Future FLD in Enzo

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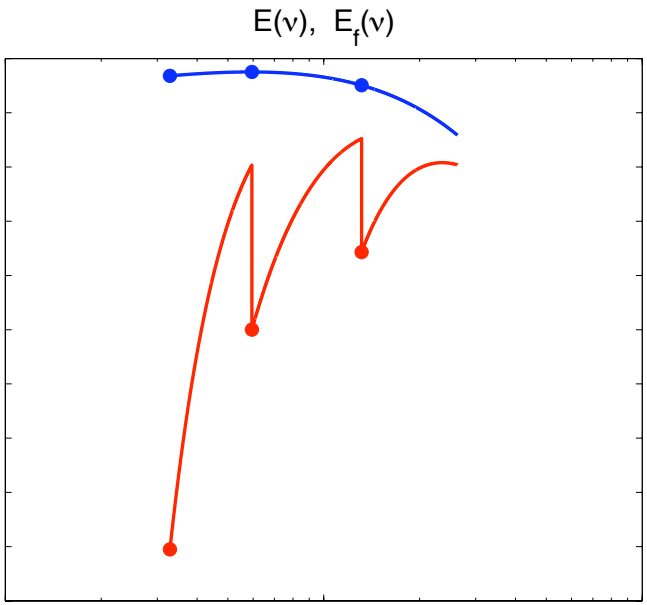
Multi-Frequency Radiation Transport

For reionization, elements absorb radiation at different frequencies. For primordial gases, important frequencies include the ionization thresholds of HI, HeI and HeII (13.6, 24.6, 54.4).

Frequencies above these thresholds participate in ionization (HI→HII, HeI→HeII→HeIII). Hence, typical spectra look like:



In other words, the spectrum is smooth except at ionization thresholds, where it experiences singularities due to absorption.

Multi-Frequency RT Approximation

Traditional MF codes discretize ν-space into a large number of bins $\nu_0 < \nu_1 < \ldots < \nu_N$, and assume a piecewise constant/linear profile.

Following [1-2], we capture these jumps directly in the approximation:

$$E(\nu, x, t) = E_f(x, t) \exp\left(\sum_{i=1}^{3} c_i \sigma_i(\nu)\right),$$

where E_f is an optically-thin radiation density, $\sigma_i(\nu)$ is the cross-section of species i, and c_i are expansion coefficients that satisfy

$$\begin{aligned} E(\nu_1, x, t) &= E_1(x, t), \\ E(\nu_2, x, t) &= E_2(x, t), \\ E(\nu_3, x, t) &= E_3(x, t), \end{aligned}$$

and where each $E_i(x, t)$ is *monochromatic* at the frequency ν_i.

[1] Gnedin & Abel, *NewAst*, 2001, [2] Ricotti, Gnedin & Shull, *ApJ*, 2002

Multi-Frequency Radiation Equations

So instead of a very large system of coupled radiation equations

$$\partial_t E_\nu - \nabla \cdot (D \nabla E_\nu) + \tfrac{1}{a} \nabla \cdot (E_\nu \mathbf{v}_b) = \nu \tfrac{\dot{a}}{a} \partial_\nu E_\nu + 4\pi\eta_\nu - c k_\nu E_\nu,$$

for $\nu = \nu_0, \nu_1, \ldots, \nu_N$, we only have the four radiation equations,

$$\begin{aligned}
\partial_t E_f &= \nabla \cdot \left(\tfrac{\nabla E_f}{|\nabla E_f|} c E_f \right) + c\mu \nabla^2 E_f - \tfrac{\dot{a}}{a} E_f + 4\pi\eta_f, \\
\partial_t E_1 &= -\tfrac{1}{a} \nabla \cdot (E_1 \mathbf{v}_b) + \nabla \cdot (D_1 \nabla E_1) + 4\pi\eta_1 - c\kappa_1 E_1, \\
\partial_t E_2 &= -\tfrac{1}{a} \nabla \cdot (E_2 \mathbf{v}_b) + \nabla \cdot (D_2 \nabla E_2) + 4\pi\eta_2 - c\kappa_2 E_2, \\
\partial_t E_3 &= -\tfrac{1}{a} \nabla \cdot (E_3 \mathbf{v}_b) + \nabla \cdot (D_3 \nabla E_3) + 4\pi\eta_3 - c\kappa_3 E_3.
\end{aligned}$$

These are then combined together to form $E(\nu, x, t)$ that is used to compute the gas photo-heating and chemical photo-ionization rates,

$$G = \tfrac{1}{\rho_b} \sum_{i=1}^{3} \mathrm{n}_i \int_{\nu_i}^{\infty} c\, E(\nu)\, \sigma_i(\nu)\, \tfrac{h\nu - h\nu_i}{h\nu}\, \mathrm{d}\nu,$$

$$\Gamma_i^{ph} = \int_{\nu_i}^{\infty} c\sigma_i(\nu) \tfrac{E(\nu)}{h\nu}\, \mathrm{d}\nu, \quad i = 1, 2, 3.$$

New Solvers

Now instead of one diffusion solve over the domain (as in grey FLD), and one set of photo-heating and photo-ionization integrals, we have:

(a) One free-streaming radiation solve for E_f (scalar-valued, non-symmetric, diagonally-dominant). We use a MG-preconditioned BiCGStab solver from HYPRE.

(b) Three decoupled diffusion solves for E_1, E_2 and E_3. These are identical to the grey equation, and solved with MG-CG.

(c) One set of ν-integrals in each cell to compute G and Γ_i^{ph}. Due to the smoothness of these in ν-space (except at ν_i thresholds), these integrals may be computed efficiently to high accuracy.

Interfacing with Enzo's existing chemistry infrastructure

Due to their development path (`gFLDProblem`→`gFLDSplit`) the FLD solvers currently implement their own chemical ionization and cooling, which provides only a subset of Enzo's chemistry options.

Since the `gFLDSplit` solver already splits off chemistry/cooling from radiation, we are completing an interface from that solver to call Enzo's existing chemistry modules (instead of it's own).

This will enable increased options, a simplified user experience, and a single location in the source code for improvements (e.g. improved rates).

Difficulties at this moment are only superficial, having to do with unit types expected/produced by each module.

Combined FLD & Ray Tracing

John Wise's ray-tracing radiation package naturally captures MF radiative transfer, and allows sources with varying spectra.

However, it can have difficulty scaling to large numbers of sources, especially when treating Lyman-Werner radiation.

We are therefore completing an interface between John's ray-tracing solvers for transfer of ionizing radiation, and the free-streaming FLD solver for transport of Lyman-Werner radiation.

Initial construction is complete but needs testing, especially in AMR contexts where the LW radiation will propagate on the root grid only.

Hybrid parallelism

Since FLD solves couple the entire domain together, it naturally takes a significant portion of the runtime, and is dominated by communication.

However, the MF solver requires significantly more computation per cell (due to the ν-integrals). These will be converted to hybrid parallelism to leverage multi-core architectures.

HYPRE is also multi-threaded (according to documentation), so this could result in increased multi-core performance. We have yet to test the parallel speedup due to multi-core HYPRE usage, but multi-core means fewer MPI tasks, which could aid in communication performance.

Extensions to Adaptive Mesh Refinement

James Bordner has created a self-gravity solver for Enzo's AMR grids using the FAC solver interface in HYPRE,

$$\nabla^2 \phi = -\frac{4\pi G}{a} \rho_b.$$

This implicit system has the same nonzero matrix structure as implicit FLD problems. Moreover, FAC methods excel on parabolic systems.

We plan to begin extensions the `gFLDSplit` to use James' new solver interface, as the `gFLDSplit` solver requires no nonlinear solver infrastructure. Eventually, these will be ported to all FLD solvers.

Difficulties include more complex matrix entries and time-stepping questions (since FLD is implicit, it need not subcycle for CFL stability).