Handling the Radiation Source Term Numerically

1. Notation and Statement of the Problem

Let's start with some notation. In the lab frame, let the gas and radiation stress-energy tensors after advection and geometrical source terms have been applied be given by T'^{μ}_{ν} and R'^{μ}_{ν}, i.e., with primes on the symbols. Correspondingly, let the gas density and internal energy at this stage of the calculation be ρ', u', the gas four velocity in the lab frame be u'^{μ}_{g}, the radiation energy density be E'_r and the radiation frame four velocity in the lab frame be u'^{μ}_{r}. For simplicity, let us ignore the magnetic field.

We wish to apply the radiation source term G_ν and solve for the final values of the various quantities. Let us describe this final state without primes: T^{μ}_{ν}, R^{μ}_{ν}, ρ, u, u^{μ}_{g}, E_r, u^{μ}_{r}.

Since the continuity equation does not involve radiation, we have one invariant quantity:

$$\rho' u'^{0}_{g} = \rho u^{0}_{g} = \text{invariant}. \tag{1}$$

For the remaining eight quantities — u, u^i_g, E_r, u^i_r — we have the following eight equations:

$$T^{0}_{\nu} - T'^{0}_{\nu} = G_\nu \Delta t = -R^{0}_{\nu} + R'^{0}_{\nu}, \tag{2}$$

where Δt is the time step in the lab frame. The above version of the equations corresponds to an implicit computation, where the radiation source term G_ν is computed based on the unprimed final solution. In the easier explicit version, we would use G'_ν.

The source term is defined in the gas rest frame. For the implicit computation, we go to an orthonormal frame in which the gas is at rest. In this frame, which we identify with a "widehat", we have

$$\begin{aligned} \widehat{G}^{0} &= \kappa_{\rm abs}(\widehat{E} - 4\pi B), & (3)\\ \widehat{G}^{i} &= \chi_{\rm tot}\widehat{F}^{i}, & (4) \end{aligned}$$

where $\widehat{E}$ is the radiation energy density in the gas frame, and $\widehat{F}^i$ is the radiation flux vector in the same frame. The four-vector G_ν in eq (2) is calculated by transforming $\widehat{G}_\nu$ from the orthonormal gas frame to the lab frame.

2. Gas Frame vs Lab Frame

Consider the following set of equations in the gas frame,

$$\widehat{T}^{0}_{\nu} - \widehat{T}'^{0}_{\nu} = \widehat{G}_\nu \Delta\tau = -\widehat{R}^{0}_{\nu} + \widehat{R}'^{0}_{\nu}, \tag{5}$$

where $\Delta\tau$ corresponds to a small interval of the gas proper time. In the gas frame, we know that the gas four velocity takes the simple form $\widehat{u}_g^0 = 1$, $\widehat{u}_g^i = 0$. Thus, we can rewrite equations (5) more generally as

$$\widehat{T}_\nu^\mu - \widehat{T}_\nu'^\mu = \widehat{G}_\nu \widehat{u}_g^\mu \Delta\tau = -\widehat{R}_\nu^\mu + \widehat{R}_\nu'^\mu. \tag{6}$$

This equation is in covariant form, so it is equally valid in the lab frame:

$$T_\nu^\mu - T_\nu'^\mu = G_\nu u_g^\mu \Delta\tau = -R_\nu^\mu + R_\nu'^\mu. \tag{7}$$

Setting $\mu = 0$ in these equations and comparing with eqs (2), we see that they are identical provided

$$\Delta t = u_g^0 \Delta\tau, \tag{8}$$

i.e., just the standard Lorentz transformation of time between frames.

The point of the above exercise is simply to demonstrate that equations (2) and equations (5) are completely equivalent. We could solve all eight equations in the lab frame, or all eight equations in the gas frame, or solve the $\nu = 0$ pieces of (5) in the gas frame and the $\nu = i$ pieces of (2) in the lab frame, or any other combination of the equations.

3. Towards a More Stable Numerical Algorithm

Why is the previous analysis important? The source term $\widehat{G}_\nu$ has the nasty property that its time and space components can differ enormously in magnitude. Because of the very steep dependence of $\kappa_{\rm abs}$ on the gas temperature T_g ($\equiv p/\rho = (\Gamma - 1)u/\rho$), it is not unusual for $\kappa_{\rm abs}$ to be eight orders of magnitude smaller than $\chi_{\rm tot}$. This is no big deal in the fluid frame because the two opacities appear in different equations. The energy equation becomes even nicer if we follow the usual replacement trick

$$\widehat{T}_0^0 \to \widehat{T}_0^0 + \rho\widehat{u}_g^0, \qquad \widehat{T}_0'^0 \to \widehat{T}_0'^0 + \rho'\widehat{u}_g'^0. \tag{9}$$

Thus, the two energy equations in the gas frame are very well-behaved and should provide the necessary information to solve for u and E_r, while the six momentum equations will have the information to solve for the gas and radiation momentum densities. The latter could be done either in the lab frame or the fluid frame, but it is safest to solve the two energy equations in the fluid frame.

What is wrong with solving all the equations in the lab frame? Because $\widehat{G}_\nu$ is defined in the moving gas frame, by the time we transform to the lab frame, all the $\kappa_{\rm abs}$ and $\chi_{\rm tot}$ terms will get mixed together. If the gas is moving reasonably quickly, say $\beta_g \sim 0.1$, and

$\chi_{\rm tot}/\kappa_{\rm abs} \gg 1$, say 10^8, there will be a huge hit in precision. It is much better to avoid this hit by simply solving the energy equation in the gas frame.

Normally, even with this loss of precision, the Newton-Raphson method would be okay. It may limp a bit, but it would not produce a crazy solution. In the present case, we have a second problem. Because $\kappa_{\rm abs}$ has a weird temperature dependence, or equivalently u-dependence, when the value of u goes a little astray during the iteration, there is a chance for things to diverge rapidly. In RN's opinion, this is a particularly serious problem when one works in the lab frame, where $\chi_{\rm tot}$ mucks up the energy equation.

Here then is the recommendation:

1. When applying the radiation source term, either solve all eight equations in the fluid frame (eqs 5 with $\Delta\tau$ given by eq 8), or use the two energy equations in the fluid frame ($\nu = 0$ in eqs 5) and the six momentum equations in the lab frame ($\nu = i$ in eqs 2).

2. As a further safeguard, during the iterations, do not let the gas temperature T_g and the radiation temperature $T_r \equiv (\widehat{E}_r/a_{\rm rad})^{1/4}$ to cross each other. That is, make sure at each step of the Newton-Raphson that $(T_g - T_r)$ has the same sign as $(T'_g - T'_r)$. This may not be essential, but it will help a lot to tame the wild behavior of $\kappa_{\rm abs}$.

The above changes are likely to solve (again in RN's opinion) a large fraction of the current problems in HARMRAD. Even if the first recommendation does not meet with the approval of team members, there is nothing lost by introducing the second recommendation into the current code. It will certainly cause no harm, and it might already (even without following the first recommendation) solve a lot of problems.

A simpler but slightly inaccurate version of this approach, based on entropy, was described in a previous note.

4. Numerical Implementation

In terms of numerical implementation, note that the primed tensors, T'^{μ}_{ν} and R'^{μ}_{ν}, are already available. The eight unknowns are u, u^i_g, E_r, u^i_r. Given a set of values for these unknowns, we can calculate ρ, T^{μ}_{ν}, R^{μ}_{ν}.

Let us suppose we plan to work with the two energy equations in the fluid frame, viz.,

$$\widehat{T}^0_0 - \widehat{T}'^0_0 = -\kappa_{\rm abs}(\widehat{E} - 4\pi B)\Delta\tau = -\widehat{R}^0_0 + \widehat{R}'^0_0. \tag{10}$$

The term $\widehat{T}^0_0$ is very straightforward,

$$\widehat{T}^0_0 + \rho\widehat{u}^0_g = u + b^2/2, \tag{11}$$

where we have included the contribution of the magnetic energy density, the various other Ts and Rs are similarly easily calculated, e.g.,

$$\widehat{R}^0_0 = R^\mu_\nu u^\nu_g (u_g)_\mu, \quad \text{etc.}, \tag{12}$$

while $\widehat{E} = -\widehat{R}^0_0$. Thus it is possible to compute all the terms in the energy equations (10) without requiring tetrads or orthonormal frames.

While everything that has been written so far is in terms of eight unknowns and eight equations, actually there are effectively only four unknowns. This is because, once we write down T^μ_ν in terms of the four gas-primitives u, u^i_g, we can immediately calculate the radiation tensor R^μ_ν:

$$R^\mu_\nu = R'^\mu_\nu + T'^\mu_\nu - T^\mu_\nu, \tag{13}$$

and invert to obtain the radiation primitives. The converse is also true. Nevertheless, solving even the resulting four non-linear equations for the four unknowns is a major problem. In fact, when we include magnetic fields, there are additional unknowns and certain analytical simplifications that help in the pure hydro problem are lost.

A dumb, brute-force approach is to compute the local Jacobian of the non-linear equations via numerical derivatives and to use the Newton-Raphson method. Jon has developed more sophisticated schemes which reduce the nine-dimensional magnetized gas problem to five or even four dimensions. Moreover, by computing the Jacobian analytically, he expects the accuracy to be greatly improved. How well these ideas will translate to the fluid-frame version of the energy equations discussed here is unclear. One should probably try the basic brute-force method first before doing anything fancy.

5. Explicit vs Implicit Solution

It would be helpful to know when we should apply the full power of the implicit method and when it is sufficient to simply carry out an explicit time step. The following simplified analysis provides an answer.

Let us consider an explicit calculation. We assume that we have completed the advection and other non-radiative updates and have calculated the tensors T'^μ_ν and R'^μ_ν and the conserved density $\rho' u'^0_g$. Since in an explicit calculation everything is referenced to this base state, it is not necessary to retain primes, so we will drop the primes hereafter. Then, in the explicit approach, the updates to the two tensors are given by

$$\Delta T^0_\nu = G_\nu \Delta t = -\Delta R^0_\nu. \tag{14}$$

Equally well, we can write this in the fluid frame of the base state as

$$\Delta \widehat{T}^0_\nu = \widehat{G}_\nu \Delta \tau = -\Delta \widehat{R}^0_\nu. \tag{15}$$

In the fluid frame, the gas has density ρ (recall we decided to drop primes), internal energy u, pressure $p = (\Gamma - 1)u$. By definition, the gas is not moving. The radiation, of course, will in general be moving and will have an energy density $\widehat{E}$ and radiation flux $\widehat{F}^i$. Let us orient our axes so that the radiative flux is parallel to the 1-axis. As a result of the interaction between the gas and the radiation, the gas will be pushed in the 1-direction and will acquire a velocity $\Delta\beta_g$. Its internal energy, or temperature, will also change because of absorption or emission of radiation.

In the spirit of linearization, which is basic to the Newton-Raphson method, $\Delta\beta_g$ can be assumed to be small and higher order terms like $(\Delta\beta_g)^2$ can be ignored. Assuming further that ρ remains unchanged (I think this is okay but it bears thinking), we thus have very simple expressions for the components of $\Delta\widehat{T}^0_\nu$:

$$\Delta \widehat{T}^0_0 = \widehat{G}_0 \Delta\tau \quad \rightarrow \quad -\Delta u = -\kappa_{\rm abs}(\widehat{E} - 4\pi B)\Delta\tau, \tag{16}$$

$$\Delta \widehat{T}^0_1 = \widehat{G}_1 \Delta\tau \quad \rightarrow \quad (\rho + u + p)\Delta\beta_g = \chi_{\rm tot}\widehat{F}_1 \Delta\tau. \tag{17}$$

The solution for the shifts is

$$\Delta u = \kappa_{\rm abs}\Delta\tau(\widehat{E} - 4\pi B), \tag{18}$$

$$\Delta\beta_g = \chi_{\rm tot}\Delta\tau \left(\frac{\widehat{E}}{\rho + u + p}\right)\beta_r, \tag{19}$$

where we have assumed that the radiation frame moves slowly with respect to the gas frame and hence written the velocity β_r of this frame as

$$\beta_r = \widehat{F}_1 / \widehat{E}. \tag{20}$$

The two radiation equations are equally simple:

$$\Delta \widehat{R}^0_0 = -\widehat{G}_0 \Delta\tau \quad \rightarrow \quad \Delta\widehat{E} = -\kappa_{\rm abs}(\widehat{E} - 4\pi B)\Delta\tau, \tag{21}$$

$$\Delta \widehat{R}^0_1 = -\widehat{G}_1 \Delta\tau \quad \rightarrow \quad \Delta\widehat{F}_1 \equiv \widehat{E}\Delta\beta_r = -\chi_{\rm tot}\widehat{F}_1 \Delta\tau. \tag{22}$$

The quantity $\Delta\beta_r$ in the second equation is defined as

$$\Delta\beta_r \equiv \Delta\widehat{F}_1/\widehat{E}. \tag{23}$$

It is a measure of how much the radiation frame velocity is changed as a result of the explicit update to the solution. Solving the two radiation equations gives

$$\begin{aligned} \Delta\widehat{E} &= -\kappa_{\rm abs}\Delta\tau(\widehat{E} - 4\pi B), && (24) \\ \Delta\beta_r &= -\chi_{\rm tot}\Delta\tau\beta_r. && (25) \end{aligned}$$

We thus have the complete solution for the updates under the explicit scheme. Now we want to know whether this solution is safe and when it must be replaced by the more elaborate implicit solution. We use a physically motivated criterion to answer this.

The interaction between gas and radiation is basically a relaxation process. Consider first the energy equations. If the radiation energy density $\widehat{E}$ exceeds the blackbody energy density $4\pi B$, then the gas gets heated up and the radiation energy density decreases. The converse is similarly true. Thus, the two quantities $\widehat{E}$ and $4\pi B$ are pushed towards each other, as verified by looking at the signs of the solutions for Δu and $\Delta\widehat{E}$. Physically, because we are dealing with a relaxation process, $\widehat{E}$ and $4\pi B$ cannot cross each other. The explicit method, however, being a local linearized representation of the problem, knows nothing about this global constraint, so it will sometimes produce large shifts which cause the two energy densities to cross. We want to avoid this. Therefore, a simple criterion for the validity of the explicit solution is that it should not cause crossing. This requirement is quantified as follows.

Recall that the gas temperature is given by $T_g = (\Gamma - 1)u/\rho$. Thus, the shift in $4\pi B$ caused by the explicit step is

$$\Delta(4\pi B) = \Delta(a_{\rm rad}T_g^4) = \frac{16\pi B}{u}\Delta u. \tag{26}$$

The net shift in $(\widehat{E} - 4\pi B)$ is then estimated to be

$$|\Delta(\widehat{E} - 4\pi B)| = \kappa_{\rm abs}\Delta\tau\left(1 + \frac{16\pi B}{u}\right)(\widehat{E} - 4\pi B). \tag{27}$$

For stability of the explicit scheme, we want the left hand side to be no more than some fraction ζ (< 1) of $(\widehat{E} - 4\pi B)$. Thus, we obtain the following criterion:

$$\text{Criterion 1}: \qquad \kappa_{\rm abs}\Delta\tau\left(1 + \frac{16\pi B}{u}\right) < \zeta. \tag{28}$$

The momentum equation is again a relaxation process. If the radiation is moving towards the positive 1-direction ($\beta_r > 0$), then the gas acquires a positive velocity ($\Delta\beta_g > 0$), while the radiation velocity decreases ($\Delta\beta_r < 0$). The two frames thus approach each other, but they cannot cross. However, as in the previous case, the explicit scheme does not know about this condition. Therefore, a second criterion is that $\Delta\beta_g - \Delta\beta_r$ should be less than ζ times β_r. This gives the following second criterion:

$$\text{Criterion 2}: \qquad \chi_{\rm tot}\Delta\tau \left(1 + \frac{\widehat{E}}{\rho + u + p}\right) < \zeta. \tag{29}$$

When both criteria (28) and (29) are satisfied, we expect the explicit scheme to be well-behaved. However, if either or both are violated, we should switch to the implicit scheme.

What value of ζ should we choose? Any value less than unity is probably fine. However, we made several approximations in our analysis, so it may be good to be conservative. A value of $\zeta = 0.5$ is probably sufficient, while $\zeta = 0.1$ should be quite safe.

An interesting sidelight of the above analysis is that, apart from the obvious factors $\kappa_{\rm abs}\Delta\tau$ and $\chi_{\rm tot}\Delta\tau$, two other factors turn out to be important: $16\pi B/u$ and $\widehat{E}/(\rho+u+p)$. This gives a clue to the behavior of the equations. Consider the energy equation first. When $16\pi B \gg u$, the explicit shift acts primarily on the gas (through u) and has only a small effect on the radiation ($\widehat{E}$). In this limit, it is preferable to use u as our primary primitive variable and to solve for $\widehat{E}$ in terms of it, rather than the other way round. On the other hand, if $16\pi B \ll u$, then it is better to use $\widehat{E}$ as the primary primitive and treat u as a derived quantity. In the case of the momentum equation, the critical ratio is $\widehat{E}/(\rho+u+p)$. If $\widehat{E} \gg (\rho + u + p)$, there is a large velocity shift in the gas and a negligible velocity shift in the radiation. We should, therefore, treat β_g as our primary primitive. In the opposite limit, we should treat β_r as the primary primitive.