Producing High-fidelity Flux Fields From N-body Simulations Using Neural Networks

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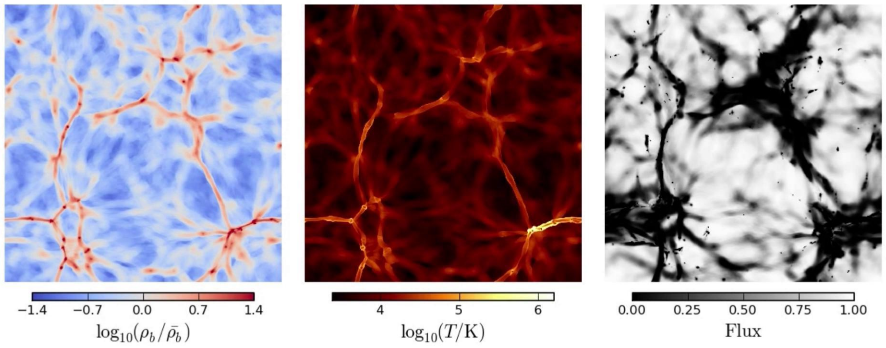
Cosmology background

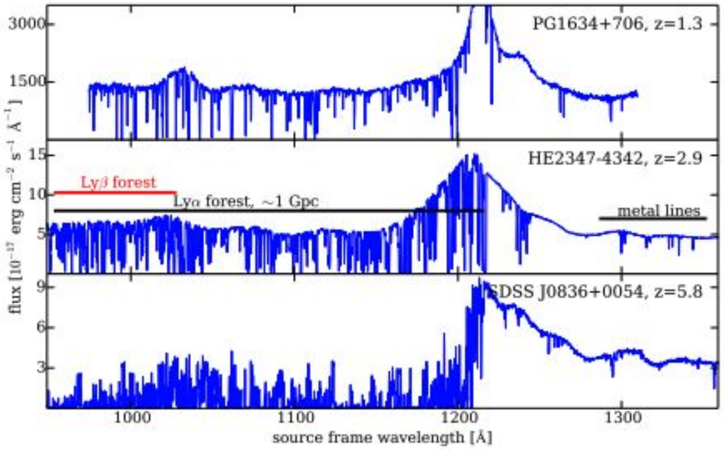
Dark matter is abundant, and a crucial component in the formation and evolution of structure in the universe, but can't see it -- only have key "observables" like **Lyman-alpha (Lya) flux**.

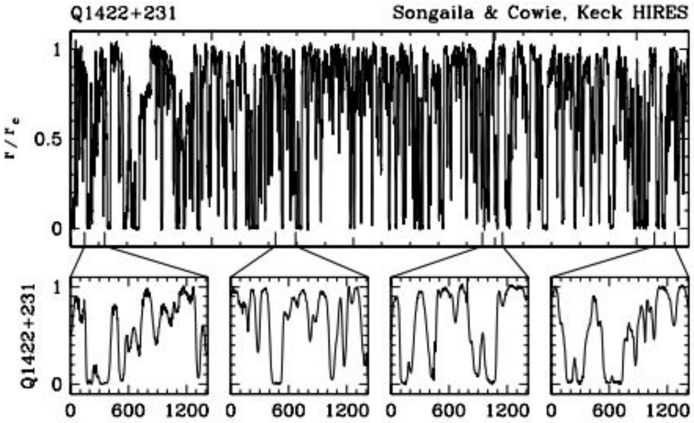
- H gas is gravitationally coupled to the filaments formed by large-scale dark matter distributions
- Additionally, the gas distribution depends on collisional (i.e., **hydrodynamic**) effects
- Density and temperature fluctuations determine how much neutral H is present, which absorbs Lya wavelengths



Cosmology background: Lyman-alpha flux

McQuinn (2016)





- Characteristic pattern of density fluctuations is "imprinted" into spectrum of observed light from distant quasars

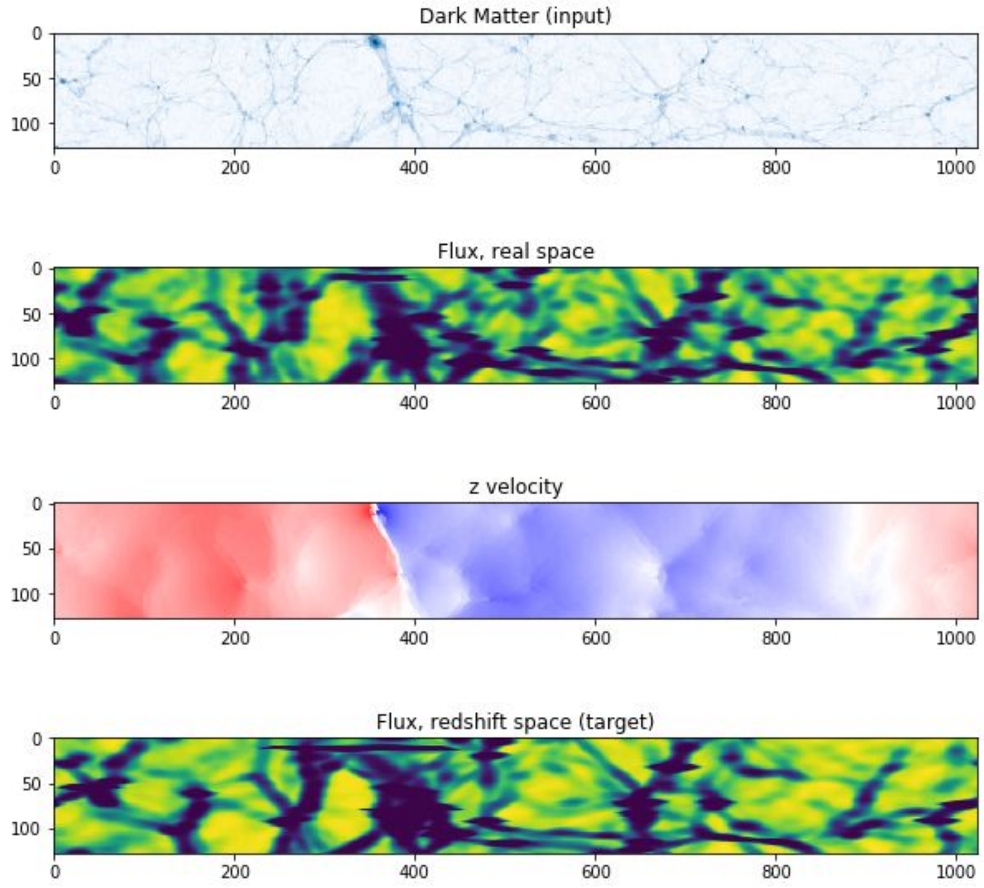
- Lots of quasars, and some are very far! Lya signal is capable of tracing density fluctuations as far back as when universe was just 1 Gyr old.

- Key point: the **redshift** of Lya absorbers is determined by their line-of-sight velocity:
    - Mainly, *cosmological redshift* due to their extreme distance (receding due to expansion of universe)
    - Also, the *local velocity* of the absorbing gas ("peculiar velocity")

Cosmology background: Lyman-alpha flux

The gas velocity along the line of sight **warps the real-space flux field** to what is observed in redshift space, which is all we can see.

This presents an additional challenge to the task of modeling Lya flux to match observations at percent-level accuracy.



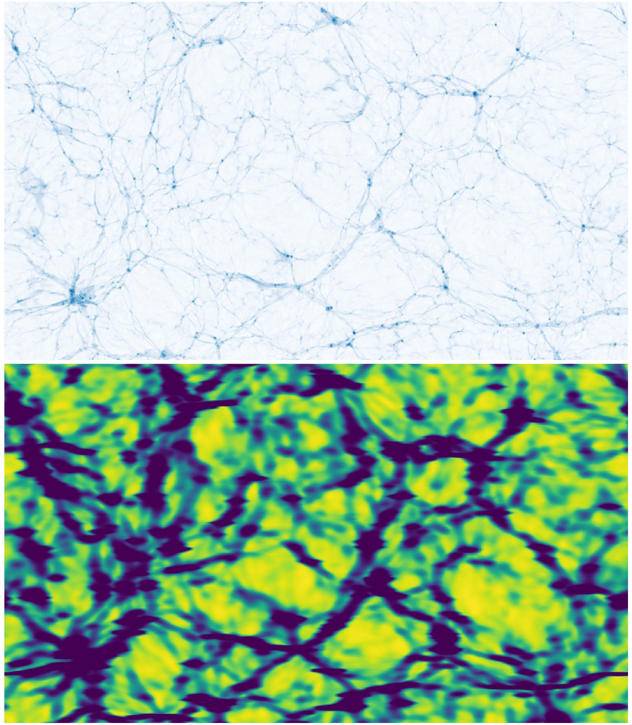
Numerical simulations: challenges in cost & scale

No analytical solution to these complex, multi-physics, multi-scale interactions -- must use numerical approaches. Challenges:

- High resolutions (spatial and temporal) required to model density fluctuations & complex physics -- cost can be $O(10^5)$ - $O(10^7)$ CPU hours

- Accurate modeling of hydrodynamic effects required to get Lya flux, which adds significant expense to simulations

- Finding a reliable method to reconstruct Lya flux from N-body simulations (non-hydrodynamic) has been a long-standing research goal



Do it with neural networks, of course!

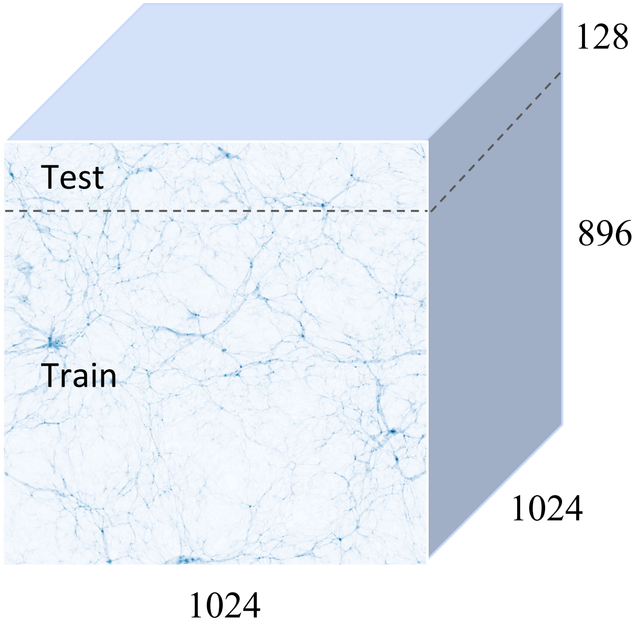
Dataset: Nyx simulation

N-body + hydrodynamic simulation, with physical fields:

- Dark matter density
- Baryon density, temperature, velocity (x,y,z)
- Lya flux, real-space
- Lya flux, redshift-space

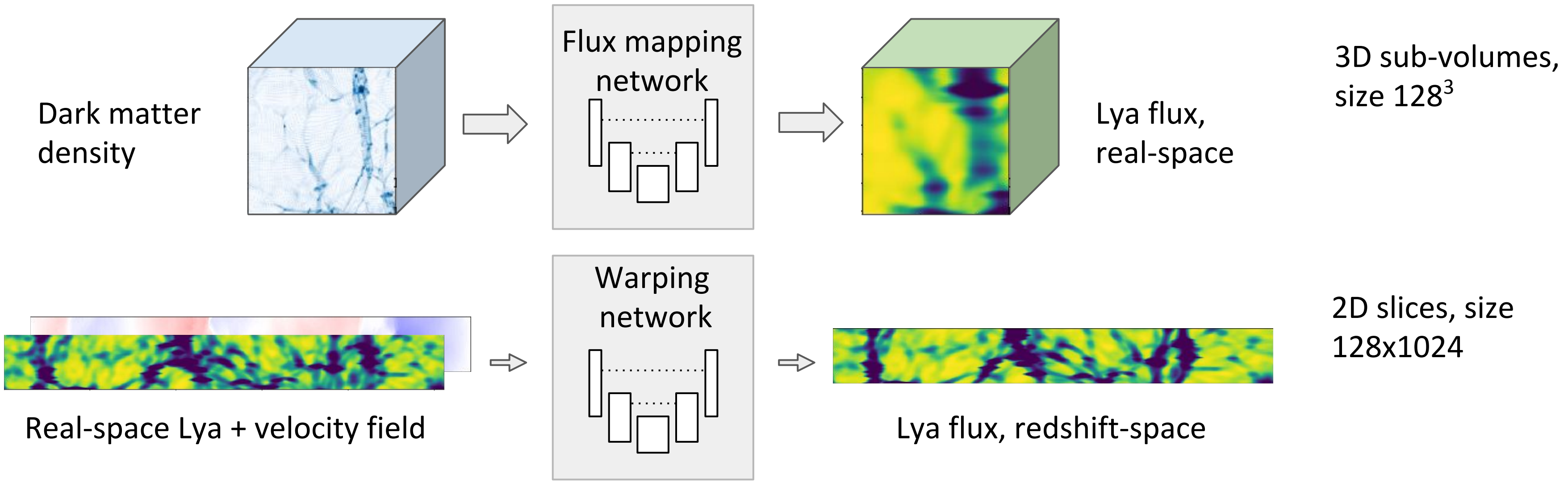
Defined on uniform grid, 1024^3 voxels, with periodic boundary conditions

Reserve top 1/8th for validation set



Dual-network pipeline

During training, randomly crop (x,y) pairs from simulation data:



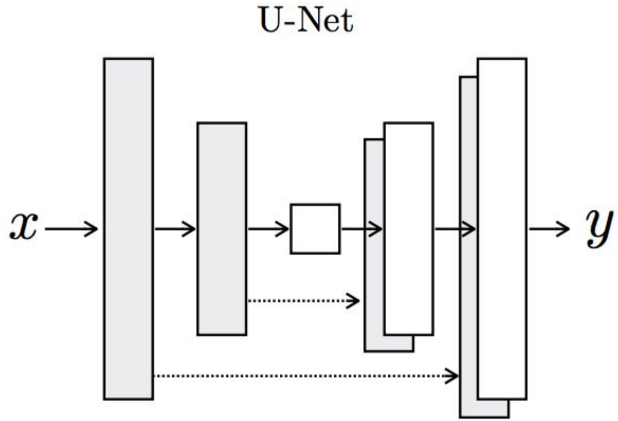
- Both networks trained with L1 loss, which is sufficient for good results
- Additional adversarial loss (given by a discriminator network) was useful in providing slight refinements to the output of the 3D flux mapping network

Network Architectures

Architecturally, networks are simple U-Nets:

- Originally developed for biological image segmentation, U-Nets are being used in many fields now -- esp. in recent cosmological deep learning applications (He et al. 2019, Ramanah et al. 2019, Zhang et al. 2019,...)

- U-Net design allows encoding/decoding of high-level features while using skip connections to pass low-level details and easily backpropagate gradients to early layers



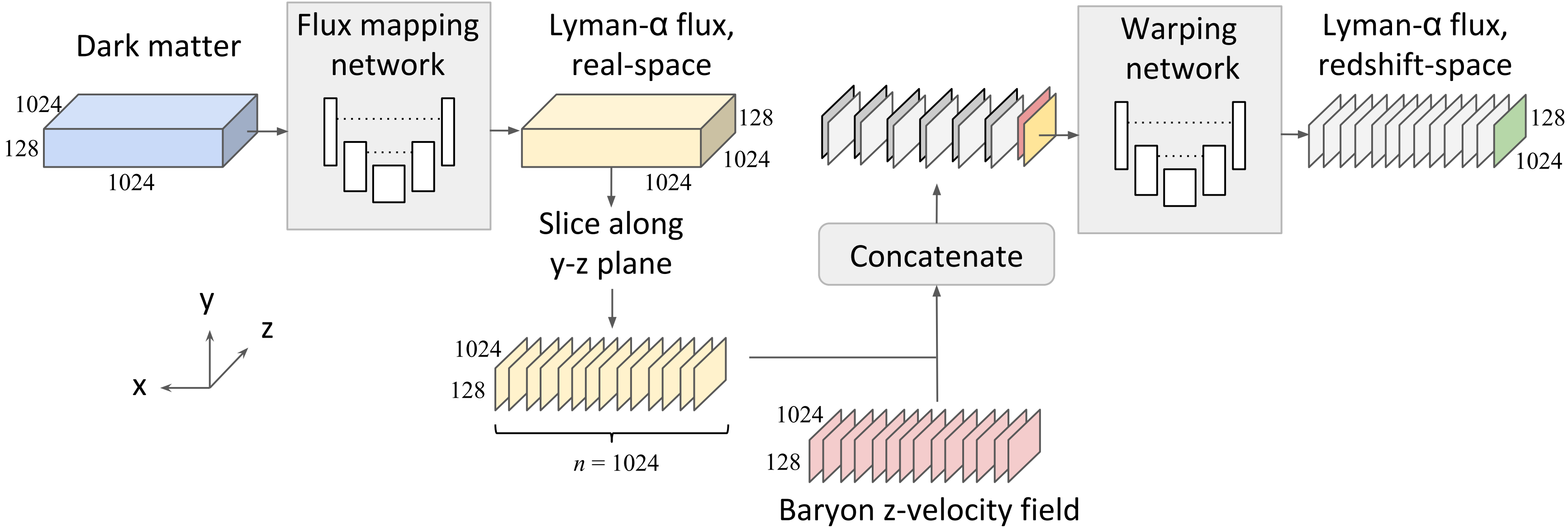
Isola et al. (2018)

- **Side note**: the "bottleneck" layer of the U-Net is not always useful …

    - After downsampling to a bottleneck layer with dimension of 1 in all spatial directions (with *N* high-level feature encoding channels), as is done in the original pix2pix mode, we found the bottleneck layer to be completely ignored by the next up-sampling layer. This happened in several datasets, so beware!

Dual-network pipeline

During inference, chain networks together:



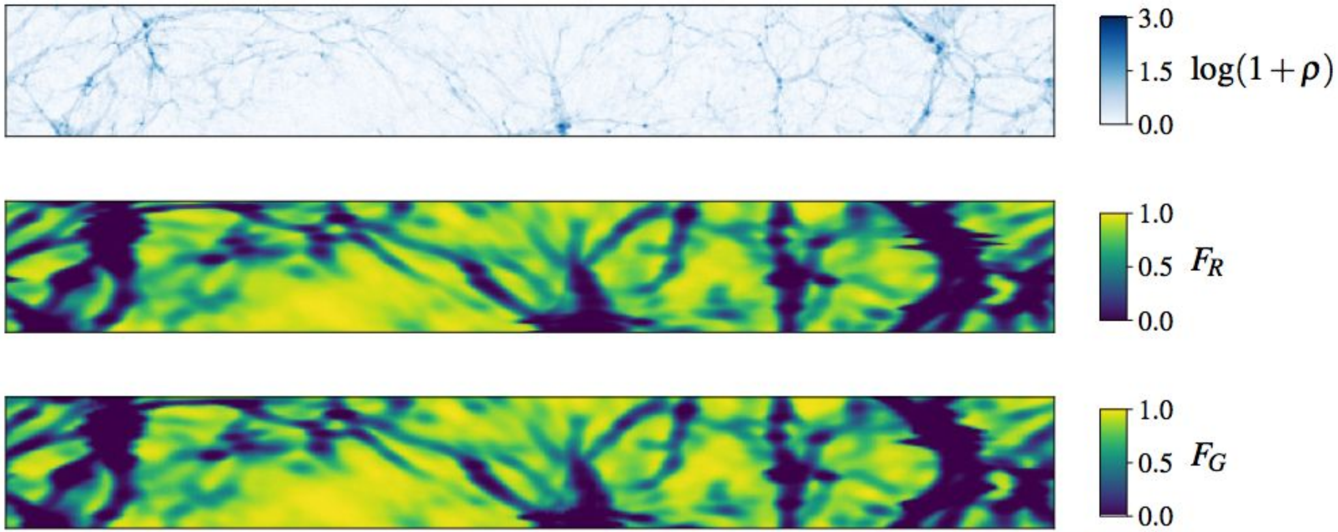
Results

- Qualitatively, the pipeline captures features well across a range of scales
- Sharp transitions and extreme redshift-space distortions seem to be the most prominent failure modes

Dark matter density (input)

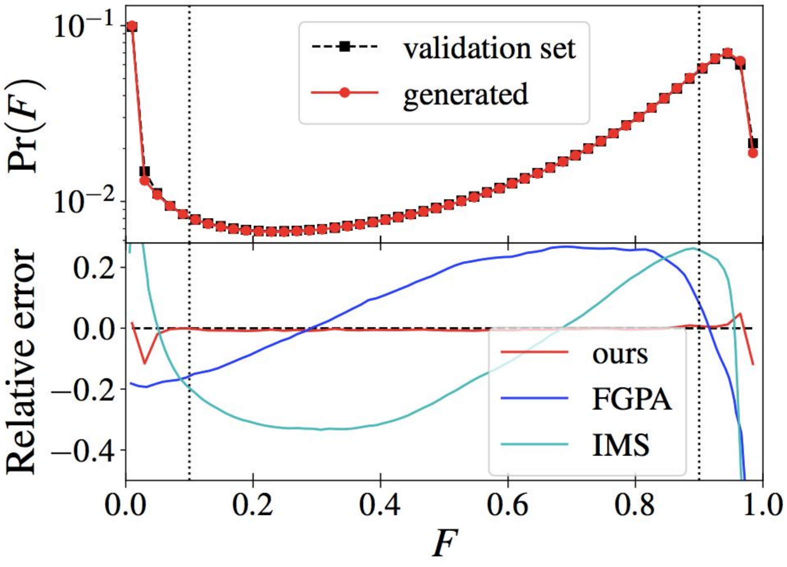
Redshift-space Lya flux (target)

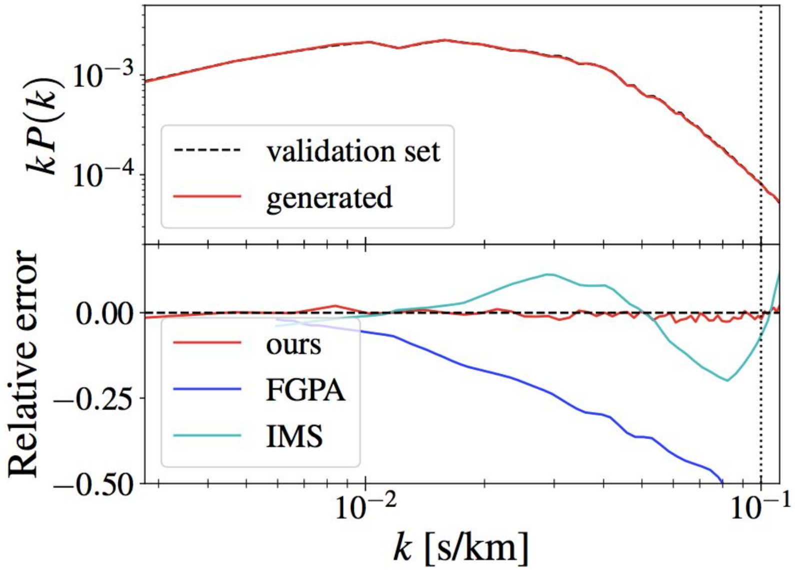
Network prediction



Results: statistical analysis

Two key statistics used in Lya flux analysis: **flux PDF** and **1D power spectrum**

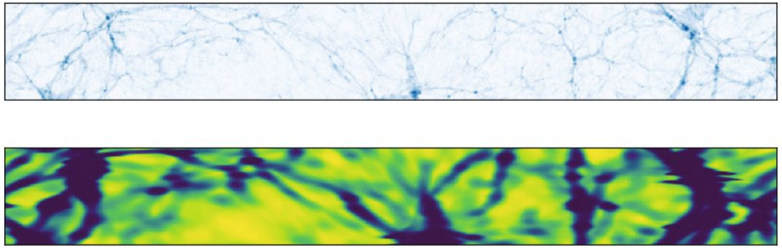




Our network **significantly reduces** the relative error incurred by existing methods

Conclusions & next steps

By training on small volumes and predicting on large ones, we have reproduced the useful characteristics of existing techniques while reducing the relative error by an order of magnitude.



These initial results open the door to several next steps:

- Re-train the networks using true N-body only simulations paired with full-physics simulations (approx. gas velocities from dark matter velocity field)

- Learn a mapping from dark matter to full gas distribution variable set (density, temperature, velocity) to **fully replace hydrodynamic component** of these simulations