The Lyman-α Forest in Cosmological Hydrodynamic Simulations

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Big picture

Observational probes

CMB
Lyα Forest
Galaxies

Very precise ICs
evolve with linear theory
simulation

Image credit: ESA / C. Carreau
The Lyα Forest

Intergalactic gas with small fraction of neutral Hydrogen.

Quasars provide distant backlights. The photons redshift on their way to us.

Neutral Hydrogen absorbs light at local Lyα wavelength.

There are many lines, but HI Lyα happens to be most prominent.

Quasar spectrum from Mike Rauch and William Keel
Lya Forest for Cosmology

The 1D flux power provides matter power estimates at smaller scales than other measurements. Most interesting for constraining spectral index and neutrino mass.

Future experiment DESI will use this to constrain sum of neutrino masses down to 17 meV.
BOSS/SDSS III is the largest galaxy and quasar spectroscopic survey to date. (Just finished last Monday!)

- 1,350,000 galaxies, 169,000 Lyα quasars.
- eBOSS survey will possibly double these numbers.

DESI is the next generation spectroscopic survey, planned for 2018.

- 20-30 million galaxies and quasars

Theory is not ready for these tiny statistical error bars!
Ly$\alpha$ Forest Simulation Challenge

Simple physics and algorithms— Computationally demanding

Simulations must resolve minimum length (Jeans) scale to capture absorption systems.

Simulations must include large linear scales to capture representative volume, $\sim$1000x larger.

“Resolving” the Jeans scale in simulations actually means covering it with $\sim$5 resolution elements, increasing the requirement to $\sim$5000 dynamic range.

Signal comes from mean density regions, which fill the volume, making AMR more expensive than larger unigrid. (SMR still interesting though)
The Nyx code

Cosmological Eulerian hydrodynamics code, developed at LBL (CCSE and C³), built on the BoxLib AMR framework.

N-body particle representation of dark matter, finite volume representation of gas, both on 3D cartesian grid.

Developed for IGM simulations, but applicable to many other problems including redshift-space distortion modeling, AGN modeling, cosmological turbulence, isolated galaxy sims...

Code paper: Almgren et al. 2013
Particle-Mesh Gravity

Standard algorithm for depositing dark matter particle mass to grid (CIC), adding gas mass, and using multigrid relaxation to solve Poisson equation.

\[ \nabla^2 \phi = \frac{4\pi G \rho_{m,0}}{a} \left( \frac{\rho - \bar{\rho}}{\bar{\rho}} \right) \]

\[ \mathbf{g} = -\nabla \phi \]

\[ \frac{d\mathbf{p}}{da} = -\mathbf{g}, \quad \frac{d\mathbf{x}}{da} = \frac{\mathbf{p}}{\dot{a}a^2} \]

Dark matter particles evolved with Kick-Drift-Kick stepping, and self-gravity included in hydro source terms.

Currently adding root grid FFT solve for scalability.
Hydrodynamics

Hydro solver is higher-order Godunov scheme, with PPM reconstruction, unsplit flux update with full corner coupling.

\[ \frac{\partial \rho}{\partial t} + \frac{1}{a} \frac{\partial \rho v_i}{\partial x_i} = 0 \]
\[ \frac{\partial (\rho v_j)}{\partial t} + \frac{1}{a} \frac{\partial (\rho v_i v_j + p \delta_{ij})}{\partial x_i} = -\frac{\dot{a}}{a} \rho v_i + \frac{1}{a} \rho g_j + S_{\rho v_j} \]
\[ \frac{\partial (\rho e)}{\partial t} + \frac{1}{a} \frac{\partial [(\rho e + p \delta_{ij}) v_i]}{\partial x_i} = -2 \frac{\dot{a}}{a} \rho e + \frac{1}{a} \rho v_i g_i + S_{\rho e} \]
\[ \frac{\partial (\rho e_{th})}{\partial t} + \frac{1}{a} \frac{\partial (\rho e_{th} v_i)}{\partial x_i} = -2 \frac{\dot{a}}{a} \rho e_{th} + S_{\rho e_{th}} \]

Assumes gamma-law equation of state since gas is primordial and atomic.

Include evolution of thermal energy density to avoid truncation errors in temperature calculation (dual-energy formalism in lit.)
Optically-thin radiative heating/cooling

Assume atomic species in photoionization equilibrium and spatially uniform ionizing/UV background radiation.

\[
\begin{align*}
(\Gamma_{e,\text{H}i} n_e + \Gamma_{\gamma,\text{H}i}) n_{\text{H}i} &= \alpha_{r,\text{H}ii} n_e n_{\text{H}ii} \\
(\Gamma_{e,\text{He}i} n_e + \Gamma_{\gamma,\text{He}i}) n_{\text{He}i} &= (\alpha_{r,\text{He}ii} + \alpha_{d,\text{He}ii}) n_e n_{\text{He}ii} \\
[\Gamma_{\gamma,\text{He}ii} + (\Gamma_{e,\text{He}ii} + \alpha_{r,\text{He}ii} + \alpha_{d,\text{He}ii}) n_e] n_{\text{He}ii} &= \alpha_{r,\text{He}iii} n_e n_{\text{He}iii} + (\Gamma_{e,\text{He}i} n_e + \Gamma_{\gamma,\text{He}i}) n_{\text{He}i}
\end{align*}
\]

Solve iteratively with closures for Hydrogen/Helium abundance, conservation of mass and charge.

Adding density-dependent heating to simulate arbitrary rho-T relation.

Katz et al. 1996
Sweeping through domain

Flux panel shows what density and temperature range the Lyα Forest signal is sensitive to.
Nyx employs hybrid MPI + OpenMP, allows scaling to higher core counts than MPI alone.

Demonstrated weak scaling up to 50k cores on Hopper at NERSC. Problem size fixed to $128^3$ cells and particles per NUMA node.

Running $4096^3$ problems on 50k cores on Edison at NERSC now.
Ongoing work

Simulations with fixed cosmology and UVB. Very high resolution small box (~100 Mpc) cosmological hydrodynamic runs.

Focusing on error control before exploring cosmological/astrophysical parameter sensitivity.

Convergence study (Lukic et al.)

Finding we get percent level flux stats with 20 kpc/h resolution and 40 Mpc/h box.

Code comparison (Stark et al.)

Comparing Nyx sims run at LBL and Gadget sims run at Brookhaven National Lab.

Gadget is a popular cosmological hydrodynamics code that uses smoothed particle hydrodynamics and features a higher resolution gravity solver.

Update to Regan++07, Bird++13 on Lyαf in SPH and grid codes.
Resolution study

Simulations with fixed cosmology, UVB, and initial perturbations (adding in new small-scale modes with increasing resolution).

Lukic et al. 2014
Box size study

Fixed resolution and increased box size.

Difficult to compare across box sizes since we cannot use the same perturbations, i.e. will always include cosmic variance.

Scaling up L10_N512 run meant performing L20_N1024, L40_N2048, L80_N4096 simulations. Largest of its kind to date!

Previous Lyα forest simulations used very small box, which is not representative, or similar size box with poor resolution, under-resolving the forest.

First simulations with large enough box and resolution.

Conclusion: 40 Mpc/h is sufficient. Inaccurate growth in 20 and 10 Mpc/h boxes is noticeable.
Comparison across codes

Slice through 10 Mpc/h simulation.

Completely independent codes with different algorithms still agree to few percent in flux stats.

Extra testing demonstrated remaining differences mostly come from star formation in Gadget and no star formation in Nyx.
The Case for Radiation Hydrodynamics

Current approach:
• input ionizing background model from analytic calculations of source luminosity function and IGM filtering.
• assume all gas in simulation is optically thin, so incident radiation is the spatially uniform.

Ideal approach:
• pick sources in simulations and use observed luminosity function.
• Directly simulate ionization fronts and ionizing background with RT.
• Capture dynamical effect of ionization heating and hydrodynamic response.

Spatially uniform ionizing background is a good approximation, but we expect some variation from distance to sources and shadowing.

Previous approximate work estimates a 10% difference in the flux 1D power — a large systematic for current and future experiments.
Rad-Hydro: Status

Exploratory work in Meiksin and Tittley 2012. First rad-hydro sim (RT in domain subset) of the IGM with HI and HeII reionization.

- Density structure
- Temperature change with RT

Shows significant scatter in density-temperature relation. Temperature differences several times the mean!

Conclusion: RT has substantial impact on thermal state following reionization. Low density regions behind high densities undergo much more heating. Results in significant change in optically-thin line widths.
Rad-Hydro: Status

RT will be more expensive than hydro even with approximations appropriate for our problem.

Ideal case for substepping RT on GPUs (or other accelerators) and everything else on host CPU.

Work in other astrophysical regimes by Umemura, Susa, and co. (RSPH/START) should be applicable here.

Example of difference between RHD simulation and RT post-processing of hydrodynamic simulation.

Table 3. Properties of simulated halos.

<table>
<thead>
<tr>
<th>Name</th>
<th>$M_{\text{halo}}$</th>
<th>$M_{\text{b}}$</th>
<th>$M_\ast$</th>
<th>$\dot{N}_{\text{int}}$ $[1/\text{s}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Halo-R (w/ UV)</td>
<td>$6.8 \times 10^9$</td>
<td>$1.2 \times 10^9$</td>
<td>$2.9 \times 10^7$</td>
<td>52</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.31</td>
</tr>
<tr>
<td>Halo-H (w/o UV)</td>
<td>$6.7 \times 10^9$</td>
<td>$1.0 \times 10^9$</td>
<td>$2.0 \times 10^8$</td>
<td>53</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.15</td>
</tr>
</tbody>
</table>

a) Escape fraction of photons ionizing H I.
b) Escape fraction of photons ionizing He I.
c) Escape fraction of photons ionizing He II.
Summary

The Lyman-α Forest offers a unique cosmological probe in time and scale.

BOSS, eBOSS, and DESI are significant experimental investments, but theory to exploit the statistical power lags behind.

The Nyx code is now well-tested for this problem and scales to required resolution demonstrated in convergence tests.

Nyx simulations are achieving percent level convergence in common flux statistics without runs being too expensive — still possible to run a grid exploring cosmological parameters.

Beginning simulation suite to explore cosmological response.

Including RT in cosmological hydrodynamic simulations still prohibitive, but we want to experiment as soon as possible.
Lyman α Forest Basic Theory

**Equation of state in diffuse IGM**

\[ T = T_0 (\frac{\rho}{\bar{\rho}})^{\gamma - 1} \]

**Photoionization equilibrium**

\[ n_{\text{HI}} = A \frac{n_e n_H}{\Gamma_{\text{HI}} T^{-0.7}} \]

**Flux stats**

\[ \tau_{\text{HI}} \propto \frac{n_{\text{HI}}}{\sqrt{T}} \]

\[ F = \exp(-\tau) \]

Flux traces matter on large scales

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2D slice through 3D Nyx simulation.

Lukic et al. 2014
Lyα Forest Observables

\textit{n-point functions}

- mean flux
  - measure of IGM opacity evolution
  - constrains ionizing sources, reionization events.

- flux PDF
  - shape sensitive to IGM thermal state.

- flux power spectrum
  - sensitive to small scale cosmological perturbations

\textbf{References}

Becker et al. 2013  
Paris et al. 2011  
Faucher-Giguere et al. 2008  
McDonald et al. 2005  
Bernardi et al. 2003  
Kim et al. 2007  
Lee et al. 2014  
Becker et al. 2007  
McDonald et al. 2000  
Rauch et al. 1997  
Palanque-Delabrouille et al. 2012  
McDonald et al. 2006  
Croft et al. 2002
Resolution study

Conclusion: resolution matching $512^3$ simulation is ideal, $256^3$ is fine for some statistics, $128^3$ fails.
Box size study

Fixed resolution and increased box size.
Difficult to compare across box sizes since we cannot use the same perturbations, i.e. will always include cosmic variance.

Conclusion: 40 Mpc/h is sufficient. Inaccurate growth in 20 and 10 Mpc/h boxes is noticeable.

Lukic et al. 2014
Modeling the Lyα Forest in simulations

Choose rays crossing the simulation domain, and compute optical depth to HI Lyman-α scattering.

The simulation provides the ingredients:

\[ \rho_b, T, J_\nu \rightarrow n_{HI} \]

\[ n_{HI}, T, v_\parallel \rightarrow \tau_\nu \]

We assume a Doppler line profile, with no extra broadening components, and integrate analytically.

Future directions include modeling realistic quasar positions and continua, and casting rays at speed of light (currently fixed time approximation).
Adaptive Mesh Refinement

BoxLib features well-tested and scalable AMR infrastructure.

Refinement process:
1. Tag cells for refinement on a desired criteria.
2. Group cells into optimal rectangular grids.
3. Split grids and distribute them to processes.

Refinement factor of 2 or 4.

No strict parent-child relation between patches.
Rad-Hydro: Previous IGM Work

Norman et al. 1998, Abel et al. 1999:

Split radiation into two components

\[ I_\nu = I_{\nu}^{pts} + I_{\nu}^{diff} \]

and solve point contribution with simple ray-casting (long characteristic) scheme.

Bolton et al. 2004:

extended method to HeII heating.

Tittley and Meiksin 2007:

coupled RT to PM code (gravity only).

McQuinn et al. 2009:

RT only on hydrodynamic sim. snapshot.

grayscale: initial HI density. contours: I-front.
Particle overloading

1 particle per cell

8 particles per cell

$P(\rho_{\text{dm}})$