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Simulating the Lyman-α Forest with Nyx

Abstract

We recently developed the cosmological hydrodynamics code Nyx to perform simulations of the intergalactic medium (IGM) and model the Lyman-α forest (LyAF). The scalability of Nyx allows us to simulate dynamic ranges that capture enough linear modes while resolving the Jeans scale in the IGM for redshifts relevant to LyAF observations (z=2–3). As part of the SCIDAC-3 project, "Computation-Driven Discovery for the Dark Universe", we work on providing accurate and robust predictions of the various LyAF statistics including the mean flux, the flux PDF, and the 1D power spectrum. On large scales, we aim to accurately determine the bias b and the redshift-space distortion parameter β. On small scales, our ultimate goal is to emulate the anisotropic power spectrum $P_F(k, \mu)$.

Simulating the IGM

Nyx is a cosmological Eulerian hydrodynamics code, built on the BoxLib AMR framework. Nyx models the baryonic content of the universe as an inviscid, gamma-law gas, gravitationally coupled to dark matter:

$$\begin{aligned}
\frac{\partial\rho}{\partial t} &= -\frac{1}{a}\frac{\partial\rho v_i}{\partial x_i}\\
\frac{\partial(a\rho v_j)}{\partial t} &= -\frac{\partial(\rho v_j v_i)}{\partial x_i} - \frac{\partial p}{\partial x_j} + \rho g_j\\
\frac{\partial(a^2\rho e)}{\partial t} &= -\frac{\partial(\rho e v_i + p v_i)}{\partial x_i} + a\rho v_i g_i + a\Lambda_{\rm HC}\\
\nabla^2\phi &= \frac{4\pi G}{a}\left(\rho_{\rm b} + \rho_{\rm dm} - \rho_{\rm crit}\right)\\
\mathbf{g} &= -\nabla\phi
\end{aligned}$$

Nyx evolves baryon quantities using an advanced unsplit, higher-order Godunov scheme. Dark matter is modeled as collisionless particles, evolved with a standard particle-mesh scheme. The Poisson equation is solved via a multigrid method.

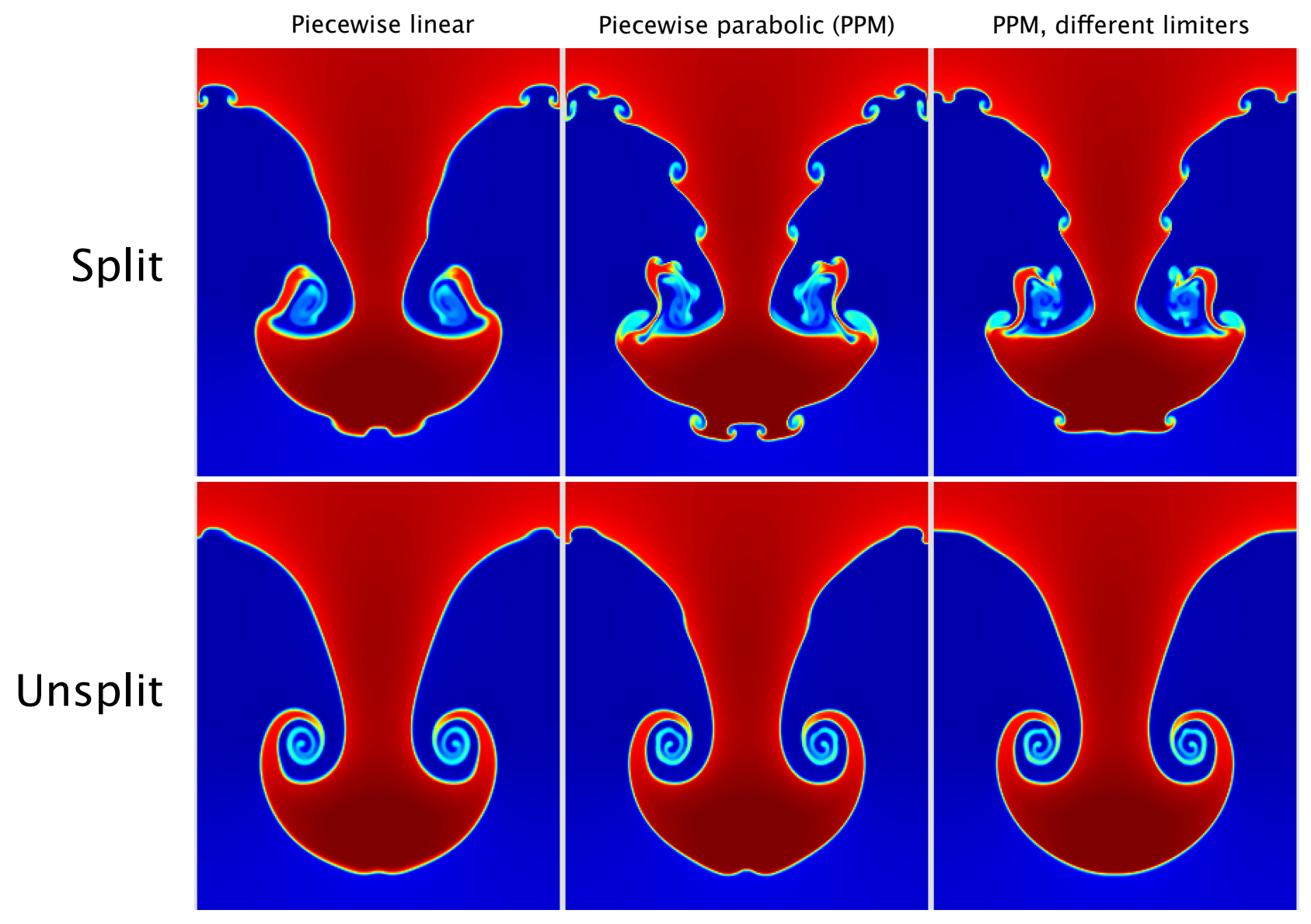


Fig. 1. Unsplit methods better model fluid flow, as shown in this Rayleigh-Taylor instability example. Dimensional splitting produces secondary instabilities, regardless of the reconstruction method (Almgren et al. 2010).

The radiative heating and cooling rates are a critical component of simulating the IGM. These terms include photoionization, recombination, and collisional excitation of the primordial species, Compton cooling off the CMB and bremsstrahlung. Assuming ionization equilibrium, the total heating/cooling rate is reduced to a function of the baryon density, temperature, and the redshift-dependent uniform ionizing background.

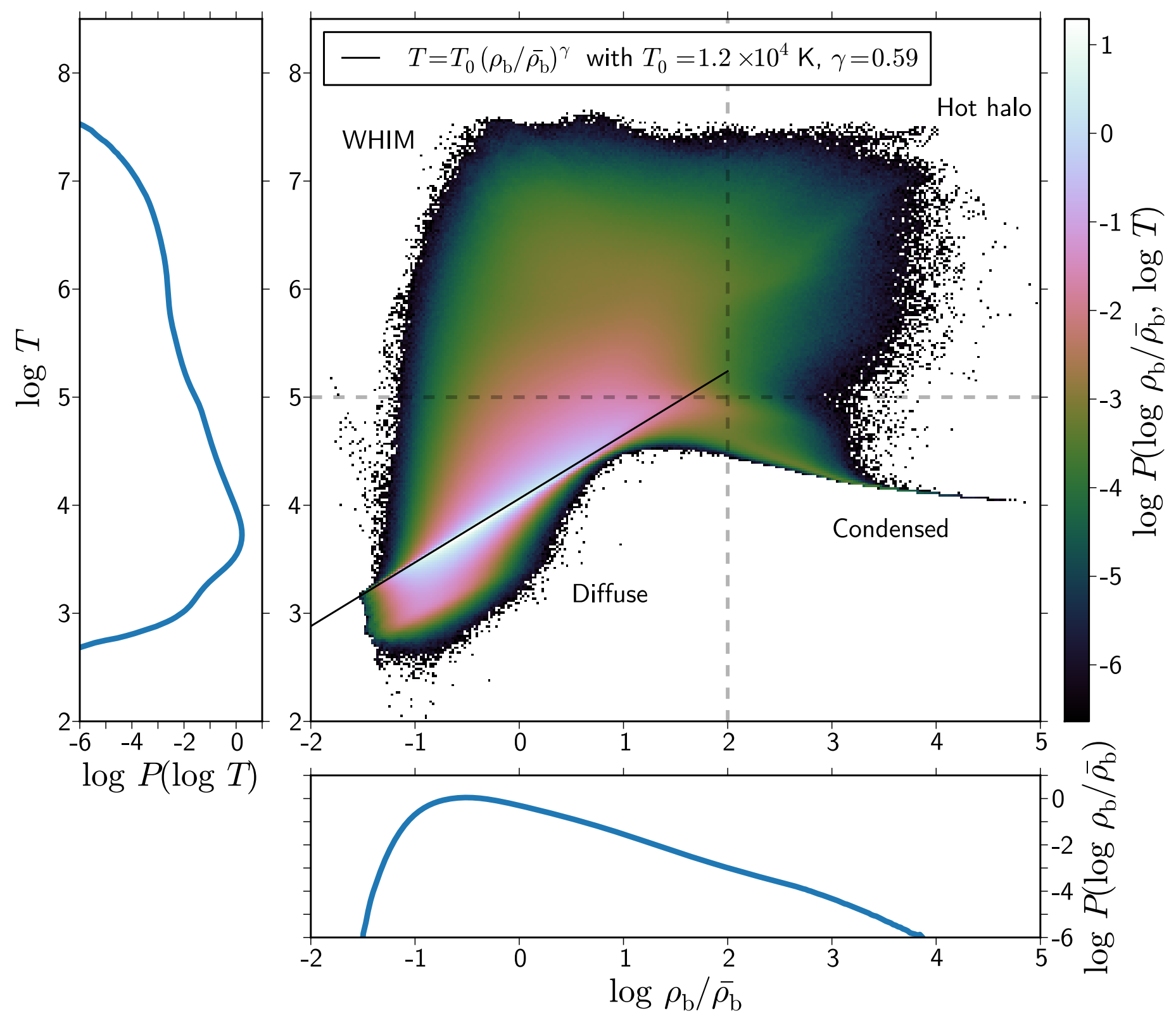


Fig. 2. Two-dimensional PDF of baryon density (in units of mean density) and temperature (in K), taken from a L=100 Mpc/h, 2048³ simulation at z=2.5. We illustrate the four phases of the IGM with cuts at a density of 100 times mean and a temperature of 10⁵ K. The diffuse phase is what provides the LyAF signal and comprises most of the IGM by volume.

Modeling the Lyman-α Forest

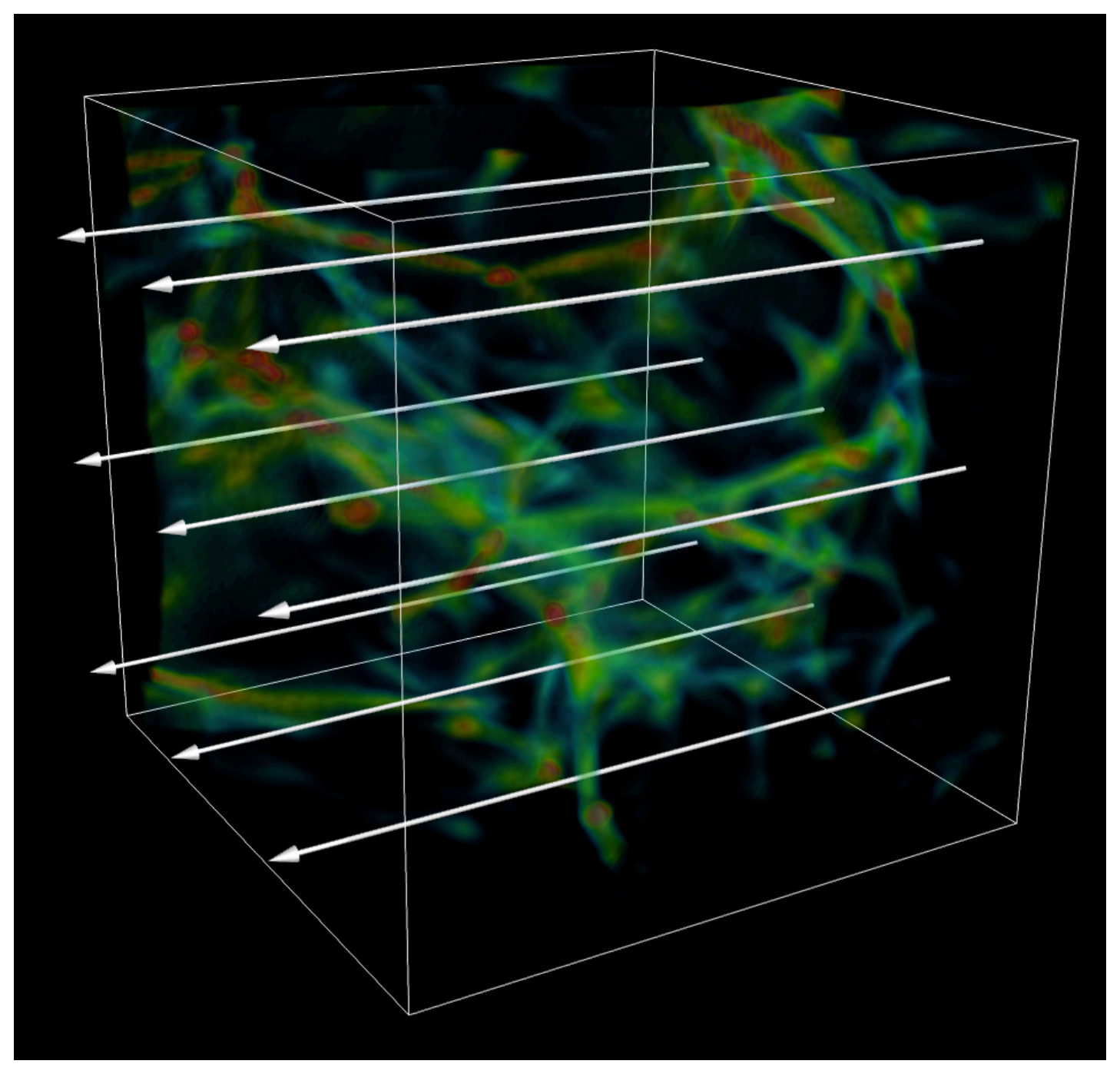


Fig. 3. Illustration of how the skewers cross the simulation domain, over a volume rendering of the logarithm of HI number density (cm⁻³, spanning −10.2 to −8.2). For illustration purposes, we have taken a small piece of a larger simulation and subsampled the skewers.

The LyAF is made up of many redshifted absorption features from HI Lyman-α scattering along the line of sight (LOS) to a QSO. To create simulated spectra, we use the HI number density, temperature, and line of sight velocity component provided by the simulations to compute the optical depth.

$$\tau_\nu = \int_{s_0}^{s} n_{\rm HI}(s')\sigma_\nu(s')ds'$$

$$\tau_v = \frac{\sigma_0\lambda_0}{2H(z)}\sum_i n_{\rm HI,i}\left[\mathrm{erf}\left(\frac{v - v_{{\rm los},i} - \dot{a}x_{i+1/2}}{v_{\rm th}}\right) - \mathrm{erf}\left(\frac{v - v_{{\rm los},i} - \dot{a}x_{i-1/2}}{v_{\rm th}}\right)\right]$$

We use the standard Doppler cross section and integrate analytically. We noticed significant differences between our analytic integration and the midpoint expression. We calculate the optical depth along rays piercing the box face and crossing the domain (see Figure 3). This provides us with N² evenly-spaced spectra with N pixels.

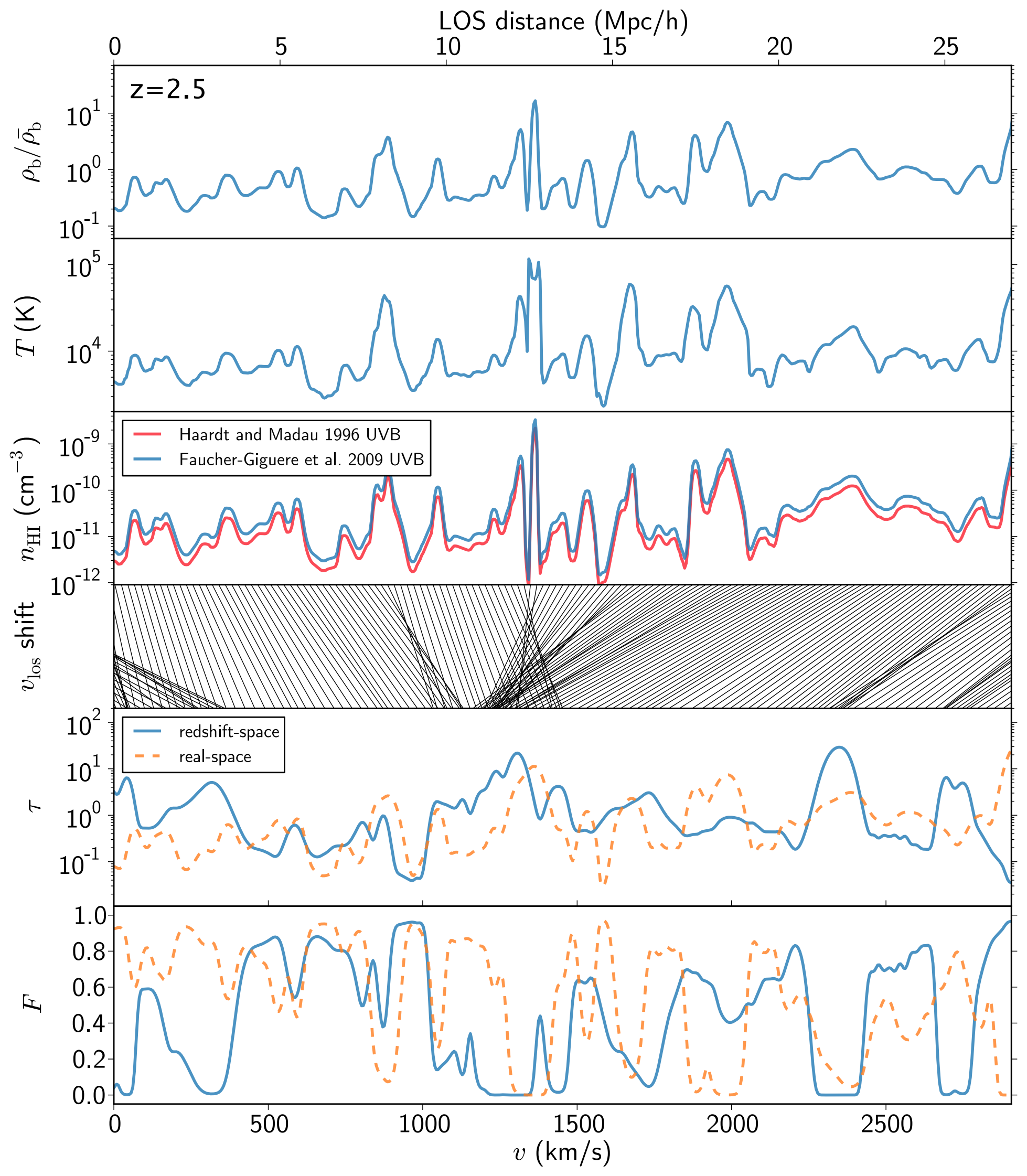


Fig. 4. A sample skewer from a 100 Mpc/h simulation with 50 kpc/h resolution. We ran this simulation with the FG09 ultraviolet background (UVB), but also show the HI number density derived from the HM96 UVB in post-processing. The LOS velocity subplot demonstrates how the line center is shifted by peculiar velocities. The redshift-space optical depth includes the effects of thermal broadening and peculiar velocities, while the real-space version ignores peculiar velocities.

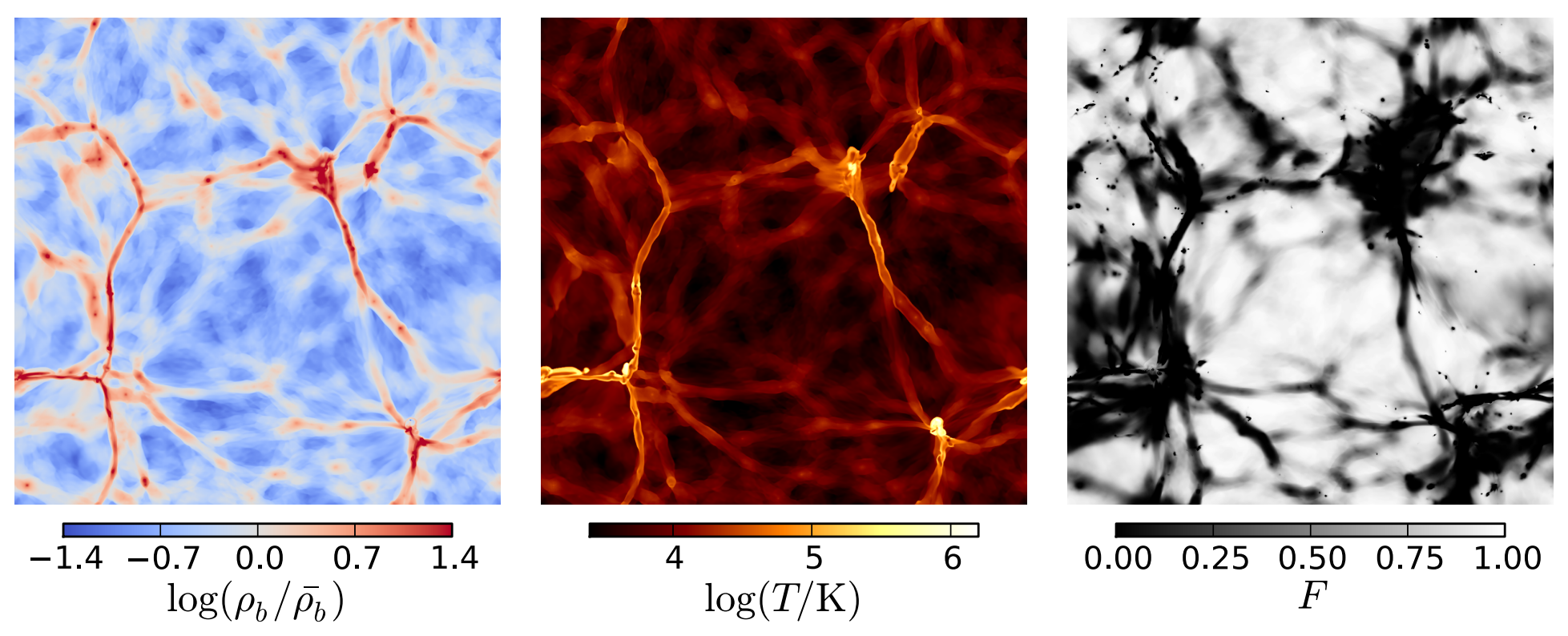


Fig. 5. A slice (one cell thick) through a L=10 Mpc/h simulation at z=2.5. The flux LOS is into the page.

Nyx's Performance

The scalability of Nyx allows us to run large problems with very quick turnaround. We are able to run 2048³ simulations down to z=2 on 32k cores on Hopper at NERSC in a matter of hours rather than days. Preliminary tests on the Edison Phase I machine indicate that Nyx runs about 3 times faster than on Hopper.

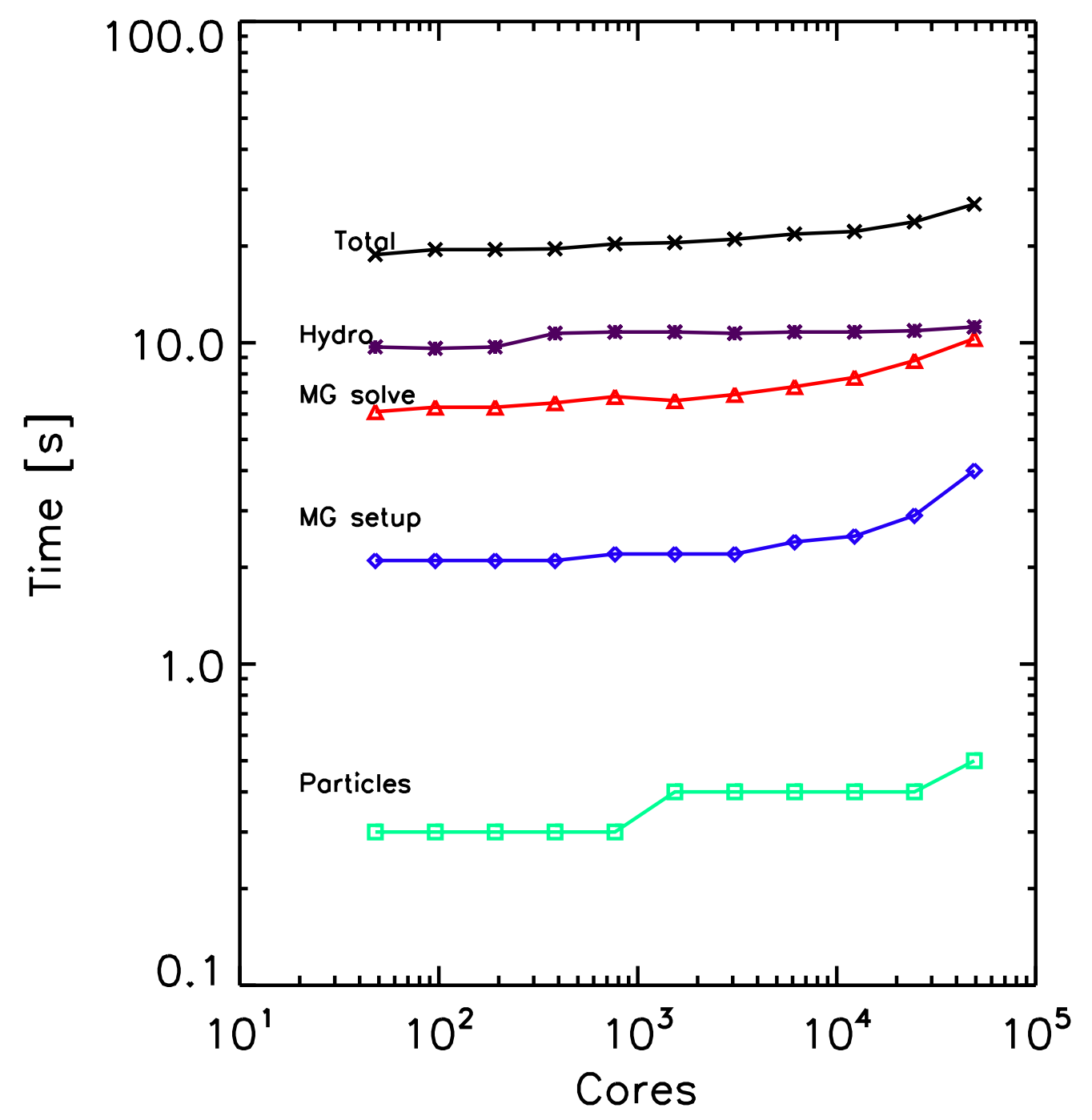
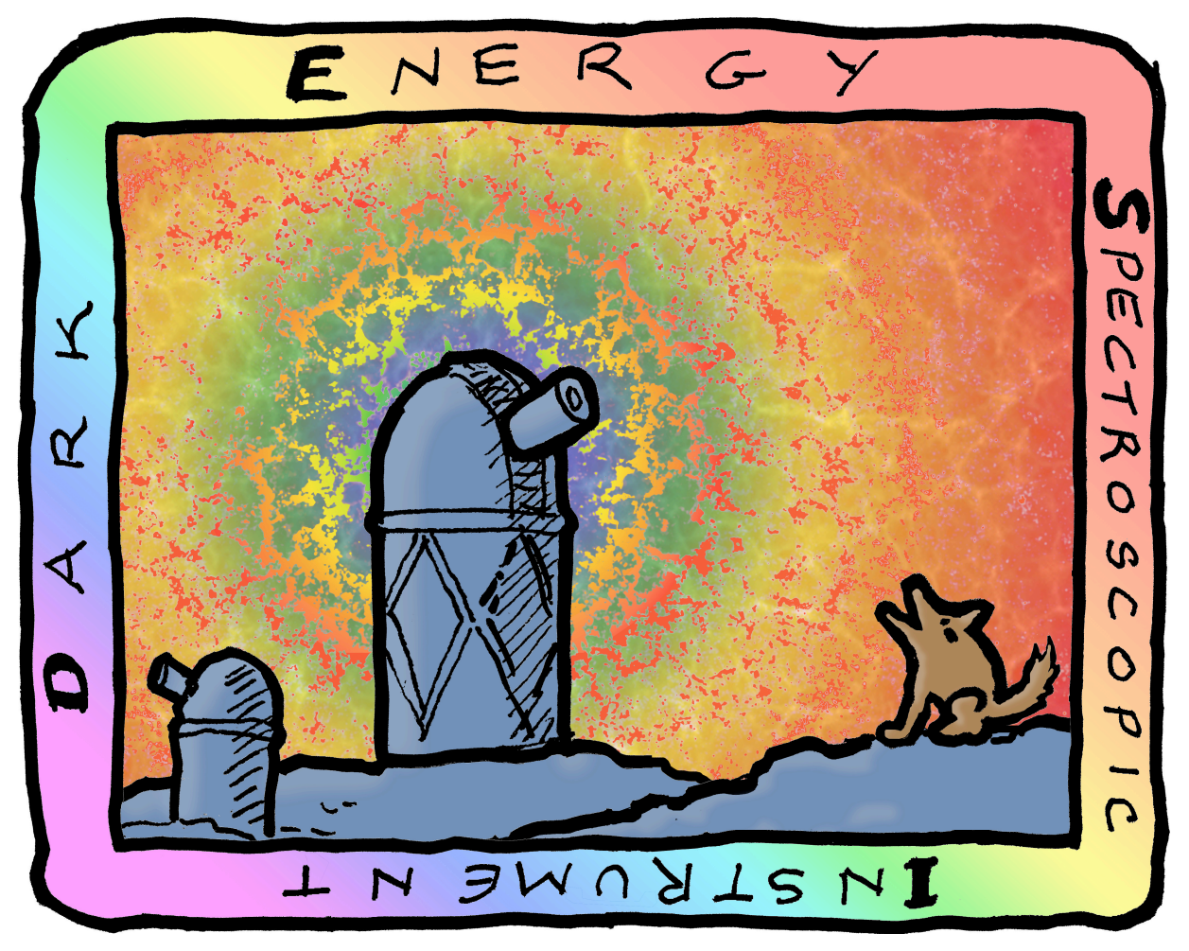


Fig. 6. Weak scaling of Nyx up to 50k cores on Hopper, based on the average walltime per timestep, broken down by task. We fixed the problem size such that each NUMA node (6 cores) held 128³ cells and particles.

Relation to FastMath

Nyx is built on BoxLib, and fully relies on BoxLib capabilities to manipulate Adaptive Mesh Refinement (AMR) grid structures, as well as on the linear solvers implemented. I/O and almost all parallelization is handled in BoxLib rather than Nyx itself, enabling Nyx to focus on the physics of the LyAF and different cosmological models, effectively "outsourcing" many difficult mathematical and computational tasks to BoxLib.

Observational Motivation



The last decade has seen increasing use of LyA absorption to investigate large scale structure of the universe. This is crucial for understanding the nature of the dark energy. BOSS, and the upcoming DESI experiments, represent a massive increase in data volume and provide new windows on a host of astrophysical and cosmological issues. To effectively utilize such an increase in observational capability demands a corresponding increase in our theoretical understanding of, and ability to simulate the LyAF. BOSS, and in the future DESI, also represent the first 3D maps of the LyAF. The traditional approach utilizing purely high-resolution LOS measurements are more sensitive to parameters that impact correlations on Mpc scales or smaller. However, 3D correlation measurements allow detection of the BAO feature, large-scale intensity and temperature fluctuations from hydrogen and helium reionization.

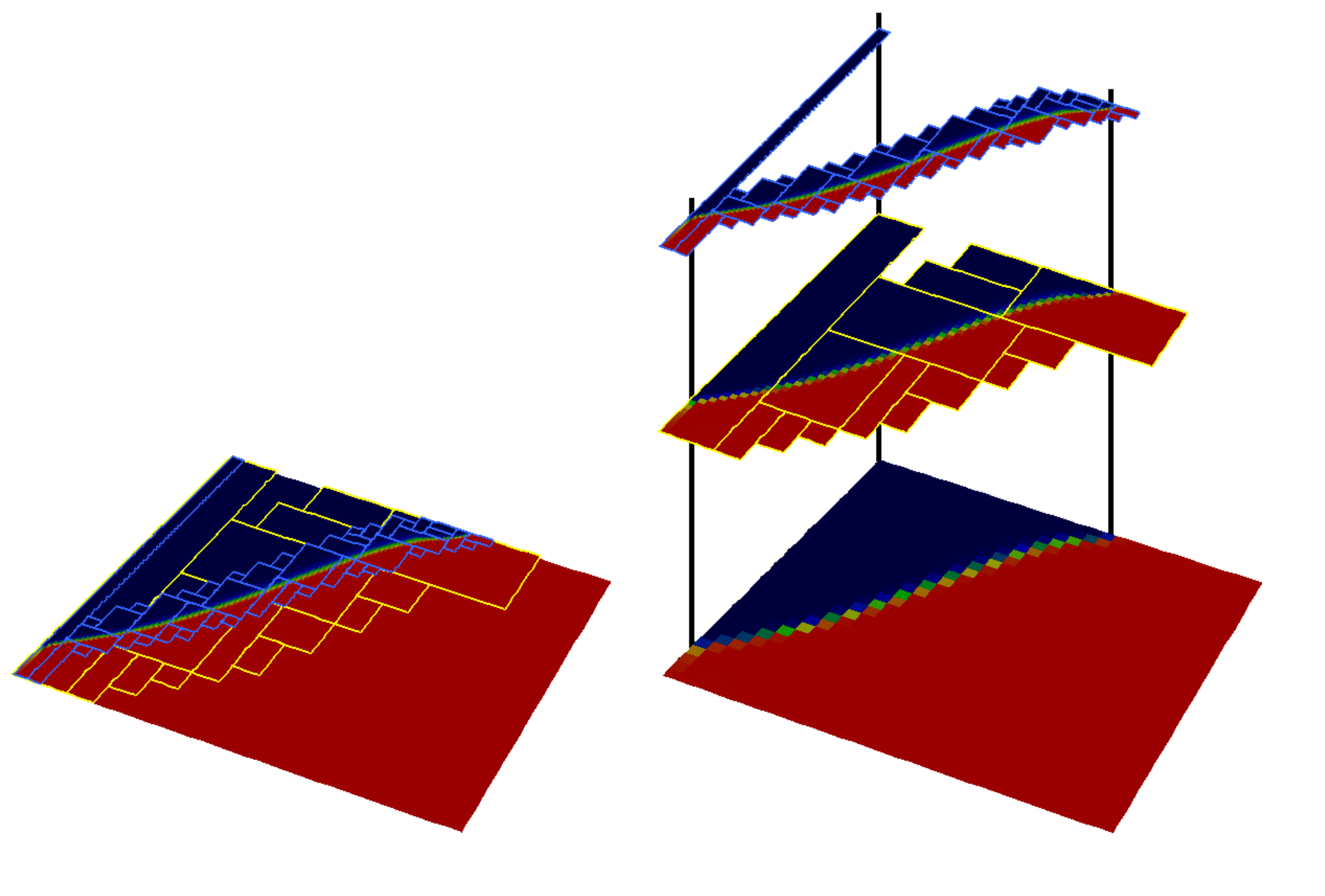


Fig. 7. Sample grid structure with base grid and two levels of refinement in BoxLib. Nyx fully relies on BoxLib to manage all grids, specifying only the criterion for the refinement.

Convergence of Flux Statistics

Common statistics extracted from the LyAF are the flux mean, PDF, and power spectrum. Here we show results from a 10 Mpc/h box simulations with varying resolution to demonstrate convergence of these statistics with respect to grid size. We also demonstrate an important point that under-resolving the forest produces incorrect predictions on all scales (middle panel). This is not the case for most other quantities in cosmological simulations, like the matter power spectrum (right), making Ly-α simulations challenging.

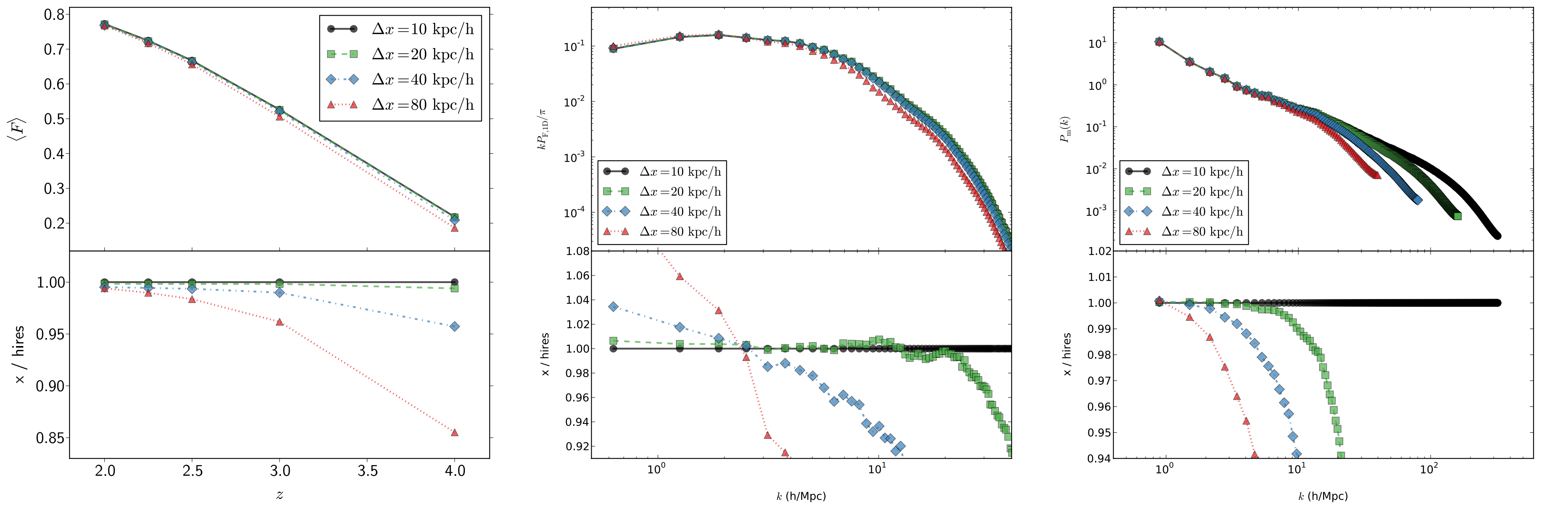


Fig. 8. From left to right, the mean flux as a function of redshift, the flux PDF at z=2.5, and the 1D flux power spectrum at z=2.5. The physical resolution of the simulations is about 80, 40, and 20 kpc.

In addition to testing convergence with respect to physical resolution, we are investigating convergence with respect to domain size, number of particles, initial redshift, etc. These studies are essential for establishing the accuracy of our predictions and are conducted as precursors to our large production runs on Edison Phase II. Our simulation campaign will consist of L~100 Mpc/h, 4096³ runs with varying cosmological parameters and UV backgrounds.

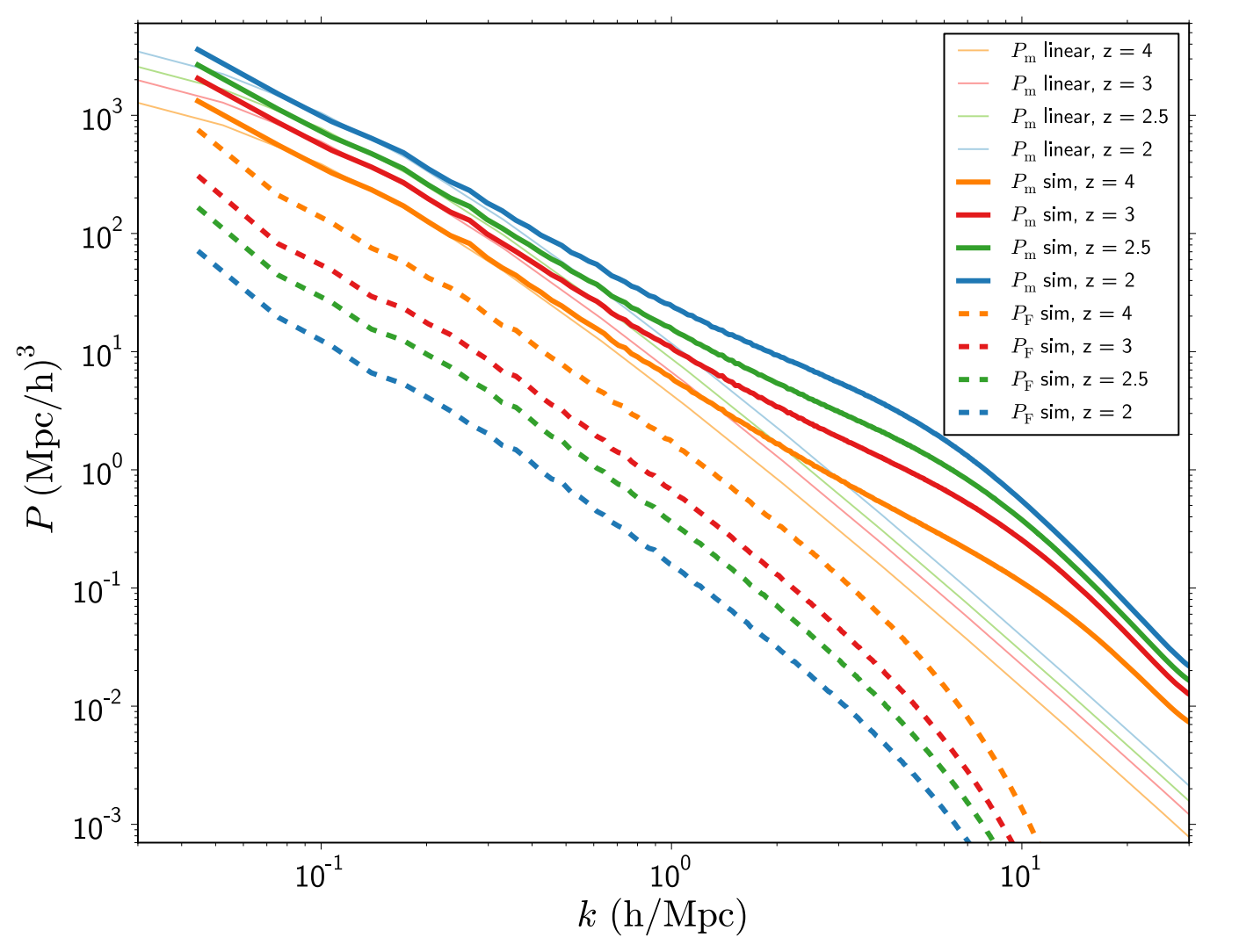


Fig. 9. Combined plot of the isotropic power spectra of the linear prediction for matter, and the simulated matter and flux in a L=200 Mpc/h, 2048³ simulation.

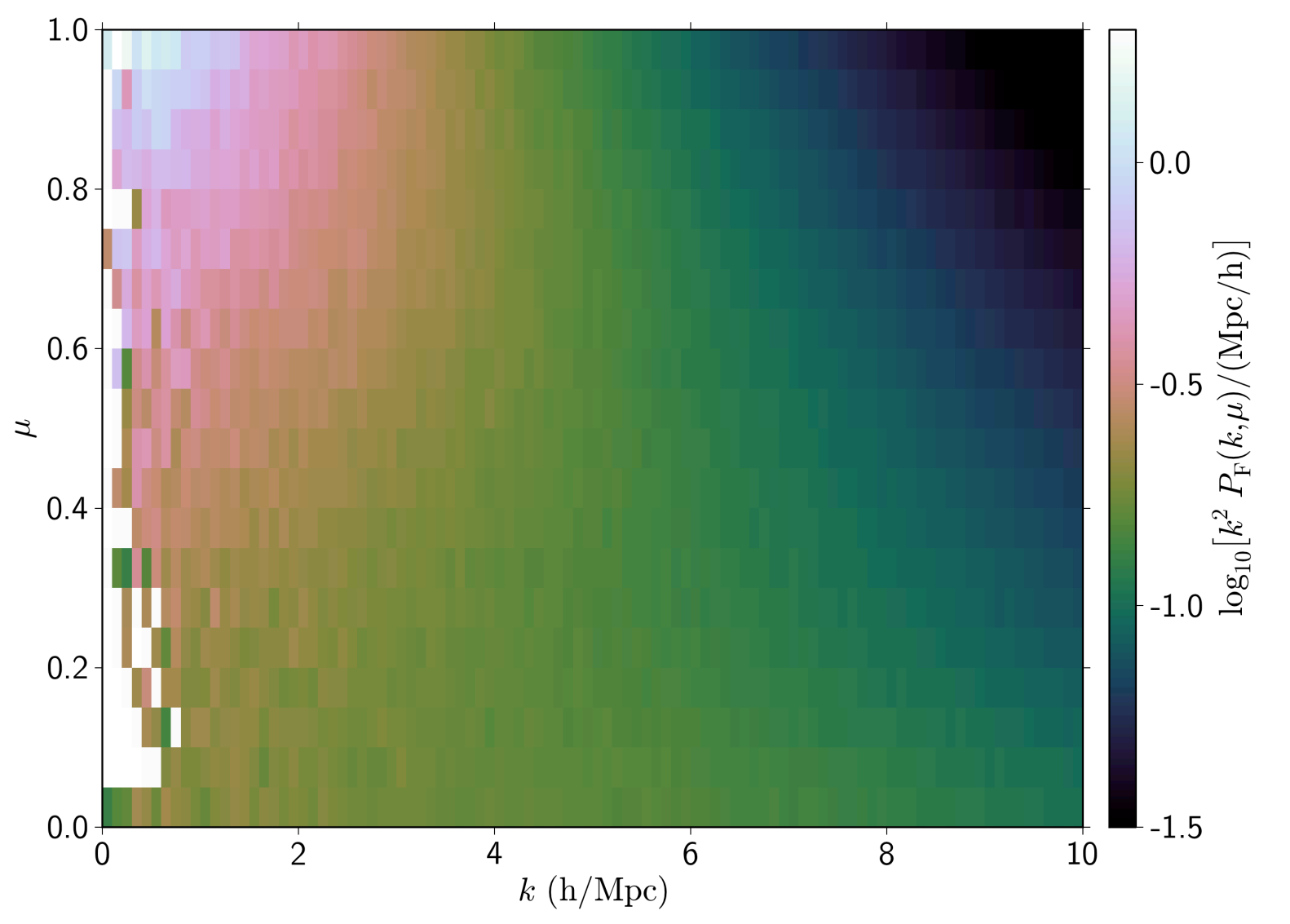


Fig. 10. The anisotropic redshift-space flux power spectrum, multiplied by k² for better visualization, from a L=100 Mpc/h, 2048³ simulation at z=2.5.