Self-Consistent Cosmological Radiation Hydrodynamics

(or how and why we put radiative transfer into Enzo)

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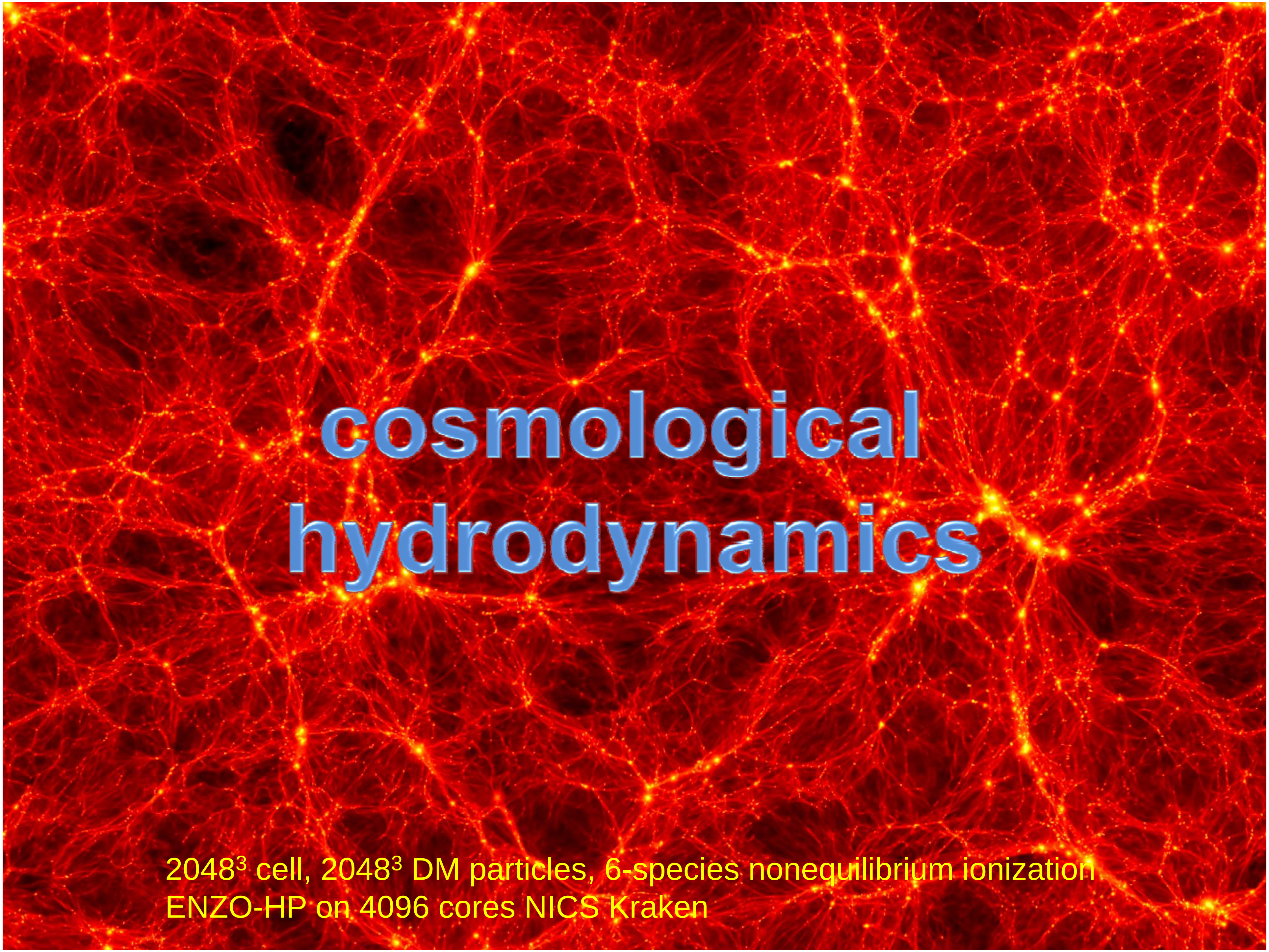
My Career as a Code Developer

- get interested in some physics
- develop a code
- apply and write some papers
- make code public
- repeat

- Thesis code (1980)
- ZEUS (w/D. Clarke; 1988)
- ZEUS-2D (w/J. Stone; 1992)*
- ZEUS-3D (w/D. Clarke; 1992)*
- KRONOS (w/G. Bryan; 1994)*
- ENZO-SMP (w/ G. Bryan; 1995)
- ENZO-MPI (w/G. Bryan; 1997)
- ZEUS-MP/1 (w/R. Fiedler; 1999)*
- ENZO-V1.0 (w/B. O'Shea; 2004)*
- ZEUS-MP/2 (w/J. Hayes; 2006)*
- ENZO-V1.5 (w/R. Harkness; 2008)*
- ZEUS-MP/2-MFRT (w/D. Whalen; 2010)
- ENZO-HP (w/R. Harkness; 2010)
- ENZO-MHD (w/D. Collins & H. Xu; 2010)
- ENZO-RT (w/ D. Reynolds; 2010)

***available at lca.ucsd.edu/portal/software**


radiative transfer
+
ionization



cosmological hydrodynamics

2048^3 cell, 2048^3 DM particles, 6-species nonequilibrium ionization
ENZO-HP on 4096 cores NICS Kraken

Algorithm Requirements

- Independent of N(sources)→O(1)
- Scalable WRT N(cells)→O(N)
- Scalable WRT N(processors)→O(log(Np))
- Extensible to AMR
- Extensible to multifrequency
- Not too slow to use
- *Success! parallel multigrid*

Outline

- Scientific motivation
- Photo-ionization, I-fronts, & Ionized Flows
- 3D cosmological radiative transfer
- Self-consistent cosmological radiation hydrodynamics (algorithm)
- The ENZO-RT code & results
- Conclusions and future work

Eagle Nebula

TWiki resources

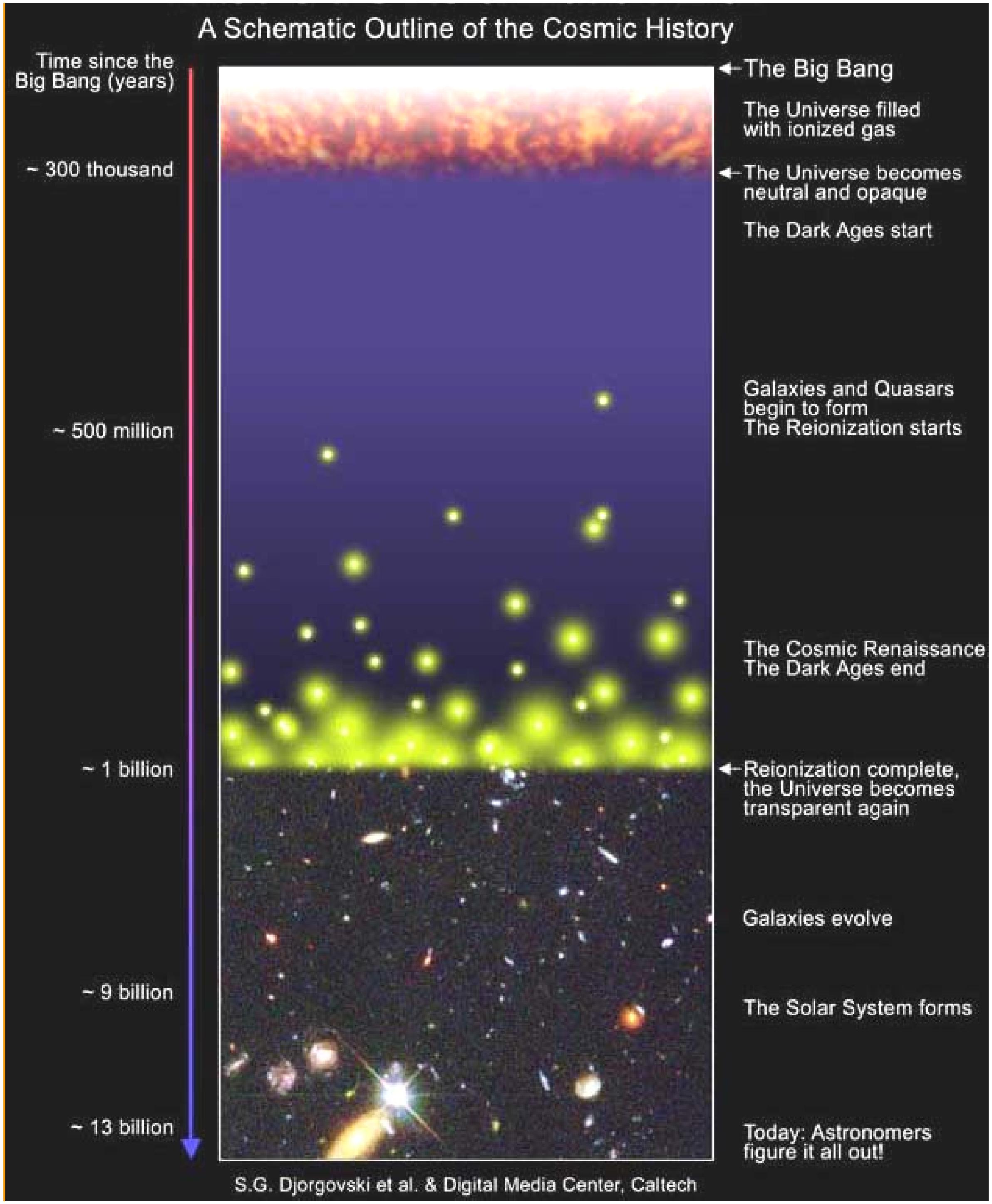
- Background reading
  - Observational Constraints on Reionization: Fan, Carilli & Keating, ARAA, 45, 415 (2006)
  - Ionization Basics: Whalen PhD thesis Ch. 2
  - Methods for solving 3D radiative transfer equation
  - Code comparison papers: Iliev et al. 2006, 2009
  - Whalen & Norman (2006) algorithm
  - Reynolds et al. (2009) algorithm

Scientific Motivation

- Effect of energetic radiation (UV, X) on cosmological structure formation
  - Cosmic reionization
  - depletion of baryons in low mass halos
  - Suppression of star formation due to heating
  - Escape fractions of internally generated radiation in galaxies/QSOs
- Evolution of radiation backgrounds and effect on IGM properties
  - Reheating of the IGM by Quasars

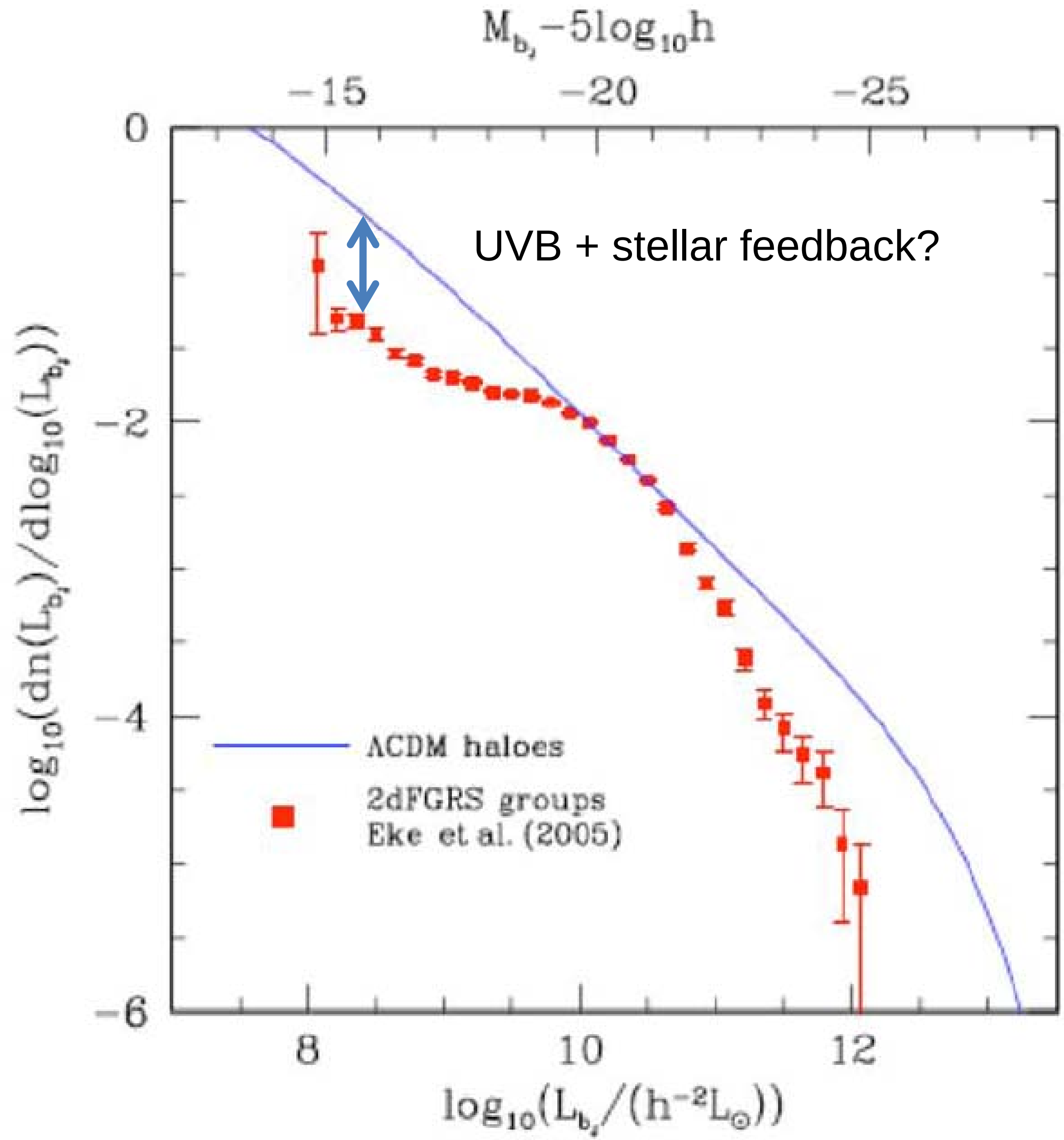
Reionization Questions

- Timing:
  - when did reionization begin and end?
- History:
  - How does the ionized fraction of the intergalactic medium evolve with redshift?
- Topology:
  - What is the topology of ionized gas before overlap?
  - What is the shape of the "last neutral surface"?
- Astrophysics:
  - What are the ionizing sources?

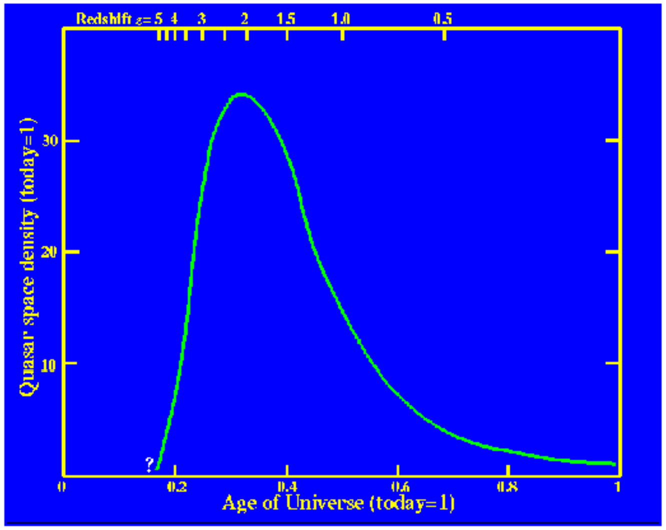


Baryon depletion in low-mass halos

Solution to the galaxy LF discrepancy with ΛCDM?



Late He II Reionization by Quasars



Shaver (1996)

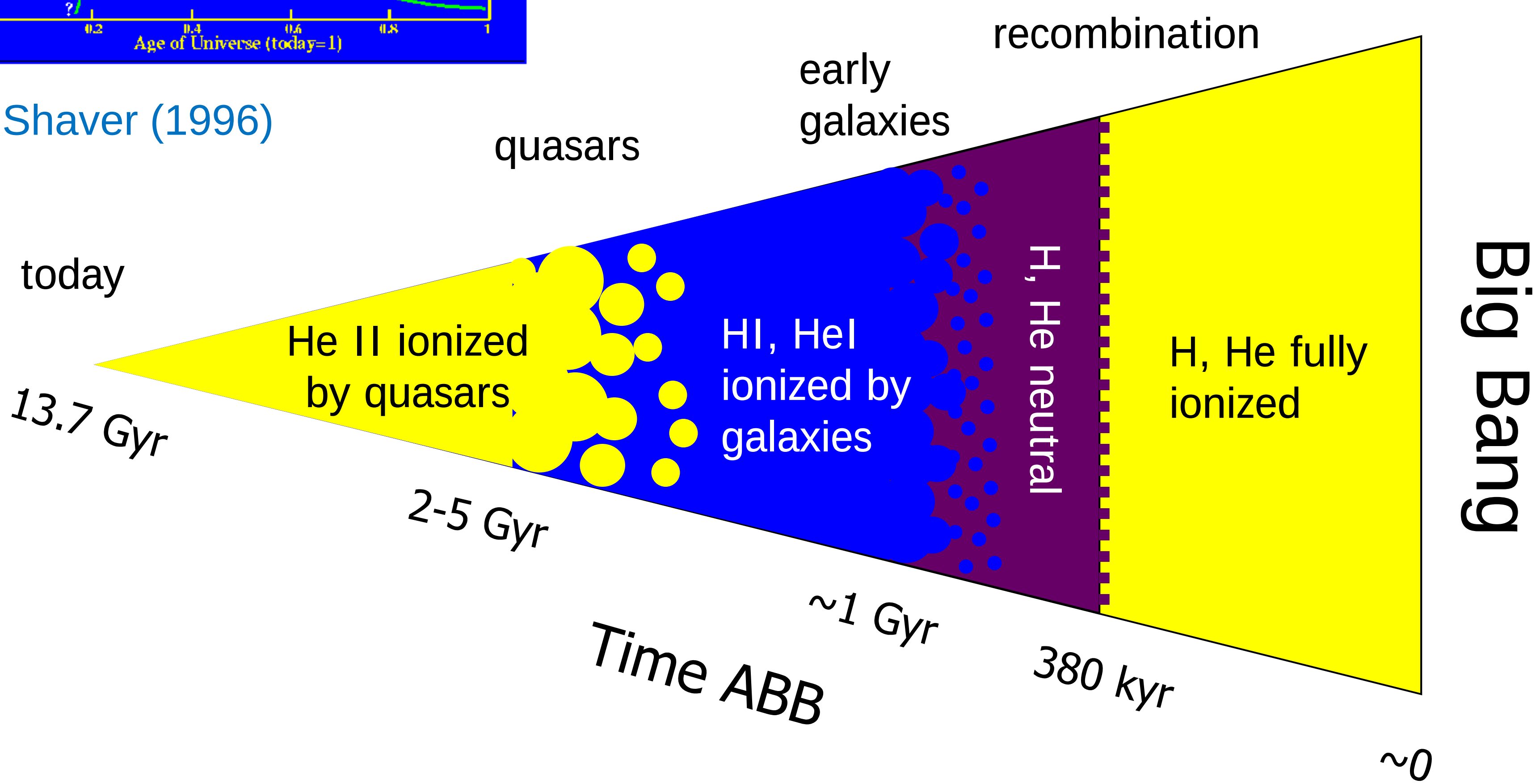
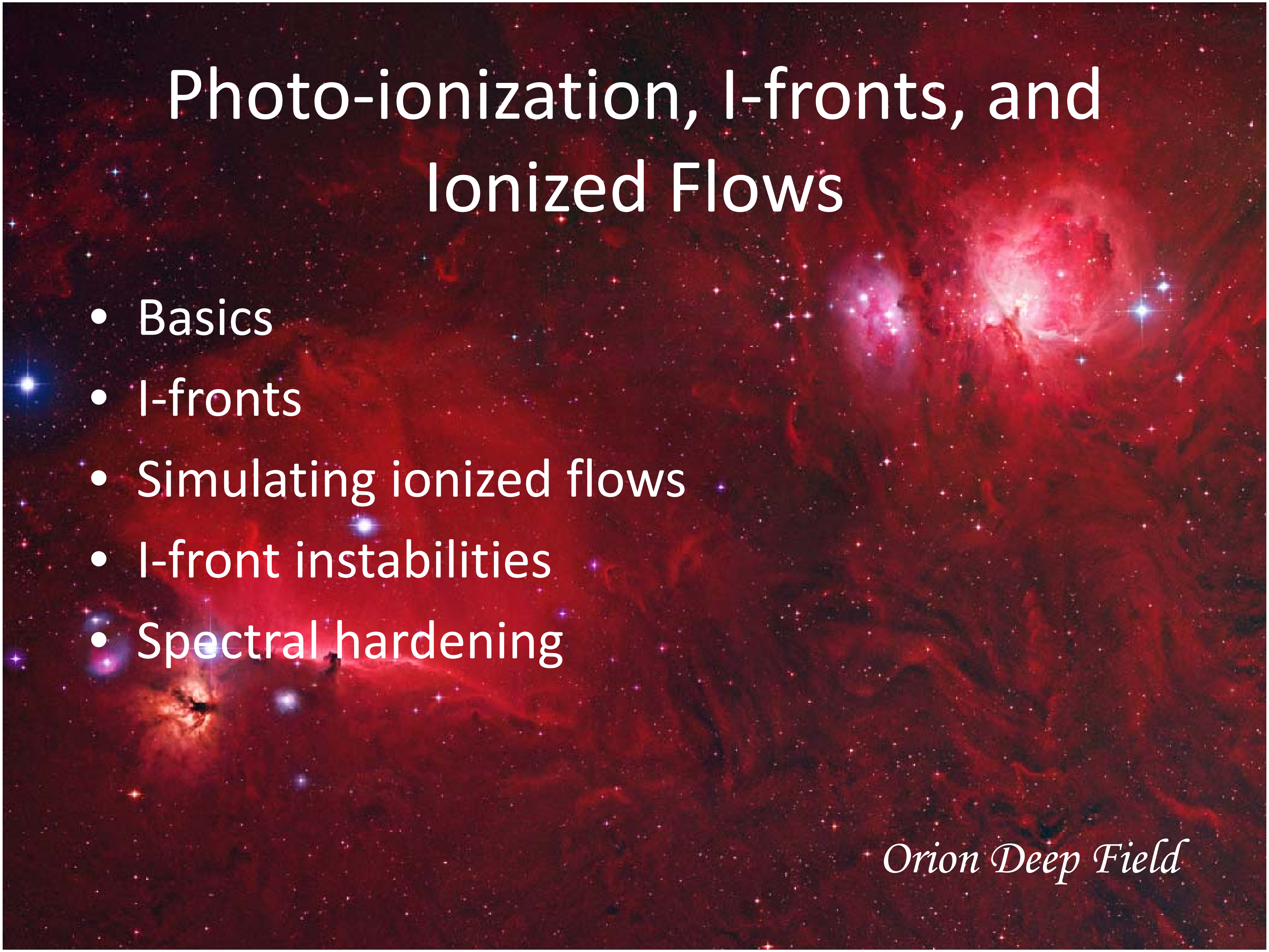


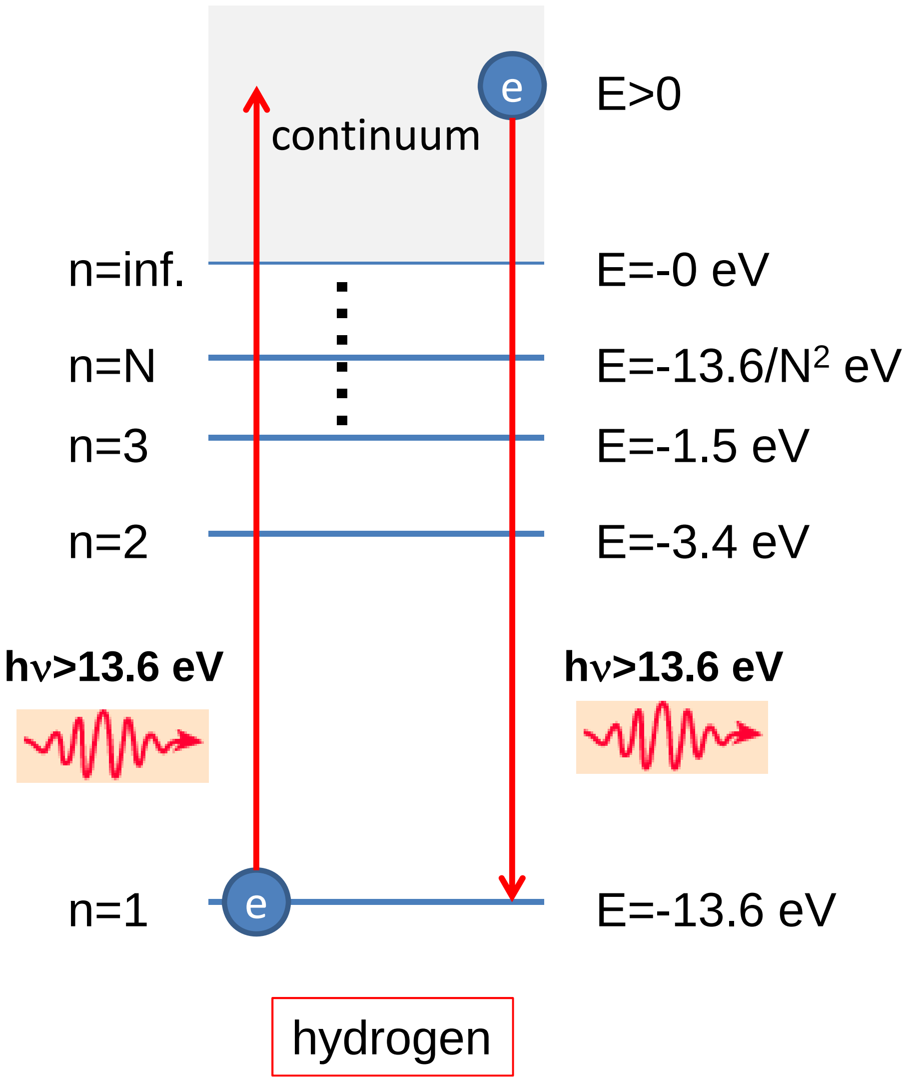
Photo-ionization, I-fronts, and Ionized Flows

- Basics
- I-fronts
- Simulating ionized flows
- I-front instabilities
- Spectral hardening



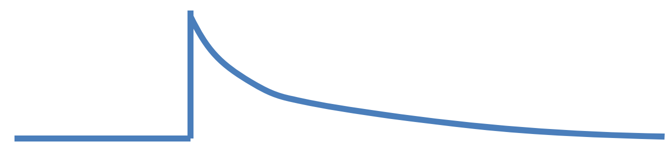
Orion Deep Field

Basics: Microphysical



Photoionization

$$\sigma_{PI}(\nu) \approx \begin{cases} \sigma_{th}(\nu/\nu_{th})^{-3}, & \nu \geq \nu_{th} \\ 0 & , \nu < \nu_{th} \end{cases}$$



Radiative recombination

$$\sigma_{rec}(\varepsilon - 13.6eV) \approx \sigma_{PI}(\varepsilon / h)$$

most recombinations from $\varepsilon \sim h\nu_{th}$

Case A: to n=1

ionizing photon emitted

Case B: to n>1

non-ionizing photon emitted

Basics: Macrophysical

radiation field

specific intensity

$$I_\nu(\vec{x},\hat{n}) \equiv I(\vec{x},\hat{n},\nu)$$

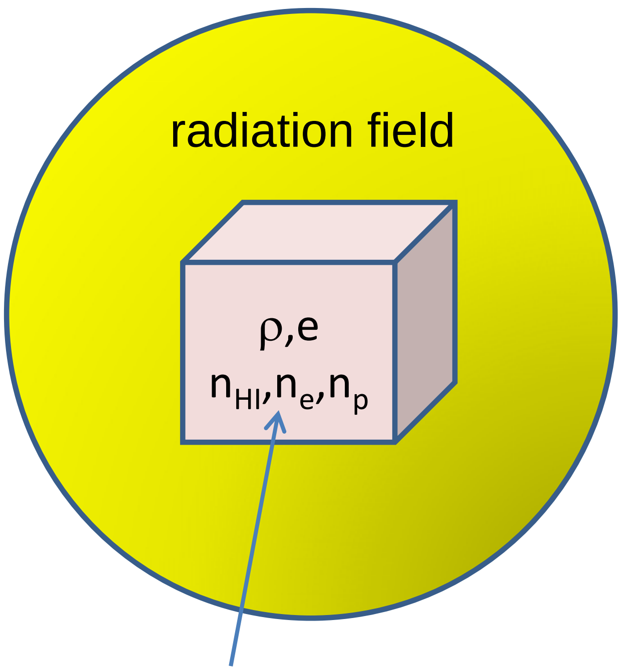
energy density

$$E_\nu(\vec{x}) = \frac{1}{c}\oint_{4\pi} I_\nu(\vec{x},\hat{n})\,d\Omega$$

photon number density

$$n_\nu(\vec{x}) = \frac{E_\nu(\vec{x})}{h\nu}$$

Basics: Macrophysical



- pure hydrogen plasma
- optically thin

Photoionization kinetics

$$\frac{\mathrm{dn_{HI}}}{\mathrm{dt}} = (\alpha_{rec}^{n=1} + \sum_{n>1} \alpha_{rec}^{n}) n_e n_p - I_{HI} n_{HI}$$

$$\alpha_{rec}^{n} \equiv \alpha_{rec}^{n}(T) \qquad \text{recombination rate to level } n$$

$$I_{HI} = \int_{\nu_{th}}^{\infty} d\nu \cdot \sigma_{PI}(\nu) \frac{E_\nu}{h\nu} \qquad \text{photo-ionization rate}$$

On-The-Spot (OTS) approximation

$$\frac{\mathrm{dn_{HI}}}{\mathrm{dt}} \approx \sum_{n>1} \alpha_{rec}^{n} n_e n_p - I_{HI} n_{HI} \equiv \alpha_B(T) n_e n_p - I_{HI} n_{HI}$$

$$\alpha_B \equiv \text{case B recombination coefficient}$$

Gas photoheating

$$\frac{\mathrm{de}}{\mathrm{dt}} = n_{HI} G_{HI} - \Lambda(T)$$

$$G_{HI} = \int_{\nu_{th}}^{\infty} d\nu \cdot \sigma_{PI}(\nu) \frac{E_\nu}{h\nu} (h\nu - h\nu_{th})$$

Strömgren Spheres

Strömgren (1939)

- For a uniform medium, balancing ionizations and recombinations to n>1

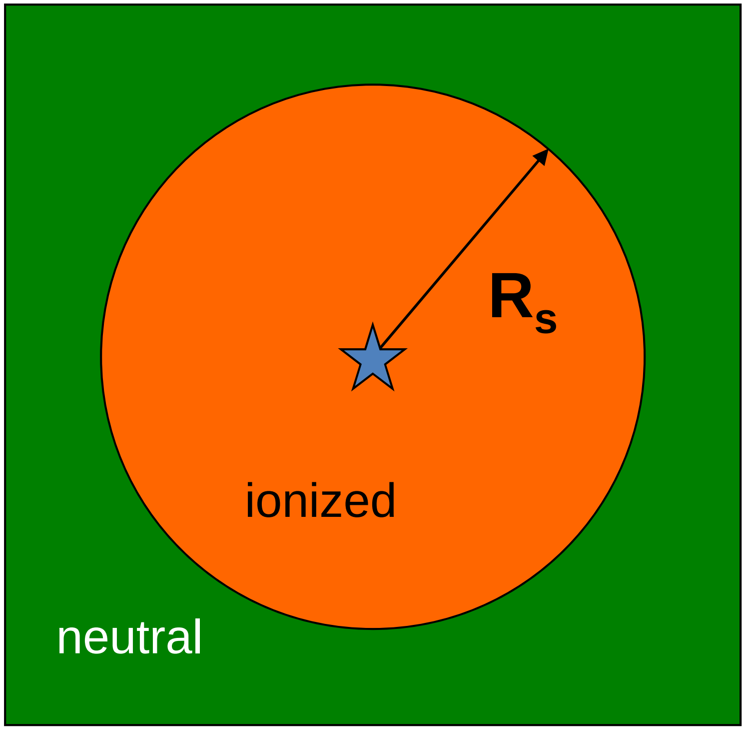
$$\frac{4\pi}{3} R_S^3 n_p n_e \alpha_B = \dot{N}_\gamma$$

$$R_S = \left(3\dot{N}_\gamma \Big/ 4\pi n_{\mathrm{H}}^2 \alpha_B \right)^{1/3}$$

$$n_p = n_e = n_H$$

R_S is Strömgren radius

~ 20 pc for O star in ISM



Strömgren Sphere Expansion Phase

in frame of the I-front

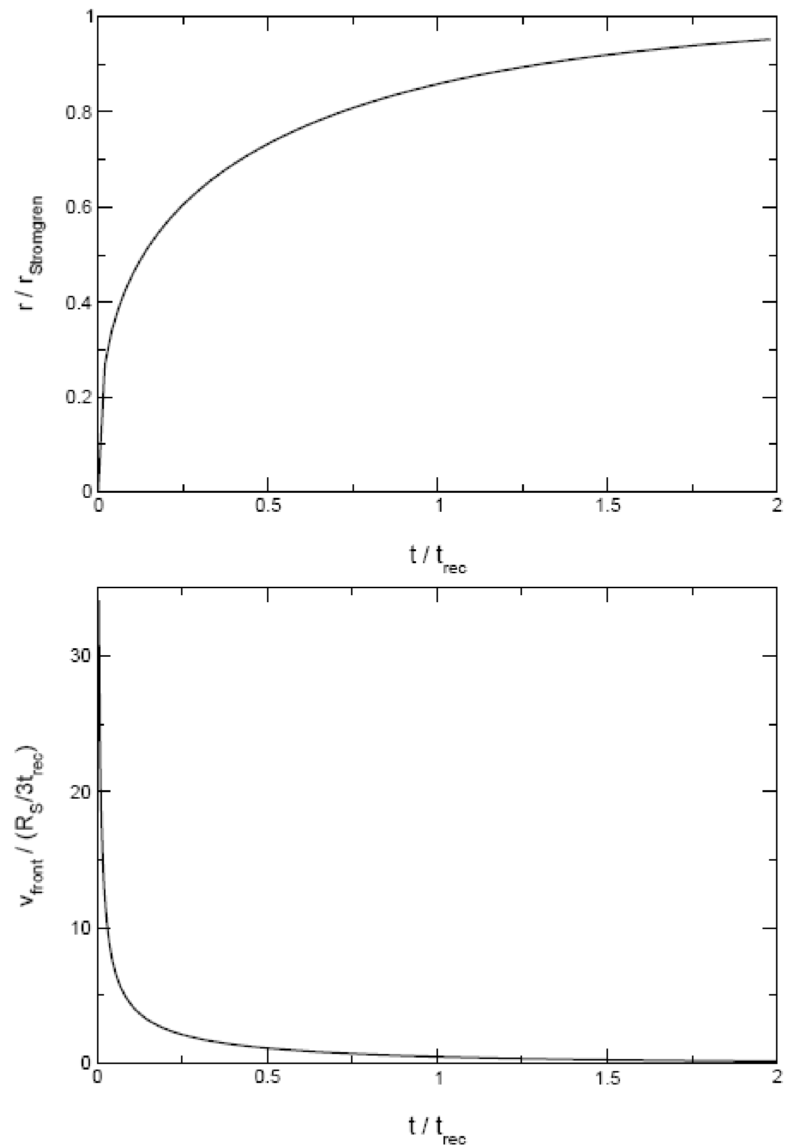
$$\mathrm{n_H} V_f = j_{ph}$$

$$\therefore V_f = \frac{1}{n_H} \frac{j_{ph@\,front}}{4\pi r_f^2}$$

$$= \frac{1}{n_H} \frac{1}{4\pi r_f^2} \left[\dot{N}_\gamma - \frac{4\pi}{3} r_f^3 n_e n_p \alpha_B \right]$$

$$\frac{\frac{d}{dt}(r_f^3)}{R_\mathrm{S}^3 - r_f^3} = n_H \alpha_B \equiv t_{rec}^{-1}$$

$$\Rightarrow r_f(t) = R_S[1 - \exp(t / t_{rec})]$$



Assumes α_B is a constant (isothermal)

Cosmological Stromgren Spheres

Shapiro & Giroux (1987)

- In an expanding universe

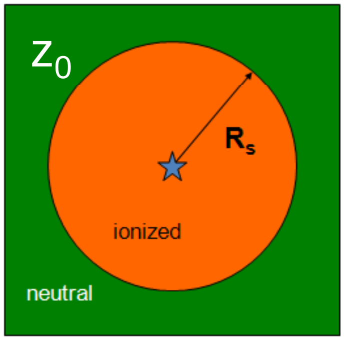
$$n_H = n_{H,0}\left(\frac{a_0}{a}\right)^3 = n_{H,0}\left(\frac{1+z}{1+z_0}\right)^3$$

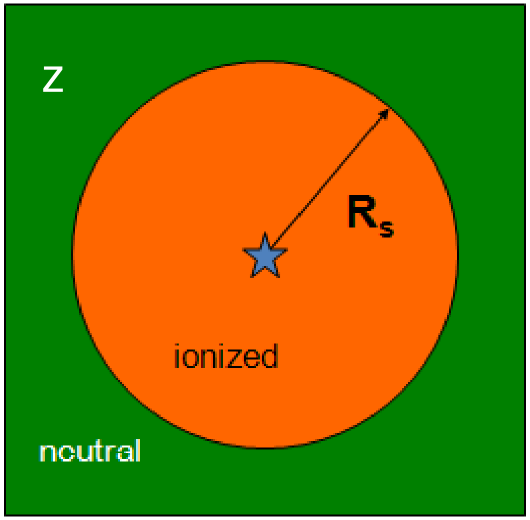
$$\frac{4\pi}{3}R_S^3 n_H^2 \alpha_B = \dot{N}_\gamma$$

$$R_S = \left(3\dot{N}_\gamma \Big/ 4\pi n_{\rm H}^2 \alpha_B\right)^{1/3} = R_{S,0}\left(\frac{a(t)}{a_0}\right)$$

many Mpc for luminous QSO

all quantities are *proper*





CSS Time-dependent Solution

Shapiro & Giroux (1987)

No. 2, 1987 COSMOLOGICAL H II REGIONS L109

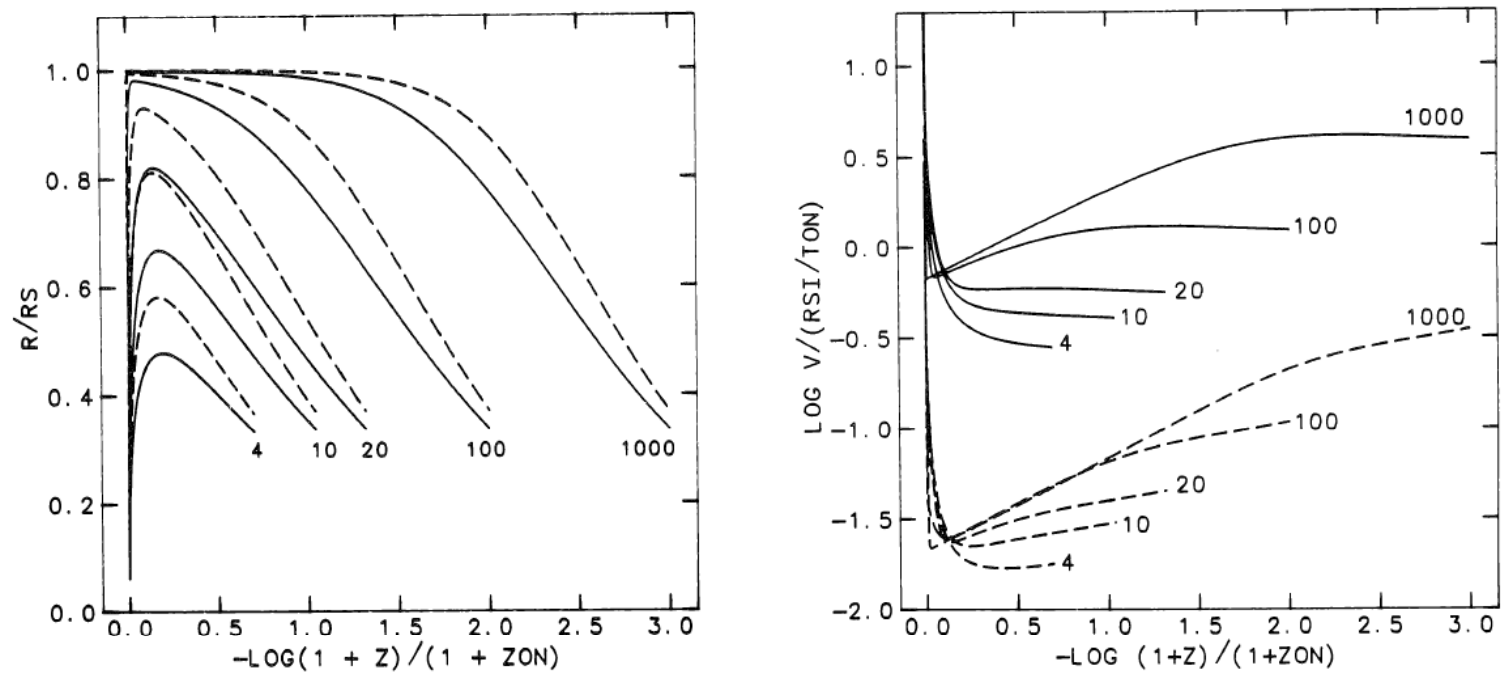


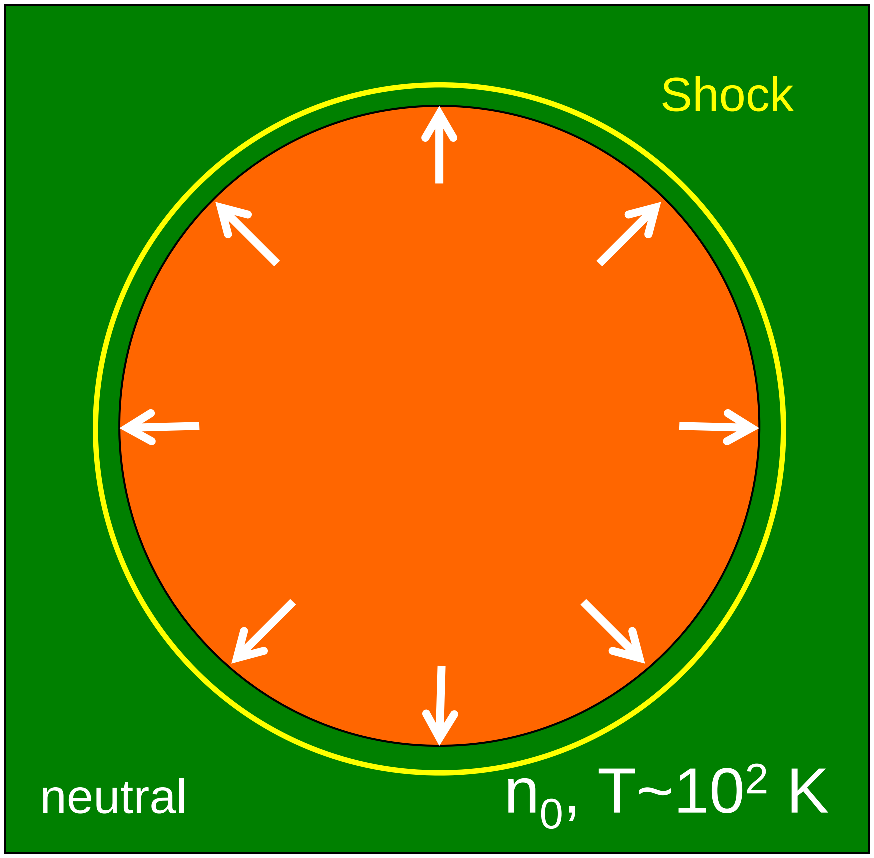
FIG. 1*a* FIG. 1*b*

FIG. 1.—(*a*) $r_I(t)/r_S(t)$ is plotted against redshift, where "ZON" is z_i, and $c_l\Omega_b h = 0.1$ is assumed. We take $\alpha_2 = 2.6 \times 10^{-13}$ cm^3 s^{-1} and $\chi_{\rm eff} = 1$ for all of the figures in this *Letter*. Curves are labeled with the value of z_i. Solid lines correspond to $q_0 = 0.5$, dashed to $q_0 = 0.05$. (*b*) Same as (*a*), except $v_{\rm pec}/(r_{S,i}/t_i)$ is plotted. Curves for $q_0 = 0.05$ case have been displaced downward for visual clarity, so quantity plotted is $\log_{10}[v_{\rm pec}/(r_{S,i}/t_i)] - 1.5$.

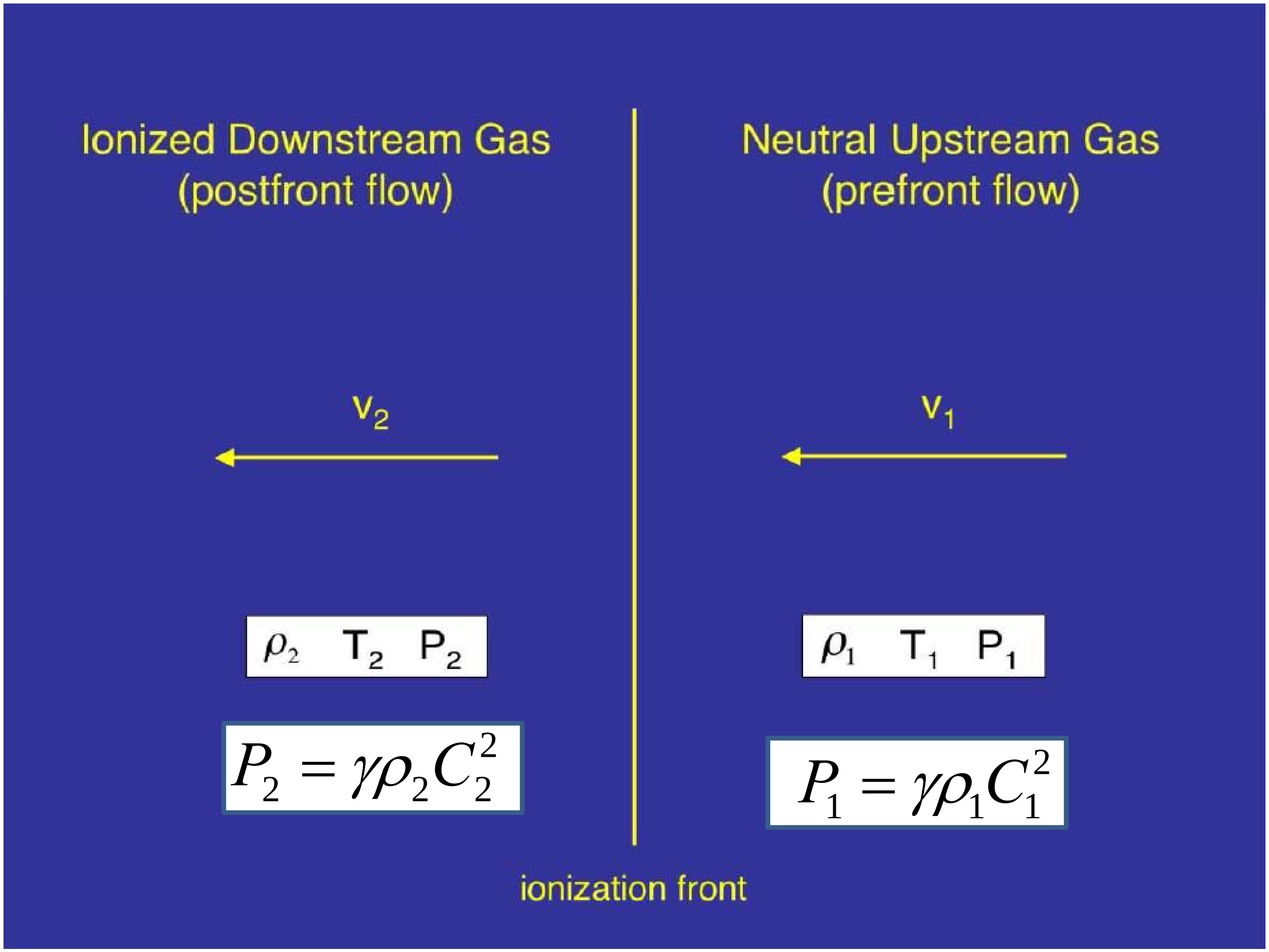
- Analytical solution; ignores cosmological redshift of ionizing source
- Most QSO I-fronts never reach their Stromgren radius

Dynamic HII Regions

- Stromgren sphere is manifestly out of pressure equilibrium
- $P_{inside}/P_{outside}$~200
- Drives expansion
- As HII region expands, mean density drops, reducing internal recombinations
- $R_s \sim (n_e n_p)^{-1/3}$ increases



I-front jump conditions



Types of I-fronts

Kahn (1954)

$$\rho_2 \upsilon_2 = \rho_1 \upsilon_1 (= \overline{m} j_{ph}) \qquad \text{conservation of mass and photons}$$

$$\rho_2 \upsilon_2^2 + P_2 = \rho_1 \upsilon_1^2 + P_1 \qquad \text{conservation of fluid moment}$$

$$\rho_2 (\upsilon_2^2 + C_2^2) = \rho_1 (\upsilon_1^2 + C_1^2)$$

$$\upsilon_2^2 - \left(\upsilon_1 + \frac{C_1^2}{\upsilon_1} \right) \upsilon_2 + C_2^2 = 0 \Rightarrow \text{real solutions only if } \left(\upsilon_1 + \frac{C_1^2}{\upsilon_1} \right) > 2C_2$$

$$\upsilon_1^2 - 2C_2 \upsilon_1 + C_1^2 = f(\upsilon_1) > 0 \quad \text{quadratic equation for } \upsilon_1$$

2 roots:

$$\upsilon_D = C_2 - (C_2^2 - C_1^2)^{1/2} \approx \frac{C_1^2}{2C_2} \qquad \text{D - type} \quad \text{(Dense)}$$

$$\upsilon_R = C_2 + (C_2^2 - C_1^2)^{1/2} \approx 2C_2 \qquad \text{R - type} \quad \text{(Rarified)}$$

Properties of I-fronts

- weak R-type
  - Propagate *supersonically* WRT to both upstream and downstream gas
  - Essentially *no hydrodynamic coupling* to gas
- weak D-type
  - Propagate *supersonically* WRT to upstream gas but *subsonically* WRT downstream gas
  - Therefore pressure difference *drives a shockwave* into the upstream gas
  - *Strongly coupled hydrodynamically*

In Pictures

Weak R-type

I-front →

ionized

$$\rho_2 \approx \rho_1, T_2 \approx 10^4 K, \quad \upsilon_2 \approx 0$$

neutral

$$\rho_1, T_1, \quad \upsilon_1 = 0$$

Weak D-type

I-front → S-front →

ionized

$$\rho_2 << \rho_3, T_2 \approx 10^4 K, \quad \upsilon_2 < \upsilon_3$$

neutral

neutral

$$\rho_1, T_1, \quad \upsilon_1 = 0$$

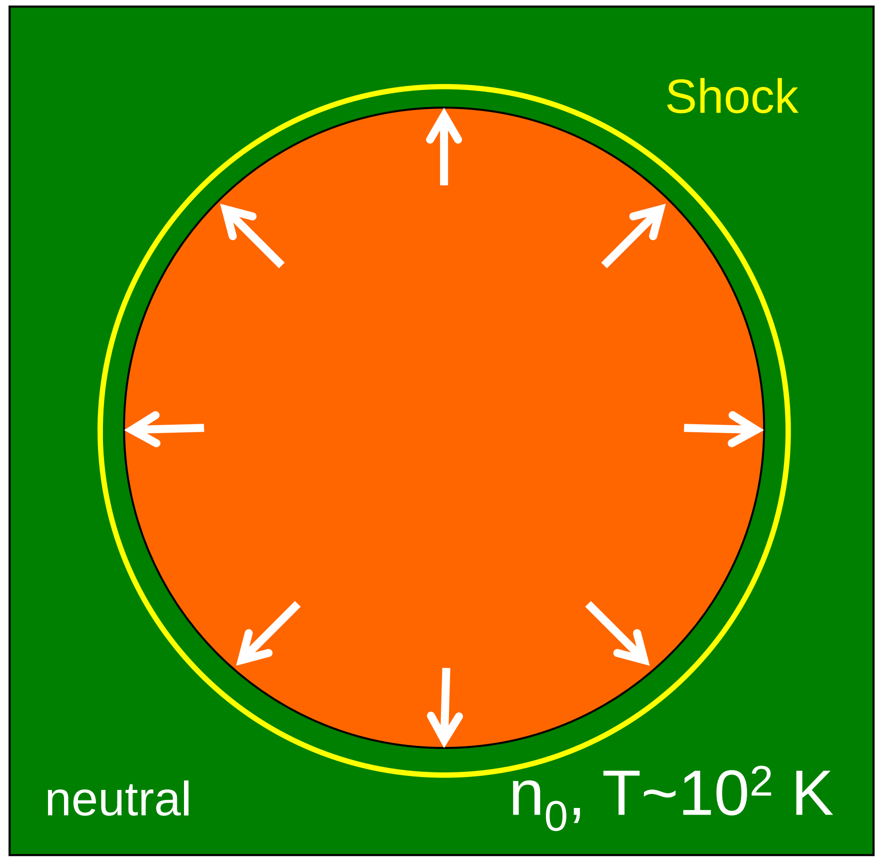
$$\rho_3 > \rho_1, T_3 > T_1, \quad \upsilon_S > \upsilon_3 > 0$$

Dynamic HII Regions:
Pressure-driven expansion phase

- Offset power-law solution (Spitzer 1978)

$$r_i(t) = R_S\left(1 + \frac{4}{7}\frac{C_2 t}{R_S}\right)^{4/7}$$

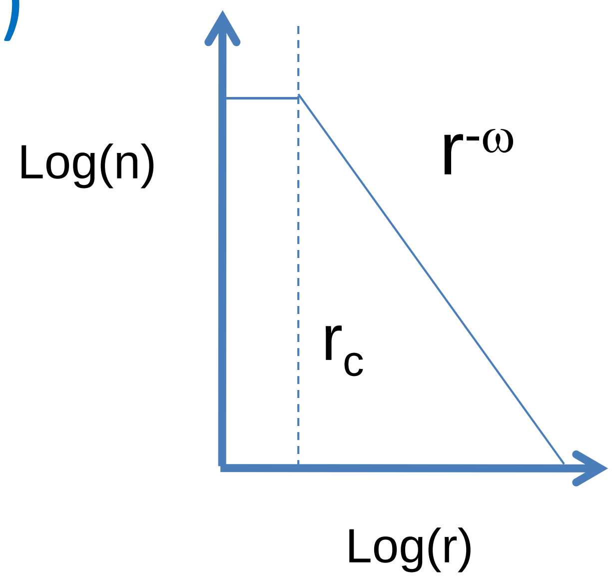
- Summary of I-front phases
  - Weak R ➔
  - Critical R ➔
  - Critical D ➔
  - Weak D ➔
  - Pressure equilibrium with ISM



I-fronts in Power-law Density Fields

Franco et al. (1990)

$$n_H(r) = \begin{cases} n_c & r \le r_c \\ n_c (r/r_c)^{-\omega} & r > r_c \end{cases}$$



$$\omega_{crit} = \frac{3}{2}\left[1 - \left(\frac{r_c}{R_S}\right)^3\right]^{-1}$$

$\omega < \omega_{crit}$ I-front becomes D-type at modifed Stromgren radius

$$R_\omega = R_S \left[\frac{3-2\omega}{3} + \frac{2\omega}{3}\left(\frac{r_c}{R_S}\right)^3\right]^{1/(3-2\omega)} \left(\frac{R_S}{r_c}\right)^{2\omega/(3-2\omega)}$$

$\omega > \omega_c$ I-front remains R-type and "flash ionizes" the cloud

However, if $r_c \approx R_s$, can have R $\Rightarrow$ D $\Rightarrow$ R

Expansion of the "core shock"

- For $\omega > \omega_c$, after the cloud has been "flash ionized", it has a huge pressure gradient since $P(r)=n(r)k*10^4$ K
- Leads to an expansion wave at ~14 km/s which steepen into a shock "core shock"

$$\omega_{crit} < \omega < 3$$

$$r_c(t) \approx r_c + \left[1 + \left(\frac{3}{3-\omega}\right)^{1/2}\right] C_{II} t$$

$$\omega = 3$$

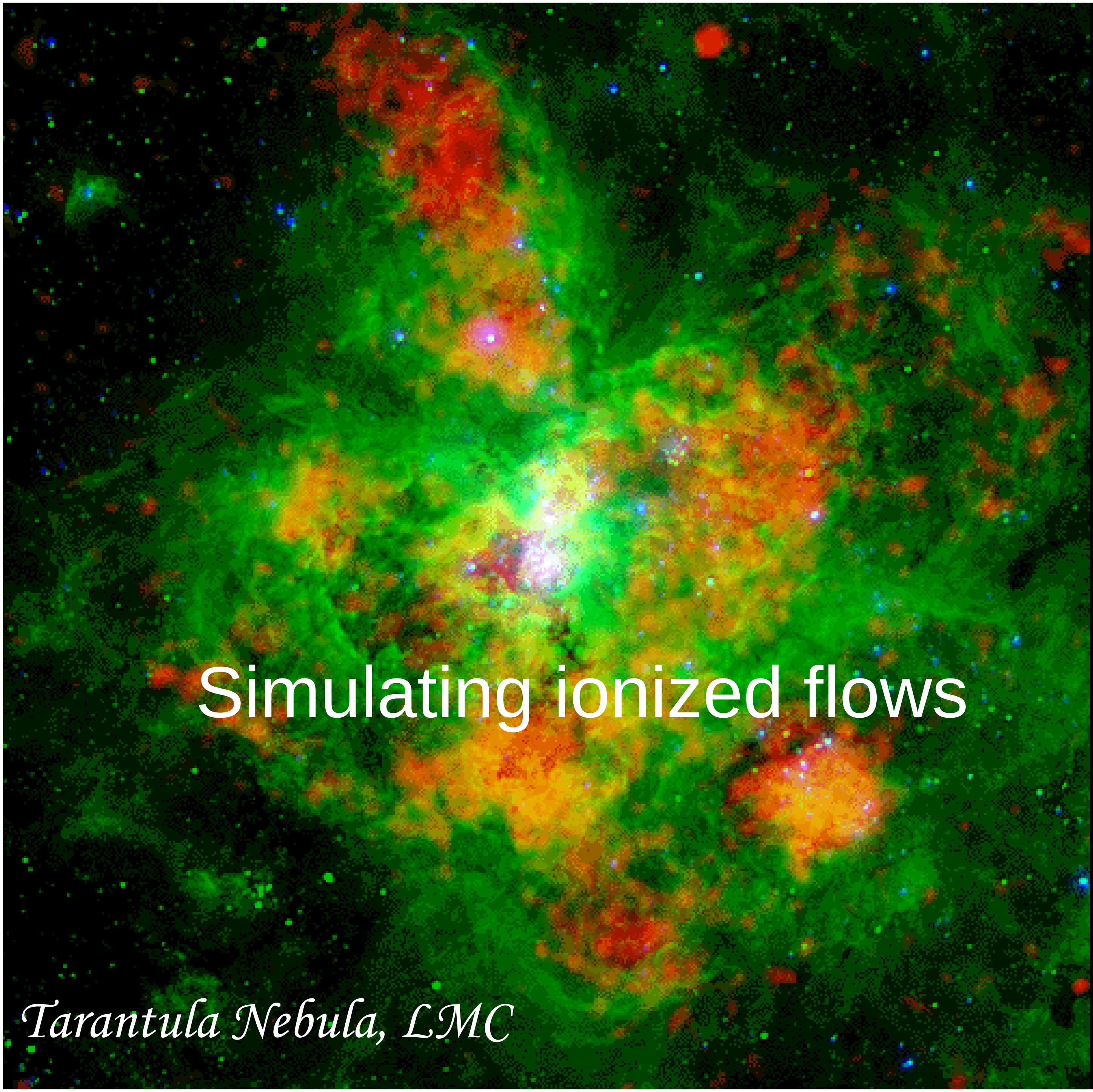
$$r_c(t) \approx 3.2 r_c \left(\frac{C_{II} t}{r_c}\right)^{1.1}$$

$$\omega > 3$$

$$r_c(t) \approx r_c \left[1 + \left(\frac{4}{\omega-3}\right)^{1/2} \left(\frac{\delta+2-\omega}{2}\right)\left(\frac{C_{II} t}{r_c}\right)\right]^{2/(\delta+2-\omega)}$$

$$\delta \approx 0.55(\omega-3) + 2.8$$

Franco et al. (1990)



X-ray emitting
hot gas (shocks)

Ionized hydrogen

UV sources

Simulating Ionized Flows: Governing Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{\upsilon}) = 0$$ mass conservation

$$\frac{\partial \rho \vec{\upsilon}}{\partial t} + \nabla \cdot (\rho \vec{\upsilon} \vec{\upsilon}) = -\nabla P - \rho \nabla \phi$$ momentum conservation

$$\frac{\partial e}{\partial t} + \nabla \cdot (e \vec{\upsilon}) = -P \nabla \cdot (\vec{\upsilon}) + \rho (G - \Lambda)$$ energy conservation

$$\frac{d\rho_i}{dt} + \nabla \cdot (\rho_i \vec{\upsilon}) = \pm \sum_j \sum_l \alpha_{jl}(T) \rho_j \rho_l \pm \sum_j I_j \rho_j$$ species advection-reaction

$$\nabla^2 \phi = 4\pi G \rho$$

$$I_j = \int_{\nu_{th},j}^{\infty} d\nu \cdot \sigma_{PI,j}(\nu) \frac{E_\nu}{h\nu}, \quad G_j = \int_{\nu_{th},j}^{\infty} d\nu \cdot \sigma_{PI,j}(\nu) \frac{E_\nu}{h\nu} (h\nu - h\nu_{th,j})$$

$$P = (\gamma - 1) e = k_B T \sum_i n_i \ , \quad \rho = \sum_i m_i n_i, \quad \Lambda = \Lambda(T) \ \text{ cooling curve}$$

$\alpha_{jl}(T)$ are 2-body reaction rates (temperature-dependent)

Solution Methods: ZEUS-MP/2-MFRT

Whalen & Norman (2006)

Transport Step

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{\upsilon}) = 0$$

$$\frac{\partial \rho \vec{\upsilon}}{\partial t} + \nabla \cdot (\rho \vec{\upsilon} \vec{\upsilon}) = 0$$

$$\frac{\partial e}{\partial t} + \nabla \cdot (e \vec{\upsilon}) = 0$$

$$\frac{d\rho_i}{dt} + \nabla \cdot (\rho_i \vec{\upsilon}) = 0$$

done in integral form using finite volumes as described in Stone lecture 2

Source Step

$$\frac{\partial \rho \vec{\upsilon}}{\partial t} = -\nabla P - \nabla \cdot \overleftrightarrow{Q} - \rho \nabla \phi$$

$$\frac{\partial e}{\partial t} = -P\nabla \cdot (\vec{\upsilon}) + \rho (G - \Lambda)$$

$$\nabla^2 \phi = 4\pi \mathrm{G} \rho$$

$$\frac{d\rho_i}{dt} = \pm \sum_j \sum_l \alpha_{jl}(T) \rho_j \rho_l \pm \sum_j I_j \rho_j$$

rate equations for stiff system of ODEs; semi-implicit scheme of Anninos et al. (1997)

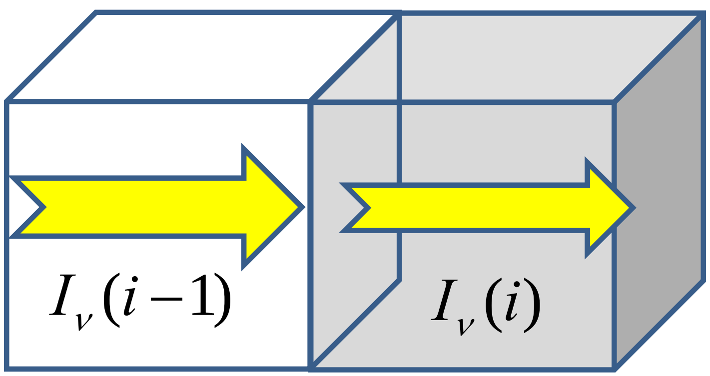
Photon-conserving radiative transfer and ionization

Abel, Norman & Madau (1999), Whalen & Norman (2006)

Idea: convert each photon removed from the beam into an ionized atom
Benefit: I-fronts propagate at the correct speed *independent of resolution*

$$\tau_\nu(i) = n_H(i)\sigma_H^{ion}(\nu)\Delta x$$

$$\Delta I_\nu(i) = 1 - e^{-\tau_\nu(i)}$$



cell i-1 cell i

$$I_\nu(i) = I_\nu(i-1) - \Delta I_\nu(i)$$

Ionization accounting in cell i

#ionizing photons absorbed

$$N_{abs} = \int_{\nu_{th}}^{\infty} \frac{\Delta \mathrm{I}_\nu}{h\nu} d\nu \times Area$$

photon conservation

$$N_{ion} = N_{abs}$$

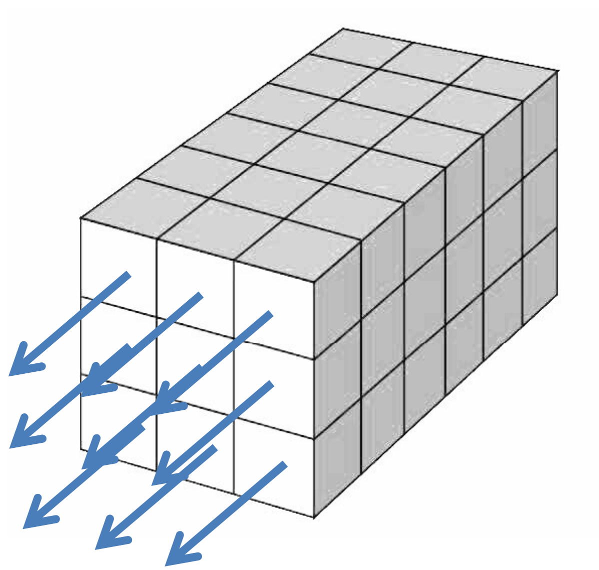
rate equation

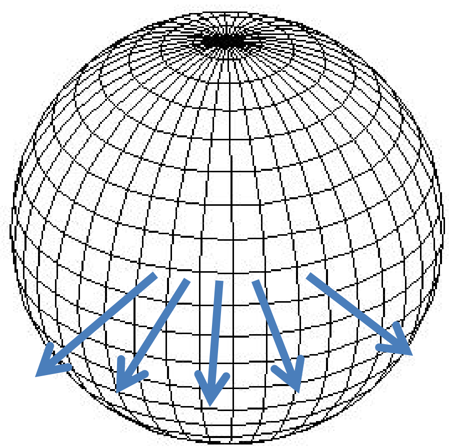
$$\frac{\mathrm{dn_H}}{\mathrm{dt}} = -k_{PI}\mathrm{n_H} \Rightarrow \frac{n_H^{n+1} - n_H^n}{\Delta t} = \frac{N_{ion} / Volume}{\Delta t}$$

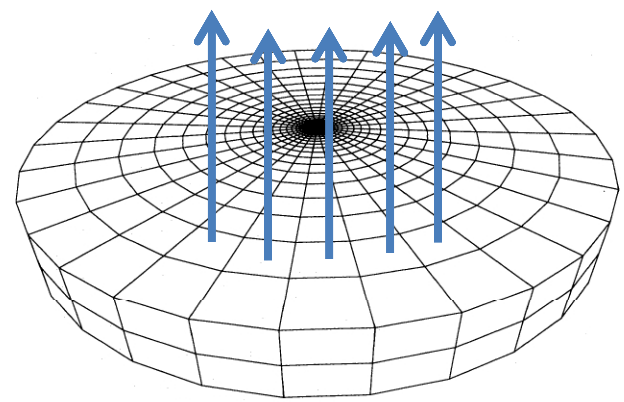
$$\therefore k_{PI} = \frac{N_{ion} / Volume}{n_H^n \Delta t} = \int_{\nu_{th}}^{\infty} \frac{1 - e^{-\tau_\nu}}{h\nu} d\nu \times \frac{1}{n_H^n \Delta x \Delta t}$$

ZEUS-MP/2 grid options: 1D, 2D, 3D

http://lca.ucsd.edu/portal/codes/zeusmp2



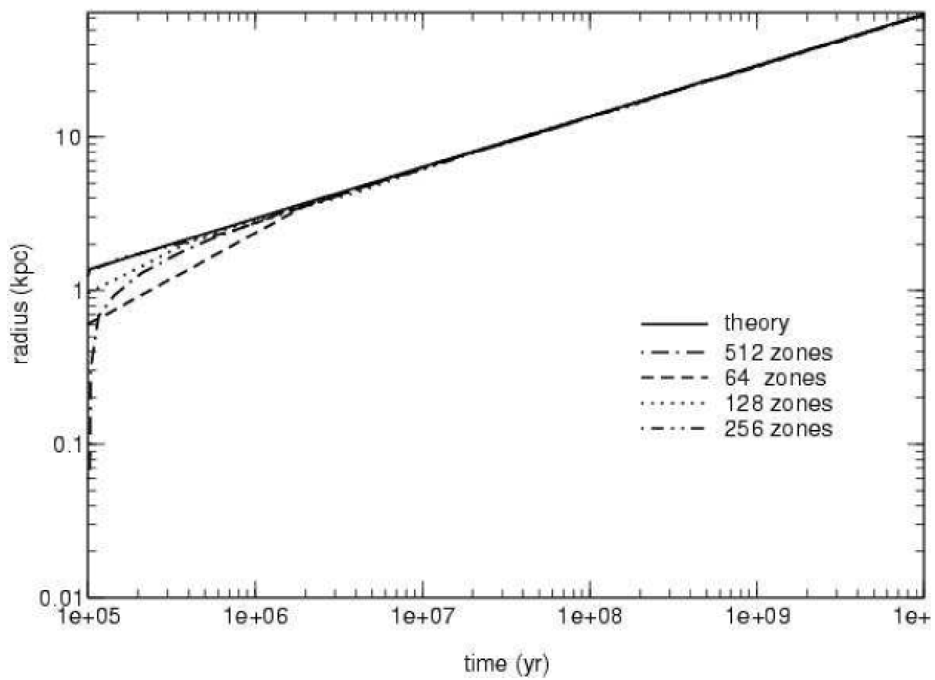




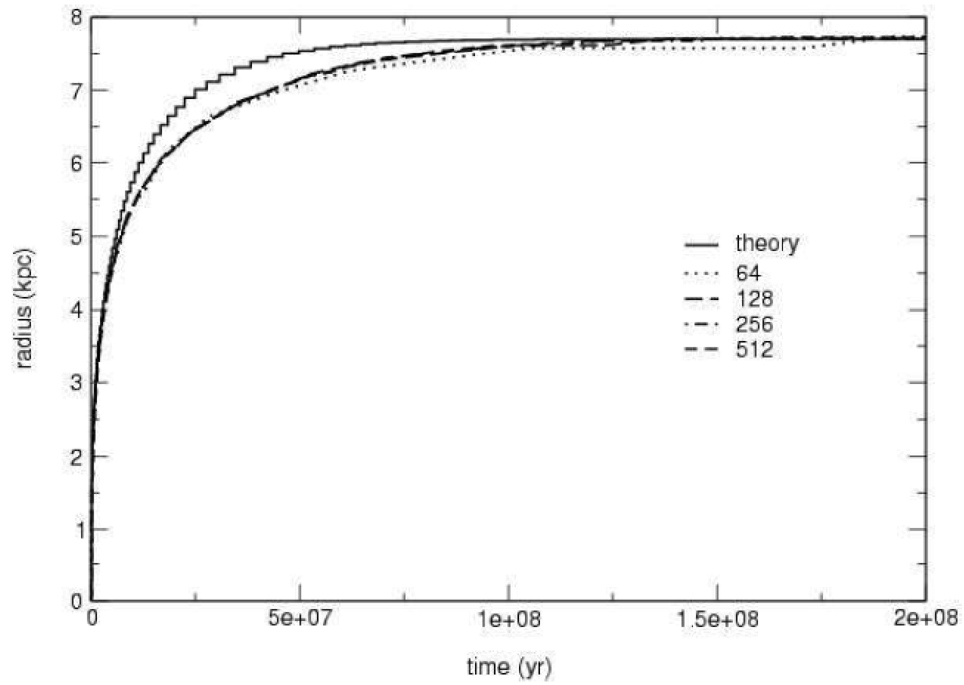
- rays are cast parallel to radial coordinate for point source radiation
- rays are cast parallel x or z axis for plane wave illumination

Uniform Static Medium Verification Tests

no recombinations

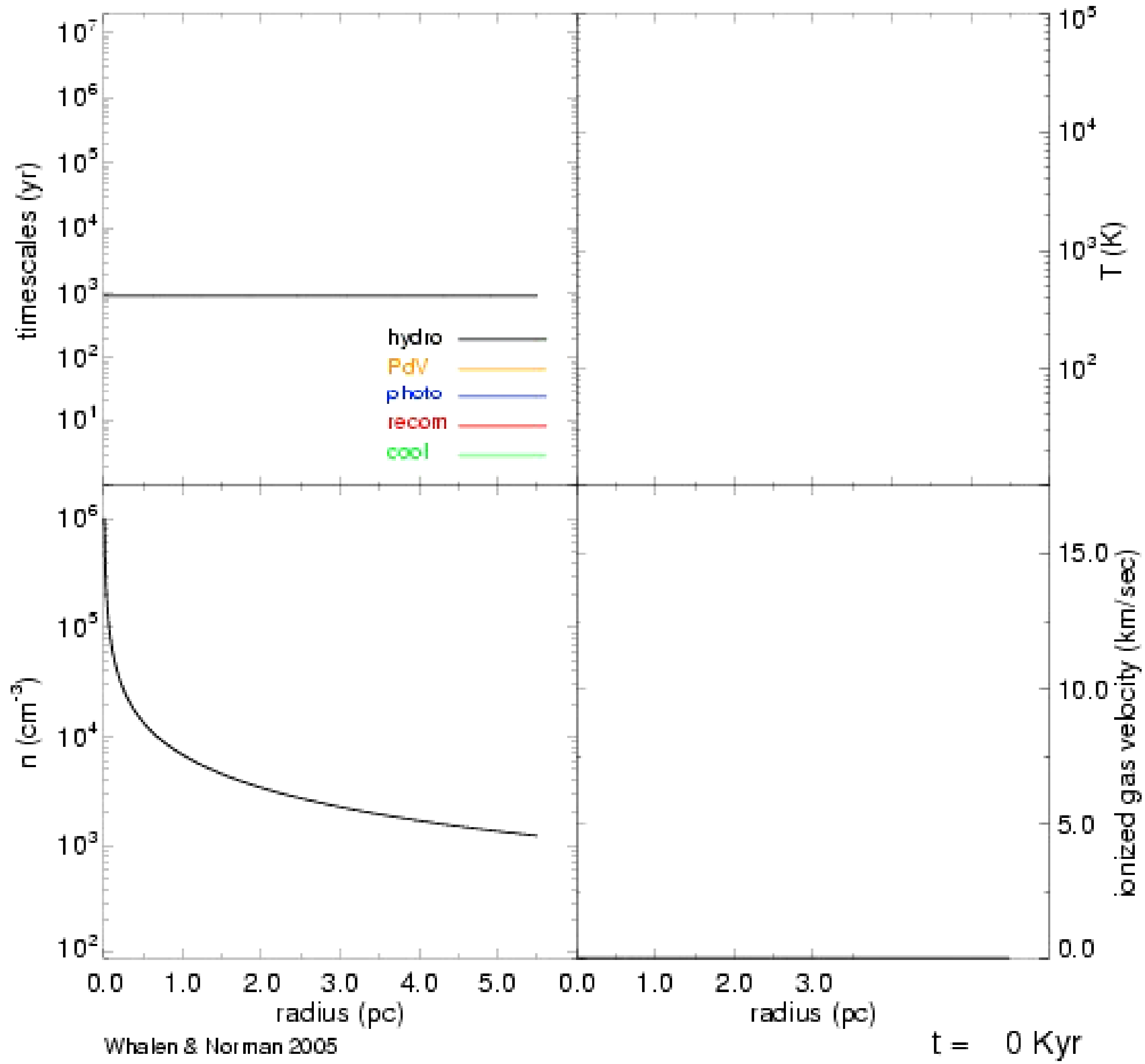


recombinations



Whalen & Norman (2006)

Ionized Flow Dynamics: r^{-1} Density Field



Adaptive Subcycling

Whalen & Norman (2006)

THREE TIMESCALES FOR A CELL

$$t_{chem} = \frac{n_e}{\dot{n}_e}, \quad t_{heat/cool} = \frac{e_{gas}}{\dot{e}_{rad}}, \quad t_{CFL} = \frac{\Delta x}{|c_s + \upsilon|}$$

ALGORITHM

1. radiative transfer solver to compute $k_{ph}\{i\}$
2. compute $t_{heat/cool} = 0.1 * \min\{t_{heat/cool}(i)\}$
3. compute $t_{CFL} = C * \min\{t_{CFL}(i)\}$
4. $t_{hydro} = \min\{t_{heat/cool}, t_{CFL}\}$
5. compute $t_{chem} = 0.1 * \min\{t_{chem}(i)\}$
6. if $(t_{chem} < t_{hydro})$

   then a) subcycle over RT and chemistry/heating until $t = t_{hydro}$

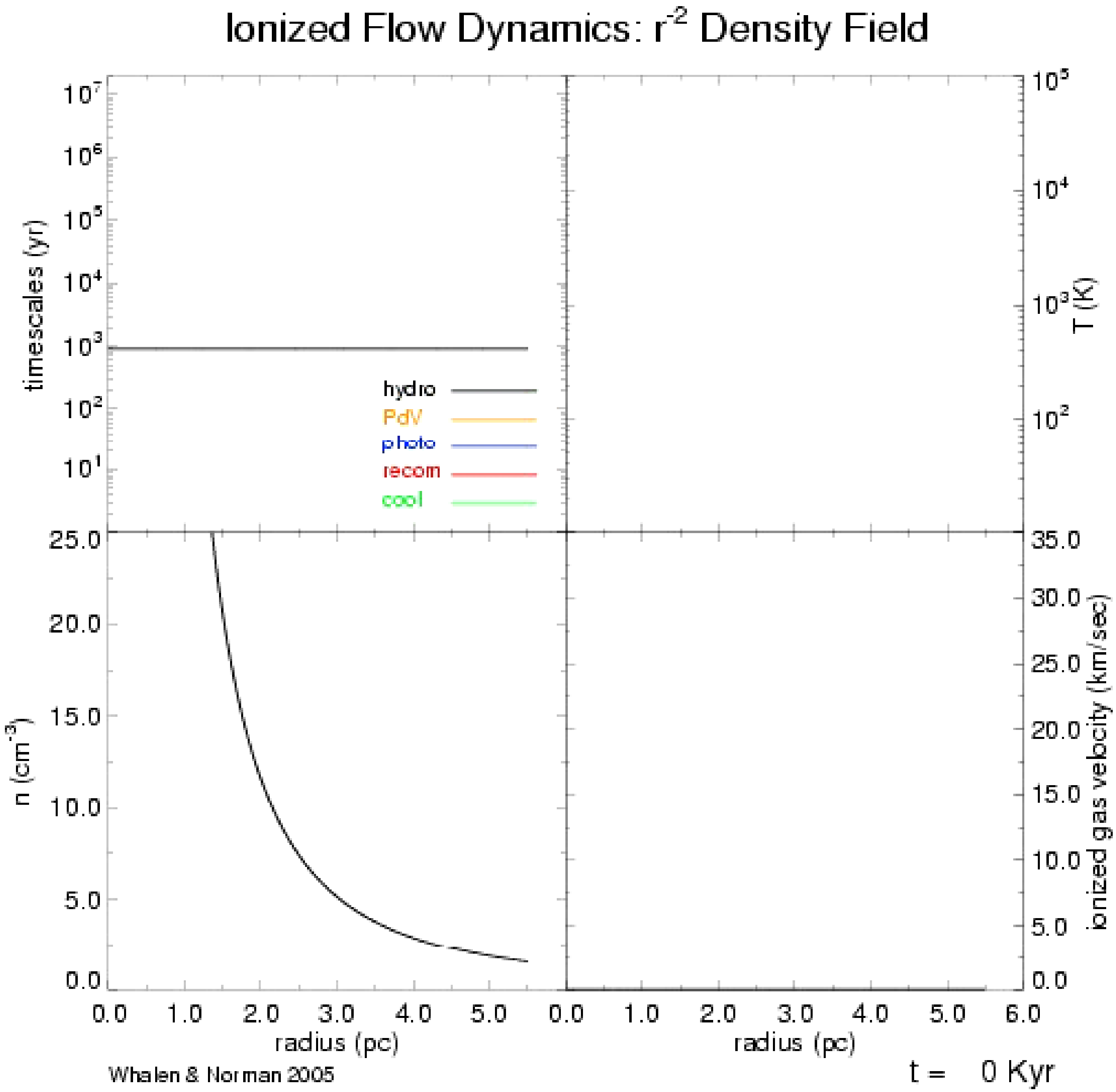
   b) take next hydro step

   c) go to 1.

   else a) take one chemistry/heating step using t_{hydro}

   b) take next hydro step

   c) go to 1.

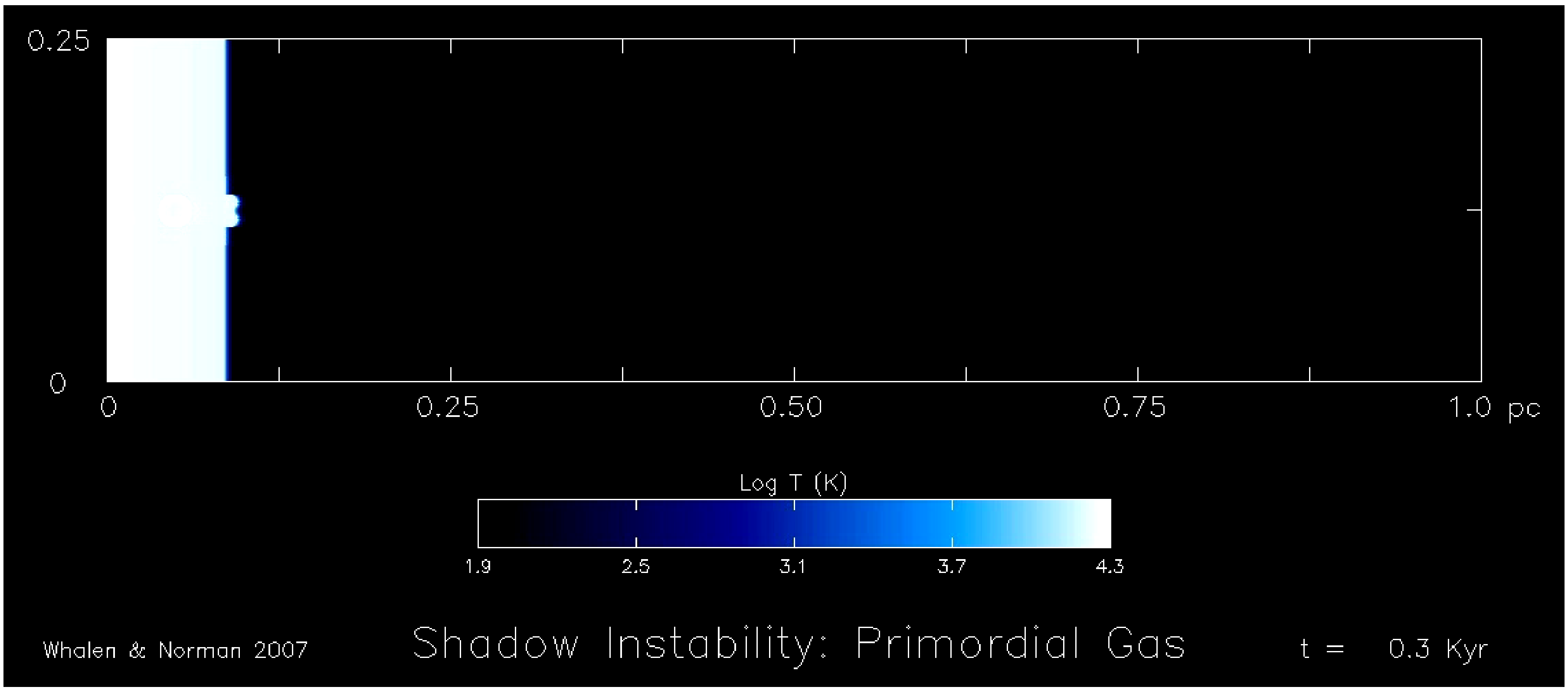

Ionized Flow Dynamics: r^-2 Density Field
timescales (yr)
10^7
10^6
10^5
10^4
10^3
10^2
10^1
hydro
PdV
photo
recom
cool
10^5
10^4
10^3
10^2
T (K)
n (cm^-3)
25.0
20.0
15.0
10.0
5.0
0.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
ionized gas velocity (km/sec)
0.0 1.0 2.0 3.0 4.0 5.0
radius (pc)
0.0 1.0 2.0 3.0 4.0 5.0 6.0
radius (pc)
Whalen & Norman 2005
t = 0 Kyr


Tarantula Nebula, LMC
I-front instabilities

Shadow Instability (R-type)

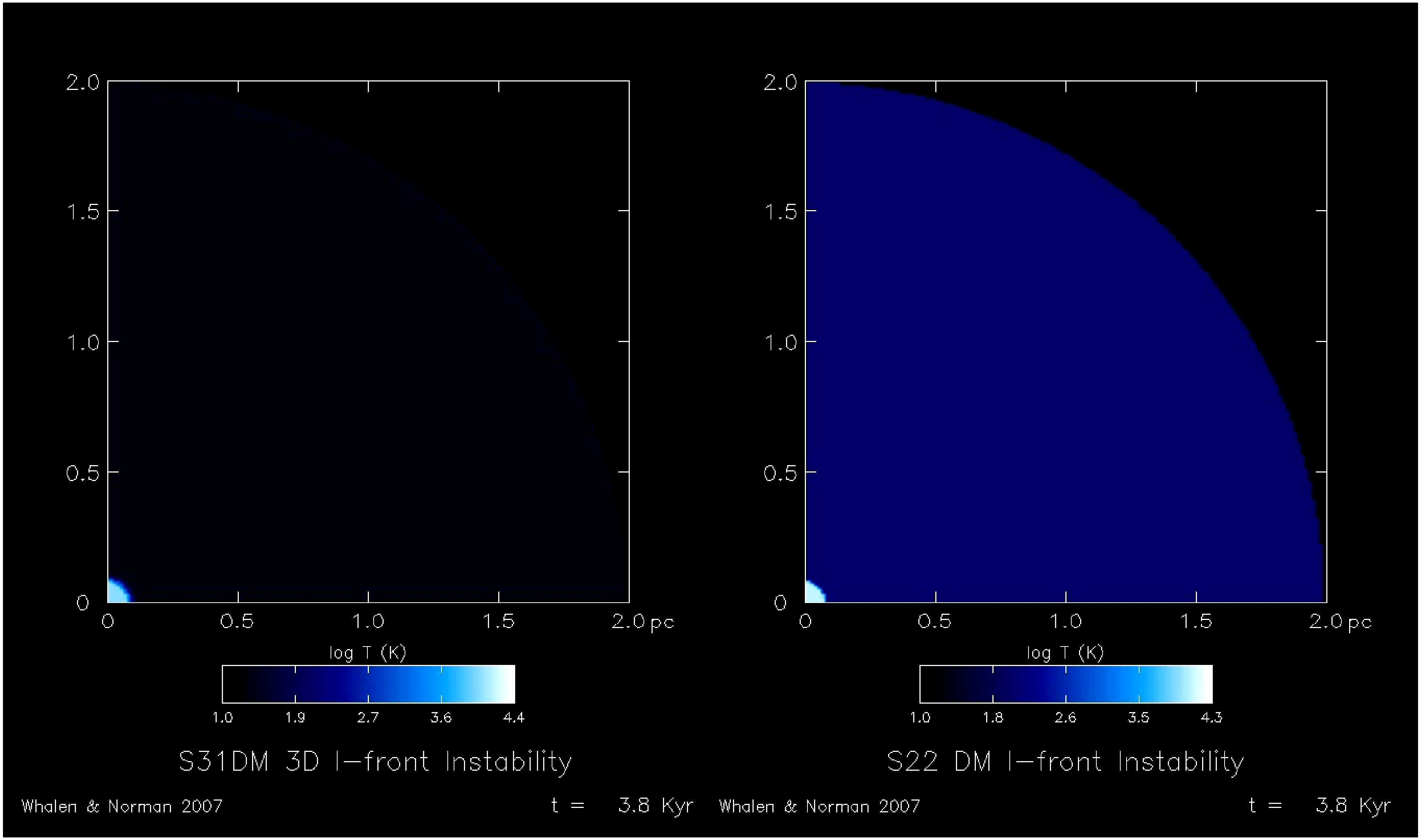
O(1) density inhomogeneities modulate speed of R-type fronts rippling surface

Violent instabilities ensue when front transitions to D-type



Whalen & Norman (2008)

Thin Shell Instability (D-type)



Whalen & Norman (2008)

I-Front Structure

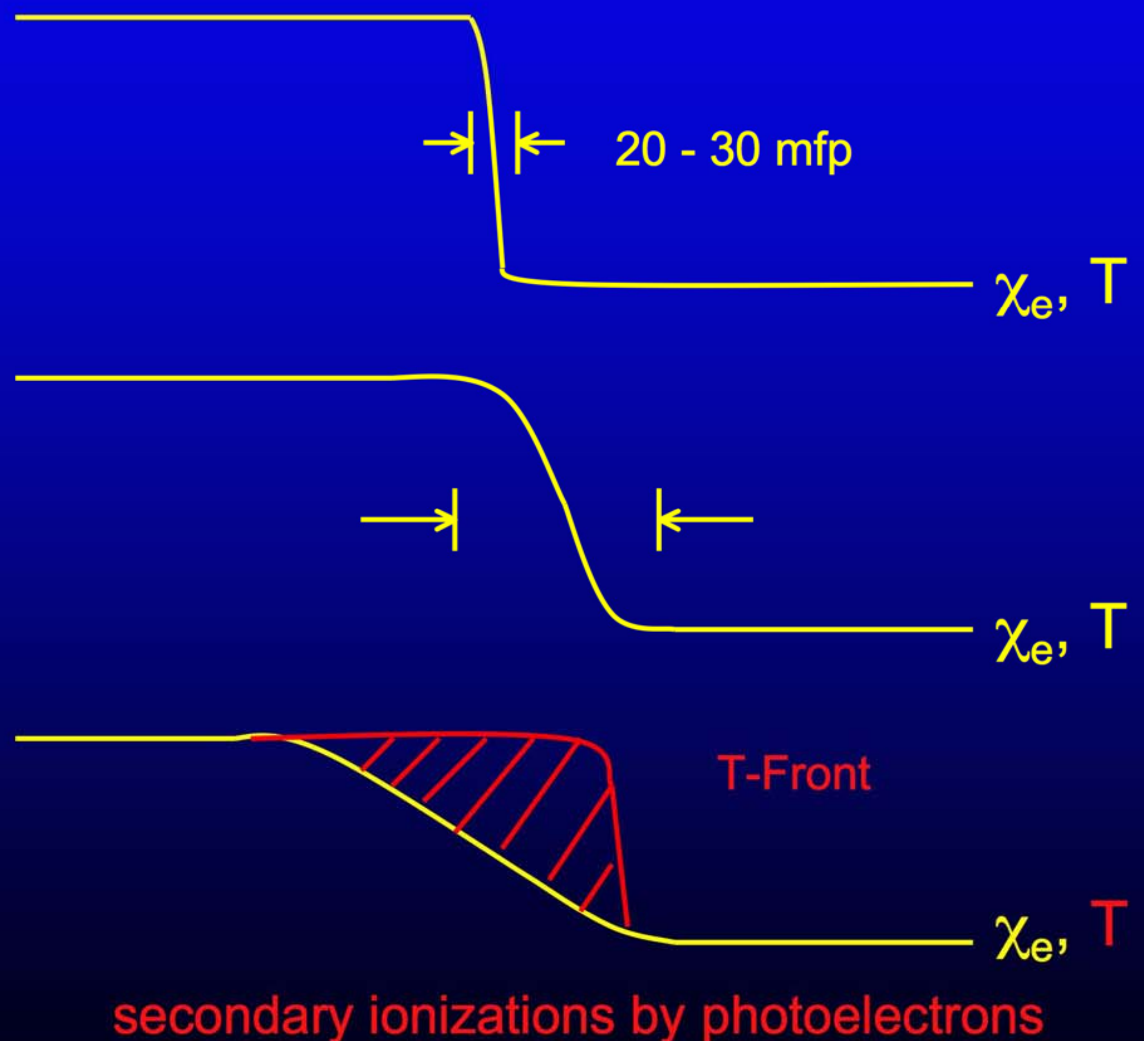
$$H + e^- \rightarrow H^- + \gamma \qquad H^- + H \rightarrow H_2 + e^-$$

$$H^+ + H \rightarrow {H_2}^+ + \gamma \qquad {H_2}^+ + H \rightarrow H_2 + H^+$$

monoenergetic:

10^5 K blackbody:

quasar:



3D Cosmological Radiative Transfer

Cosmological Radiative Transfer Equation

cosmological redshift

cosmological expansion

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \frac{\hat{n}\cdot\nabla I_\nu}{a} - \frac{H(t)}{c}\left(\nu\frac{\partial I_\nu}{\partial \nu} - 3I_\nu\right) = \eta_\nu - \chi_\nu I_\nu$$

$$a(t) \equiv \frac{1}{1+z} \quad \text{cosmic scale factor}$$

$$H(t)^2 \equiv \left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3}\rho - \frac{k}{a^2} + \frac{\Lambda}{3} \quad \text{Friedmann Eq.}$$

Spatial gradients WRT coordinates comoving with expanding universe

Local Approximation

- Prior to complete reionization, size of individual ionized bubbles small compared with cosmic horizon

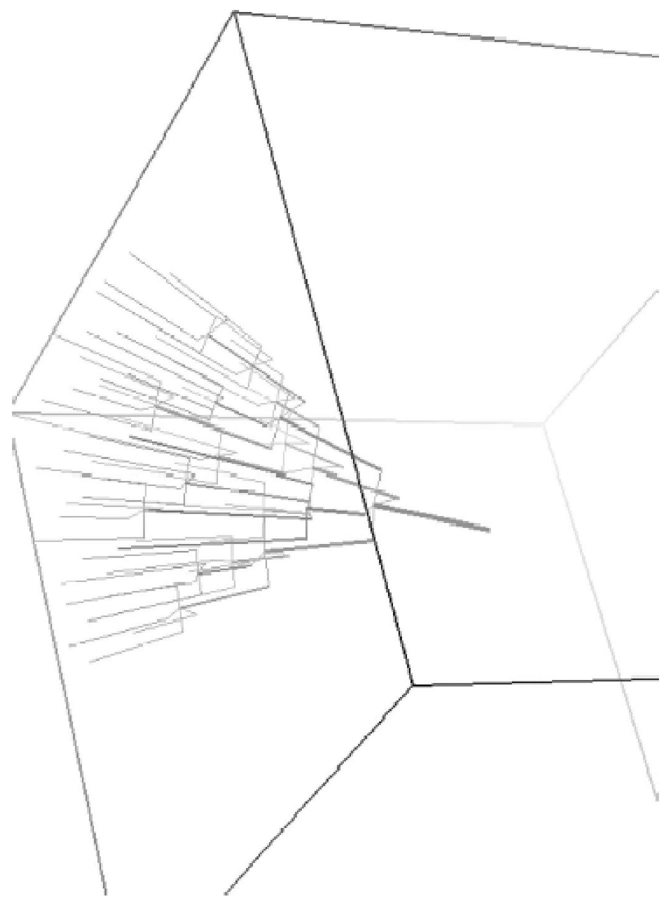
$$\left[\nabla_x\right] \propto \lambda_{mfp}^{-1}, \quad \left[\frac{H(t)}{c}\right] = L_H^{-1} << \lambda_{mfp}^{-1}$$

$$\bar{a} \approx 1$$

$$\therefore \frac{1}{c}\frac{\partial I_\nu}{\partial t} + \hat{n} \cdot \nabla_x I_\nu = \eta_\nu - \chi_\nu I_\nu$$

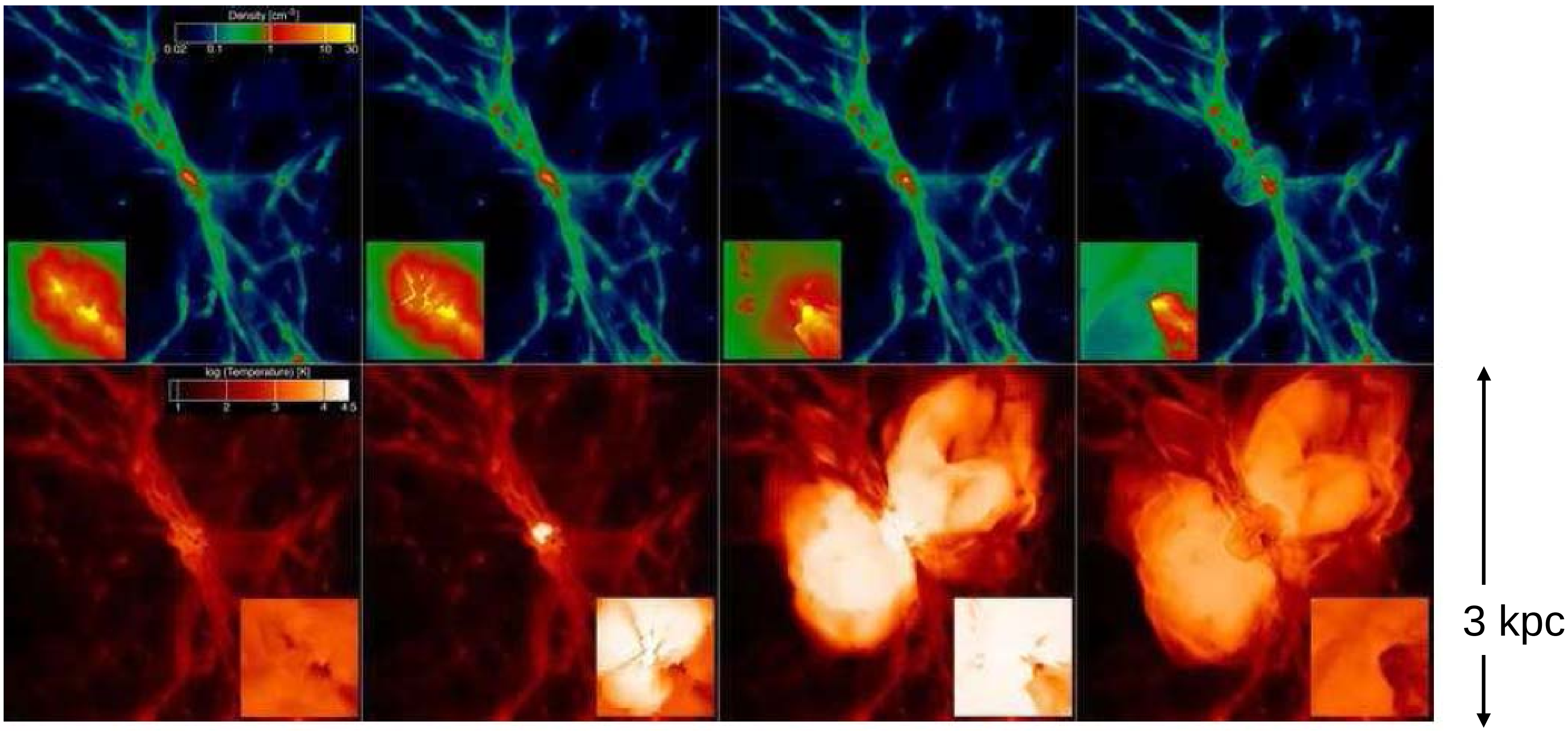
Methods for 3D RT used in Reionization Simulations

- Adaptive Ray-tracing
  - Abel & Wandelt (2002)
  - Razoumov & Cardall (2005)
  - Mellema et al. (2006)
- Monte Carlo
  - Ciardi et al. (2001)
  - Maselli et al. (2003)
- Moment Methods
  - Gnedin & Abel (2001)
  - Paschos, Norman & Bordner (2006)



Abel & Wandelt (2002)

HII Region in AMR Simulation of Pop III Star Formation



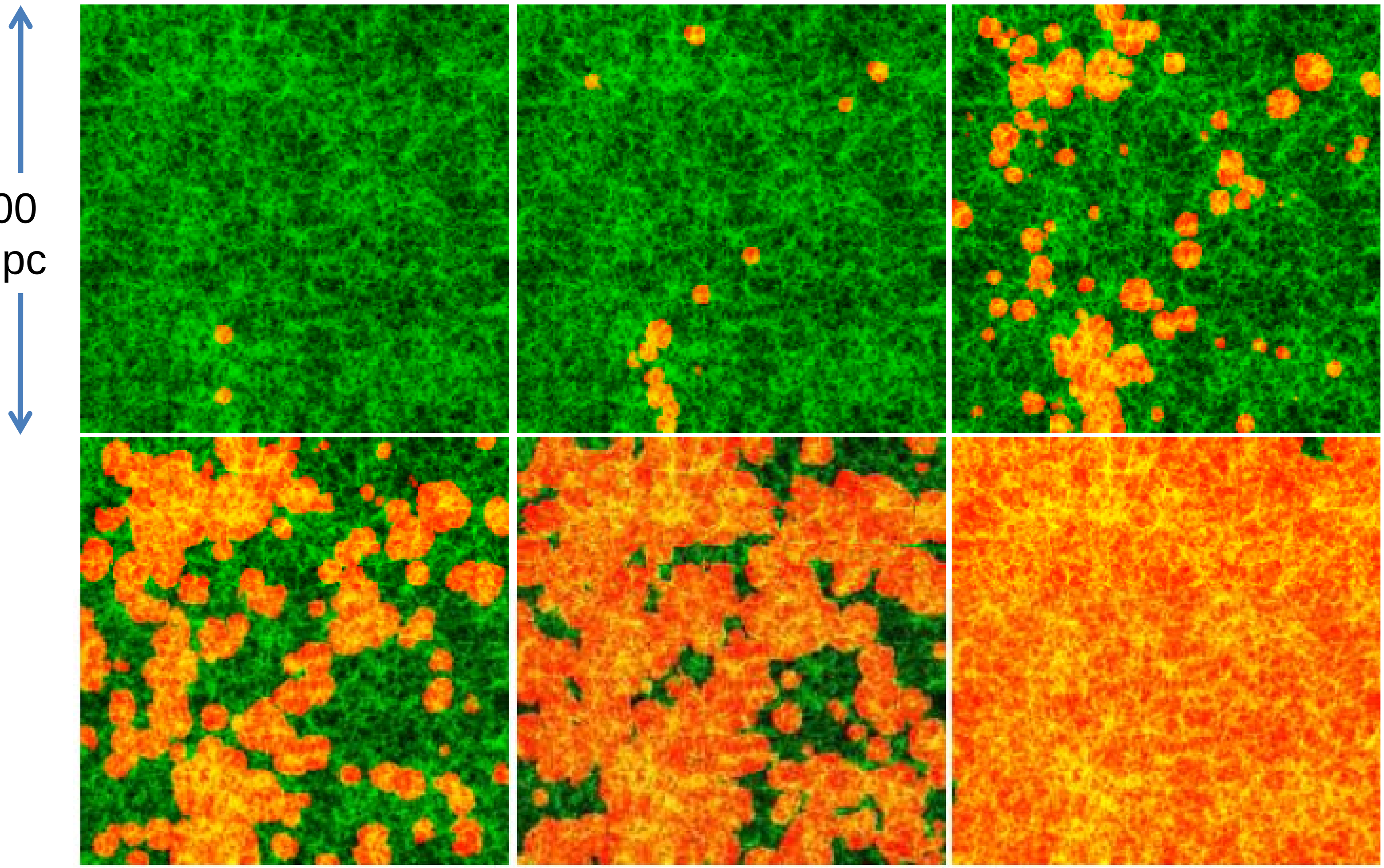
Abel, Wise & Bryan (2006)

Post-processing N-body density fields

(large volumes)

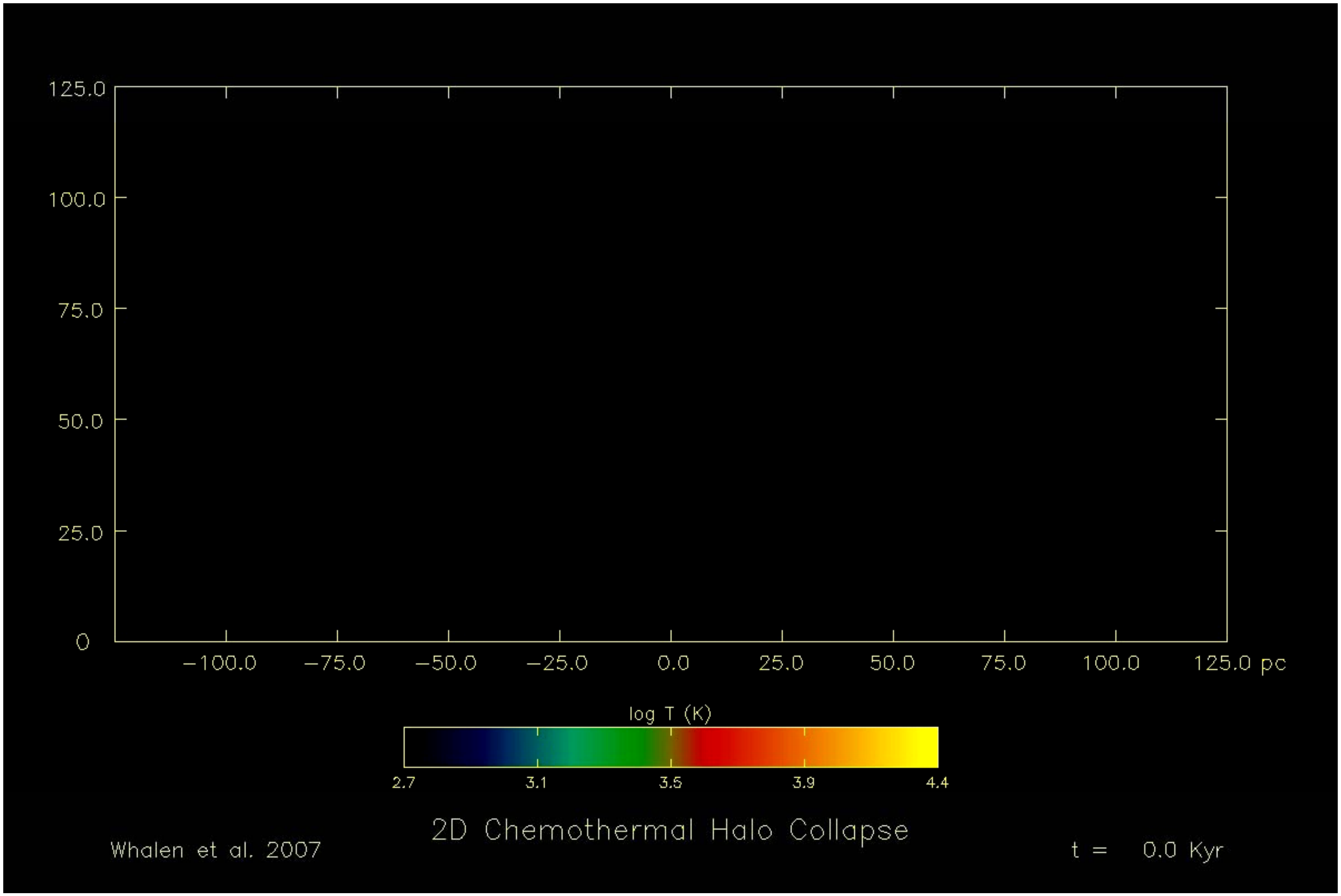
- I-fronts are assumed to be weak R-type everywhere
- Cost is proportional to N_{source}

200 Mpc



Iliev et al. (2006)

I-front "trapping"



Moment Methods: VTEF

- combine 0^{th} + 1^{st} angular moments of the time-dependent monochromatic transfer equation
- second order closure using Eddington tensor

$$\frac{\partial E_\nu}{\partial t} = \nabla \cdot \left(\frac{c}{\chi_\nu} \nabla \cdot \overleftrightarrow{P}_\nu\right) + \eta_\nu - c\kappa_\nu E_\nu$$

$$\overleftrightarrow{P}_\nu = \overleftrightarrow{f} E_\nu \quad \text{Eddington closure}$$

$$\Rightarrow \frac{\partial E_\nu}{\partial t} = \nabla \cdot \left(\frac{c}{\chi_\nu} \nabla \cdot \overleftrightarrow{f}_\nu E_\nu\right) + \eta_\nu - c\kappa_\nu E_\nu$$

$$f_{ij}(\vec{x}) = \frac{\oint_\Omega I(\vec{n},\vec{x}) n_i n_j \, d\Omega}{\oint_\Omega I(\vec{n},\vec{x}) \, d\Omega}, \quad \text{Eddington tensor}$$

Casting Shadows: VTEF vs FLD

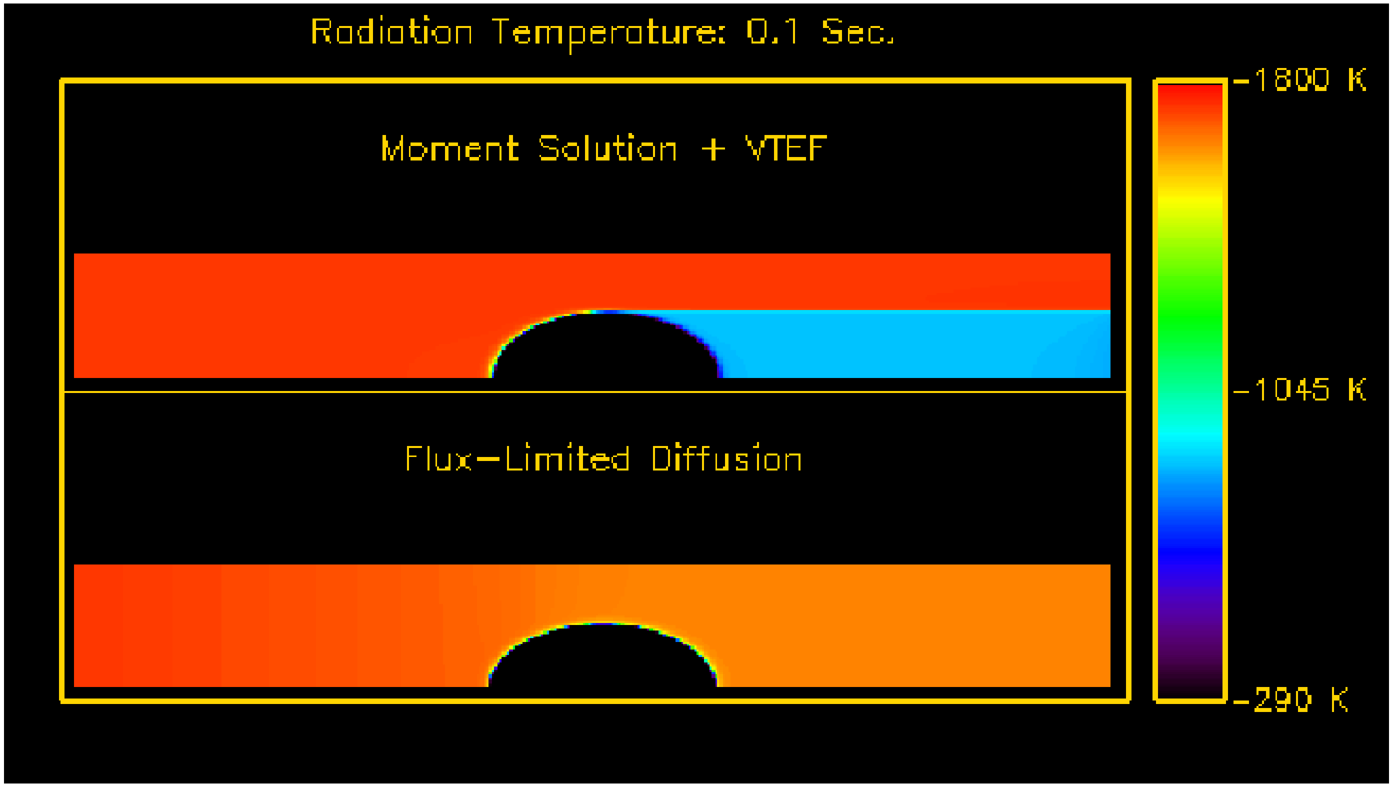
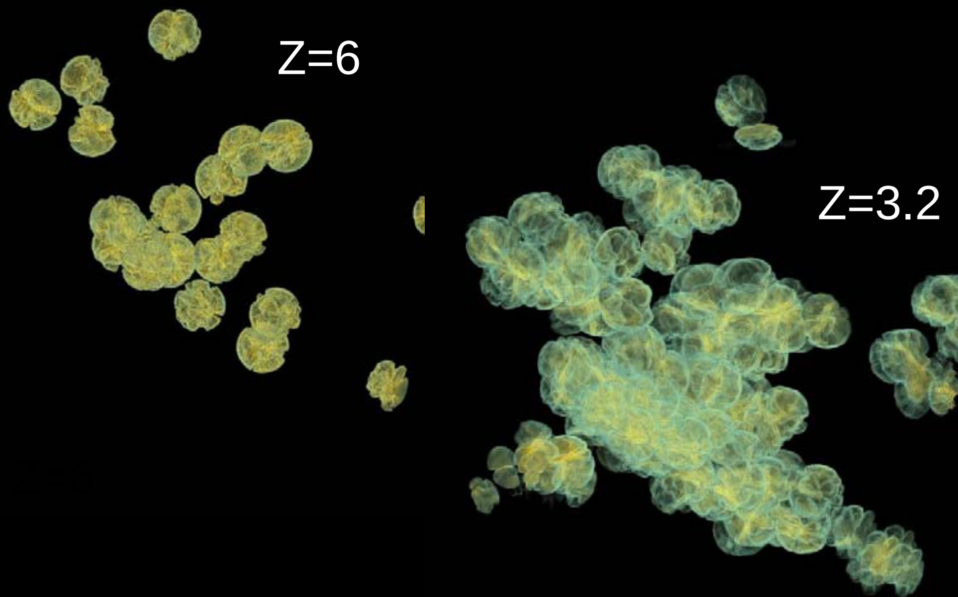


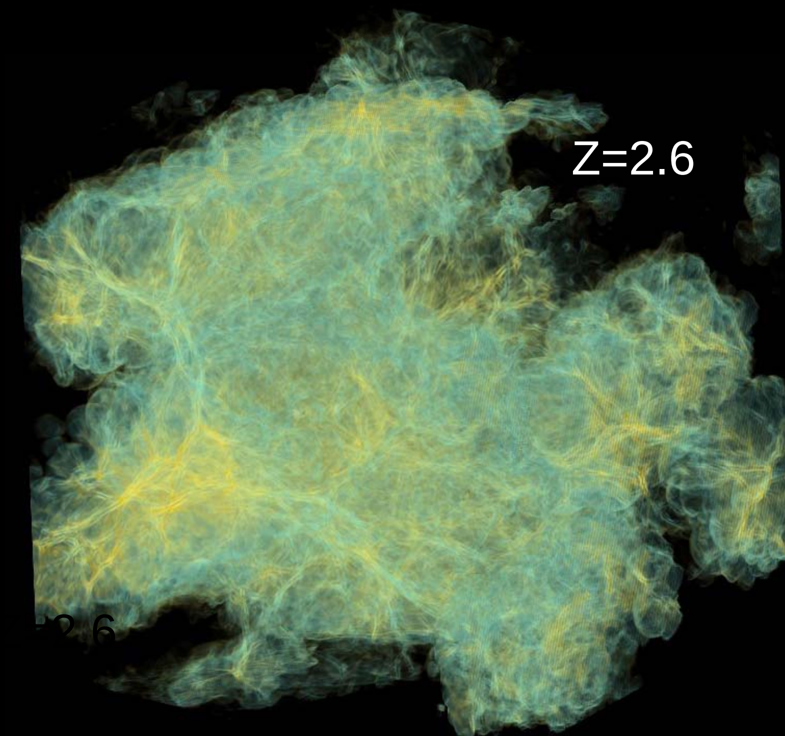
Fig. 9.— VTEF vs. FLD: the radiation energy density at 0.1 seconds (3×10^9 light-crossing times) for the VTEF calculation (top) and the FLD calculation (bottom). Note that the VTEF calculation has remained essentially unchanged from its asymptotic state in figure 7.

Hayes & Norman (2003)

He II Reionization by QSOs

Paschos, Norman & Bordner (2007)





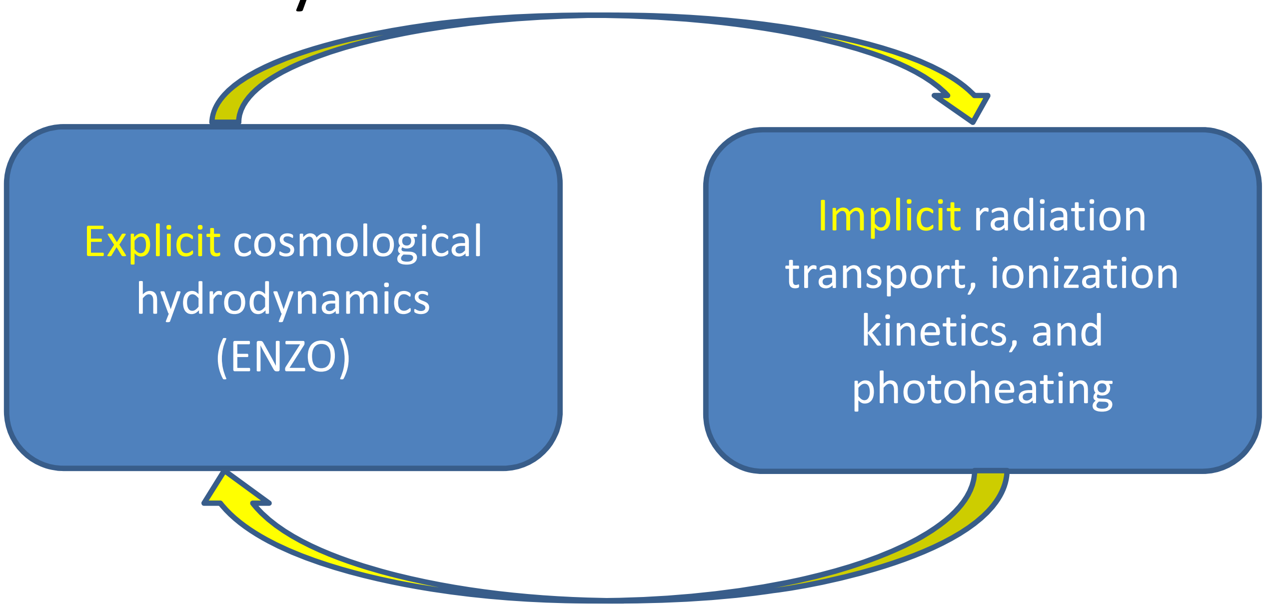
3 frequency groups
OTVET Eddington tensor
gas photoheating calculated
not dynamically self-consistent (postprocessing)

Self-Consistent Cosmological Radiation Hydrodynamics

Self-consistent Cosmological Radiation Hydrodynamics/Ionization

Reynolds et al. (2009)

- Goal
  - Create a parallel scalable solver that couples cosmological hydrodynamics, radiation transport, chemical ionization, and gas photoheating self-consistently



Cosmological Radiative Transfer Equation

cosmological redshift   cosmological expansion

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t}+\frac{\hat{n}\cdot\nabla I_\nu}{a}-\frac{H(t)}{c}\left(\nu\frac{\partial I_\nu}{\partial \nu}-3I_\nu\right)=\eta_\nu-\chi_\nu I_\nu$$

$$a(t)\equiv\frac{1}{1+z}\quad \text{cosmic scale factor}$$

$$H(t)^2\equiv\left(\frac{\dot{a}}{a}\right)^2=\frac{8\pi G}{3}\rho-\frac{k}{a^2}+\frac{\Lambda}{3}\quad \text{Friedmann Eq.}$$

Spatial gradients WRT coordinates comoving with expanding universe

Flux-Limited Diffusion Radiation Transfer

We approximate the radiative flux as a function of the energy density gradient,

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

where $D : \Omega \to I\!R^{3\times 3}$ is the *flux-limiter**, $D = D(e, E_\nu, \nabla E_\nu)$.

With this approximation, the radiation energy equation becomes

$$\partial_t E_\nu + \frac{1}{a}\nabla\cdot(E_\nu \mathbf{v}_b) - \frac{1}{a^2}\nabla\cdot(D\nabla E_\nu) - \frac{1}{ca^3}(\nabla(D\nabla E_\nu)):(\nabla \mathbf{v}_b)$$
$$= \nu\frac{\dot{a}}{a}\partial_\nu E_\nu - 3\frac{\dot{a}}{a}E_\nu + 4\pi\eta_\nu - ck_\nu E_\nu.$$

$$\partial_t E_\nu + \frac{1}{a}\nabla\cdot(E_\nu \upsilon_b) = \frac{1}{a^2}\nabla\cdot(D\nabla E_\nu) + \frac{\dot{a}}{a}\left(\nu\partial_\nu E_\nu - 3E_\nu\right) + 4\pi\eta_\nu - c\kappa_\nu E_\nu$$

Reduces to standard equation setting a=1

Spectral Modeling

$$E_\nu(\mathbf{x},t,\nu) = \tilde{E}(\mathbf{x},t)\,\chi_E(\nu)$$

$$\chi_E(\nu) = \begin{cases} \delta(\nu - \nu_0) & monochromatic \\ \mathrm{B}_\nu(T) & blackbody \\ \chi_0(\nu/\nu_0)^\alpha & powerlaw \end{cases}$$

<u>Comoving radiation energy density</u>

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

$$\partial_t E + \frac{1}{a}\nabla\cdot(E\upsilon_b) = \frac{1}{a^2}\nabla\cdot(D\nabla E) + m\frac{\dot{a}}{a}E + 4\pi\eta - c\kappa E$$

Why use FLD?

- Invented by my thesis adviser Jim Wilson
- Simple and easy (no formal solution needed)
- Correct behavior in limiting regimes
- Causal propagation of radiation energy
- I am interested in large volumes and many sources, where diffuse radiation backgrounds dominate local effects (i.e., shadows)
- SPD matrix➔efficient solution methods
- Extenstion to VTEF with analytic EFs straightforward

System of Equations

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

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

$$\partial_t e + \frac{1}{a}\mathbf{v}_b \cdot \nabla e = -\frac{2\dot{a}}{a}e - \frac{1}{a\rho_b}\nabla \cdot (p\mathbf{v}_b) - \frac{1}{a}\mathbf{v}_b \cdot \nabla \phi + G - \Lambda \tag{3}$$

$$\partial_t \mathbf{n}_i + \frac{1}{a}\nabla \cdot (\mathbf{n}_i \mathbf{v}_b) = \alpha_{i,j}\mathbf{n}_e \mathbf{n}_j - \mathbf{n}_i \Gamma_i^{ph}, \qquad i = 1, \ldots, N_s \tag{4}$$

$$\partial_t E + \frac{1}{a}\nabla \cdot (E\mathbf{v}_b) = \nabla \cdot (D\nabla E) - m\frac{\dot{a}}{a}E + 4\pi\eta - c\kappa E. \tag{5}$$

$$\nabla^2 \phi = \frac{4\pi g}{a}(\rho_b + \rho_{dm} - \langle\rho\rangle), \tag{6}$$

$$e = \frac{p}{\rho_b(\gamma - 1)} + \frac{1}{2}|\mathbf{v}_b|^2, \tag{7}$$

$$\Gamma_i^{ph} = \int_{\nu_i}^{\infty} c\,\sigma_{\mathbf{n}_i}(\nu)\,\frac{E_\nu}{h\nu}\,d\nu$$

Operator Splitting

let

$$e = e_h + e_c$$

where

e_h is gas energy due to hydrodynamic motions

e_c is energy correction due to coupling with radiation/ionization

Gas energy equation

$$\partial_t(e_h + e_c) + \frac{1}{a}\mathbf{v}_b \cdot \nabla(e_h + e_c) = - \frac{2\dot{a}}{a}(e_h + e_c) - \frac{1}{a\rho_b}\nabla \cdot (p\mathbf{v}_b) - \frac{1}{a}\mathbf{v}_b \cdot \nabla\phi + G - \Lambda. \quad (13)$$

Explicit hydrodynamics

$$\partial_t \rho_b + \frac{1}{a}\mathbf{v}_b \cdot \nabla \rho_b = -\frac{1}{a}\rho_b \nabla \cdot \mathbf{v}_b, \tag{14}$$

$$\partial_t \mathbf{v}_b + \frac{1}{a}\left(\mathbf{v}_b \cdot \nabla\right)\mathbf{v}_b = -\frac{\dot{a}}{a}\mathbf{v}_b - \frac{1}{a\rho_b}\nabla p - \frac{1}{a}\nabla\phi, \tag{15}$$

$$\partial_t e_h + \frac{1}{a}\mathbf{v}_b \cdot \nabla e_h = -\frac{2\dot{a}}{a}e_h - \frac{1}{a\rho_b}\nabla \cdot (p\mathbf{v}_b) - \frac{1}{a}\mathbf{v}_b \cdot \nabla\phi \tag{16}$$

$$\partial_t \mathrm{n}_i + \frac{1}{a}\nabla \cdot (\mathrm{n}_i \mathbf{v}_b) = 0, \tag{17}$$

$$\partial_t E + \frac{1}{a}\nabla \cdot (E\mathbf{v}_b) = 0, \tag{18}$$

This is what ENZO already does

Implicit Coupled System

- non-equilibrium multispecies model

$$\partial_t e_c = -\frac{2\dot{a}}{a} e_c + G - \Lambda, \qquad (19)$$

$$\partial_t \mathrm{n}_i = \alpha_{i,j} \mathrm{n}_e \mathrm{n}_j - \mathrm{n}_i \Gamma_i^{ph}, \qquad (20)$$

$$\partial_t E = \nabla \cdot (D \nabla E) - m\frac{\dot{a}}{a} E + 4\pi\eta - c\kappa E, \qquad (21)$$

- LTE (2 temperature) model

$$\partial_t e_c = -\frac{2\dot{a}}{a} e_c + G - \Lambda, \qquad (19)$$

$$\partial_t E = \nabla \cdot (D \nabla E) - m\frac{\dot{a}}{a} E + 4\pi\eta - c\kappa E, \qquad (21)$$

Temporal Discretization

<u>Generalized Crank-Nicholson (theta scheme)</u>

$$e_c^{n+1} + \Delta t \theta \mathcal{L}_e^{n+1} = e_c^n + \Delta t(\theta - 1)\mathcal{L}_e^n, \tag{22}$$

$$\mathrm{n}_i^{n+1} + \Delta t \theta \mathcal{L}_{\mathrm{n}_i}^{n+1} = \mathrm{n}_i^n + \Delta t(\theta - 1)\mathcal{L}_{\mathrm{n}_i}^n, \tag{23}$$

$$E^{n+1} + \Delta t \theta \left[\mathcal{D}_E^{n+1} + \mathcal{L}_E^{n+1}\right] = E^n + \Delta t(\theta - 1)\left[\mathcal{D}_E^n + \mathcal{L}_E^n\right]. \tag{24}$$

$$\mathcal{D}_E = \mathcal{D}_E(E, \mathrm{n}_i) \equiv -\nabla \cdot (D \nabla E), \tag{25}$$

and we have defined the local "reaction" operators as

$$\mathcal{L}_e = \mathcal{L}_e(e_c, E, \mathrm{n}_i) \equiv \frac{2\dot{a}}{a} e_c - G + \Lambda \tag{26}$$

$$\mathcal{L}_{\mathrm{n}_i} = \mathcal{L}_{\mathrm{n}_i}(\mathrm{n}_i, e_c, E) \equiv \mathrm{n}_i \Gamma_i^{ph} - \alpha_{i,j} \mathrm{n}_e \mathrm{n}_j \tag{27}$$

$$\mathcal{L}_E = \mathcal{L}_E(E, e_c, \mathrm{n}_i) \equiv m \frac{\dot{a}}{a} E - 4\pi\eta + ckE. \tag{28}$$

Nonlinear Solver

- Global inexact Newton

$$f(U) \equiv U + \Delta t\,\theta \begin{pmatrix} \mathcal{L}_e(U) \\ \mathcal{L}_{\mathrm{n}_i}(U) \\ \mathcal{D}_E(U) + \mathcal{L}_E(U) \end{pmatrix} - \begin{pmatrix} g^n_{e_c} \\ g^n_{\mathrm{n}_i} \\ g^n_E \end{pmatrix}, \qquad (29)$$

$$U = (e_c, \mathrm{n}_i, E)^T$$

$f(U) = 0$ for the updated vector of unknowns U^{n+1}

The Schur Complement

- For our systems that couple (e, $\mathbf{n}$, E), the Jacobian matrices have the form

$$J(U) = I + \Delta t \theta \begin{bmatrix} J_{e,e} & J_{e,\mathrm{n}} & J_{e,E} \\ J_{\mathrm{n},e} & J_{\mathrm{n},\mathrm{n}} & J_{\mathrm{n},E} \\ J_{E,e} & J_{E,\mathrm{n}} & J_{E,E} \end{bmatrix}$$

- All of these blocks are local in space, except for $J_{E,E}$, which includes the linearized diffusion operator. We therefore group these blocks into the system,

$$\begin{bmatrix} M & U \\ L & D \end{bmatrix} \begin{pmatrix} x_M \\ x_E \end{pmatrix} = \begin{pmatrix} b_M \\ b_E \end{pmatrix}$$

where $D = I + \Delta t\ \theta J_{E,E}$ is a scalar-valued reaction-diffusion matrix.

- Since M^{-1} is easy to compute (block diagonal), we use the Schur complement to solve for (x_e, $x_{\mathbf{n}}$) in terms of x_E, to obtain the solution through a pair of solves:

$$Mx_M + Ux_E = b_M \quad \rightarrow \quad x_M = M^{-1}(b_M - Ux_E),$$

so

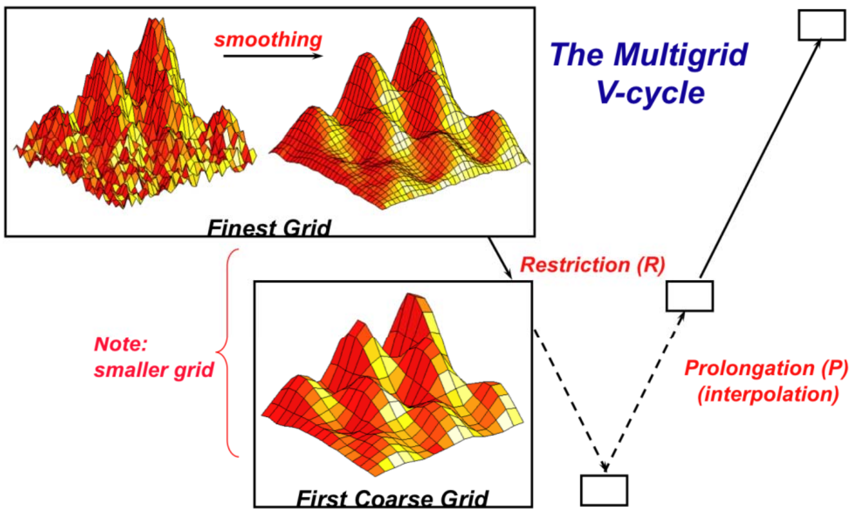
$$Lx_M + Dx_E = b_E \quad \rightarrow \quad (D - LM^{-1}U)\, x_E = b_E - LM^{-1}b_M.$$

Multigrid-Preconditioned Conjugate Gradient

- The primary difficulty in solving these systems lies in the Schur complement system

$$(D - LM^{-1}U)\, x_E = b_E - LM^{-1}b_M$$

- Due to the diffusion approximation, and the spatial locality of M and L, this matrix is symmetric and positive definite.
- SPD systems are often solved using the *conjugate-gradient* method; a robust, low-memory Krylov iterative solver. Unfortunately, CG convergence rates depend on the eigenvalues of the matrix, which here spread rapidly with mesh refinement, resulting in slower convergence as the mesh is refined.
- We therefore *precondition* the CG solver, i.e. $Ax = b \;\rightarrow\; (P^{-1}AP^{-1})(Px) = P^{-1}b$, where the symmetric operator P^{-1} comes from a *geometric multigrid* (MG) solver.
- MG methods, while less robust, exhibit convergence rates that are independent of the matrix spectrum, resulting in near optimal log-linear algorithm complexity, and scalability to thousands of processors.
- This MG-CG combination results in a robust, scalable solver for the inner Schur systems.



Free Streaming Radiation

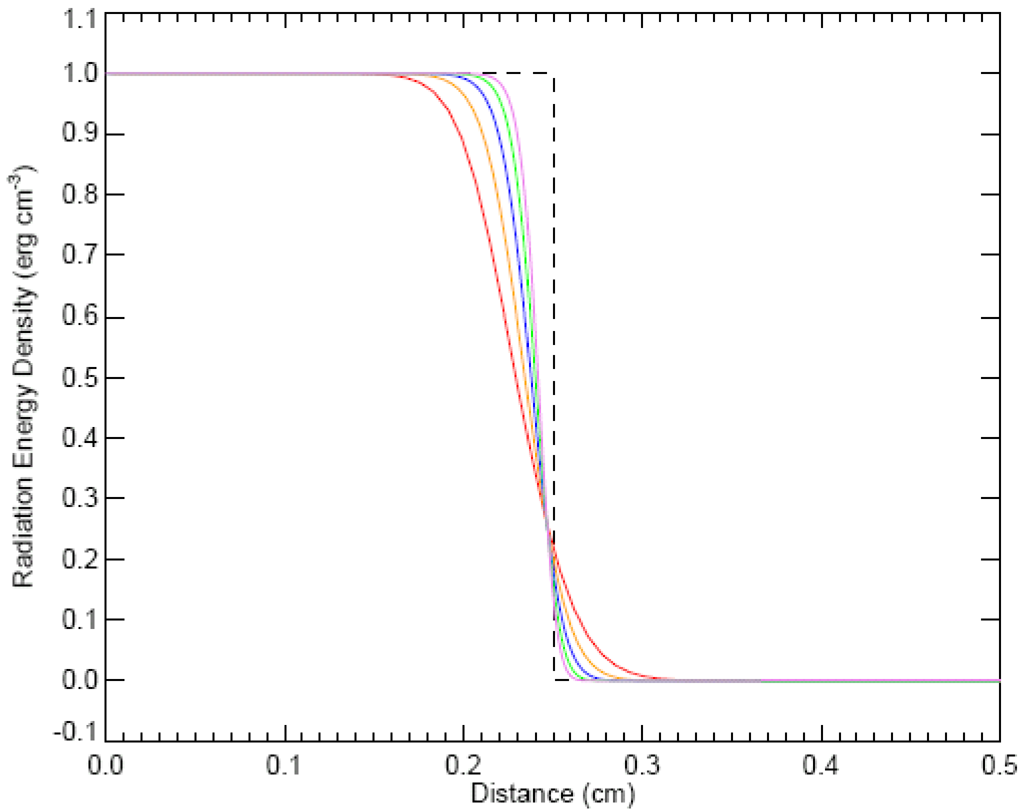
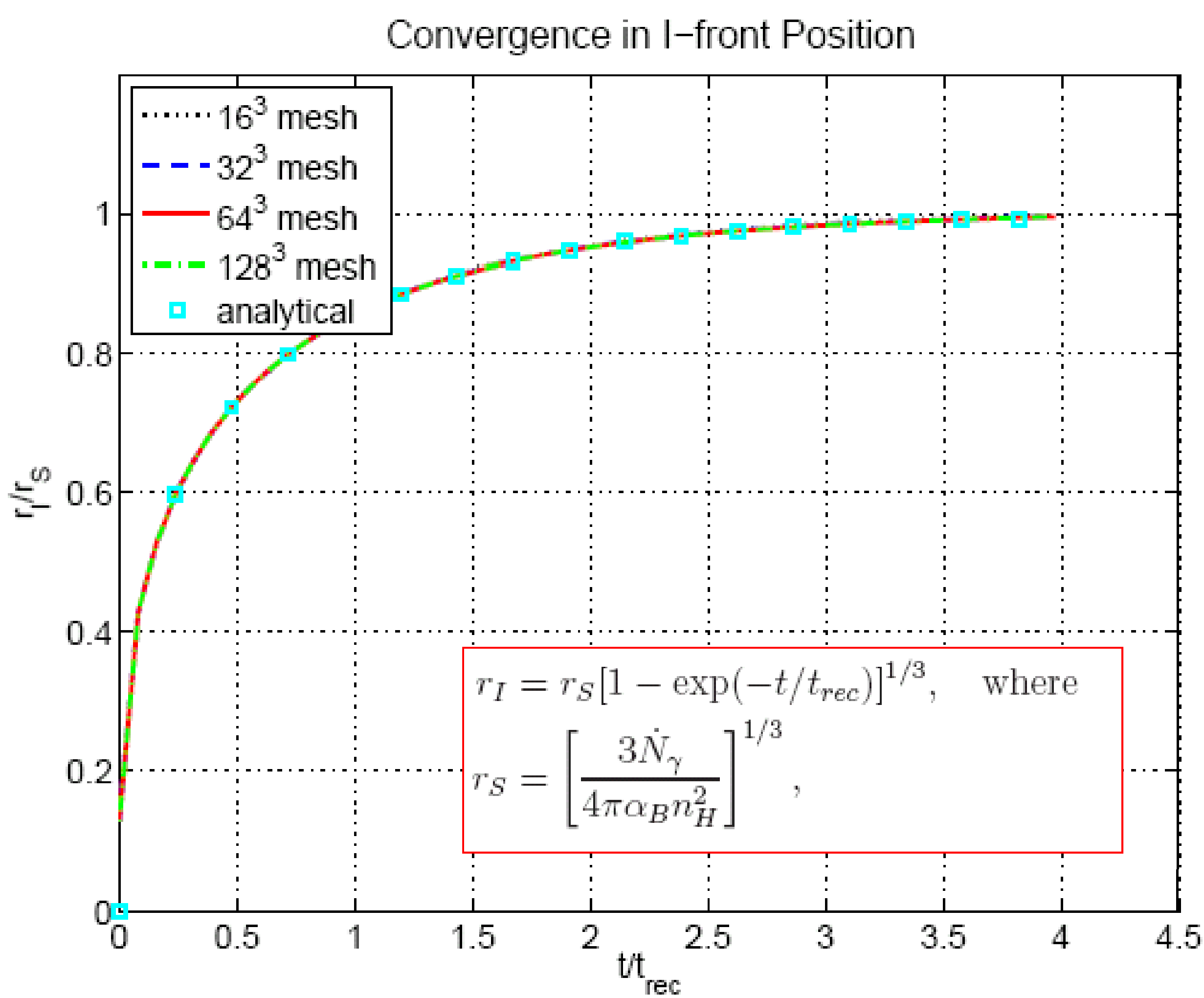


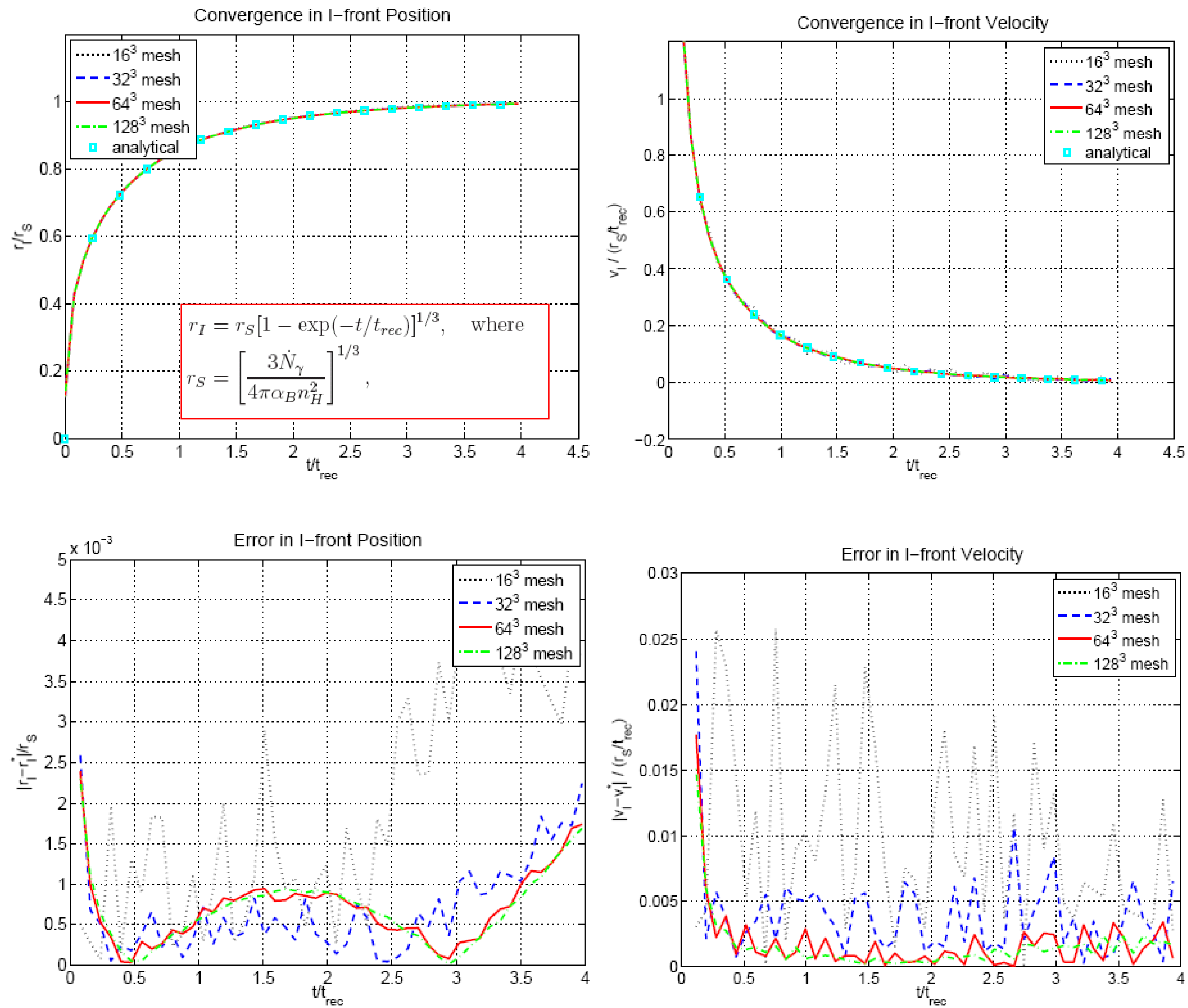
Fig. 1. Curves of E vs. x for mesh sizes of 128 (red), 256 (orange), 512 (blue), 1024 (green), and 2048 (violet) zones. The analytical solution (black dashed line) is a step function centered at $x = 0.25$cm.

HII Region Expansion in static, homogeneous, isothermal medium (Stromgren sphere test)

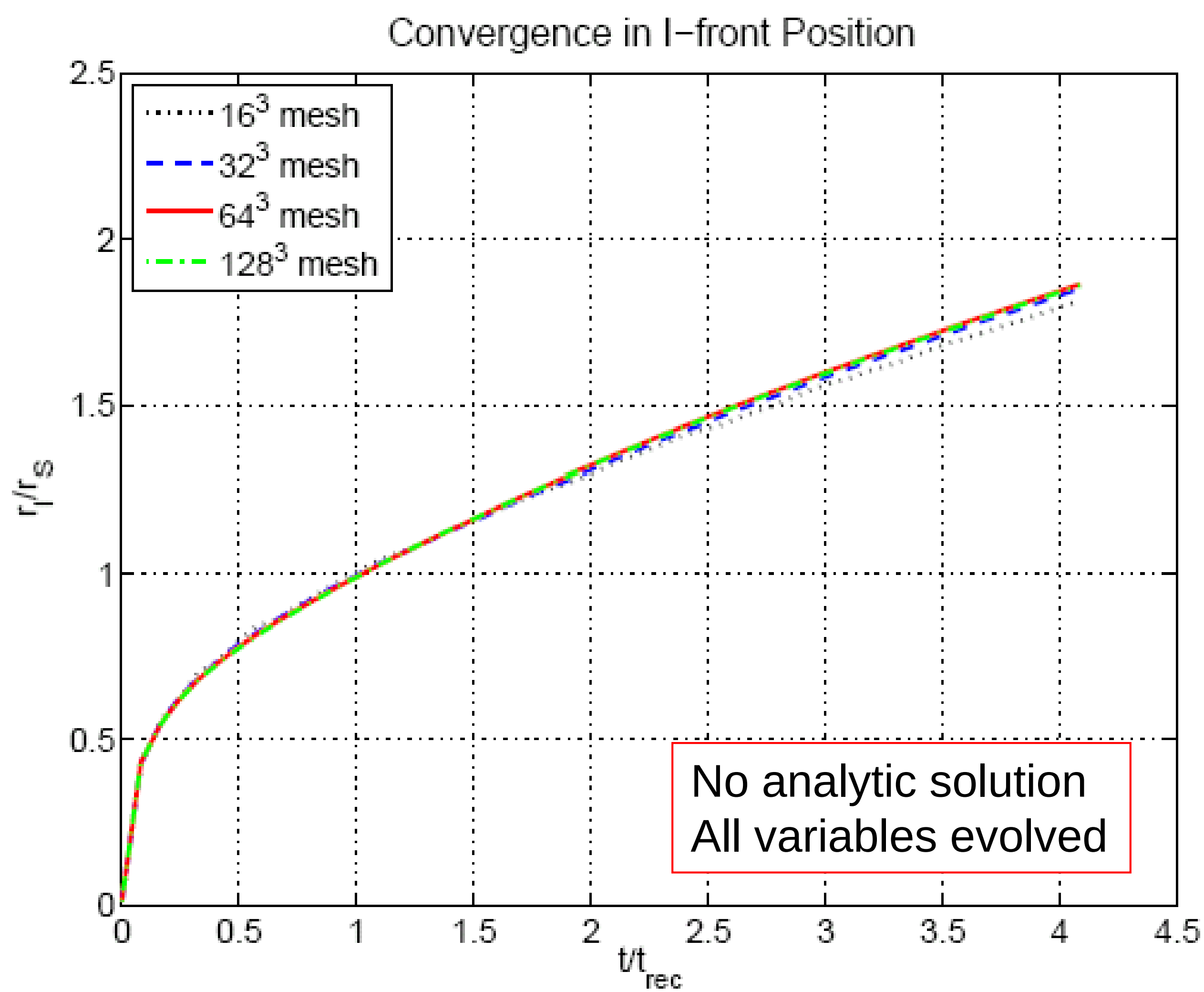


$$r_I = r_S[1 - \exp(-t/t_{rec})]^{1/3}, \quad \text{where}$$

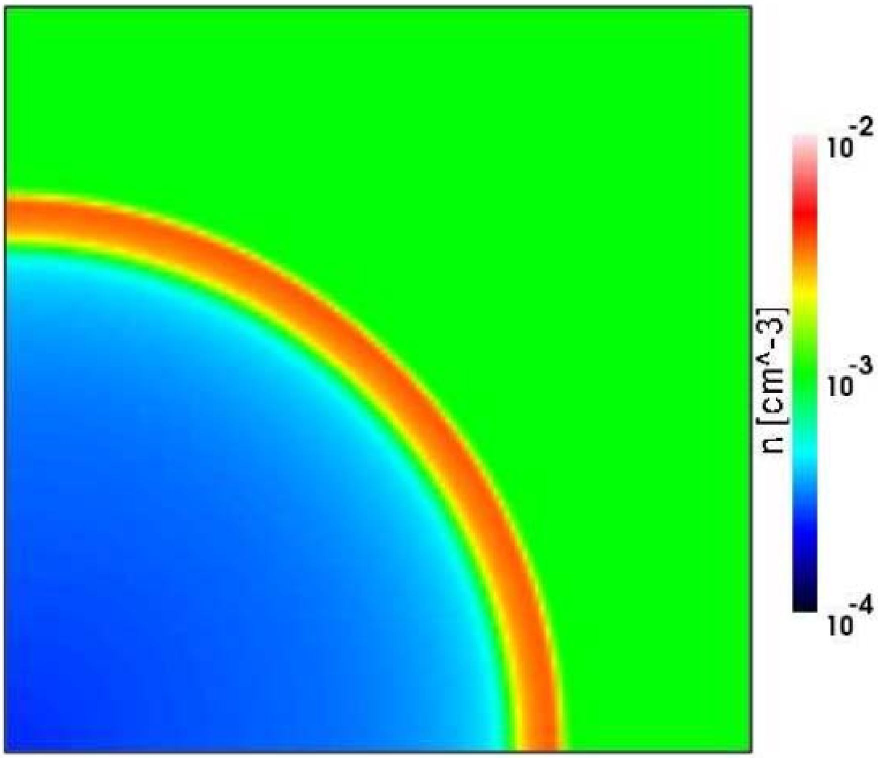
$$r_S = \left[\frac{3\dot{N}_\gamma}{4\pi\alpha_B n_H^2}\right]^{1/3},$$


Convergence in I−front Position
16^3 mesh
32^3 mesh
64^3 mesh
128^3 mesh
analytical
r_I/r_S
t/t_rec
$r_I = r_S[1 - \exp(-t/t_{rec})]^{1/3}$, where
$r_S = \left[\frac{3\dot{N}_\gamma}{4\pi\alpha_B n_H^2}\right]^{1/3}$,
Convergence in I−front Velocity
16^3 mesh
32^3 mesh
64^3 mesh
128^3 mesh
analytical
v_I / (r_S/t_rec)
t/t_rec
Error in I−front Position
x 10^-3
16^3 mesh
32^3 mesh
64^3 mesh
128^3 mesh
|r_I−r_I^*|/r_S
t/t_rec
Error in I−front Velocity
16^3 mesh
32^3 mesh
64^3 mesh
128^3 mesh
|v_I−v_I^*| / (r_S/t_rec)
t/t_rec

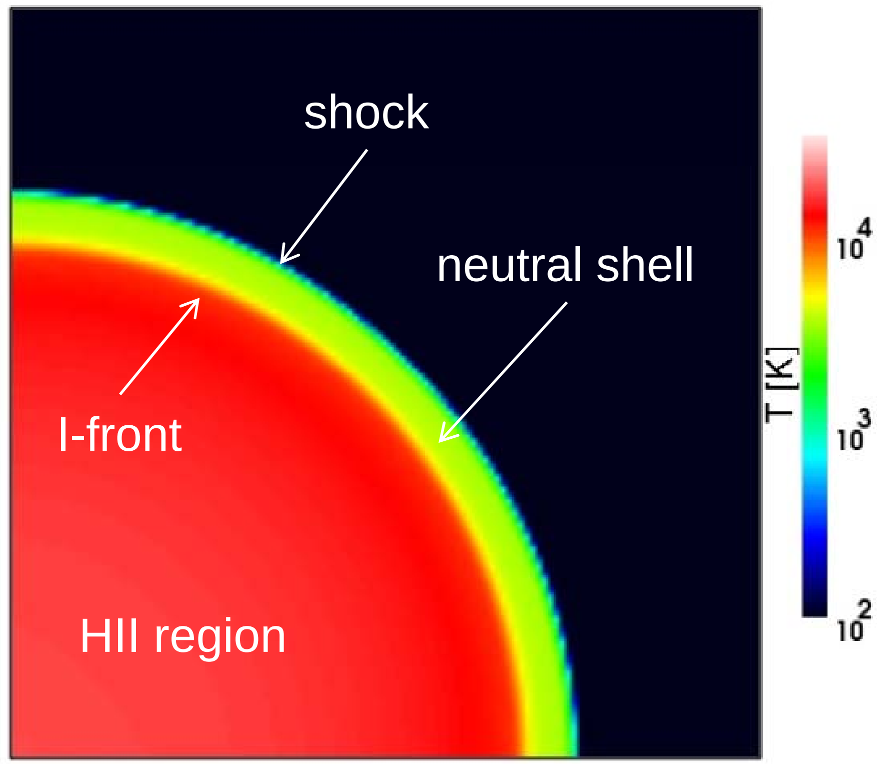
Hydrodynamic HII Region Expansion
(Whalen & Norman test problem)



Hydrodynamic HII Region Expansion

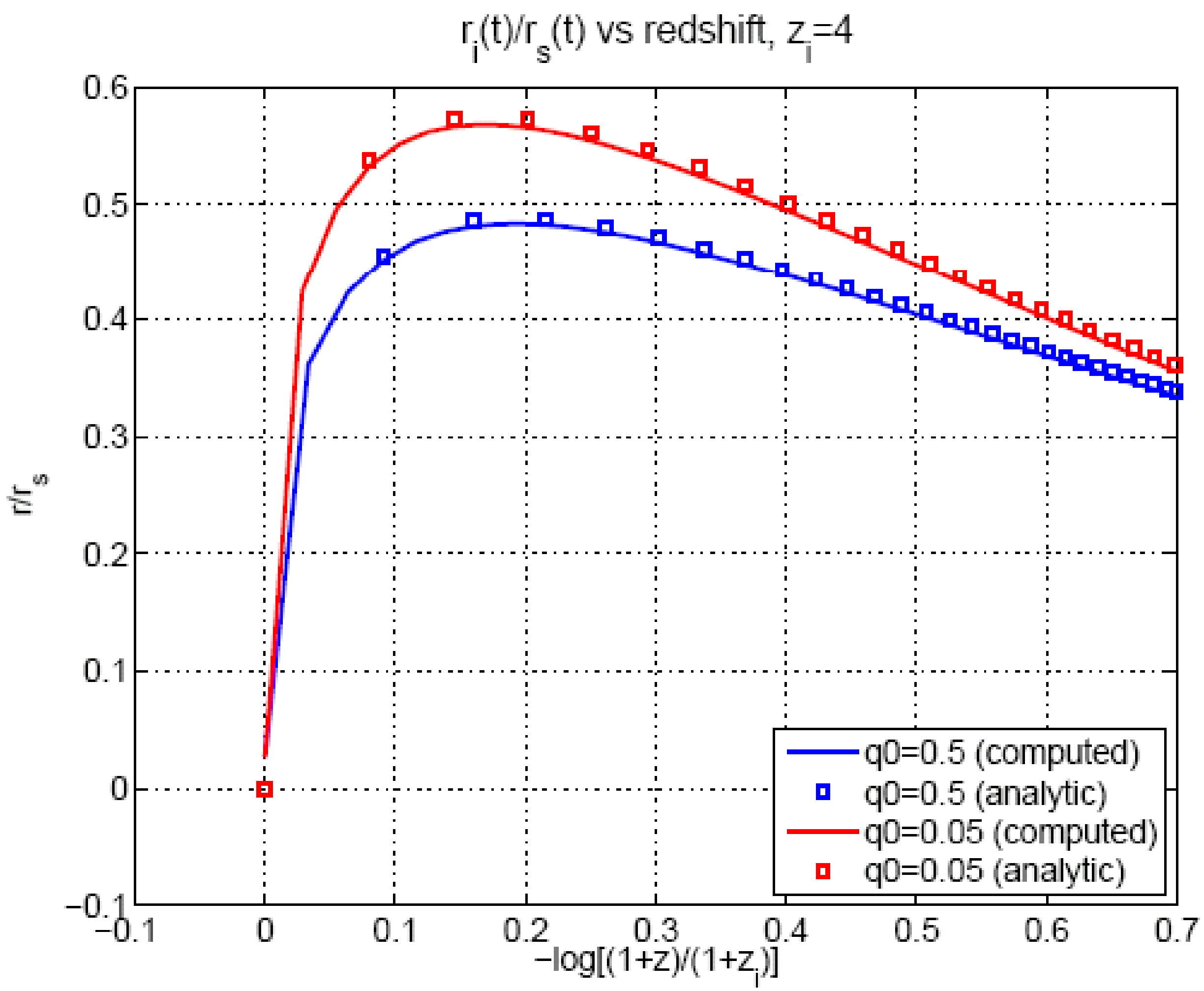


density



temperature

Cosmological HII Region Expansion
(Shapiro & Giroux test problem)



Scalability, algorithmic and parallel

Weak scaling test: lattice of HII regions

Geometric multigrid is optimally scalable

HYPRE parallel implemenation also scalable

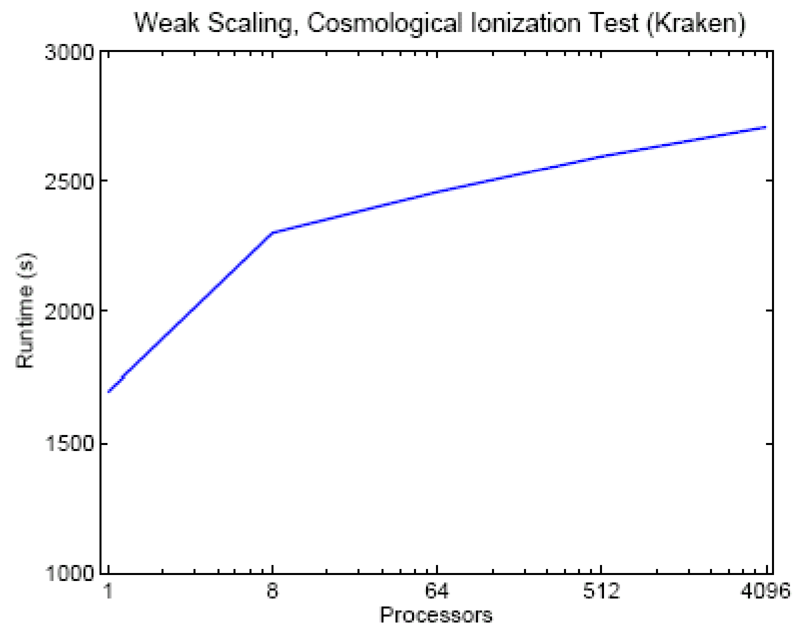


Fig. 13. Weak scaling results for the cosmological HII-region expansion test.

Mesh	Processors	Time Steps	Run Time	Newton Its	CG Its	MG V-cycles
64^3	1	266	1694.38	322	914	2991
128^3	8	265	2299.60	274	799	2575
256^3	64	265	2456.58	268	787	2524
512^3	512	264	2594.50	265	780	2510
1024^3	4096	264	2707.30	265	780	2510

Free-Streaming Multi-source Test

ENZO Cosmological AMR Code

Bryan & Norman 1997, 1999; O'Shea et al. 2004; Norman et al. (2007)

http://lca.ucsd.edu/projects/enzo

- Berger-Oliger AMR
- PPM and ZEUS hydro solvers
- PM dark matter solver
- FFT/multigrid gravity solver
- 6, 9, 12 multispecies ionization/chemistry
- UV and X-ray backgrounds
- Various star formation and feedback recipes
- MPI parallel; C++/C/F90
- Coming 2010: MHD, RHD, hybrid parallel

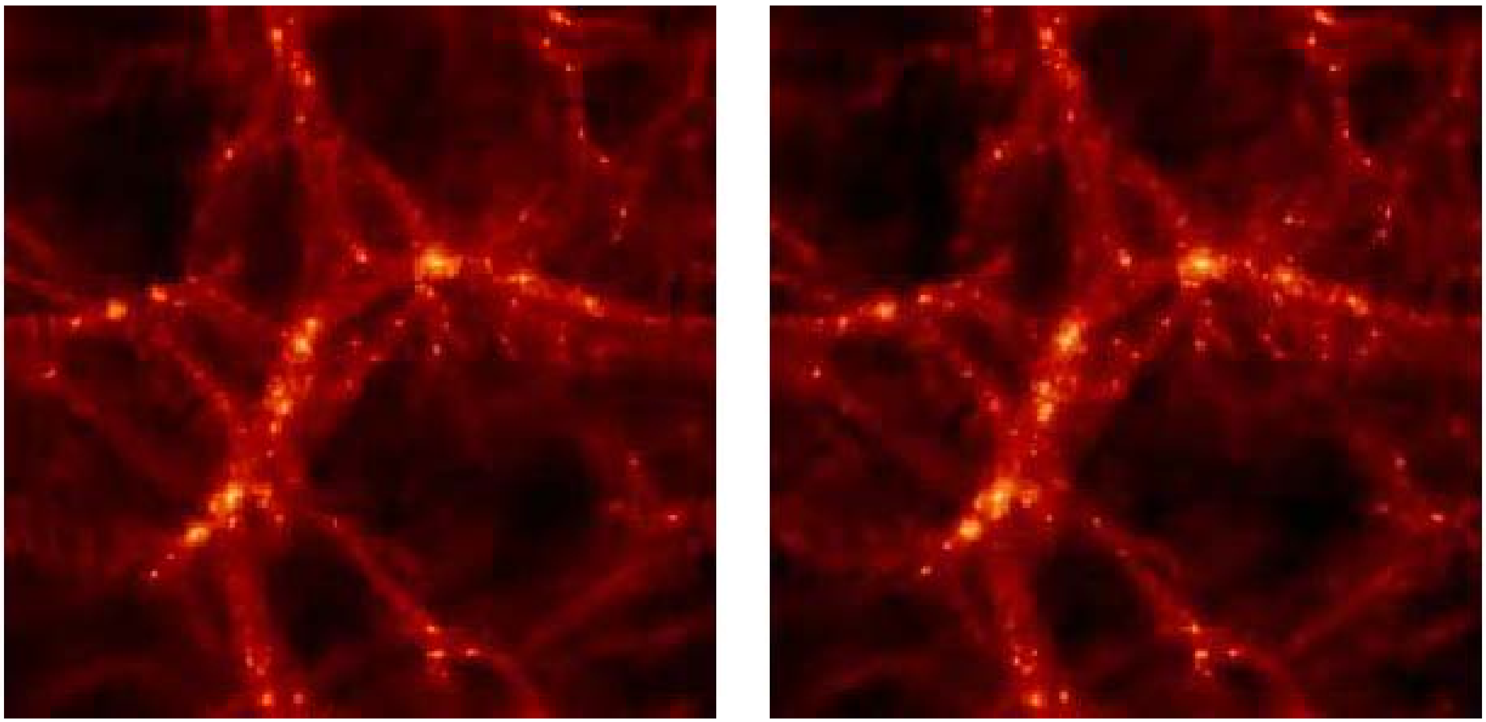
Dark Matter: Tree vs. AMR-PM

O'Shea et al. (2005)

For comparable dark matter halo mass function GADGET is much (10x) faster

GADGET | ENZO

DM

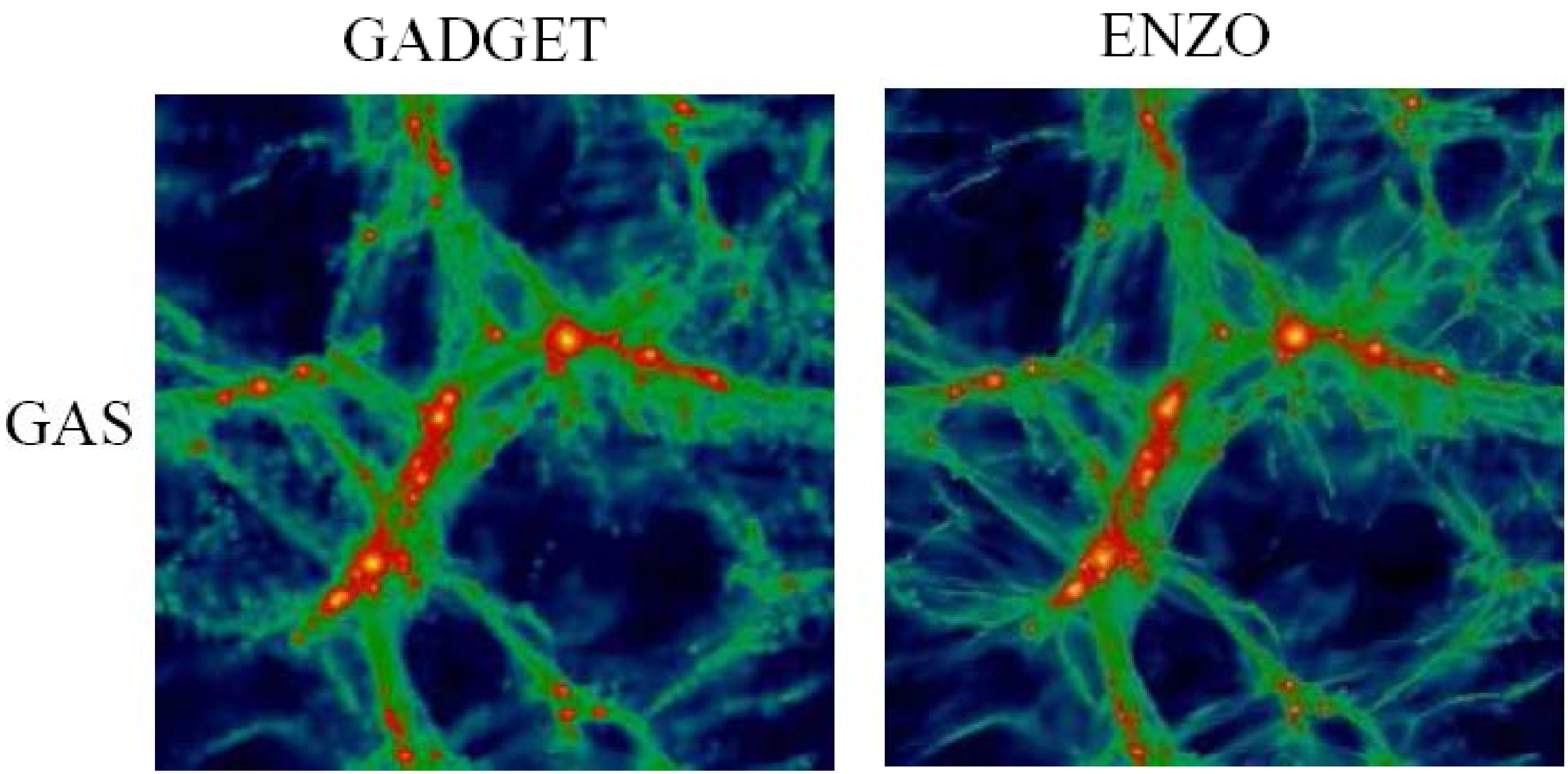


$N = 64^3$ | $M = 128^3, N = 64^3$

Gas: Tree vs. AMR-PM

O’Shea et al. (2005)

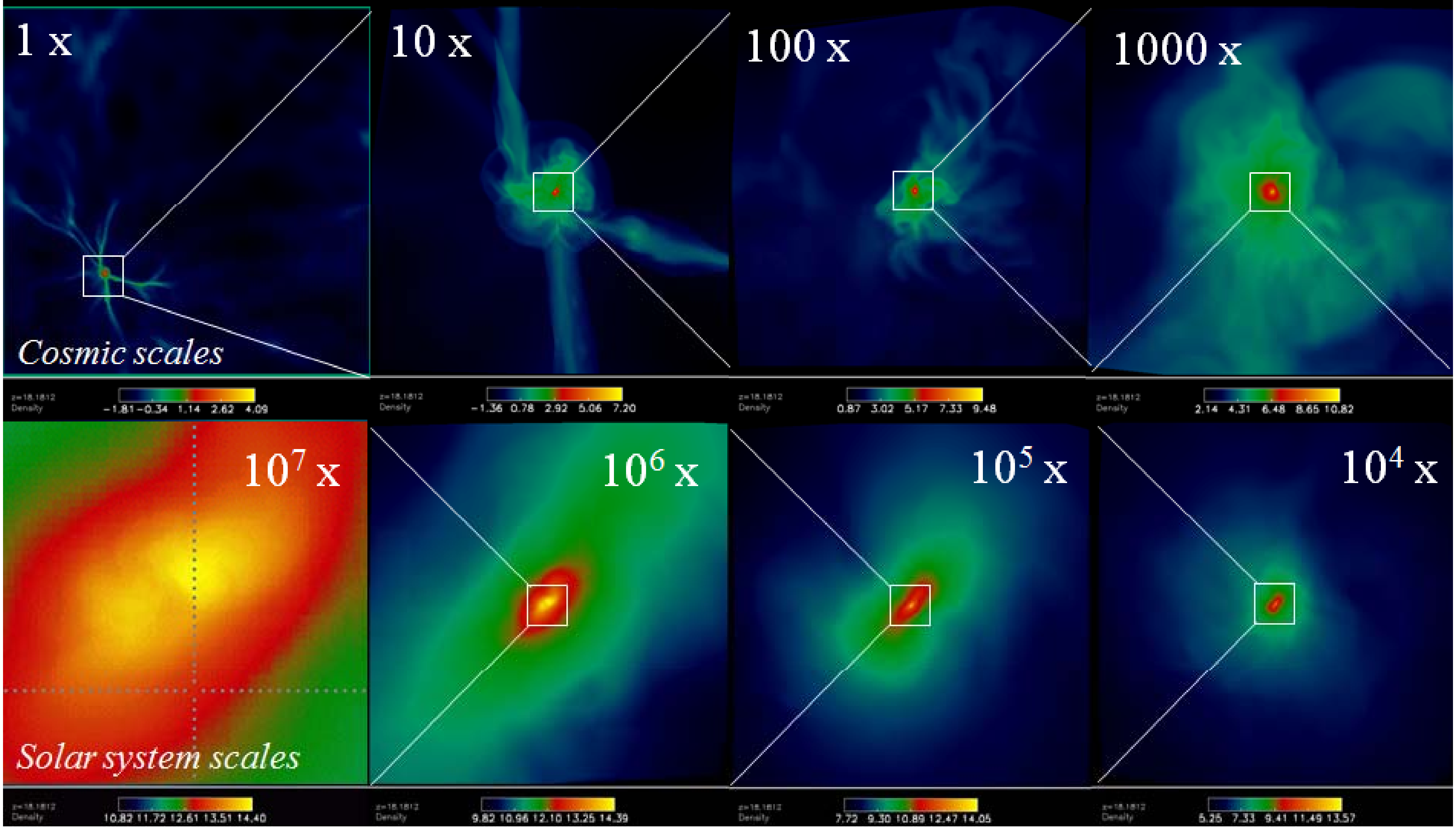
SPH a little “ragged” in the filaments and voids; entropy profiles different in halo cores

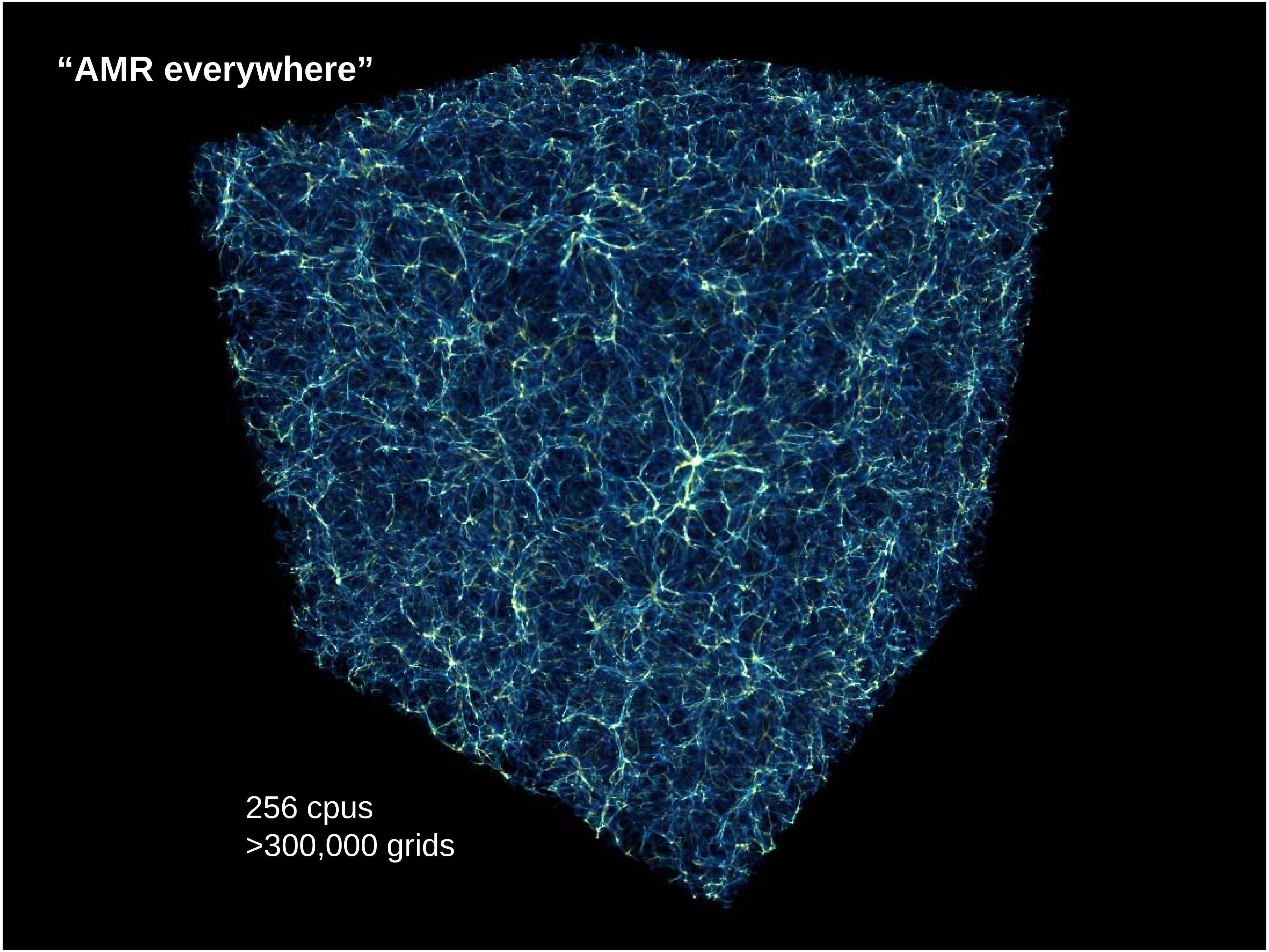


$N = 64^3$ $\qquad$ $M = 128^3, N = 64^3$

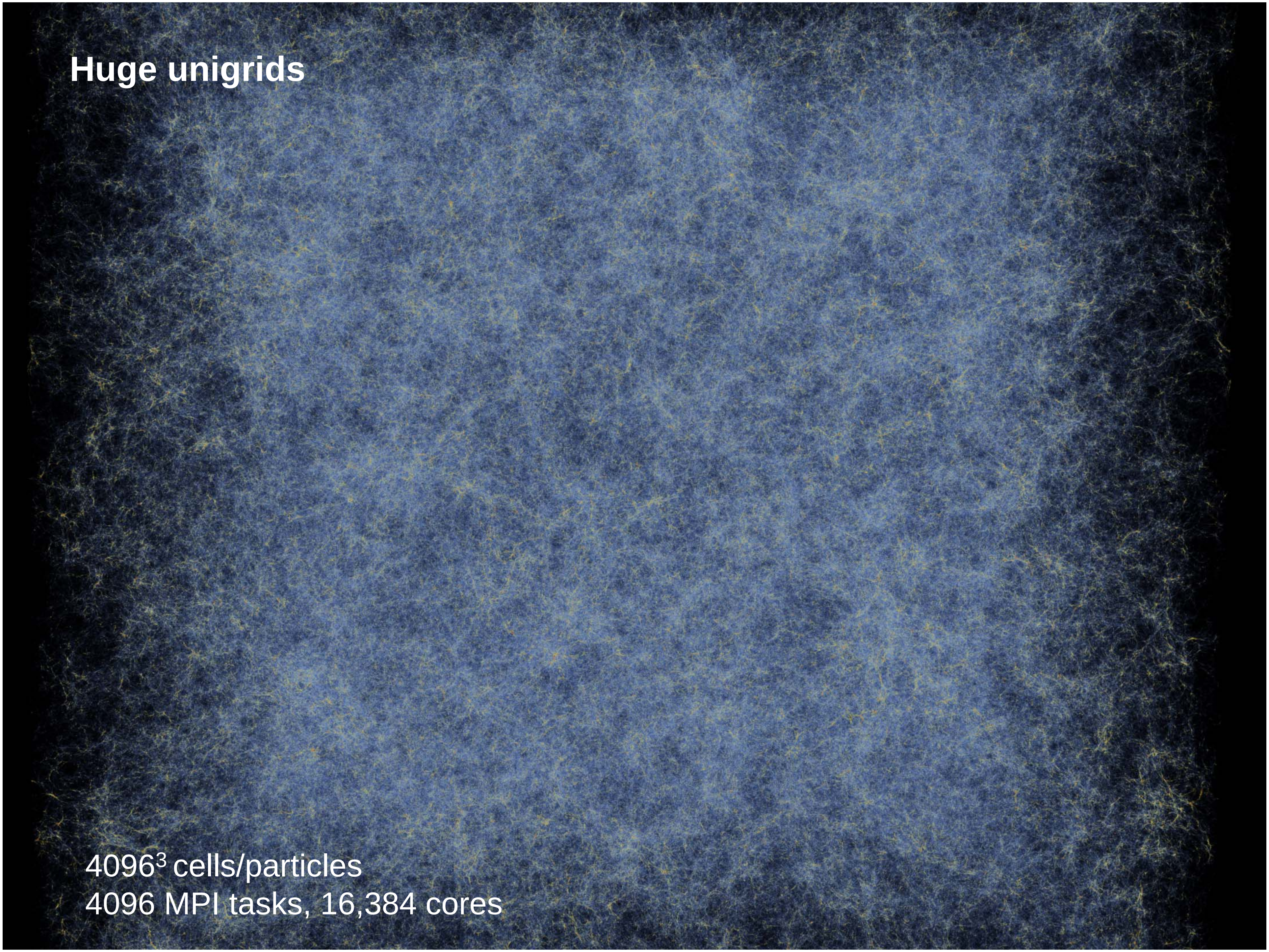
Formation of First Stars

Abel, Bryan & Norman (2001) *Science*




"AMR everywhere"
256 cpus
>300,000 grids

Huge unigrids



4096^3 cells/particles

4096 MPI tasks, 16,384 cores

Maiden Voyage of Combined Solver: Self-Consistent H Reionization

(done last week!)

ΛCDM WMAP5 parameters

8 comoving Mpc box

$z_{\text{initial}} = 100$

256^3 cells/particles (no AMR)

$\Rightarrow m_{\text{dm}} = 10^6 M_S$

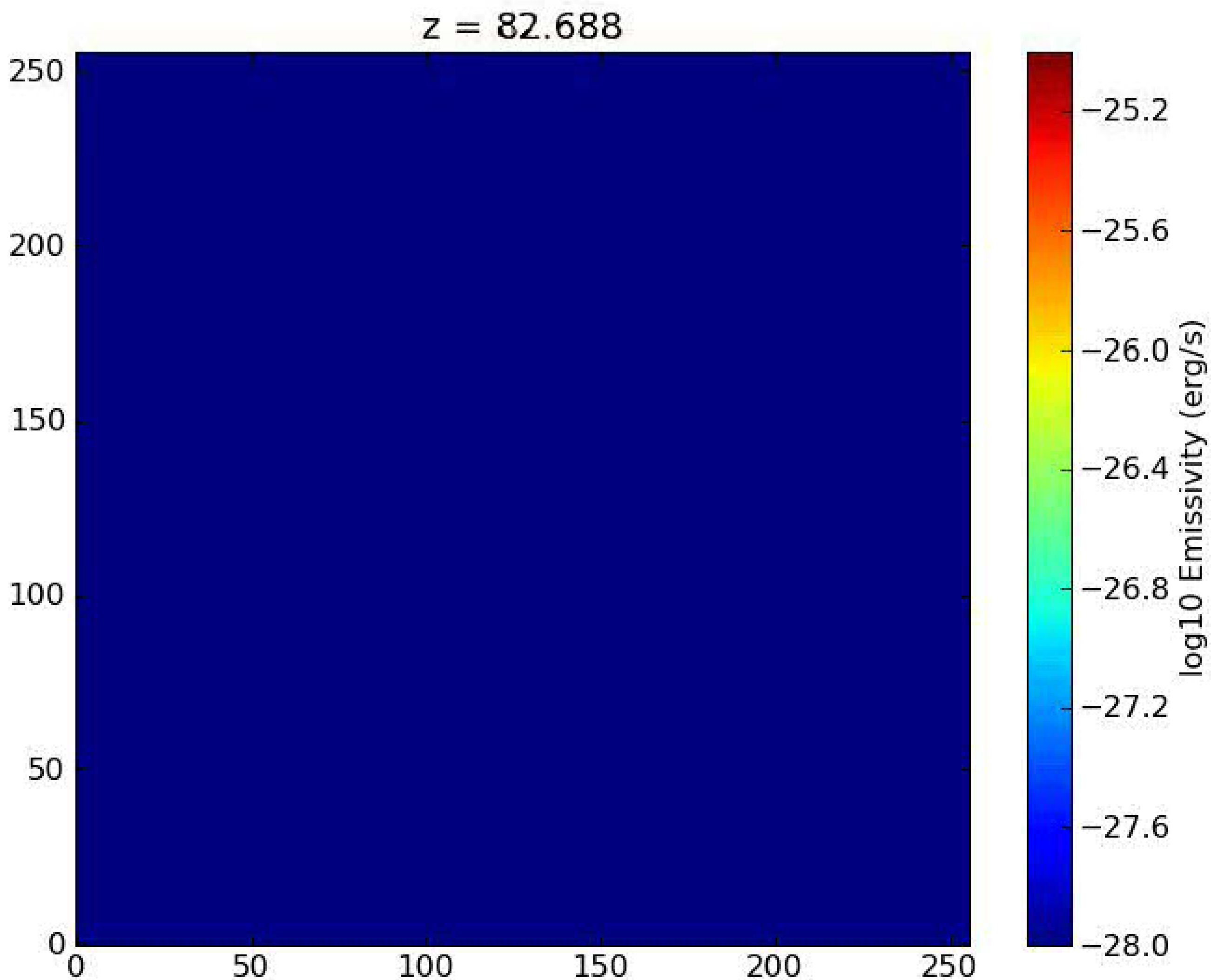
$\Rightarrow \Delta x_{\text{proper}}(z = 7) = 4kpc$

modified Cen & Ostriker starmaker

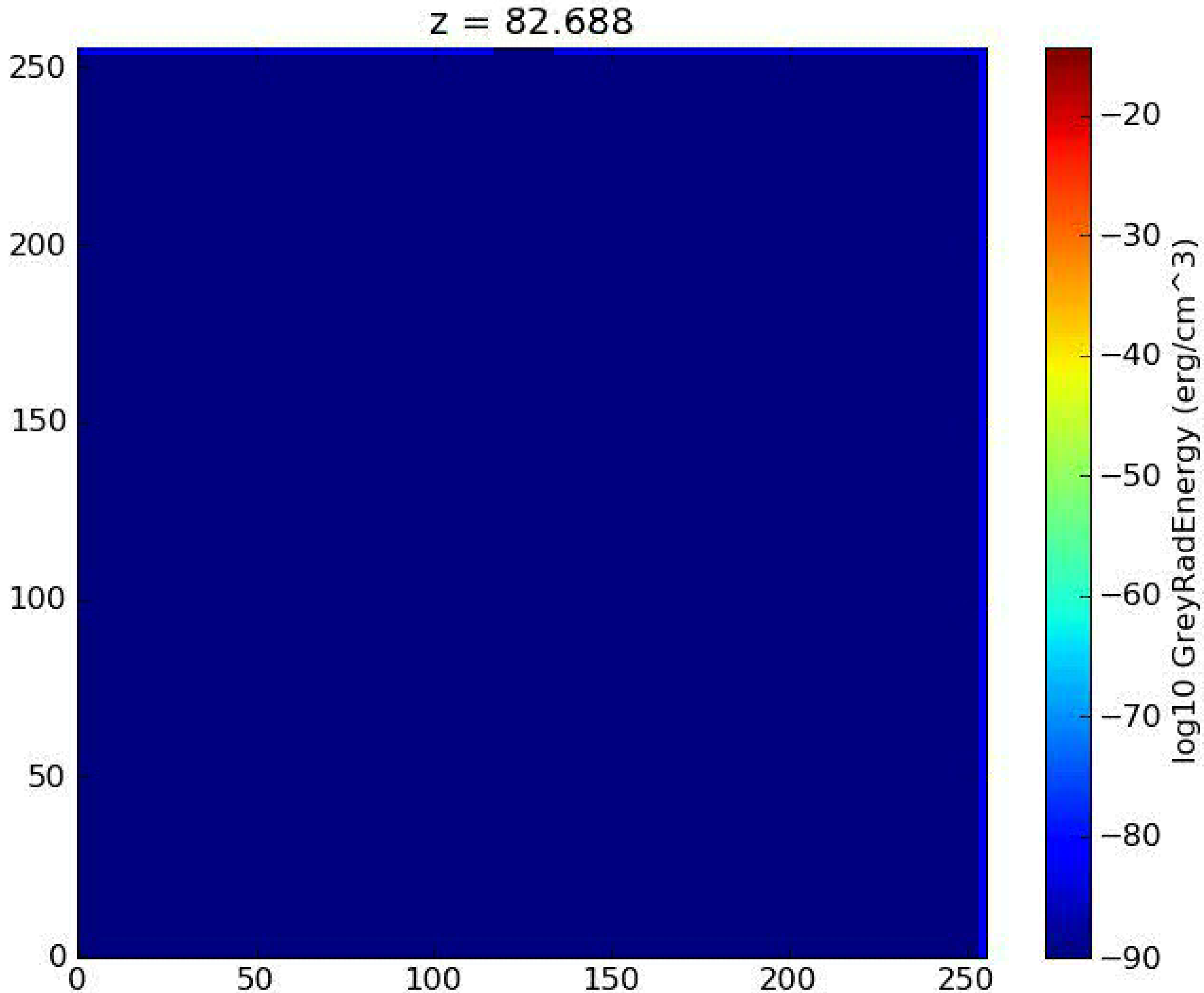
$\eta_{\text{UV}} = 3\times10^{-6} \dot{M}_{SF} c^2$

- Emissivity movie
- Radiation movie
- Ionization movie
- Density movie

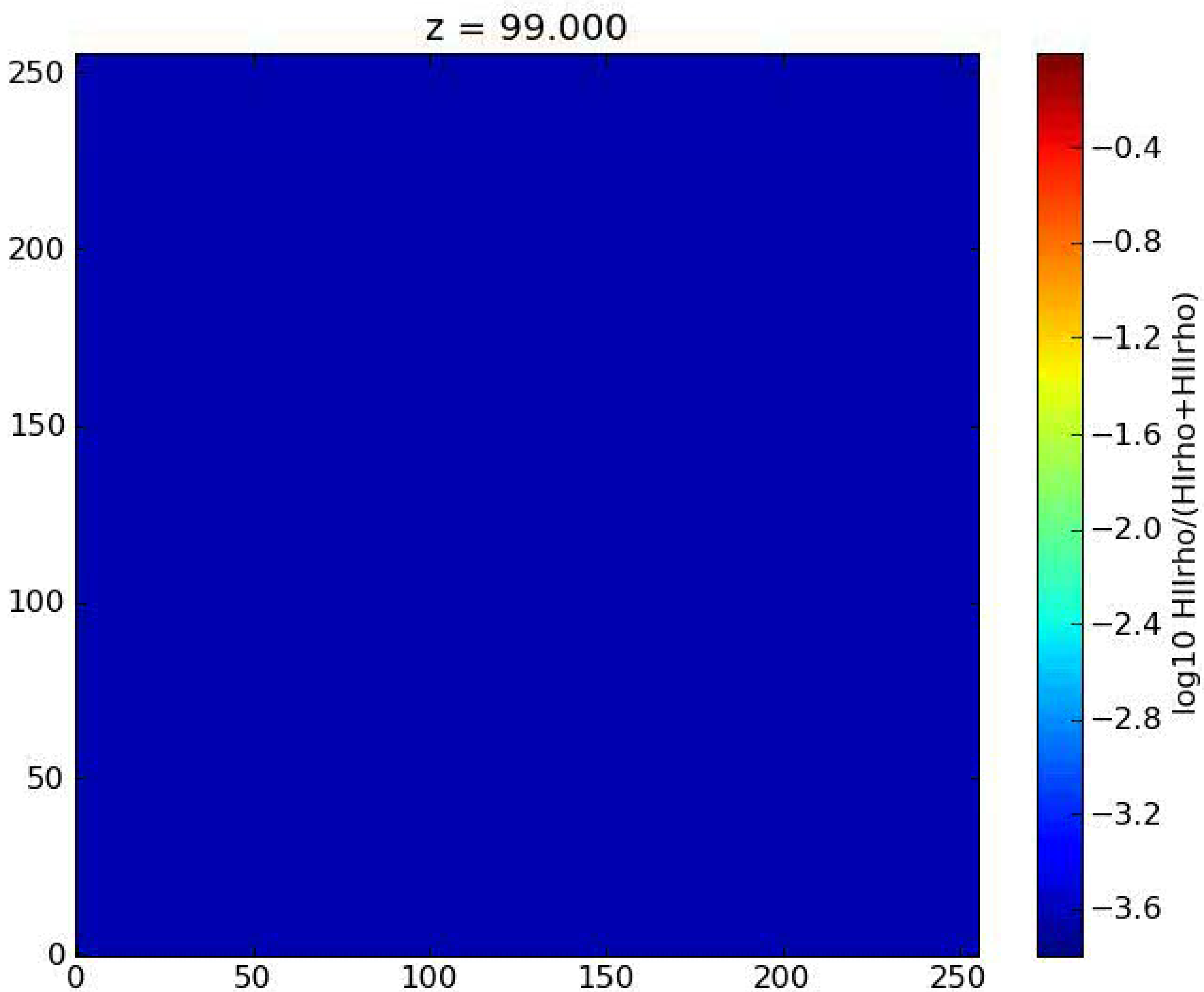
Emissivity Evolution



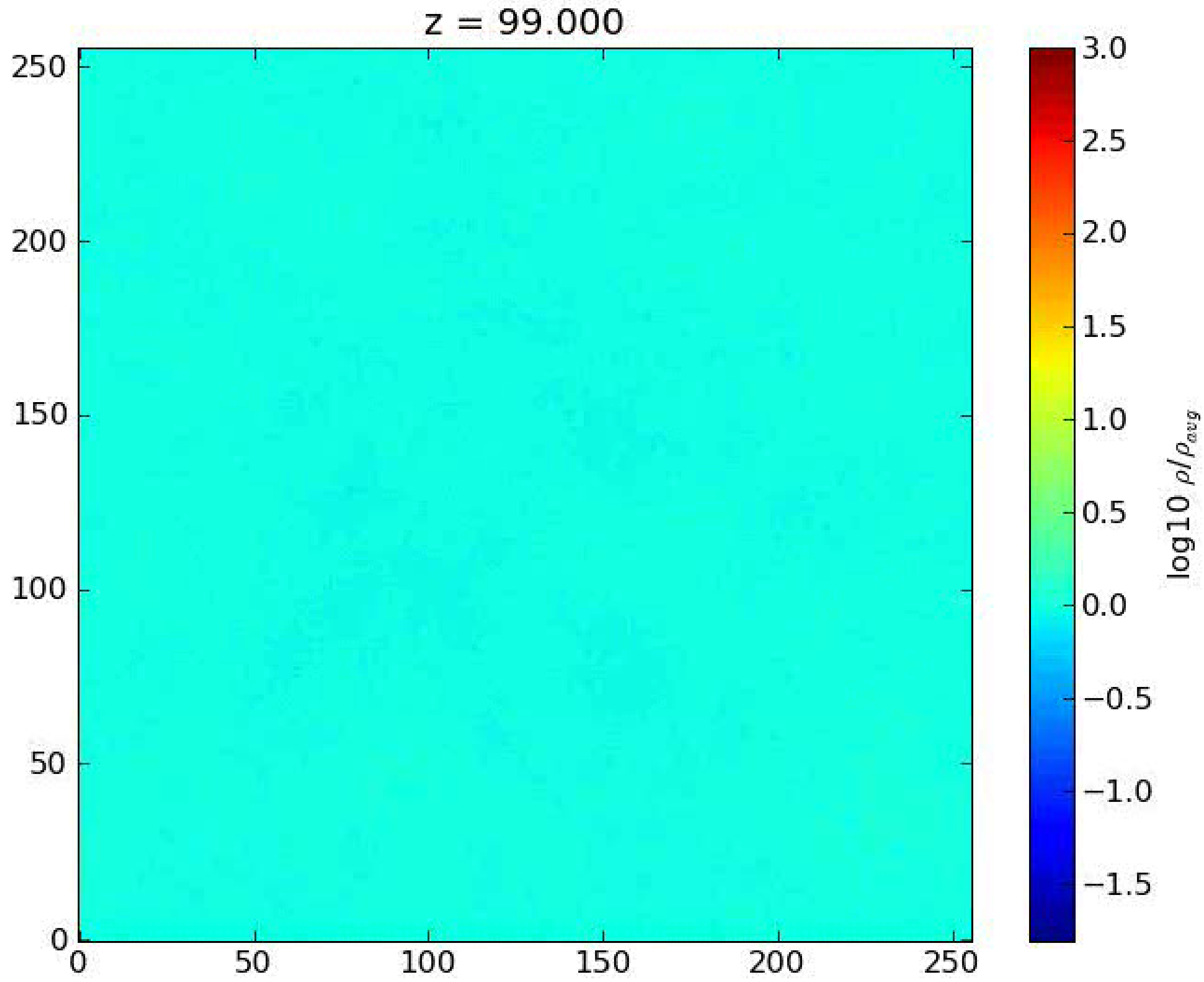
Radiation Energy Density



Ionization Fraction Evolution



Overdensity Evolution



What’s it all mean?

- Dunno, just got movies 2 days ago
- Looks like code is working
- It’s like first light on a new telescope
  - Need to spend some time getting to know it
  - Exciting though!
- Hints of substantial modification of baryon distribution in filaments and voids
  - Photoevaporation flows
- Regulated cosmic star formation?
  - Next 12 months should be fun

Conclusions

- Self-consistent radiation hydro cosmological simulations are now feasible due to
  - Some physical simplifications (FLD)
  - Scalable linear solvers (multigrid)
  - Implicit time integration (hydro timestep)
- Radiation solves takes about 50% of runtime (doubles the cost)

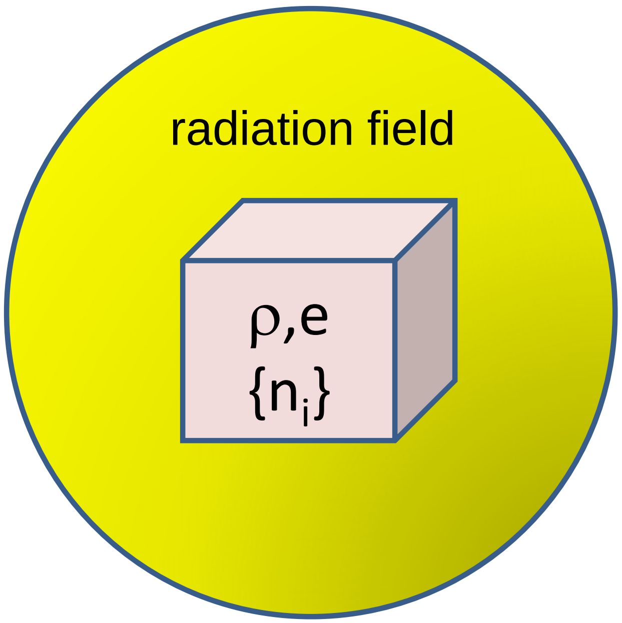
Next steps

- Extend to AMR
  - switch to FAC multigrid solver
  - explore timestepping issues
- Extend to multifrequency/multigroup
  - H and He ionization, H_2 chemistry
- Develop hybrid FLD/ray tracing solver (w/ John Wise)
  - Ray tracing for AMR and shadowing
  - FLD for diffuse background radiation fields


Let’em shine!

Reserve slides

Basics: Macrophysical



Photoionization kinetics

$$\frac{\mathrm{dn_i}}{\mathrm{dt}} = \pm\sum_j\sum_l \alpha_{jl} n_j n_l \pm \sum_j I_j n_j$$

$$\alpha_{jl} \equiv \alpha_{jl}(T) \qquad \text{2-body reaction rates}$$

$$I_j = \int_{\nu_{th,j}}^{\infty} d\nu \cdot \sigma_{PI,j}(\nu)\frac{E_\nu}{h\nu} \qquad \text{1-body ionization rates}$$

Gas photoheating

$$\frac{\mathrm{de}}{\mathrm{dt}} = \Gamma_{PI} - \Lambda(T)$$

$$\Gamma_{PI} = \sum_j n_j m_j G_j$$

$$G_j = \int_{\nu_{th,j}}^{\infty} d\nu \cdot \sigma_{PI,j}(\nu)\frac{E_\nu}{h\nu}(h\nu - h\nu_{th,j})$$

Moments of the Specific Intensity

- radiation energy density (0th)

$$E_\nu = E(\mathbf{x},t;\nu) = \frac{1}{c}\oint d\omega I(\mathbf{x},t;\mathbf{n},\nu)$$

- radiation flux (1st)

$$F_\nu^i = F^i(\mathbf{x},t;\nu) = \oint d\omega n^i I(\mathbf{x},t;\mathbf{n},\nu)$$

- radiation pressure tensor (2nd)

$$P_\nu^{ij} = P^{ij}(\mathbf{x},t;\nu) = \frac{1}{c}\oint d\omega n^i n^j I(\mathbf{x},t;\mathbf{n},\nu)$$