

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

Simon Bolding^a, Joshua Hansel^a, Jarrod D. Edwards^b, Jim E. Morel^a,
Robert B. Lowrie^c

^a*Department of Nuclear Engineering, 337 Zachry Engineering Center, TAMU 3133,
Texas A&M University, College Station, Texas, 77843*

^b*Phenomenology and Sensor Science Department, Sandia National Laboratory,
Albuquerque, NM*

^c*Computational Physics Group CCS-2, Los Alamos National Laboratory, P.O. Box 1663,
MS D413, Los Alamos, NM 87545*

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:

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

$$\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2) + \frac{\partial}{\partial x} (p) = \frac{\sigma_t}{c} \mathcal{F}_0, \quad (1b)$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x} [(E + p) u] = -\sigma_a c (aT^4 - \mathcal{E}) + \frac{\sigma_t u}{c} \mathcal{F}_0, \quad (1c)$$

$$\frac{1}{c} \frac{\partial \psi^+}{\partial t} + \frac{1}{\sqrt{3}} \frac{\partial \psi^+}{\partial x} + \sigma_t \psi^+ = \frac{\sigma_s}{4\pi} c \mathcal{E} + \frac{\sigma_a}{4\pi} a c T^4 - \frac{\sigma_t u}{4\pi c} \mathcal{F}_0 + \frac{\sigma_t}{\sqrt{3}\pi} \mathcal{E} u, \quad (1d)$$

$$\frac{1}{c} \frac{\partial \psi^-}{\partial t} - \frac{1}{\sqrt{3}} \frac{\partial \psi^-}{\partial x} + \sigma_t \psi^- = \frac{\sigma_s}{4\pi} c \mathcal{E} + \frac{\sigma_a}{4\pi} a c T^4 - \frac{\sigma_t u}{4\pi c} \mathcal{F}_0 - \frac{\sigma_t}{\sqrt{3}\pi} \mathcal{E} u, \quad (1e)$$

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, \mathcal{E} is the radiation energy density,

$$\mathcal{E} = \frac{2\pi}{c} (\psi^+ + \psi^-) , \quad (2)$$

\mathcal{F} is the radiation energy flux,

$$\mathcal{F} = \frac{2\pi}{\sqrt{3}} (\psi^+ - \psi^-) \quad (3)$$

and \mathcal{F}_0 is an approximation to the comoving-frame flux,

$$\mathcal{F}_0 = \mathcal{F} - \frac{4}{3}\mathcal{E}u . \quad (4)$$

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

$$\frac{\partial \mathcal{E}}{\partial t} + \frac{\partial \mathcal{F}}{\partial x} = \sigma_a c (aT^4 - \mathcal{E}) - \frac{\sigma_t u}{c} \mathcal{F}_0 , \quad (5a)$$

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:

$$\frac{1}{c^2} \frac{\partial \mathcal{F}}{\partial t} + \frac{1}{3} \frac{\partial \mathcal{E}}{\partial x} = -\frac{\sigma_t}{c} \mathcal{F}_0 . \quad (5b)$$

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

$$p = \rho e (\gamma - 1) , \quad (6a)$$

$$T = \frac{e}{c_v} , \quad (6b)$$

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

2. Solution method for nonlinear equations

2.1. Elimination of material equations

Within each solution time step, first the hydro variables are advected (either using local predicted fluxes or a Riemann solver). Then, a non-linear system must be solved. 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 affect the choice of Δt , the end time state, and the known source terms on the right hand side, which come from known previous states in time. The non-linear equations to be solved in this case are, neglecting spatial differencing indices,

$$\frac{\rho^{n+1} (u^{n+1,k} - u^*)}{\Delta t} = \frac{1}{2} \left[\sigma_t \frac{u}{c} \left(\mathcal{F} - \frac{4}{3} \mathcal{E} u \right) \right]^{n+1,k} + \frac{1}{2} \left[\sigma_t \frac{u}{c} \left(\mathcal{F} - \frac{4}{3} \mathcal{E} u \right) \right]^n \quad (7)$$

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

plus the S_2 equations. To simplify the algebra, define a source term Q_E for all the known, lagged quantities in the above equation as

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

First, Eq. (7) is solved for a new velocity, using lagged radiation energy and flux densities. For the initial solve, these can be taken at t_n . We then linearize the Planckian function about some temperature near T^{n+1} , denoted T^k . The linearized Planckian is

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

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:

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

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

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

Solution of the main equation for the desired quantity then gives

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

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).

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

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

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

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

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

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

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

The above expression can be substituted for the emission source in the S_2 equations, including 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). It is important to use this linearized equation to ensure energy conservation. This process can now be repeated until convergence, beginning with a solve of Eq. (7) with updated radiation quantities. Once the system is converged, the EOS can be used to update p^{n+1} .

2.2. Constructing sources for S_2 equations

Without spatial discretization, the S_2 equations can be written as