Cosmic Structure in the Age of Machine Learning: Rethinking Hydrodynamical Simulations

Benjamin Horowitz
Kavli Fellow IPMU

View online with animations here

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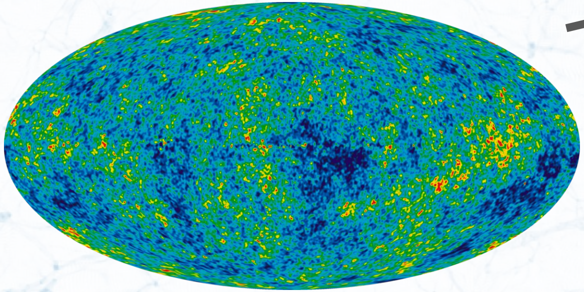
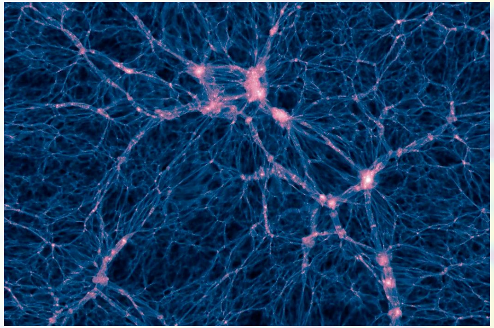
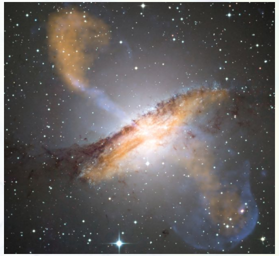
Initial Conditions



Dark Matter Distribution



Galaxies + Gas



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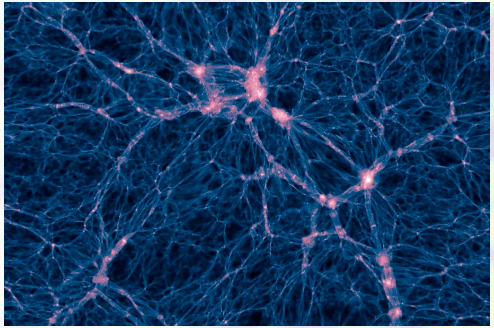

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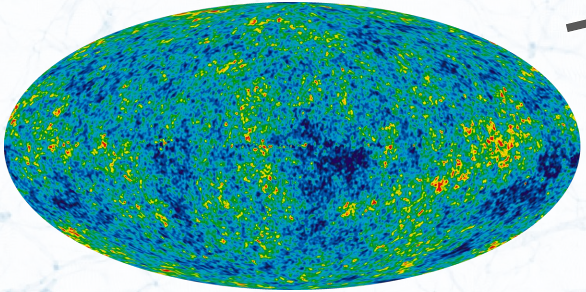

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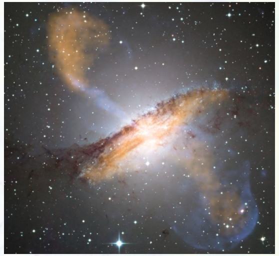

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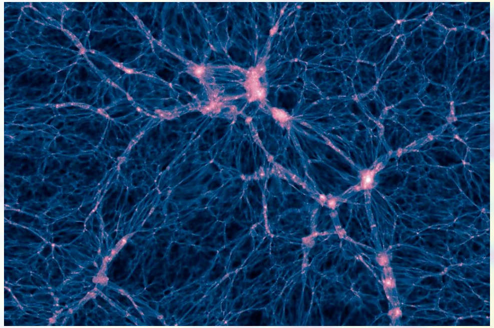
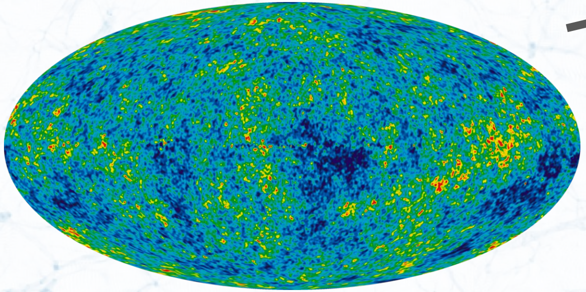


Dark Energy Nature/Evolution
General Relativity

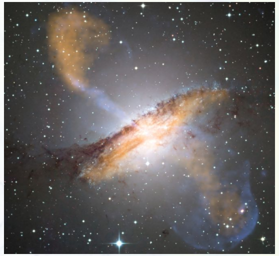
Initial Conditions



Inflation Models
Primordial Non-Gaussianity

Galaxy Evolution/Formation
Thermal History of Gas

Galaxies + Gas



Outline

1) Large-Scale Structure and Baryons: A high-z (Lyman-ɑ)and low-z example (tSZ)

2) Cosmological Hydrodynamical Simulations

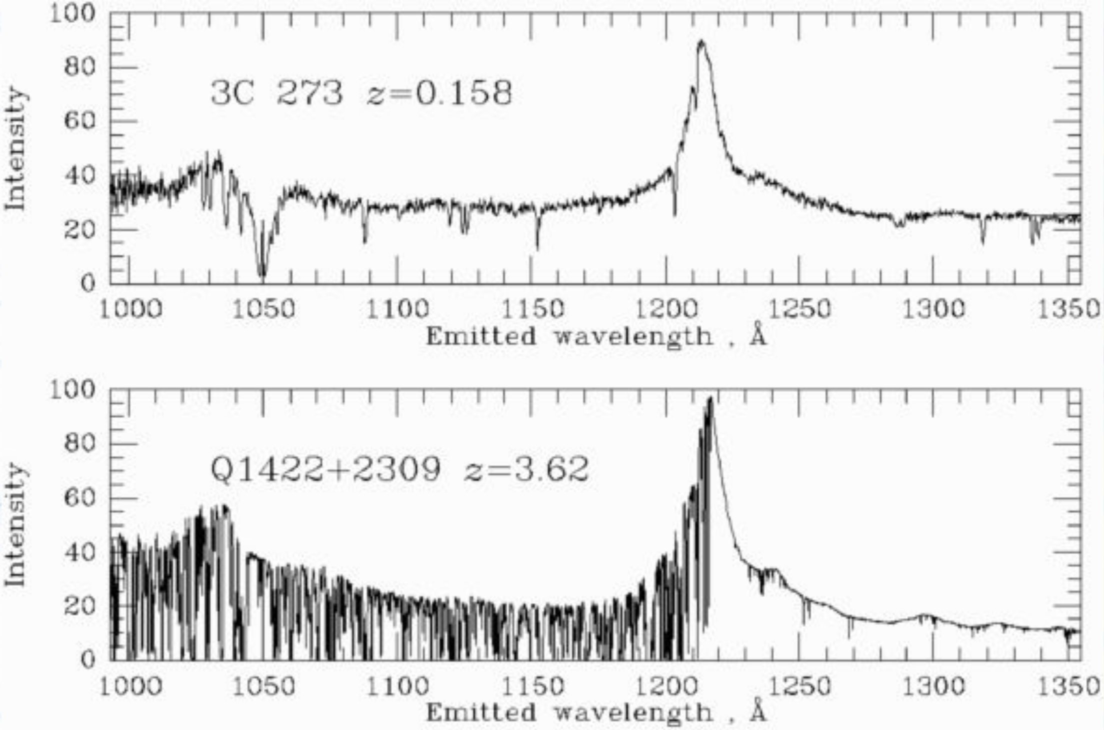
3) Machine Learning as a New Computational Paradigm

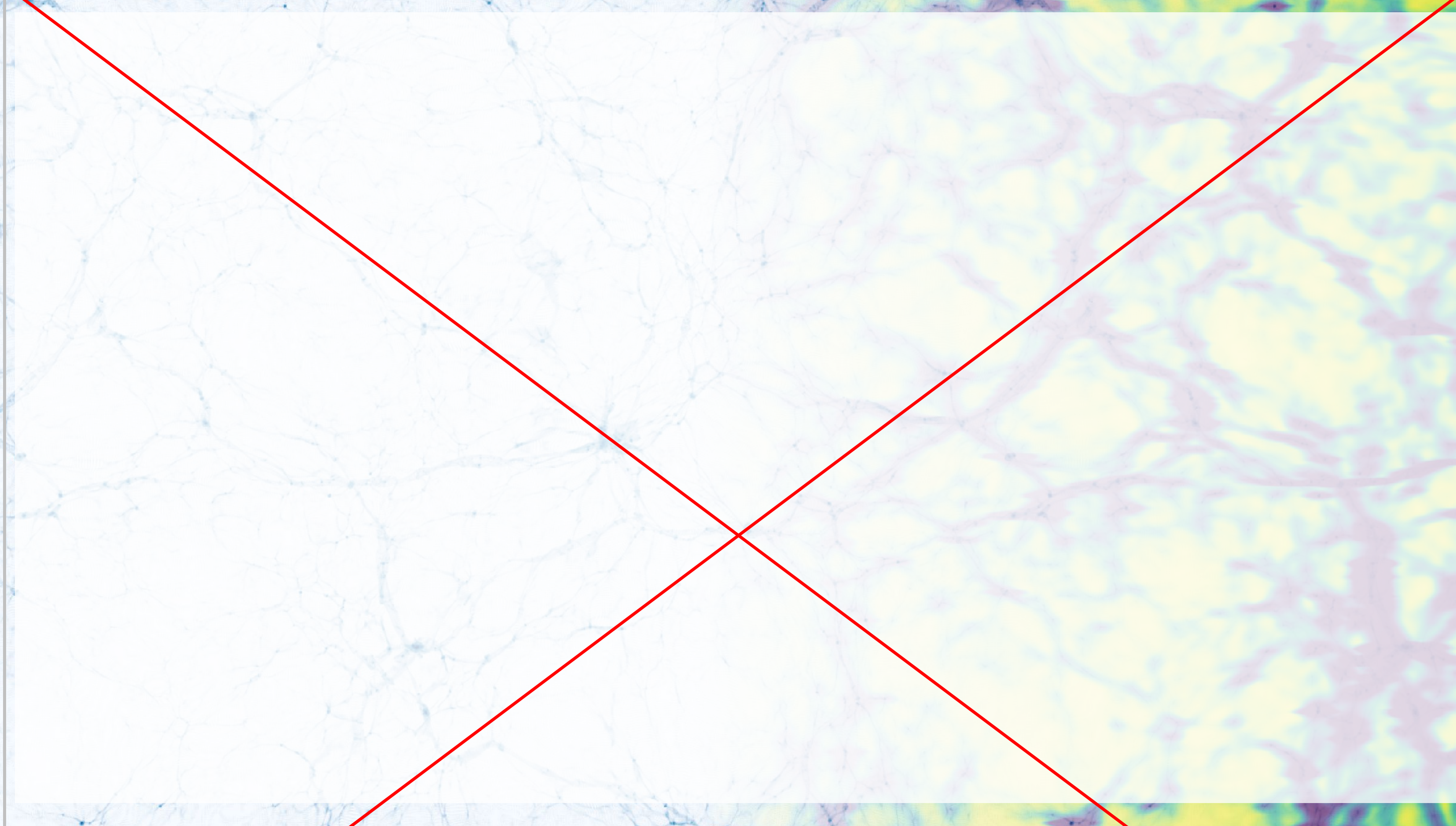
4) Unifying ML and Hydrodynamical Simulations with a Field Level Approach

A High Redshift Example: Lyman-α Forest

From Bill Keel

Nearby (low-z) quasars have fewer absorption lines than distant (high-z) quasars

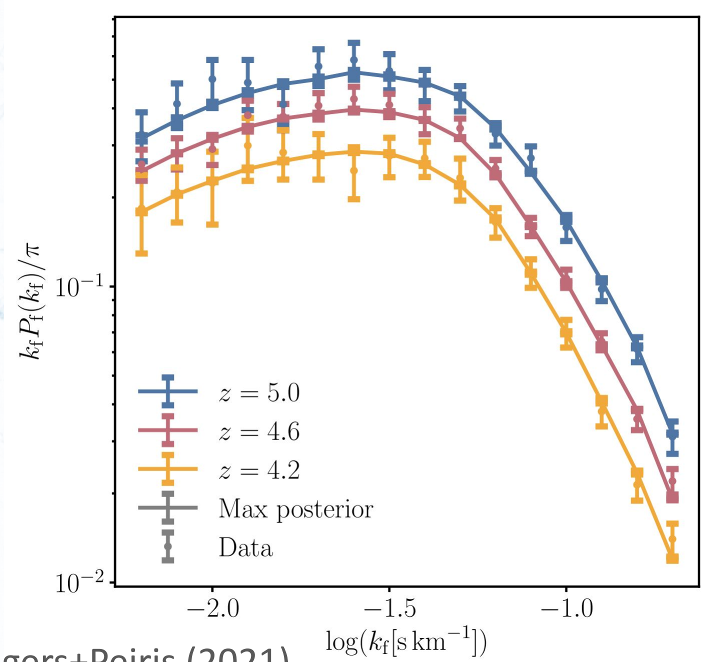




Lyman Alpha as a Cosmological Probe

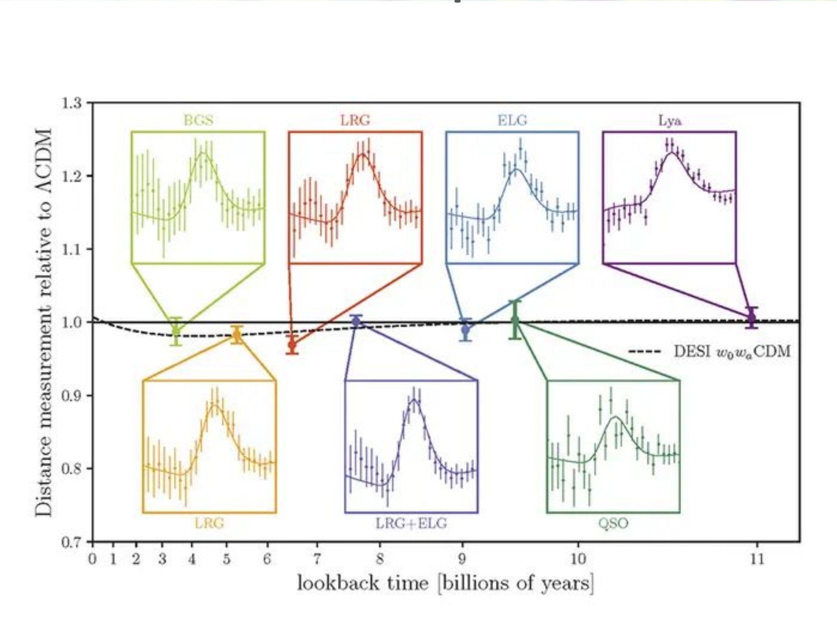
If neutral hydrogen/flux is a function of density, can use absorption as a tracer of clustering
$\longrightarrow$ constrain physics which effects clustering

Warm Dark Matter



Rogers+Peiris (2021)

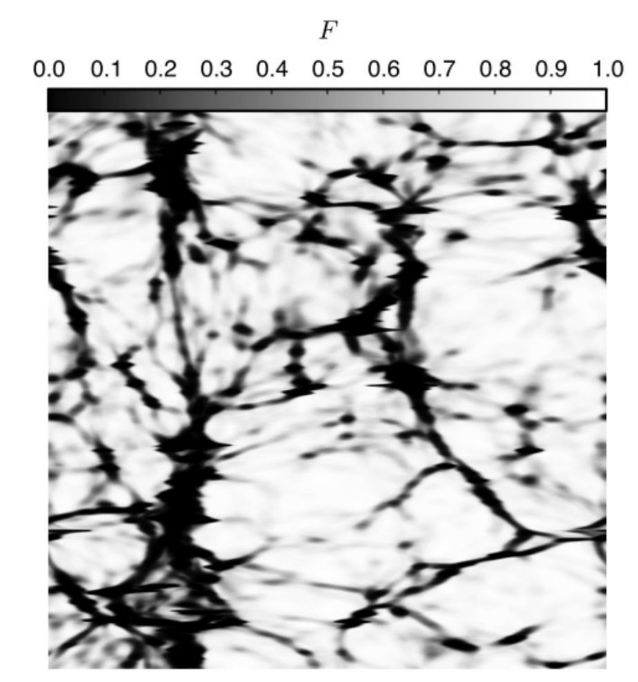
Cosmic Expansion



DESI (2024)

Lyman Alpha Tomography: Unique Probe of z~2 Universe

Basic Idea: Observe lots of lines of sight in small area and then interpolate/extrapolate between absorptions on various of lines of sight.
(Pichon+2001, Caucci+2008, Lee+2014)



From Casey Stark

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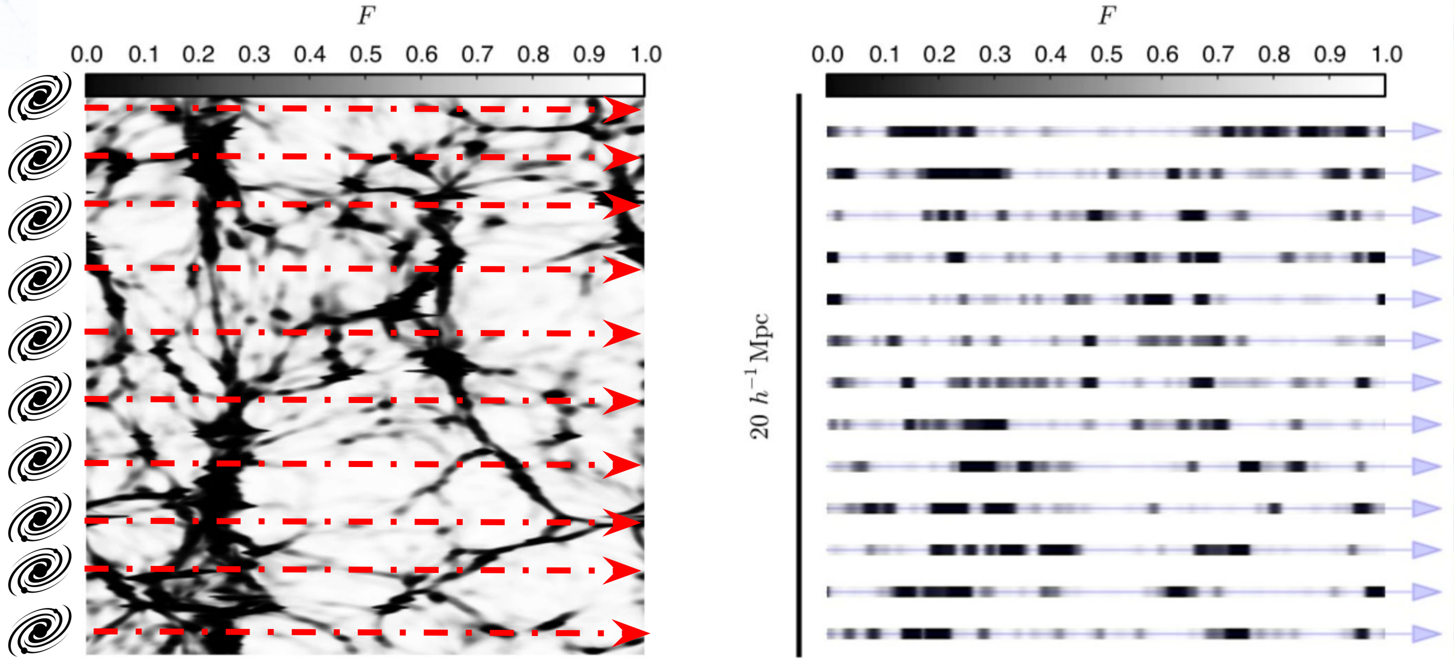
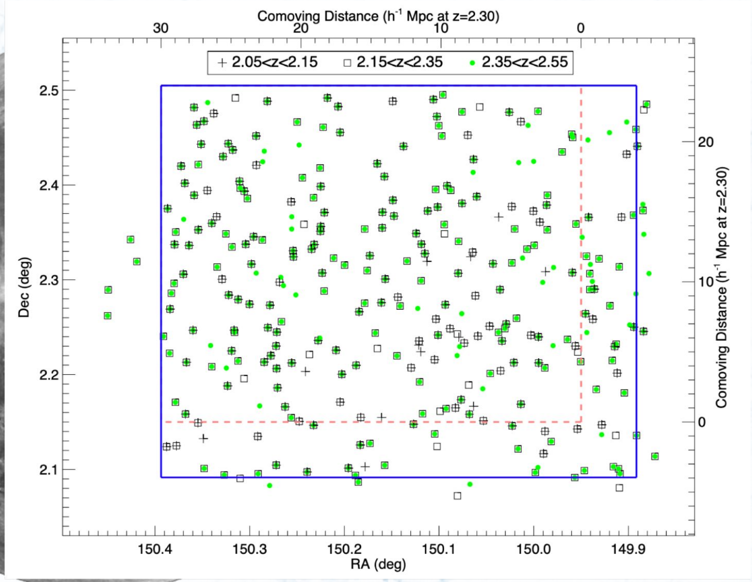


From Casey Stark

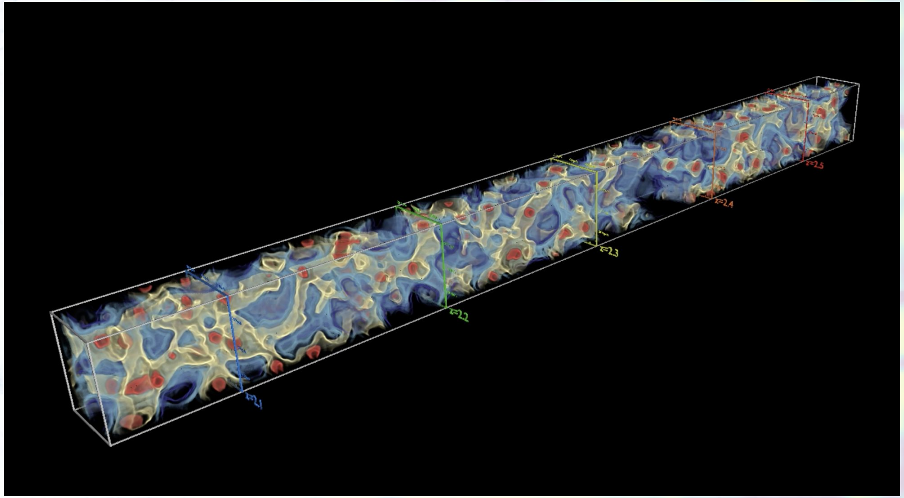
Applied to Data: COSMOS Field

COSMOS Lyman Alpha Mapping and Tomography Observations (CLAMATO)

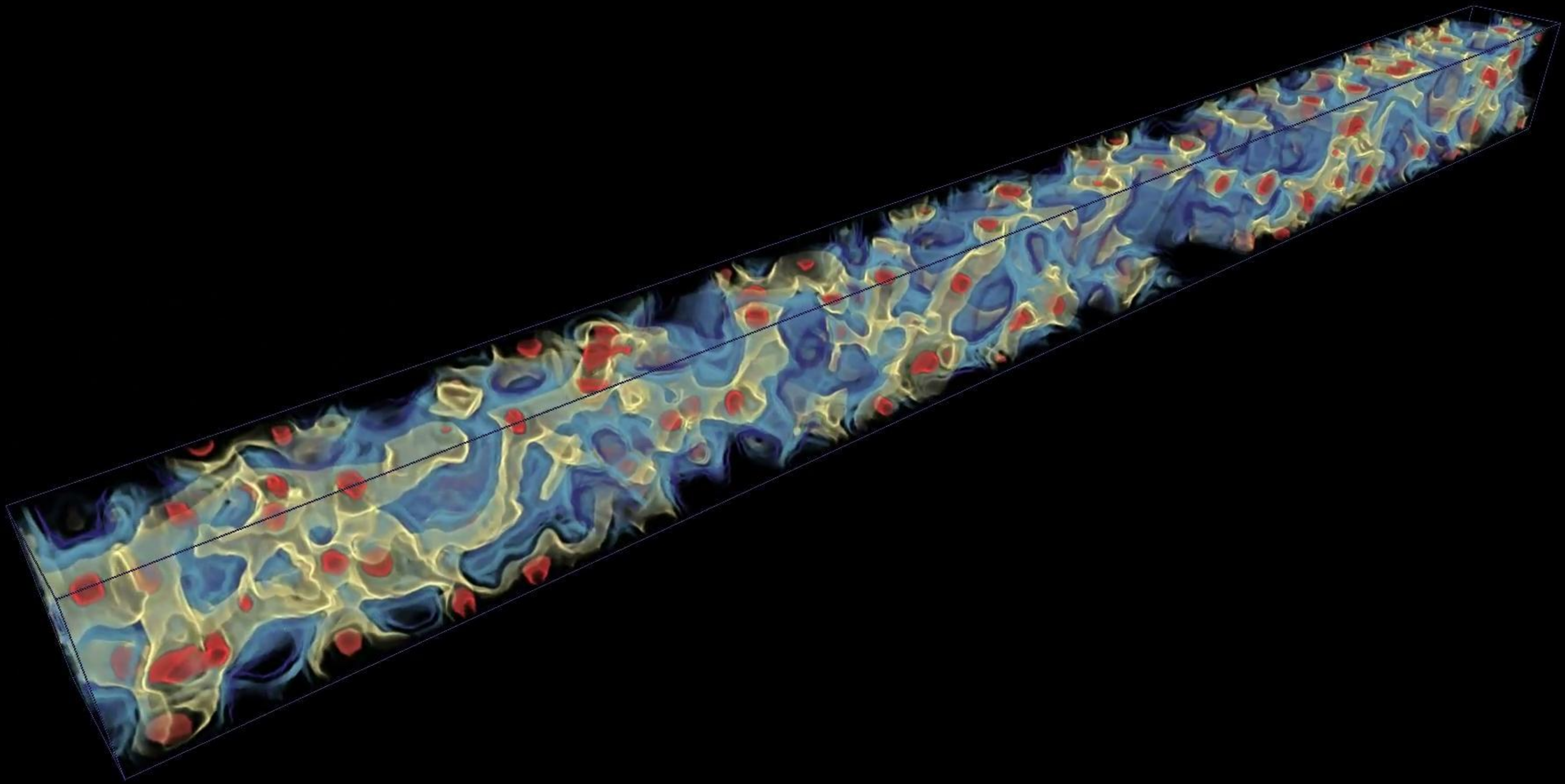


320 background sources in COSMOS field

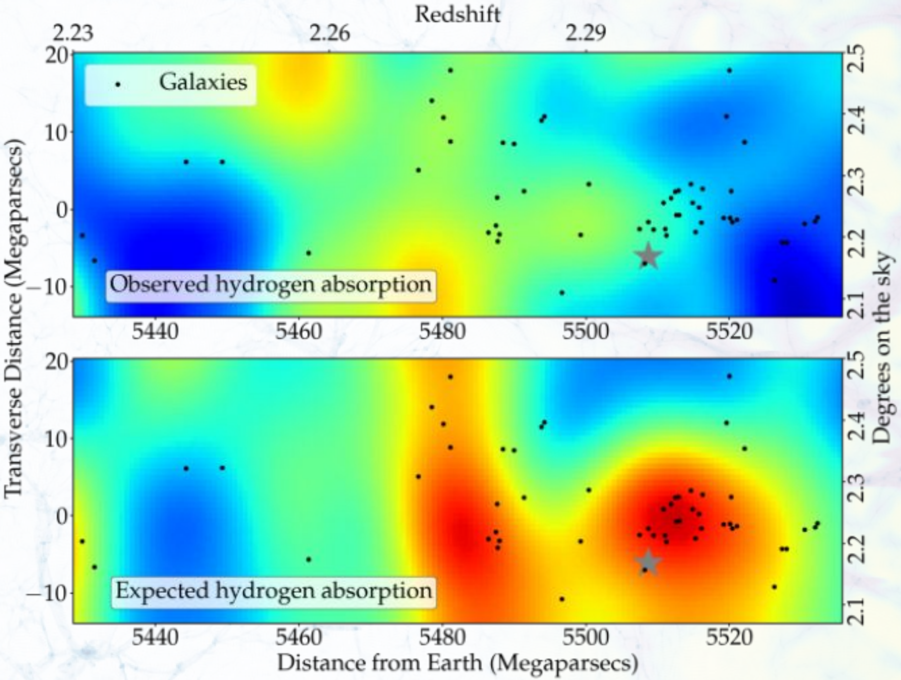
Three Dimensional Map of Cosmic Web



Lee et al. (2016), BH et al. (2023)



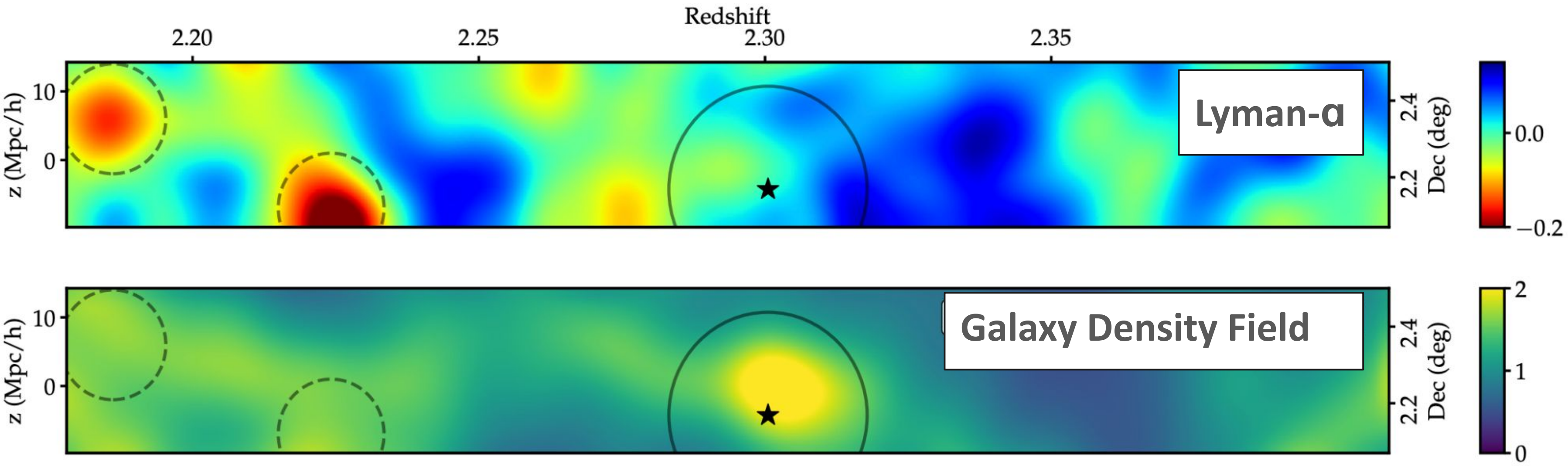
Discrepancy between Galaxy Fields and Flux Fields



There exist a lot of clusters which appear in either galaxy or Lyman-α, but not both!

Dong + BH et al. (2023

Discrepancy between Galaxy Fields and Flux Fields



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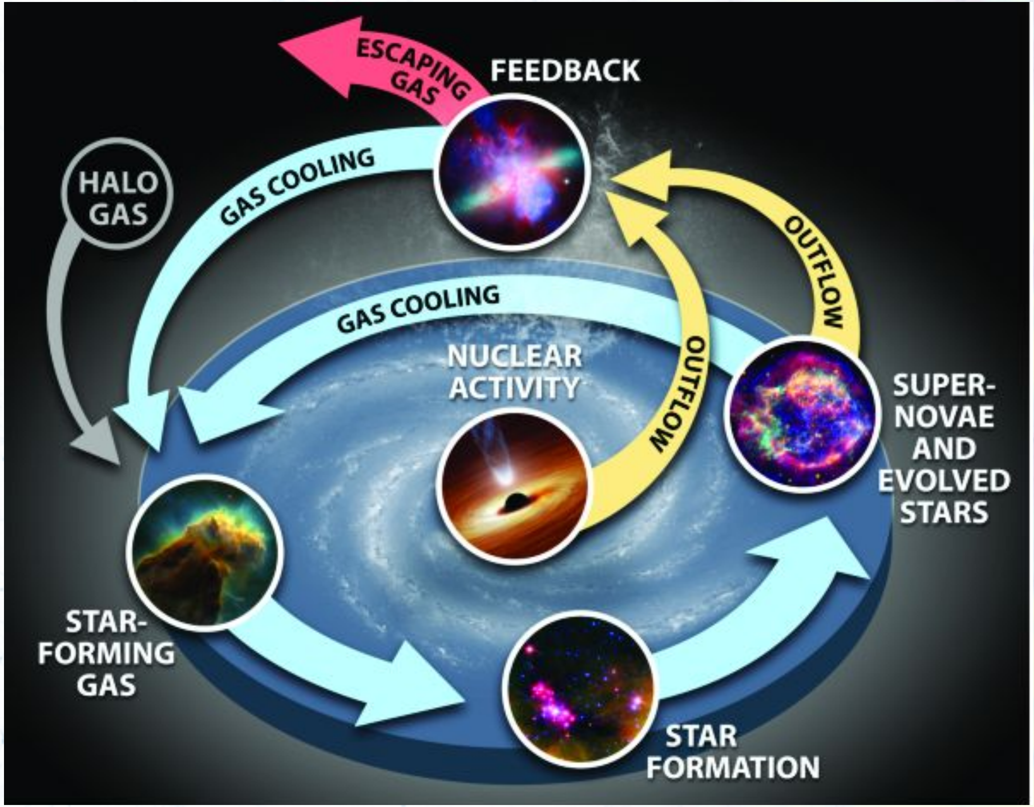
Dong + BH et al. (2023

Feedback and Baryon Cycle

Leisawitz et al (2019)

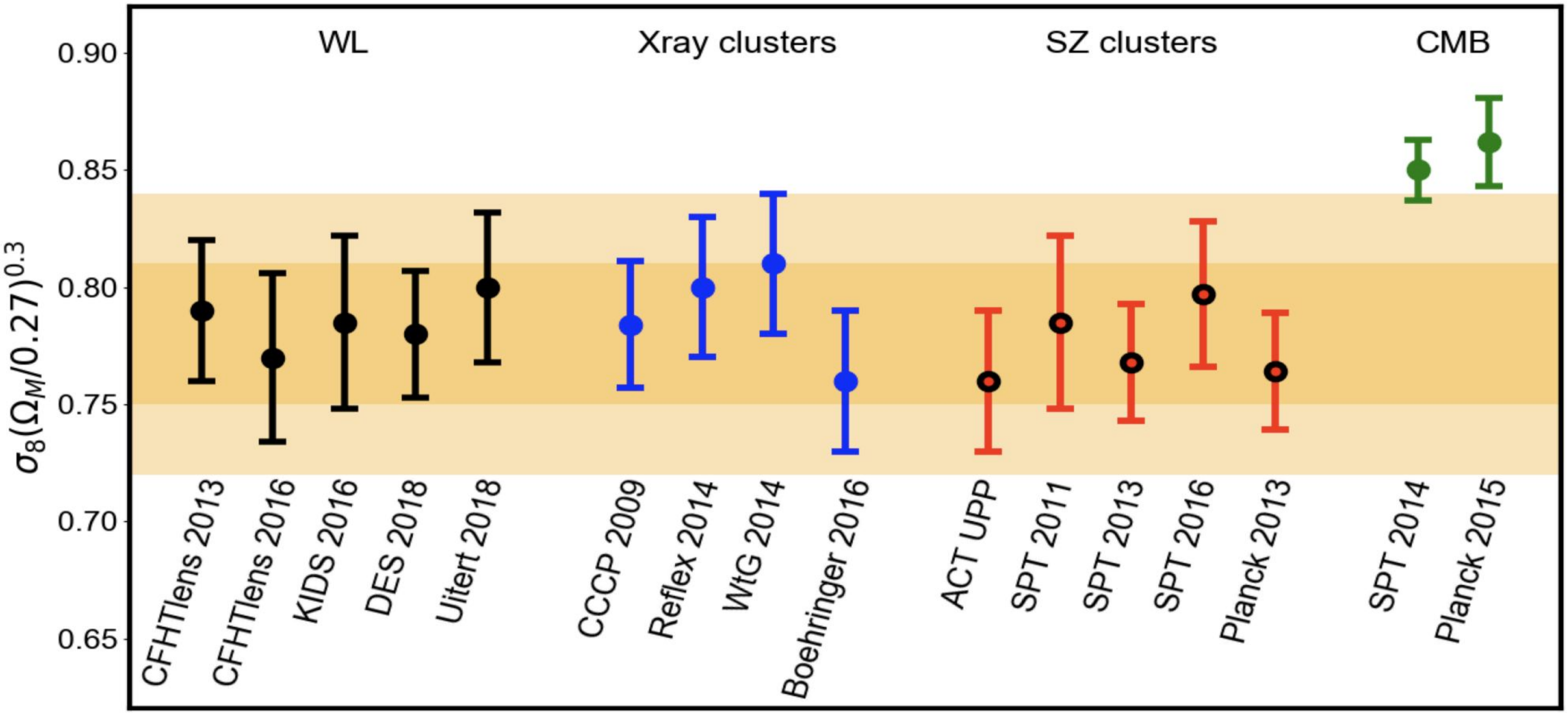


(from M. Douspis)

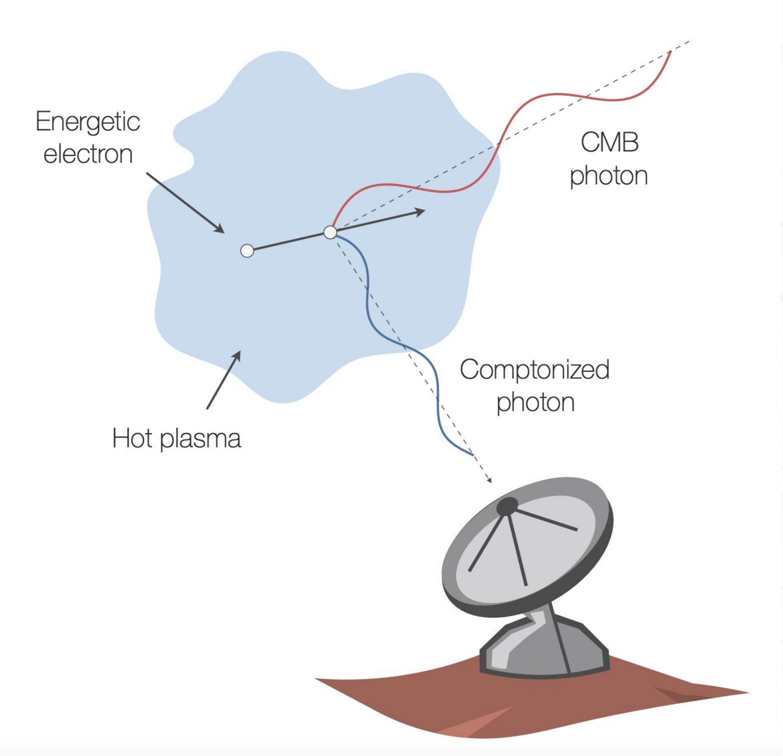
A low-z Example : Sigma 8 Tension and tSZ

Low Redshift

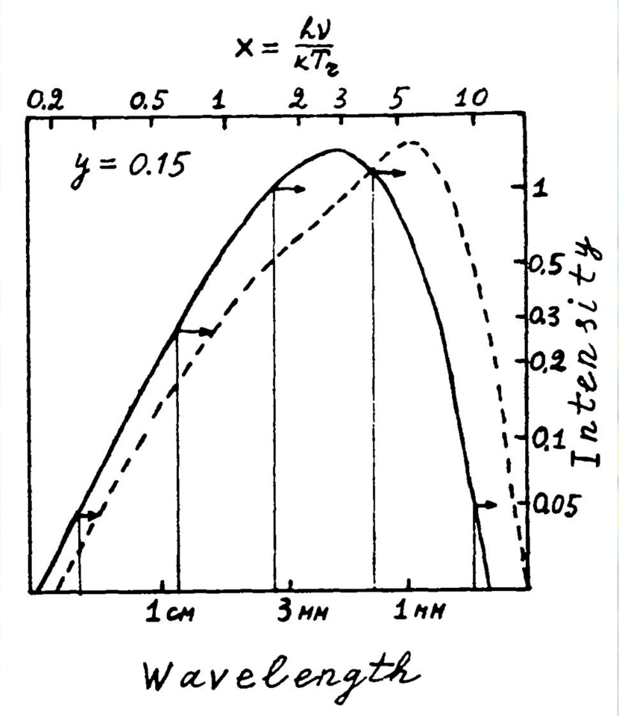
Inferred from High Redshift



One Example: Thermal Sunyaev Zeldovich Effect



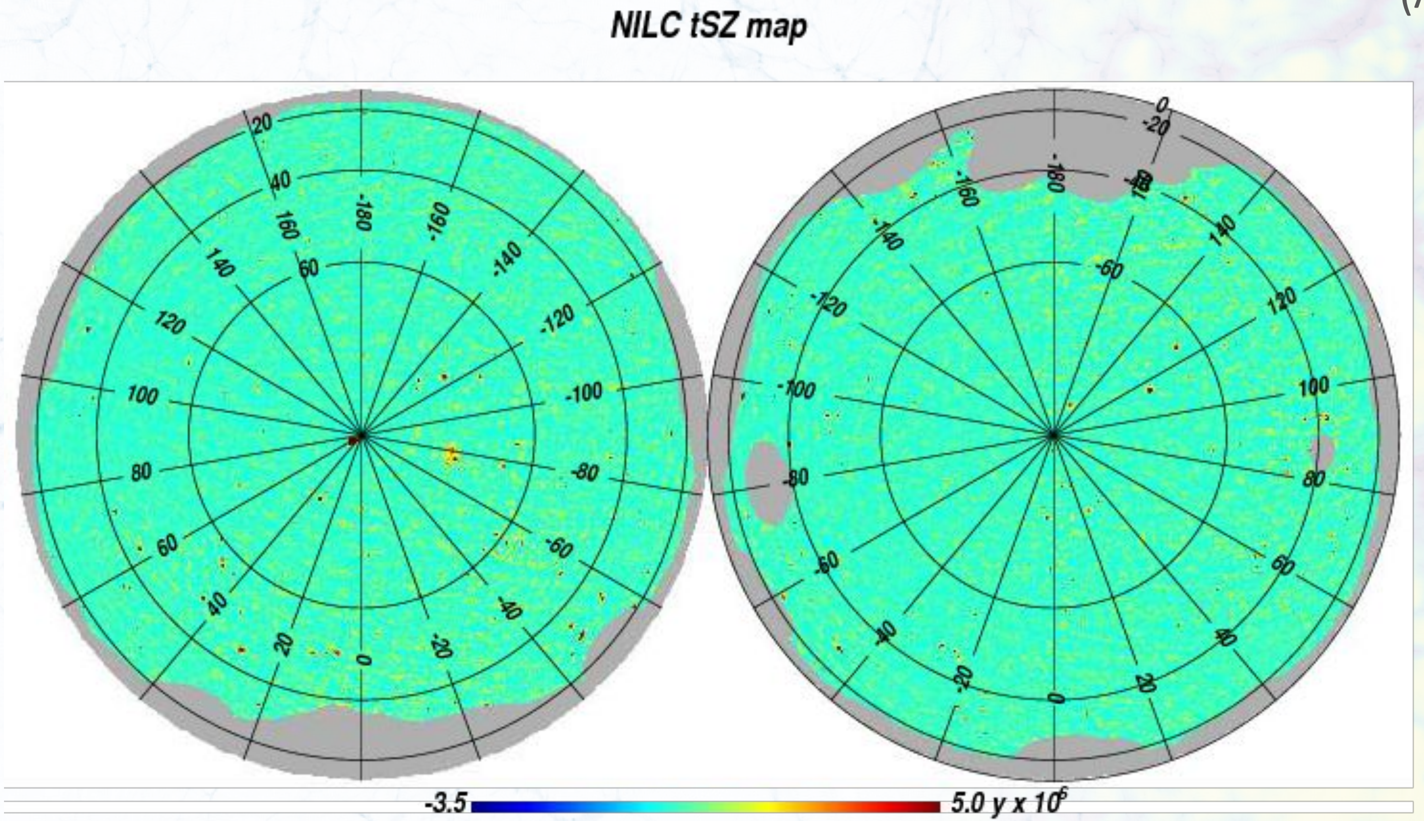
Mroczkowski, Nagai, Basu, Chluba et al. (2019)

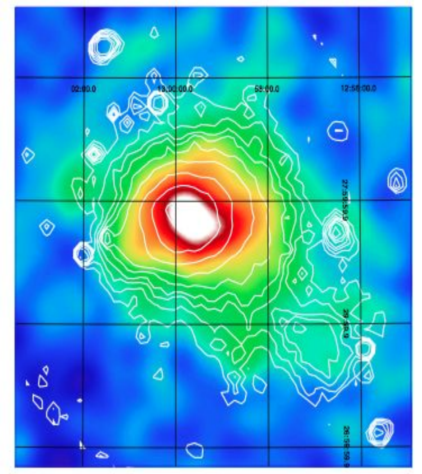


from Sunyaev + Zeldovich (1980)

tSZ Effect : Compton y-map

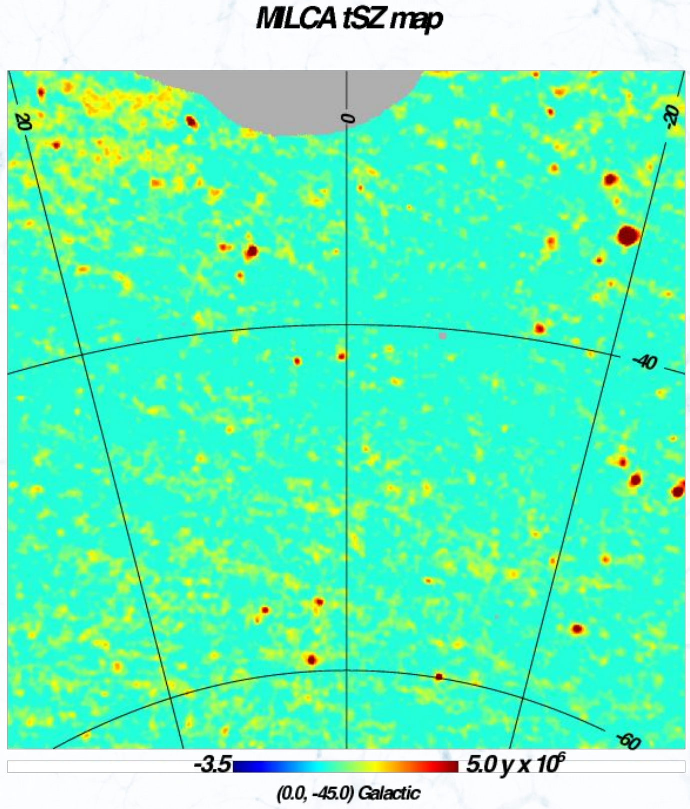
Planck 2015
(Aghanim, et al.)





Coma Cluster tSZ

Thermal Sunyaev Zeldovich Effect : Halo Model

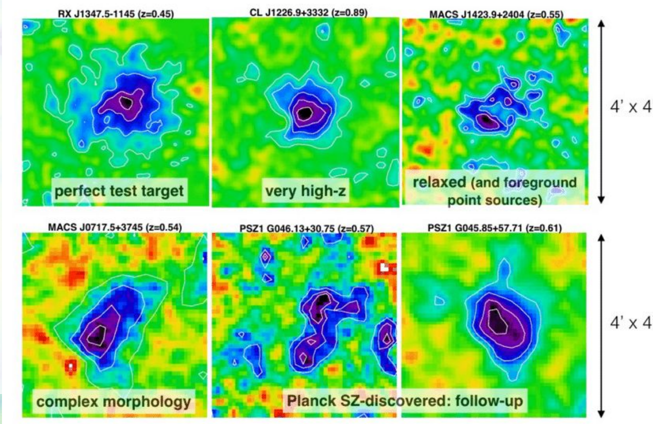


Total “power” of tSZ comes from clusters across different masses at different redshifts:

$$\frac{dn(M,z)}{dM}\,|\tilde{y}_l(M,z)|^2$$

Halo Mass Function (Cosmology)

Halo Pressure Profile



NIKA (Macías-Pérez et al. 2019)

BH, Seljak (2017)

Thermal Sunyaev Zeldovich Effect : Power Spectra

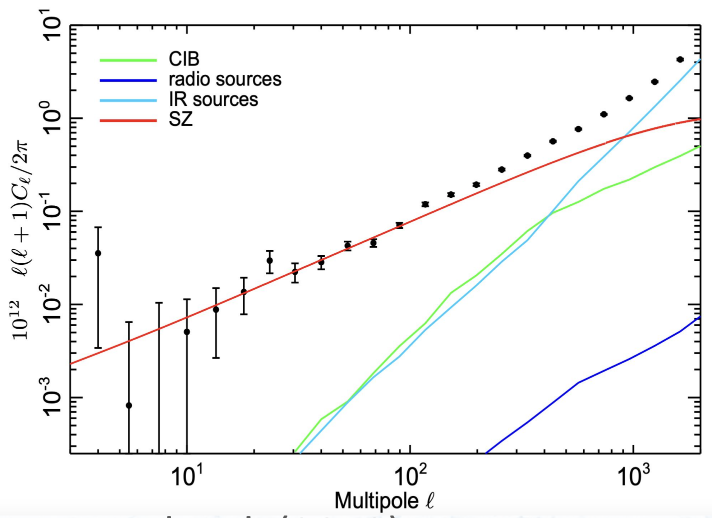
Add up all halos across all redshifts and mass ranges, weighted by pressure/geometry

$$C_l^{1-halo} = \int_{z_{low}}^{z_{max}} dz \frac{d^2V}{d\Omega dz} \int_{M_{min}}^{M_{max}} dM \frac{dn(M,z)}{dM} \left|\tilde{y}_l(M,z)\right|^2$$

Volume Factor (Geometry)

Halo Mass Function (Cosmology)

Halo Pressure Profile (Baryon Physics)



Planck (2013)

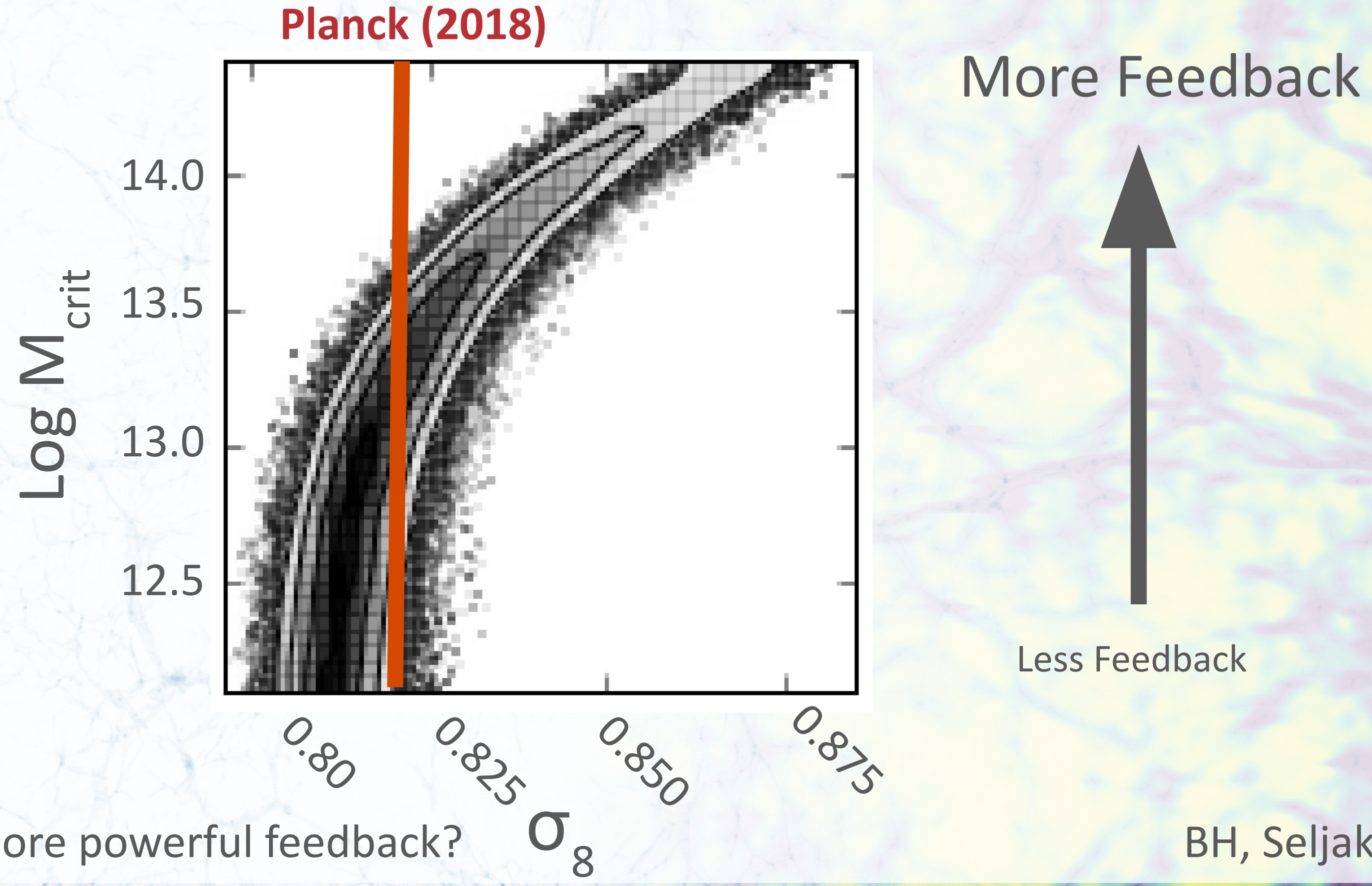
Modelling Pressure Profile with Feedback:

$$y_l^{\mathrm{new}}(x, r_{\mathrm{vir}}) = f_{\mathrm{gas}} y_l^0(x) + (1 - f_{\mathrm{gas}}) y_l^{\mathrm{feedback}}(x, r_{\mathrm{vir}})$$

Parametrization:

$$f_{\mathrm{gas}}(M_{halo}, M_{crit}) = \frac{1}{1 + \left(\frac{M_{crit}}{M_{halo}}\right)^2}$$

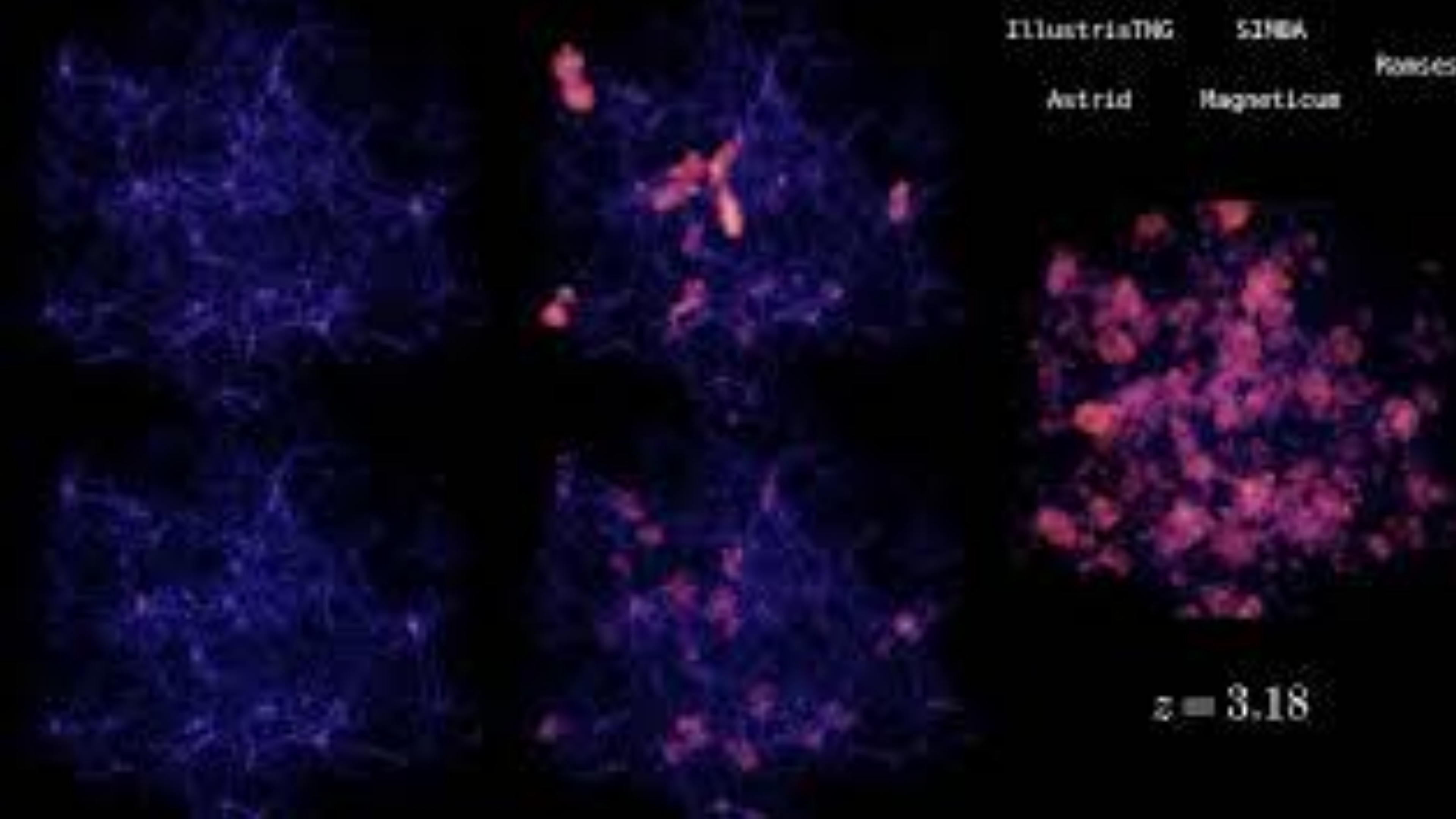
tSZ: Likelihood analysis with Planck Data



Preference for more powerful feedback?

BH, Seljak (2017)

Can simulations provide insight?


IllustrisTNG
SIMBA
Ramses
Astrid
Magneticum
$z = 3.18$

Components of a Hydrodynamical Simulation

1) Dark Matter evolution

2) Gas evolution

3) “Subgrid Physics” (i.e. anything not in Navier-Stokes Equations)

Dark Matter Evolution

Collisionless Boltzmann Equation/Vlasov Equation for phase space distribution (f):

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

Can solve this numerically by sampling phase space and using Hamilton's Equations:

Position:

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

Velocity:

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

Lots of tricks to calculate g efficiently (particle-mesh, octotree, etc.)

Hydrodynamics

Euler Equations:

(Comoving coordinates, single energy formalism)

Density

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

Momenta

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

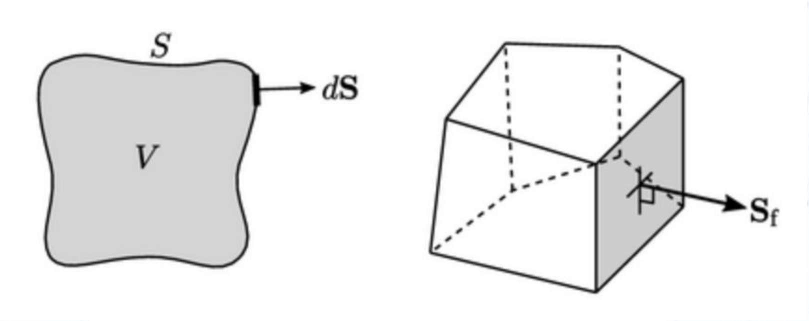
Energy

$$\frac{\partial (a^2 \rho_b E)}{\partial t} = -a\nabla \cdot (\rho_b U E + pU) + a(\rho_b U \cdot \mathbf{g})$$

Describes the change in density, pressure/internal energy, and momenta of a gas

Discretize and Solve (Eulerian)

Break up domain into discrete blocks:



$$\int_S (d\mathbf{S} \cdot \Psi) \rightarrow \sum_f \mathbf{S}_f \cdot \Psi_f$$

State Vector (Density, Momentum, Energy)

Turns every timestep into a series of linear operations:

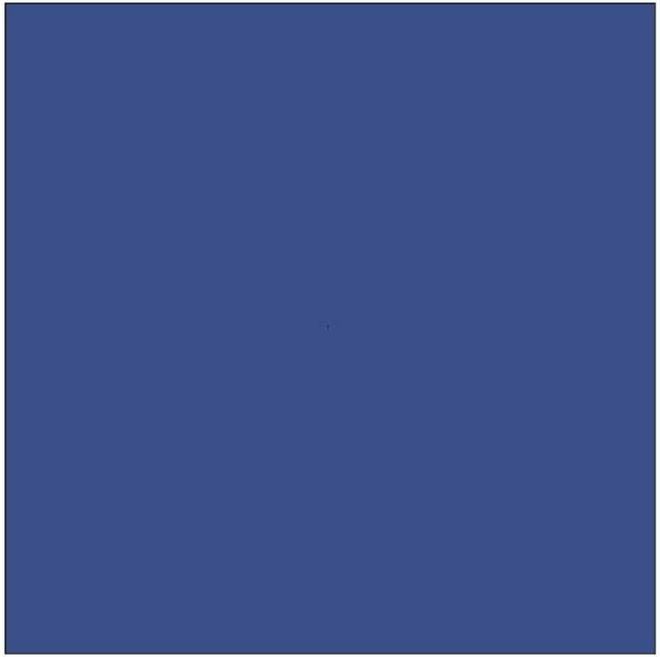
$$\frac{\partial \Psi}{\partial t} + \nabla \cdot (\mathbf{u}\Psi) + \nabla \cdot (\Gamma \nabla \Psi) = S_\Psi$$

$$\begin{bmatrix} \star & \star & & \star \\ \star & \star & \star & \\ & \star & \star & \star \\ \star & & \star & \star \end{bmatrix} \begin{bmatrix} \Psi \end{bmatrix} = \begin{bmatrix} \star \\ \circledast \\ \star \\ \star \end{bmatrix}$$

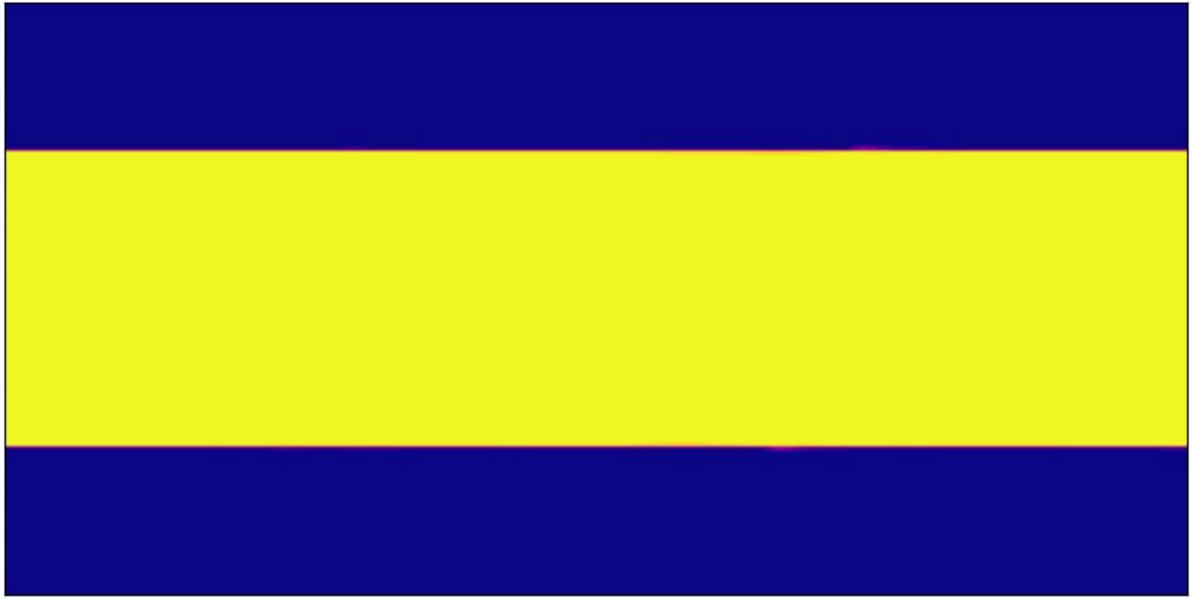
Actual choices of how to best break up these terms are quite complex…

Hydrodynamics

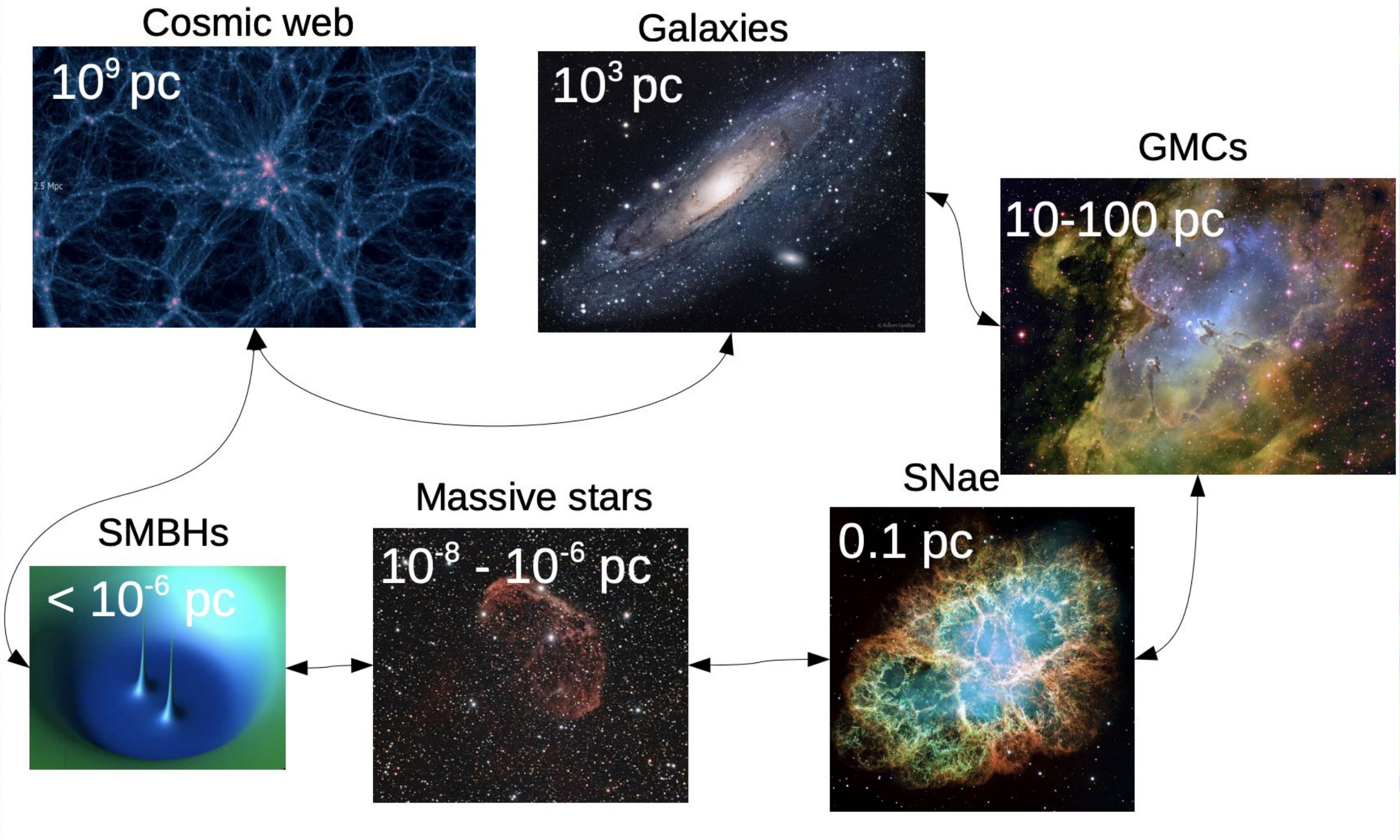
Shocks



Fluid Instabilities



Subgrid Physics



From Debora Sijacki

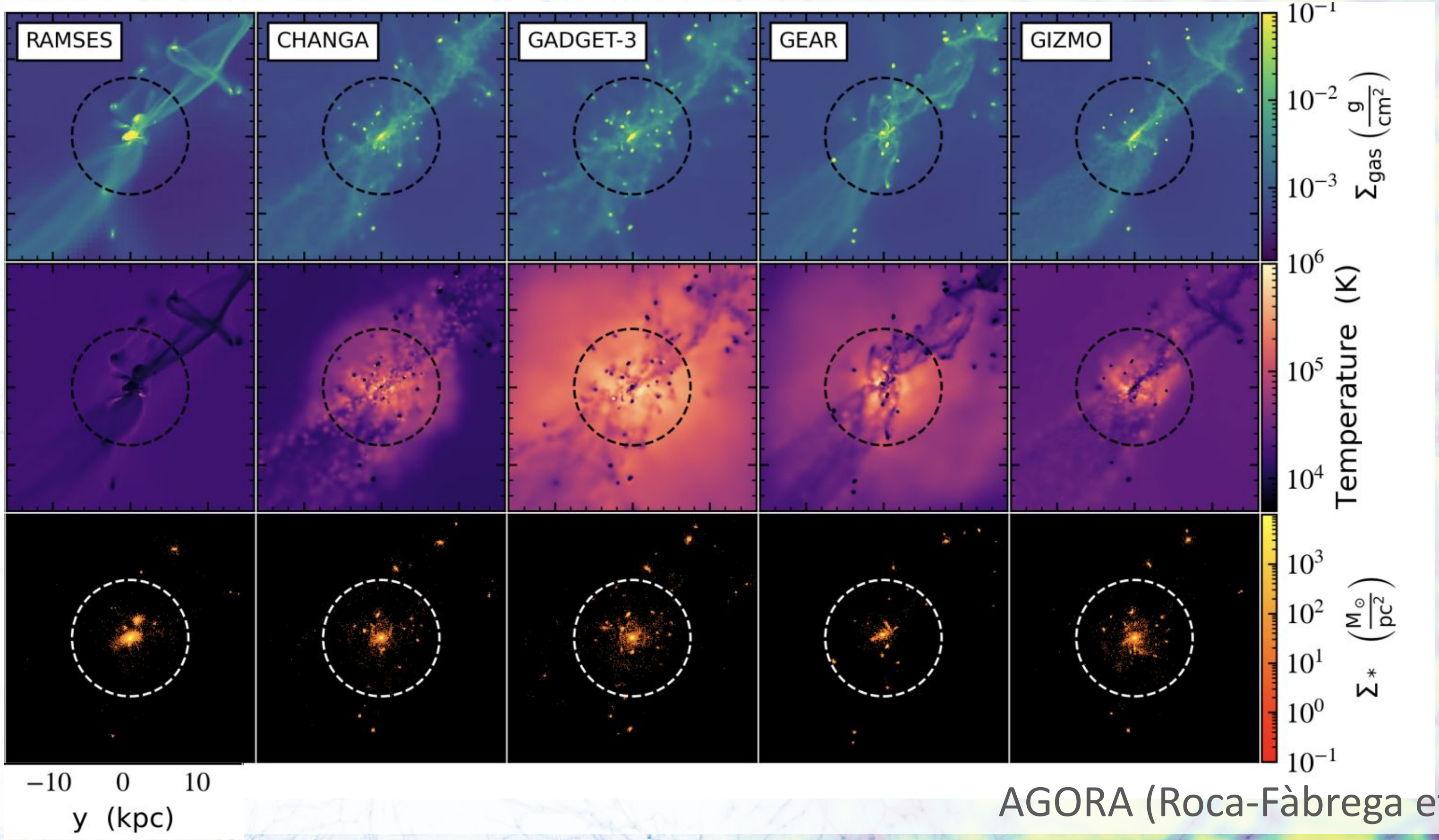
Subgrid Physics

Lots of possible subgrid physics to include:

1) Metal heating/cooling
2) Star Formation
3) Active Galactic Nuclei
4) MHD
5) Cosmic Rays
6) Galactic Inflow/Outflow
7) Subgrid turbulence

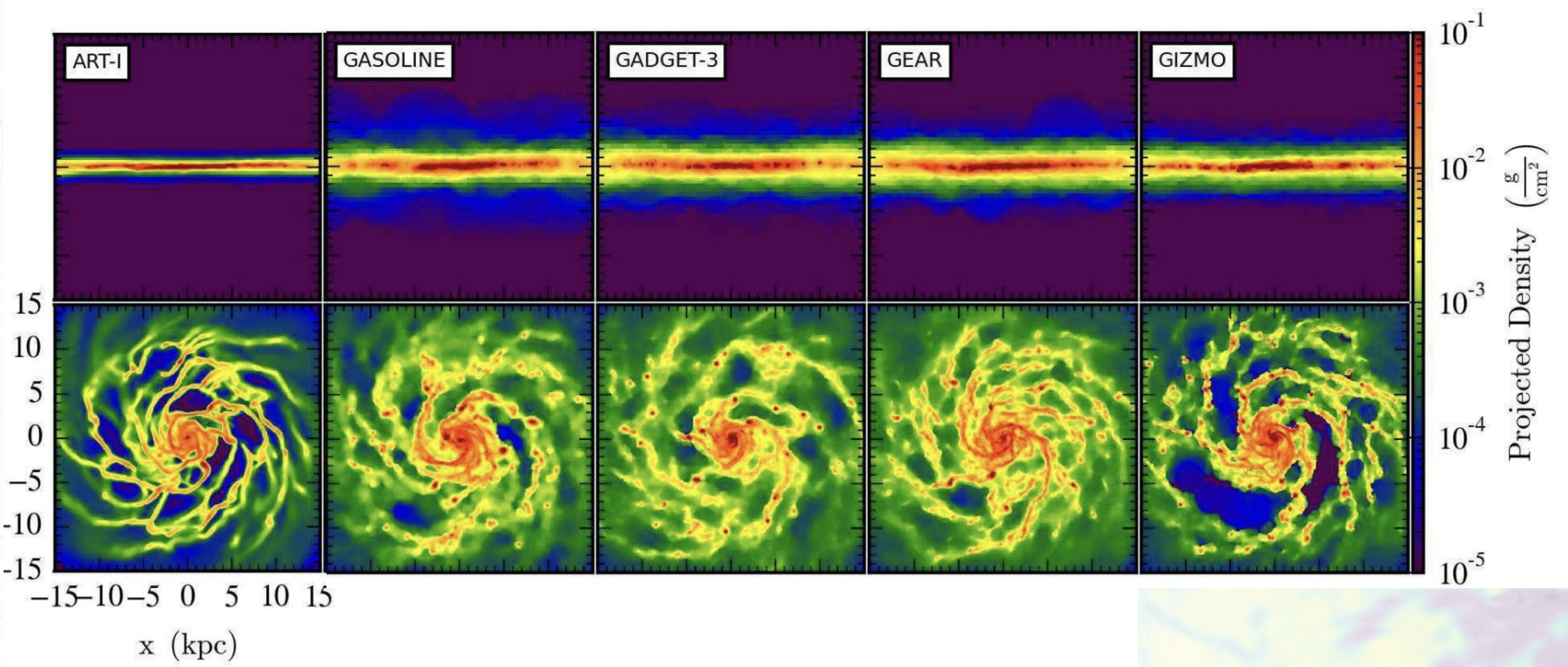
Many others…

Hydrodynamical Simulations : Inconsistencies at Small Scales



AGORA (Roca-Fàbrega et al. 2021)

Hydrodynamical Simulations : Inconsistencies at Small Scales



AGORA (Kim et al. 2019)

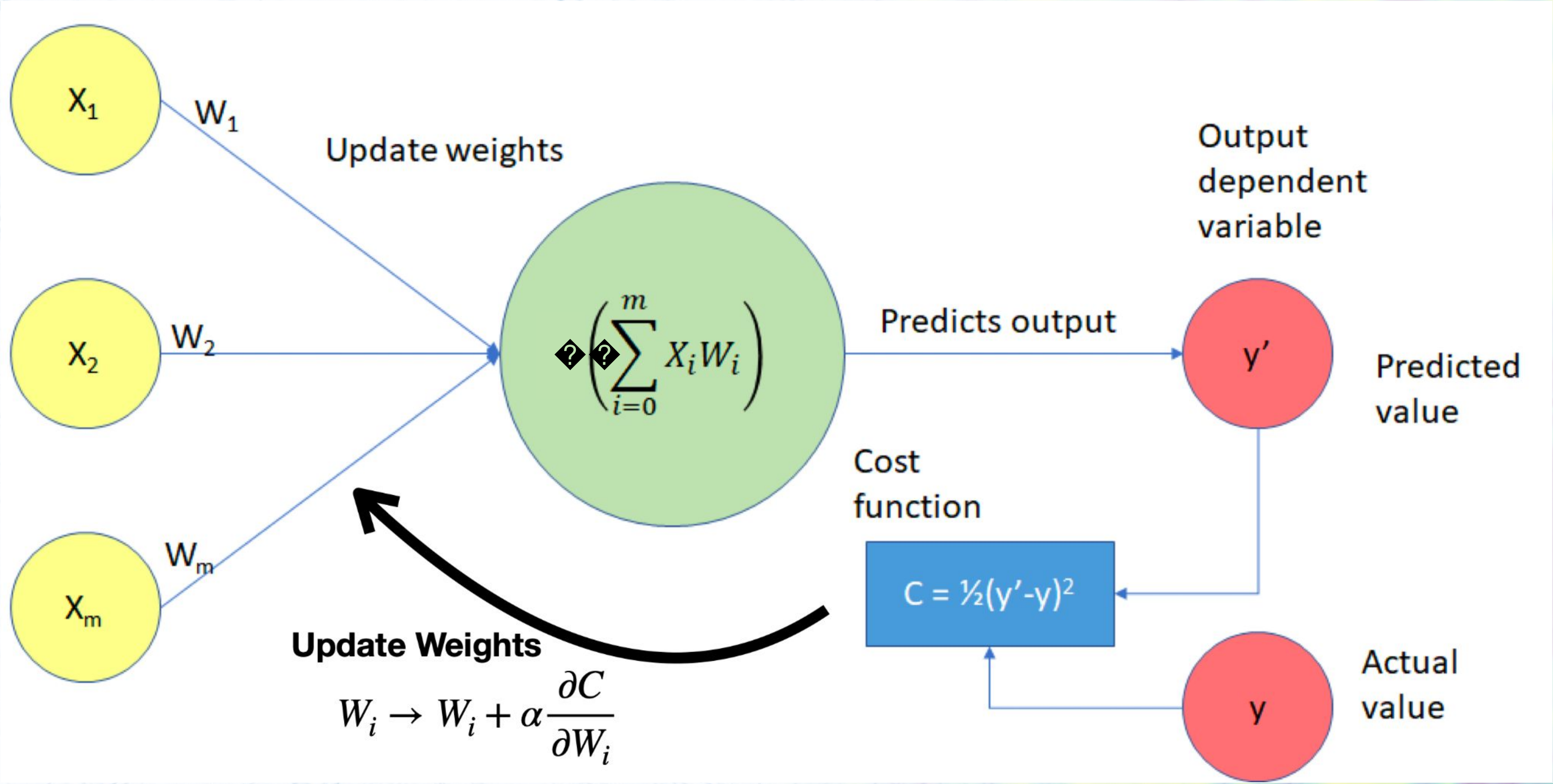
Can machine learning help?

Machine Learning Revolution

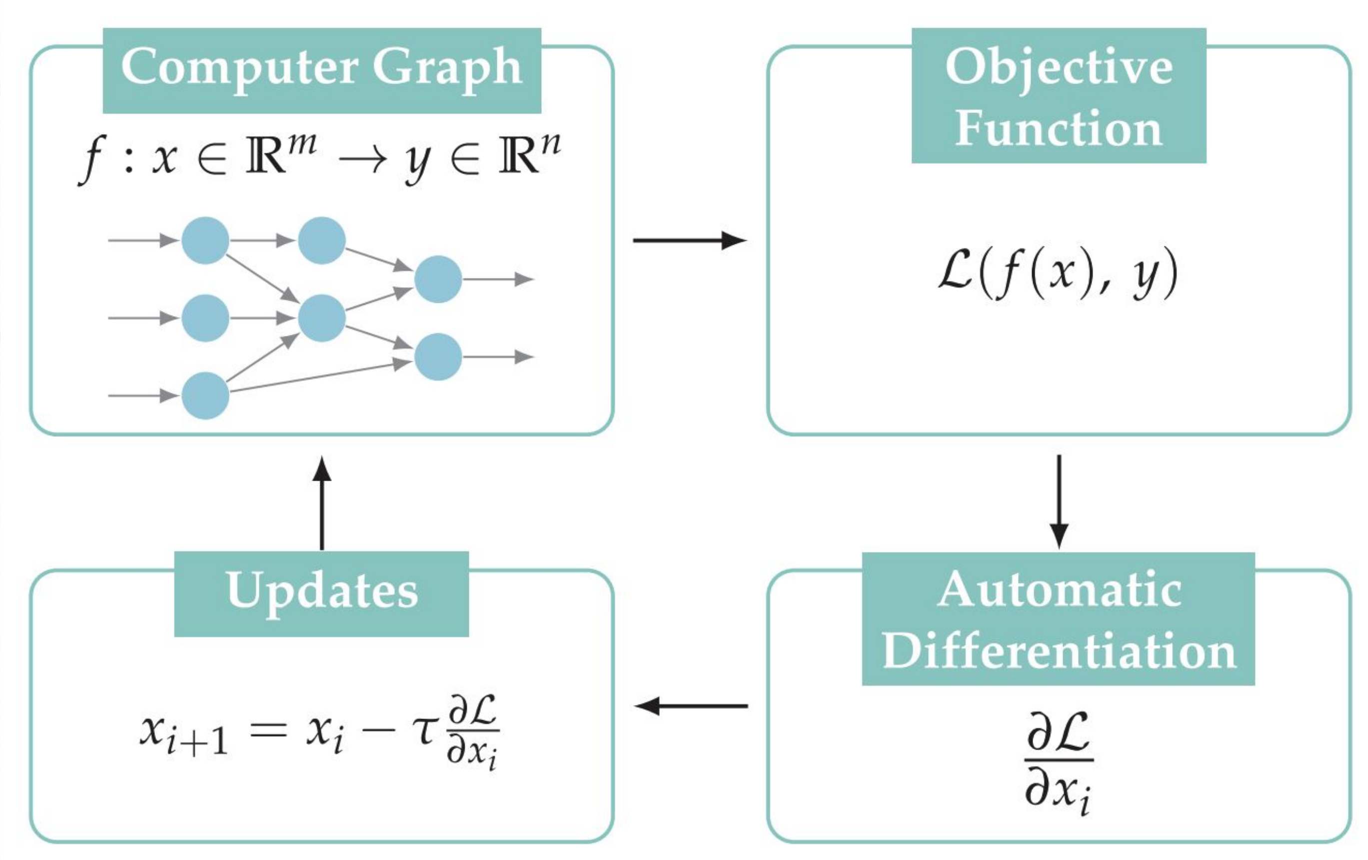
https://github.com/georgestein/ml-in-cosmology

A First Look at creating mock catalogs with machine learning techniques	SVM, kNN	https://arxiv.org/abs/1303.1
Machine Learning Etudes in Astrophysics: Selection Functions for Mock Cluster Catalogs	SVM, GMM	https://arxiv.org/abs/1409.1
PkANN I&2. Non-linear matter power spectrum interpolation through artificial neural networks	NN	https://arxiv.org/abs/1203.1 https://arxiv.org/abs/1312.2
Machine learning and cosmological simulations I.&II.	kNN, DT, RF, EXT	https://arxiv.org/abs/1510.06 https://arxiv.org/abs/1510.07
Estimating Cosmological Parameters from the Dark Matter Distribution	CNN	https://arxiv.org/abs/1711.02
Painting galaxies into dark matter haloes using machine learning	SVR, kNN, MLP, DT, RF, EXT, AdR	https://arxiv.org/abs/1712.03
Modeling the Impact of Baryons on Subhalo Populations with Machine Learning	RF	https://arxiv.org/abs/1712.04
Fast cosmic web simulations with generative adversarial networks	GAN	https://arxiv.org/abs/1801.09
Machine learning cosmological structure formation	RF	https://arxiv.org/abs/1802.04
A Machine Learning Approach to Galaxy-LSS Classification I: Imprints on Halo Merger Trees	SVM	https://arxiv.org/abs/1803.11

Neural Network : Training a Regression Model



More Broadly: Differentiable Programming



Role of (Deep) ML in Simulation-Based Cosmology

1) **Direct Regression/Inference** : Train models on existing simulations and apply directly to data.
   - Models don't know what they aren't trained on… need to know systematics EXACTLY (see BH, Melchior 2022)

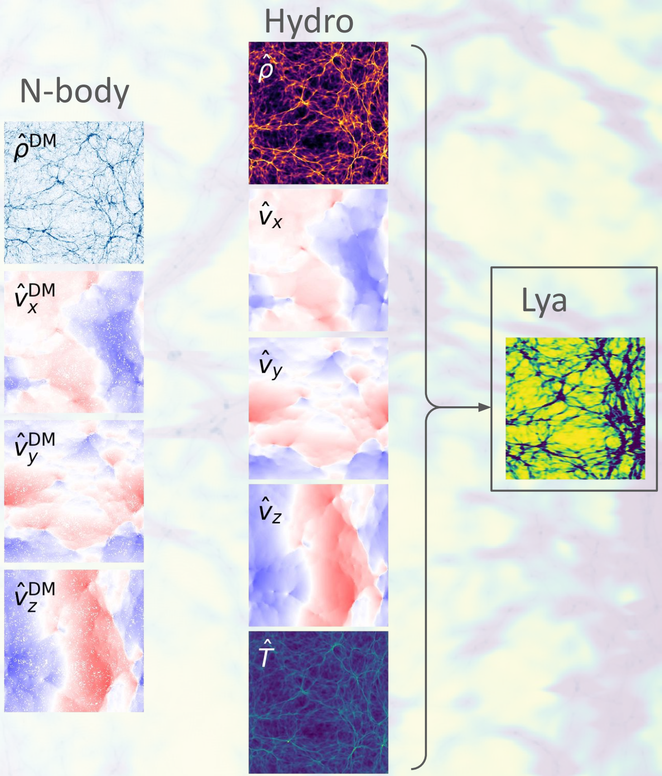
2) **Generation/Surrogate Modelling** : Use ML tools to generate additional simulations to apply "traditional" techniques.

3) **Integrated Approach** : Leverage ML tools within traditional simulations to allow new types of inference.

Surrogate Model Approach

Hydrodynamic reconstruction from N-body simulations

Finding a reliable method to reconstruct hydrodynamic quantities from N-body simulations has been a long-standing research goal



Hydrodynamic reconstruction from N-body simulations

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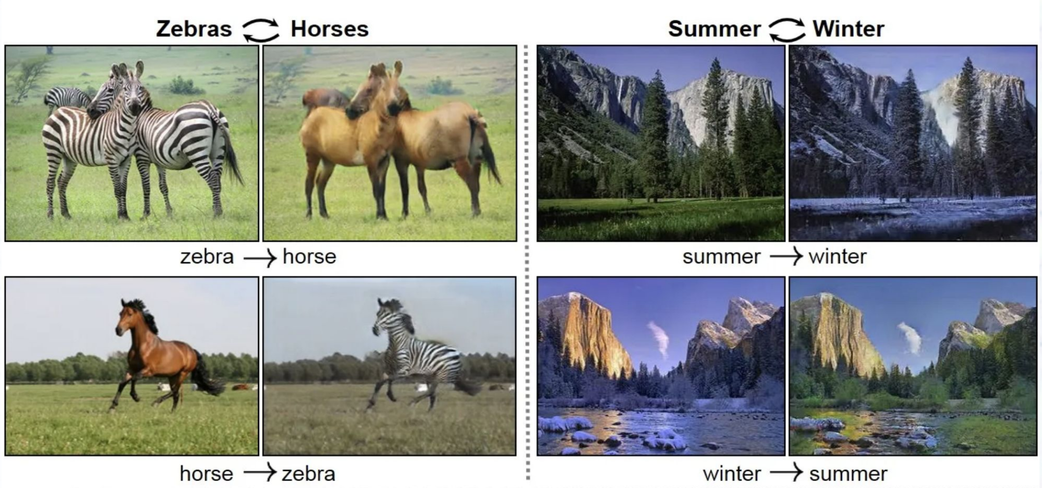
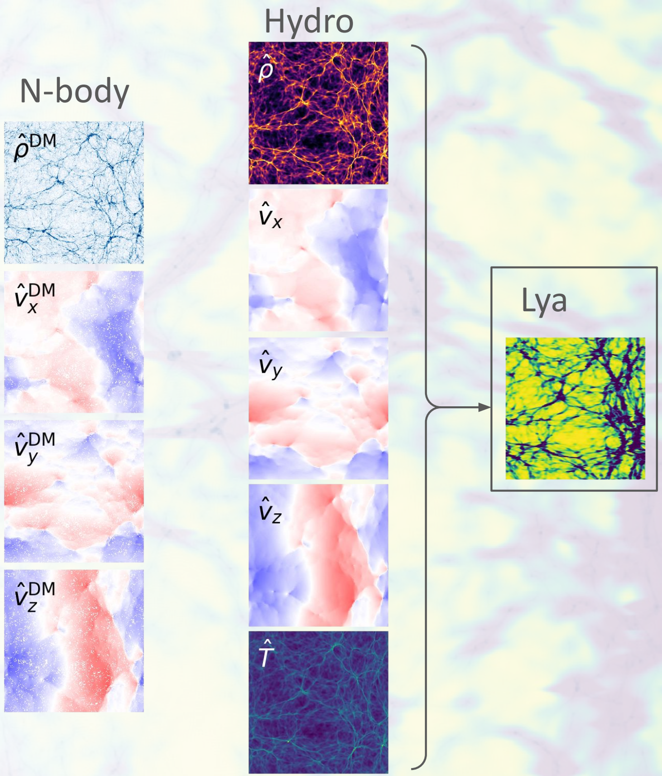
Do it with neural networks of course!
Image translation models are great candidates

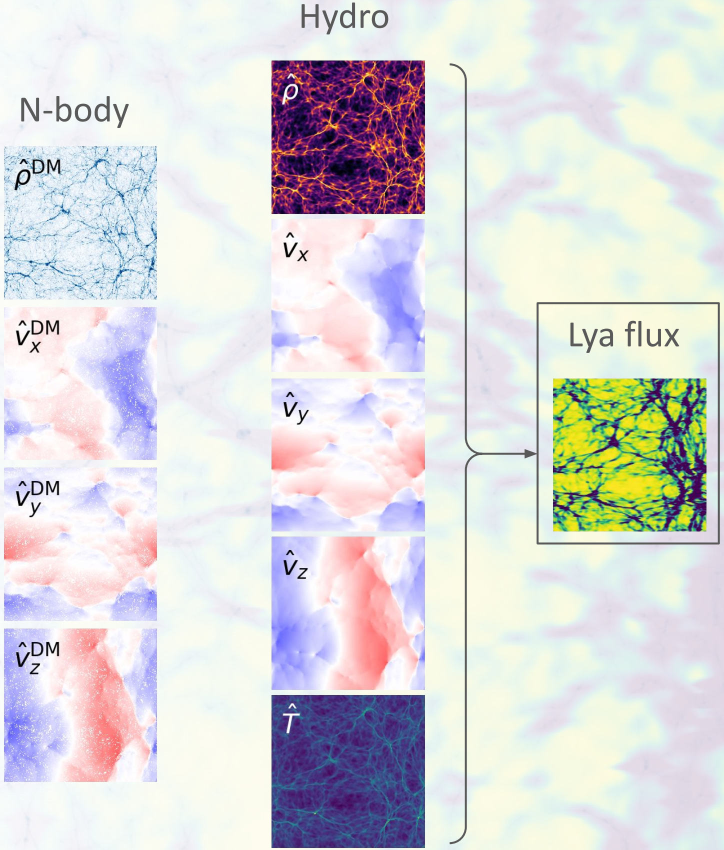




Hydrodynamic reconstruction from N-body simulations

Three approaches:

1. **Adversarial U-Net: deterministic approach**
   Reconstruct hydro fields, focus on accuracy in Lya
   (Harrington ++ BH, 2021)



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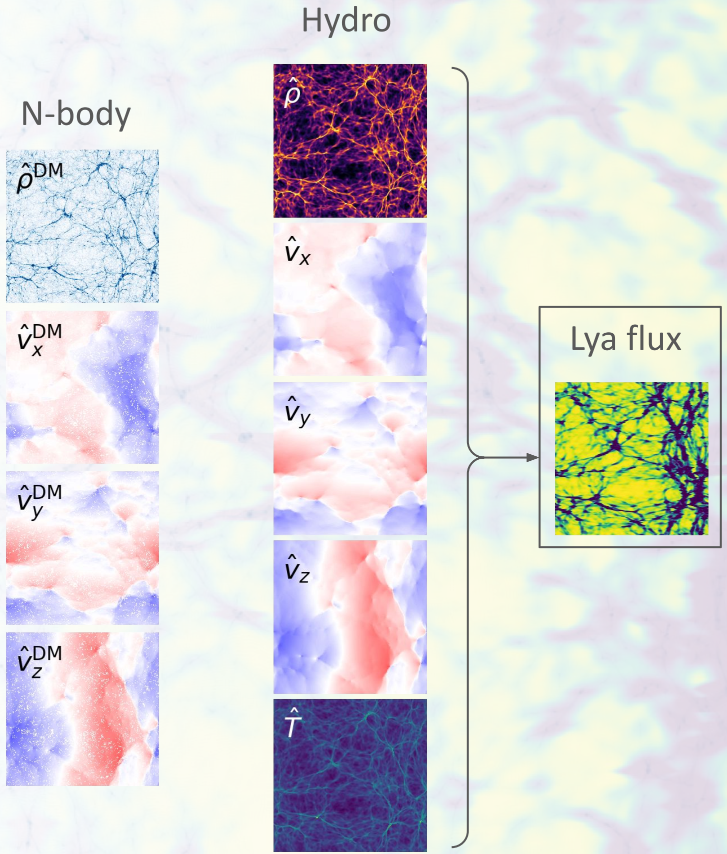
   (BH+ 2022)



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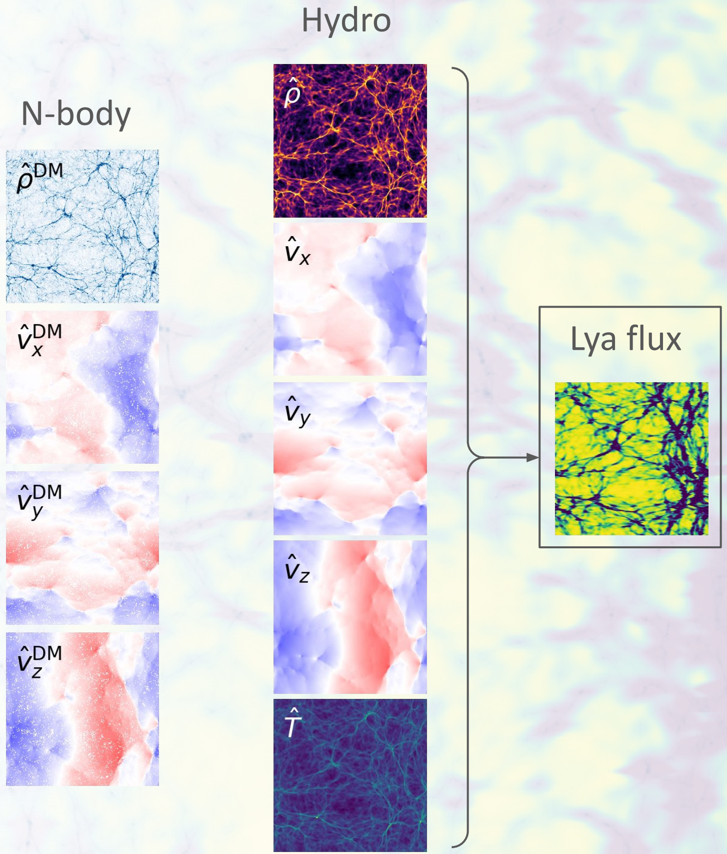
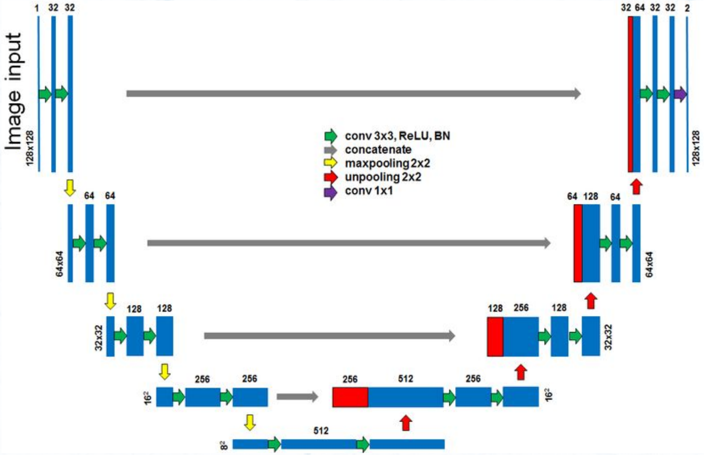
3. **Stochastic Interpolants Model**
   Uncertainty estimation + better reconstruction fidelity
   (BH + 2025)

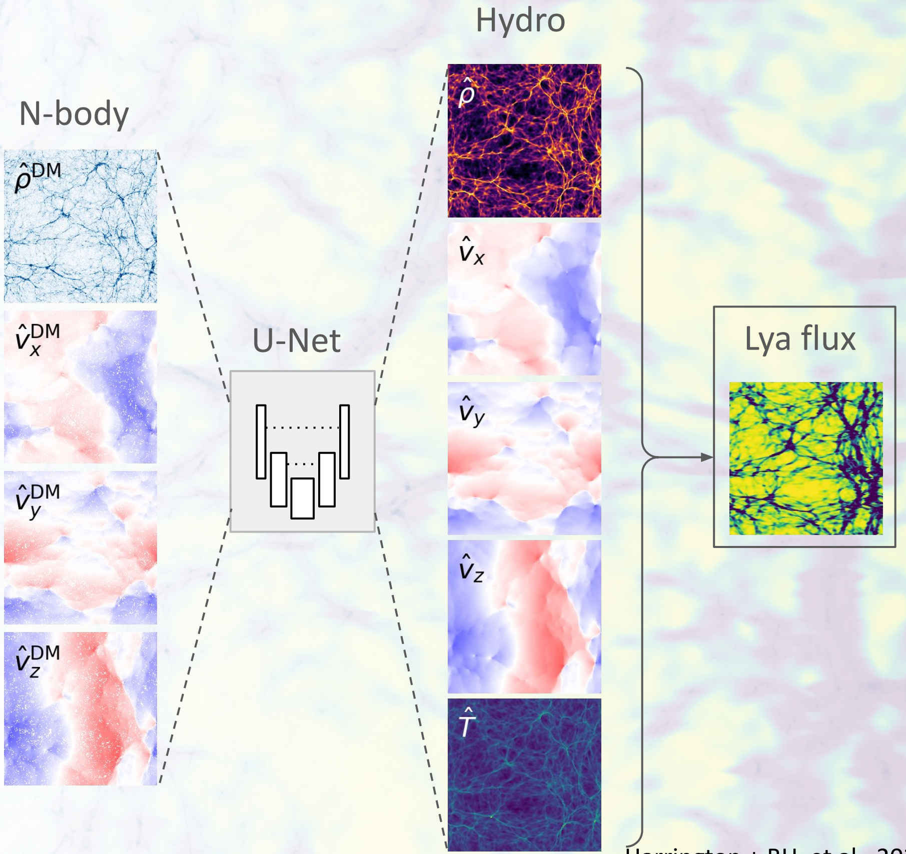


N-body → Hydro

Generative modeling task:
Accurately reproduce Lya flux from N-body simulation

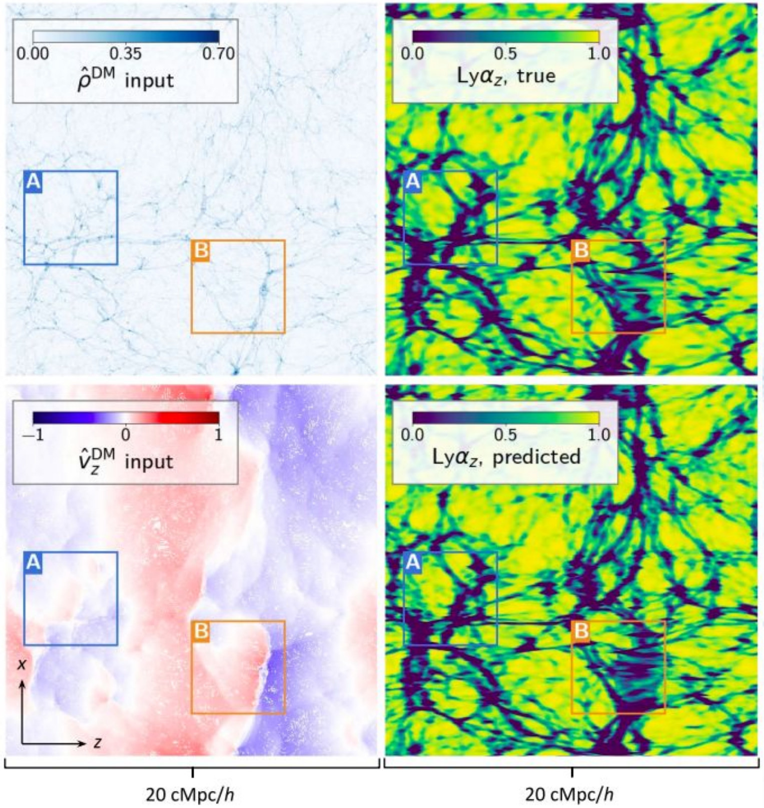
Following pix2pix design, generation of output fields handled by U-Net architecture:





Harrington + BH et al., 2021

N-body → Hydro: Lya reconstructions



Harrington + BH et al., 2021

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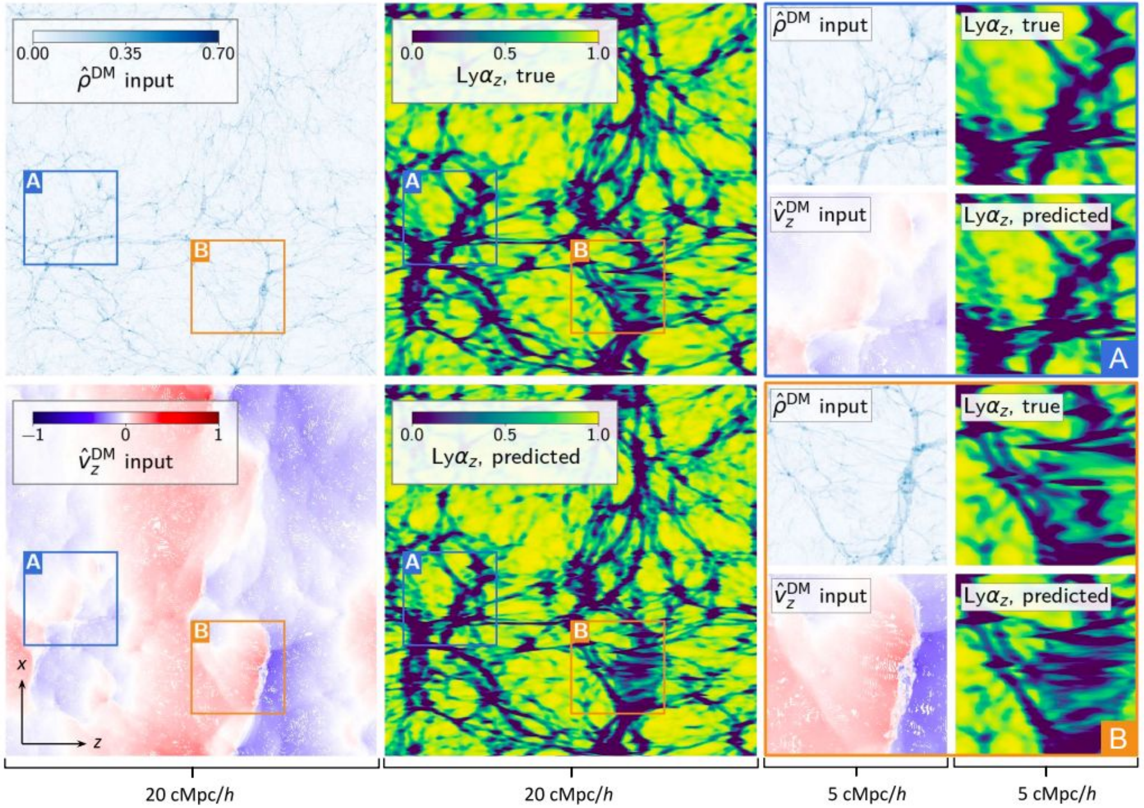
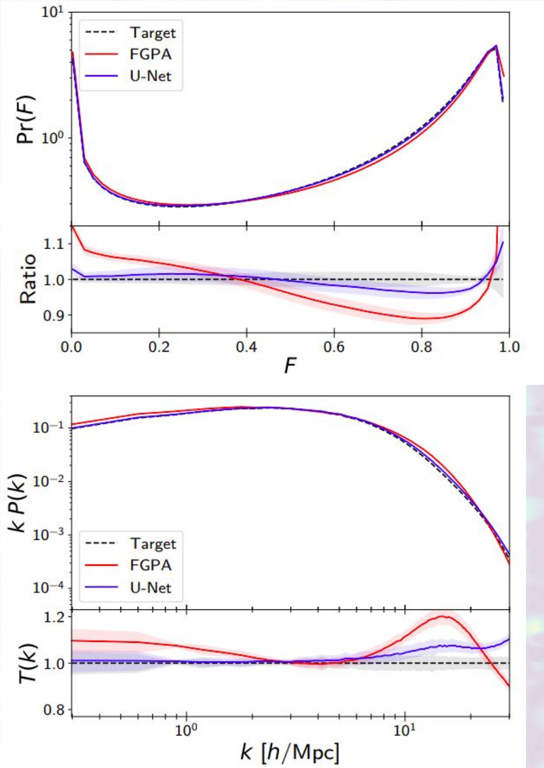


Summary Statistics



Harrington + BH et al., 2021

Extend to Include Uncertainty Estimation: HyPhy

BH et al. (2022)

Can implement latent space implementation in variational auto-encoder or diffusion model approach.

Target Distribution

DM Image in Latent Space

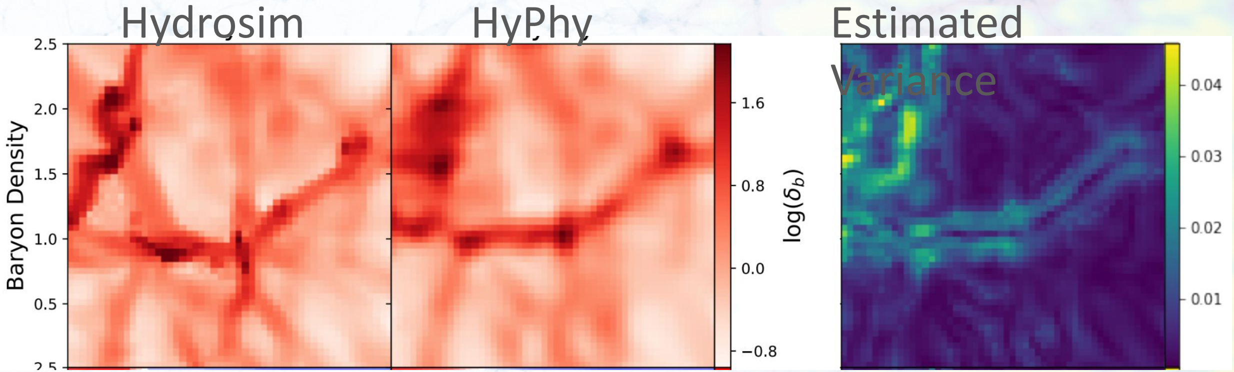
$$\underbrace{p(\tau|\delta)}_{\text{Target Distribution}} = \int \underbrace{p(\tau|z,\delta)}_{\text{Decoder}}\, p(z|\delta)\, dz$$

Hydro

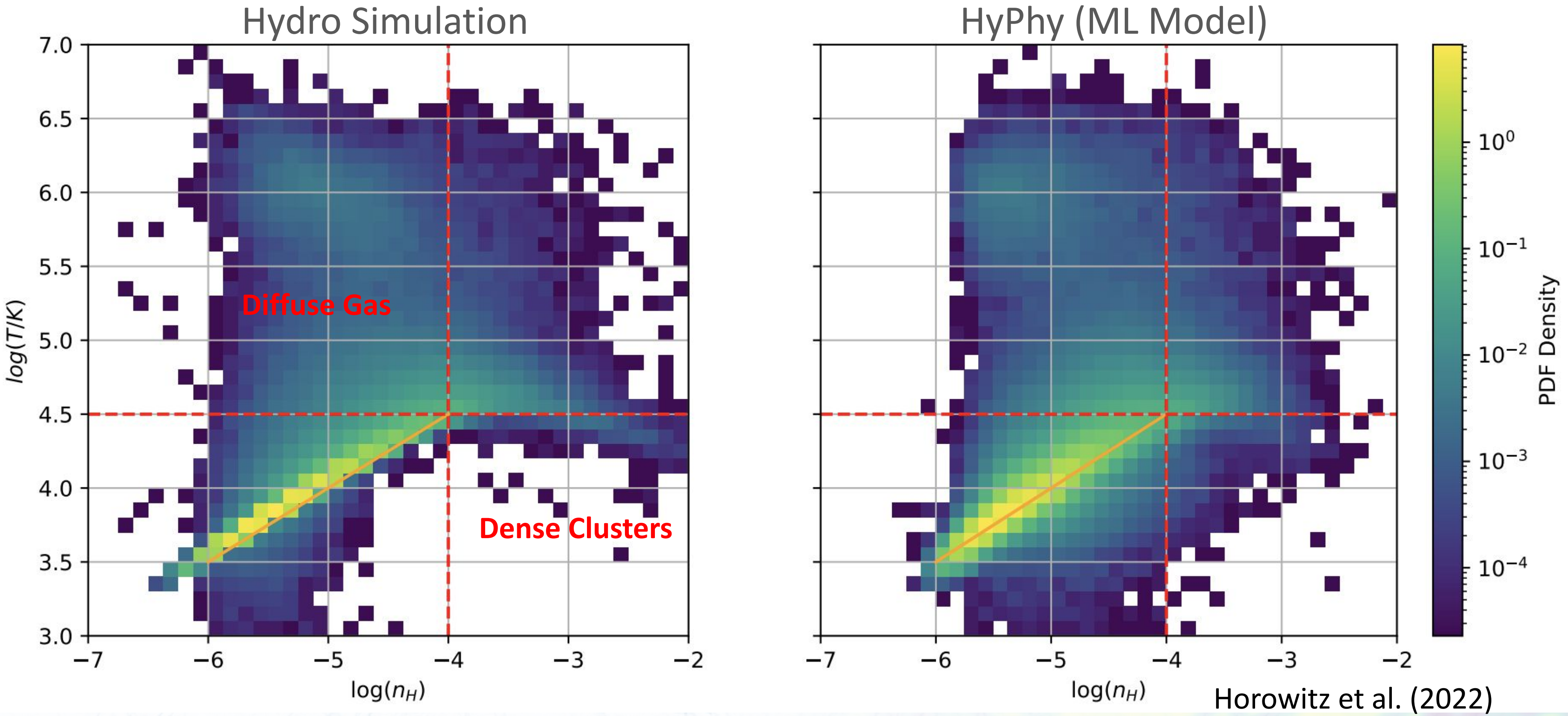
Dark Matter

Decoder

Latent Space Parameter



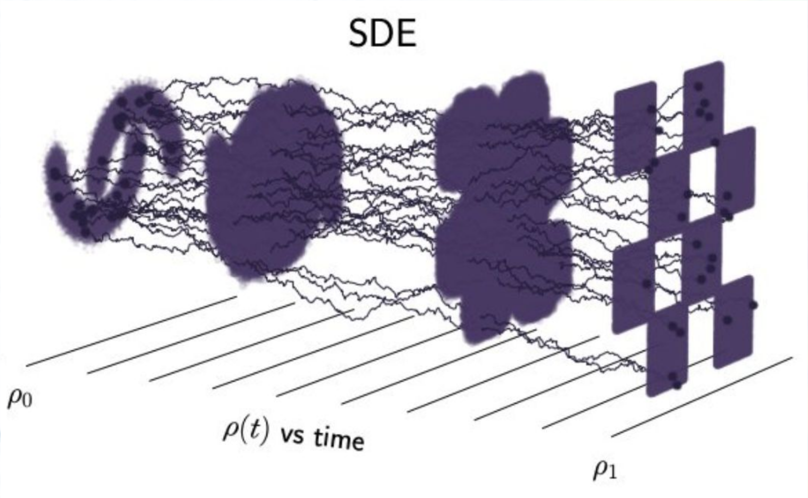
Uncertainty Quantification Allows Diffuse Gas Recon



Horowitz et al. (2022)

The Future: Stochastic Interpolants with Score-Based Diffusion

Learn the solution to a stochastic differential equation mapping from an input to a target distribution.



w/ Omar Yehia (IPMU),
Carolina Cuesta (MIT)

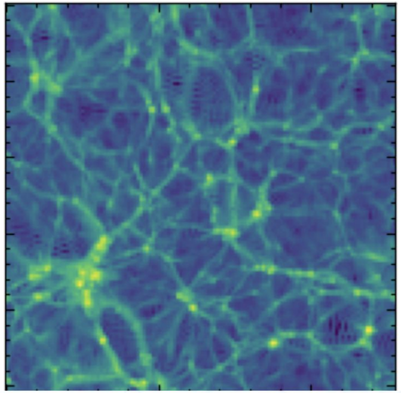
Preliminary

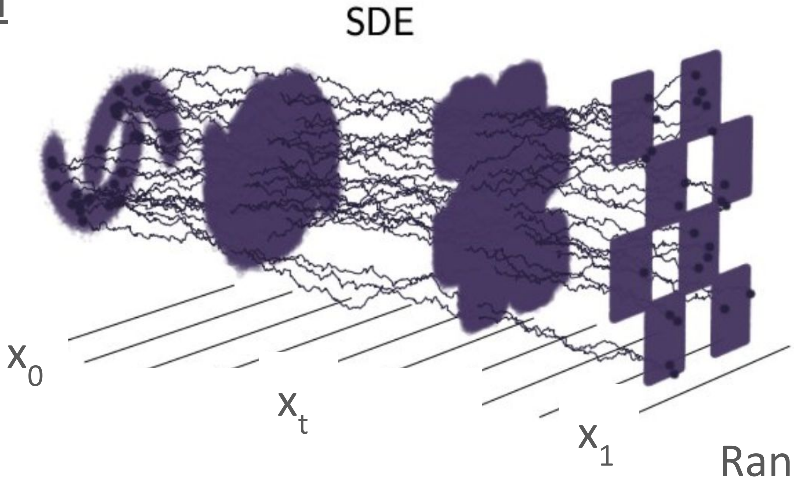
BaryonBridge: Stochastic Interpolants

Learn the solution to a stochastic differential equation mapping from an input to a target distribution.

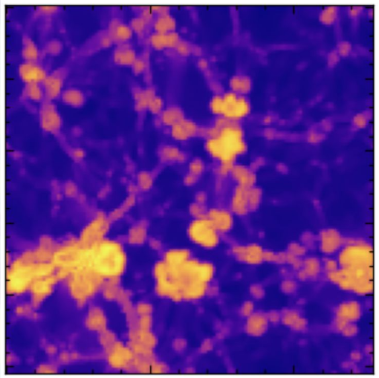
We will map to fully hydrodynamic CAMELS simulations from particle-mesh realizations generated from same ICs. Conditional on cosmological and astrophysical parameters.

Particle-Mesh IC-matched





Gas Temperature



Random/latent variables

$$x_t = (1-t)x_0 + t x_1 + \sqrt{2t(1-t)}z$$

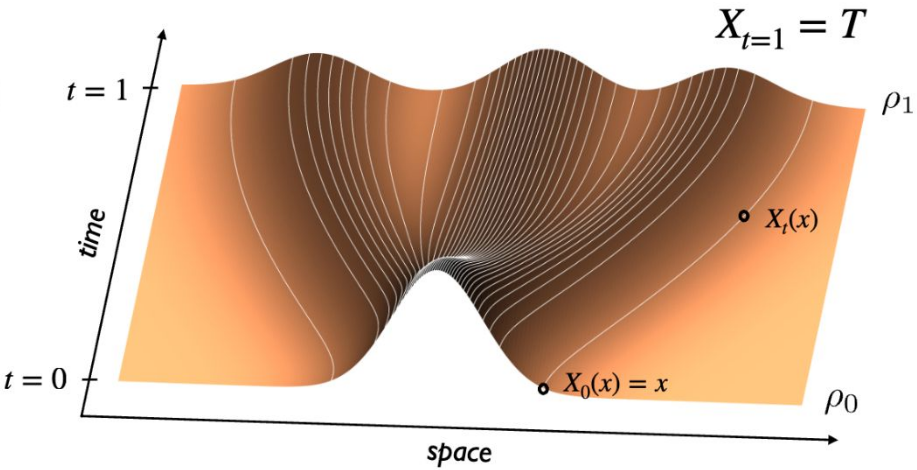
w/ Omar Yehia (IPMU),
Carolina Cuesta (MIT)

Continuous Transport Realizations

X_t flow map given by velocity field $b(t, x)$

$$X_{t=0}(x) = x \in \mathbb{R}^d$$

$$\dot{X}_t(x) = b(t, X_t(x))$$



Transport equation

$$\partial_t \rho(t, x) + \nabla \cdot \big(b(t, x) \rho(t, x) \big) = 0, \quad \rho(t = 0, \cdot) = \rho_0$$

If $\rho(t)$ solves TE, **then** $\rho(t = 1, \cdot) = \rho_1$

Stochastic case generalizes to Fokker-Planck Equation

(Albergo++ 2022, 2023)

Interpolant Function

Interpolant Function $I(t, x_0, x_1)$

- A function of x_0, x_1, and time t with b.c.'s: $I_{t=0} = x_0$ and $I_{t=1} = x_1$
- Example: $I(t, x_0, x_1) = (1 - t)x_0 + tx_1$

If x_0, x_1 drawn independently, then $I(t, x_0, x_1)$ is a **stochastic process which samples** $x_t \sim \rho(t, x)$

$$\rho(t, x) = \mathbb{E}_{\rho_0, \rho_1}\left[\delta\big(x - I(t, x_0, x_1)\big)\right]$$

Interpolant Density

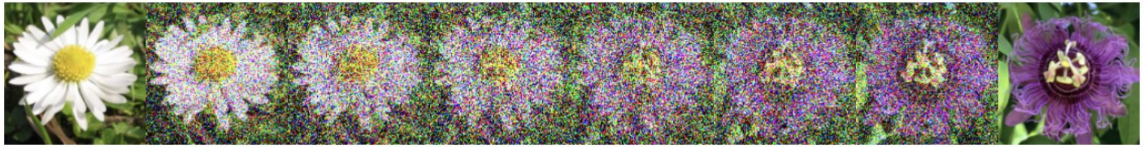
(Albergo++ 2022, 2023)

(Albergo++ 2022, 2023)

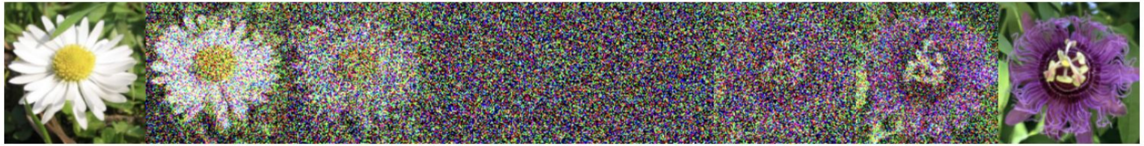
Interpolant Function

Without latent variable $x_t = (1-t)x_0 + tx_1$

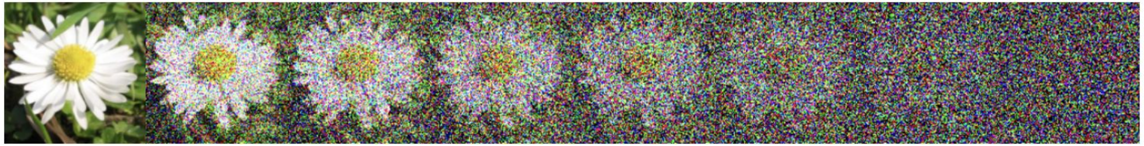
With latent variable $x_t = (1-t)x_0 + tx_1 + \sqrt{2t(1-t)}z$



Gaussian encoding-decoding $x_t = \cos^2(\pi t)(1_{[0,\frac{1}{2})}(t)x_0 + 1_{(\frac{1}{2},1]}(t)x_1) + \sqrt{2t(1-t)}z$



One-sided $x_t = (1-t)x_0 + tz$



Training Interpolant Functions

The PDF $\rho(t, x)$ satisfying the continuity equation has a velocity field $b(t, x)$ which is the minimizer of a simple quadratic objective

$$L[\hat{b}] = \min_{\hat{b}(t,x)} \int_0^1 \mathbb{E}\left[\,|\,\hat{b}(t, x_t) - \partial_t I(t, x_0, x_1)\,|^2\right] dt$$

$$= \left(\,|\,\hat{b}(t, x_t)\,|^2 - 2\partial_t I(t, x_0, x_1) \cdot \hat{b}(t, x_t)\right) dt + \text{const}$$

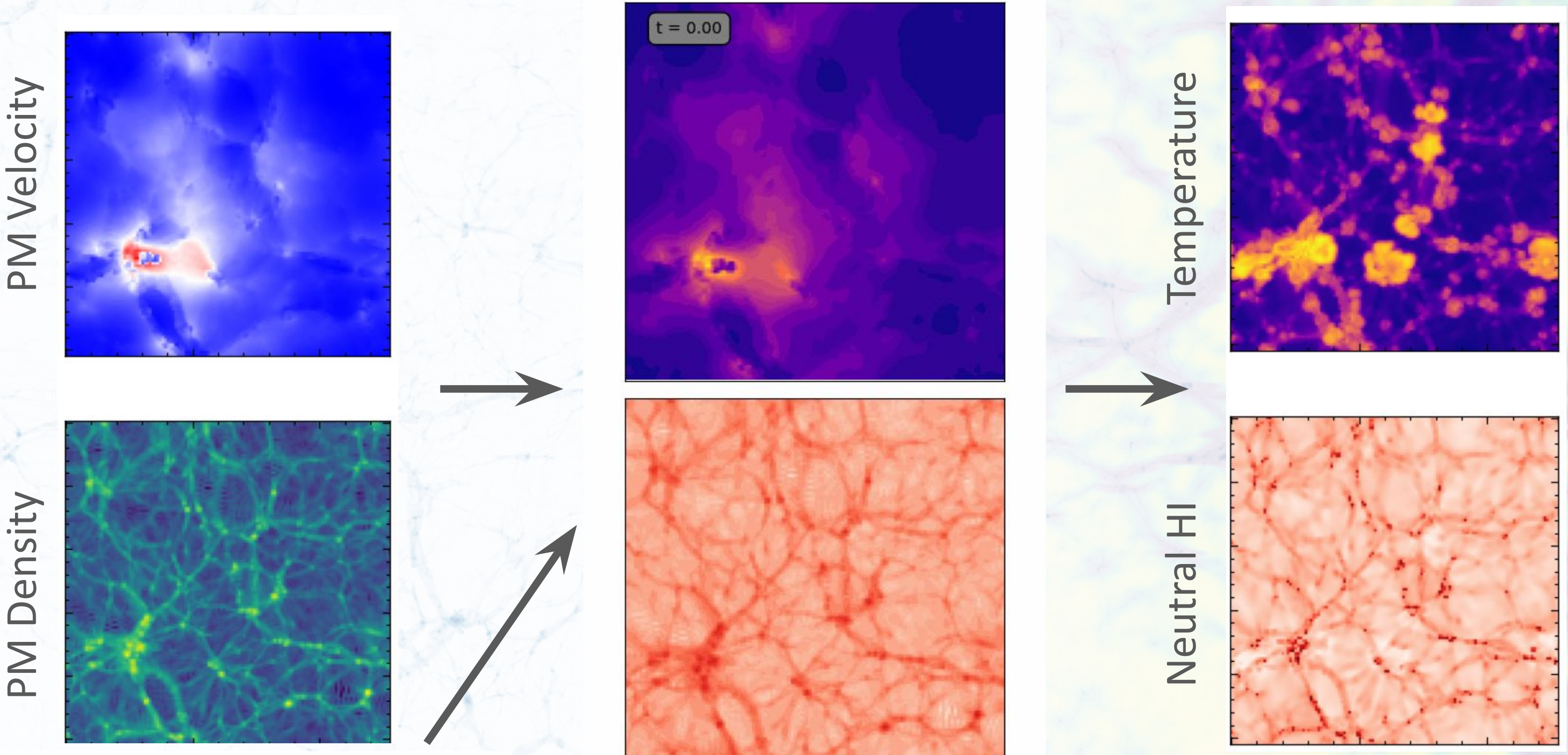
where $x_t = I(t, x_0, x_1)$.

- Loss is directly estimable over ρ_0, ρ_1
- Likelihood and sampling available via fast ODE integrators

(Albergo++ 2022, 2023)

Stochastic Interpolation Model: Conditional with CAMELS sims

Preliminary



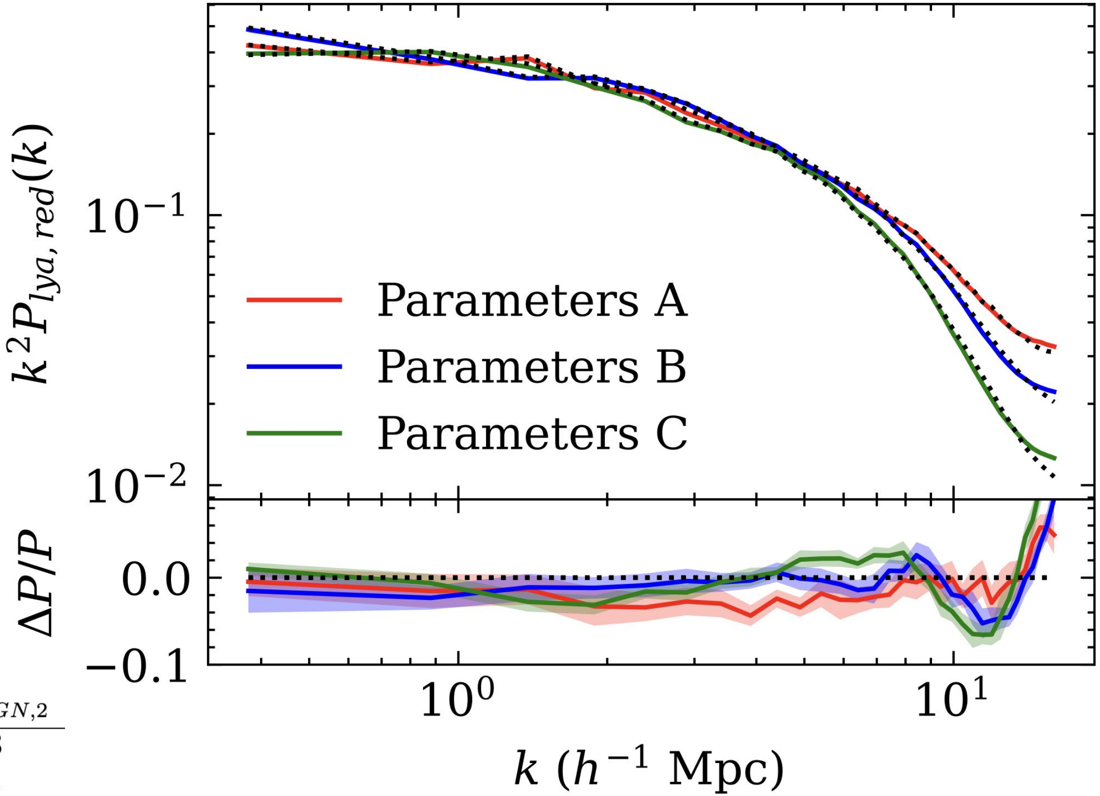
$(\Omega_m, \sigma_8, A_{SN1}, A_{SN2}, A_{AGN1}, A_{AGN2})$

Generalized Across Cosmology/Astrophysics

Preliminary

Map to 3d Lyman Alpha Forest w/ THALAS (Ding, BH, Lukic (2024))

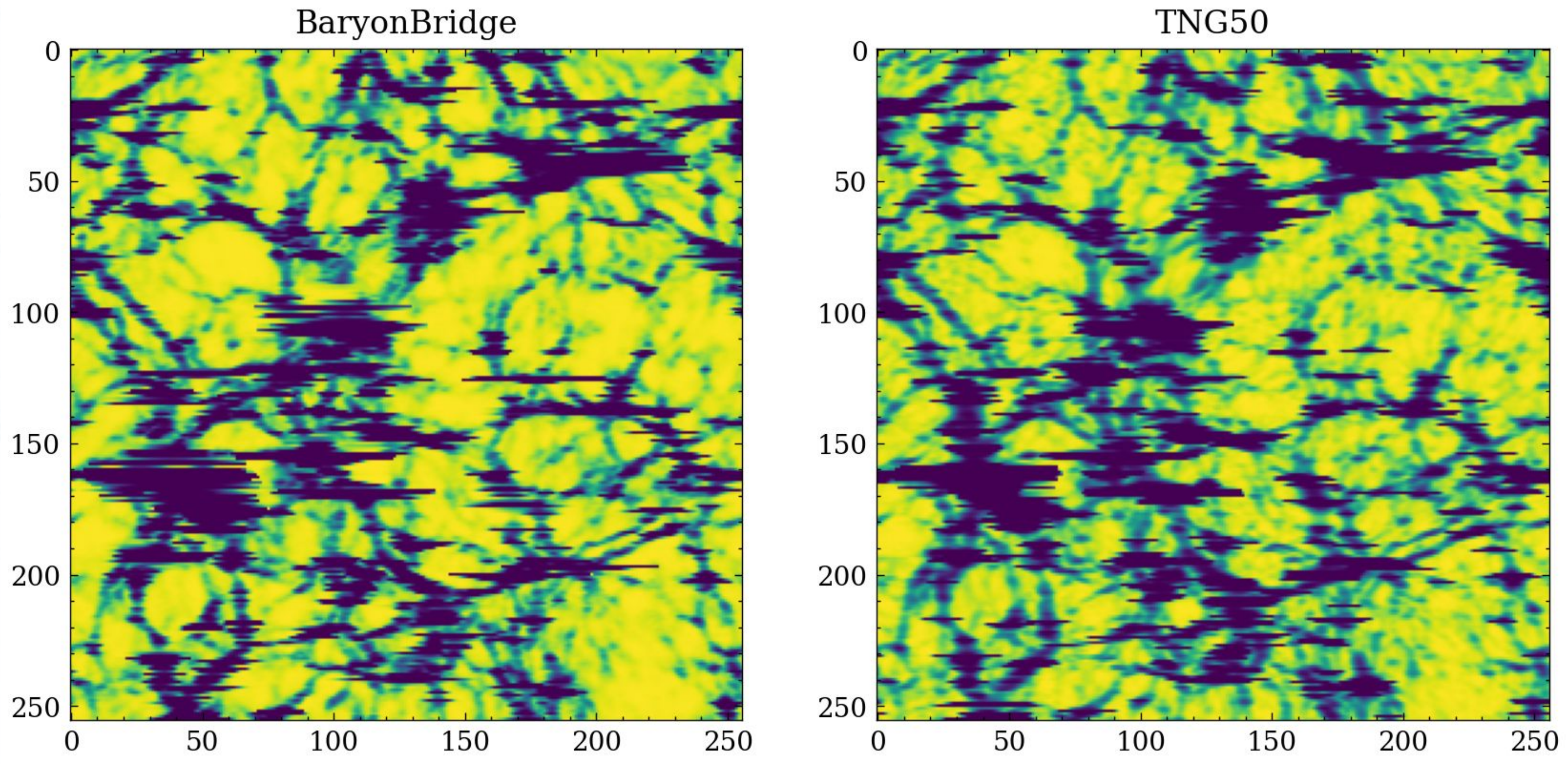
Can also be used for field level inference, since ML model is differentiable…



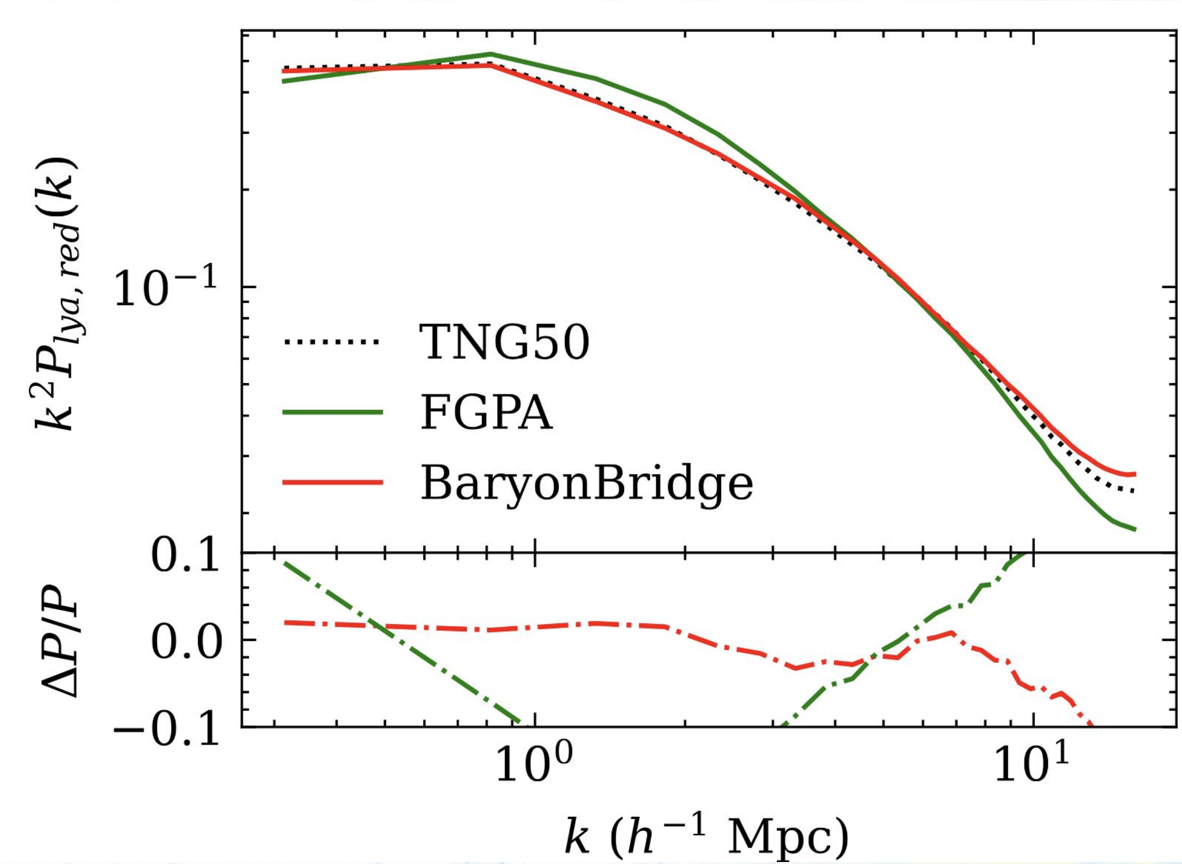
	Ω_m	σ_8	$A_{SN,1}$	$A_{SN,2}$	$A_{AGN,1}$	$A_{AGN,2}$
Parameters A	0.46	0.87	3.81	0.70	1.50	1.78
Parameters B	0.22	0.79	0.82	0.27	0.55	1.11
Parameters C	0.14	0.68	2.34	2.83	0.79	0.54

Applied to Arbitrarily Large Volumes : CAMELS -> TNG50

Preliminary



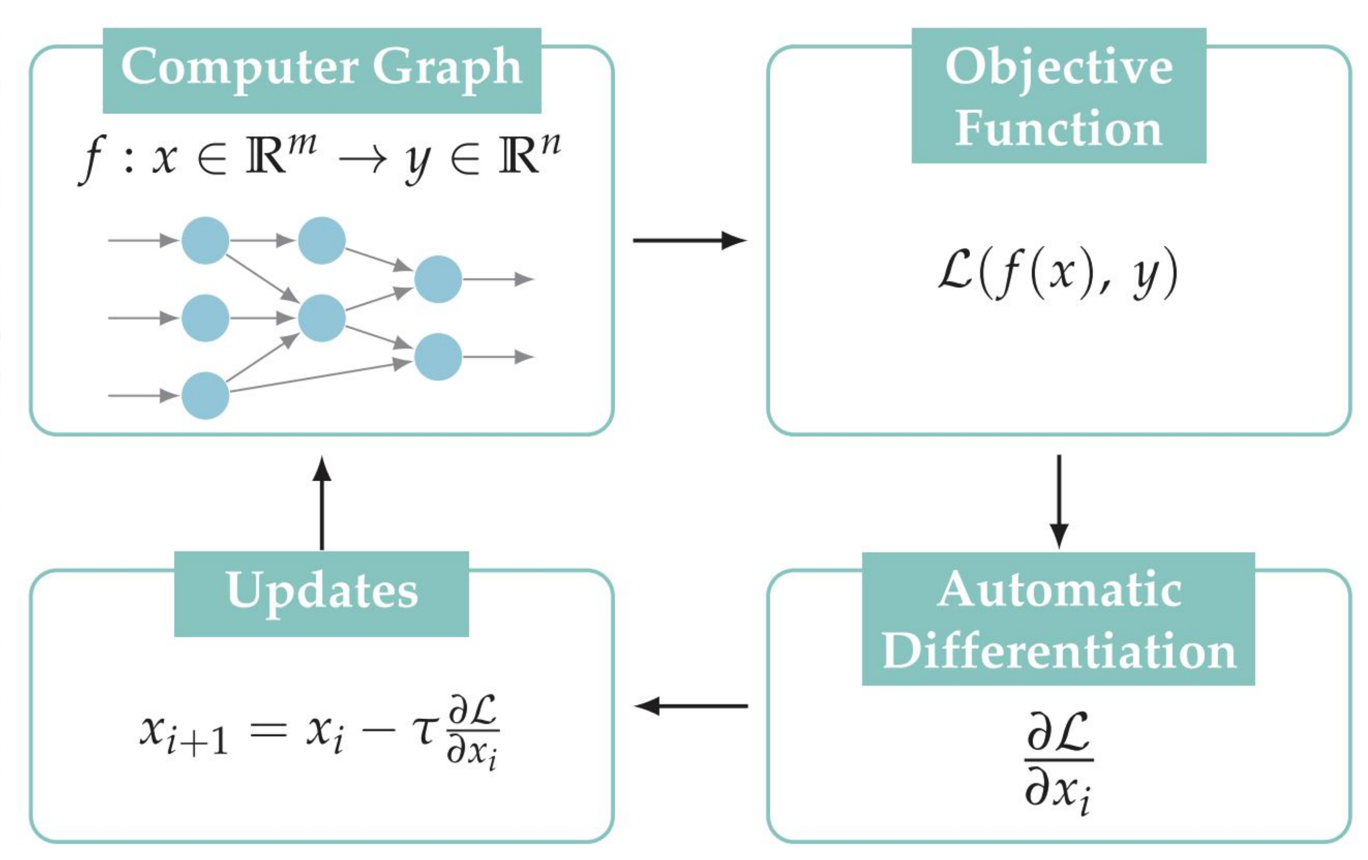
Power Spectrum on TNG50 (large separate hydrosim)



Field Level Inference
w/ Differentiable Programming

Differentiable Programming

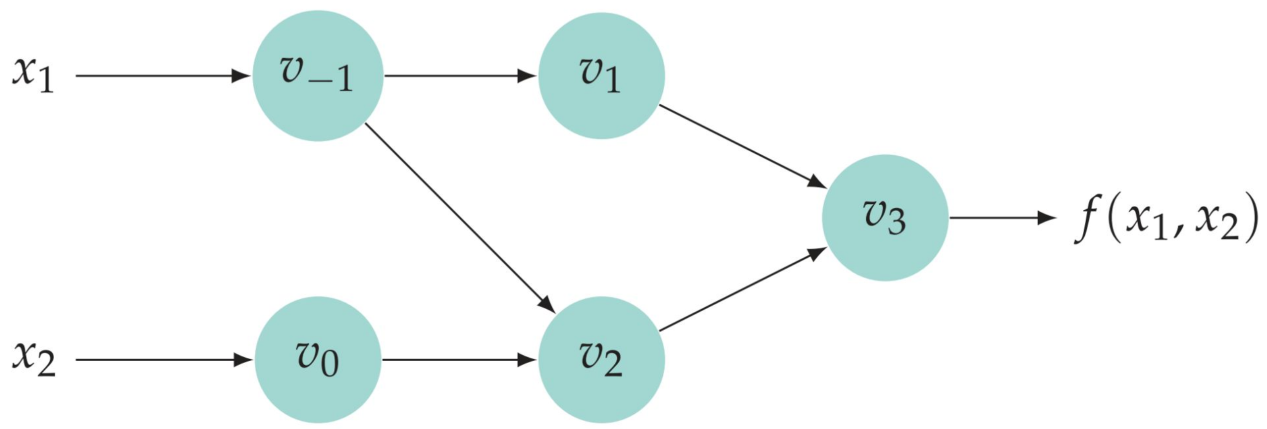
Chen et al. (2023)



Automatic Differentiation

Chen et al. (2023)

Computational graph for simple function: $y = f(x_1, x_2) = \sin(x_1) + x_1 x_2$



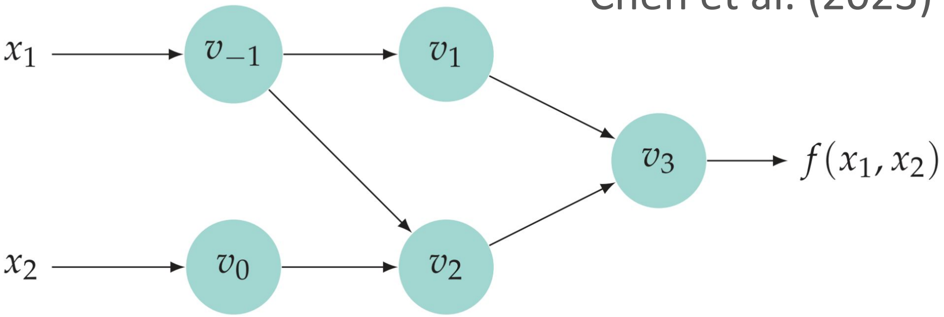
Forward primal trace

v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 1$
v_1	$= \sin v_{-1}$	$= \sin 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 1$
v_3	$= v_1 + v_2$	$= 0.909 + 2$
y	$= v_3$	$= 2.909$

Automatic Differentiation

$$f(x_1,x_2) = \sin(x_1)+x_1x_2$$

Chen et al. (2023)



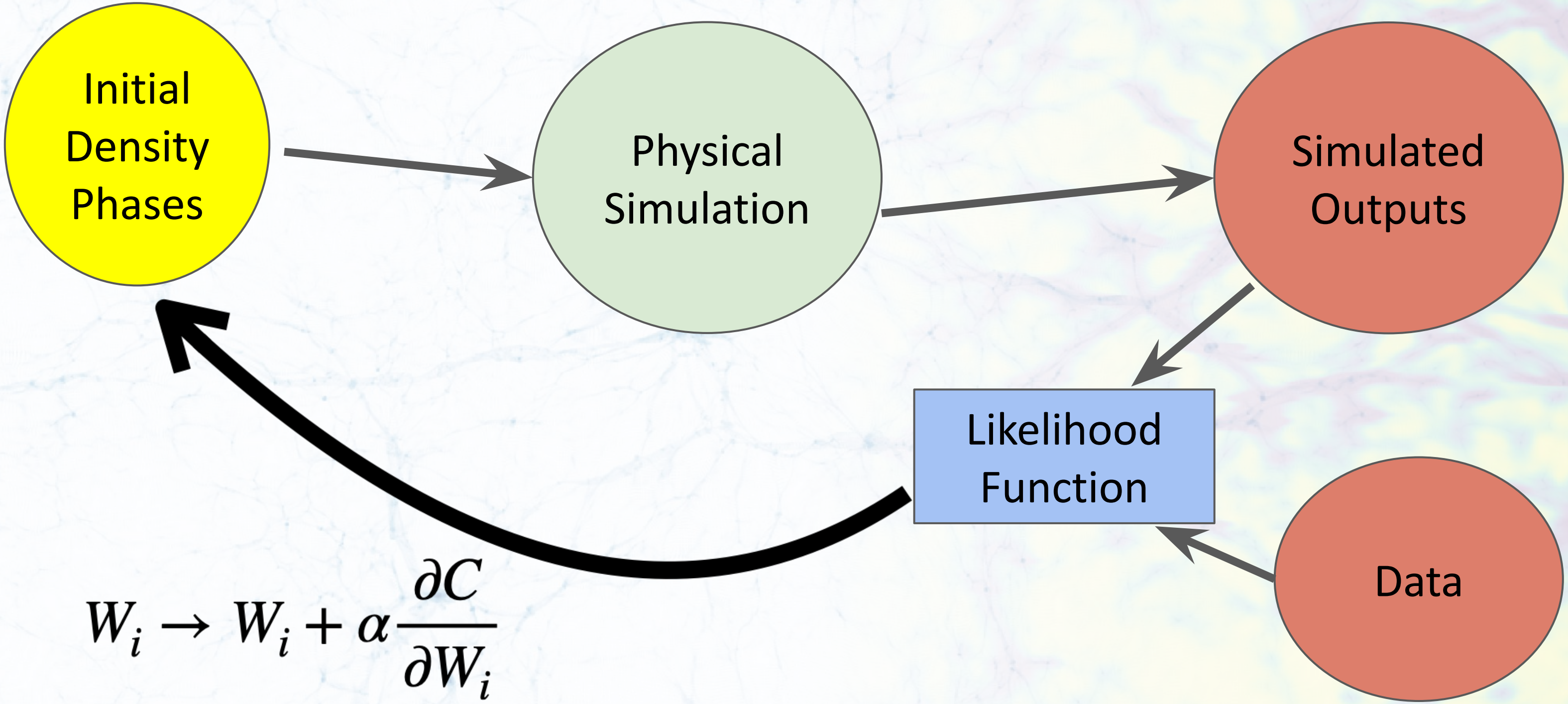
Forward primal trace

$$\begin{aligned}
v_{-1} &= x_1 &&= 2 \\
v_0 &= x_2 &&= 1 \\
\hline
v_1 &= \sin v_{-1} &&= \sin 2 \\
v_2 &= v_{-1} \times v_0 &&= 2 \times 1 \\
v_3 &= v_1 + v_2 &&= 0.909 + 2 \\
\hline
y &= v_3 &&= 2.909
\end{aligned}$$

Reverse derivative trace

$$\begin{aligned}
\boldsymbol{\bar{x}_1} &= \boldsymbol{\bar{v}_{-1}} && && = \mathbf{0.584} \\
\boldsymbol{\bar{x}_2} &= \boldsymbol{\bar{v}_0} && && = \mathbf{2} \\
\hline
\bar{v}_{-1} &= \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}} + \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}} &&= \bar{v}_1 \cos(v_{-1}) + \bar{v}_0 &&= 0.584 \\
\bar{v}_0 &= \bar{v}_2 \frac{\partial v_2}{\partial v_0} &&= \bar{v}_2 v_{-1} &&= 2 \\
\bar{v}_1 &= \bar{v}_3 \frac{\partial v_3}{\partial v_1} &&= \bar{v}_3 \times 1 &&= 1 \\
\bar{v}_2 &= \bar{v}_3 \frac{\partial v_3}{\partial v_2} &&= \bar{v}_3 \times 1 &&= 1 \\
\hline
\bar{v}_3 &= \bar{y} &&= 1
\end{aligned}$$

Differentiable Cosmological Simulations



$$W_i \rightarrow W_i + \alpha \frac{\partial C}{\partial W_i}$$

Update Phases/Parameters

Differentiable Dark Matter Evolution

Small industry has developed for differentiable particle mesh codes:

code	OSS	gradient	mem efficient	hardware	
BORG		analytic		CPU	(Jasche & Wandelt 2013)
ELUCID		analytic		CPU	(Wang et al. 2014, …)
`FastPM-vmad`	✓	AD		CPU	(Feng et al. 2016, …)
`FlowPM`	✓	AD		GPU/CPU	(Modi et al. 2020)
pmwd	✓	adjoint	✓	GPU/CPU	(Li et al. 2022)

Particle Mesh codes are lots of linear operations (including fast fourier transforms), so straightforward to differentiate.

From Li et al. (2022)

Differentiable Particle Mesh Dark Matter

```python
import tensorflow as tf
import numpy as np
import flowpm

cosmo = flowpm.cosmology.Planck15()
stages = np.linspace(0.1, 1.0, 10, endpoint=True)

initial_conditions = flowpm.linear_field(32,          # size of the cube
                                         100,         # Physical size of the cube
                                         ipklin,      # Initial power spectrum
                                         batch_size=16)


# Sample particles
state = flowpm.lpt_init(cosmo, initial_conditions, a0=0.1)

# Evolve particles down to z=0
final_state = flowpm.nbody(cosmo, state, stages, 32)

# Retrieve final density field
final_field = flowpm.cic_paint(tf.zeros_like(initial_conditions), final_state[0])
```

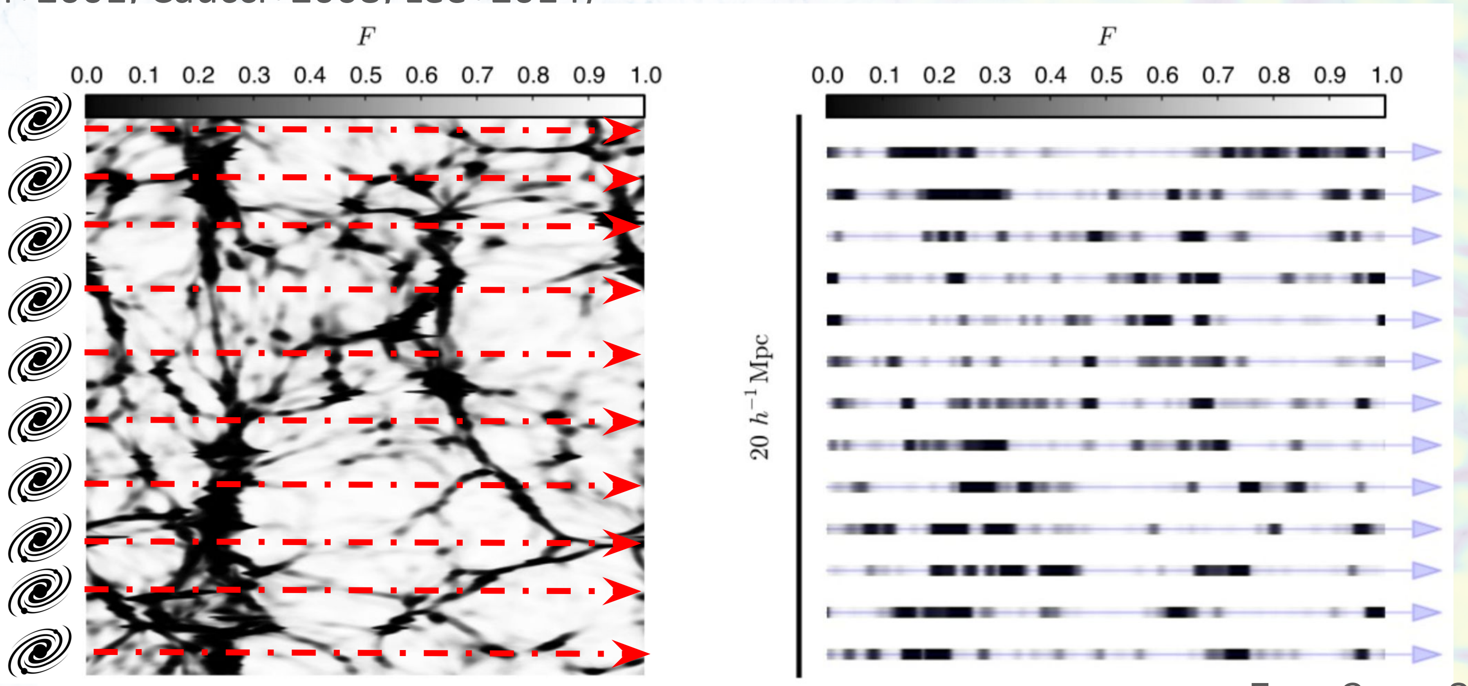
https://github.com/modichirag/flowpm

Modi et al. (2020)

Lyman Alpha Tomography: Unique Probe of z~2 Universe

Basic Idea: Observe lots of lines of sight in small area and then interpolate/extrapolate between absorptions on various of lines of sight.

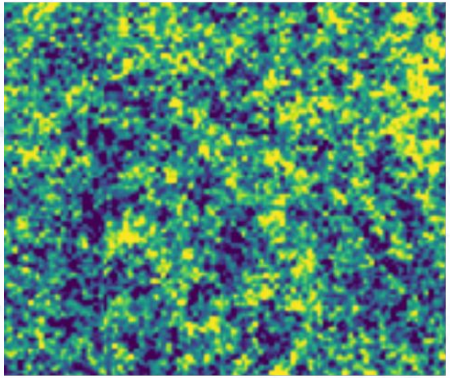
(Pichon+2001, Caucci+2008, Lee+2014)

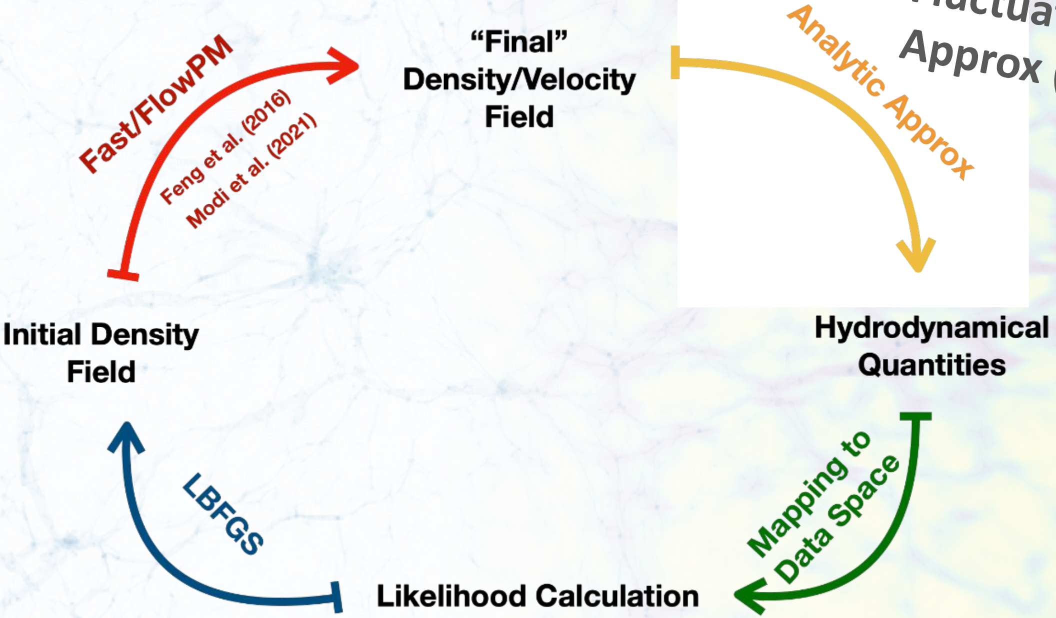


From Casey Stark

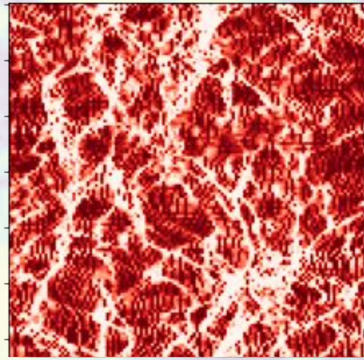
Tomographic Absorption Density Inference Scheme (TARDIS)

Forward modeling approach to reconstruct the initial density field given the observed Lyman alpha forest.





Fluctuating Gunn-Peterson Approx (exp mapping)

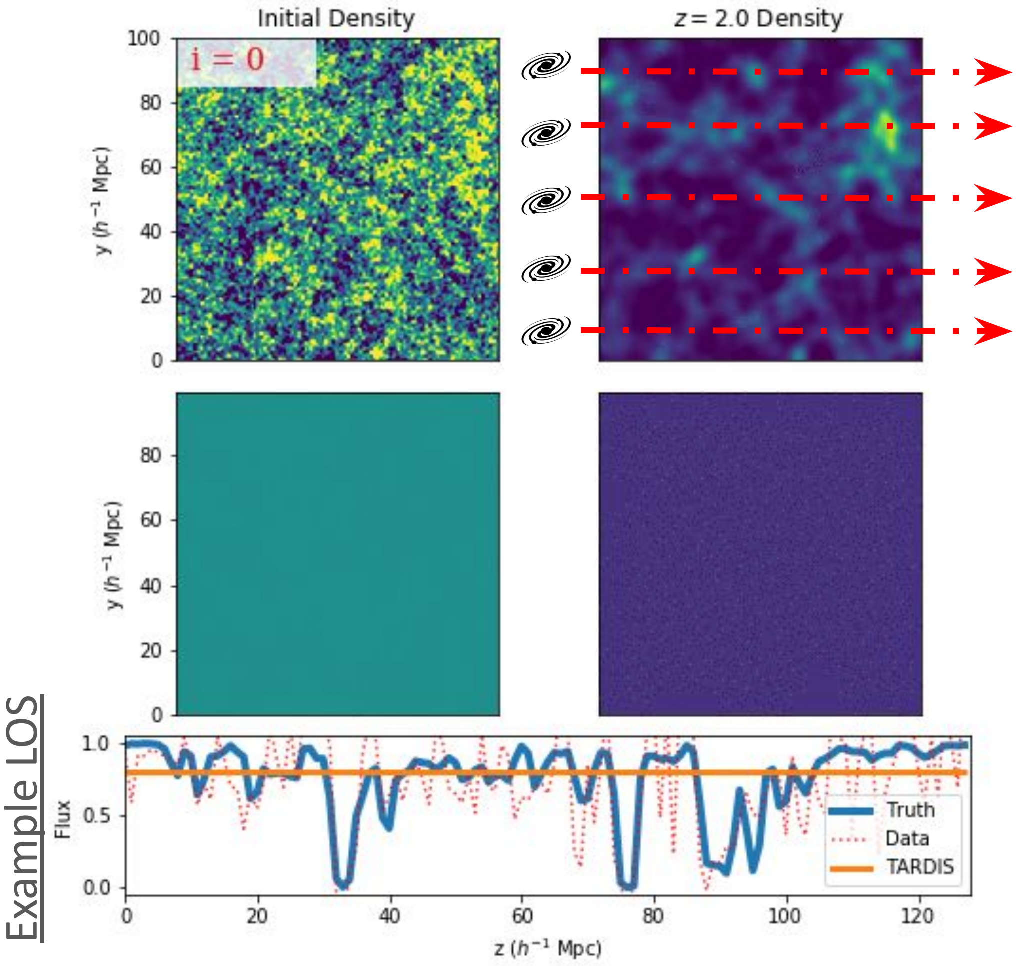


Neutral Hydrogen

$$\mathcal{L}_{\mathrm{Ly}\alpha}(\delta_i|\delta_{\mathrm{Ly}\alpha,\mathrm{obs}}) = \sum_n \frac{(\delta_{\mathrm{Ly}\alpha,obs}(n) - \delta_{\delta_{\mathrm{Ly}\alpha,rec}}(n))^2}{\sigma_{obs}(n)^2}$$

BH et al. (2019, 2020)

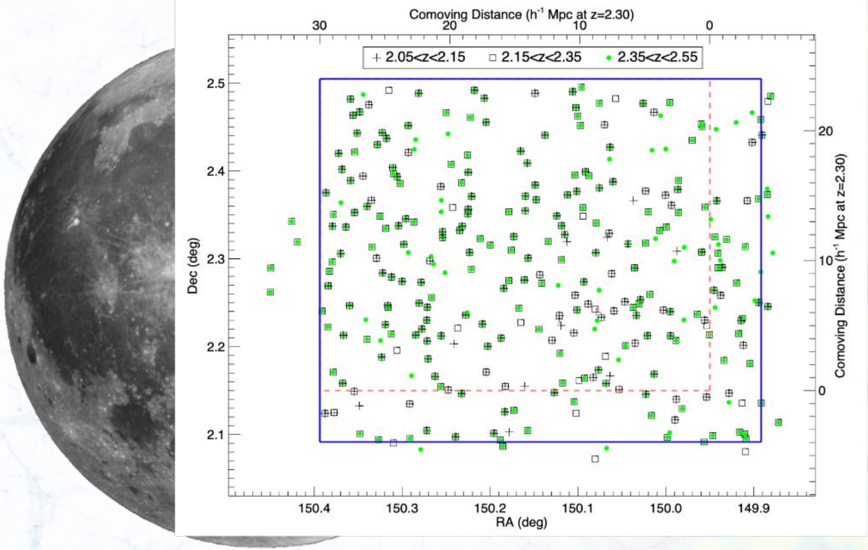
Data to Initial Conditions



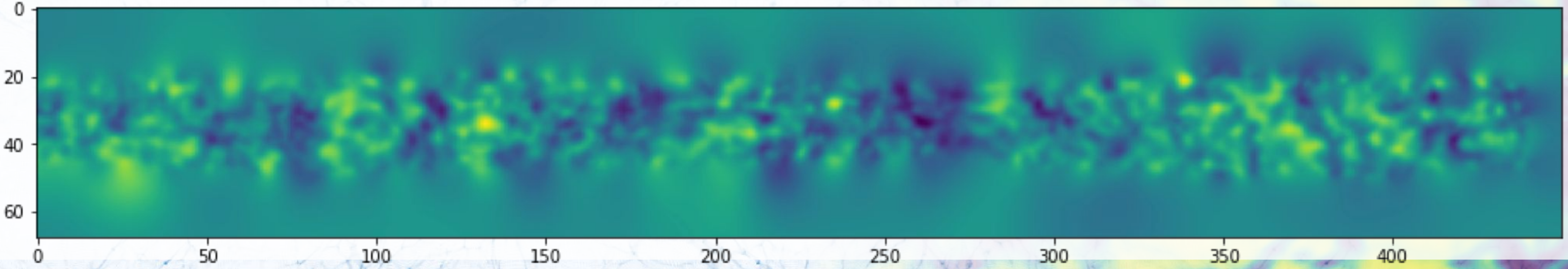
BH et al. (2019, 2020)

BH et al. (2023)

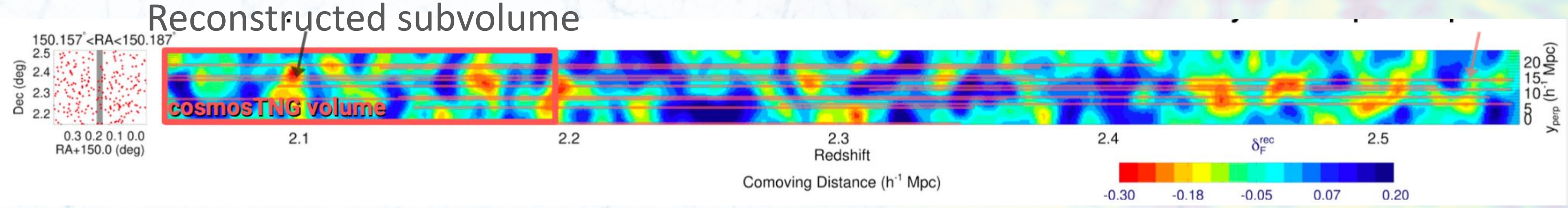
Applied to Data: COSMOS Field



Initial Gaussian Field



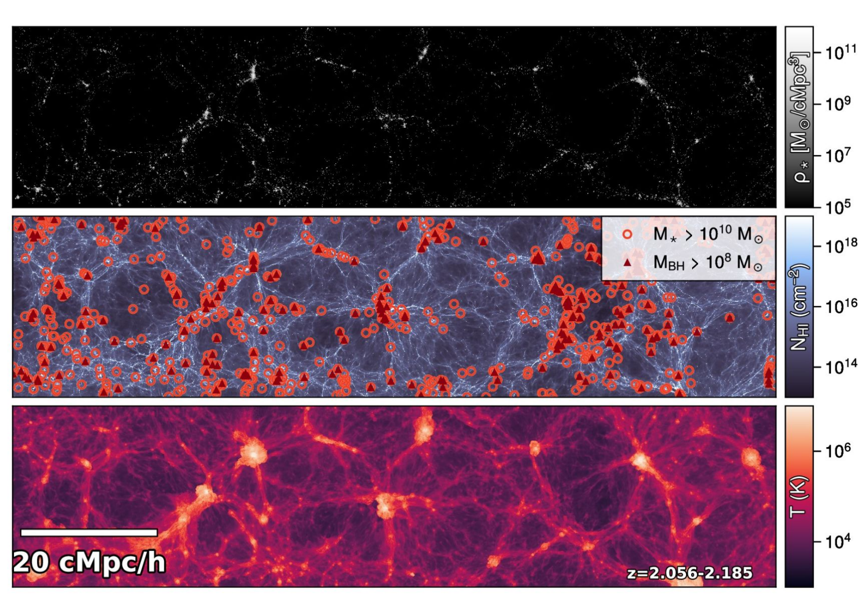
Run Illustris With Same Initial Conditions: cosmosTNG



Design a constrained simulation in the COSMOS field at z~2 using the AREPO code + TNG galaxy formation model

Good qualitative match between field level observations and constrained hydrosim run

Lots of limitations, particularly in centers of massive clusters… **Can we plug in AREPO/TNG to TARDIS?**



Byrohl ++ BH (2024)

Fully Differentiable Hydrodynamics

Fully Differentiable Hydrodynamical Simulations

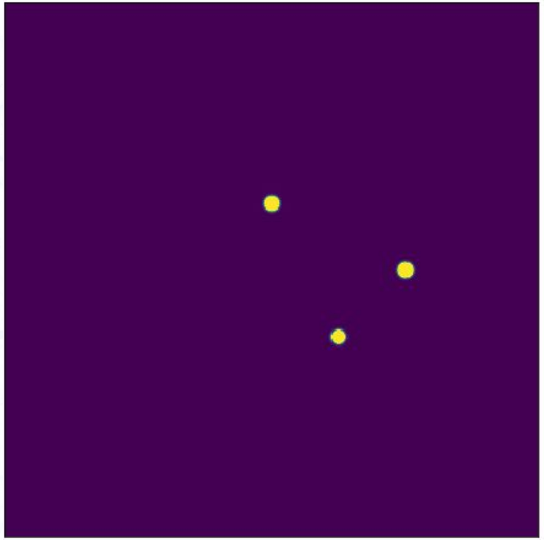
Toy Example: Taylor–von Neumann–Sedov blast waves in 2D

<u>Euler Eq.</u>

$$\frac{D\rho}{Dt} = -\rho\nabla\cdot\mathbf{u}$$

$$\frac{D\mathbf{u}}{Dt} = -\frac{\nabla p}{\rho} + \mathbf{g}$$

$$\frac{De}{Dt} = -\frac{p}{\rho}\nabla\cdot\mathbf{u}$$



No gravity, constant medium

2nd order TVD scheme

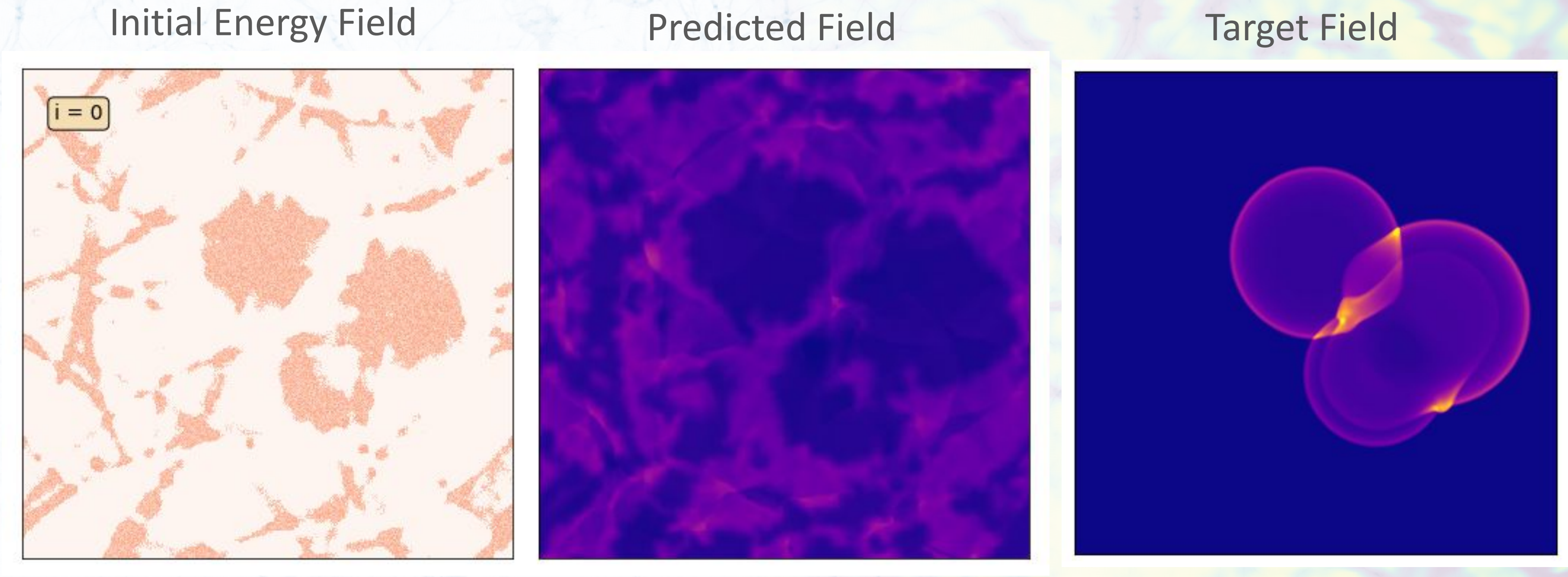
Based on fortran code from Trac & Pen (2003)

- In some cases can just import a different library to get automatic differentiability (i.e. JAX vs numpy).
- Care needed for full hydro-sims for memory reasons; can't save all states!
  - Adjoint method: Pontryagin (1962), McNamara et al. (2004), Li et al. (2022)

BH + Lukic (2025)

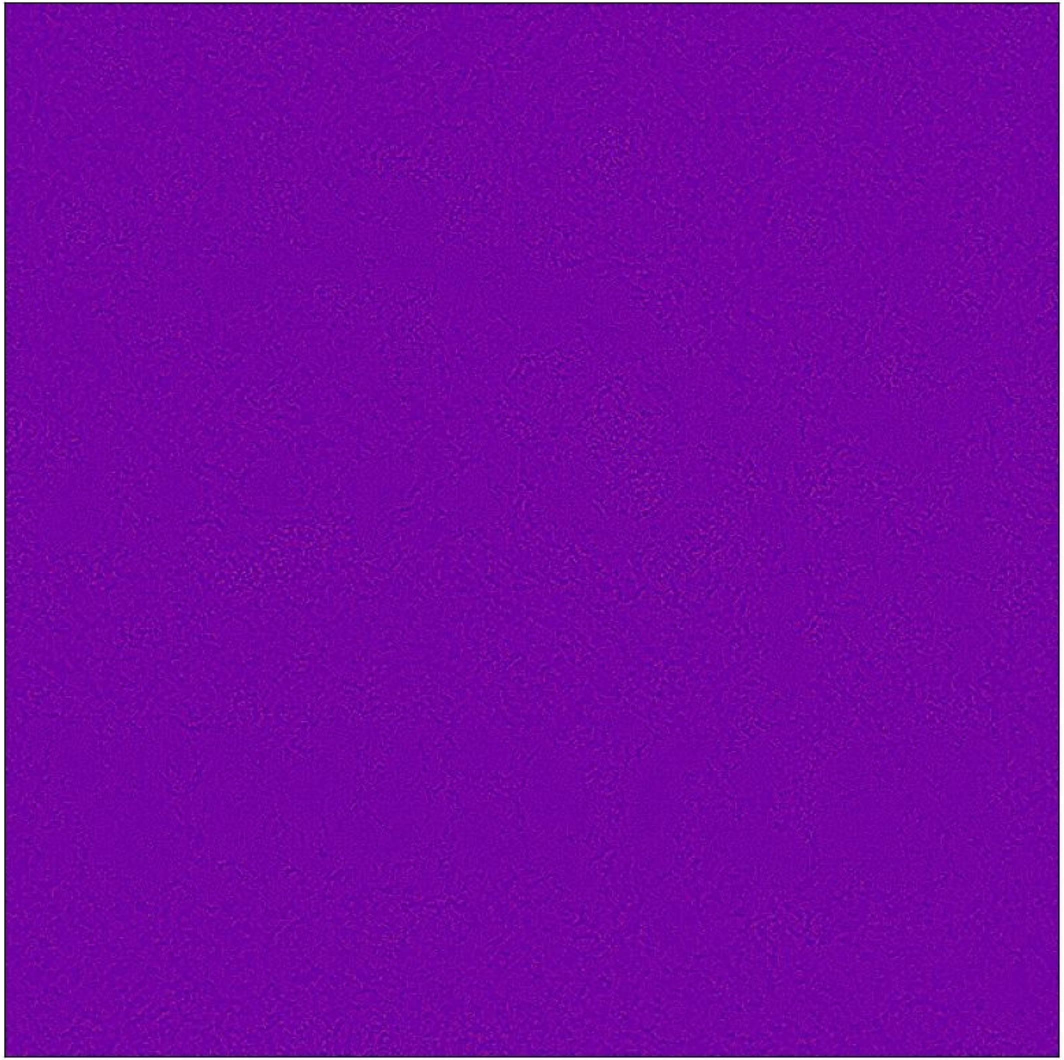
The Future? Fully Differentiable Hydrodynamical Simulations

Toy Example: Taylor–von Neumann–Sedov blast wave in 2D Optimization!

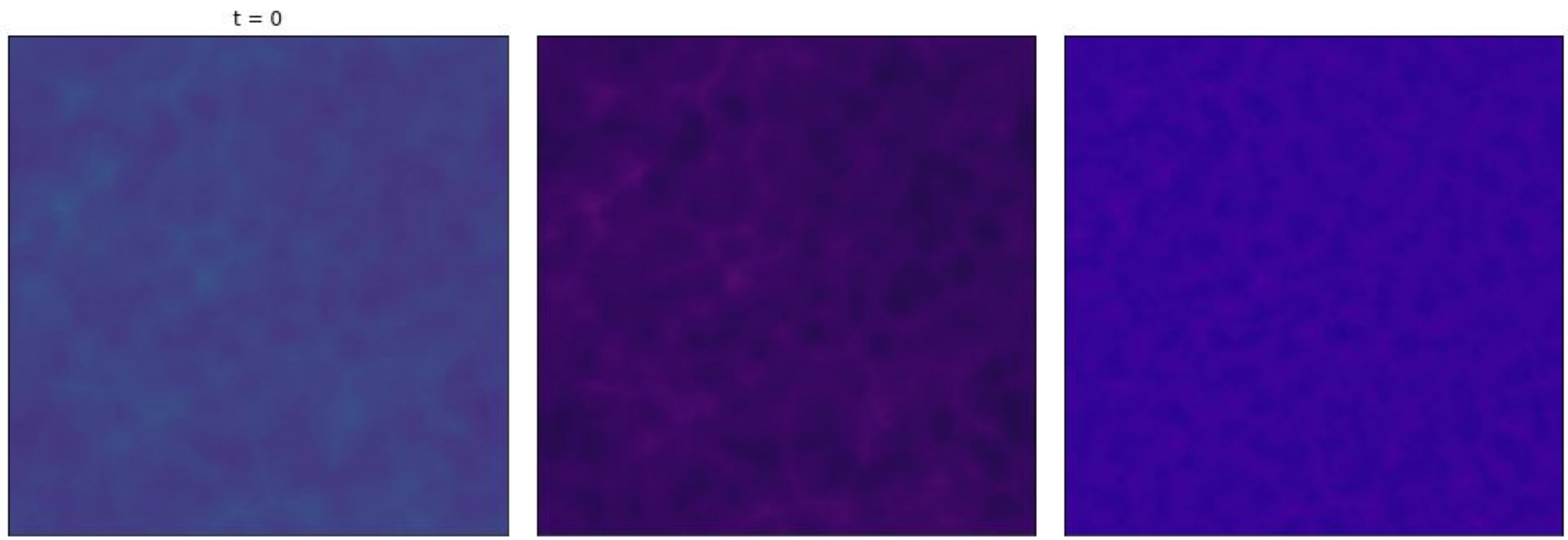


BH + Lukic (2025)

800x800 resolution
on 4 gpus (V100)



Couple Dark Matter to Hydro Gravitationally



Dark Matter Gas Density IE (Temp)

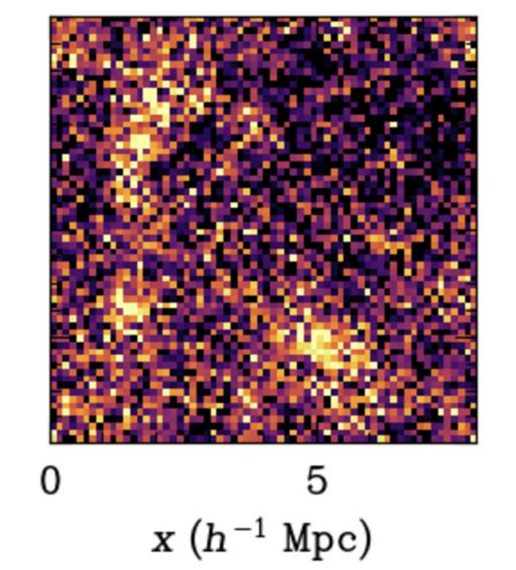
BH + Lukic (2025)

Field Level Inference through Hydrosims

Mock observable inspired by thermal SZ: Noisy 3d map of thermal pressure

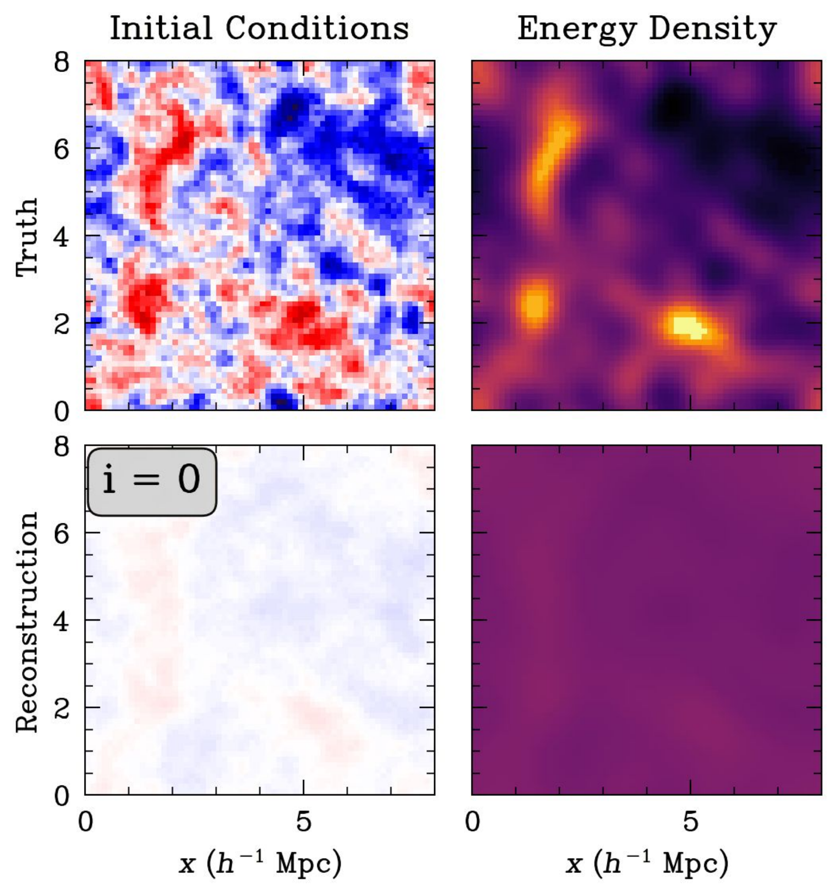
64^3 box, 8 h^{-1} Mpc, evolved till z=2.98 (240 timesteps of hydrosim)

Mock Data Slice

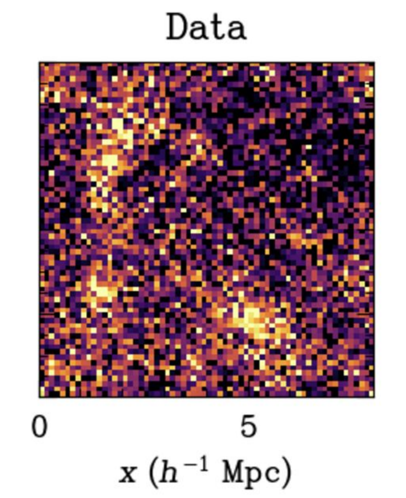


BH + Lukic (2025)

Field Level Inference : Baryons + Dark Matter

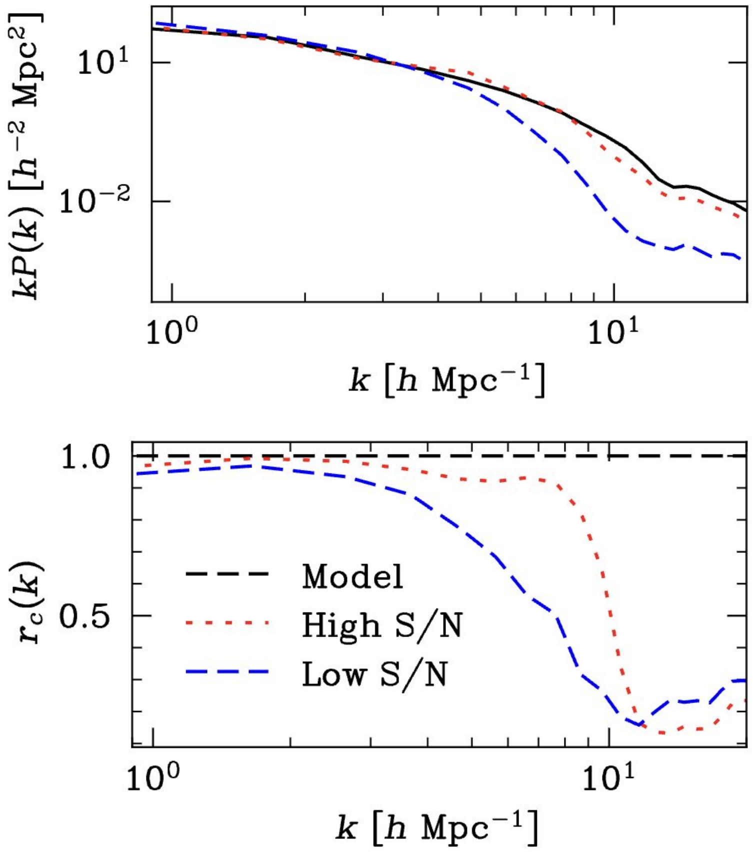


Joint optimization of initial dark matter + baryon distribution!



BH + Lukic (2025)

Field Level Inference : Recovered Summary Statistics



Applications

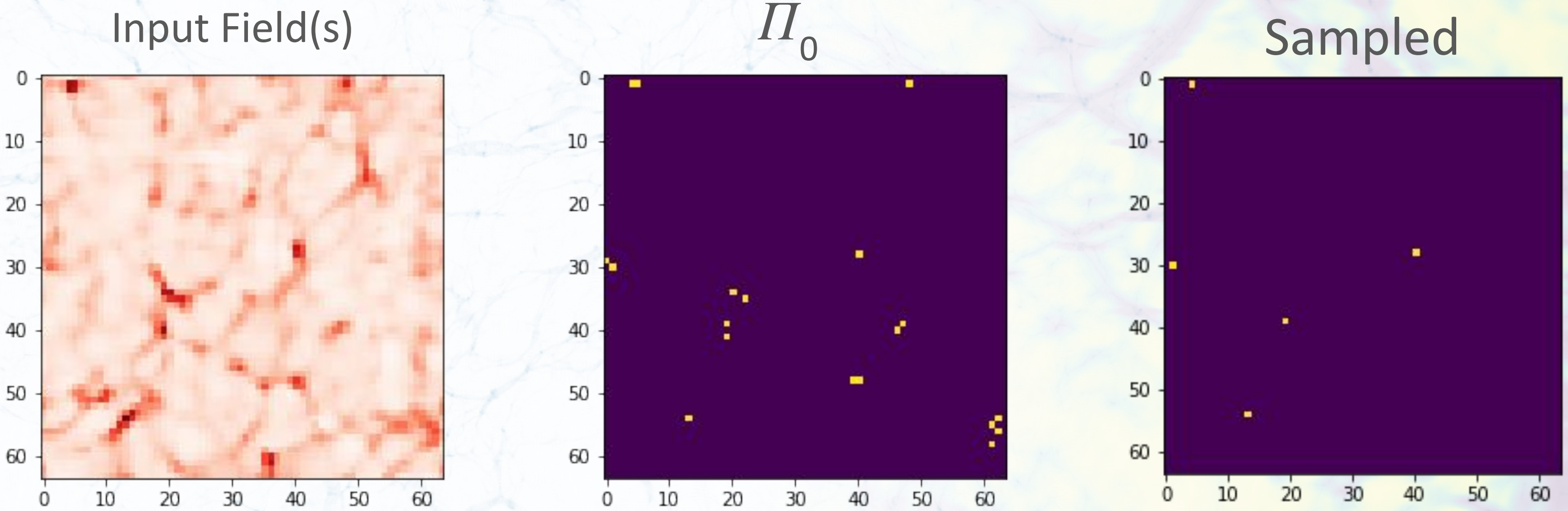
- **The Dream**: Full field level inverse modelling including galaxy formation down to z=0, marginalizing over all possible subgrid physics, including all CMB secondaries, etc.

- **The near-term**: Map hydrodynamical fields and work in summary statistic space, optimizing for cosmology/subgrid/bias jointly. (i.e. Lanzieri+ (BH) (2022) for weak lensing)

In either case, could also use some tricks like MUSE (BH+2018, Millea+Seljak 2022) to avoid sampling.

Subgrid physics modelling example: Supernova feedback

A simple model: Stochastic formation of a star particle with probability Π_0 if $T < T_c$, and the density $\boldsymbol{\delta} > \boldsymbol{\delta}_c$. Stars release energy, E_0, at once.

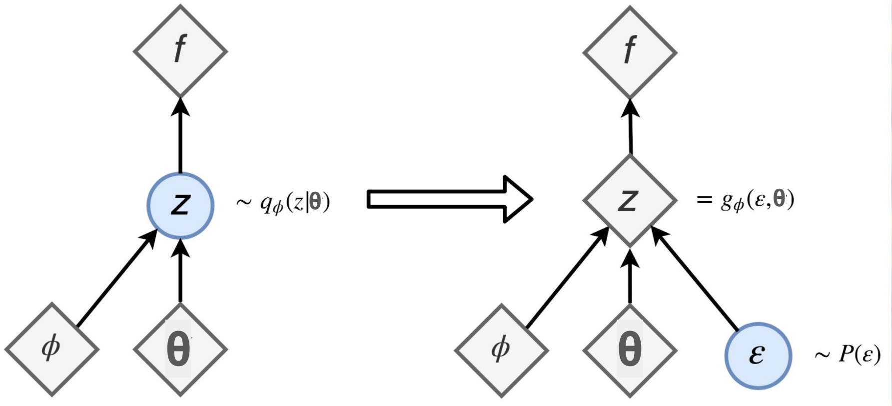


Dealing with Stochasticity and Discreteness

Taking derivatives through random variables

$$z = f(\theta, \epsilon) \text{ with } \epsilon \sim \mathbb{P}_\epsilon$$

Reparametrization Trick… Common with VAEs



From F. Errica

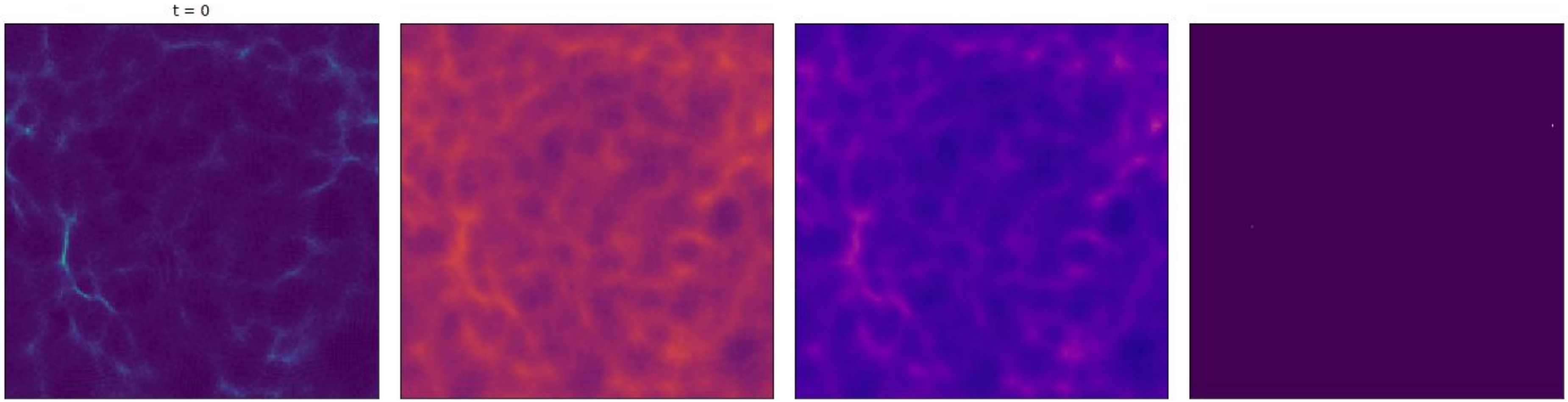
$$\frac{\partial}{\partial \theta} \mathbb{E}_{z \sim p_\theta}\left[h(z)\right] = \mathbb{E}_{\epsilon \sim p_\epsilon}\left[\frac{\partial}{\partial \theta} h(f(\theta, \epsilon))\right]$$

Gumbel Softmax (Maddison+2016, Jang+2016) : Introduce a temperature parameter to control "discreteness" w/ one-hot encoding

$$z = \frac{1}{1 + \exp(-(\log \pi + \epsilon)/\tau)} \text{ with } \epsilon \sim \text{Logistic}(0, 1)$$

Same technique for Differentiable Halo Occupancy Distribution in BH+ (2022)

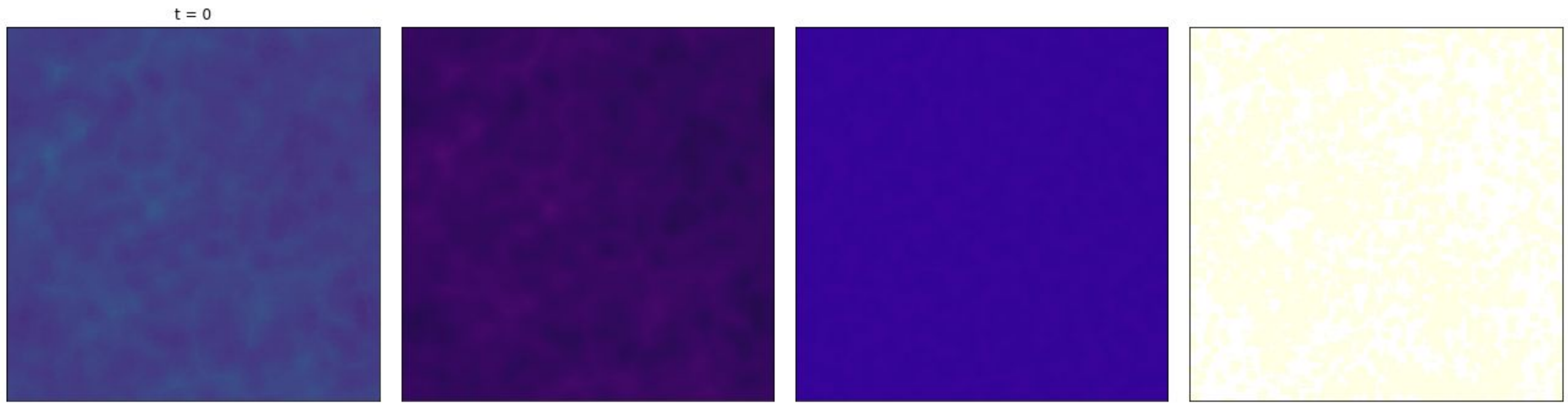
Subgrid Physics in Motion



Dark Matter IE (Temp) Gas Density Star Formation

More Realistic Simulation

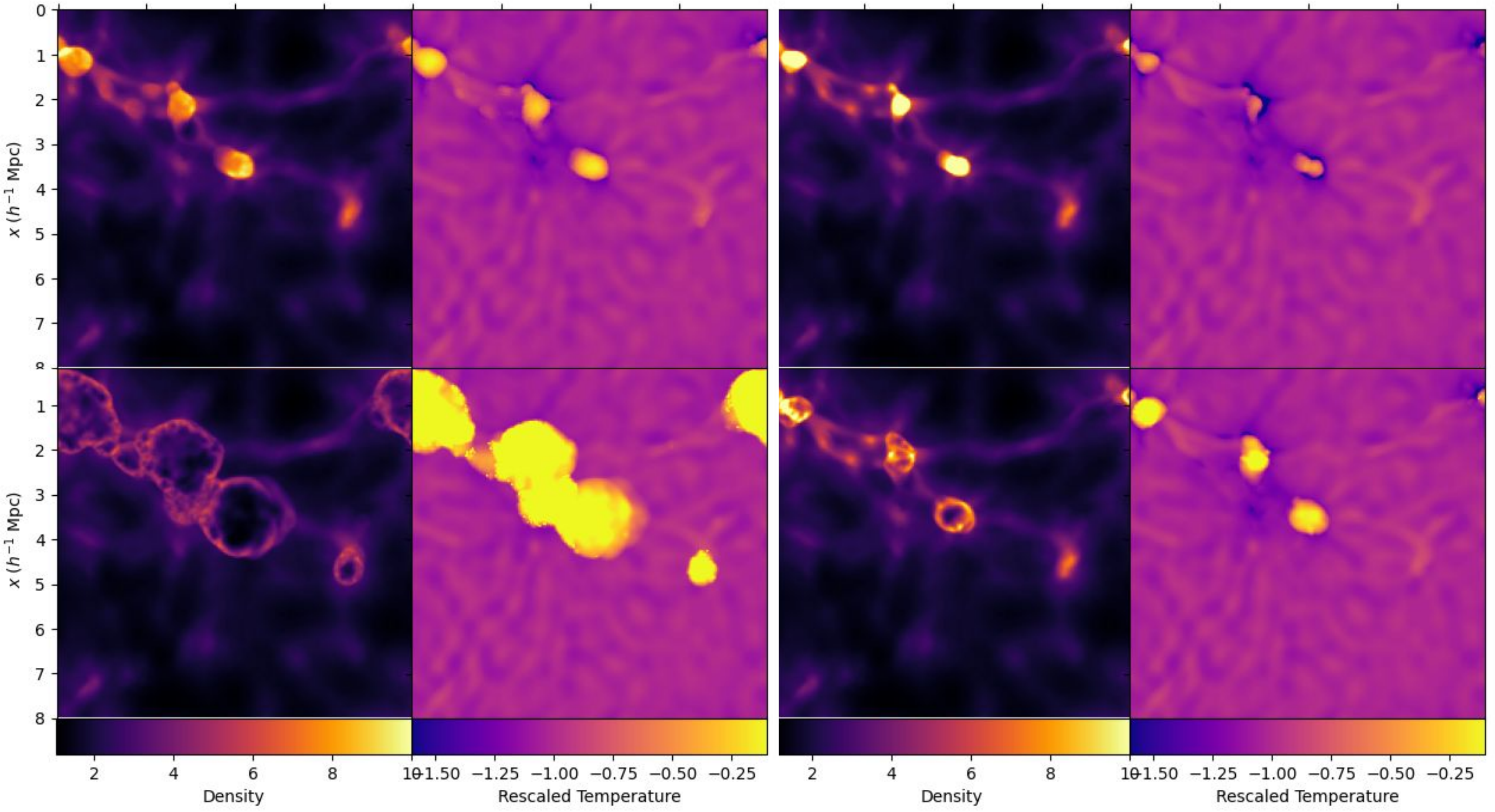
Simplifying assumption, track stellar particles with dark matter particles.



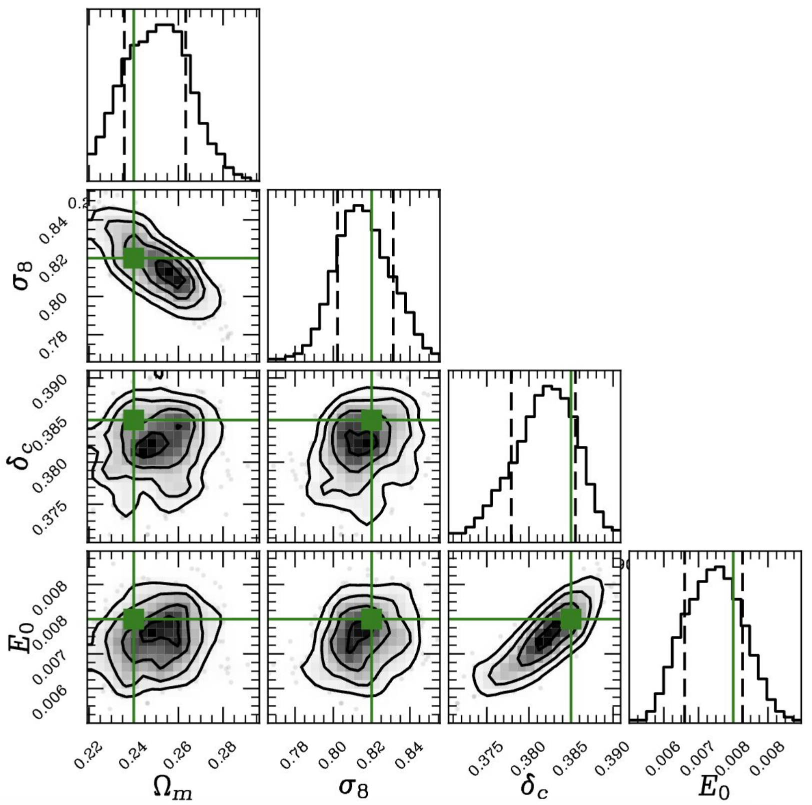
Dark Matter | Gas Density | IE (Temp) | Star Field

Increasing □$_c$

Increasing E_0



Parameter Constraints via Hamiltonian Monte Carlo



Rapidly explore combined parameter space based on mock power spectra data!

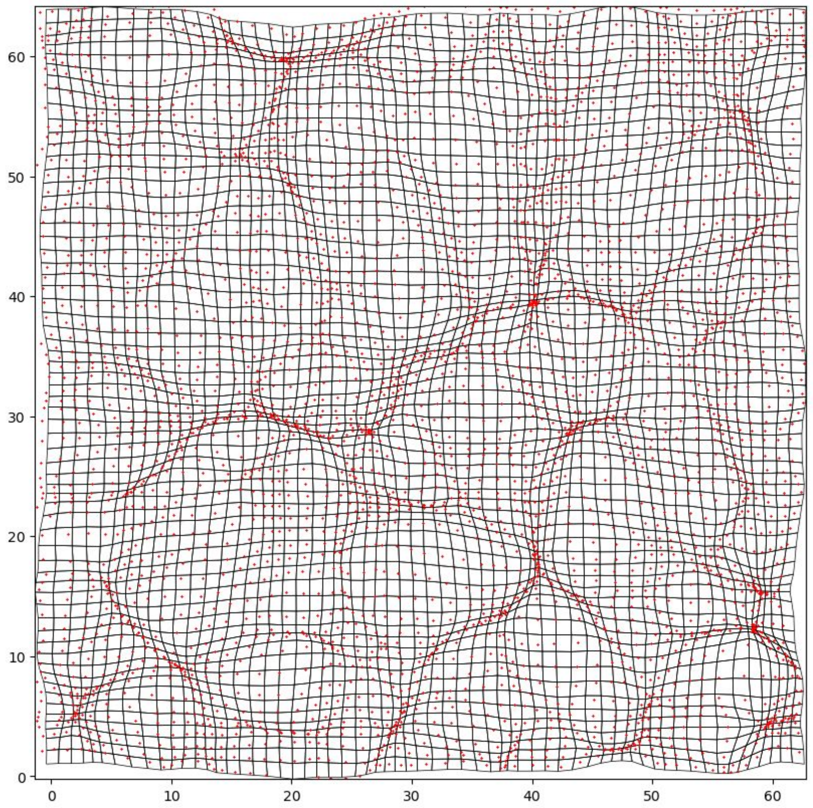
- HMC highly efficient, 500 samples with effective sample size of 6000!

Going to Smaller Scales/Faster Sims

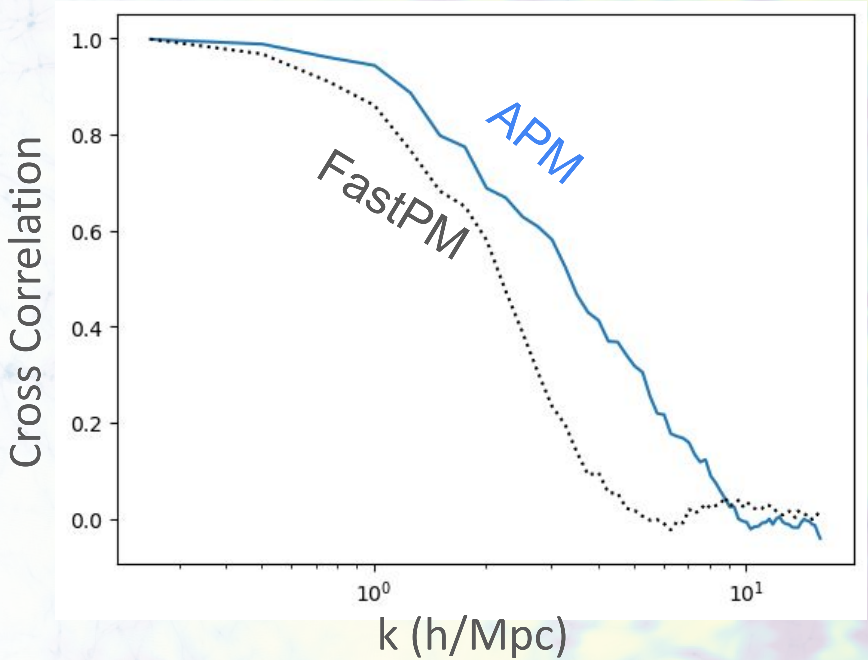
Going Beyond Standard Particle Mesh : Adaptive Approach

Preliminary

Use adaptive mesh which maintains same rectangular topology (easy for GPU, easy for autodiff)



Can't use standard FFTs, instead directly solve for potential



Inspired by U. Pen (1997)

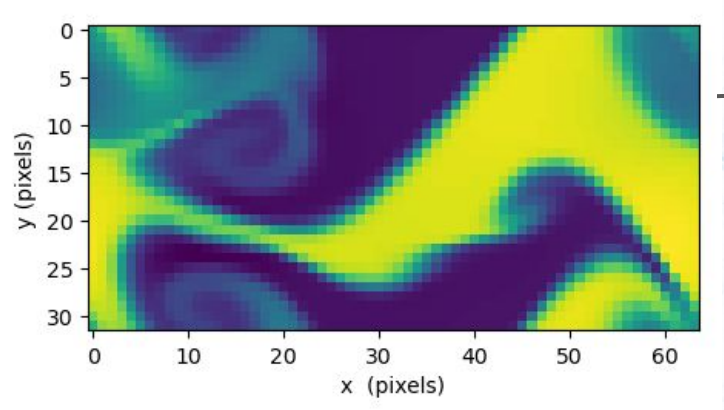
The Future… Solver-in-Loop Models

Inspired by Um et al. (2020)

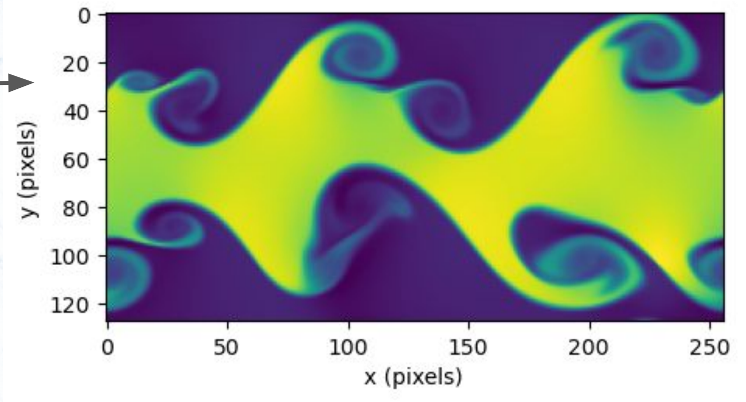
Best of both worlds?

Speed/accuracy of ML models with the generalizability of hydrodynamical simulations!

Low Resolution



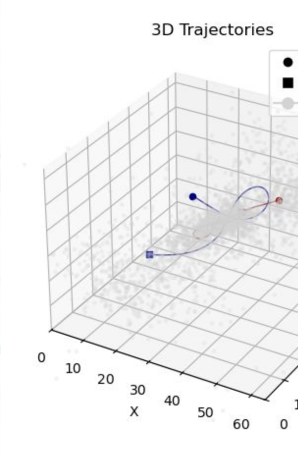
High Resolution

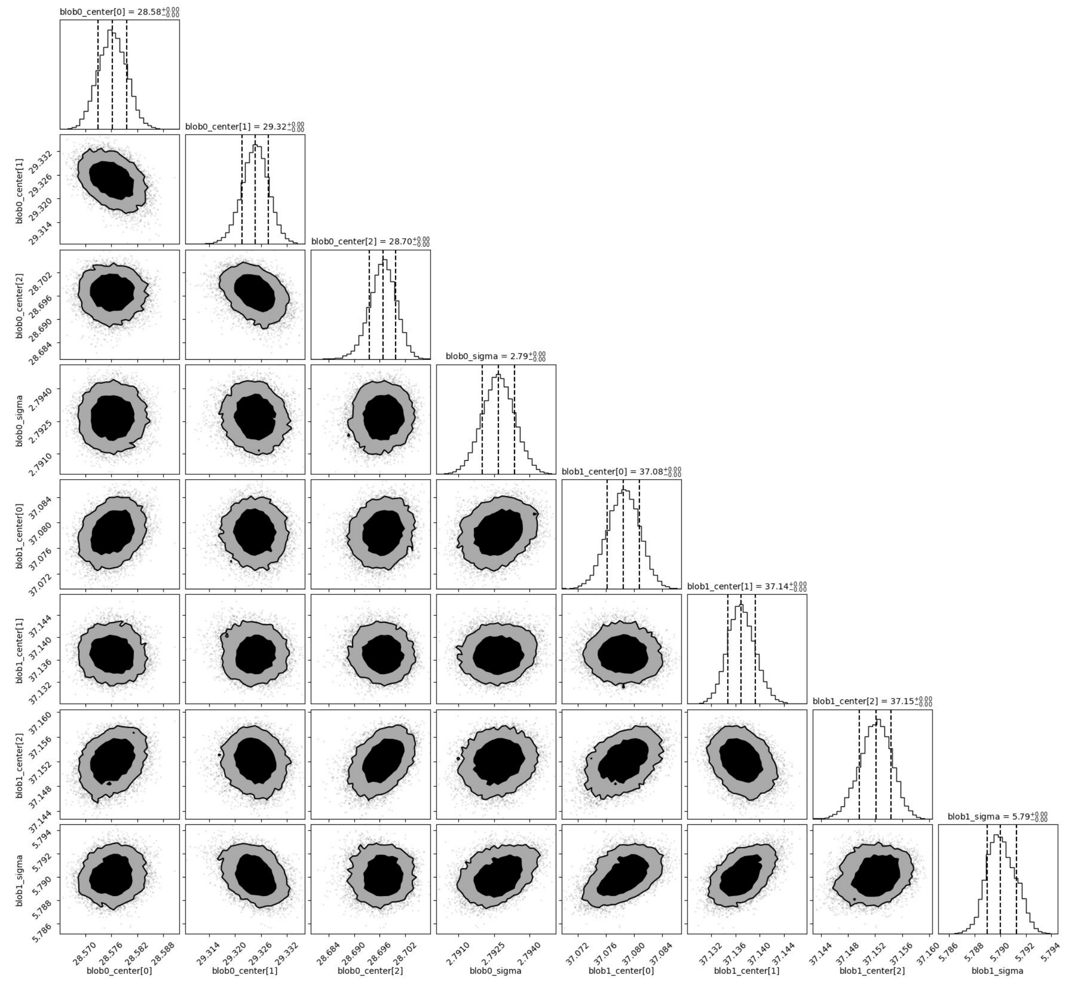


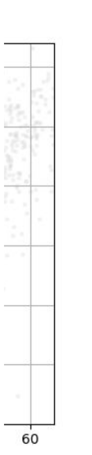
"Resolution" could mean many things… (mesh size, adaptive mesh refinement, memory intensive Riemann solvers, larger timesteps, additional (subgrid) physics, etc.)

Going Bey... proach

Can also bac... n.







w/ Lucas Mebille

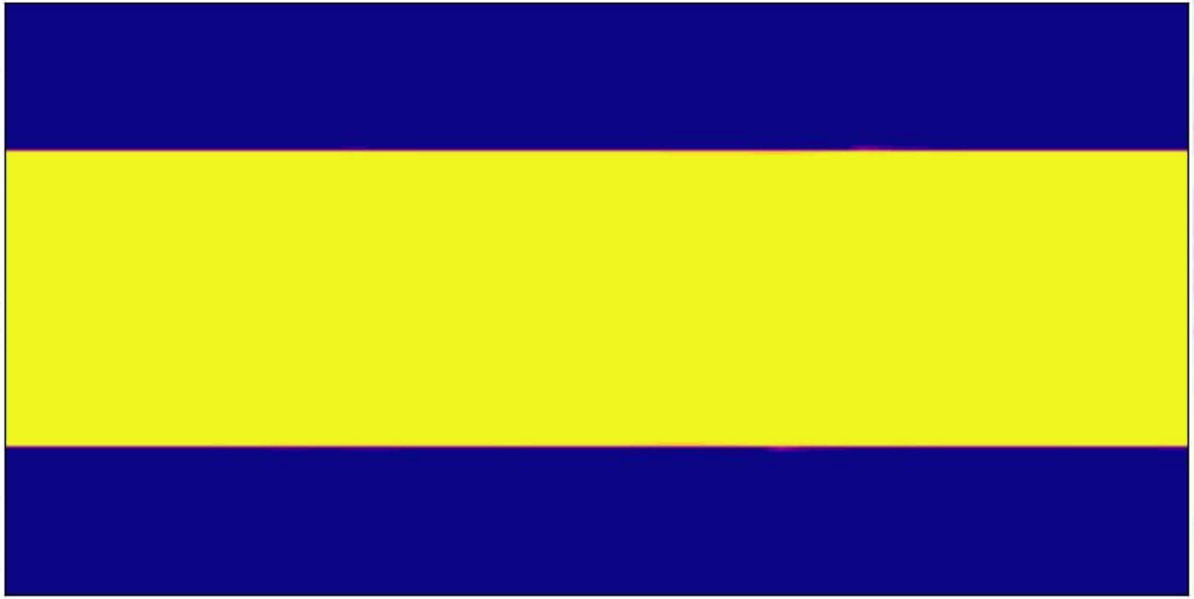
Individual orb... bles (i.e. halos)

can be recon...

Inspired by Um et al. (2020)

The Future… Solver-in-Loop Models

Even with GPU, some simulations are computationally expensive…

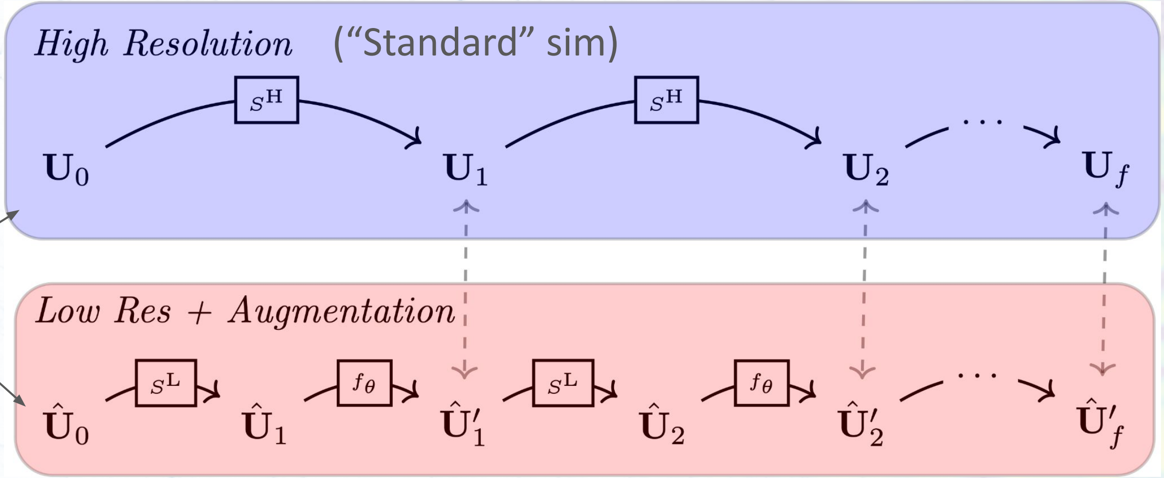


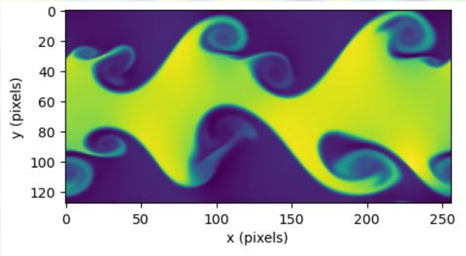
Inspired by Um et al. (2020)

The Future? Solver-in-Loop Models

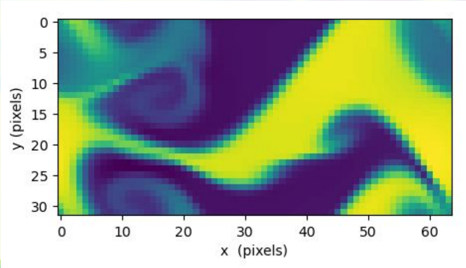
Setup neural network to augment each timestep: f_θ

Initial Condition





Final State



Train model by minimizing loss over all timesteps:

$$\mathcal{L}_\theta = \sum_i (\hat{\mathbf{U}}'_i(\theta) - \mathbf{U}_i)^2$$

Could also include it at the level of flux and/or source calculations

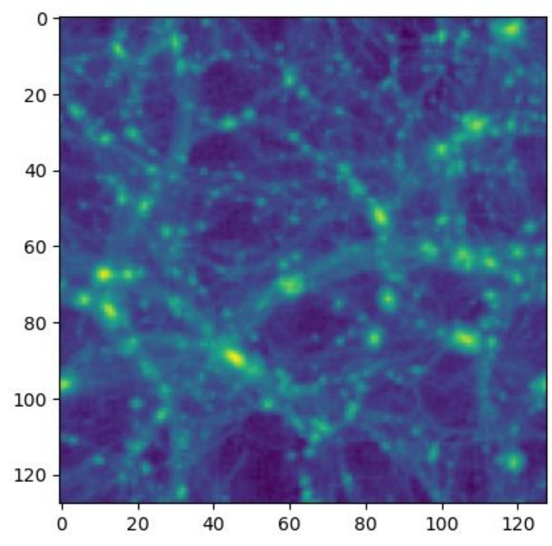
IN PROGRESS

Solver-in-Loop Models : Star Formation

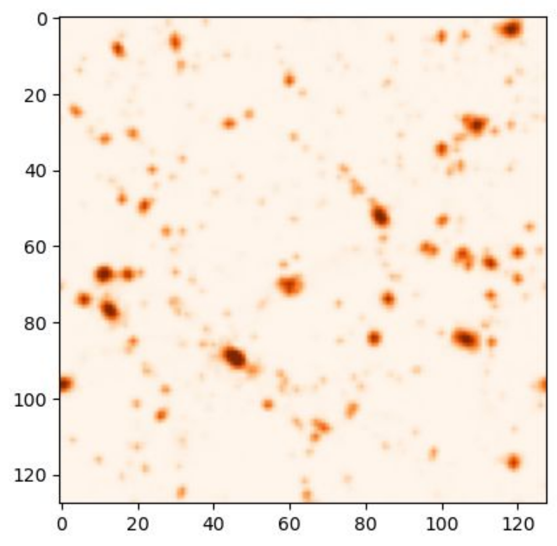
w/ Lillie Szemraj

Train star formation field iteratively in loop to capture star formation history. Trained on “standard” hydrodynamical simulations, CAMELS simulations (Villaescusa-Navarro et al).

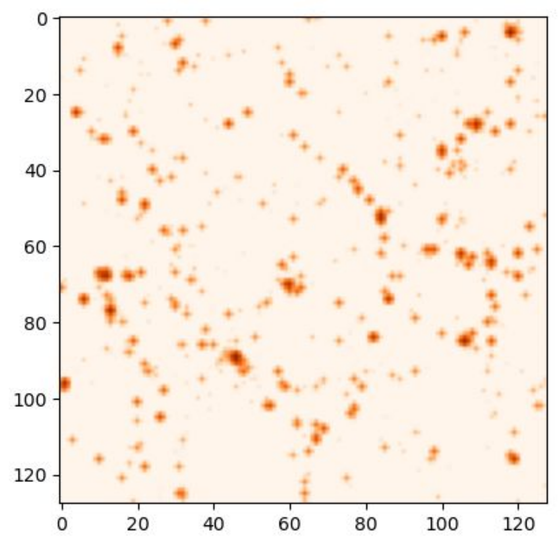
PM Dark Matter



PM Stellar Component



Hydrosim Reference



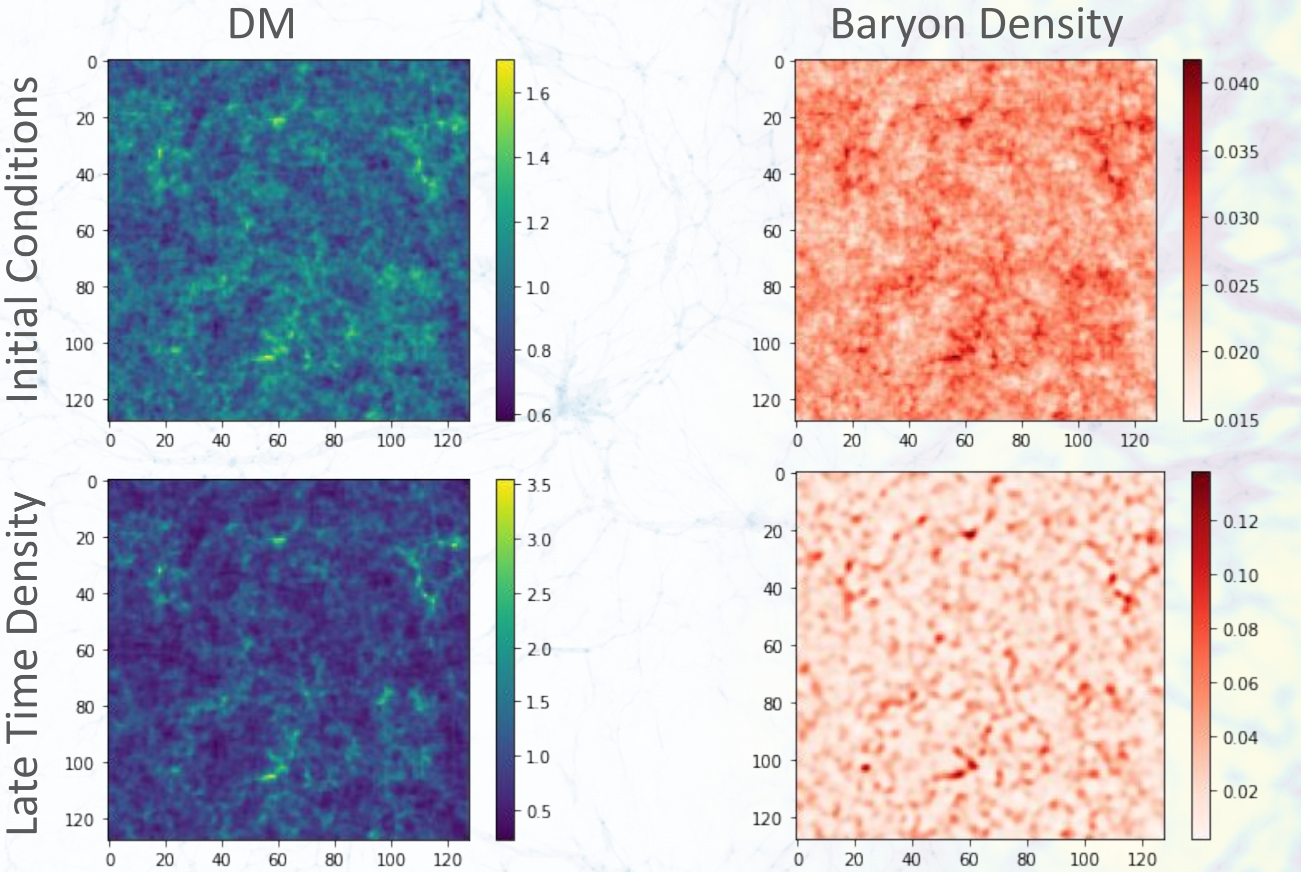
Summary

The “machine learning revolution” is useful beyond making complex black-box models! Optimization methods, available GPUs, etc. have opened new doors for analysis.

- Machine learning can be used a surrogate model for realistic hydrodynamical physics in a forward model.
- Hydro-sims themselves can be able to be constructed in a differentiable fashion, even with complex stochastic feedback.
- In the future, ML-assisted hydrosims could maintain generalizability while vastly outperforming current classes of simulations.

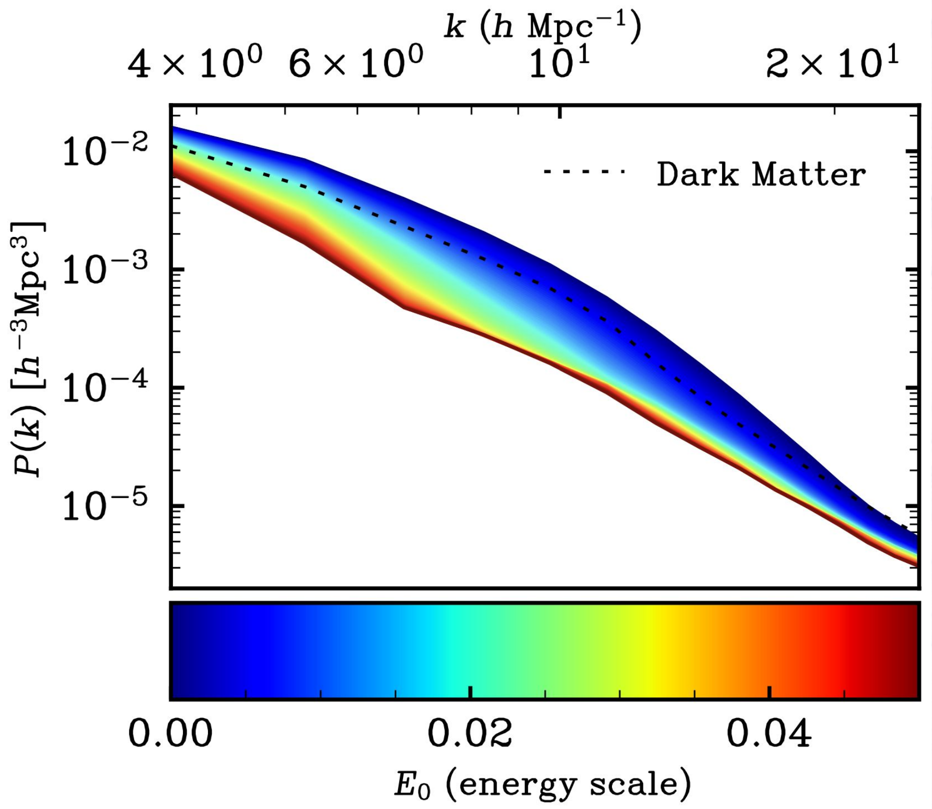
Backup Slides

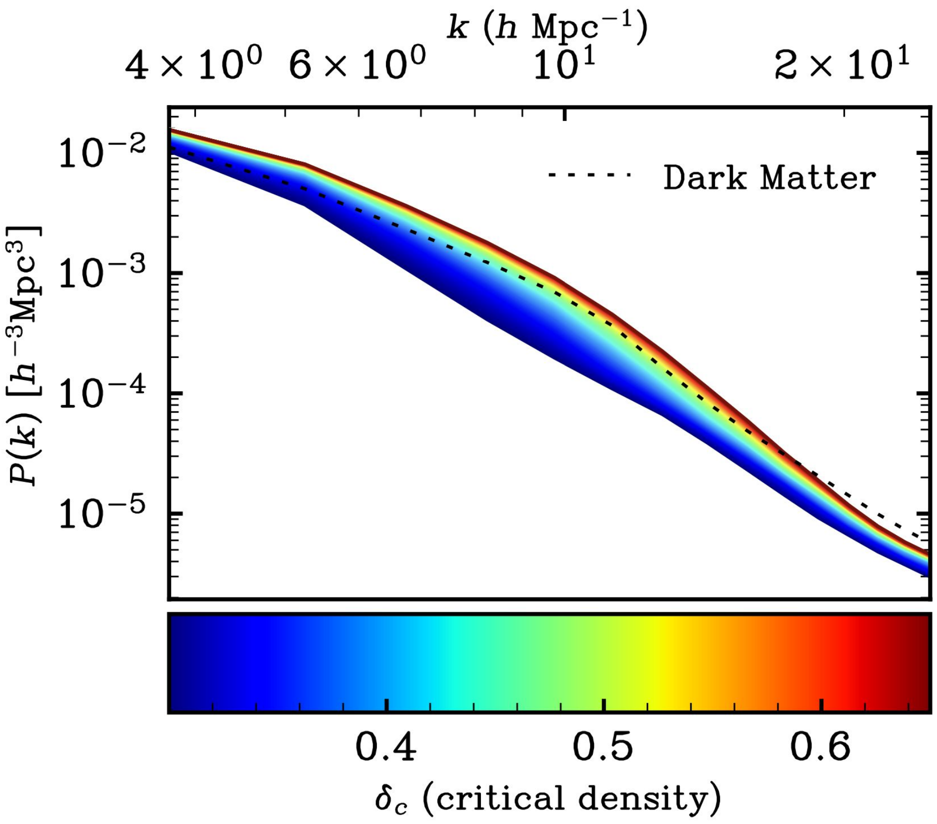
Couple to dm-solver (PMWD)



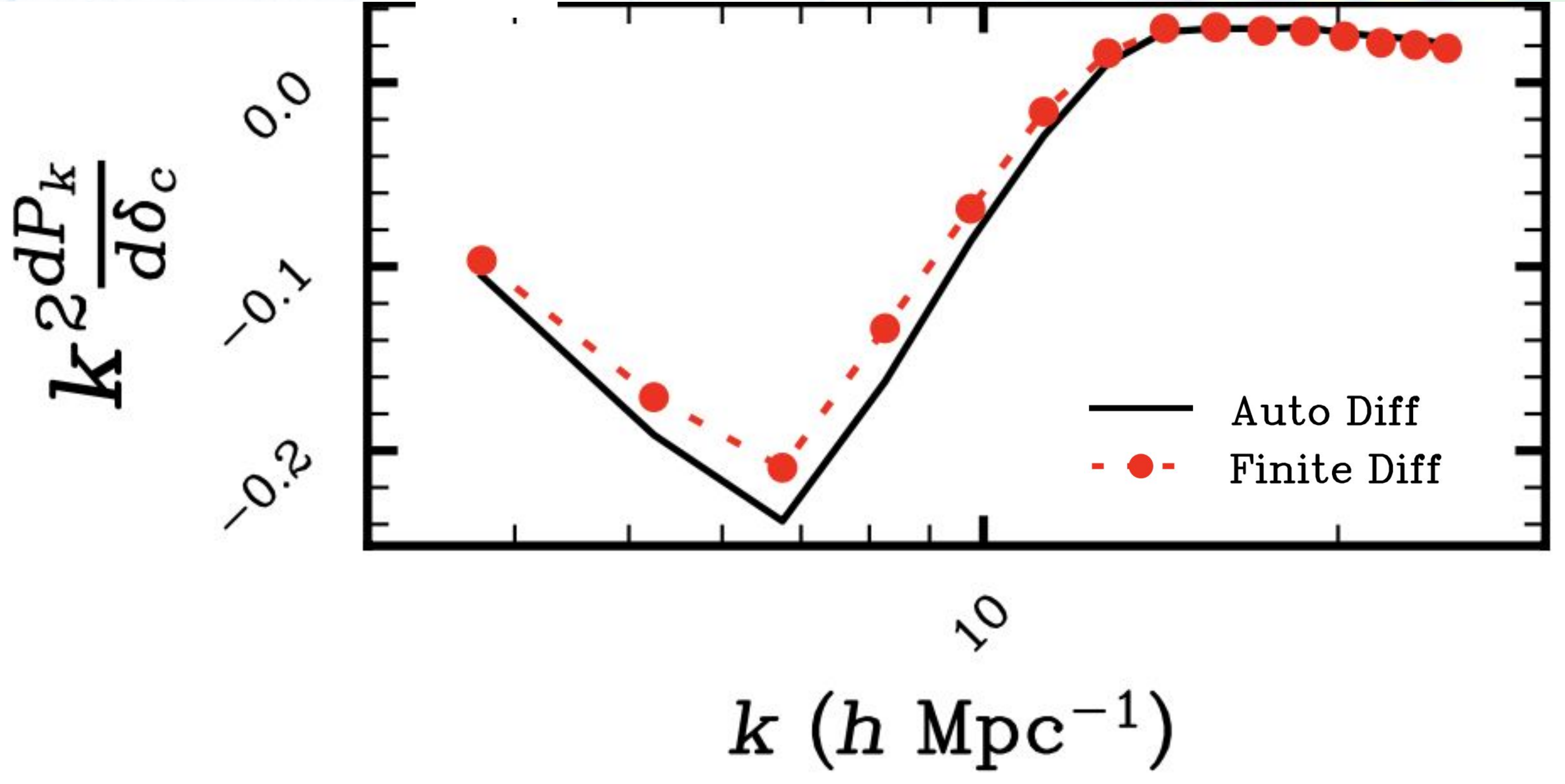
BH + Lukic (2025)

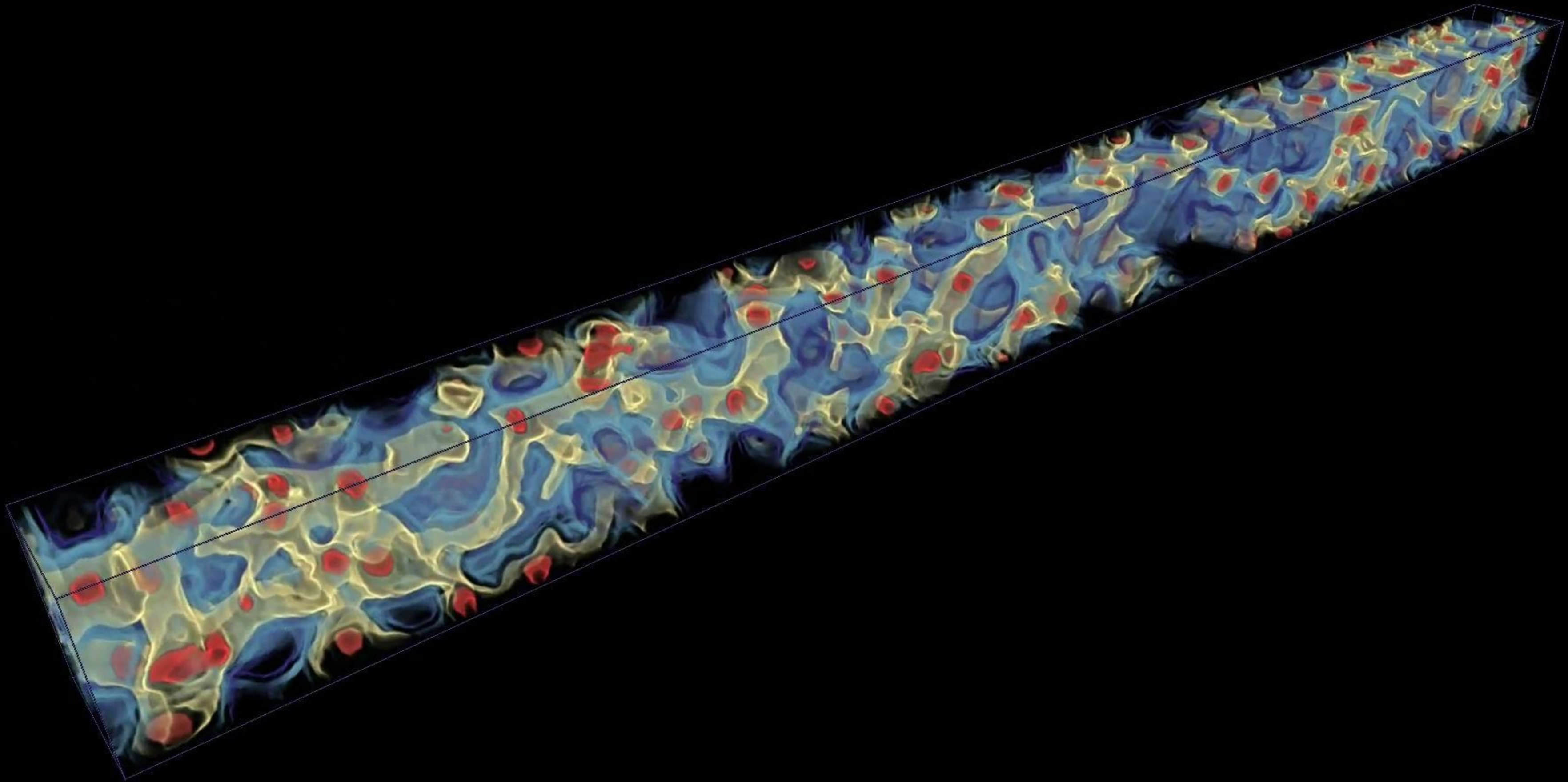
Power Spectra : Varying Critical Density

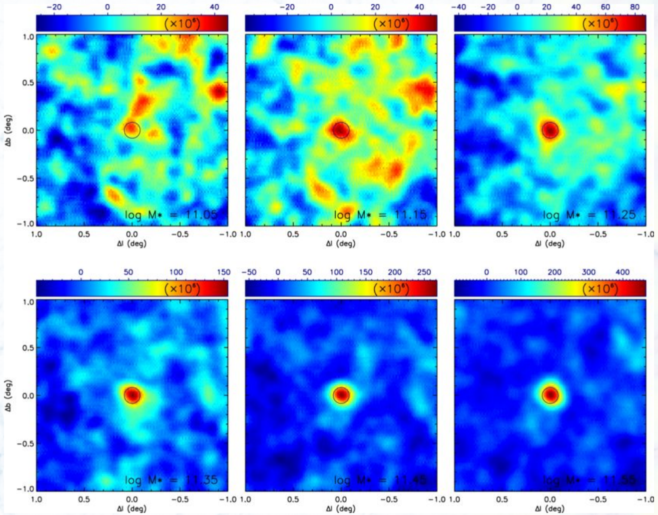




Derivatives of Summary Statistics







log M* = 11.05
log M* = 11.15
log M* = 11.25
log M* = 11.35
log M* = 11.45
log M* = 11.55
Δl (deg)
Δb (deg)

Hydrodynamics

State vector:

$$\mathbf{U} = (\rho_b, a\rho_b U, a^2\rho_b E)$$

Combined Conservation Equation:

$$\frac{\partial \mathbf{U}}{\partial t} = -\nabla \cdot \mathbf{F} + S_e + S_g$$

Flux Term:

$$\mathbf{F} = ((1/a)\rho_b U, \rho_b U U, a(\rho_b U E + pU))$$

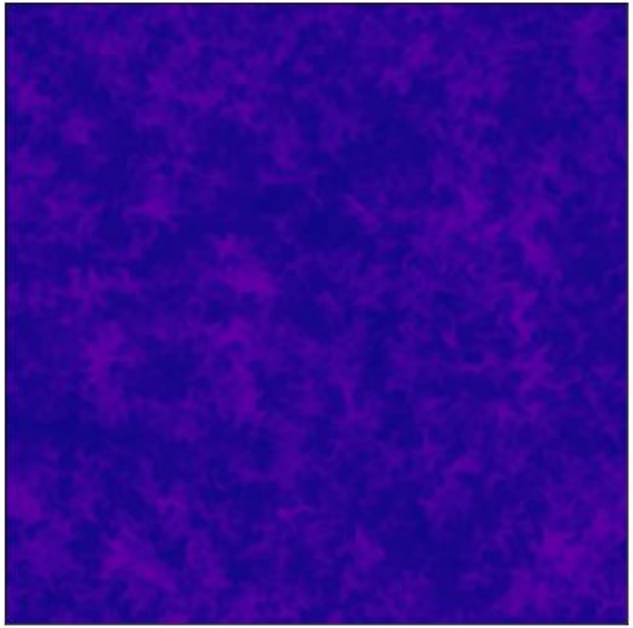
Source Terms:

$$S_e = (0, 0, -ap\nabla \cdot U)$$

$$S_g = (0, \rho_b \mathbf{g}, a\rho_b U \cdot \mathbf{g})$$

Can solve numerically time-step by timestep on a grid.

Optimization in Progress

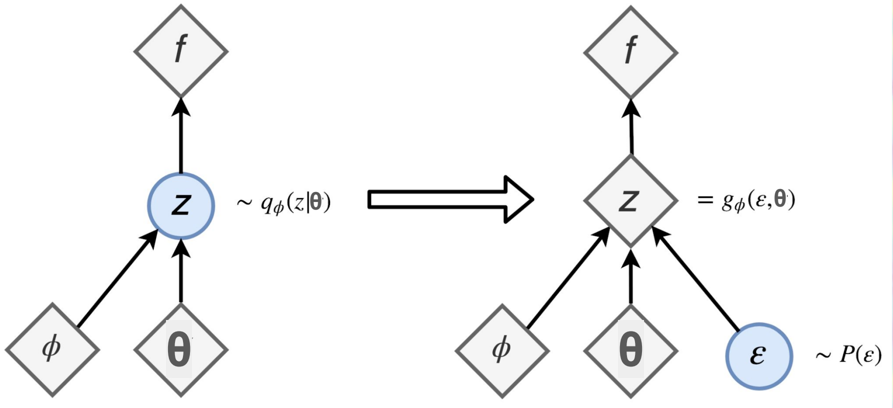


(used fewer timesteps, so easier than 3 blast example…)

Dealing with Stochasticity and Discreteness

Taking derivatives through random variables

$$z = f(\theta, \epsilon) \text{ with } \epsilon \sim \mathbb{P}_\epsilon$$



From F. Errica

Reparametrization Trick… Common with VAEs

$$\frac{\partial}{\partial\theta}\mathbb{E}_{z\sim p_\theta}\left[h(z)\right] = \mathbb{E}_{\epsilon\sim p_\epsilon}\left[\frac{\partial}{\partial\theta}h(f(\theta,\epsilon))\right]$$

Classic Multivariable Gaussian example

$$z \sim N(\mu, \sigma^2) \qquad z = \mu + \sigma\epsilon \qquad \epsilon \sim N(0, I)$$

Same technique for Differentiable Halo Occupancy Distribution in BH+ (2022)

Taking Derivative Through Discrete Stochastic Process

In Progress!

Sampling a discrete random variable differentiably with a Gumbel random g_i

$$z = \text{onehot}\left(\text{argmax}_i \left[g_i + \log(\pi_i)\right]\right)$$

Introduce tau, temperature relaxation parameter: (Maddison+2016, Jang+2016)

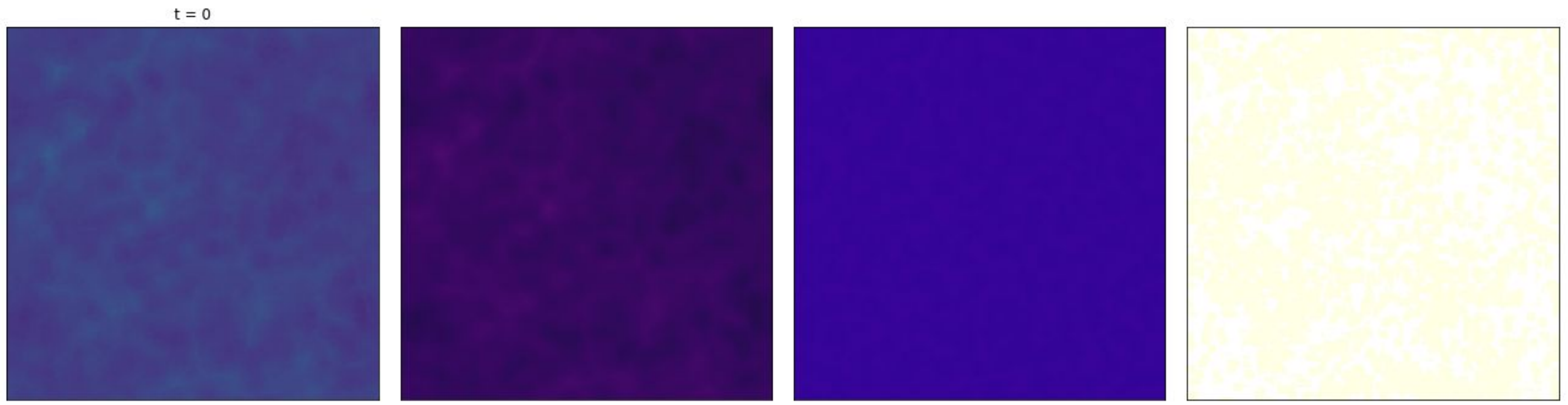
$$\hat{z}_i = \frac{\exp((\log(\pi_i) + g_i)/\tau)}{\sum_j \exp((\log(\pi_j) + g_j)/\tau)}$$

Simplifies a bit for one class:

$$z = \frac{1}{1 + \exp(-(\log \pi + \epsilon)/\tau)} \quad \text{with } \epsilon \sim \text{Logistic}(0, 1)$$

Same technique for Differentiable Halo Occupancy Distribution in BH+ (2022)

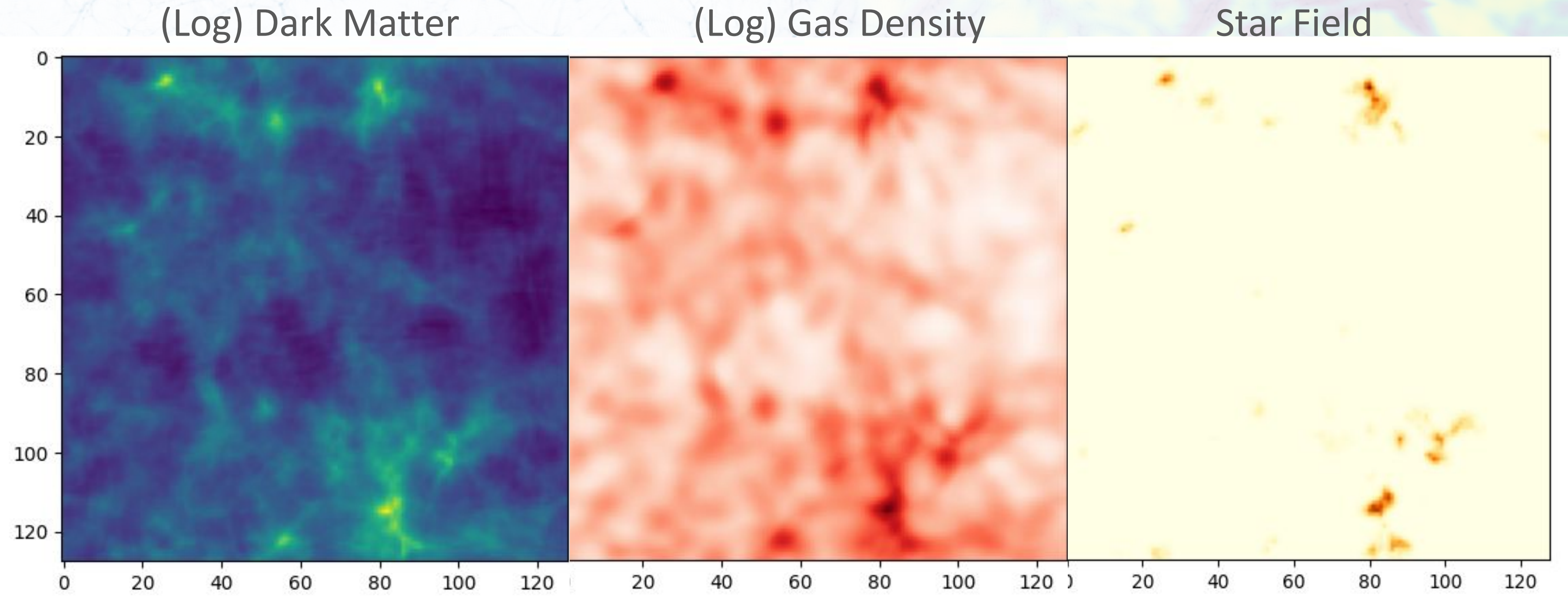
More Realistic Simulation

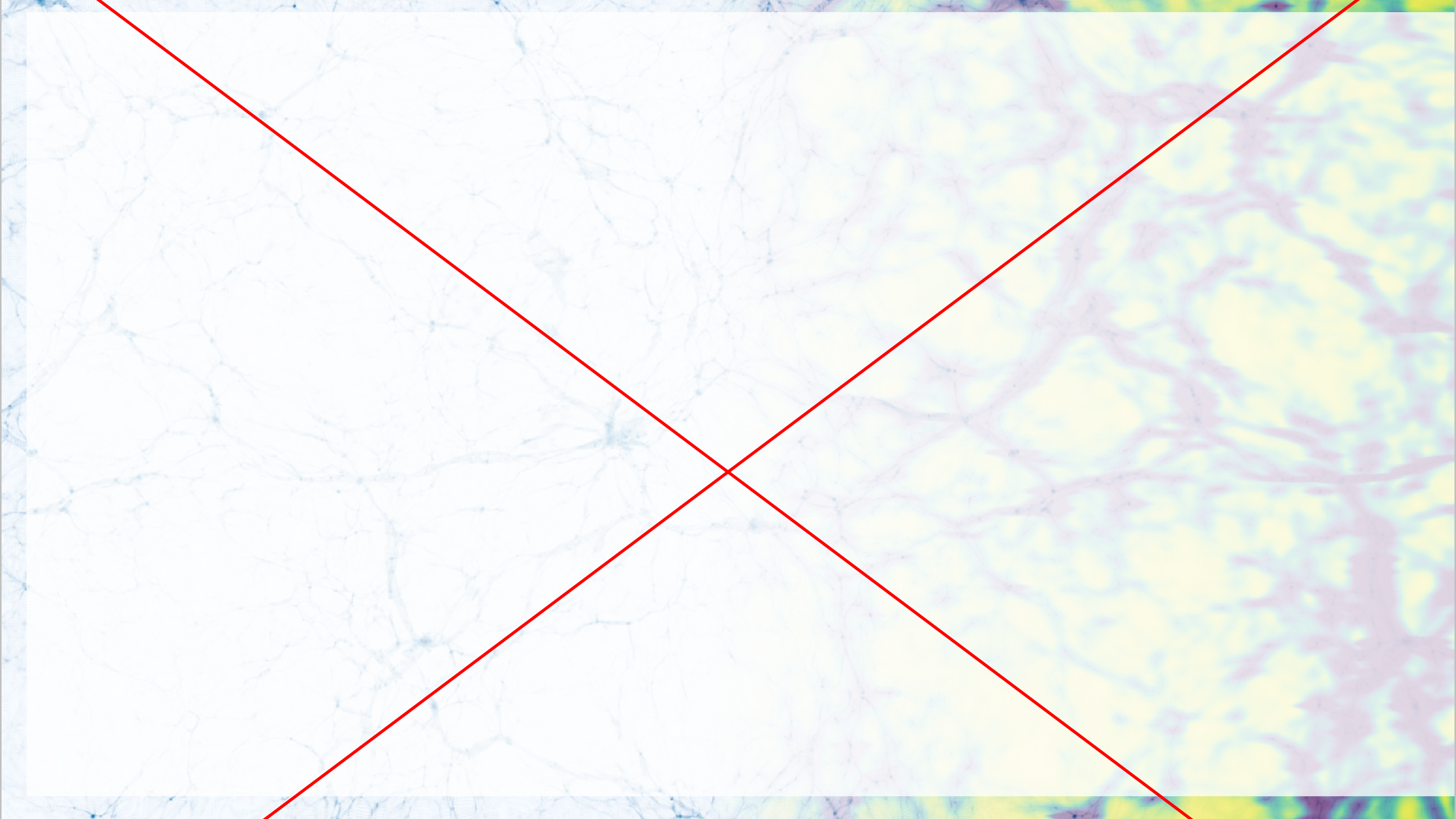


Dark Matter Gas Density IE (Temp) Star Field

Slice Through (more realistic) Simulation

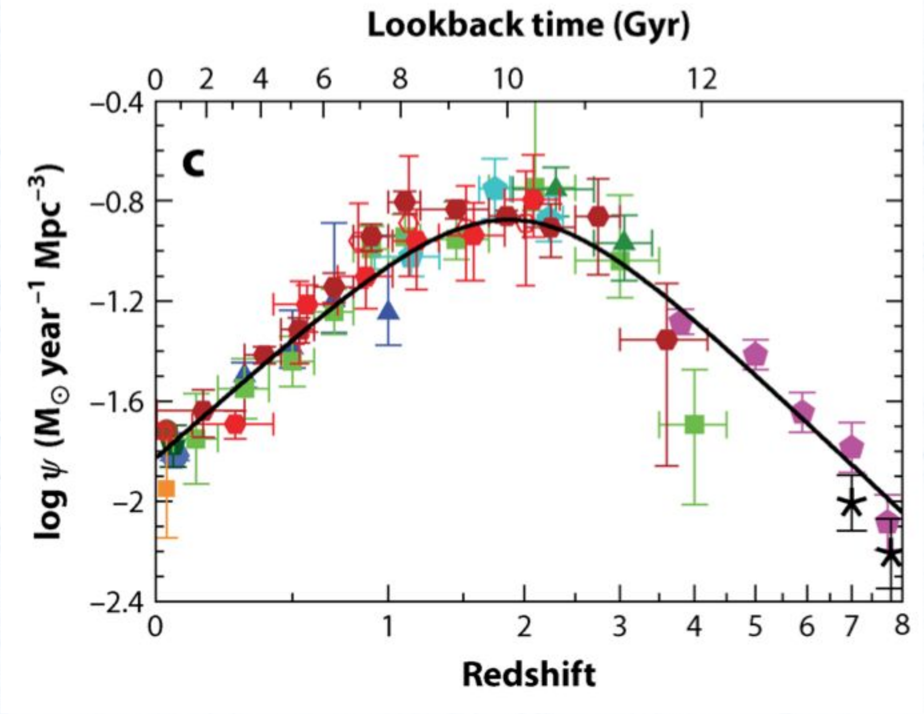
In Progress!



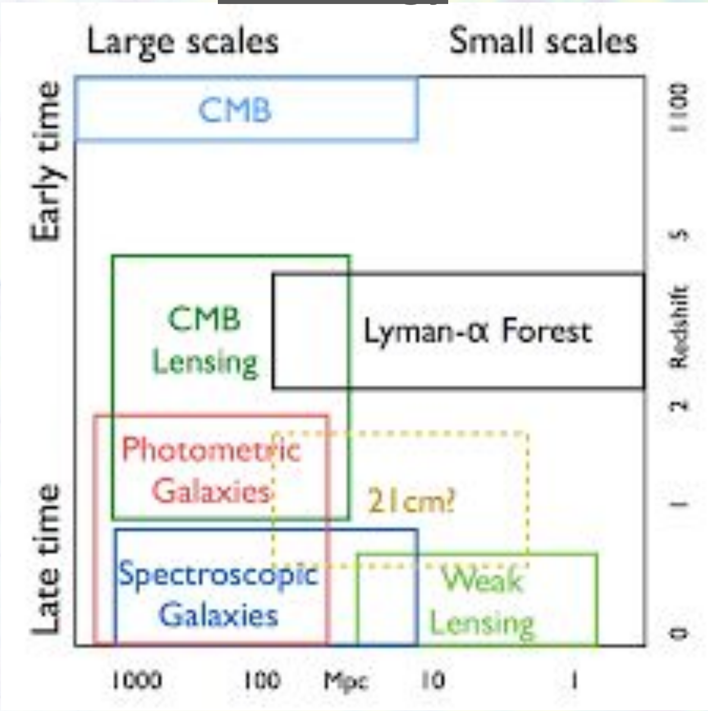


Lyman Alpha Forest: Astrophysics and Cosmology

Astrophysics



Cosmology



[Madau and Dickenson, 2014](#)

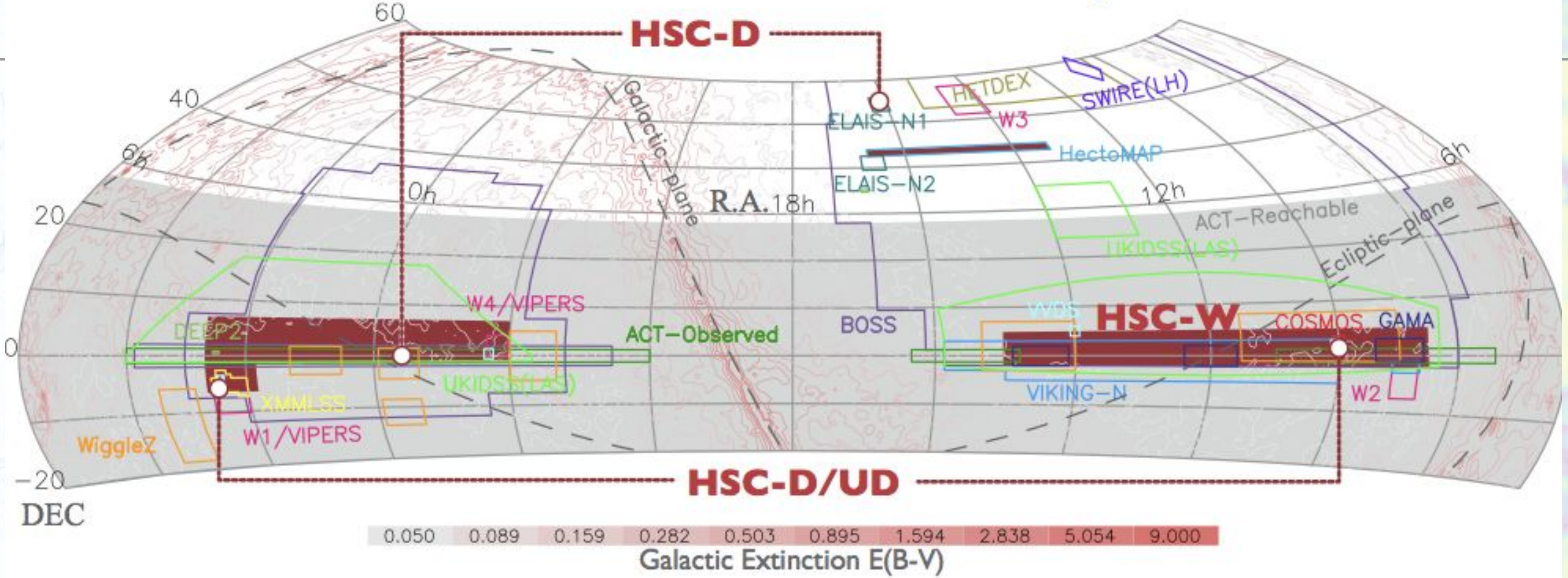
Andreu Font-Ribera

PFS - Fast facts

- Subaru *Prime Focus Spectrograph*:
  The spectroscopy part of the "SuMIRe" project.
  - Wide field: *~1.4 deg* diameter
  - High multiplicity: *2394 fibers*
    - Fiber diameter: ~1.05 arcsec
    - Fiber positioner pitch: ~85 arcsec
    - Minimum fiber separation: ~30 arcsec

  - Quick fiber reconfiguration: *~60-120 sec* (TBC)
  - VIS-NIR coverage: *380-1260nm simultaneously*
    - Low resolution mode: ~2.5 A resolution
    - Medium resolution mode (around 800nm): ~1.6 A resolution

Subaru HSC/PFS Survey fields



HSC-SSP: 8 years, 300 nights, completed

Wide: ~1200 sq deg to 26, Deep: 30 sq deg to 27, Ultra-Deep 3 sq deg to 28

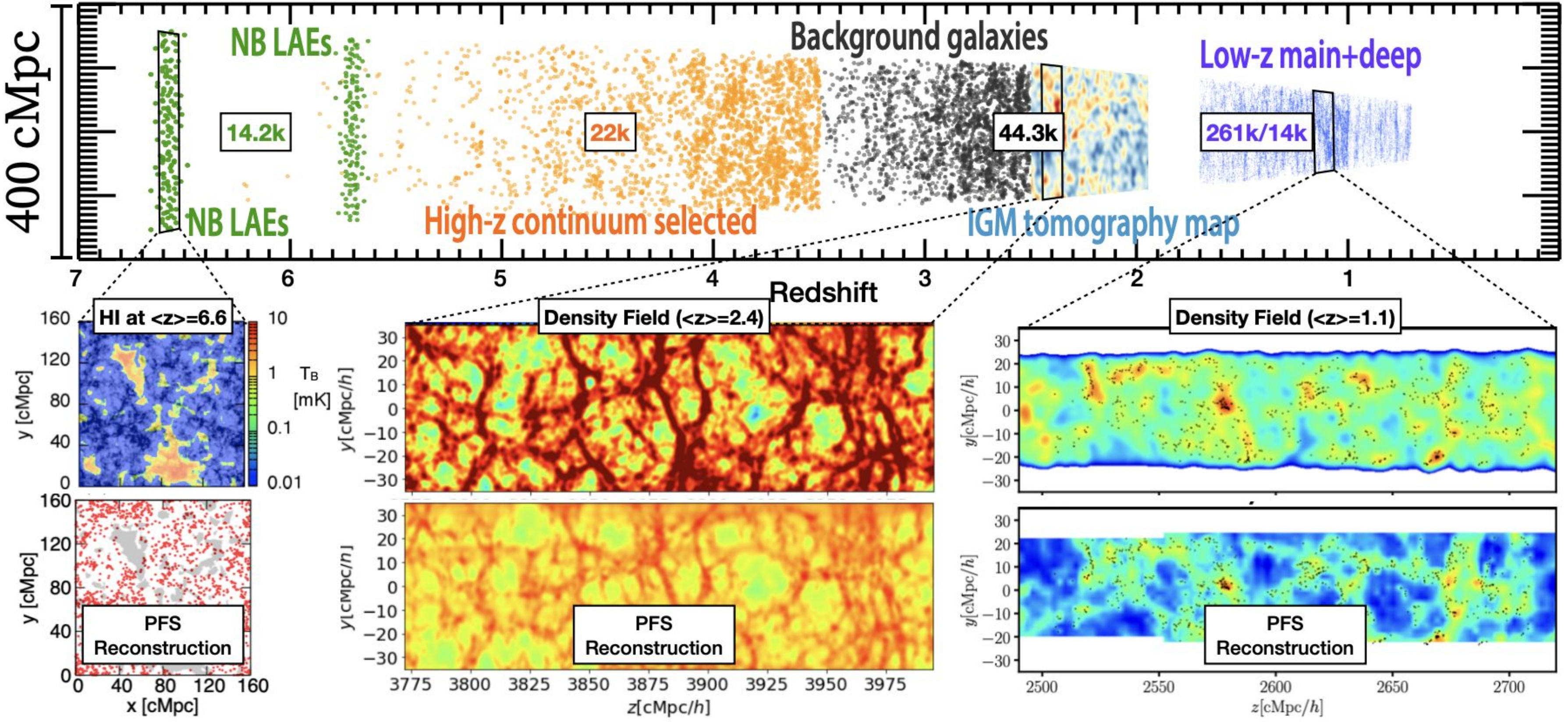
PFS-SSP: 5 years, 360 nights, starting S2025

Key Pillars of the PFS-SSP

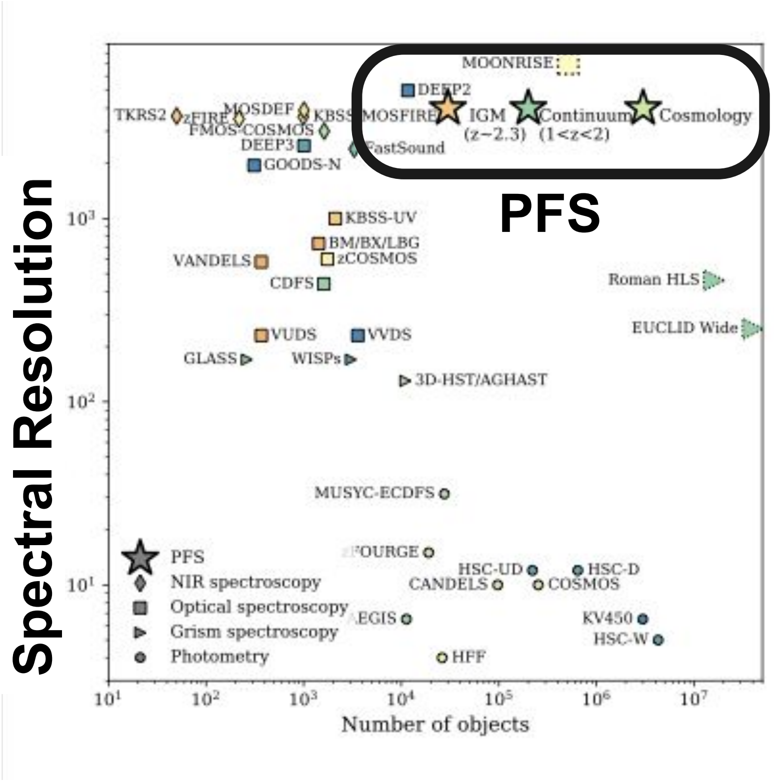
- CO - Cosmology
- GA - Galactic Archaeology
- GE - Galaxy Evolution

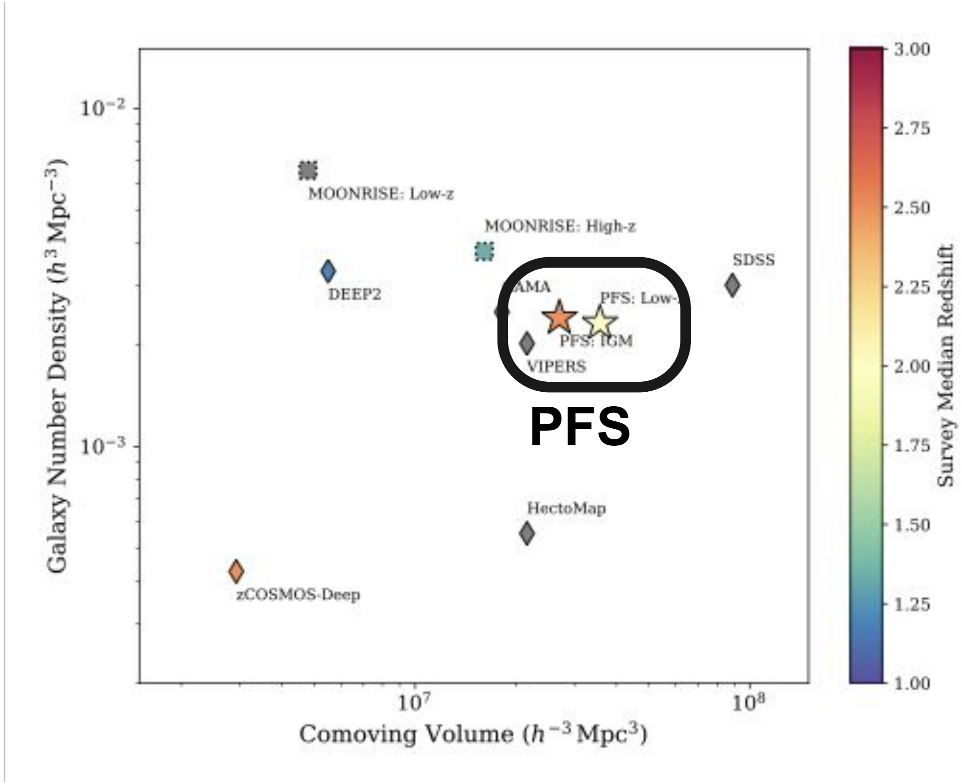
	Testing ΛCDM	Assembly history of galaxies	Importance of IGM
CO	• Nature & role of neutrinos • Expansion rate via BAO up to z=2.4 • PFS+HSC tests of GR • Curvature of space: Ω_K • Primordial power spectrum	• PFS+HSC synergy • Absorption probes with PFS/SDSS QSOs around PFS/HSC host galaxies	• Search for emission from stacked spectra
GA	• Nature of DM (dSphs) • Structure of MW dark halo	• Stellar kinematics and chemical abundances – MW & M31 assembly history	• dSph as relic probe of reionization feedback • Past massive star IMF from element abundances
GE	• Small-scale tests of structure growth	• Halo-galaxy connection: $M_*/M_{\rm halo}$ • Outflows & inflows of gas • Environment-dependent evolution	• Physics of cosmic reionization via LAEs & 21cm studies • Tomography of gas & DM

Prime Focus Spectraph: Redshift Evolution of the Galaxy - Environment Relation



Unprecedented combination:
spectral resolution, wavelength coverage, multiplex





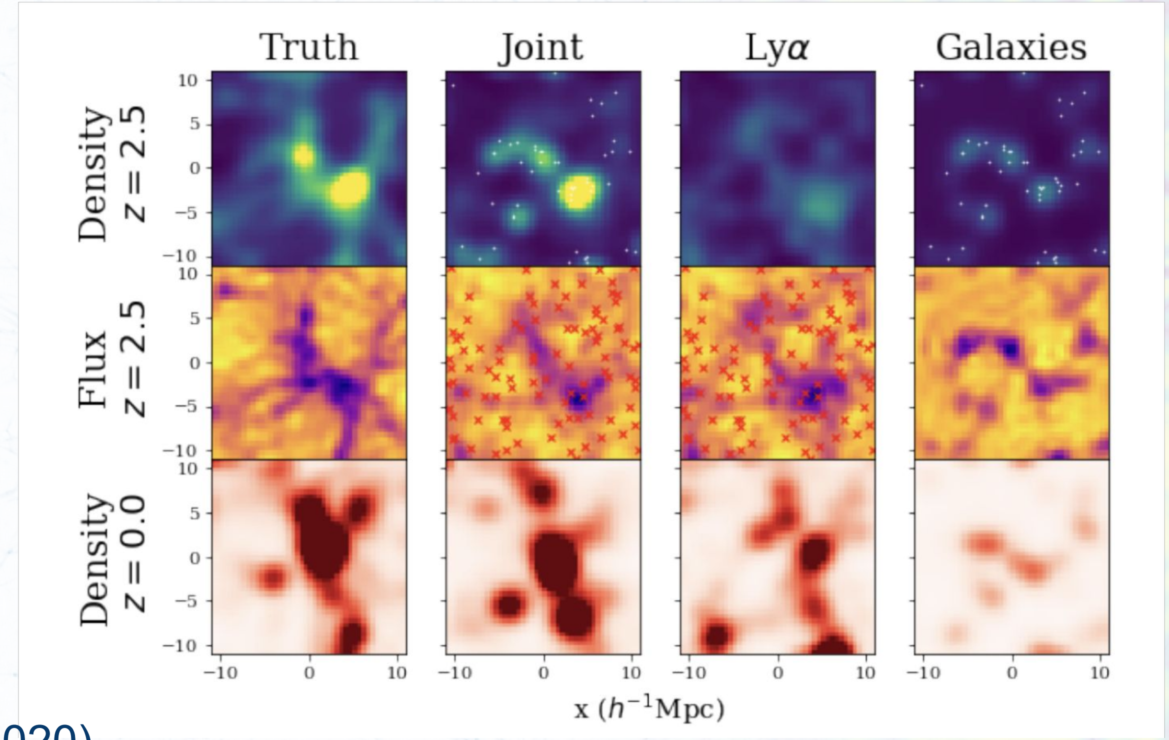
Differentiable Simulations

How Derivatives Help : Sampling

https://chi-feng.github.io/mcmc-demo/app.html

Protocluster Science

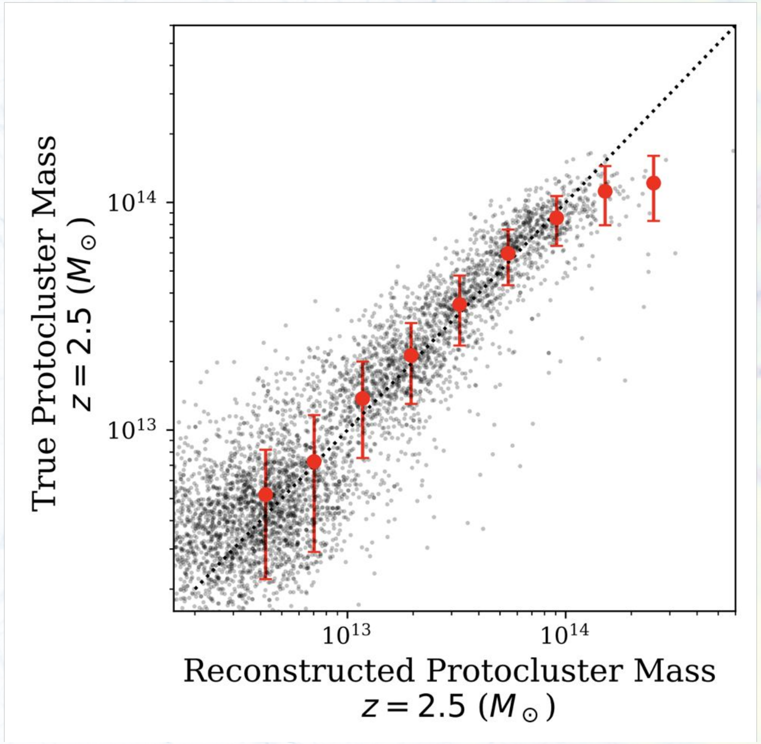
Continue to evolve reconstructed field to z=0, identify clusters using standard methods, then look at corresponding Lagrangian volume at observed redshift!



BH et al. (2019, 2020)

Protocluster Science

Continue to evolve reconstructed field to z=0, identify clusters using standard methods, then look at corresponding Lagrangian volume at observed redshift!



BH et al. (2019, 2020)