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U.S. DEPARTMENT OF ENERGY

NYX: A New Massively Parallel AMR Code for Cosmology

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NYX at a glance

- 3-D Eulerian, Cartesian grid, finite volume code
- Evolve dark matter as collisionless Lagrangian fluid
- Evolve baryons as ideal gas using unsplit Godunov-type methodology
- Adaptive mesh refinement (AMR) to extend dynamic range
- Built on BoxLib software framework developed and maintained in CCSE
- Code paper to appear in The Astrophysical Journal

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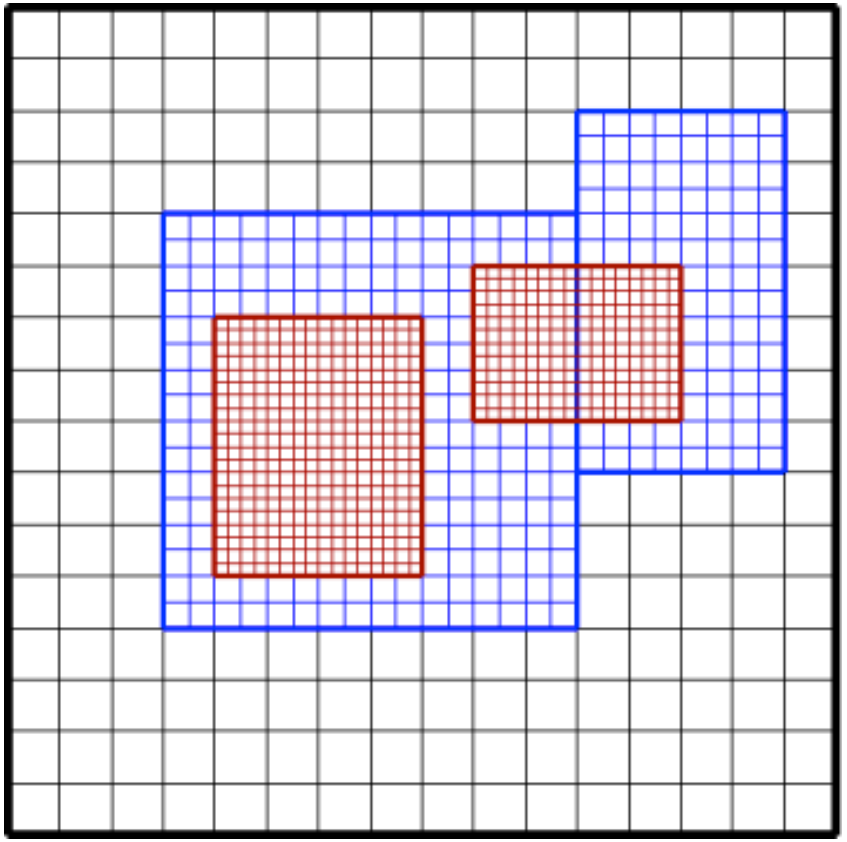
AMR

- Block refinement: nested hierarchy of rectangular grids
- Refinement by factor 2 or 4
- No strict parent-child relation
- Regridding procedure:
  1. Tag cells on given criteria
  2. Group into rectangular grids
  3. Break into large patches if needed



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Dark Matter

- Dark matter is a collisionless fluid

$$\frac{\partial f}{\partial t} + \frac{1}{ma^2}\mathbf{p}\cdot\nabla f - m\nabla\phi\cdot\frac{\partial f}{\partial \mathbf{p}} = 0$$

$$\nabla^2\phi = \frac{4\pi G}{a}(\rho_{tot} - \rho_0)$$

- Solve as an N-body system

$$\frac{d\mathbf{x}_i}{dt} = \frac{1}{a}\mathbf{u}_i$$

$$\frac{d(a\mathbf{u}_i)}{dt} = \mathbf{g}_i$$

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Baryonic matter

- Model “ordinary” matter as inviscid ideal gas

$$\frac{\partial \rho_b}{\partial t} = -\frac{1}{a}\nabla \cdot (\rho_b \mathbf{u})$$

$$\frac{\partial (a\rho_b \mathbf{u})}{\partial t} = -\nabla \cdot (\rho_b \mathbf{u}\mathbf{u}) - \nabla p + \rho_b \mathbf{g}$$

$$\frac{\partial (a^2 \rho_b E)}{\partial t} = -a\nabla \cdot (\rho_b \mathbf{u} E + p\mathbf{u}) + a\rho_b \mathbf{u} \cdot \mathbf{g} + a\dot{a}\left((2 - 3(\gamma - 1))\rho_b e\right) + a\Lambda_{HC}$$

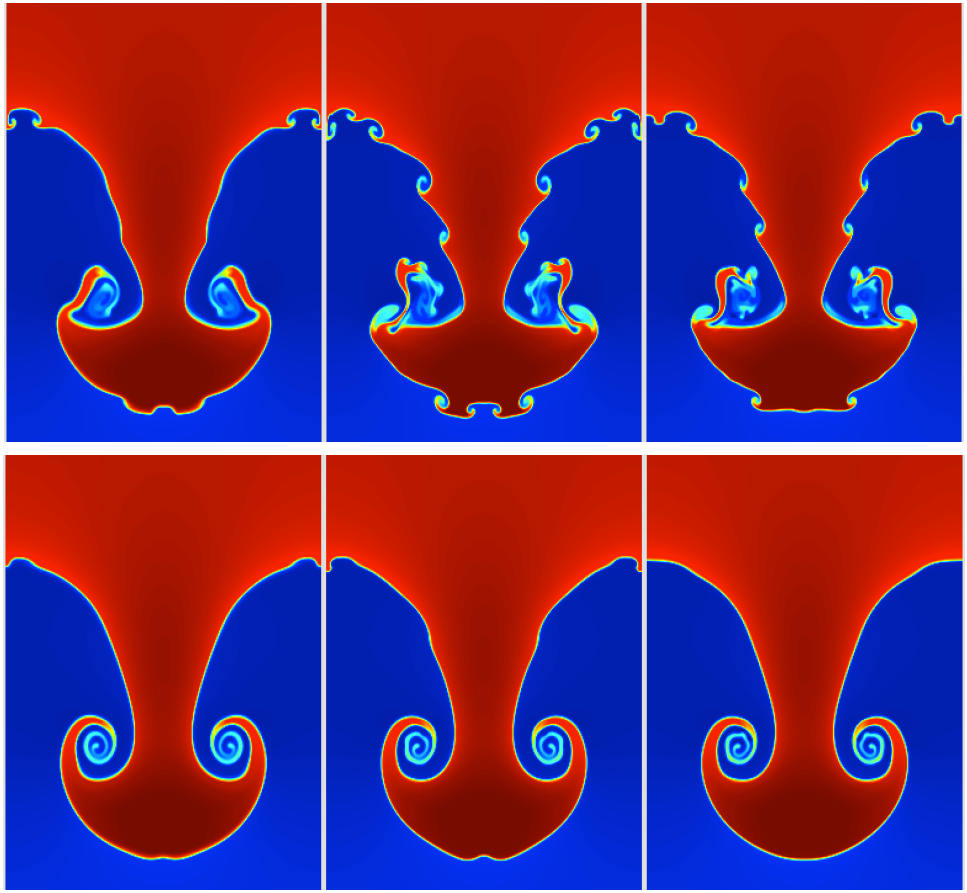
Euler equations:
- Mass
- Momentum
- Energy

$$p = (\gamma - 1)\rho e$$

Equation of state

Hydro: Split vs. Unsplit

- Rayleigh-Taylor instability: denser fluid on top of less dense
- Operator-split methods produce secondary instabilities.
- Price: unsplit methods are factor of ~2 slower in 3D



Almgren et al. 2010

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Gravity Calculation

- Particle masses deposited on a grid to define density – we use standard cloud-in-cell scheme
- Dark matter density and baryonic density added to form RHS of Poisson equation, which is solved on grid hierarchy
- Gravity used as source term for fluid equations on grid
- Gravitational forces interpolated back to particle locations for use in kick-drift-kick scheme

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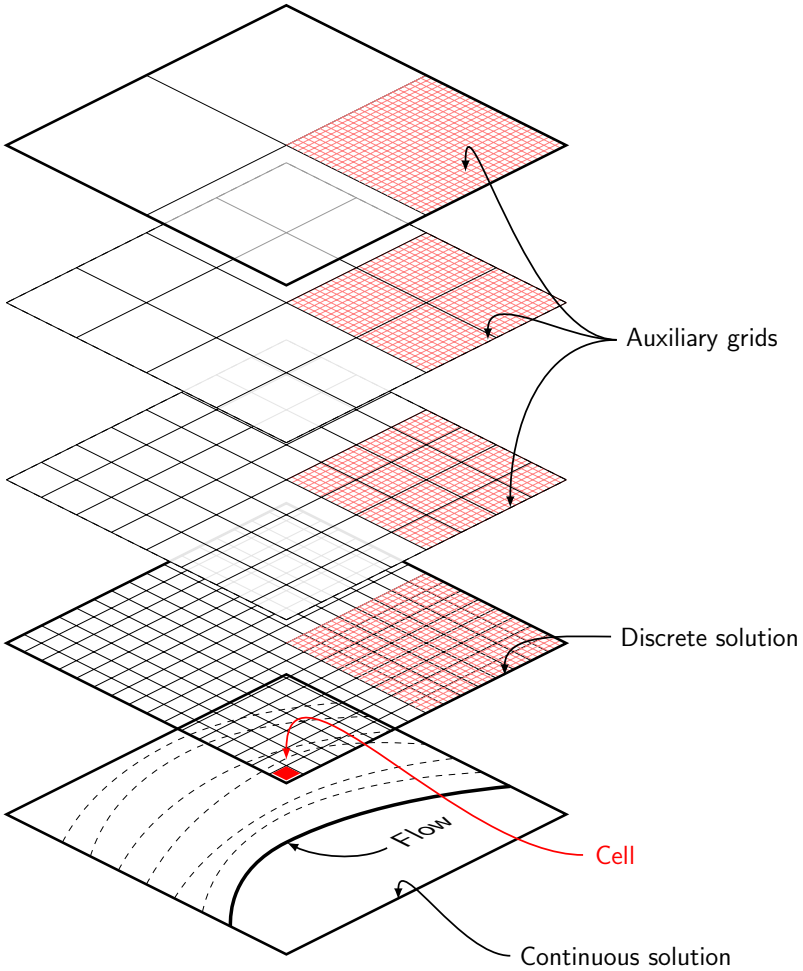
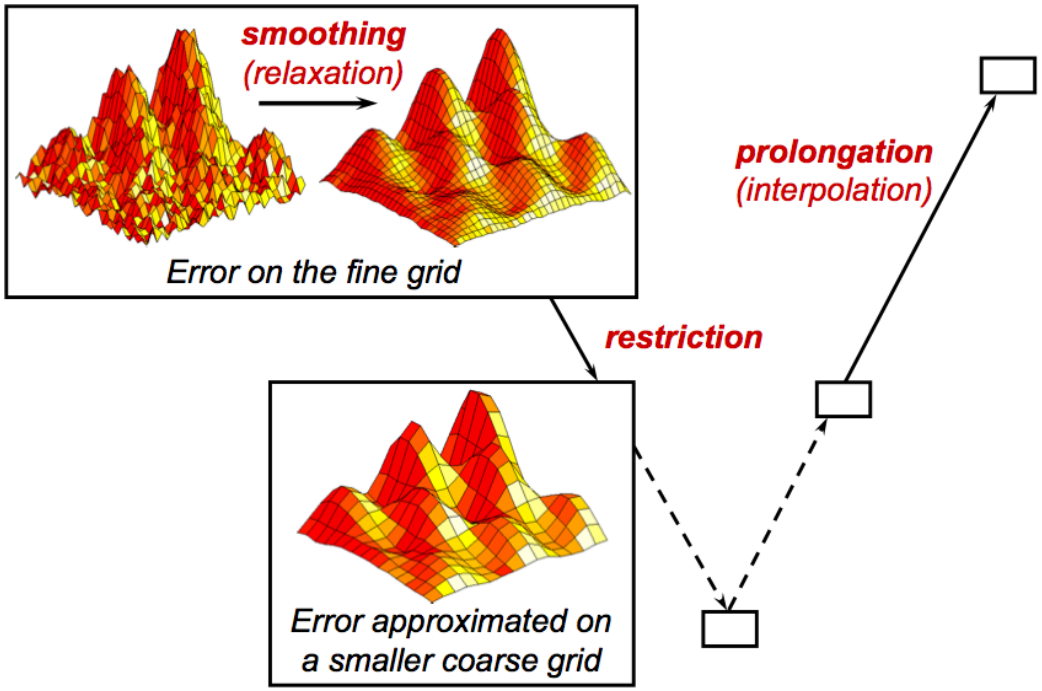
Solving Poisson equation

- Geometric multigrid with red-black GSRB and V-cycles

$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} = \rho_i$$





O(N) scaling!

BoxLib

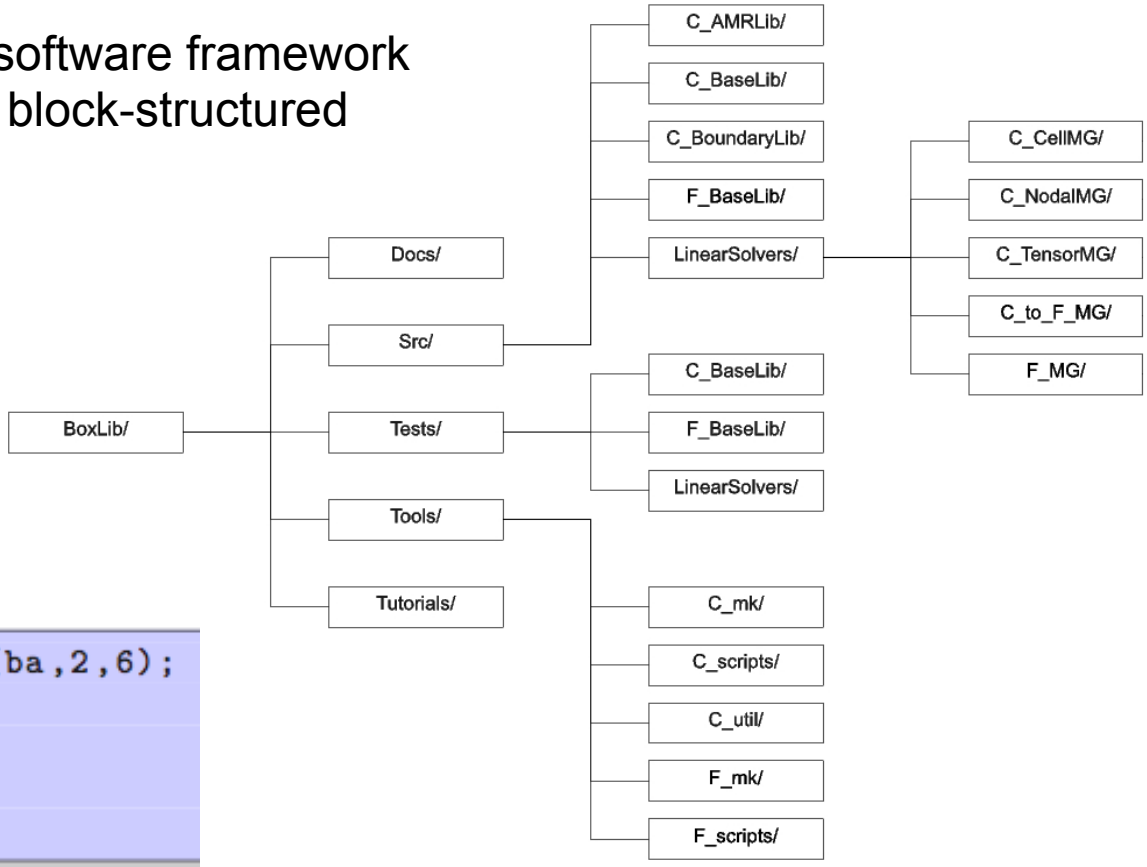
BoxLib is a publicly available software framework for building massively parallel block-structured AMR applications.

```
IntVect lo(0,0), hi(15,15);
Box bx(lo,hi);
BoxArray ba(bx);   // the Box
ba.maxSize(8);     // the Box
```

```
MultiFab* data = new MultiFab(ba,2,6);

...

delete data;
```



BoxLib (p2)

- Pure F90 as well as hybrid C++ / F90 versions of basic BoxLib functionality

•BoxLib contains extensive software support for grid-based operations as well as particles on adaptive hierarchical meshes. Particles are stored on same node as underlying grid for fast communication.

- Multilevel multigrid solvers are included for cell-based and node-based data.

- Multiple time-subcycling modes supported for AMR simulations

- Parallelism is achieved using the distribution of grids to nodes using MPI as well as on-node parallelism using OpenMP

- Native BoxLib format for checkpoint files and plotfiles – I/O speeds comparable to NERSC benchmark – format supported by Visit

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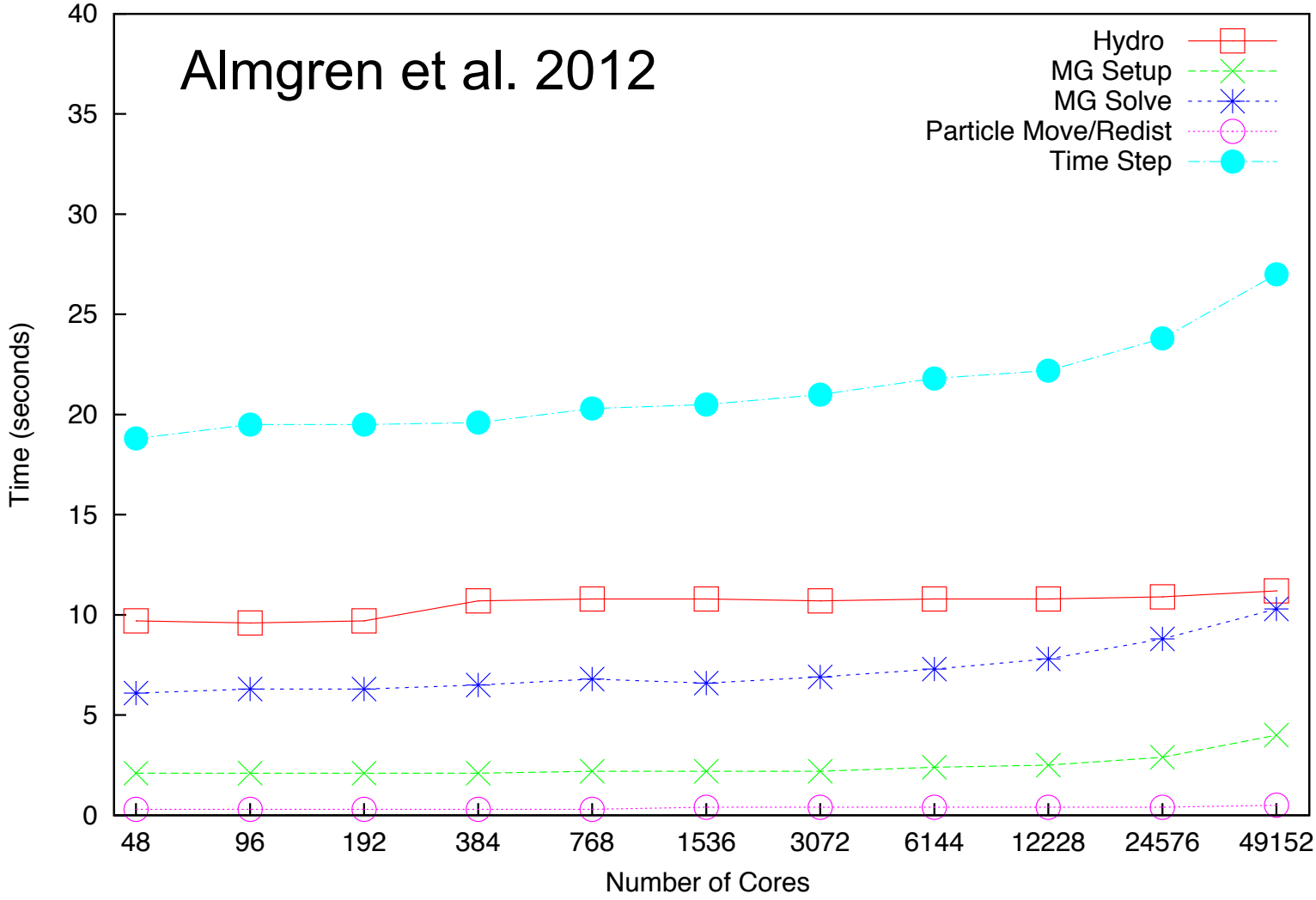
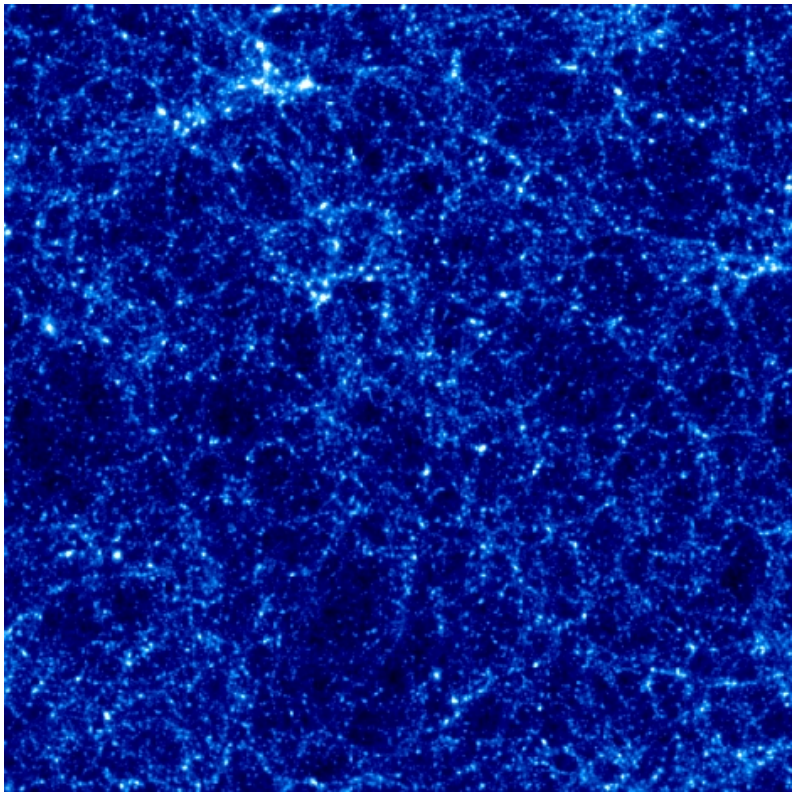
Scaling


Almgren et al. 2012
Hydro
MG Setup
MG Solve
Particle Move/Redist
Time Step
Time (seconds)
0
5
10
15
20
25
30
35
40
48
96
192
384
768
1536
3072
6144
12228
24576
49152
Number of Cores

Validating gravity

- 256Mpc/h box, with 256^3 particles
  - $\Omega_{tot} = 0.314$
  - $\Omega_{Lambda} = 0.686$
  - $\Omega_{Baryon} = 0.044$
  - $H = 71$ km/s/Mpc
  - $\sigma_8 = 0.84$
  - $n_s = 0.99$
  - $z_{init} = 50$



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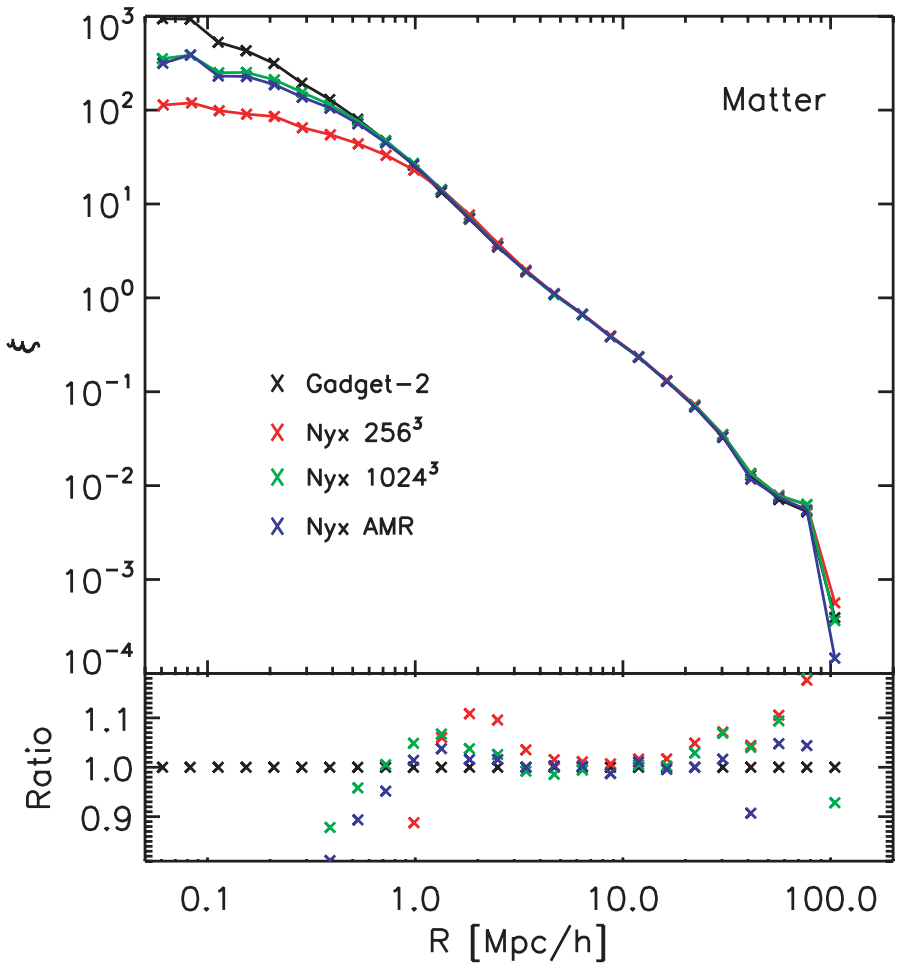
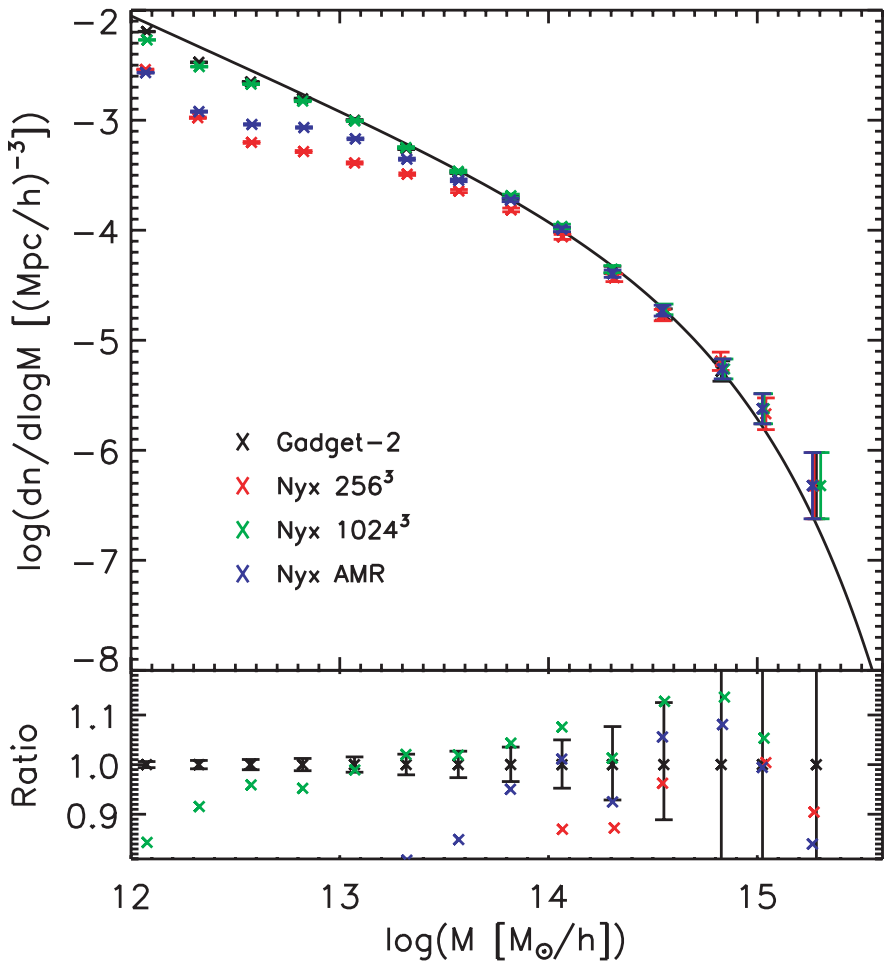
Matter correlation function

- Good agreement to Gadget-2, ran at much higher resolution.
- AMR converges to fixed-grid at highest refinement



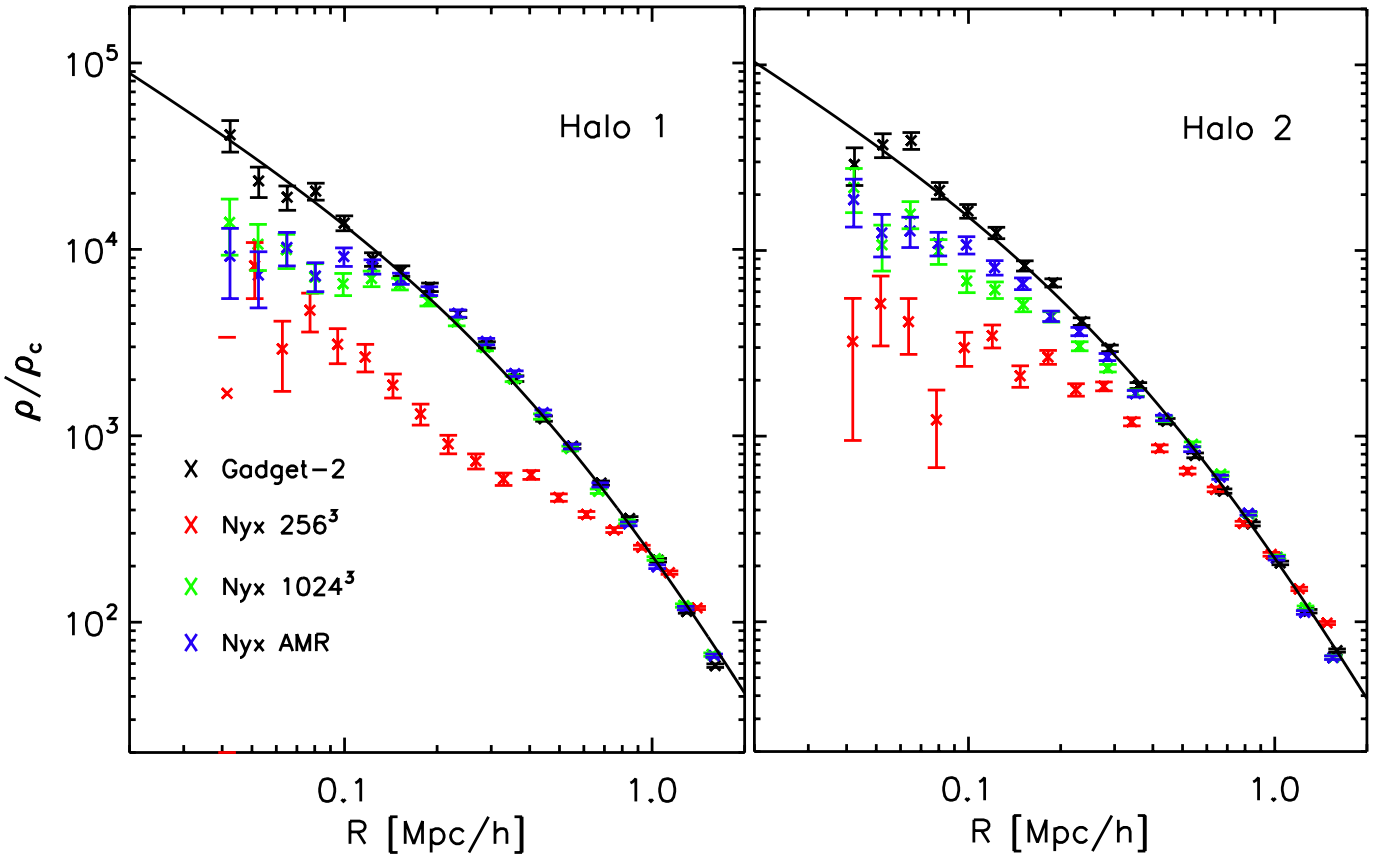
Halo mass function

- AMR codes commonly do not get small halos in the field; that would require aggressive refinement criteria.
- Studied in Lukić et al. 2007, and Heitmann et al. 2008

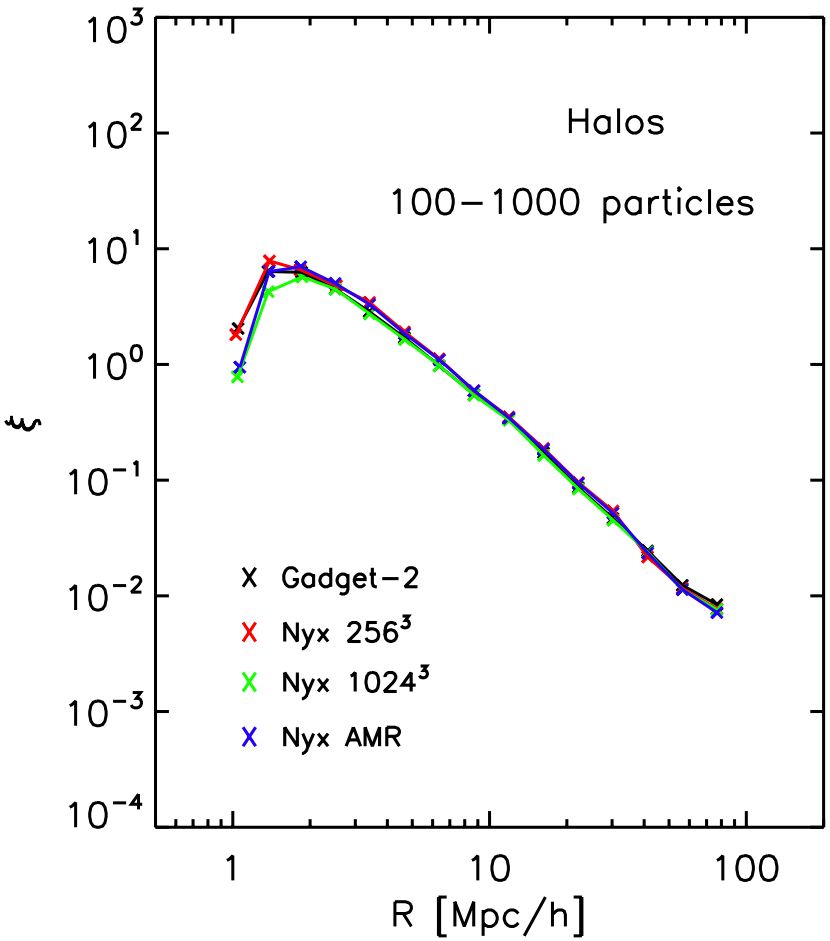


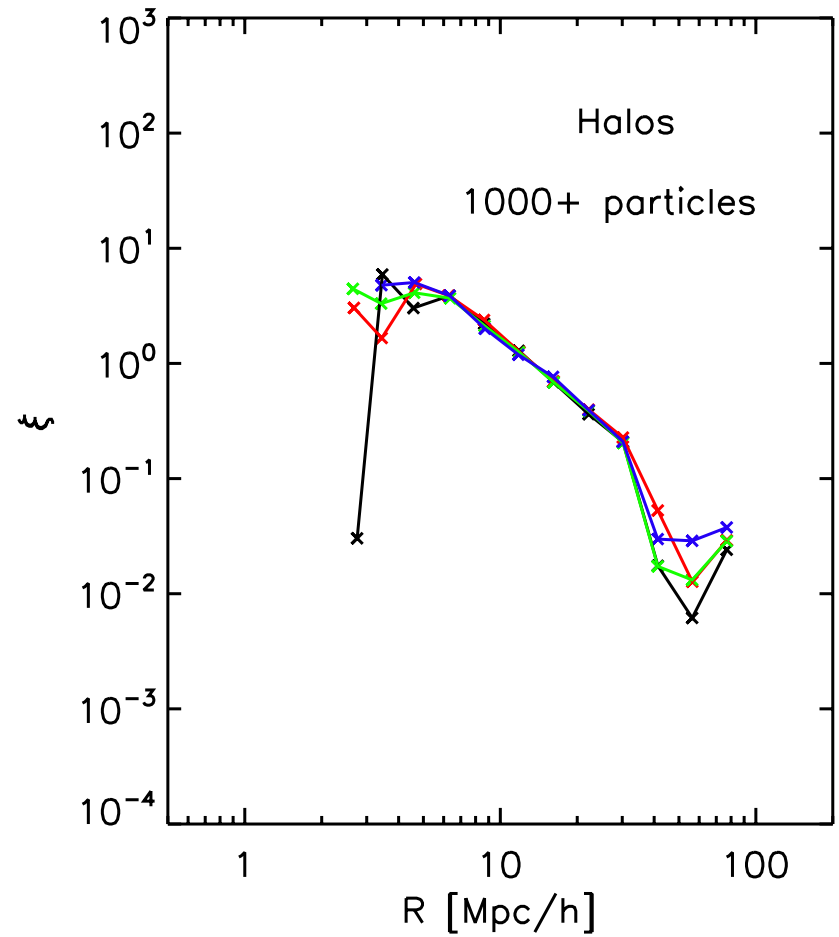
Halo profiles

- AMR helps a lot in this case!



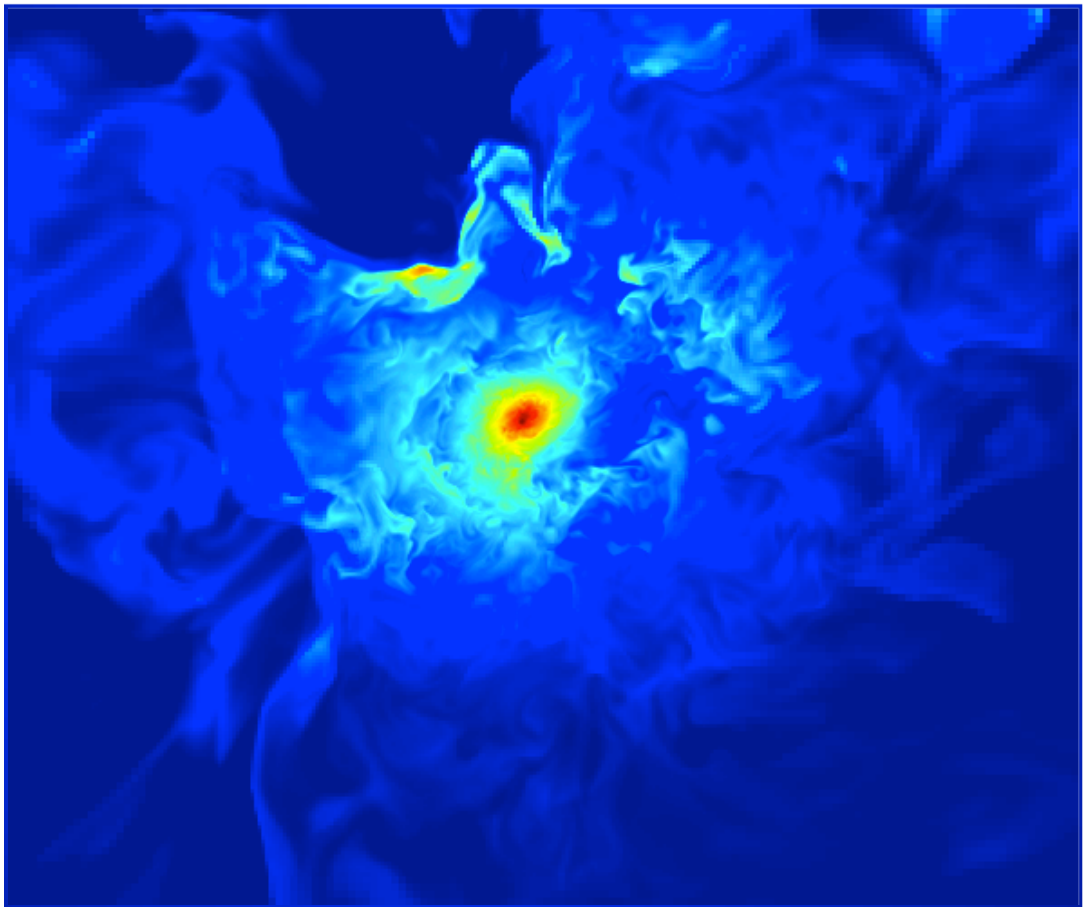
Halo correlation function





Validating gas dynamics

- Santa Barbara cluster
- $\Omega_{tot} = 1$
- $\Omega_{lambda} = 0$
- $\Omega_{Baryon} = 0.1$
- H = 50 km/s/Mpc
- Boxsize = 64Mpc
- $z_{ini} = 63$



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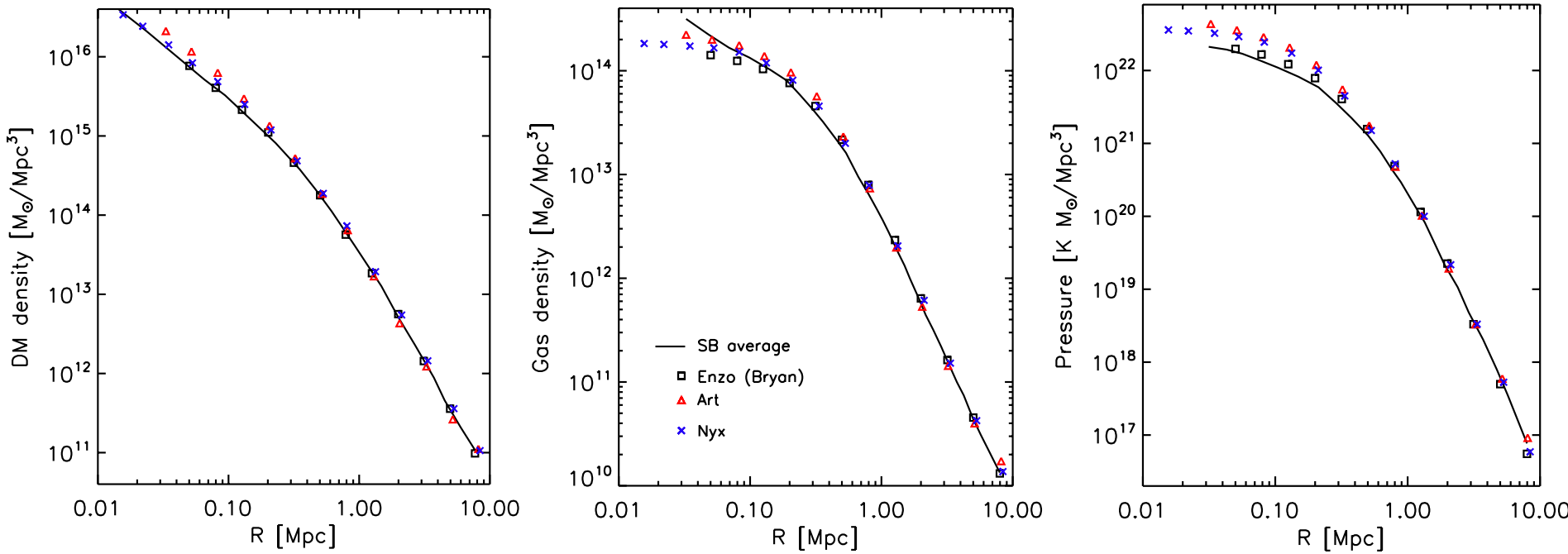
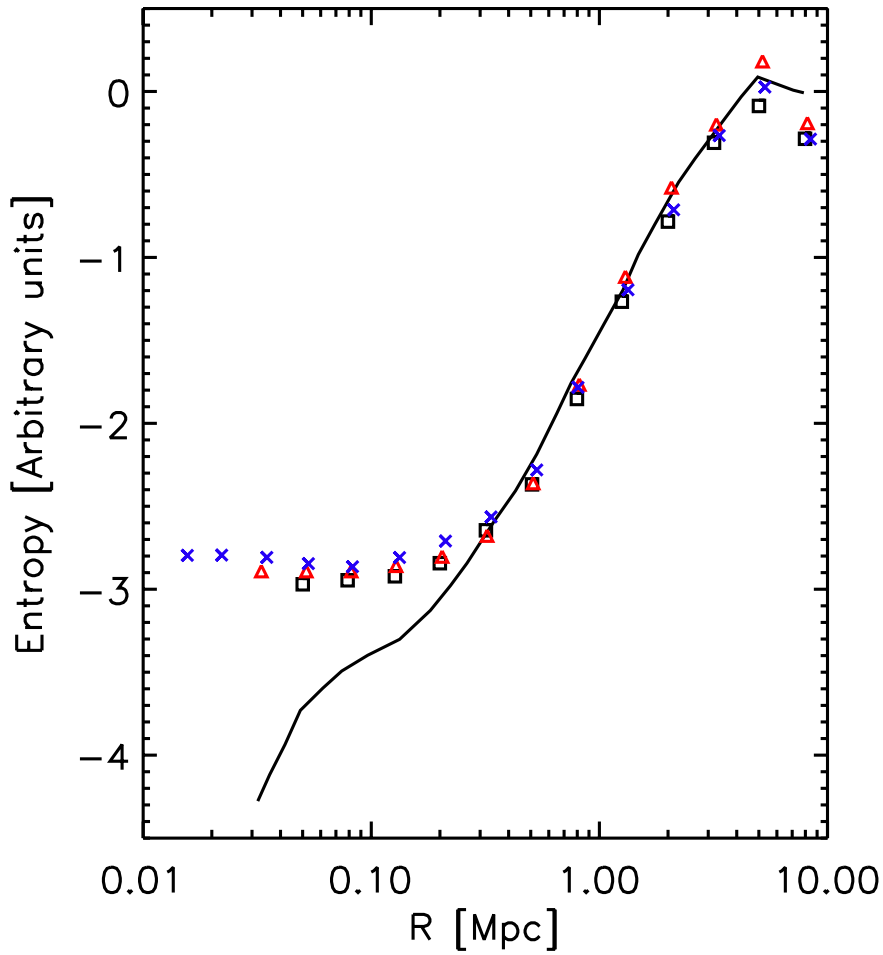
Profiles

- Agreement with other AMR codes

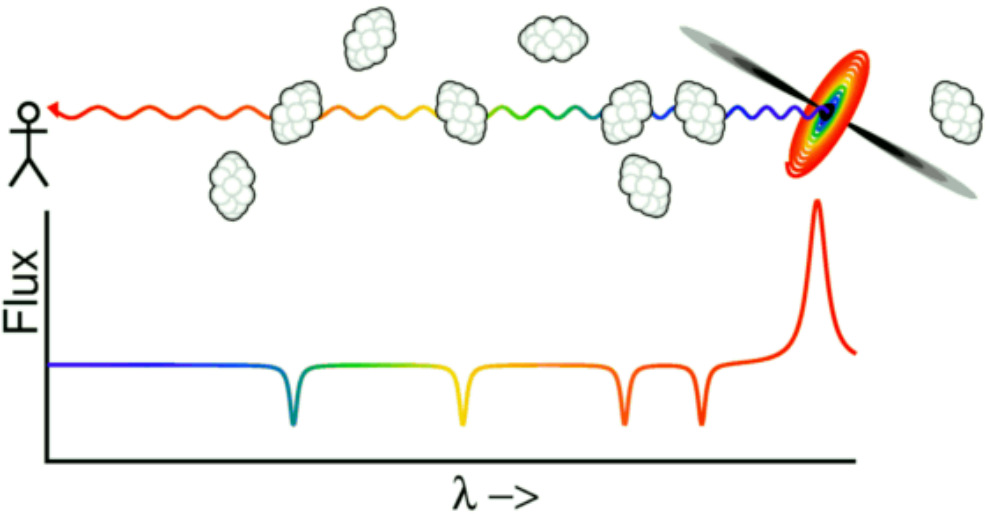


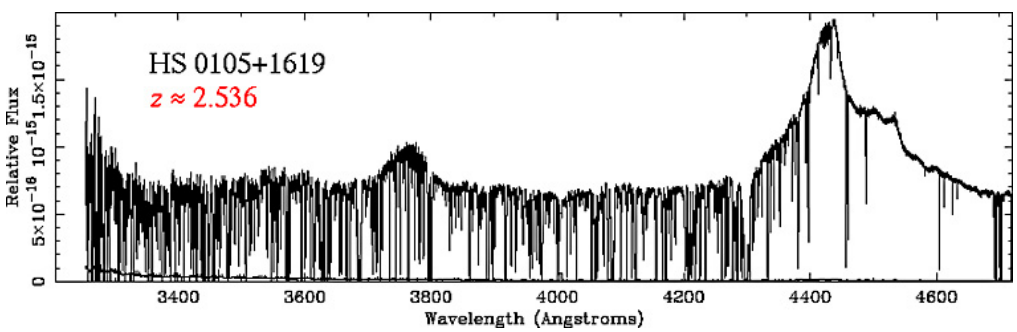
Central cluster entropy

- SPH and Eulerian codes give different answers
- This does not depend on resolution, number of particles, etc. (Mitchell 2009)
- Standard SPH formulation suppresses fluid instabilities and mixing



Ly-A





- Main SciDac target is Ly-A
  - Scalability allows for having large contiguous grids, capturing volumes of gas close to mean density
  - “A”MR allows for bridging the gap between Jeans length (~10kpc), and linearity scale (~100Mpc)
  - On-the-fly analysis for skewers (or τ at least)

Ly-A modeling challenges

- Need to know distributions of HI and HeII, rather than just "gas" density
- Photo-ionizing background is research topic in itself
- Hydrogen reionization (z~10) details likely do not matter at z~3-2 (Hui & Haiman 2003)
- He second reionization at z~3 relevant (McQuinn et al. 2011)
  - full radiation transport?
  - sources?
- First thing: optically thin medium

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Cooling and heating

- Model gas as a mixture of Hydrogen and Helium in their primordial abundances
- Atomic processes: excitations, ionizations, recombinations, free-free
- Ionization states for each element calculated assuming statistical equilibrium
- 6 species: HI, HII, HeI, HeII, HeIII and e^-
- In addition, cooling of e^- on CMB photons
- UV background heating (Faucher-Giguere et al. 2009)

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Ionization equilibrium

- Equations for 6 species:

$$\Gamma_{eH_0} n_{H_0} n_e + \Gamma_{\gamma n_{H_0}} n_{H_0} = \alpha_{H_+} n_{H_+} n_e$$

$$\Gamma_{eHe_0} n_{He_0} n_e + \Gamma_{\gamma n_{He_0}} n_{He_0} = (\alpha_{H_+} + \alpha_d) n_{He_+} n_e$$

$$\Gamma_{eHe_+} n_{He_+} n_e + \Gamma_{\gamma n_{He_+}} n_{He_+} + (\alpha_{H_+} + \alpha_d) n_{He_+} n_e =$$

$$= \alpha_{He_{++}} n_{He_{++}} n_e + \Gamma_{eHe_0} n_{He_0} n_e + \Gamma_{\gamma n_{He_0}} n_{He_0}$$

$$\alpha_{He_{++}} n_{He_{++}} n_e = \Gamma_{eHe_+} n_{He_+} n_e + \Gamma_{\gamma n_{He_+}} n_{He_+}$$

are solved self-consistently with EOS temperature

$$T = (\gamma - 1) \frac{m_p \mu}{k_B} e$$

using Newton-Raphson iterations

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Handling source terms

- Strang split:
  - integrate H/C contribution to ρe & ρE over 0.5Δt
  - advance the solution over Δt (all terms, but H/C)
  - integrate H/C for another 0.5Δt
- Positive: flexibility in time-stepping for H/C, accuracy & stability dealt separately (grain of salt), modularization…
- Negative: processes *are* coupled ➔ possible misinterpretation of the flow
- Adaptive midpoint integration of $\int \Lambda_{HC}\, dt$

  (experimental)

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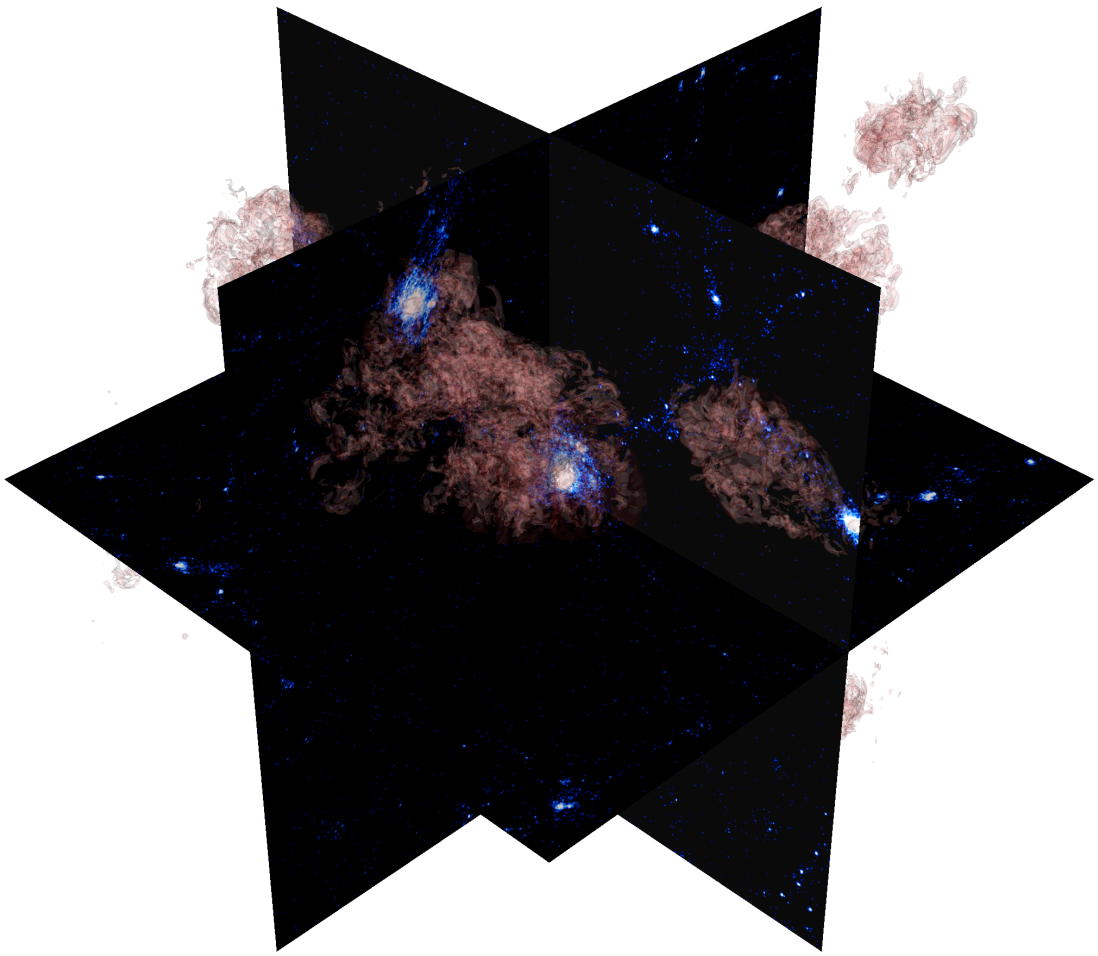
Viz/Analysis

- Data format readable by VisIt and yt
- Plotfile header describes number of AMR levels, the grid boxes at each level, the problem size, step time, etc.
- In situ analysis: isodensity halo finder, skewers…



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