Simulating Reionization: A New Code for Photon-Conserving Transport of Ionizing Radiation

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Outline

- Cosmological I-Fronts
- New cosmological radiative transfer code
- Structure formation at high-z
- Simulations of the Epoch of Reionization
- Radiative transfer codes comparison project

Propagating ionization fronts

- Whenever a source of ionizing radiation turns on in a neutral medium, it creates a propagating I-front
- General theory and classification of I-fronts exists (e.g. Spitzer).
- I-fronts start as weak, fast R-type fronts, propagating faster than gasdynamic response until slowing down due to recombinations and geometric dilution, or increased local density, converting to slower, D-type I-front, often preceded by a shock, in which case hydrodynamics becomes important.
- The I-front propagation is described by "jump condition", $v=F/n$, which expresses the balance at the front of ionizing photon flux and opposite neutral atoms flux (assuming a sharp transition).
- First cosmological I-front solutions derived in Shapiro & Giroux 87

Analytical vs. Numerical I-front solutions

Analytical:

- fast and efficient
- large dynamic range
- can handle only simple situations (symmetric, constant clumping and temperature, sharp I-fronts, etc.)

Numerical:

- general
- can include complex physics and chemistry
- works for any density field
- limited dynamic range

Photon-Conserving Transport of Ionizing Radiation

(Mellema, Iliev, Alvarez & Shapiro, in prep.)

We have developed a new radiative transfer method:

- explicitly photon-conserving. Rates calculated as in Abel, Norman & Madau 00 + averaging in time following non-equilibrium chemistry => much faster, does not require small time-steps to follow fast I-fronts)
- Tested in detail (multiple tests with exact analytical solutions performed, samples on next slides):
  - correctly evolves I-fronts even at very low spatial and time resolutions
  - non-equilibrium chemistry, energy equation
- fast and efficient, easily coupled to hydro and N-body dynamics
- applicable in either cosmological or non-cosmological situations

Simplified Transfer Scheme

- Consider the evolution of the ionized fraction x:
- Ideally you want the number of ionizations plus recombinations during one time step to match the number of photons available.
- Note: All quantities are tied to a given point in space

$$\frac{\mathrm{d}x}{\mathrm{d}t} = (1-x)\Gamma - x n_{\mathrm{e}} \alpha$$

With photo-ionization rate

$$\Gamma = \frac{1}{4\pi r^2} \int_{\nu_0}^{\infty} \frac{L_\nu a_\nu e^{-\tau_\nu}}{h\nu} \mathrm{d}\nu$$

and optical depth

$$\tau_\nu = a_\nu \int_0^r (1-x) n \mathrm{d}r$$

Solving for Ionization

- The photo-ionization equation is a stiff equation: solution between 0 and 1, time scale for change can be small.
- Solutions:
  - Very small time steps.
  - Implicit solver (iteration).
  - Analytical (relaxation) solution.
- The latter is possible, and extendable to other species then H, if $\boldsymbol{n}_{\mathrm{e}}$ is assumed given (so still some iteration needed to find a consistent solution).

Analytical Relaxation Solution

$$\frac{\mathrm{d}x}{\mathrm{d}t} = (1 - x)\Gamma - x n_\mathrm{e} \alpha$$

Solution: $$x(t) = x_\mathrm{eq} + (x_0 - x_\mathrm{eq}) e^{-\Delta t / t_\mathrm{i}}$$

with relaxation time $t_\mathrm{i} = 1/(\Gamma + n_\mathrm{e}\alpha)$

and equilibrium value: $$x_\mathrm{eq} = \frac{\Gamma}{\Gamma + n_\mathrm{e}\alpha}$$

Weak Points

- Hydrodynamic time step (sound speed): only tracks D-type IFs accurately.
- Problem for inhomogeneous medium: wide range of IF velocities, fast R-type and slow D-type.
- Following R-types is expensive: small time steps, but no hydrodynamic evolution.
- Numerical solution depends on spatial and temporal resolution (cell size and time step).
- No guarantee that photons are conserved.

Photon-Conservation: Space

- Conservative approach: a cell is a **volume** in space.
- Instead of using one ionizing flux for the whole cell, consider the difference between the one entering and the one leaving the cell (cf. Abel, Norman, Madau 1999).

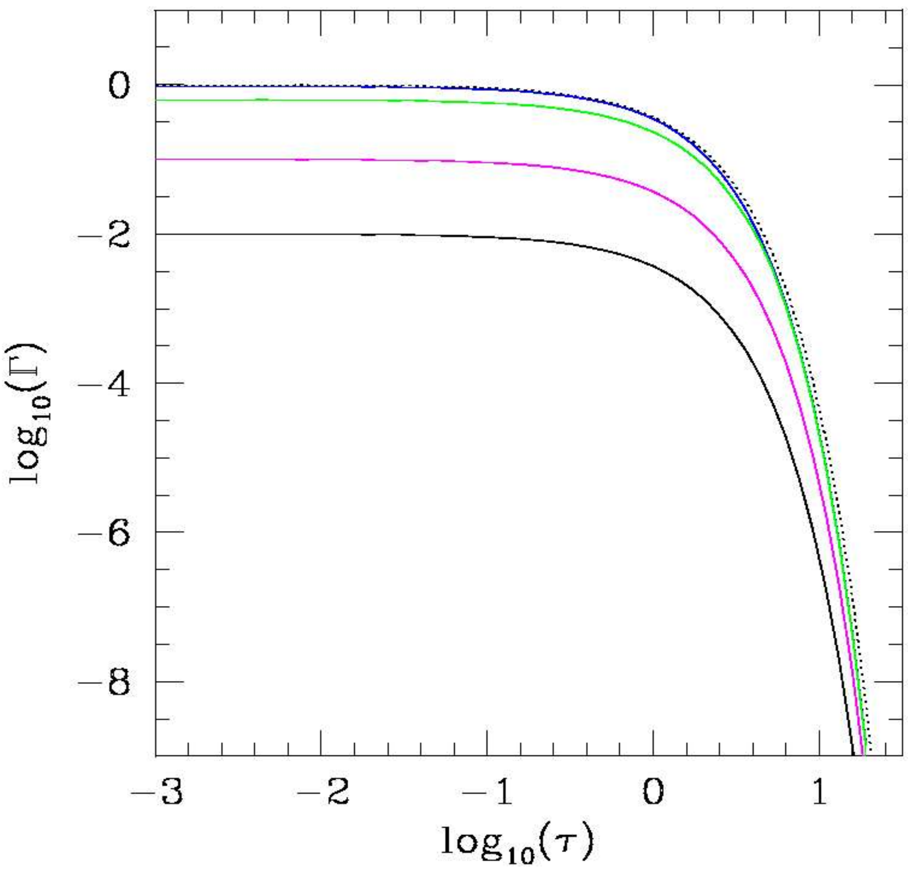
$$(1-x)nV\Gamma = N_{\rm in} - N_{\rm out}$$

$$\Gamma = \frac{1}{4\pi r^2}\int_{\nu_0}^{\infty}\frac{L_\nu a_\nu e^{-\tau_\nu}}{h\nu}\,{\rm d}\nu$$

$$\Gamma = \int_{\nu_0}^{\infty}\frac{L_\nu e^{-\tau_\nu}}{h\nu}\,\frac{1-e^{-\Delta\tau_\nu}}{(1-x)nV}\,{\rm d}\nu$$

Photon conservation: space II

- When applied to finite-size cells the local photoionization rates give the correct value (black dotted) only for optically-thin cells (blue) and progressively more incorrect for larger $\Delta\tau$ per cell (green-black)



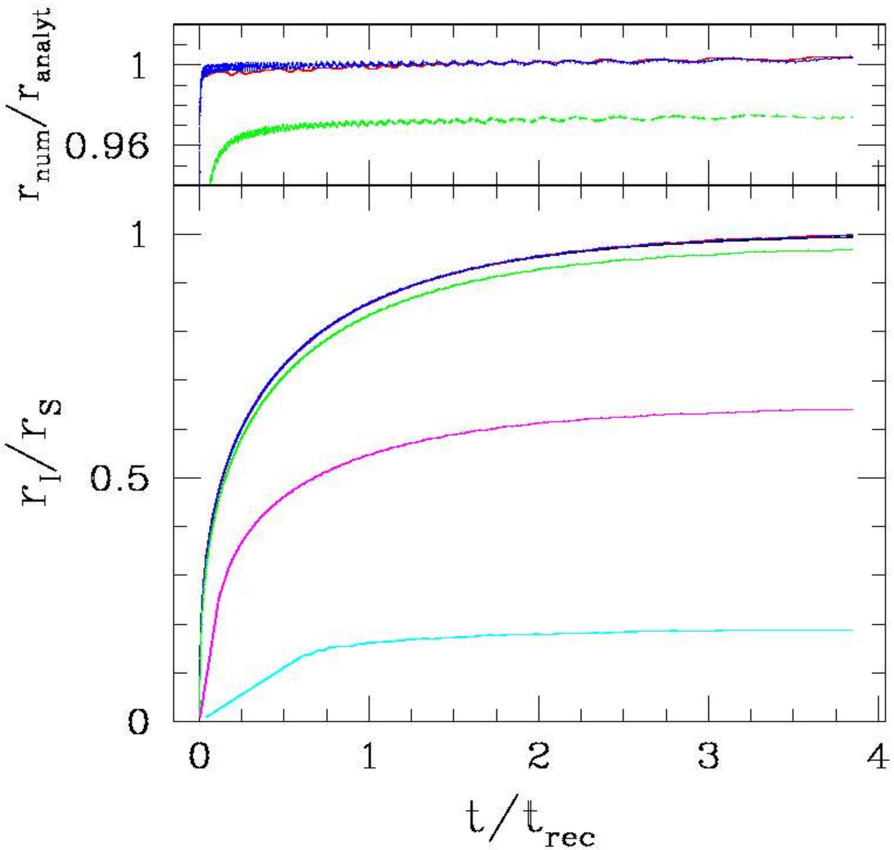
Photon-Conservation: Time

- During a time step, the optical depth of a cell can change. Which value to use for τ?
  - – Initial value: over-estimate the optical depth.
  - – Final value: under-estimate the optical depth.
- Traditional solution: Choose small time steps to limit the change. Expensive!
- New solution: find the time-averaged

$$\langle \Delta\tau_\nu \rangle = a_\nu \Delta r \left(1 - x_{\mathrm{eq}} + (x_{\mathrm{eq}} - x_0)(1 - e^{-\Delta t / t_{\mathrm{i}}}) \frac{t_{\mathrm{i}}}{\Delta t} \right)$$

Photon-Conservation: Time II

- Non-time-averaged rates require large number of timesteps to find the correct solution.
- HII region evolution: time-averaged (100 steps, red), and not averaged ones for, bottom to top: 100, 1,000, 10,000 and 100,000 time-steps.



Energy Conservation

- Photon-conservation automatically leads to energy conservation.
- Heating = (photon energy in – photon energy out) / Δt.

$$H = n_{\mathrm{HI}} \int_{\nu_{\mathrm{HI}}}^{\infty} h(\nu - \nu_{\mathrm{HI}}) \frac{L_\nu a_\nu e^{-\tau_\nu}}{h\nu} \mathrm{d}\nu \,,$$

$$H = \int_{\nu_{\mathrm{HI}}}^{\infty} h(\nu - \nu_{\mathrm{HI}}) \frac{L_\nu e^{-\langle \tau_\nu \rangle}}{h\nu} \frac{1 - e^{-\langle \Delta\tau_\nu \rangle}}{V_{\mathbf{shell}}} \mathrm{d}\nu \,,$$

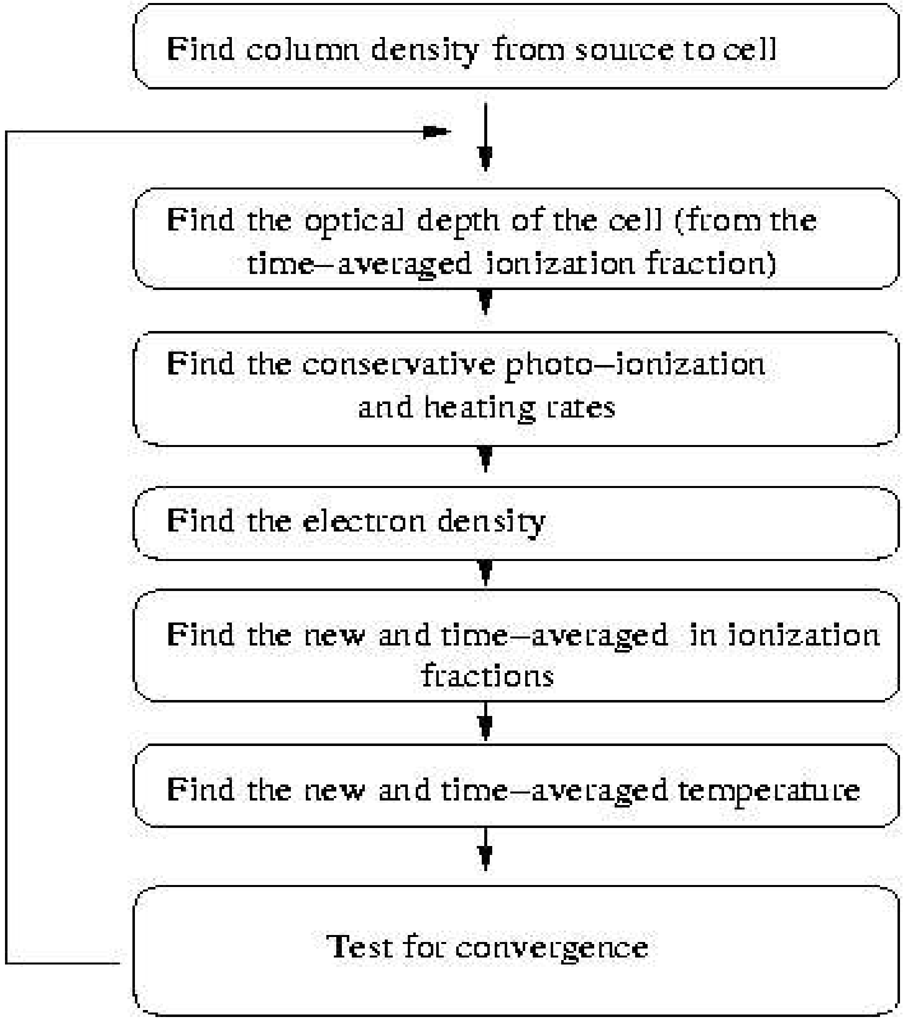
Energy Conservation

- Photon-conservation automatically leads to energy conservation.
- Heating = (photon energy in – photon energy out) / Δt.
- For long time-steps there are still some issues with distributing the energy correctly between the cells. Nevertheless, generally the method works quite well, and gives the correct solution.

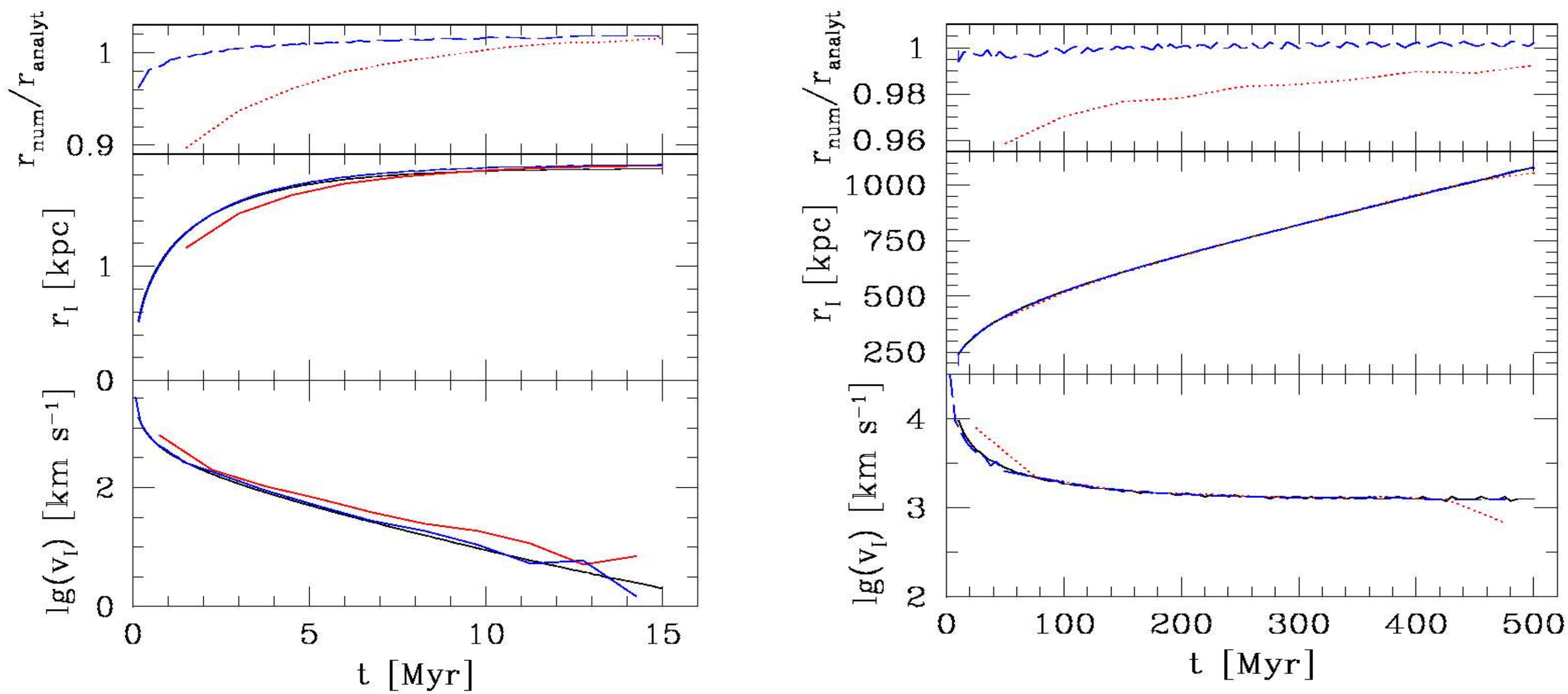
Thermal Update

- Using the photon-conserving heating rate, we update the temperature by applying it together with a cooling rate.
- The cooling rate is determined from a look-up table. Currently, a standard collisional ionization equilibrium cooling rate (H+He). This could be composition dependent.
- In order to deal with this stiff equation we subdivide the time step into smaller sub-time steps within which the energy change is limited to a fraction $\eta<1$.

Code Flow Chart

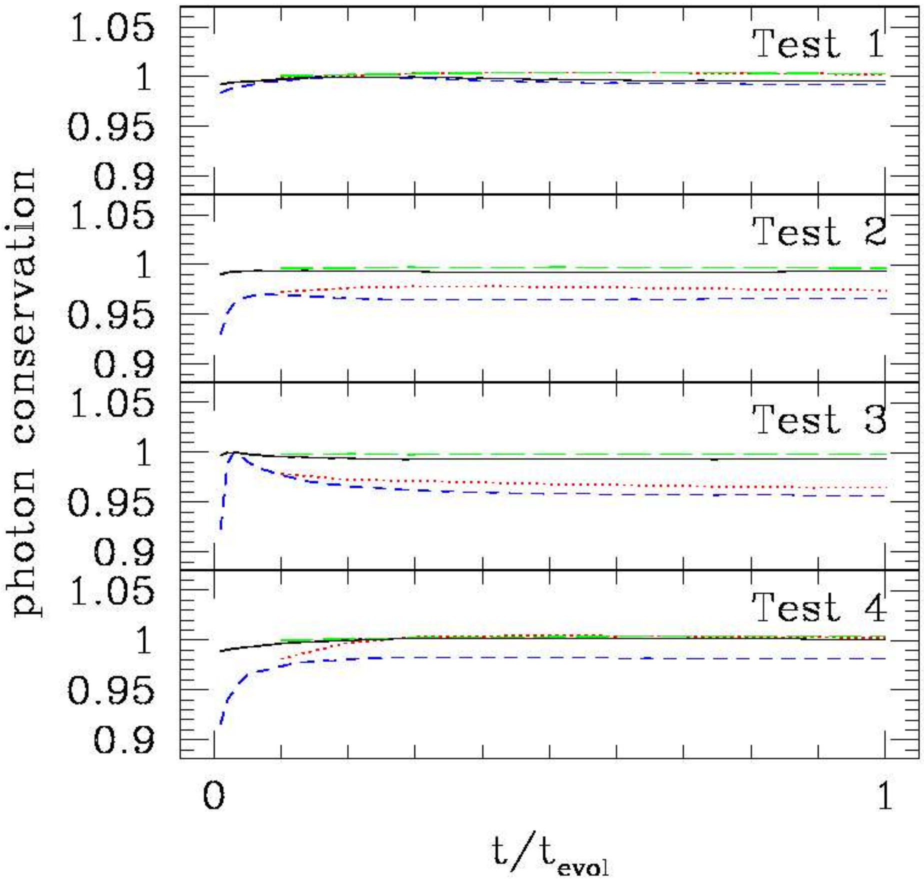


Tests: I-front propagation in 3-D
(sample)



Examples: I-front propagation in (a) 1/r density profile and (b) expanding, uniform IGM with mean clumping and fixed temperature (analytical solutions=black). Correct I-front tracking regardless of the resolution in space and time (even very coarse).

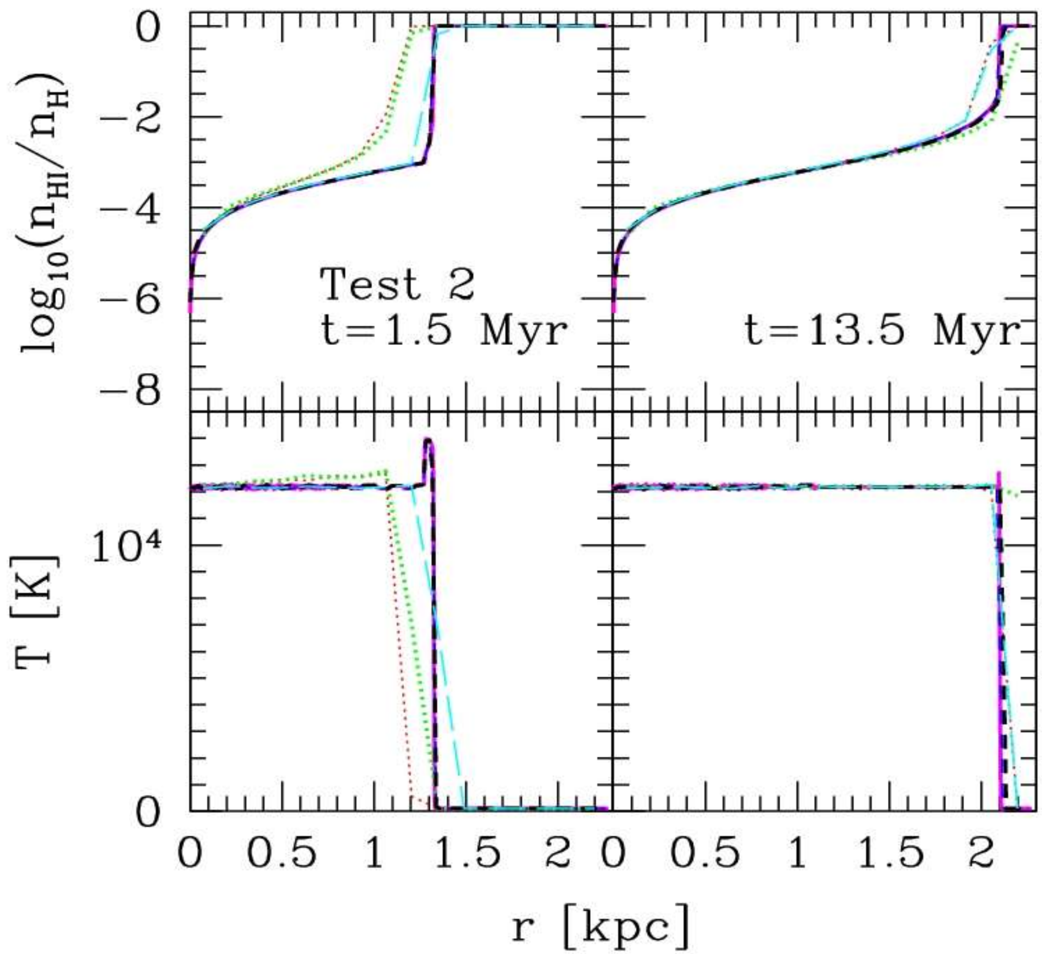
Photon Conservation



Photons are conserved to within few percent at very low resolution and small fraction of 1% at higher resolution

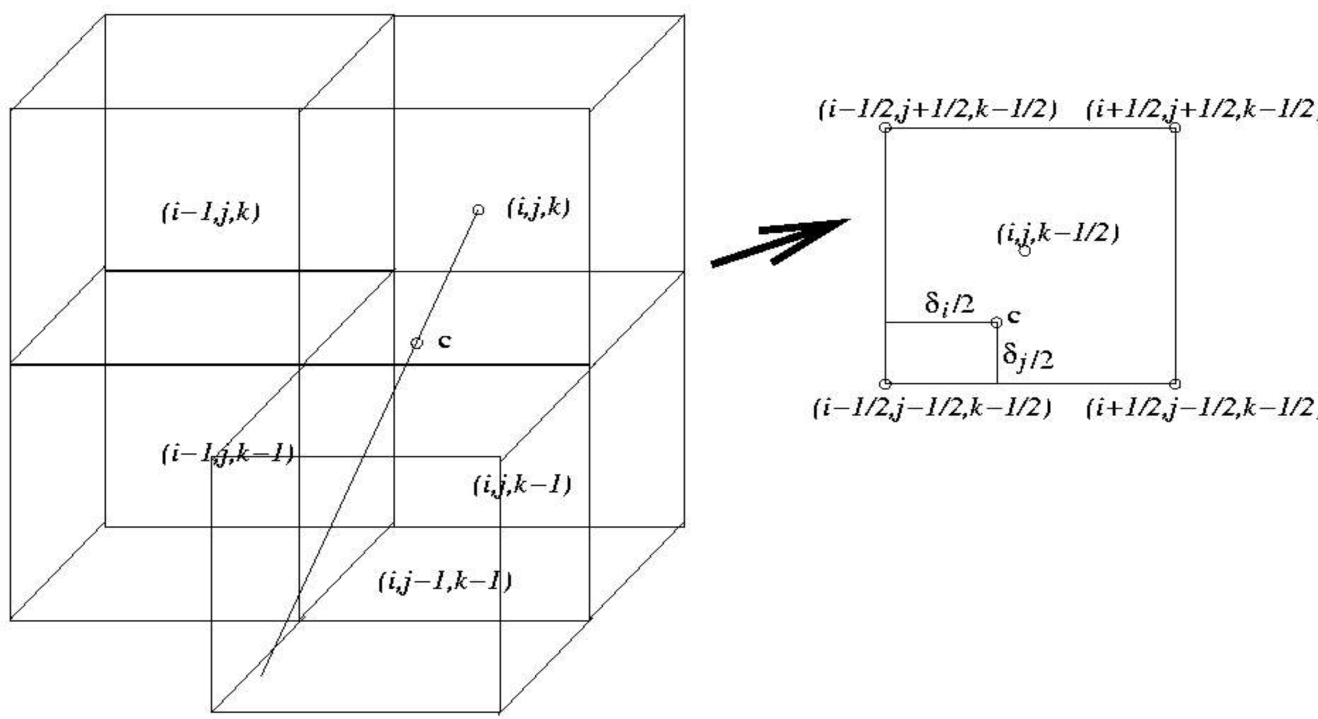
Temperature tests (sample)

- 1/r density profile (NFW-like)
- Stromgren sphere reached
- 1-D, 3-D and “analytical” agree, regardless of space/time resolution



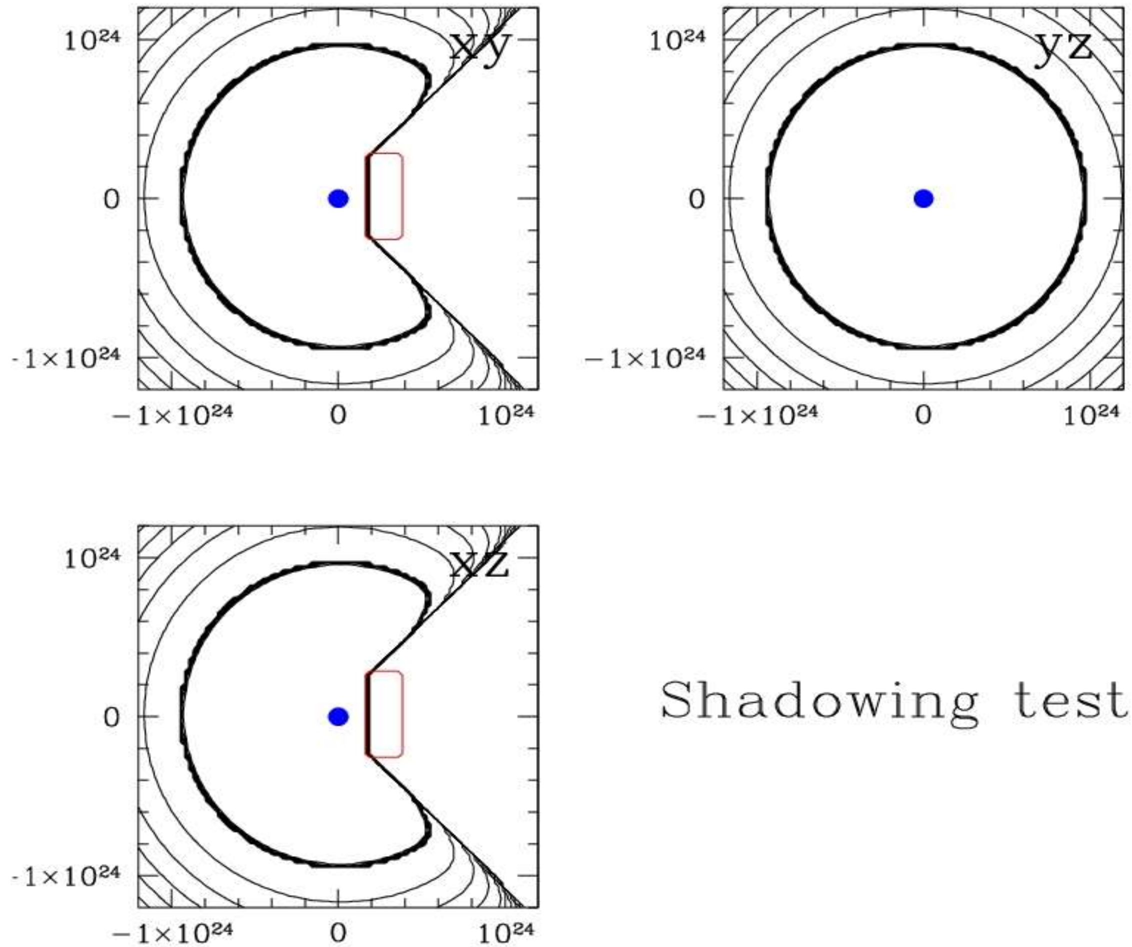
Multi-dimensional Ray-tracing

- We developed an efficient 3D ray-tracer for this, based on the technique of short characteristics.
- Optical depth is constructed from the solutions of cells closer to the source.

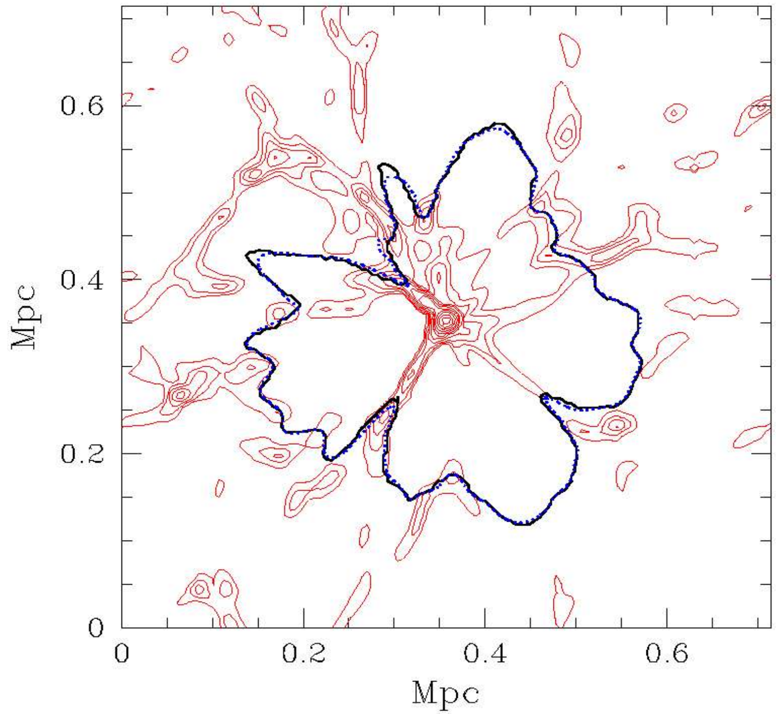


Shadowing Test

- ionizing source (blue)
- dense obstacle (red)
- 256^3 cells
- contours: time-sequence of 50% ionized fraction, every 20 Myr
- I-front is spherical, shadows are at the correct place, there is slight diffusion around the shadow's edges



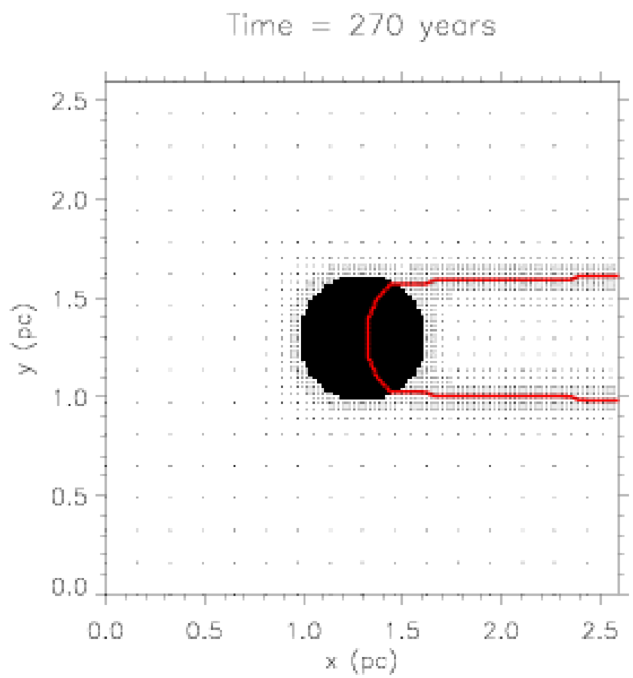
Long- vs. Short-characteristics



- Long-characteristics is more precise, but often slower and more difficult to implement for multiple sources
- Short-characteristics is faster and gives same results as LC.

Adaptive Mesh Refinement

- Coupled to AMR structure of *Yguazu-a* (cell-structured AMR)
- Currently only plane-parallel transport is implemented, but method is fully-compatible with arbitrary point sources

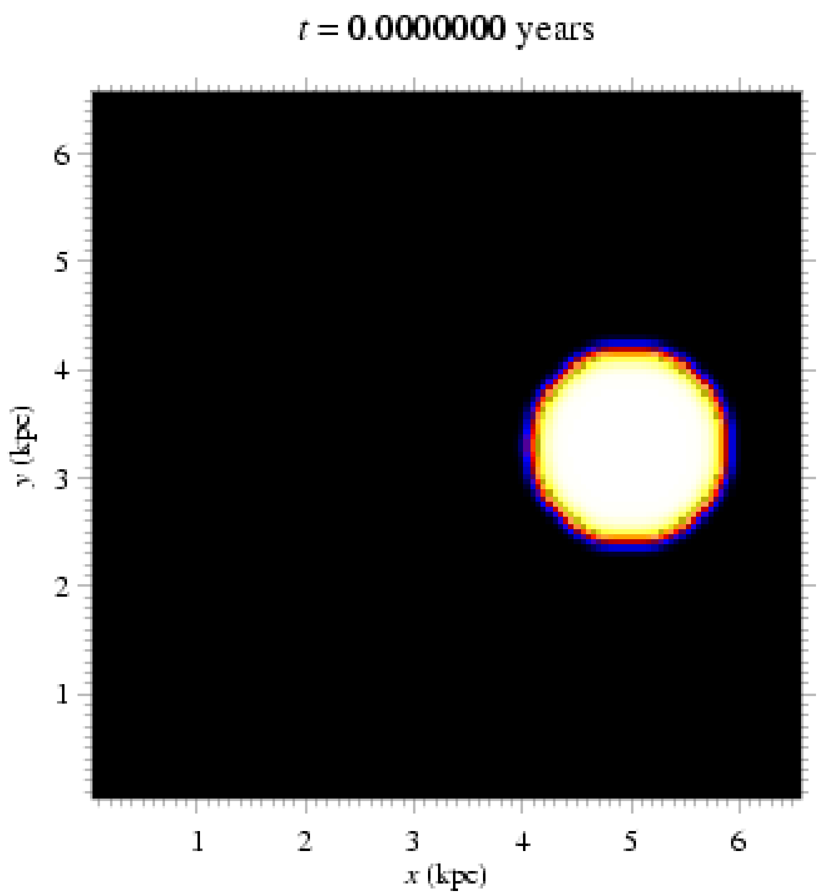


Coupling to gasdynamics: fixed grid

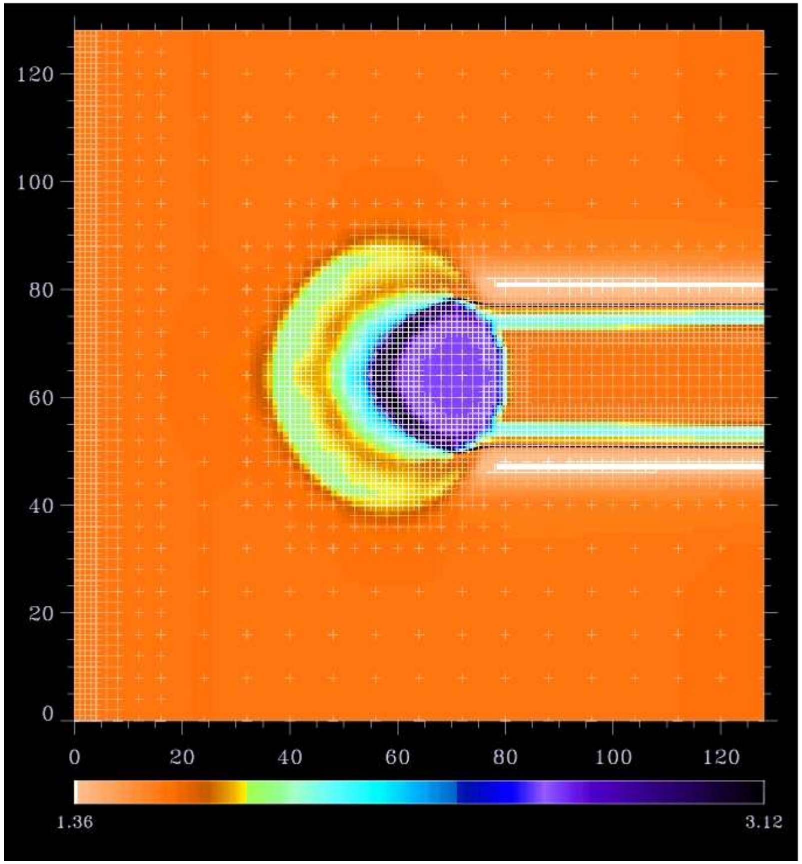
Currently coupled to:

Capreole3D= massively-parallel regular grid hydro code *(*by G. Mellema) (full RT)

Left: photoevaporation of an uniform dense clump



Coupling to AMR gasdynamics



Code is now coupled to adaptive mesh refinement (AMR) hydrodynamics code yguasu-a (by A. Raga).

Example: plane-parallel I-front encounters a dense clump and starts photoevaporating it

Summary of Features

- Hydrogen ionization (photo + collisional).
- Frequency-dependent opacity.
- Heating by photo-ionization (no secondary ionizations), cooling by specified cooling table.
- Small number of source types (lookup tables).
- Multiple sources, limited by computational resources.
- No diffuse field (OTS/case B approximation).
- On typical workstation: box sizes up to 256^3 (RAM-limited). With a few ionizing sources takes minutes to an hour runtime.
- Designed for use with both regular and adaptive meshes (AMR).

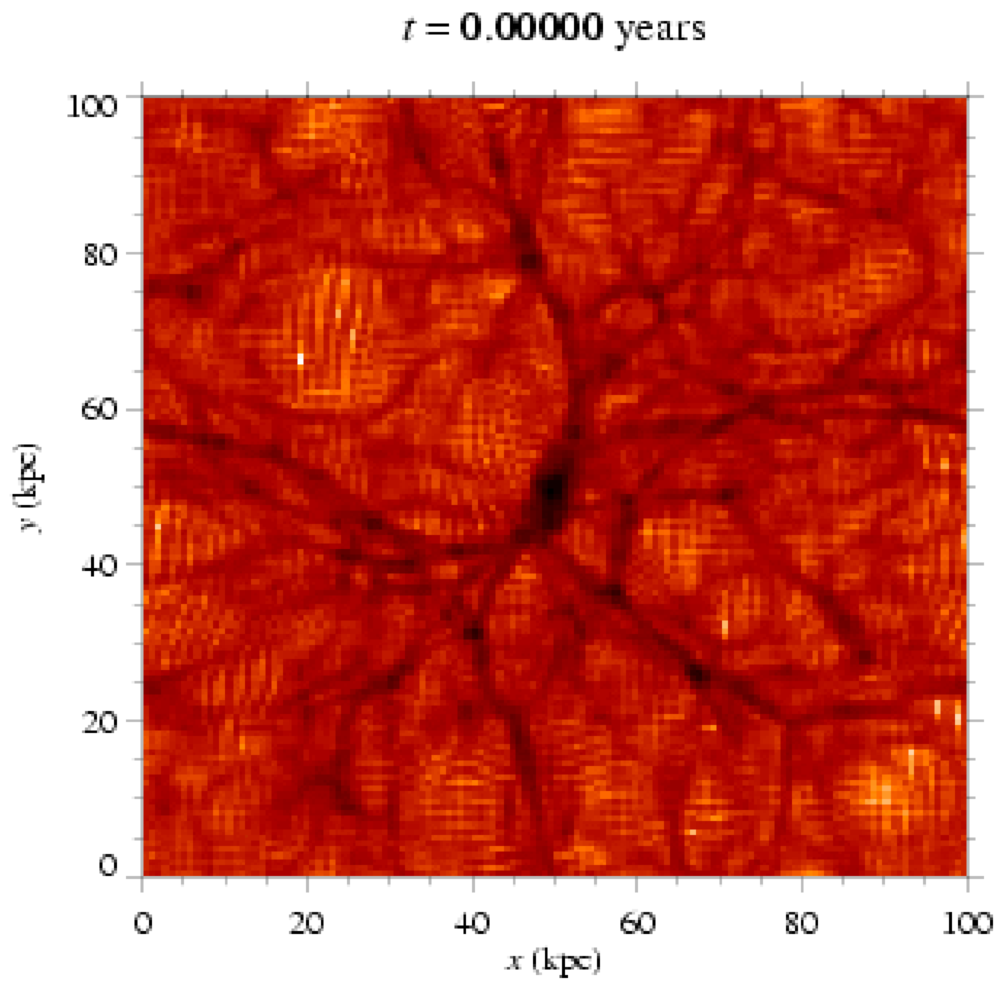
Cosmological I-front Evolution

1 Mpc box

1 source

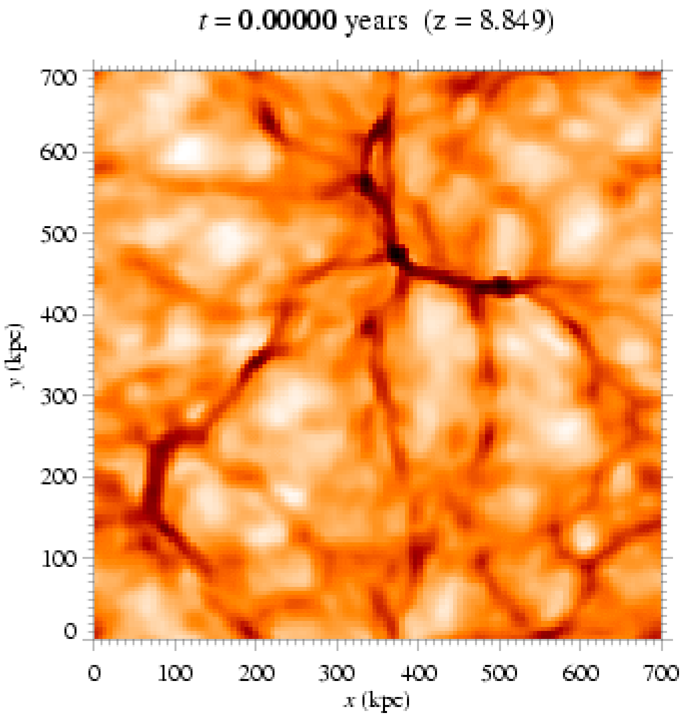
x-y cross-section

The evolution is complex (neither low-density first, not high-density first) dense filaments and halos cast long shadows

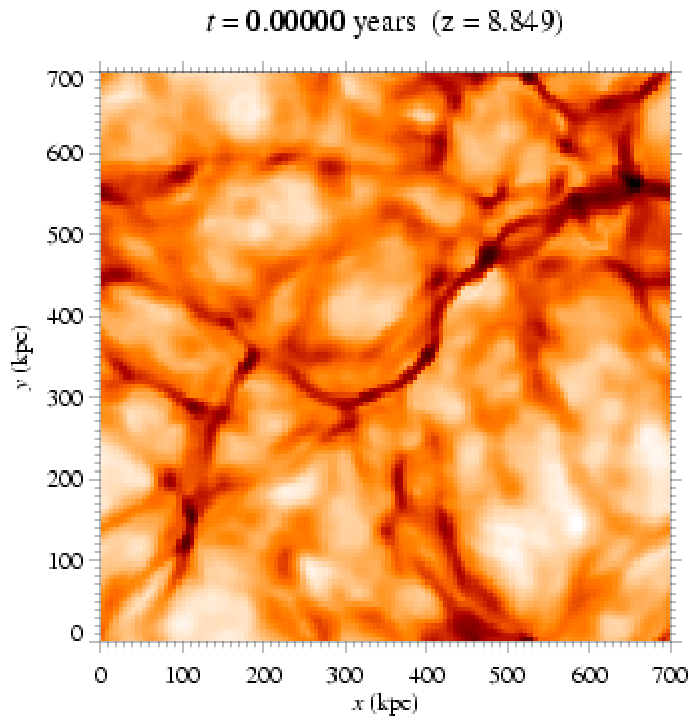


Multiple-source run

x-y slice



y-z slice



16 ionizing sources

Structure Formation at High-z

We performed very high-resolution N-body simulations of structure formation at high-z using PMFAST code developed at CITA

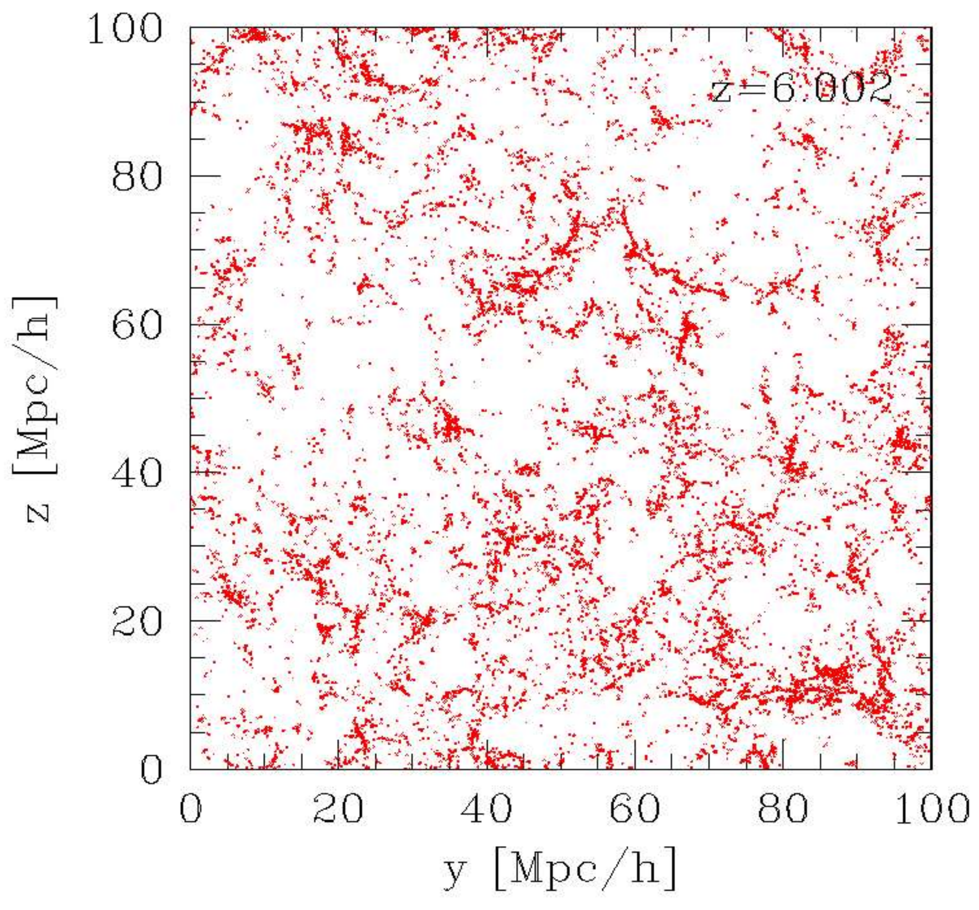
(Merz, Pen & Trac 2004)

Simulation parameters:

- 100/h Mpc box (other box sizes, from 3/h up to 35/h Mpc also completed)
- 1624^3 particles=4.3 billion (up to 1836^3 = 6.4 billion particles possible on available hardware), 3248^3 (3712^3) cells.
- Code is very efficient: each run takes few days to a week.
- Identified up to 1.3 million halos (at z=3) (>100 particles/halo=2.5e9 M_solar)

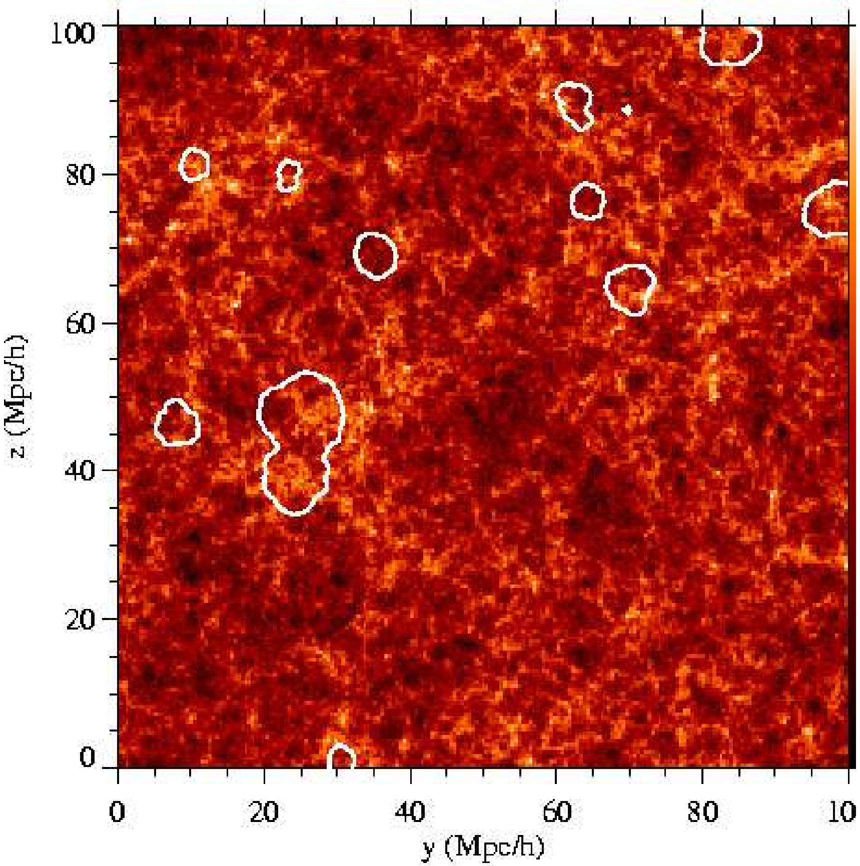
High-resolution N-body simulations

- 2/h Mpc slice=1/50 of boxsize
- z=6
- red=resolved halos (16,205 halos in this slice)

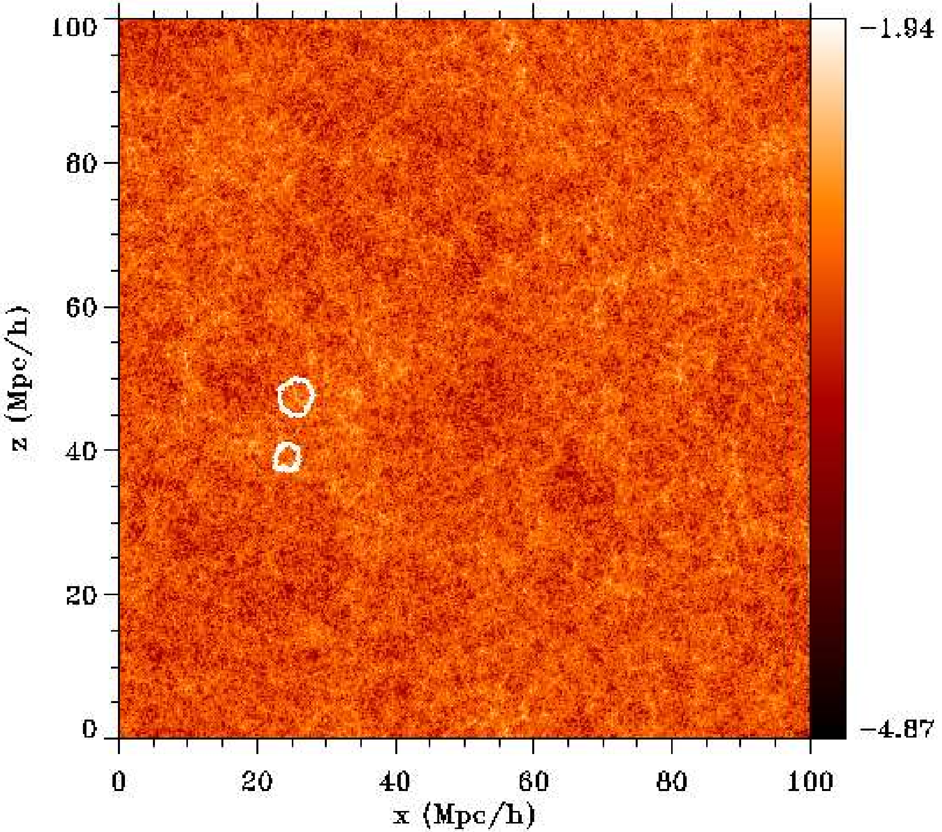


Application: first high-resolution reionization simulations
(preliminary results, running now)

203^3 box, z=15

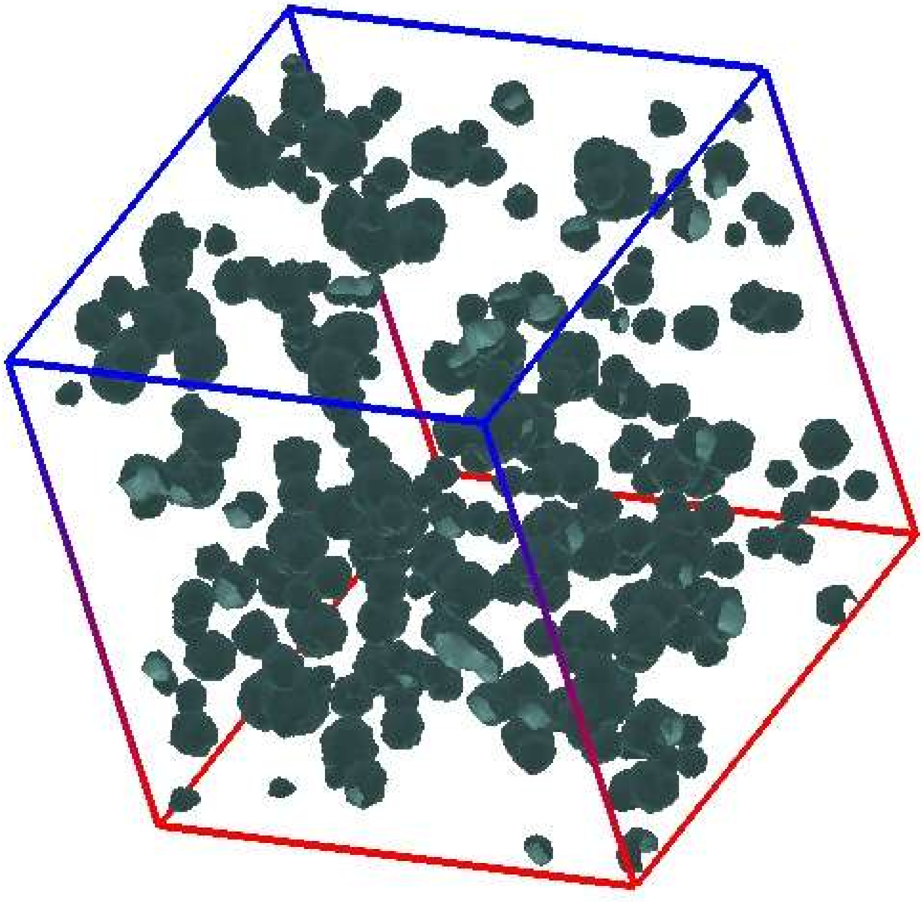


812^3 box, z=16.6



Universe at z=14.5

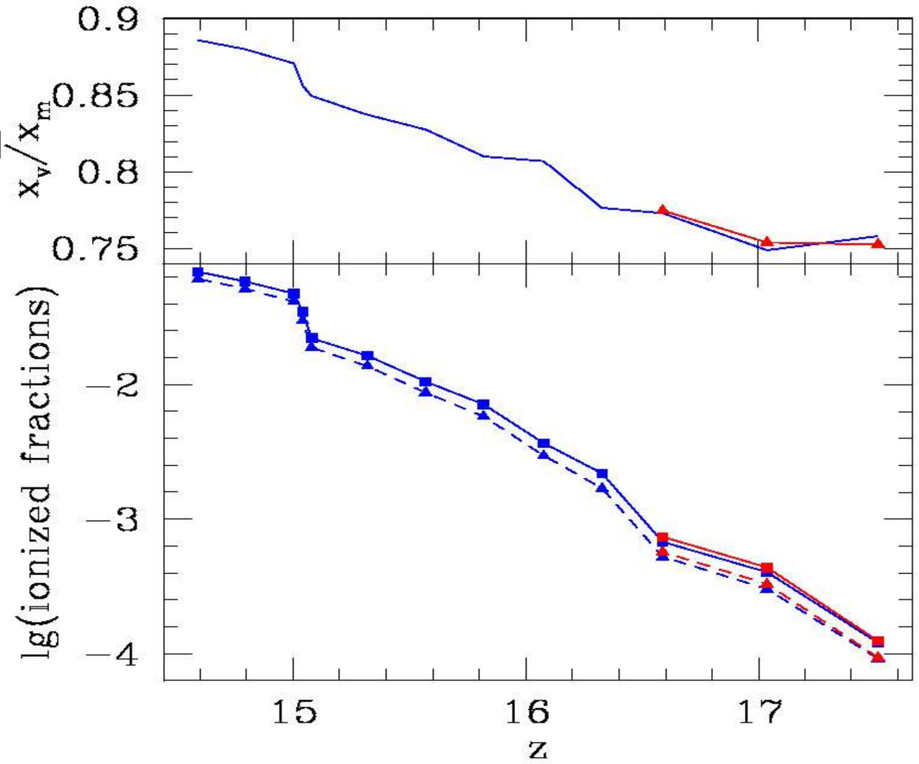
- HII regions of individual sources and groups start overlapping.
- The topology of the ionized/neutral regions is complex.



(visualized using Ifrit package by N.Gnedin)

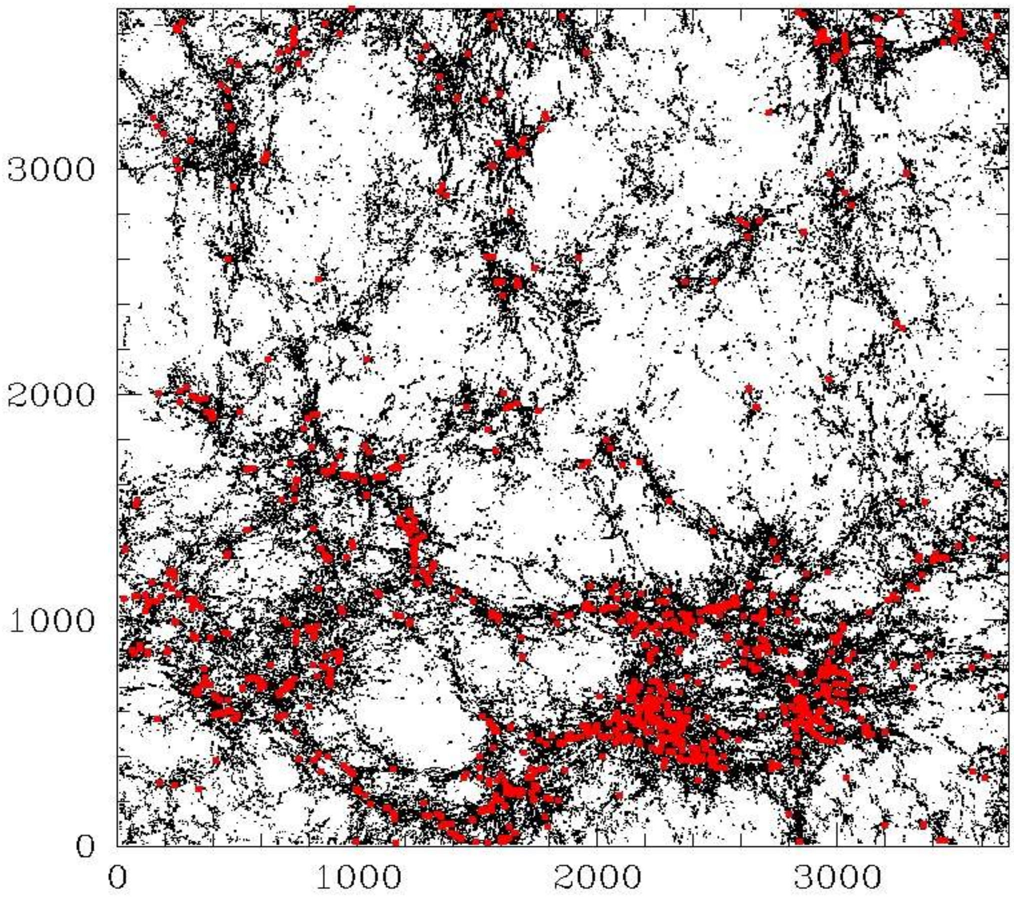
Evolution of the ionized fractions

- Mass-weighted ionized fraction starts higher than volume-weighted (dense regions around sources ionized first)
- The high- and low-res results roughly agree but there are noticeable, and growing, discrepancies (~10% at z~16.5-17).



High-resolution N-body simulations: smaller box

- 10/h Mpc box
- 1 Mpc slice
- z=9.42
- red=sources (1077 halos)
- black=minihalos (124,121 halos)



Radiative transfer code comparison project

- Verification of current codes
- Testbed for future radiative transfer code development
- 9 codes
- 8 tests, 5 pure RT and 3 with gas-dynamics
- results still being collected, project to be finalized by Fall 2005
- preliminary results show general agreement, but also some interesting differences, to be studied.

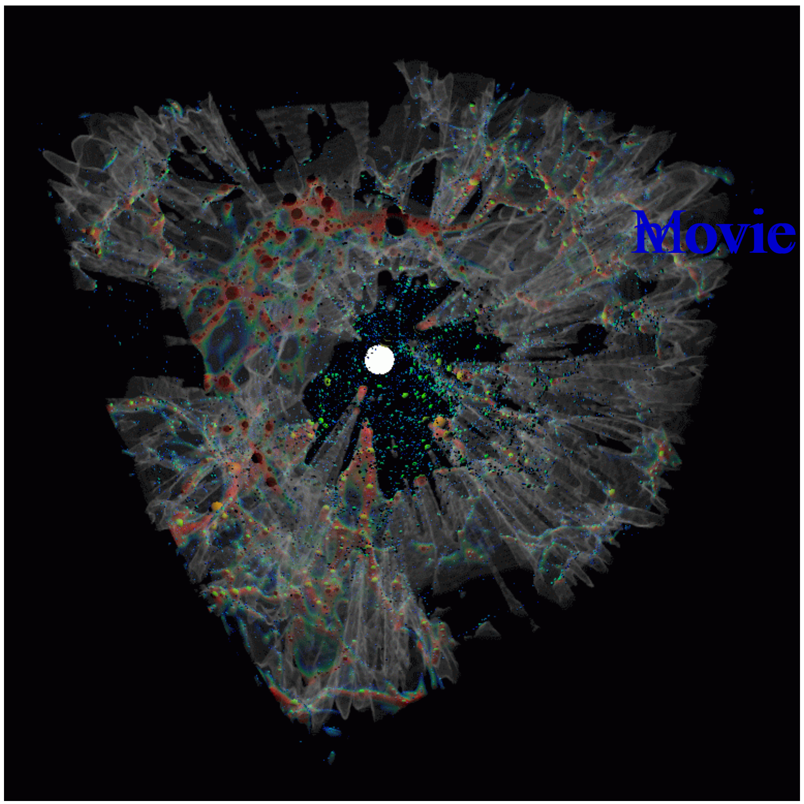
Looking Ahead

- Easy additions:
  - Helium (He^0, He^+, He^{2+}) photo-ionization.
  - Other atomic species (C, N, O, Ne, S): ionization and cooling (no opacity).
  - Secondary ionizations ($h\nu > 25$ eV).
- Harder additions:
  - Molecular hydrogen.
  - True diffuse field

Conclusions

- A photon-conserving (finite-volume) approach using time-averaged optical depths along rays allows an efficient and accurate treatment of ionization fronts.
- This efficiency allows the photo-ionization to be calculated inside a hydrodynamics simulation. Code is already coupled to gasdynamics codes, both fixed-grid and AMR.
- Combination with adaptive mesh refinement makes it possible to handle a large dynamic range.
- Detailed predictions for reionization observations with e.g. next-generation radio arrays at 21-cm now possible

I-front propagation in a cosmological density field with minihalos



Visualization of an I-front propagation in a cosmological density field (LCDM)

box : 0.5/h Mpc

redshift: z=9

Movie