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Solution of the nonlinear multifrequency radiation diffusion equations using pseudo transient continuation[1]

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Computer codes simulating high energy density physics consist of modules for distinct physical processes, e.g., compressible hydrodynamics and radiation transport. For the latter, one model assumes tight coupling between radiation and matter. The dependent variables are the spectral radiation energy density $u(x,\nu,t)$ and the matter temperature $T(x,t)$, where x, ν, and t denote position, frequency, and time, respectively. The system is of parabolic form,

$$\partial_t u = \nabla\cdot(D\nabla u) + c\,\rho\,\kappa\,(B-u)\,, \tag{1}$$

$$\rho\,c_{\rm v}\,\partial_t T = -c\,\rho\int_0^\infty d\nu\,\kappa\,(B-u)\,. \tag{2}$$

In (1)-(2), c is the speed of light, ρ the mass density, κ the opacity, and $c_{\rm v}$ the specific heat. The Planck function $B \propto y^3/(e^y-1)$, where $y \propto \nu/T$. In our context, $\rho(x,t)$ is a known function. The opacity is a complicated function of ρ, T, and ν. For "free-free transitions", $\kappa \propto \nu^{-3}$. The coefficient D depends on the mean free path $\ell \doteq 1/\rho\,\kappa$ and, to mitigate unphysical propagation speeds, a flux limiter is introduced. One common description is $D = c/[f(u)+3/\ell]$, where $f = |\nabla u|/u$.

Equations (1)-(2) are solved by discretizing the spectrum $0 \le \nu \le \infty$ into G *groups* defined by $\{\nu_j\}_{j=0}^G$. Integration over each interval (ν_{j-1},ν_j), yields the multigroup equations in which the integral over ν is replaced by a sum of G terms. The system is difficult to solve because of its nonlinearity and wide ranges of time and spatial scales. The ranges are evidenced by the coupling $c\,\rho\,\kappa$ $(= c/\ell)$ and diffusion $D \sim c\ell$ terms. High frequency radiation is characterized by $\ell \gg 1$, i.e., slow coupling and fast transport. The opposite holds for low frequencies. In simulations, the coefficients can vary over 10 to 30 orders of magnitude. The difficulty is compounded by nonlinearity and material composition since the coefficients depend on ρ and T.

In this talk we describe a scheme to solve (1)-(2) for multiphysics codes containing a separate hydrodynamic module. Since such codes typically run at the

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Courant-limited *sound* speed, for our applications, the time step Δt is arbitrarily large. Hence, we use backward Euler temporal differencing. After multiplying through by Δt, we obtain,

$$0 = u_j^0 - u_j + \nabla \cdot (D_j' \nabla u_j) + k_j \, (B_j - u_j) \; , \quad j = 1, \ldots , G \; , \tag{3}$$

$$0 = \rho \, c_{\rm v} \, (T^0 - T) - \sum_{j-1}^{G} k_j \, (B_j - u_j) \; , \tag{4}$$

where $D_j' = \Delta t \, D_j$, $k_j = c \, \Delta t \, \rho \, \kappa_j$, and the superscript 0 denotes the solution at the prior time level. The index j replaces the frequency dependence. Thus, $u_j = \int d\nu \, u$ and similarly for B, where the integration is over (ν_{j-1}, ν_j). The coefficients D_j and κ_j denote averages over the interval.

Viewing (3)-(4) as a nonlinear elliptic system, we introduce pseudo transient continuation (Ψtc). On the LS of (3), we place $(u_j - u_j^*)/\Delta\tau$, where $\Delta\tau$ is the Ψtc parameter and u_j^* is the solution at the previous *pseudo* time. Similarly, the LS of (4) becomes $\rho \, c_{\rm v} \, (T - T^*)/\Delta\tau$. The desired solution is the pseudo time steady-state.

For each Ψtc step, we linearize B_j about the previous iterate, $B_j = B_j^* + (\partial B_j/\partial T)|_{T=T^*}(T - T^*)$. Remaining coefficients, e.g., k_j, are evaluated at $T = T^*$. We avoid a full Newton linearization in order to maintain robustness. (Coefficients such as κ_j are only known approximately and are given in tabular form.) For the first Ψtc step, $u_j^* = u_j^0$ and $T^* = T^0$.

The energies u_j are directly coupled to T through the coefficients k_j. The equation for T does not contain any spatial derivatives. After linearizing, we solve for T analytically and substitute the result into the u_j equations, (Schur complement). This yields G equations in which each u_j is explicitly coupled to the rest. The linear system is of order $N \, G$, where N is the number of spatial points and is of the form

$$(\Lambda - M_1 - M_2) \, u = b \; . \tag{5}$$

In (5), Λ is diagonal, M_1 contains the offdiagonal terms stemming from diffusion and M_2, from intergroup coupling. The parameter $1/\Delta\tau$ appears in both Λ and b; in both places, it contributes to robustness.

We derive conditions on $1/\Delta\tau$ that yield diagonal dominance and non-negative RS, $b \geq 0$. The conditions determine the initial value of $1/\Delta\tau$. Our strategy ensures that each Ψtc iterate, yields a physically reasonable result. In "real" problems, the requirement is crucial since the solution of (5) is used to obtain T, which in turn determines updates of k_j, B_j, etc. A conventional Newton iteration may generate an unphysical value, e.g., $T = -1$, causing the code to halt.

The scheme has been implemented in a radiation-hydrodynamic code. Results will be presented comparing the Ψtc scheme with a more conventional one.