarize them. For the lower yield, gray

⁹Inputs are tailored so that our EOS returns equal pressures for both materials, approximately 1 bar.

¹⁰Using the conversion $4.18 \cdot 10^{19}$ erg/kT, the actual yields are 10.9731 kT, 0.9870682 MT, 10.9665 kT, and 0.9862604 MT for the two gray and two MGD runs, respectively.

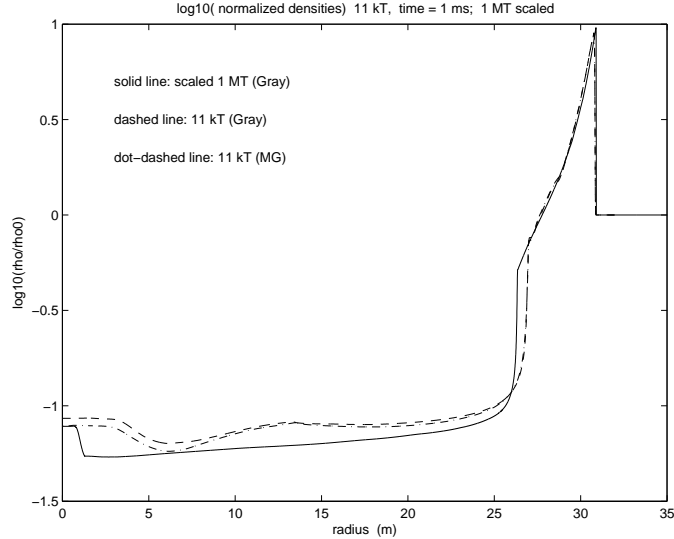


Figure 6: Hot sphere problem. Log of normalized densities; $Y = 11$ kT yield, $t = 1$ ms, gray and multigroup diffusion; $Y = 1$ MT gray curve is scaled.

and MGD simulations are very similar. However, for $Y = 1$ MT, the gray and MGD simulations differ significantly and this, we feel, is a new result. Although it contradicts established theory (Brode [5]) we believe it to be correct since it is explained by examining spectra of the radiation field (see below). Furthermore, our MGD result is corroborated by the trusted computer code LASNEX [20].

Figures 6, 7 and 8 display densities, temperatures and velocities, respectively. Each figure contains three curves. Two are from gray and MGD simulations with $Y = 11$ kT. The third curve is from a simulation using gray diffusion and a yield $Y = 1$ MT. The 1 MT curves are drawn after implementing Sachs scaling, i.e., by scaling time and radii by the cube root of the yield ratio $R_Y = (Y_1/Y_2)^{1/3}$, where $Y_1 = 11$ and $Y_2 = 1000$. Hence, while the $Y = 11$ results are taken at $t = 1$ ms, the 1 MT results are at $t = 4.48$ ms and the 1 MT radii have been divided by R_Y . Figure 6 displays $\log_{10}(\rho/\rho_0)$, where $\rho_0 = 0.00129$ g/cm³ is the ambient air density. Although the close agreement displayed in Figs. 6, 7 and 8 may not surprise, it is indeed remarkable how well the gray scaled 1 MT curves compare with the lower yield results. The similarity of the $Y = 11$ kT gray and MGD curves indicates that gray diffusion is adequate for small Y .

The results in Figs. 6, 7 and 8 are characteristic of an event transitioning from a radiation dominated regime to one dominated by hydrodynamics. Figures 6 and 7 depict a strong shock at $r = 31$ m separating from a fireball of radius 26-27 m.

In order to validate our gray $Y = 1$ MT simulation, we continue the run to $t = 7$ ms and find good qualitative agreement when we compare with Brode

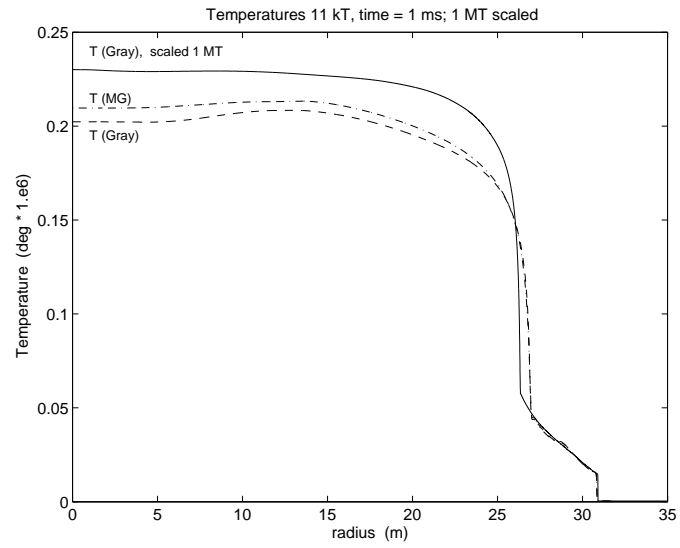


Figure 7: Hot sphere problem. Matter temperatures T ; $Y = 11$ kT yield, $t = 1$ ms, gray and multigroup diffusion; $Y = 1$ MT gray curve is scaled.

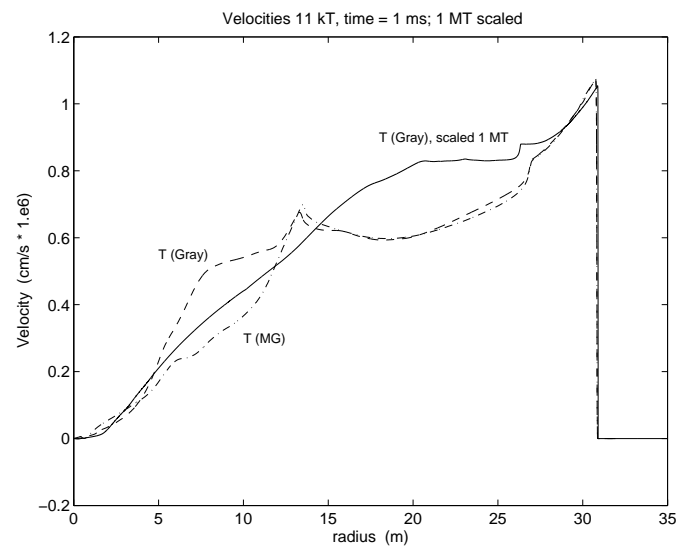


Figure 8: Hot sphere problem. Velocities; $Y = 11$ kT yield, $t = 1$ ms, gray and multigroup diffusion; $Y = 1$ MT gray curve is scaled.

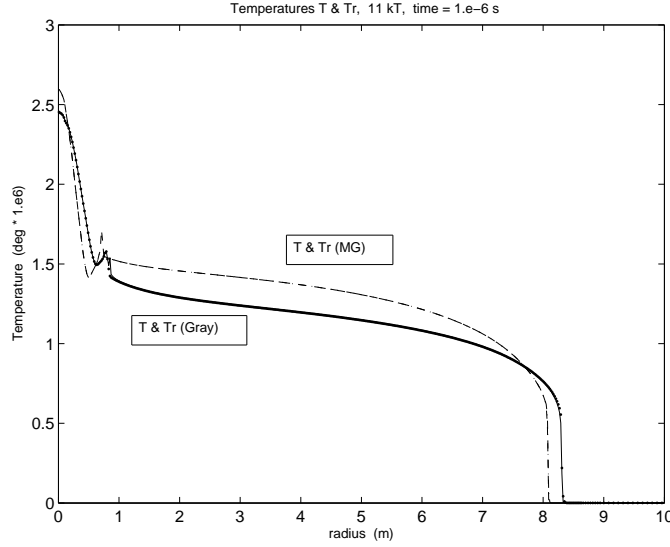


Figure 9: Hot sphere problem. Gray and multigroup temperatures T and T_r , $Y = 11$ kT, $t = 1\mu\text{s}$.

[5]. Quantitatively, at $t = 7$ ms, we find a strong shock at $r = 164$ m, whereas Brode finds it at $r \approx 190$ m. Both simulations show a nearly tenfold density rise at the shock, while inside the fireball, $\rho \approx 5 \cdot 10^{-5} \text{ cm}^3$. For the central ($r = 0$) temperature we have $T = 2.04 \cdot 10^5$ K at $t = 7$ ms vs. $\approx 2 \cdot 10^5$ K for Brode. Our fireball radius is 138 m (≈ 160 for Brode), and our shock temperature is $1.65 \cdot 10^4$ K ($\approx 1.6\text{--}1.7 \cdot 10^4$ K for Brode).

We now compare the gray and MGD results for $Y = 11$ kT yield at the earlier time, $t = 1 \mu\text{s}$, when the solution is dominated by radiation. At this time, since the thermal wave is supersonic, it suffices to only examine the temperatures T and T_r , where, for both gray and MGD simulations, $T_r \doteq (E_r/a)^{1/4}$ and a is the radiation constant. (Although the Al ball has ballooned to nearly 1 m, which launches a strong shock at the Al/air interface, there is little separation between the interface and the shock. Thus, beyond 1 m, the air density is nearly the same as it was initially.) Figure 9, which displays the temperatures, shows little difference between gray and MGD. Both models display a fireball extending to $r = 8.1\text{--}8.4$ m and a central $T \approx 2.5 \cdot 10^6$ K; both also display the start of the shock at the Al/air interface, as evidenced by the spike at $r \approx 0.8$ m.

However, for high yield, the gray and MGD simulations differ dramatically. Figure 10 displays T and T_r for $Y = 1$ MT at $t = 1\mu\text{s}$.¹¹ We see that for gray

¹¹The spatial scale of Figure 10 cannot resolve the small, but nevertheless significant hydrodynamic effects which expand the Al sphere to $r \approx 80$ cm. For MGD, the temperature is not monotone w.r.t. to r near the origin. It falls from a central value of $2.6 \cdot 10^6$ deg to $1.8 \cdot 10^6$ at the edge of the sphere (due to the rarefying Al) then rises to $2.06 \cdot 10^6$ in the air.

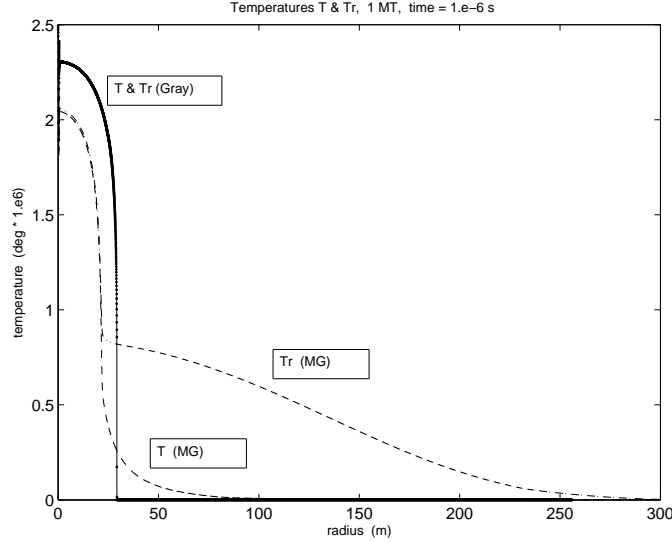


Figure 10: Hot sphere problem. Gray and multigroup temperatures T and T_r , $Y = 1$ MT, $t = 1\mu\text{s}$.

diffusion, $T = T_r$; just as for $Y = 11$ kT. The gray diffusion thermal wave, which is still supersonic, has a front at $r \approx 30$ m. However, the MGD result is strikingly different. Multigroup diffusion lowers the central temperatures by more than 10%. More surprisingly, for MGD, T and T_r are tightly coupled only out to $r \approx 20$ m. Beyond that, at $T \approx 8.5 \cdot 10^5$ K, T and T_r decouple. The radiation temperature extends to $r \approx 300$ m, which is the free-streaming limit.

To examine why the high yield gray and MGD simulations differ, we turn off hydrodynamics and heat conduction, repeat the simulation, and find temperatures similar to Fig. 10. This is not surprising since the dynamics are radiation-dominated. To gain more insight, we examine spectra. Figure 11 displays the spectral radiation energy vs. frequency at 5–160 m. Evidently, the frequency-dependent air opacity is responsible. High frequency (30–200 keV) photons travel largely unimpeded whereas near the origin, the spectrum develops a hole at 10 keV. Moving away from the center, the hole progresses to lower frequencies so that at 100–200 m, the spectrum consists of two peaks, one at the high frequencies, another near the visible range. Since the latter contains little energy, the protruding radiation “tongue” of Fig. 10 is due to the high frequencies.

We believe that the difference between the $Y = 11$ kT and $Y = 1$ MT MGD simulations is due to the factor of 100 between the yields. Because the energy is added with a Planckian spectrum, the initial maximum temperatures differ by roughly the fourth root, or approximately 3. Since the initial temperatures are of order 3–5 keV, the high frequencies have a nearly Wien distribution, $\nu^3 e^{-\nu/T}$.

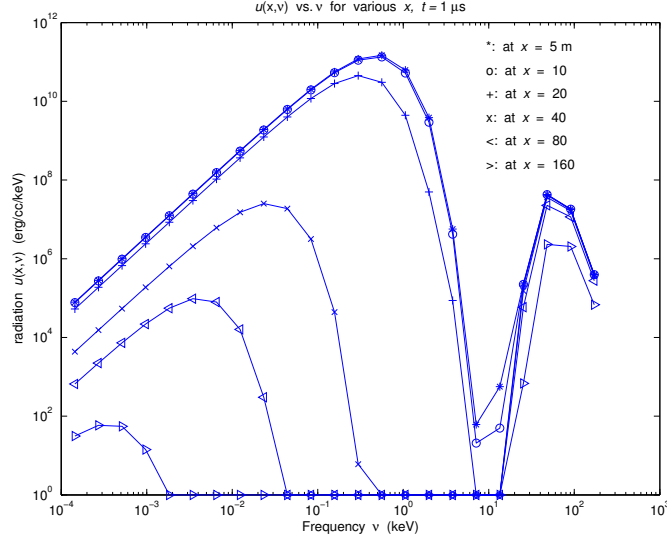


Figure 11: Hot sphere problem. Spectral radiation energy (erg/cc/keV) vs. frequency (keV) at various radii; multigroup physics only; $Y = 1$ MT, $t = 1 \mu\text{s}$.

Hence, we expect the $Y = 11$ kT spectrum to be $e^{-\nu/T}/e^{-\nu/3T}$ or $e^{-2\nu/3T}$ times smaller than the high yield case. Substituting $T = 3$ and $\nu = 100$ keV gives a very small number. The conclusion is that the $Y = 11$ kT case has an insignificant number of those energetic photons that are not absorbed by air.

We conclude the section by comparing results of the 1D spherical and 3D Cartesian versions of our code. We return to running with full functionality, i.e., with hydrodynamics, heat conduction, as well as with two AMR levels. For the Cartesian simulation, the Al “sphere” is a cube 31 cm per side (in contrast to the 1D, 31 cm diameter ball.) The difference in volumes implies that the initial central, Cartesian temperatures are necessarily smaller in order to have the same yield. Figure 12 displays the radial 1D results and a x axis lineout of the Cartesian run. The agreement of the profiles is self-evident.

To summarize, we have simulated real-life problems, viz., air bursts with yields $Y = 11$ kT and 1 MT. We’ve shown that for low Y , gray and MGD give similar results. However, for large Y , they differ for early times when the dynamics are dominated by radiation. Our high yield MGD simulation contradicts results of Brode [5]. However, Brode’s pioneering simulations were done many years ago when the relatively limited computational resources precluded using sophisticated modules such as MGD.

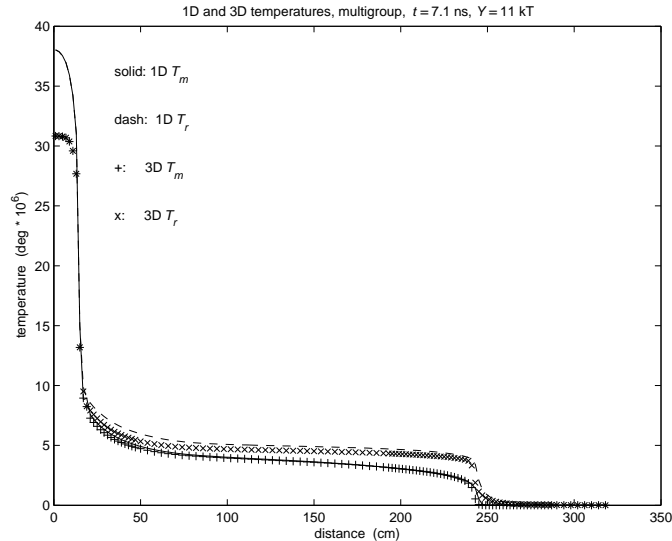


Figure 12: Hot sphere problem. Comparison of T and T_r for Cartesian and spherical multigroup runs; $Y = 11$ kT, $t = 7.1$ ns.

6 Conclusion/Summary

We have described a numerical scheme to solve the radiation multigroup diffusion equations. The scheme is implemented in a radiation-hydrodynamic code with the patch-based AMR methodology, originally proposed by Berger and Olinger [3] for hyperbolic partial differential equations. Our scheme consists of two parts. The first, described in Sections 2 and 3, is applied on a *level* of the AMR grid layout and may be adapted to any code. This part consists of adding $\Psi\tau c$ to the “fully-implicit” iterative scheme of Axelrod et al [2]. $\Psi\tau c$ brings an extra degree of robustness and enhances convergence of the Axelrod scheme. We have developed lemmas that determine the minimum magnitude for the $\Psi\tau c$ parameter τ to ensure that the iterations converge and the result is physically meaningful. The appropriate magnitude depends on the problem.

Our implementation of $\Psi\tau c$ is not optimal—at least for our AMR code architecture. In our code, for each AMR level, we compute a *single* scalar parameter τ . However, the levels consist of a collection of grids (rectangles in 2D) that need not be connected. If the grids are not connected, they form independent problems. Hence, it would be more efficient to use different τ for disconnected grids.

The second part of our scheme, the sync-solve (SS), addresses a specific need of our code, viz., the requirement of having an energy-conserving result on the composite grid of multiple AMR levels. For the multigroup equations, this part reduces to a coupled system of elliptic equations on the unstructured grid com-

binning all levels. Since the SS is intended to be a small correction to the result of the level solves, we adapted the key element of the “partial temperature” scheme of Lund and Wilson [9]. This allowed reducing the multigroup SS to a collection of scalar SS’s. We were then able to reuse existing software.

This paper included simulations of three problems. The first two are idealized tests of only the multigroup module. The third is a “real” problem, which uses the full capability of the code: AMR, multiple materials, etc. The first problem was chosen because of its non-triviality and the availability of analytic results with which to compare. We obtained excellent agreement and verified the convergence properties of the scheme. The second problem illustrated the benefits brought by Ψ_{tc} . We compared the conventional scheme of Axelrod et al [2] with our Ψ_{tc} -modified version. For hard problems, Ψ_{tc} either decreased run times or ensured convergence in regimes where the conventional scheme diverged. The third problem showed that our multigroup module has been fully integrated into the code and has already extended the scientific frontier. For a high yield air burst at STP, we found that gray diffusion gives an incorrect result during the radiation-dominated regime because gray fails to capture the frequency-dependent effects of the air opacity.

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A Revised S&B table

x	T	E_r	$\epsilon(T)$	$\epsilon(E_r)$
0.000000E+00	9.9373253E-01	5.6401674E-03	5.4E-09	5.9E-11
2.000000E-01	9.9339523E-01	5.5646351E-03	1.8E-08	7.0E-11
4.000000E-01	9.8969664E-01	5.1047352E-03	6.0E-09	6.2E-11
4.600000E-01	9.8060848E-01	4.5542134E-03	9.8E-09	6.4E-11
4.700000E-01	9.7609654E-01	4.3744933E-03	1.3E-08	6.9E-11
4.800000E-01	9.6819424E-01	4.1294850E-03	8.2E-09	6.3E-11
4.900000E-01	9.5044751E-01	3.7570008E-03	6.7E-09	6.3E-11
5.000000E-01	4.9704000E-01	2.9096931E-03	7.7E-09	2.8E-11
5.100000E-01	4.3632445E-02	2.0623647E-03	1.2E-08	6.3E-11
5.200000E-01	2.5885608E-02	1.6898183E-03	1.3E-08	6.3E-11
5.300000E-01	1.7983134E-02	1.4447063E-03	1.8E-08	7.0E-11
5.400000E-01	1.3470947E-02	1.2648409E-03	1.5E-08	6.5E-11
6.000000E-01	4.3797848E-03	7.1255738E-04	1.1E-08	6.4E-11
8.000000E-01	6.4654865E-04	2.3412650E-04	2.3E-08	6.8E-11
1.000000E+00	1.9181546E-04	1.0934921E-04	1.0E-08	6.1E-11

Revised S&B table (Bolstad [4]); time $t = 1.0$, $T_f = 0.1$. Columns 4 and 5 give maximum, absolute error estimates. Hence, at $x = 0$, entry T is correct to $\pm 5.4E-09$, i.e., has 8 trustworthy digits.

B Diagonal dominance; large mean-free-paths

As noted in the footnote of Section 3.2 (and remarked by a referee), long mean free paths may lead to diffusion coefficients that overwhelm the other matrix terms. Thus, the estimate for σ , obtained in Lemma 2, may be insufficient. The matrix diagonal contains three terms of various magnitudes. The first stems from the discretization of the $\partial/\partial t$ derivative. Because we multiply by Δt , the term equals 1. The second term is due to the coupling coefficient, a_g ; the term equals $\Delta t c/l_g$, where $l_g = (\rho \kappa_g)^{-1}$ is the mean free path. The third term is the diffusion coefficient, which after including the time step and discretization of $\partial^2/\partial x^2$, is of the form $\Delta t c l'_g/3 h^2$, where l'_g is the flux-limiter-modified mean free path;

$$l'_g = 1/[(l_g)^{-1} + (3h)^{-1}(\beta + |\Delta u_g|/u_g)],$$

where β is a small, user-set constant, whose utility will become evident and $\Delta u_g/u_g$ is a normalized difference of adjoining cell-centered values.

In the limit $l_g \rightarrow \infty$, the coupling term a_g is negligible. Hence, we compare the diffusion term with unity. As $l_g \rightarrow \infty$, l'_g no longer depends on l_g . After factoring a factor of h , the diffusion term is of magnitude,

$$(\Delta t c/h) / (\beta + |\Delta u_g|/u_g).$$

The quantity β^{-1} plays the role of the maximum number of mean free paths allowed, in units of h . If the gradient of u_g is not negligible, $|\Delta u_g|/u_g$ dominates

the diffusion term. If both $l_g \gg 1$ and $|\Delta u_g|/u_g \ll 1$, β dominates. In that case, we are left comparing 1 to $\Delta t c/h \beta$. The parameter β is small; we often use 10^{-4} . Using $c = 3 \cdot 10^{10}$ cm/s gives a diffusion term of order

$$3 \cdot 10^{14} \Delta t/h. \quad (37)$$

If this exceeds machine precision, the σ estimate of Lemma 2 does not guarantee diagonal dominance. We are now left with problem-specific estimates. Clearly, simulations requiring small h or large Δt are problematic. Luckily, our envisioned applications yield reasonable $\Delta t/h$ ratios.

Consider two topics, ICF hohlraums and simulations of the type described in Section 5.3. For the former, mesh sizes are rarely less than 0.1 microns, i.e., $\min(h) = \mathcal{O}(10^{-5})$ cm. Luckily, in ICF, typical total simulation times are of order of tens of ns, requiring significantly smaller timesteps. Using $\max(\Delta t) = \mathcal{O}(10^{-9})$ s, makes (37) of order 10^{10} , which, when compared to unity, is six orders of magnitude above double precision.

For applications of the type presented in section 5.3, while timesteps vary enormously, so do mesh sizes; hence, the ratio $\Delta t/h$ remains moderate. For long-time simulations requiring Δt exceeding 1 s, it is unlikely that it is necessary to resolve details less than 100 cm. Substituting these values into (37) leaves $3 \cdot 10^{12}$, which, is also resolved by double precision, but just barely.

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