[Toward] Simulating Cosmological Reionization with Enzo

Texas Cosmology Network Meeting 2009

29 October 2009

Daniel R. Reynolds

M.L. Norman, P. Paschos, G. So [UCSD]

J.C. Hayes [LLNL]

Sponsor: NSF Astronomy & Astrophysics

Personal Introduction

- Assistant professor in Mathematics at SMU.
- Computational/applied math background; expertise in nonlinear and linear solvers for multi-scale problems in computational physics.
- This work focuses on collaborations with UCSD's Laboratory for Computational Astrophysics (M. Norman et al.).
- Goal is to develop high-accuracy, scalable solvers for coupled simulations of radiation, hydrodynamics and ionization.
- Efforts focused on developing solver modules for *Enzo*, an open-source code for cosmological hydro., dark-matter, gravity and chemical ionization (advertised by Kim Tran earlier).
- Target applications are mainly in cosmological reionization, though goal is to develop numerical methods that span to other regimes as well.

Enzo-RT Goals

I. Extend Enzo to include radiation transport & ionization, to enable:

- studies of self-regulated star formation,
- predictions on the epoch of cosmic reionization, and
- predictions on the observed properties of early galaxies.

II. Accurately model stiff cosmological RT and chemical ionization processes.

III. Integrate new solver in Enzo code so that coupling respects hydrodynamics approach (shocks), but tightly couples physics.

IV. Enable very-large-scale simulations ($\mathcal{O}(10^6)$ processors).

Coupled Matter-Radiation System

We consider the coupled cosmological PDE system,

$$\nabla^2\phi = \frac{4\pi G}{a}\left(\rho_b + \rho_{dm} - \rho_0\right),$$

$$\partial_t \rho_b + \frac{1}{a}\mathbf{v}_b \cdot \nabla \rho_b = -\frac{1}{a}\rho_b \nabla \cdot \mathbf{v}_b,$$

$$\partial_t \mathbf{v}_b + \frac{1}{a}\left(\mathbf{v}_b \cdot \nabla\right)\mathbf{v}_b = -\frac{\dot a}{a}\mathbf{v}_b - \frac{1}{a\rho_b}\nabla p - \frac{1}{a}\nabla\phi,$$

$$\partial_t e + \frac{1}{a}\mathbf{v}_b \cdot \nabla e = -\frac{2\dot a}{a} e - \frac{1}{a\rho_b}\nabla \cdot \left(p\mathbf{v}_b\right) - \frac{1}{a}\mathbf{v}_b \cdot \nabla\phi + G - \Lambda,$$

$$\partial_t \mathbf{n}_i + \frac{1}{a}\nabla \cdot \left(\mathbf{n}_i \mathbf{v}_b\right) = -3\frac{\dot a}{a}\mathbf{n}_i - \mathbf{n}_i \Gamma_i^{ph} + \alpha_{i,j}^{rec}\,\mathbf{n}_e \mathbf{n}_j,$$

$$\partial_t E_\nu + \frac{1}{a}\nabla \cdot \left(E_\nu \mathbf{v}_b\right) = \nabla \cdot \left(D\,\nabla E_\nu\right) + \nu\frac{\dot a}{a}\partial_\nu E_\nu + 4\pi\eta_\nu - ck_\nu E_\nu.$$

Here, $G(E, \mathtt{n}_i)$ and $\Lambda(E, \mathtt{n}_i)$ are the heating and cooling rates. The E_ν equation approximates the radiative flux as a function of the energy density gradient,

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

where $D(E_\nu, \nabla E_\nu) \in \mathbb{R}^{3\times 3}$ is the *flux limiter*.

[Bryan et al., *Comp. Phys. Comm.*, 1995; R. et al., *J. Comput. Phys.*, 2009]

Enzo Operator-Split Numerics

We solve this coupled system in an operator-split framework, solving one component of the system at a time within a time step:

(i) Project dark matter particles onto mesh to generate ρ_{dm}.

(ii) Solve for the gravitational potential ϕ via FFT or MG methods.

(iii) Advect dark matter particles via Particle-Mesh method.

(iv) Explicitly evolve $(\rho_b, \mathbf{v}_b, e)$ and advect $(E_\nu, \mathtt{n}_i)$ with a high-order PPM method.

(v) Implicitly evolve a stiffreaction-di ffusion PDE system that updates $(E_\nu, e, \mathtt{n}_i)$.

Enzo Operator-Split Numerics

We solve this coupled system in an operator-split framework, solving one component of the system at a time within a time step:

(i) Project dark matter particles onto mesh to generate ρ_{dm}.

(ii) Solve for the gravitational potential ϕ via FFT or MG methods.

(iii) Advect dark matter particles via Particle-Mesh method.

(iv) Explicitly evolve $(\rho_b, \mathbf{v}_b, e)$ and advect $(E_\nu, \mathtt{n}_i)$ with a high-order PPM method.

(v) Implicitly evolve a stiffreaction-di ffusion PDE system that updates $(E_\nu, e, \mathtt{n}_i)$.

Gray FLD Radiation Transfer Equation

Prior to investigating the multi-frequency case, we begin using a single, frequency-integrated ("grey") radiation energy,

$$E(x,t) = \int_{\nu_0}^{\infty} E_\nu(x,t,\nu)\, d\nu = \tilde{E}(x,t) \int_{\nu_0}^{\infty} \chi_E(\nu)\, d\nu,$$

where $\chi_E : I\!R \to I\!R$ is an assumed radiation energy density spectrum.

With this approximation, the integrated radiation energy equation becomes

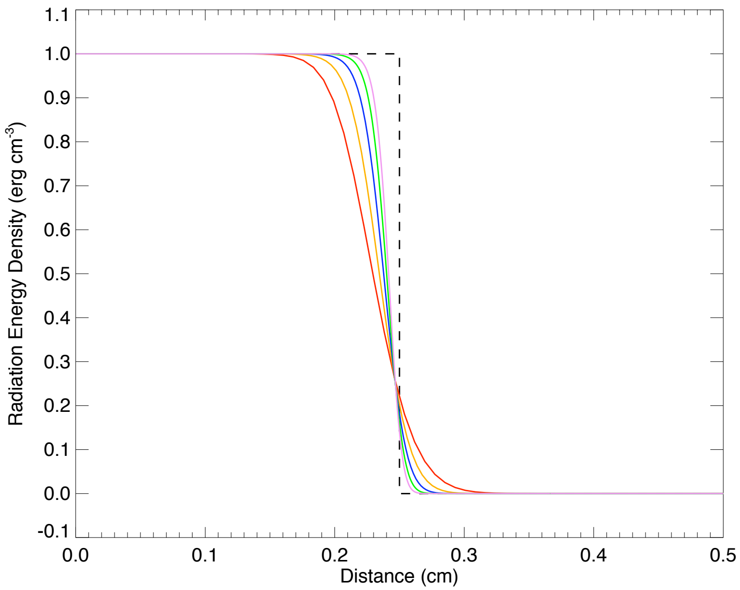
$$\partial_t E + \frac{1}{a}\nabla \cdot (E\mathbf{v}_b) \;=\; \nabla \cdot (D\,\nabla E) - \frac{\dot{a}}{a} E + 4\pi\eta - ckE,$$

where the new coupling terms are integrated over frequency:

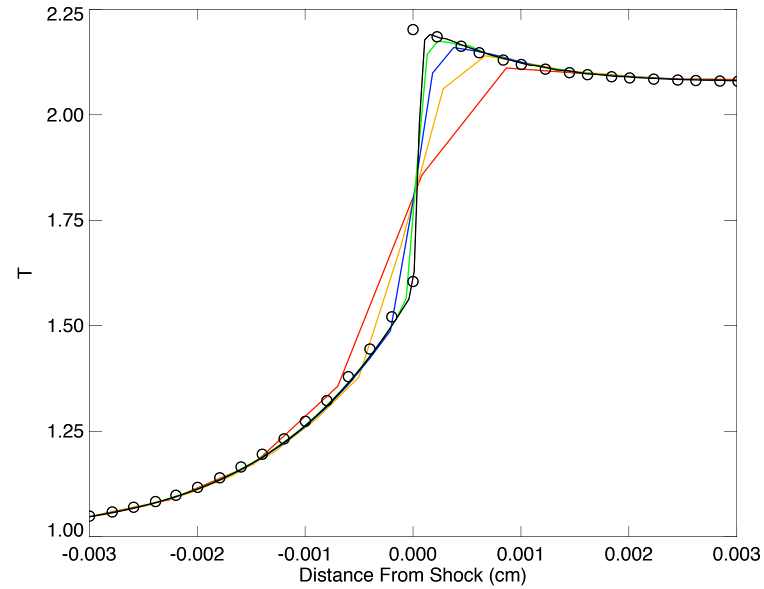
$$\eta = \int_{\nu_0}^{\infty} \eta_\nu\, d\nu$$

$$k = \left(\int_{\nu_0}^{\infty} k_\nu E_\nu\, d\nu\right) \Big/ \left(\int_{\nu_0}^{\infty} E_\nu\, d\nu\right).$$

Rad-Hydro Verification Results



Smearing of a radiation front in a vacuum due to FLD approximation (convergence wrt Δx).



Radiating shock front convergence wrt Δx. [Lowrie & Edwards, *ShWav*, 2008].

Thermal equilibration: energy conserv. error,

$$\left(\int |\Delta E_{\text{tot}}|\,\mathrm{d}x\right) \Big/ \left(\int E_{\text{tot}}(0)\,\mathrm{d}x\right),$$

L→H and H→L equilibration, under various nonlinear and linear tolerances (ε, δ). [Turner & Stone, *ApJ*, 2001]

ε	δ	$L \rightarrow H$	$H \rightarrow L$
1e-7	1e-9	7.0e-12	1.4e-12
1e-10	1e-9	3.1e-13	3.5e-14
1e-4	1e-9	3.6e-11	1.8e-11
1e-7	1e-12	7.0e-12	1.4e-12
1e-7	1e-3	7.0e-12	1.4e-12

Isothermal Radiative Ionization Test

Tests of isothermal ionization of a static, initially-neutral hydrogen region:

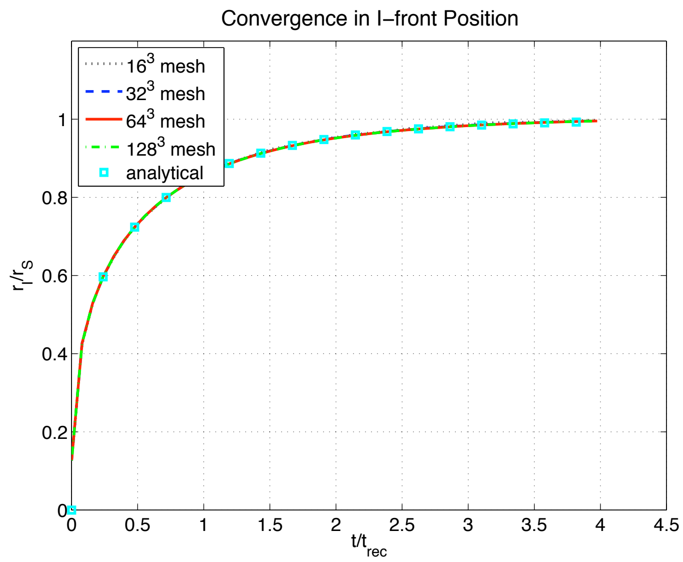
- $L = 6.6$ kpc.
- Monochromatic emission: $\dot{N}_\gamma = 5 \cdot 10^{48}$ photons s^{-1}, at $h\nu = 13.6$ eV.
- Fixed gas temperature, $T = 10^4$ K.
- Case-B recombination rate, $\alpha_B = 2.59 \cdot 10^{-13}$ cm^3 s^{-1}.
- Constant number density $n = 10^{-3}$ cm^{-3}.

Analytical solution given by

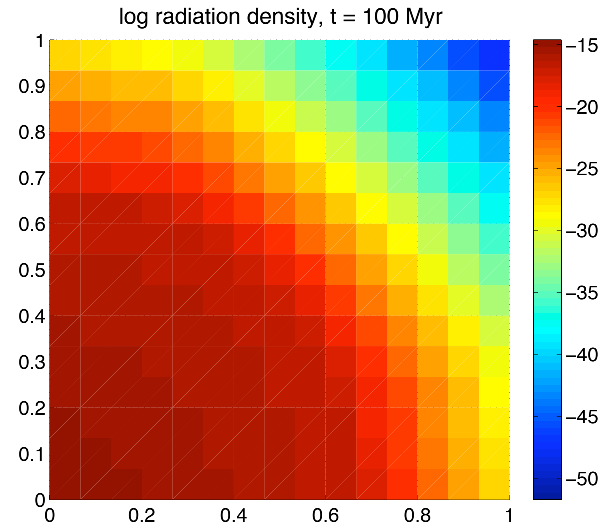
$$\begin{aligned} r_I &= r_S\left[1 - e^{-t\alpha_B n_H}\right], \quad \text{where} \\ r_S &= \left[\frac{3\dot{N}_\gamma}{4\pi\alpha_B n_H^2}\right]^{1/3}. \end{aligned}$$

[Iliev et al., *MNRAS*, 2006]

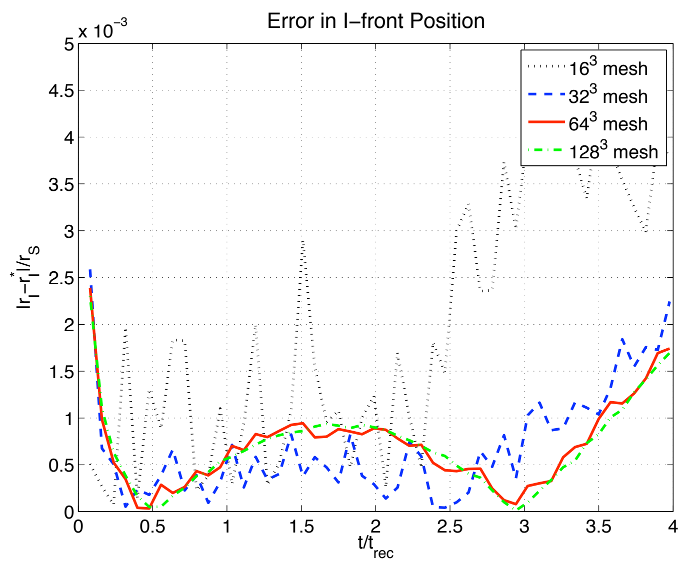
Isothermal Ionization Results



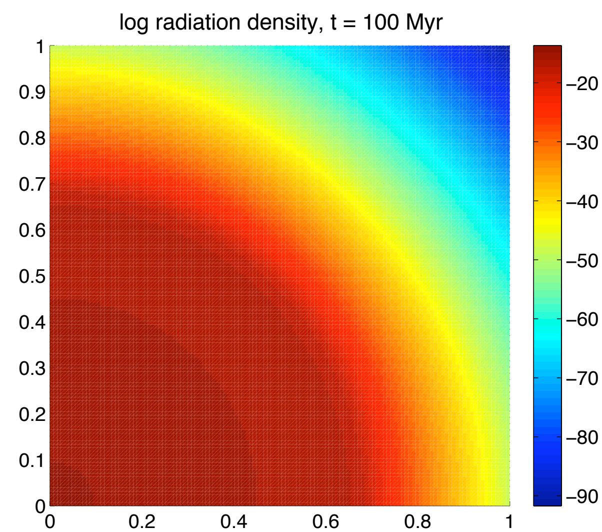
NW:
I-front position history.



NE:
Coarse radiation field ($N_x = 16$).



SW:
r_I convergence vs Δx.



SE:
Fine radiation field ($N_x = 128$).

Isothermal Cosmological Ionization Test

Repeat of previous test, but in a cosmologically expanding universe.

Four tests:

q_0	z_i	L_i [kpc]	$\rho_{b,i}$ [g cm^{-3}]	H_0	Ω_m	Ω_Λ	Ω_b
0.5	4	80	1.18e-28	0.5	1.0	0	0.2
0.05	4	60	2.35e-28	1.0	0.1	0	0.1
0.5	10	36	1.18e-28	0.5	1.0	0	0.2
0.05	10	27	2.35e-28	1.0	0.1	0	0.1

Analytical solution given by

$$r_I(t) = r_{S,i}\left(\lambda e^{-\tau(t)}\int_1^{a(t)} e^{\tau(b)}\left[1-2q_0+2q_0(1+z_i)/b\right]^{-1/2}\mathrm{d}b\right)^{1/3},$$

where

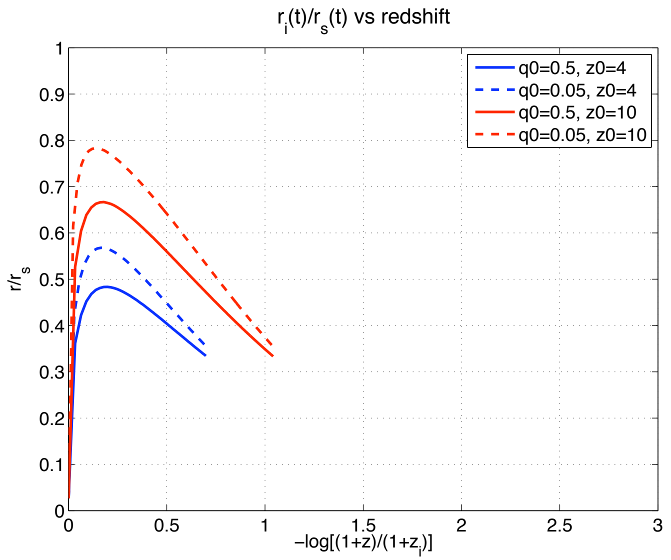
$$\tau(a) = \lambda\left[F(a)-F(1)\right]\left[6q_0^2(1+z_i)^2\right]^{-1},$$

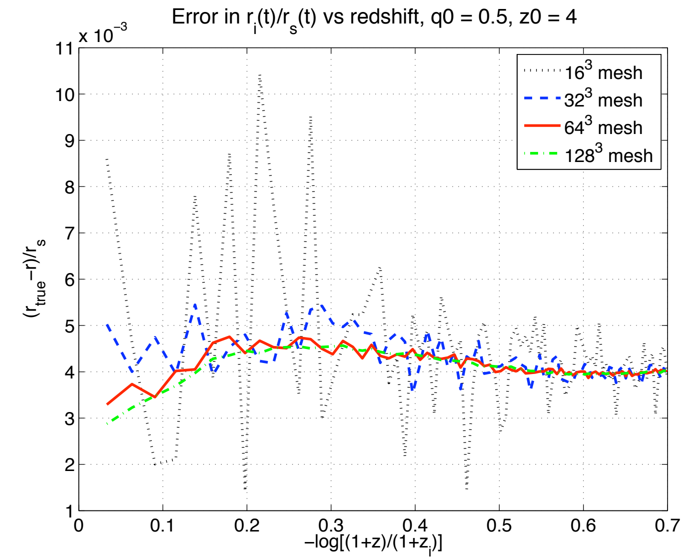
$$F(a) = \left[2-4q_0-2q_0\frac{1+z_i}{a}\right]\left[1-2q_0+2q_0\frac{1+z_i}{a}\right]^{1/2},$$

$$\lambda = \alpha_B n_{H,i}/H_0/(1+z_i).$$

[Shapiro & Giroux, *ApJ*, 1987]

Cosmological Ionization Results



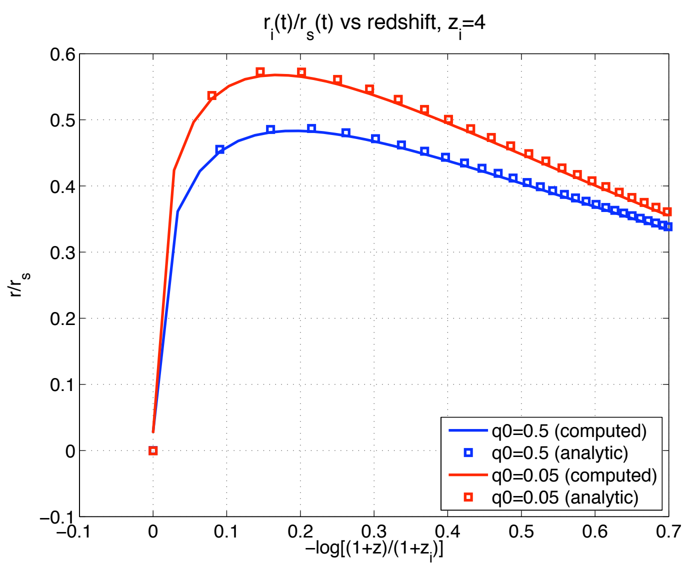


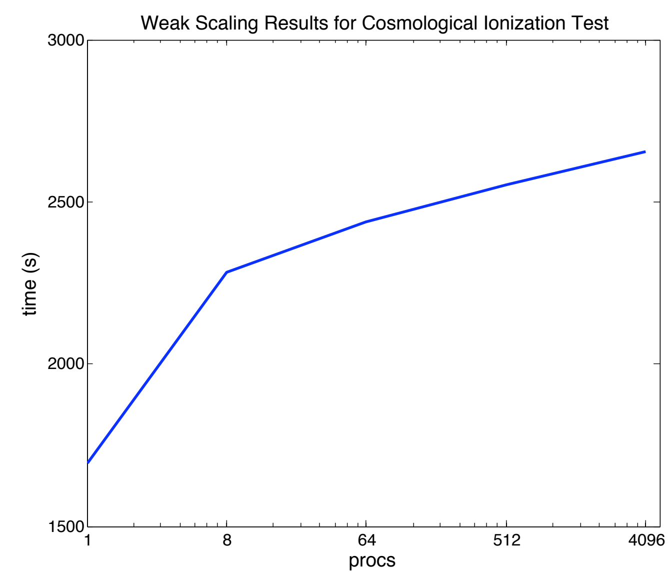
NW:
I-front radii
vs scaled z.

NE:
I-front error
vs scaled z.

SW:
I-front radii
for $z_i = 4$.

SE:
Weak CPU
scaling [*Kraken*]
$N_{\mathrm{src}} \propto N_{\mathrm{CPU}}$
$(\mathcal{O}(N \log N))$





Hydrodynamic Radiative Ionization Test

Re-do first test in a dynamic medium ($L = 15$ kpc); combines radiation, hydrodynamics and hydrogen ionization:

- Emission source has a $T = 10^5$ K blackbody spectrum.
- Initial temperature set to $T = 10^2$ K.
- Front transitions from R-type to D-type as it reaches Strömgren radius.
- Eventually stalls at $r_f = r_S \left(\frac{2T_i}{T_e}\right)^{2/3}$, where T_i and T_e are the temperatures behind and ahead of the i-front.

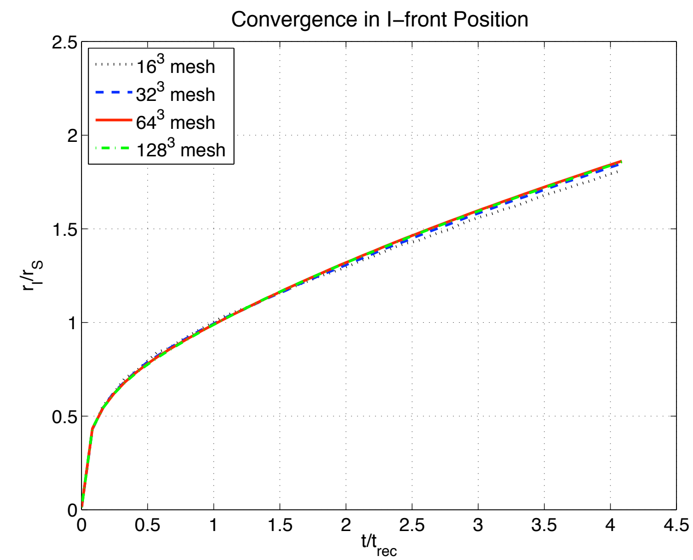
R-type and D-type propgation have different analytical solutions,

$$r_I^R = r_S \left[1 - e^{-t\alpha_B(T_i)n_H}\right]^{1/3}, \qquad r_I^D = r_S \left[1 + \frac{7c_s t}{4r_S}\right]^{4/7},$$

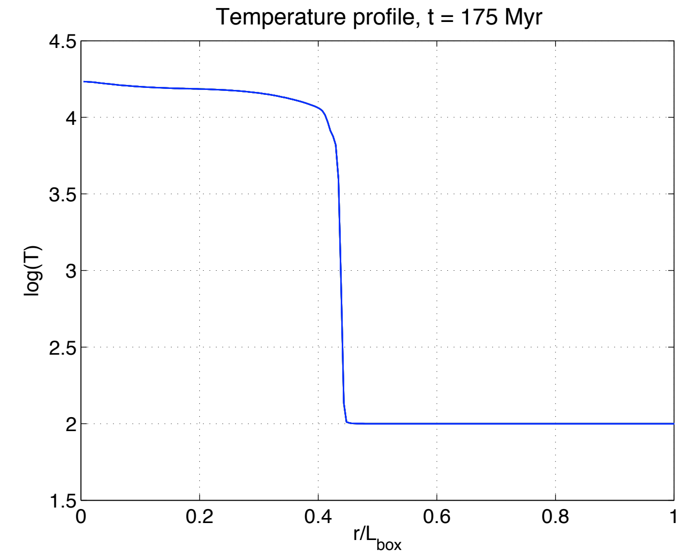
with true solution somewhere between the two.

[Whalen & Norman, *ApJS*, 2006; Iliev et al., *MNRAS*, 2009]

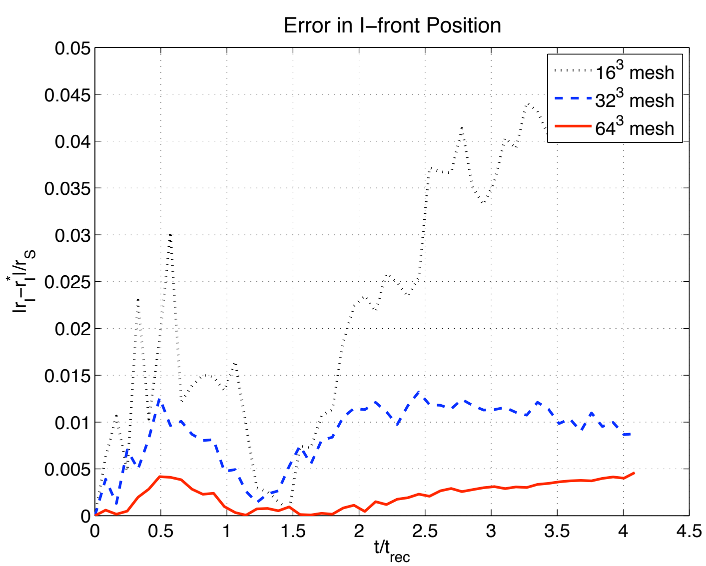
Hydrodynamic Radiative Ionization Results



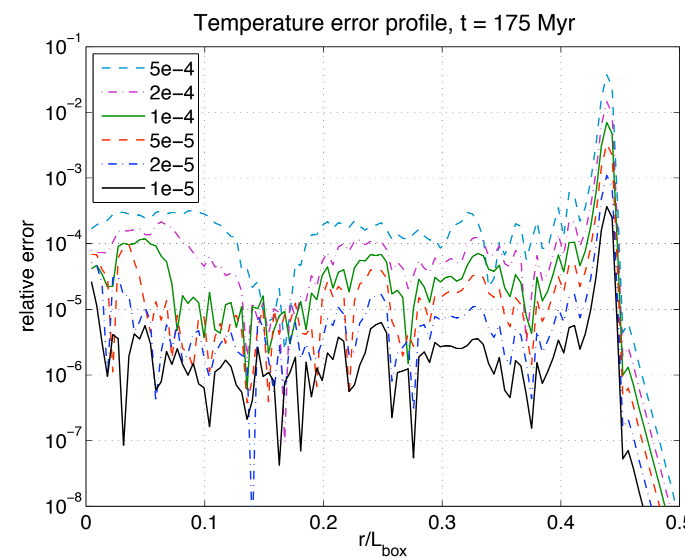
NW:
I-front position history.



NE:
T profile at 200 Myr.



SW:
r_I convergence wrt Δx.



SE:
T convergence wrt Δt.

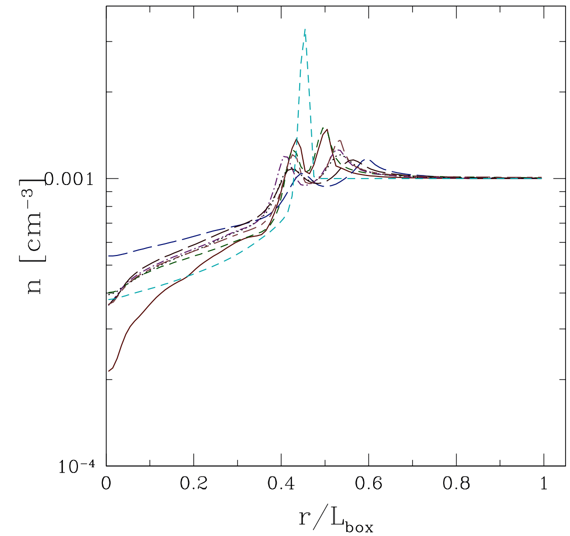
The Need for Multi-Frequency

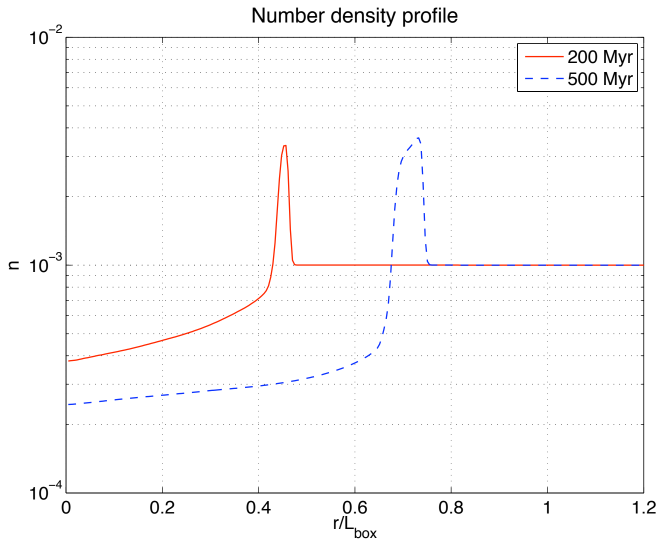
However, in comparison with other RT codes, we get peculiar results:

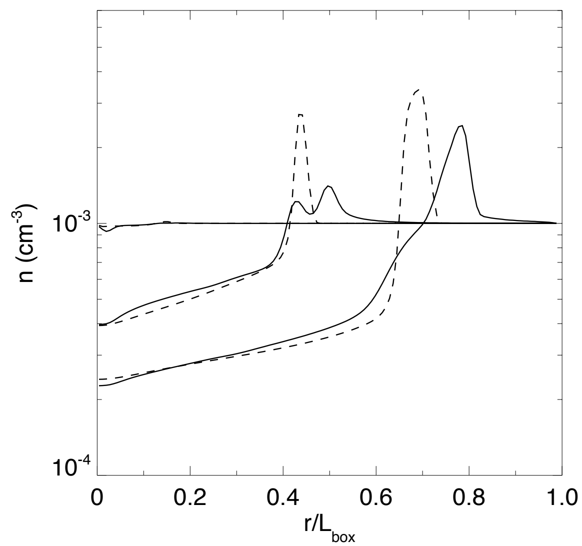
Right: $\mathbf{n}$ profiles at 250 Myr (cyan is Enzo) [1].

Below: Enzo $\mathbf{n}$ profiles results at 200, 500 Myr.

Lower right: Zeus-MP results (solid is MF, dashed is monochromatic).







Summary of Current Results

We've achieved a second-order accurate (space and time) coupled solver for cosmological radiation, hydrodynamics, self gravity and chemical ionization.

- Captures shock fronts due to trusted PPM hydrodynamics approach.
- Accurately solves couplings between radiation, ionization and gas energy, due to implicit formulation and coupled solvers.
- Highly scalable, with current tests using > 4000 processors, thanks to reliance on optimal multigrid methods.

However, the grey radiation approximation has its shortcomings:

- Single radiation field allows full absorption by hydrogen, even though higher-frequency radiation should pass through.
- Leads to increased absorption in optically-thick regions, with no pre-heating ahead of I-fronts.

Continuing Work

- Enhance stability of chemistry computations at large Δt
  - Fastest dynamics occur in ionization, ostensibly allowing complete ionization of a volume in a single step $[\mathcal{O}(1) \to \mathcal{O}(10^{-5})]$.
  - Time inaccuracy can over-shoot to give negative densities.
- Extend radiation approximation to multi-frequency case, $E \to E_\nu$
  - New physical couplings and interpolation of ν-space, based offof [Ricotti, Gnedin & Shull, *ApJ*, 2002]
  - Large-scale solvers for coupled reaction-diffusion systems
- Extend implicit solver software to AMR grids
  - Regular-grid geometric multigrid $\to$ AMG or FAC methods