Second-Order Discretization in Space and Time for Radiation-Hydrodynamics

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1. Introduction

In this work, we derive, implement, and test a new IMEX scheme for solving the equations of radiation hydrodynamics that is second-order accurate in both space and time. We consider a RH system that combines a 1-D slab model of compressible fluid dynamics with a grey radiation S_2 model, given by:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(\rho u\right) = 0\,, \tag{1a}$$

$$\frac{\partial}{\partial t}\left(\rho u\right) + \frac{\partial}{\partial x}\left(\rho u^2\right) + \frac{\partial}{\partial x}\left(p\right) = \frac{\sigma_t}{c}F_{r,0}\,, \tag{1b}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}\left[\left(E+p\right)u\right] = -\sigma_a c\left(aT^4 - E_r\right) + \frac{\sigma_t u}{c}F_{r,0}\,, \tag{1c}$$

$$\frac{1}{c}\frac{\partial \psi^+}{\partial t} + \frac{1}{\sqrt{3}}\frac{\partial \psi^+}{\partial x} + \sigma_t\psi^+ = \frac{\sigma_s}{4\pi}cE_r + \frac{\sigma_a}{4\pi}acT^4 - \frac{\sigma_t u}{4\pi c}F_{r,0} + \frac{\sigma_t}{\sqrt{3}\pi}Eu\,, \tag{1d}$$

$$\frac{1}{c}\frac{\partial \psi^-}{\partial t} - \frac{1}{\sqrt{3}}\frac{\partial \psi^-}{\partial x} + \sigma_t\psi^- = \frac{\sigma_s}{4\pi}cE_r + \frac{\sigma_a}{4\pi}acT^4 - \frac{\sigma_t u}{4\pi c}F_{r,0} - \frac{\sigma_t}{\sqrt{3}\pi}Eu\,, \tag{1e}$$

where ρ is the density, u is the velocity, $E = \frac{\rho u^2}{2} + \rho e$ is the total material energy density, e is the specific internal energy density, T is the material temperature, E_r is the radiation energy density,

$$E_r = \frac{2\pi}{c}\left(\psi^+ + \psi^-\right) \,, \tag{2}$$

F_r is the radiation energy flux,

$$F_r = \frac{2\pi}{\sqrt{3}}\left(\psi^+ - \psi^-\right) \tag{3}$$

and $F_{r,0}$ is an approximation to the comoving-frame flux,

$$F_{r,0} = F_r - \frac{4}{3}E_r u \,. \tag{4}$$

Note that if we multiply Eqs. ((1d)) and ((1e) by 2π and sum them, we obtain the radiation energy equation:

$$\frac{\partial E_r}{\partial t} + \frac{\partial F_r}{\partial x} = \sigma_a c(aT^4 - E_r) - \frac{\sigma_t u}{c}F_{r,0} \,, \tag{5a}$$

and if we multiply Eq. (1d) by $\frac{2\pi}{c\sqrt{3}}$, multiply Eq. (1e) by $-\frac{2\pi}{c\sqrt{3}}$ and sum them, we get the radiation momentum equation:

$$\frac{1}{c^2}\frac{\partial F_r}{\partial t} + \frac{1}{3}\frac{\partial E_r}{\partial x} = -\frac{\sigma_t}{c}F_{r,0} \,. \tag{5b}$$

Equations (1a) through (1e) are closed in our calculations by assuming an ideal equation of state (EOS):

$$p = \rho e(\gamma - 1) \,, \tag{6a}$$

$$T = \frac{e}{C_v} \,, \tag{6b}$$

where γ is the adiabatic index, and C_v is the specific heat. However, our method is compatible with any valid EOS.

2. Linearization of Equations

Consider the case of the non-linear system to be solved for Crank Nicolson over a time step from t_n to t_{n+1}. The changes to the non-linear system for the predictor and corrector time steps will only effect the choice of Δt, the end time state, and the known source terms on the right hand side from previous states in time. The non-linear equations to be solved in this case are

$$\frac{\mathcal{E}^{n+1} - \mathcal{E}}{\Delta t} = \tag{7}$$

$$\begin{aligned}\frac{E^{n+1} - E^*}{\Delta t} &= -\frac{1}{2}\left[\sigma_a c\left(aT^4 - \mathcal{E}\right)\right]^{n+1,k+1} - \frac{1}{2}\left[\sigma_a c\left(aT^4 - \mathcal{E}\right)\right]^n \\ &\quad - \frac{1}{2}\left[\sigma_t \frac{u}{c}\left(\frac{4}{3}\mathcal{E}u - \mathcal{F}\right)\right]^{n+1,k} - \frac{1}{2}\left[\sigma_t \frac{u}{c}\left(\frac{4}{3}\mathcal{E}u - \mathcal{F}\right)\right]^n\end{aligned} \tag{8}$$

To simplify the algebra, define a source term Q_E for all the known, lagged quantities in the above equation as

$$Q_E^k = \frac{1}{2}\left[\sigma_a c\left(a(T^n)^4 - \mathcal{E}\right)\right]^n - \frac{1}{2}\left[\sigma_t \frac{u}{c}\left(\frac{4}{3}\mathcal{E}u - \mathcal{F}\right)\right]^{n+1,k} - \frac{1}{2}\left[\sigma_t \frac{u}{c}\left(\frac{4}{3}\mathcal{E}u - \mathcal{F}\right)\right]^n \tag{9}$$

We then linearize the Planckian function about some temperature near T^{n+1}, denoted T^k. The linearized Planckian is

$$\sigma_a ac\left(T^{n+1,k+1}\right)^4 = \sigma_a ac\left[(T^k)^4 + \frac{4(T^k)^3}{c_v^k}\left(e^{n+1,k+1} - e^k\right)\right]. \tag{10}$$

For the initial iteration $T^k = T^n$. The above equation is substituted into Eq. (8) and we define $\beta^k = \frac{4a(T^k)^3}{c_v^k}$ for clarity. The resulting equation can be solved for $(e^{n+1,k+1} - e^k)$ through algebraic manipulation:

$$\begin{aligned}\frac{E^{n+1} - E^*}{\Delta t} &= -\frac{1}{2}\left[\sigma_a^{n+1,k} c\left(a(T^{n+1,k+1})^4 - \mathcal{E}^{n+1,k+1}\right)\right] + Q_E^k \\ \frac{E^{n+1} - E^*}{\Delta t} &= -\frac{1}{2}\left[\sigma_a^{n+1,k} c\left(a(T^k)^4 + \beta^k(e^{n+1} - e^k) - \mathcal{E}^{n+1,k+1}\right)\right] + Q_E^k \\ \frac{E^{n+1} - \rho^{n+1}e^k + \rho^{n+1}e^k - E^*}{\Delta t} &= -\frac{1}{2}\left[\sigma_a^{n+1,k} c\left(a(T^k)^4 + \beta^k(e^{n+1} - e^k) - \mathcal{E}^{n+1,k+1}\right)\right] + Q_E^k\end{aligned}$$

We drop the superscript on ρ because $\rho^{n+1} = \rho^*$. Then, the left hand side can be simplified as

$$\frac{E^{n+1} - \rho e^k + \rho e^k - E^*}{\Delta t} = \frac{\rho}{\Delta t}\left[(e^{n+1} - e^k) + \frac{1}{2}(u^{n+1,2} - u^{*2}) + (e^k - e^*)\right] \tag{11}$$

Solution of the main equation for the desired quantity then gives

$$e^{n+1} - e^k = \frac{\Delta t\left(\frac{1}{2}\sigma_a c(\mathcal{E}^{n+1,k+1} - a(T^k)^4) + Q_E^k\right) - \rho(e^k - e^*) - \frac{\rho}{2}(u^{n+1,2} - u^{*2})}{\left[\rho + \frac{1}{2}\sigma_a c\Delta t\beta\right]} \tag{12}$$

We then multiply the above equation by $\sigma_a c\beta^k$ and divide the RHS by ρ/ρ; this will simplify substitution back into Eq. (10).

$$\begin{aligned}\sigma_a c\beta(e^{n+1} - e^k) = &\frac{\frac{1}{2}\sigma_a ac\Delta t\frac{\beta}{\rho}}{1 + \frac{1}{2}\sigma_a c\Delta t\frac{\beta}{\rho}}\left(\sigma_a c\left[\mathcal{E}^{n+1,k+1} - a(T^k)^4\right] + 2Q_E^k\right)\\ &- \left(\frac{\frac{1}{2}\sigma_a c\frac{\beta}{\rho}\Delta t}{1 + \frac{1}{2}\sigma_a c\Delta t\frac{\beta}{\rho}}\right)\left(\frac{2\rho}{\Delta t}\right)\left[(e^k - e^*) + \frac{1}{2}(u^{n+1,2} - u^{*2})\right]\end{aligned} \tag{13}$$

The effective scattering fraction $\nu_{1/2}$, for the case of Crank Nicolson, is defined as

$$\nu_{1/2} = \frac{\sigma_a c\frac{\beta^k}{\rho}}{\frac{2}{\Delta t} + \sigma_a c\frac{\beta^k}{\rho}}. \tag{14}$$

Substituting back into the main equation, the result can be simplified as.

$$\sigma_a c\beta(e^{n+1} - e^k) = \nu_{1/2}\left(\sigma_a c\left[\mathcal{E}^{n+1,k+1} - a(T^k)^4\right] + 2Q_E^k\right) - \frac{2\nu_{1/2}\rho}{\Delta t}\left[(e^k - e^*) + \frac{1}{2}(u^{n+1,2} - u^{*2})\right]$$

Finally, this can be substituted into Eq. (10) and the $(T^k)^4$ terms simplified, giving the source term

$$\begin{aligned}\sigma_a ac\left(T^{n+1,k+1}\right)^4 = &\left(1 - \nu_{1/2}\right)\sigma_a ac(T^k)^4 + \sigma_a c\nu_{1/2}\mathcal{E}^{n+1,k+1} +\\ &2\nu_{1/2}Q_E^k - \frac{2\rho\nu}{\Delta t}\left[(e^k - e^*) + \frac{1}{2}(u^{n+1,2} - u^{*2})\right].\end{aligned} \tag{15}$$

The above expression can be substituted for the emission source in the S_2 equations, includeing an effective scattering cross section given by $\sigma_a \nu$. After solving for $\mathcal{E}^{n+1,k+1}$, a new internal energy can be estimated using Eq. (12).

Because we have only considered problems with constant densities and heat capacities, the following derivation is depicted in terms of temperature T rather than material energy for simplicity. Application of the first order Taylor expansion in time of the gray emission source $B(T)$, about some temperature T^* at some time near t^{n+1} gives

$$\sigma_a^* ac T^{4,n+1} \simeq \sigma_a^* ac \left[T^{*4} + (T^{n+1} - T^*) 4 T^{*3} \right] \tag{16}$$

where σ_a^* is evaluated at T^*. Substitution of this into the material energy equation given by Eq. (**??**) yields

$$\rho c_v \left(\frac{T^{n+1} - T^n}{\Delta t} \right) = \sigma_a^* \phi^{n+1} - \sigma_a^* ac \left[T^{*4} + (T^{n+1} - T^*) 4 T^{*3} \right]. \tag{17}$$

Further manipulation to solve for the unkown temperature at the next time step T^{n+1} yields

$$\begin{aligned}
\rho c_v \left(\frac{T^{n+1} - T^* + T^* - T^n}{\Delta t} \right) &= \sigma_a^* \phi^{n+1} - \sigma_a^* ac \left[T^{*4} + (T^{n+1} - T^*) 4 T^{*3} \right] \\
\left(T^{n+1} - T^* \right) \left\{ \rho c_v + \sigma_a^* ac 4 T^{*3} \Delta t \right\} &= \Delta t \sigma_a^* \phi^{n+1} - \Delta t \sigma_a^* ac T^{*4} + \rho c_v (T^n - T^*) \\
\left(T^{n+1} - T^* \right) &= \frac{(\Delta t \sigma_a^* \phi^{n+1} - \Delta t \sigma_a^* ac T^{*4} + \rho c_v (T^n - T^*))}{\left\{ \rho c_v + \sigma_a^* ac 4 T^{*3} \Delta t \right\}} \\
\left(T^{n+1} - T^* \right) &= \frac{\frac{\sigma_a^* \Delta t}{\rho c_v} \left[\phi^{n+1} - ac T^{*4} \right] + (T^n - T^*)}{1 + \sigma_a^* ac \Delta t \frac{4 T^{*3}}{\rho c_v}}.
\end{aligned}$$

This provides an expression for T^{n+1} as a function of T^* and the radiation scalar intensity ϕ^{n+1}, i.e.,

$$T^{n+1} = \frac{1}{\rho c_v} f \sigma_a^* \Delta t \left(\phi^{n+1} - ca T^{*4} \right) + f T^n + (1 - f) T^*. \tag{18}$$

If $T^* = T^n$, then this produces the standard IMC temperature update equation. The expression for T^{n+1} can be substituted back into Eq. (**??**) to form an explicit approximation for the emission source at t_{n+1} as

$$\sigma_a ac T^{4,n+1} \simeq \sigma_a^* (1 - f^*) \phi^{n+1} + f^* \sigma_a^* ac T^{4,n} + \rho c_v \frac{1 - f^*}{\Delta t} (T^N - T^*) \tag{19}$$

where $f^* = (1 + \sigma_a^* c\Delta t \beta^*)^{-1}$ is the usual Fleck factor with

$$\beta^* = \frac{4aT^{*3}}{\rho c_v} \tag{20}$$

The material temperature is updated at the end of the time step using Eq. **??**.

Now, the above equation for U_r^{n+1} must be discretized in space. Taking the left spatial moment yields

$$\langle \sigma_a^* acT^{4,n+1} \rangle_L = \frac{2}{h_i} \int_{x_{i-1/2}}^{x_{i+1/2}} b_L(x) \left[\sigma_a^*(1-f^*)\phi^{n+1} + f^* \sigma_a^* acT^{4,n} \right] \mathrm{d}x. \tag{21}$$

To keep the derivation general, we look at the two terms on the right side seperately: $f^*\sigma_a^* acT^{4,n}$ can be evaluated explicitly because the spatial dependence over a cell of $T^{4,n}$ is already assumed LD. The ϕ^{n+1} term is divided and multiplied by a normalization integral to form the appropriate average

$$\left\{ \frac{\dfrac{2}{h_i} \displaystyle\int_{x_{i-1/2}}^{x_{i+1/2}} b_L(x) \sigma_a^*(1-f^*)\phi^{n+1}}{\dfrac{2}{h_i} \displaystyle\int_{x_{i-1/2}}^{x_{i+1/2}} b_L(x)\phi(x)\mathrm{d}x} \right\} \int_{x_{i-1/2}}^{x_{i+1/2}} b_L(x)\phi(x)\mathrm{d}x = \langle \sigma_a^*(1-f^*) \rangle_L \langle \phi^{n+1} \rangle_L \tag{22}$$

where the quotient in braces is defined as $\langle \sigma_a^*(1-f^*) \rangle_L$ and $\langle \phi \rangle_L^{n+1} = \langle \phi \rangle_L^{+,n+1} + \langle \phi \rangle_L^{-,n+1}$ is in terms of the desired unknowns.

The evaluation of $\langle \sigma_a^*(1-f^*) \rangle_L$ is performed based on the assumed spatial dependence over a cell of σ_a and f^*. If f^* and σ_a^* are assumed constant over a cell (i.e., the dependence of these terms on temperature is assumed constant over a cell), Eq. (**??**) reduces to

$$\langle \sigma_a^* acT^{4,n+1} \rangle_L = \sigma_a^*(1-f^*) \langle \phi^{n+1} \rangle_L + f^* \sigma_a^* \langle acT^{4,n} \rangle_L \tag{23}$$

where

$$f^* = f(T^*_{avg,i}) = f\left(\sqrt[4]{\frac{T^{*4}_{L,i} + T^{*4}_{R,i}}{2}} \right) \tag{24}$$

and $\sigma^* = \sigma_a(T^*_{avg,i})$. Constant cross sections over a cell have been assumed for the first iteration of the code. If an LD dependence of the cross sections and temperature is used, $\langle \sigma_a^*(1-f^*) \rangle_L$ can be evaluated without truncation via a Gaussian quadrature or analytical integration and use of the previous (in the HOLO context) HO fine mesh solution; this is the same procedure used for evaluation of the consistency terms. It will likely be easier to use the full non-linear NK solve to handle the LD case than to try to define an LD dependence of f.

Based on a guess for T^*, the above equation gives an expression for the Planckian emission source on the right hand side of Eq. (**??**) with an additional effective scattering source. This allows for four linear equations for the four remaining radiation unknowns to be fully defined. The final equation for the left basis moment and positive flow, for constant f^* and σ_a^* over a cell, becomes

$$-2\mu_{i-1/2}^{n+1,+}\phi_{i-1/2}^{n+1,+}+\langle\mu\rangle_{L,i}^{n+1,+}\langle\phi\rangle_{L,i}^{n+1,+}+\langle\mu\rangle_{R,i}^{n+1,+}\langle\phi\rangle_{R,i}^{n+1,+}+\left(\sigma_t^*+\frac{1}{c\Delta t}\right)h_i\langle\phi\rangle_{L,i}^{n+1,+} - \frac{h_i}{2}\left(\sigma_s^*+\sigma_a^*(1-f^*)\right)\left(\langle\phi\rangle_{L,i}^{n+1,+}+\langle\phi\rangle_{L,i}^{n+1,-}\right) = \frac{1}{2}h_i\sigma_a^*acf^*\left(\frac{2}{3}T_{L,i}^{4,n}+\frac{1}{3}T_{R,i}^{4,n}\right)+\frac{h_i}{c\Delta t}\langle\phi\rangle_{L,i}^{n,+} \quad (25)$$

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Once these linear equations have been solved for ϕ^{n+1}, a new estimate of T^{n+1} can be determined. To conserve energy, the same linearization used to solve the radiation equation must be used in the material energy equation. Substitution of Eq. (**??**) into the material energy equation yields

$$\rho c_v\frac{T^{n+1}-T^n}{\Delta t}=\sigma_a^*\phi^{n+1}-\left(\sigma_a^*(1-f)\phi^{n+1}+f\sigma_a^*acT^{4,n}\right), \quad (26)$$

which gives a temperature at the end of the time step as

$$T^{n+1}=\frac{f^*\sigma_a^*\Delta t}{\rho c_v}\left(\phi^{n+1}-caT^{n4}\right)+T^n, \quad (27)$$

This is how the IMC method estimates the temperature at the end of the time step, following the MC solve. Here, the LO radiation equations have taken the place of the Monte Carlo solve. To account for spatial dependence, the above equation can simply be evaluated using ϕ_L^{n+1} and T_L^* to get T_L^{n+1}.

Based on these equations, the algorithm for solving the LO system with constant f^* and cross sections over a cell is defined as

1. Guess T_L^* and T_R^*, typically using T^n.

2. Build the LO system based on the effective scattering $(1 - f^*)$ and emission terms (i.e., evaluation of Eq. (**??**)).
3. Solve the linearized LO system to produce an estimate for ϕ^{n+1}.
4. Evaluate a new estimate of the $T_{L,i}$ and $T_{R,i}$ at the end of the time step $\tilde{T}^{n+1}$ using Eq. (**??**).
5. $T^* \leftarrow \tilde{T}^{n+1}$.
6. Repeat 2-5 until $\tilde{T}^{n+1}$ and ϕ^{n+1} are converged.

Because of the chosen linearization, the convergence primarily takes place in the lagged material properties and factor f.