Realistic Simulations of the Intergalactic Medium: The Search for **Missing Physics**

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Observing the intergalactic medium in quasar absorption line spectra

Lyman $\alpha$ forest
What is Observed

Kirkman & Tytler (1997)
The Cosmic Web: Origin of the Ly α forest absorption

Cosmic web formed by gravitational clustering of dark matter and baryons (H and He)

Hundreds of millions of lightyears
Simulation v. observation: amazing agreement

Kirkman & Tytler (1997)

Zhang et al. (1997)
Physical Origin of the Lyman Alpha Forest

- intergalactic medium exhibits cosmic web structure at high z
- models explain observed hydrogen absorption spectra

Zhang, Anninos, Norman (1995)
a $4096^3$ hydro-cosmology simulation
L=614 Mpc, Cell=150 kpc
A small but persistent discrepancy has emerged between sim. & obs. as higher precision has been achieved

<table>
<thead>
<tr>
<th>Possible Explanation</th>
<th>Finding</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observational systematics</td>
<td>NO</td>
</tr>
<tr>
<td>Simulation not converged</td>
<td>NO</td>
</tr>
<tr>
<td>Simulation box size too small</td>
<td>NO</td>
</tr>
<tr>
<td>Missing IGM physics</td>
<td>MAYBE</td>
</tr>
<tr>
<td>Missing galaxy HI absorption</td>
<td>MAYBE</td>
</tr>
</tbody>
</table>

This PRAC project
Quantifying the discrepancy: 

*Flux PDF*

![Graph showing flux PDF with labels for high and low transmission, indicating too many and not enough.](image-url)
Fiddling with the standard LAF model does not improve agreement

Curves have wrong shape
What we are exploring with Blue Waters

**Standard model**
IGM ionized by homogeneous UVB

**Quasar model**
IGM ionized by quasar point sources
Why Blue Waters is Needed

• Quasar model requires *3D time-dependent multifrequency radiative transfer*
  – Very computationally intensive

• Scale separation requires *very large grids*
  – Must resolve Ly $\alpha$ forest absorbers (25 kpc) in a box large enough to contain hundreds of quasars (100 Mpc) $\rightarrow$ 4000$^3$ grids (target)

• Model development requires high throughput for experimentation at scale

*Progress requires combination of capacity and capability that only Blue Waters can provide*
Why Multifrequency RT?
A: QSOs have hard UV spectrum

- [54.4, 65] eV
- [65, 75] eV
- [75, 125] eV
- [125, 155] eV
- [155, 400] eV

Photoheating

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Blue Waters Symposium 2016
Progress

• Quasar model implemented and tested at low-resolution ($512^3$ and $1024^3$ grids)
  – 100’s of time-dependent quasar sources
  – 5 group implicit flux limited diffusion
  – **Enzo** code + **yt** for inline halo finding

• High resolution science run underway
  – 2-3 month completion time
  – 1-2 month for data analysis
Helium reionization by time-dependent quasars: Enzo MGFLD simulation on Blue Waters

186 Mpc

Projected He+ fraction

z = 3.343805

z = 3.087600

z = 2.918258
Redshift Evolution of $\chi(\text{He}^{++})$ and T

He++ volume fraction

Temperature

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Inhomogeneous heating of the IGM by quasars

$1024^3$ Enzo-MGFLD on Blue Waters

Baryon density

$Z=3.41$

Baryon temperature

118 Mpc
Inhomogeneous heating of the IGM by quasars

$1024^3$ Enzo-MGFLD on Blue Waters

He$^+$ fraction

$Z=3.41$

Photoheating rate

118 Mpc
Rollup

- **Key Challenges**: high fidelity simulation of the IGM including inhomogeneous quasar ionization and heating
- **Why it Matters**: may explain discrepancy between theory and observation
- **Why Blue Waters**: capability and capacity to develop and run very large, computationally and memory intensive simulations
- **Accomplishments**: low-res runs completed; high-res run in progress
- **Blue Waters team contributions**: assistance with topology-aware scheduling
- **Broader Impact**: drove the development of MGFLD capability for the **Enzo** community code
- **Shared Data**: none yet
- **Products**: MGFLD capability in **Enzo** code