Constructing the finite-volume equations for cosmological FLD

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1 Base cosmological FLD equation

The radiation energy density, flux, and pressure tensor are related to the specific intensity moments via the relations

$$E_\nu = \frac{4\pi}{c} J_\nu = \frac{1}{c} \oint I_\nu \, d\Omega, \tag{1}$$

$$\mathbf{F}_\nu^i = 4\pi H_\nu^i = \oint \vec{n}^i I_\nu \, d\Omega, \tag{2}$$

$$\overline{\mathbf{P}}_\nu^{ij} = \frac{4\pi}{c} K_\nu^{ij} = \frac{1}{c} \oint \vec{n}^i \vec{n}^j I_\nu \, d\Omega, \tag{3}$$

where each of these are defined in proper, CGS units. For frequencies $\nu \in \mathbb{R}^+$, times $t \in \mathbb{R}$ and spatial locations $\mathbf{r} \in \mathbb{R}^3$, we denote the domain of these functions as $\bar{\Omega} = \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}^3$. Then $I_\nu : \bar{\Omega} \to \mathbb{R}$ is the specific radiation intensity,$E_\nu : \bar{\Omega} \to \mathbb{R}$ is the radiation energy density, $\mathbf{F}_\nu : \bar{\Omega} \to \mathbb{R}^3$ is the radiation energy flux, and $\overline{\mathbf{P}}_\nu : \bar{\Omega} \to \mathbb{R}^{3\times 3}$ is the radiation pressure tensor.

The moment equations for a generalized fluid coupled with a radiation fluid for a cosmological medium are as follows (c.f. [1, 3]). The zeroth moment of the Boltzmann equation provides an evolution equation for the radiation energy density,

$$\partial_t E_\nu + \nabla \cdot (E_\nu \mathbf{v}_b) + \nabla \cdot \mathbf{F}_\nu + \overline{\mathbf{P}}_\nu : (\nabla \mathbf{v}_b) + \frac{3\dot{a}}{a} E_\nu - \frac{\nu \dot{a}}{a} \partial_\nu E_\nu = \eta_\nu - c\kappa_\nu E_\nu. \tag{4}$$

Here, $\eta_\nu : \bar{\Omega} \to \mathbb{R}$ is the emissivity source (g cm^{-1} s^{-2}). $\kappa_\nu : \bar{\Omega} \to \mathbb{R}$ is the combined opacity (cm^{-1}) due to the elemental species, and is computed as

$$\kappa_\nu = \sum_{i=1}^{N_{\text{chem}}} \sigma_i(\nu) \, \mathtt{n}_i, \tag{5}$$

where $\sigma_i(\nu)$ is the cross-section of the elemental species $\mathtt{n}_i$. We note that in the above equation (and the remainder of this document), the spatial derivatives denoted by ∇ are taken with respect to the proper position, $\mathbf{r}$.

Similarly, the first moment of the Boltzmann equation provides an evolution equation for the radiation energy flux,

$$\partial_t \mathbf{F}_\nu + \nabla \left(\mathbf{F}_\nu \cdot \mathbf{v}_b \right) + c^2 \nabla \cdot \overline{\mathbf{P}}_\nu + \left(\mathbf{F}_\nu \cdot \nabla \right) \mathbf{v}_b + \frac{3\dot{a}}{a} \mathbf{F}_\nu - \frac{\nu \dot{a}}{a} \partial_\nu \mathbf{F}_\nu = -c\kappa_\nu \mathbf{F}_\nu. \tag{6}$$

1.1 Flux Limited Diffusion approximation

For a flux limited diffusion (FLD) approximation, the radiative flux vector is computed as a function of the energy density gradient through a parameterization,

$$\mathbf{F}_\nu = -D\,\nabla E_\nu, \tag{7}$$

where $D : \bar{\Omega} \to \mathbb{R}^{3\times 3}$ is the *flux limiter* (cm^2 s^{-1}) that depends on both the opacity κ_ν, and the radiation energy density E_ν.

Using the FLD approximation, the equation (6) may be ignored, and the zeroth moment equation (4) becomes

$$\begin{aligned}\partial_t E_\nu + \nabla\cdot(E_\nu \mathbf{v}_b) - \nabla\cdot(D\,\nabla E_\nu) - \frac{1}{c}\left(\nabla(D\,\nabla E_\nu)\right) : (\nabla \mathbf{v}_b) + \frac{3\dot{a}}{a}E_\nu - \frac{\nu\dot{a}}{a}\partial_\nu E_\nu \\ = \eta_\nu - c\kappa_\nu E_\nu,\end{aligned} \tag{8}$$

where we have used the FLD-based approximation of the radiation pressure as $\overline{\mathbf{P}}_\nu = \frac{1}{c}\nabla\mathbf{F}_\nu = \frac{1}{c}\nabla\left(D\,\nabla E_\nu\right)$. Note that in general, $\overline{\mathbf{P}}_\nu$ is non-symmetric, due to the spatial dependence of the flux-limiter D. The equation (8) is an equation defining the scalar-valued variable E_ν, that may either be solved independently, or coupled with the elemental densities $\mathtt{n}_i$ and hydrodynamic quantities of the the fluid energy e, velocity $\mathbf{v}_b$ and density ρ_b.

For conditions that allow omission of the radiation pressure term, the zeroth moment equations corresponding to (4) can be simplified to

$$\partial_t E_\nu + \nabla\cdot(E_\nu \mathbf{v}_b) - \nabla\cdot(D\,\nabla E_\nu) + \frac{3\dot{a}}{a}E_\nu - \frac{\nu\dot{a}}{a}\partial_\nu E_\nu = \eta_\nu - c\kappa_\nu E_\nu. \tag{9}$$

The equation (9) is a reaction-advection-diffusion equation, that is again a function of the energy density E_ν, though here is parabolic in nature, in that it describes a diffusion-like radiation transport.

Lastly, since Enzo performs a second-order-accurate piecewise parabolic algorithm for hydrodynamic advection, with passive advection of other density-like quantities (including E_ν), in considering a new solver for evolving only the radiation field, we may consider the simpler reaction-diffusion equation

$$\partial_t E_\nu - \nabla\cdot(D_\nu\,\nabla E_\nu) + \frac{3\dot{a}}{a}E_\nu - \frac{\nu\dot{a}}{a}\partial_\nu E_\nu = \eta_\nu - c\kappa_\nu E_\nu. \tag{10}$$

1.2 Single Group Approximation

The radiation energy density equation (10) may be discretized in frequency space by integrating the energy density (or the flux) between two frequencies, namely ν_{g+1} and ν_g. This forms one radiation energy 'group', which provides an average estimate of the moment quantity as:

$$E_g(t,\mathbf{r}) = \frac{1}{\nu_{g+1}-\nu_g}\int_{\nu_g}^{\nu_{g+1}} E_\nu(\nu,t,\mathbf{r})\,\mathrm{d}\nu, \quad g = 1,\ldots,N_g.$$

We take this approximation further, through going to the limit of a single grey radiation energy density E (g cm^{-1} s^{-2}), by integrating in frequency space from the ionization threshold of hydrogen, ν_{HI}, to infinity. We accomplish this by assuming the existence of a given radiation frequency spectrum, $\chi_E(\nu)$, such that the frequency-dependent radiation energy density may be written in the form $E_\nu(\nu,t,\mathbf{r}) = \tilde{E}(t,\mathbf{r})\,\chi_E(\nu)$. We note that this is a rather strong assumption, since it requires that all radiation throughout the space-time domain has the same frequency spectrum. With this, we define a single "grey" radiation energy density,

$$E(t,\mathbf{r}) = \int_{\nu_0}^{\infty} E_\nu(\nu,t,\mathbf{r})\mathrm{d}\nu = \tilde{E}(t,\mathbf{r})\int_{\nu_0}^{\infty}\chi_E(\nu)\mathrm{d}\nu. \tag{11}$$

We note that this approximation is valid only when the assumed frequency spectrum is integrable, i.e. if it is defined only over a limited frequency bandwidth, or if it scales with frequency as $E_\nu \propto \nu^{-\beta_q}$ for some $\beta_q > 1$. The latter case holds for quasar and stellar type spectra.

Application of such an integration in equation (10) yields the following "grey" radiation diffusion equation:

$$\partial_t E - \nabla \cdot (D\,\nabla E) + \alpha \frac{\dot{a}}{a} E = \eta - c\kappa E. \tag{12}$$

In the above equation, the term $-\frac{\nu \dot{a}}{a}\partial_\nu E_\nu$ is replaced (through integration by parts) with a contribution to the cosmology expansion term by an amount equal to $\frac{\dot{a}}{a}E$. However, if the assumed spectrum $\chi_E(\nu)$ is monochromatic, i.e. $\chi_E(\nu) = \delta_{\nu_0}(\nu)$, then integration by parts does not yield this contribution. Hence, we use the parameter α to account for this difference, in that for monochromatic radiation spectra we use $\alpha = 3$, but for all other spectra we use $\alpha = 4$.

We note that through using the integrated radiation energy density E, since it is based on an *a-priori* defined function $\chi_E(\nu)$, we may compute all frequency-space integrals based on E_ν at initialization of the radiation module, and store the integrated weights for reuse throughout the simulation. This pertains to the frequency-integrated opacity κ, in which

$$\begin{aligned} c\,\kappa\,E &= c\int_{\nu_0}^{\infty} \kappa_\nu\, E_\nu \,\mathrm{d}\nu, \\ \implies & \\ \kappa &= \frac{\int_{\nu_0}^{\infty} \kappa_\nu\, E_\nu \,\mathrm{d}\nu}{\int_{\nu_0}^{\infty} E_\nu \,\mathrm{d}\nu} = \frac{\sum_{i=1}^{N_{\mathrm{chem}}} \mathtt{n}_i \int_{\nu_i}^{\infty} \chi_E\, \sigma_{\mathtt{n}_i}\,\mathrm{d}\nu}{\int_{\nu_0}^{\infty} \chi_E \,\mathrm{d}\nu}. \end{aligned} \tag{13}$$

Similarly, we may compute the integrated photoionization rate Γ_i^{ph} as

$$\Gamma_i^{ph} = c\int_{\nu_i}^{\infty} \frac{\sigma_{\mathtt{n}_i} E_\nu}{h\nu}\,\mathrm{d}\nu = \frac{cE\int_{\nu_i}^{\infty} \frac{\chi_E\,\sigma_{\mathtt{n}_i}}{\nu}\,\mathrm{d}\nu}{h\int_{\nu_0}^{\infty}\chi_E\,\mathrm{d}\nu}.$$

We note that the above two quantities, and in fact all quantities involving the frequency integrated radiation energy density, may be written in terms of

$$\int_{\nu_0}^{\infty} \chi_E\,\mathrm{d}\nu, \qquad \int_{\nu_i}^{\infty} \chi_E\,\sigma_{\mathtt{n}_i}\,\mathrm{d}\nu, \quad \text{and} \quad \int_{\nu_i}^{\infty} \frac{\chi_E\,\sigma_{\mathtt{n}_i}}{\nu}\,\mathrm{d}\nu. \tag{14}$$

Since these integrals depend only on the *a-priori* defined functions χ_E and $\sigma_{\mathtt{n}_i}$, we may compute these once at initialization and reuse them throughout any grey FLD-based simulation. To this end, we consider the integral change of variables defined through introduction of $\omega = \nu^{-1}$:

$$\begin{aligned} \int_{\nu_0}^{\infty} f(\nu)\,\mathrm{d}\nu &= \nu_0 \int_0^1 \frac{1}{\omega^2} f\left(\frac{\nu_0}{\omega}\right)\mathrm{d}\omega = \nu_0 \sum_{i=1}^{s} \int_{\omega_{i-1}}^{\omega_i} \frac{1}{\omega^2} f\left(\frac{\nu_0}{\omega}\right)\mathrm{d}\omega \\ &\approx \nu_0 \sum_{i=1}^{s} \frac{\omega_i - \omega_{i-1}}{6}\left[\frac{1}{\omega_{i-1}^2} f\left(\frac{\nu_0}{\omega_{i-1}}\right) + \frac{1}{(\omega_{i-1}+\omega_i)^2} f\left(\frac{2\nu_0}{\omega_{i-1}+\omega_i}\right) + \frac{1}{\omega_i^2} f\left(\frac{\nu_0}{\omega_i}\right)\right], \end{aligned} \tag{15}$$

where we have partitioned the interval $(0,1)$ into s subintervals, $\omega_0 < \omega_1 < \ldots < \omega_s$. Since the integrand does not exist at either of the points 0 or 1, we choose $\omega_0 = \varepsilon$ and $\omega_s = 1-\varepsilon$, pick a regular spacing $\omega_i - \omega_{i-1} = 1/s$, and choose $s = 10000$ in order to reduce the error in the numerical integration to $\mathcal{O}(\varepsilon + 1/s^4)$.

Moreover, in the case of a grey radiation energy field, we may consider a "grey" emissivity through integrating $\eta_\nu(\nu, t, \mathbf{r})$ over $\nu \in (\nu_0, \infty)$ to determine its single-group approximation

$$\eta(t, \mathbf{r}) = \int_{\nu_0}^{\infty} \eta_\nu(\nu, t, \mathbf{r})\,\mathrm{d}\nu. \tag{16}$$

We note that this approach implicitly assumes that the spectrum of η_ν matches that of E_ν.

1.3 Flux Limiter

In the grey flux-limited diffusion approximation (12), the role of the flux limiter D is one of providing a continuous transition between the isotropic and free-streaming limits. To this end, we consider the flux limiter to be of the form,

$$D(\kappa, E) = \begin{bmatrix} D_1(\kappa, E) & 0 & 0 \\ 0 & D_2(\kappa, E) & 0 \\ 0 & 0 & D_3(\kappa, E) \end{bmatrix},$$

where we employ a limiter of the form [2]:

$$D_i(\kappa, E) = \min\left\{c\left(9\kappa_f^2 + R_i^2\right)^{-1/2}, D_{\max}\right\}, \quad i = 1, 2, 3, \tag{17}$$

$$R_i = \max\left\{\frac{|\partial_{\mathbf{r}_i} E|}{E_f}, R_{\min}\right\}. \tag{18}$$

Here, the spatial derivative within R is computed at the computational face adjoining two neighboring finite-volume cells, as will be elaborated on further in section 4. We enforce bounds on D_i and R_i to ensure numerical stability due to floating-point arithmetic error, given by $D_{\max} = \infty$ and $R_{\min} = 10^{-20} l_{\text{unit}}^{-1}$, with l_{unit} the length non-dimensionalization factor in the simulation (see the next section). Moreover, the face-centered radiation energy density and opacity are computed using the arithmetic and harmonic means, respectively,

$$E_f = \frac{E_1 + E_2}{2}, \qquad \kappa_f = \frac{2\kappa_1\kappa_2}{\kappa_1 + \kappa_2},$$

where here E_1 and E_2 are the two values of E in the cells adjacent to the face, with κ_1 and κ_2 defined similarly.

2 Units in Enzo cosmology

When run with cosmological expansion enabled, Enzo modifies the units of each internal field throughout the simulation to account for cosmological expansion. We define the comoving position $\mathbf{x}$ through the relationship $\mathbf{r} = l_{\text{unit}}\mathbf{x} \propto a\mathbf{x}$ (specific details are below in equation (22)), where a is the cosmological expansion factor. This is a time-dependent (equivalently, redshift-dependent) factor, satisfying the relationship

$$z = \frac{1}{a} - 1, \tag{19}$$

where z is the current (time-dependent) redshift. We note that since z decreases as time proceeds, a increases as a function of time, since

$$a = \frac{1}{1+z}. \tag{20}$$

Enzo then defines the non-dimensionalization factors:

$$\rho_{\text{unit}} = (1.88 \times 10^{-29})\Omega_{mn} H_{cn}^2 (1+z)^3, \tag{21}$$

$$l_{\text{unit}} = \frac{(3.086 \times 10^{24}) L_c}{H_{cn}(1+z)} \qquad \left(\text{i.e.} \quad l_{\text{unit}} = \frac{(3.086 \times 10^{24}) L_c}{H_{cn}} a\right), \tag{22}$$

$$t_{\text{unit}} = \frac{2.52 \times 10^{17}}{\Omega_{mn}^{1/2} H_{cn} (1+z_I)^{3/2}}, \tag{23}$$

$$v_{\text{unit}} = (1.225 \times 10^7) L_c \sqrt{\Omega_{mn}(1+z_I)}, \tag{24}$$

$$a_{\text{unit}} = (1+z_I)^{-1}. \tag{25}$$

Here $a = a_{\rm unit}\tilde{a}$, where $\tilde{a}$ is Enzo's normalized value, Ω_{mn} is Enzo's `OmegaMatterNow` parameter, H_{cn} is Enzo's `HubbleConstantNow` parameter, z_I is Enzo's `InitialRedshift` parameter, and L_c is Enzo's `ComovingBoxSize` parameter. As a result, Enzo actually computes the current redshift via the formula

$$z = \frac{1+z_I}{\tilde{a}} - 1. \tag{26}$$

We note that under these definitions, $v_{\rm unit} \neq l_{\rm unit}/t_{\rm unit}$, since

$$\begin{aligned}\frac{l_{\rm unit}}{t_{\rm unit}} &= \frac{(3.086\times10^{24})L_c\left(\Omega_{mn}^{1/2}H_{cn}(1+z_I)^{3/2}\right)}{H_{cn}(1+z)\,(2.52\times10^{17})} \\ &= (1.2246\times10^{7})L_c\sqrt{\Omega_{mn}(1+z_I)}\frac{(1+z_I)}{(1+z)},\end{aligned}$$

which differs from $v_{\rm unit}$ both in the precision of the leading constant (minor difference) and also by a factor of $(1+z_I)/(1+z)$, that grows in magnitude as time proceeds, especially for simulations having large initial redshift (major difference).

With these units defined, we may also consider a unit normalization factor for radiation energy density, that can be defined as either

$$\rho_{\rm unit}v_{\rm unit}^2, \quad \text{or} \quad \rho_{\rm unit}\frac{l_{\rm unit}^2}{t_{\rm unit}^2},$$

since both constitute the correct CGS units. However, since in cosmological simulations $v_{\rm unit} \neq l_{\rm unit}/t_{\rm unit}$, these two definitions are not the same. We choose the first of these,

$$E_{\rm unit} = \rho_{\rm unit}v_{\rm unit}^2. \tag{27}$$

3 Recasting to comoving, normalized form

Our equations (12) and (17)-(18) are valid in proper CGS units, whereas Enzo's fields are stored in comoving, normalized form. Specifically, the terms in our equations relate to Enzo's comoving, normalized terms in the following manner:

- $\rho_b = \rho_{\rm unit}\tilde{\rho}_b$, where ρ_b is the proper, CGS density, and $\tilde{\rho}_b$ is Enzo's comoving, normalized density value,
- $\mathbf{v}_b = v_{\rm unit}\tilde{\mathbf{v}}_b$, where $\mathbf{v}_b$ is the proper peculiar baryonic CGS velocity, and $\tilde{\mathbf{v}}_b$ is Enzo's comoving, normalized velocity value,
- $e = v_{\rm unit}^2\tilde{e}$, where e is the proper baryonic energy per unit mass, and $\tilde{e}$ is Enzo's comoving, normalized energy value,
- $E = E_{\rm unit}\tilde{E}$, where E is the proper, CGS radiation energy, and $\tilde{E}$ is Enzo's comoving, normalized radiation energy value,
- $a = a_{\rm unit}\tilde{a}$, as described above in equation (25),
- $\dot{a} = (a_{\rm unit}/t_{\rm unit})\,\dot{\tilde{a}}$, where $\dot{a}$ is the true cosmological expansion rate, and $\dot{\tilde{a}}$ is Enzo's normalized value,
- $\mathbf{r} = l_{\rm unit}\mathbf{x}$, where $\mathbf{r}$ is the proper, CGS position, and $\mathbf{x}$ is Enzo's comoving normalized position,
- $t = t_{\rm unit}\tilde{t}$, where t is the CGS time, and $\tilde{t}$ is Enzo's normalized time,
- $\kappa = \tilde{\kappa}\kappa_{\rm unit}$, where κ is the proper, CGS opacity, $\tilde{\kappa}$ is Enzo's normalized value, and $\kappa_{\rm unit} \propto l_{\rm unit}^{-1}$.

We also note that in order for us to convert our equations for the proper CGS radiation energy (E) to the normalized, comoving radiation energy density ($\tilde{E}$) we must consider how our time derivative must be modified. Specifically, since $E = E_{\rm unit}\tilde{E}$, then by the product rule,

$$\partial_t E = \partial_t \left(E_{\rm unit}\tilde{E} \right) = E_{\rm unit}\, \partial_t \tilde{E} + \tilde{E}\, \partial_t E_{\rm unit}.$$

Due to our choice of $E_{\rm unit} = \rho_{\rm unit} v_{\rm unit}^2 \propto (1+z)^3$, we then have

$$\partial_t E_{\rm unit} = \frac{3\, E_{\rm unit}\, \partial_t z}{1+z}.$$

Moreover, because $z = \frac{1}{a} - 1$ we have $\partial_t z = -\frac{\dot{a}}{a^2}$, and since $a = \frac{1}{1+z}$, this becomes

$$\partial_t E_{\rm unit} = -3 E_{\rm unit} \frac{\dot{a}}{a}.$$

As a result, we have

$$\begin{aligned} \partial_t E &= E_{\rm unit}\, \partial_t \tilde{E} - 3 E_{\rm unit} \frac{\dot{a}}{a} \tilde{E} \\ &= E_{\rm unit}\, \partial_t \tilde{E} - 3 \frac{\dot{a}}{a} E, \end{aligned}$$

which will cancel a portion of the term $\alpha \frac{\dot{a}}{a} E$ in the equation (12). Specifically, after dividing through by $E_{\rm unit}$ and canceling like terms, the equation (12) may instead be written in terms of the comoving, normalized radiation energy density:

$$\partial_t \tilde{E} - \nabla \cdot \left(D\, \nabla \tilde{E} \right) + \tilde{\alpha} \frac{\dot{a}}{a} \tilde{E} = \frac{\eta}{E_{\rm unit}} - c\kappa \tilde{E}, \tag{28}$$

where now for monochromatic radiation spectra $\tilde{\alpha} = 0$ and otherwise $\tilde{\alpha} = 1$.

Similarly, since the proper position changes as a function of time, then we may consider spatial differentiation with respect to the normalized comoving position $\mathbf{x}$. Since

$$\mathbf{r} = l_{\rm unit}\mathbf{x} \quad \Longleftrightarrow \quad \mathbf{x} = \frac{\mathbf{r}}{l_{\rm unit}},$$

then the chain rule dictates that

$$\frac{\partial}{\partial \mathbf{r}} \;=\; \frac{\partial \mathbf{x}}{\partial \mathbf{r}} \frac{\partial}{\partial \mathbf{x}} \;=\; \frac{1}{l_{\rm unit}} \frac{\partial}{\partial \mathbf{x}}.$$

We therefore denote the comoving, normalized differentiation operator as $\tilde{\nabla}$, such that

$$\nabla = \frac{1}{l_{\rm unit}} \tilde{\nabla}.$$

Resultingly, upon converting to comoving, normalized units, we have the equation

$$\partial_t \tilde{E} - \frac{1}{l_{\rm unit}^2} \tilde{\nabla} \cdot \left(D\, \tilde{\nabla} \tilde{E} \right) + \tilde{\alpha} \frac{\dot{a}}{a} \tilde{E} = \frac{\eta}{E_{\rm unit}} - c\kappa \tilde{E}. \tag{29}$$

Similarly, we may consider time differentiation with respect to our normalized time value, $\tilde{t}$:

$$\frac{\partial}{\partial t} \;=\; \frac{\partial \tilde{t}}{\partial t} \frac{\partial}{\partial \tilde{t}} \;=\; \frac{1}{t_{\rm unit}} \frac{\partial}{\partial \tilde{t}},$$

resulting in the equation

$$\partial_{\tilde{t}} \tilde{E} - \frac{t_{\rm unit}}{l_{\rm unit}^2} \tilde{\nabla} \cdot \left(D\, \tilde{\nabla} \tilde{E} \right) + \tilde{\alpha} \frac{t_{\rm unit} \dot{a}}{a} \tilde{E} = \frac{t_{\rm unit} \eta}{E_{\rm unit}} - t_{\rm unit} c\kappa \tilde{E}. \tag{30}$$

Lastly, we will convert the equation (29) so that it depends only on Enzo's normalized variables, $\tilde{t}$, $\tilde{E}$, $\tilde{a}$, $\dot{\tilde{a}}$ and $\tilde{\kappa}$. To this end, we expand each variable in terms of its normalized value and unit factor,

$$\partial_{\tilde{t}}\tilde{E} - \frac{t_{\rm unit}}{l_{\rm unit}^2}\tilde{\nabla}\cdot\left(D\,\tilde{\nabla}\tilde{E}\right) + \tilde{\alpha}\frac{t_{\rm unit}a_{\rm unit}\dot{\tilde{a}}}{t_{\rm unit}a_{\rm unit}\tilde{a}}\tilde{E} = \frac{t_{\rm unit}\eta}{E_{\rm unit}} - t_{\rm unit}\kappa_{\rm unit}c\tilde{\kappa}\tilde{E}$$

$$\Leftrightarrow \tag{31}$$

$$\partial_{\tilde{t}}\tilde{E} - \frac{t_{\rm unit}}{l_{\rm unit}^2}\tilde{\nabla}\cdot\left(D\,\tilde{\nabla}\tilde{E}\right) + \tilde{\alpha}\frac{\dot{\tilde{a}}}{\tilde{a}}\tilde{E} = \frac{t_{\rm unit}\eta}{E_{\rm unit}} - t_{\rm unit}\kappa_{\rm unit}\,c\,\tilde{\kappa}\tilde{E}, \tag{32}$$

where we compute the limiter as

$$D_i(\tilde{\kappa},\tilde{E}) = \min\left\{c\left(9\kappa_f^2 + R_i^2\right)^{-1/2}, D_{\rm max}\right\}, \quad i=1,2,3, \tag{33}$$

$$R_i = \max\left\{\frac{|\partial_{\mathbf{x}_i}\tilde{E}|}{l_{\rm unit}\tilde{E}_f}, R_{\rm min}\right\}, \tag{34}$$

with

$$\tilde{E}_f = \frac{\tilde{E}_1+\tilde{E}_2}{2}, \qquad \kappa_f = \frac{2\tilde{\kappa}_1\tilde{\kappa}_2}{\tilde{\kappa}_1+\tilde{\kappa}_2}\kappa_{\rm unit}, \tag{35}$$

where again $\tilde{E}_1$ and $\tilde{E}_2$ are the two values of $\tilde{E}$ in the cells adjacent to the face, as elaborated on in the next section.

4 Finite volume PDE approximation

On a uniform (i.e. non-AMR) mesh with comoving grid spacings Δx, Δy and Δz, we define the finite volume cell centers at the grid points in comoving, normalized units as:

$$\begin{aligned}\mathbf{x}_{i,j,k} &= [\,x_i,\,y_j,\,z_k\,],\\ x_i &= \left(i+\tfrac{1}{2}\right)\Delta x,\\ y_j &= \left(j+\tfrac{1}{2}\right)\Delta y,\\ z_k &= \left(k+\tfrac{1}{2}\right)\Delta z.\end{aligned}$$

Enzo's data arrays contain the discrete values of each field over the simulation volume at each of these grid points. More specifically, Enzo uses three-dimensional data arrays to store these discretized solution values at specific points in time. We denote $\tilde{E}^n_{i,j,k}$ as our approximation to the comoving and normalized solution at the normalized time $\tilde{t}_n$ and at the comoving normalized spatial location $\mathbf{x}_{i,j,k}$ (and do similarly for the other field data). We must therefore consider how to discretize the space and time derivatives of our equation (32) so that it depends on only these discrete data values.

We first separate the space and time discretizations. First, we discretize in time using a one-step θ-method. Introducing the notation

$$\mathcal{D}(\tilde{E},\tilde{\kappa},\eta,\tilde{a},\dot{\tilde{a}}) = \frac{t_{\rm unit}}{l_{\rm unit}^2}\tilde{\nabla}\cdot\left(D\,\tilde{\nabla}\tilde{E}\right) - \tilde{\alpha}\frac{\dot{\tilde{a}}}{\tilde{a}}\tilde{E} + \frac{t_{\rm unit}\eta}{E_{\rm unit}} - t_{\rm unit}\kappa_{\rm unit}\,c\,\tilde{\kappa}\tilde{E},$$

and denoting $\tilde{E}^n$ as our approximation to the spatially continuous solution at time $\tilde{t}_n$, the θ-method may be written as

$$\tilde{E}^{n+1} - \tilde{E}^n = \theta\Delta\tilde{t}\mathcal{D}(\tilde{E}^{n+1},\tilde{\kappa}^{n+1},\eta^{n+1},\tilde{a}^{n+1},\dot{\tilde{a}}^{n+1}) + (1-\theta)\Delta\tilde{t}\mathcal{D}(\tilde{E}^n,\tilde{\kappa}^n,\eta^n,\tilde{a}^n,\dot{\tilde{a}}^n), \tag{36}$$

where in the first $\mathcal{D}$ term we lag the implicit dependence of the solution on the flux limiter D^{n+1} to the previous time, D^n to result in a linearly implicit system of equations.

We must similarly apply our finite-volume spatial discretization of the operator $\mathcal{D}$. For the discretized equation centered at the comoving normalized position $\mathbf{x}_{i,j,k}$, we have

$$\tilde{E}^{n+1}_{i,j,k} - \tilde{E}^{n}_{i,j,k} = \theta\Delta\tilde{t}\mathcal{D}^{n+1}_{i,j,k} + (1-\theta)\Delta\tilde{t}\mathcal{D}^{n}_{i,j,k}, \tag{37}$$

where

$$\begin{aligned}
\mathcal{D}_{i,j,k} = &\frac{t_{\rm unit}}{l^2_{\rm unit}\Delta x^2}\left(D_{i+1/2,j,k}\left(\tilde{E}_{i+1,j,k}-\tilde{E}_{i,j,k}\right) - D_{i-1/2,j,k}\left(\tilde{E}_{i,j,k}-\tilde{E}_{i-1,j,k}\right)\right) \\
&+ \frac{t_{\rm unit}}{l^2_{\rm unit}\Delta y^2}\left(D_{i,j+1/2,k}\left(\tilde{E}_{i,j+1,k}-\tilde{E}_{i,j,k}\right) - D_{i,j-1/2,k}\left(\tilde{E}_{i,j,k}-\tilde{E}_{i,j-1,k}\right)\right) \\
&+ \frac{t_{\rm unit}}{l^2_{\rm unit}\Delta z^2}\left(D_{i,j,k+1/2}\left(\tilde{E}_{i,j,k+1}-\tilde{E}_{i,j,k}\right) - D_{i,j,k-1/2}\left(\tilde{E}_{i,j,k}-\tilde{E}_{i,j,k-1}\right)\right) \\
&- \tilde{\alpha}\frac{\dot{\tilde{a}}}{\tilde{a}}\tilde{E}_{i,j,k} + \frac{t_{\rm unit}\eta_{i,j,k}}{E_{\rm unit}} - t_{\rm unit}\kappa_{\rm unit}\, c\,\tilde{\kappa}_{i,j,k}\tilde{E}_{i,j,k},
\end{aligned} \tag{38}$$

and where, following equations (33)-(35), we similarly discretize the limiter as, e.g.

$$\begin{aligned}
D_{i+1/2,j,k}(\tilde{E},\kappa) &= \min\left\{c\left(9\kappa^2_{i+1/2,j,k} + R^2_{i+1/2,j,k}\right)^{-1/2}, D_{\max}\right\}, \\
R_{i+1/2,j,k} &= \max\left\{\frac{2}{l_{\rm unit}\Delta x}\frac{|\tilde{E}_{i+1,j,k}-\tilde{E}_{i,j,k}|}{\tilde{E}_{i+1,j,k}+\tilde{E}_{i,j,k}}, R_{\min}\right\}, \\
\kappa_{i+1/2,j,k} &= \frac{2\tilde{\kappa}_{i+1,j,k}\tilde{\kappa}_{i,j,k}}{\tilde{\kappa}_{i+1,j,k}+\tilde{\kappa}_{i,j,k}}\kappa_{\rm unit}.
\end{aligned} \tag{39}$$

We note that in many of the above factors, the unit values change as a function of time. As a result, all quantities are converted using the unit evaluated at the appropriate time step, t_{n+1} or t_n.

References

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