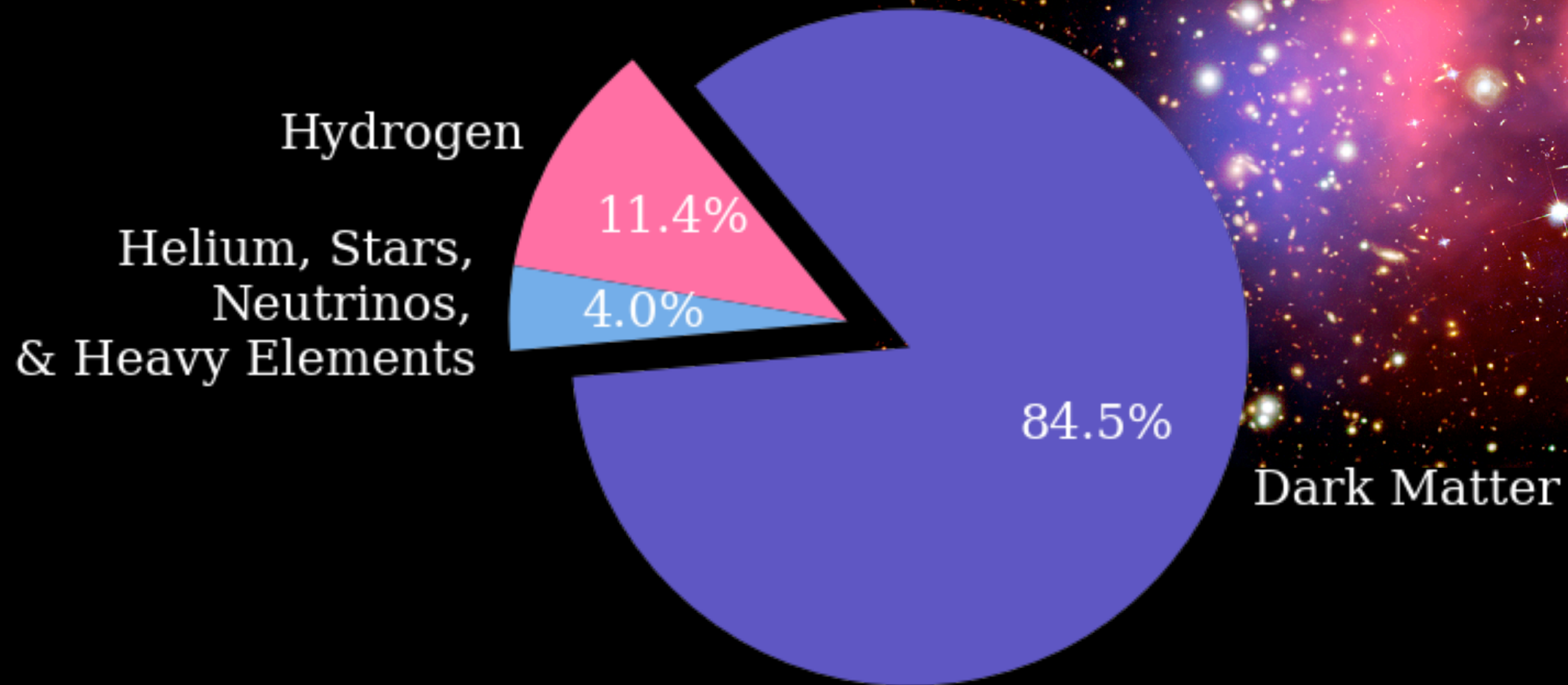


PHYSICS– INFORMED MACHINE LEARNING FOR COSMOLOGICAL SIMULATIONS

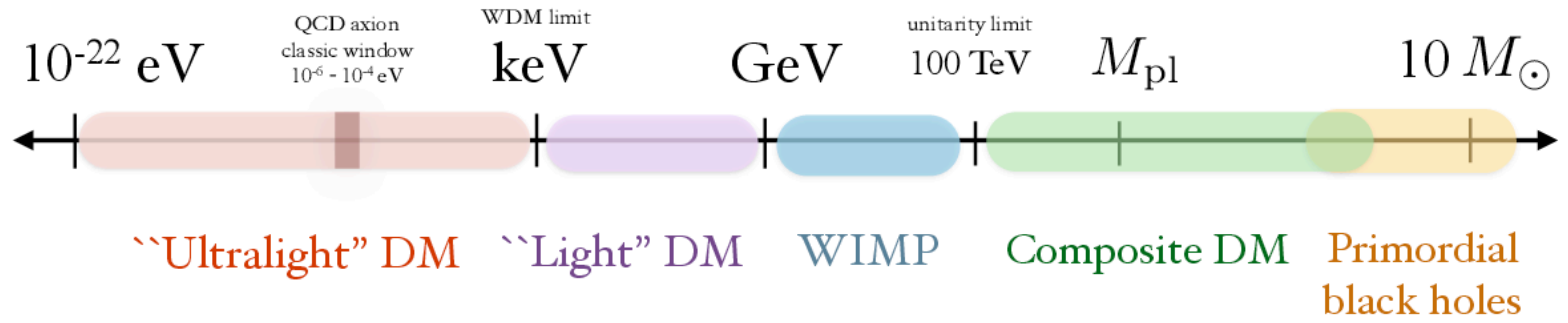
Emma Tolley

AI+ Astronomy
Hangzhou, China
22 October 2025

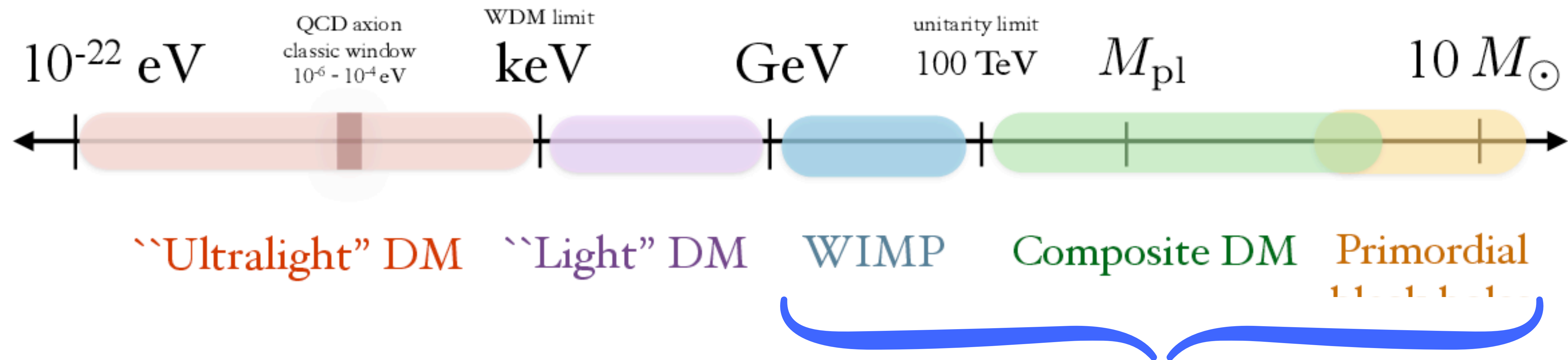
MATTER CONTENT OF THE UNIVERSE



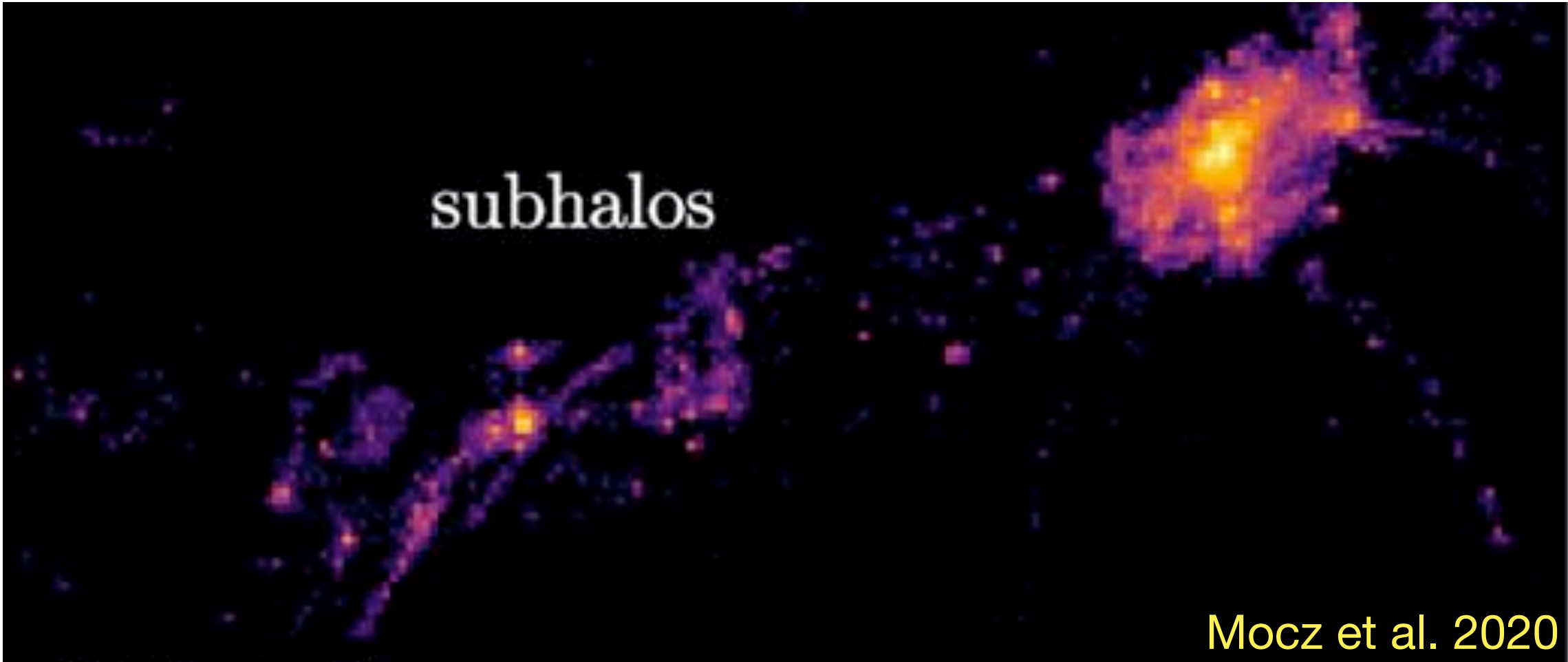
NATURE OF DARK MATTER



NATURE OF DARK MATTER

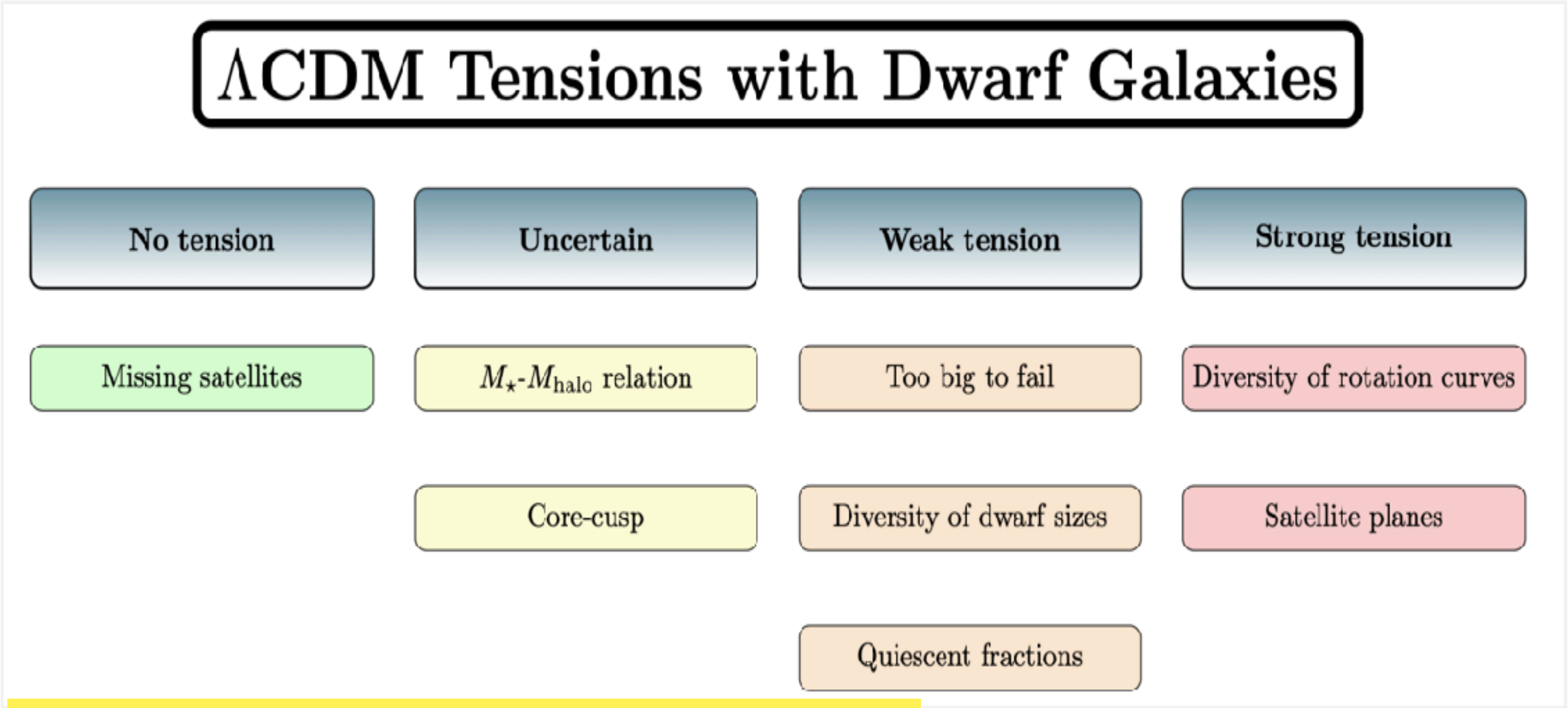


Cold Dark Matter (CDM): dark matter is a cold, collisionless fluid



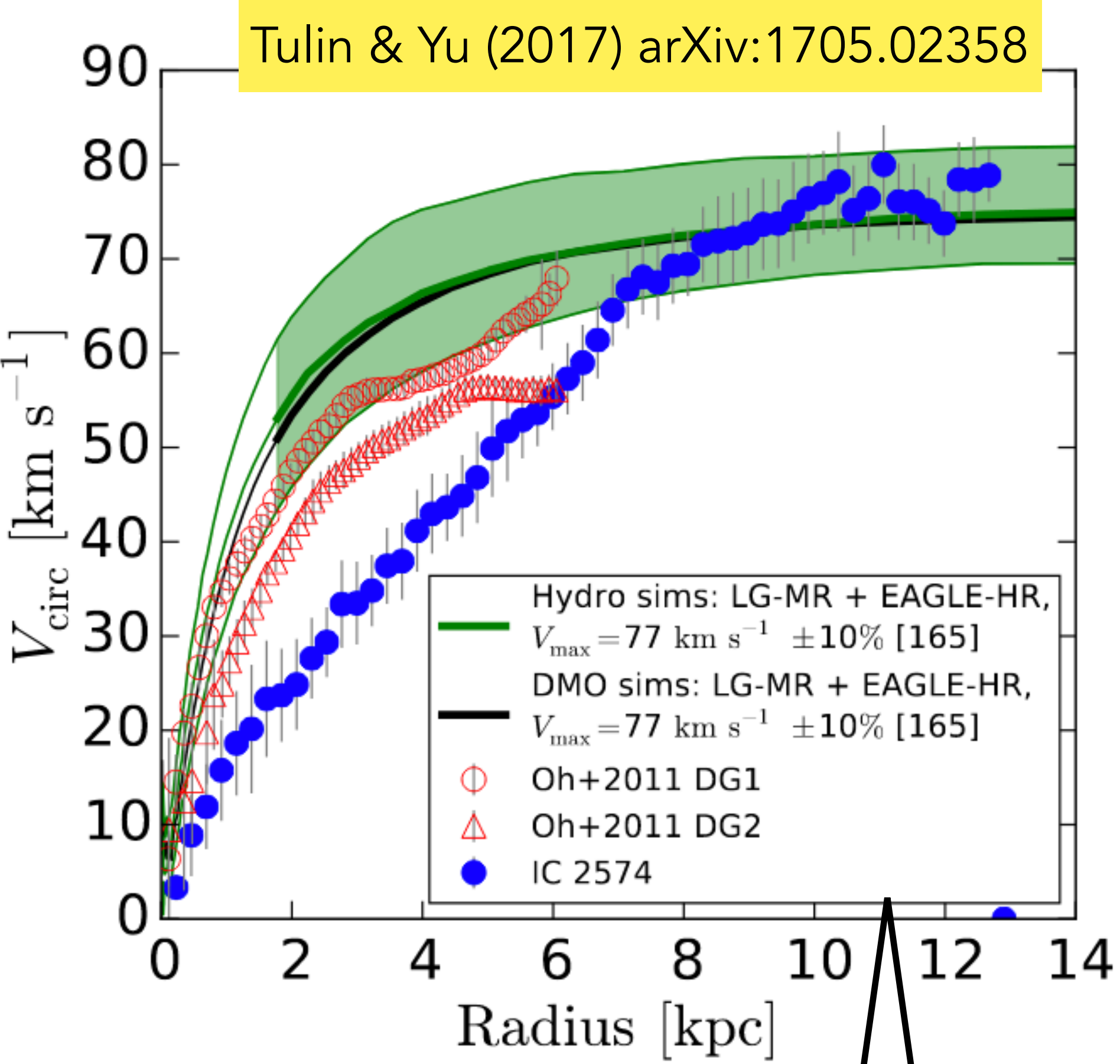
PROBLEMS WITH COLD DARK MATTER

Cold DM Predicts the large scale structure very well, but has some problems at smaller scales



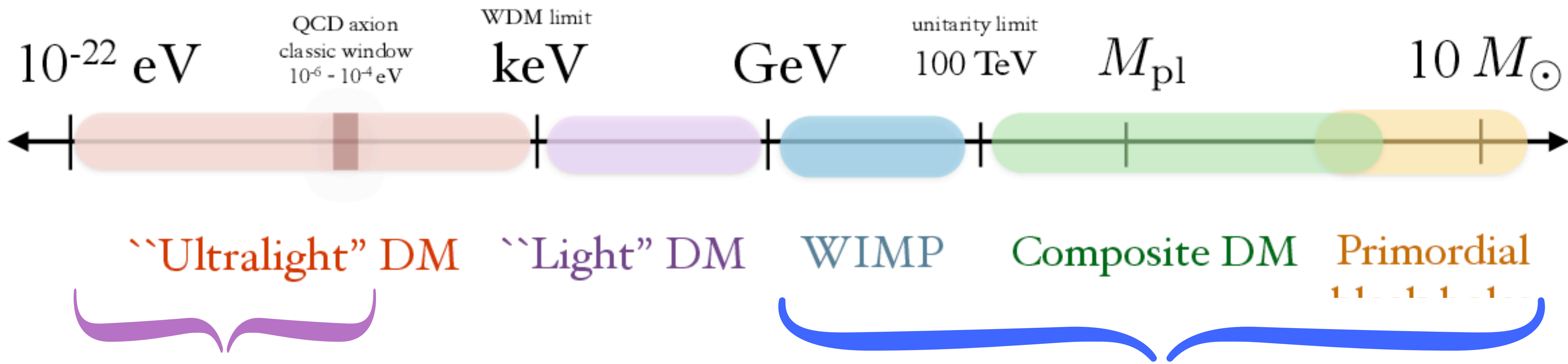
Bullock & Boylan-Kolchin (2017) arXiv:1707.04256

Sales et al (2022) arXiv:2206.05295



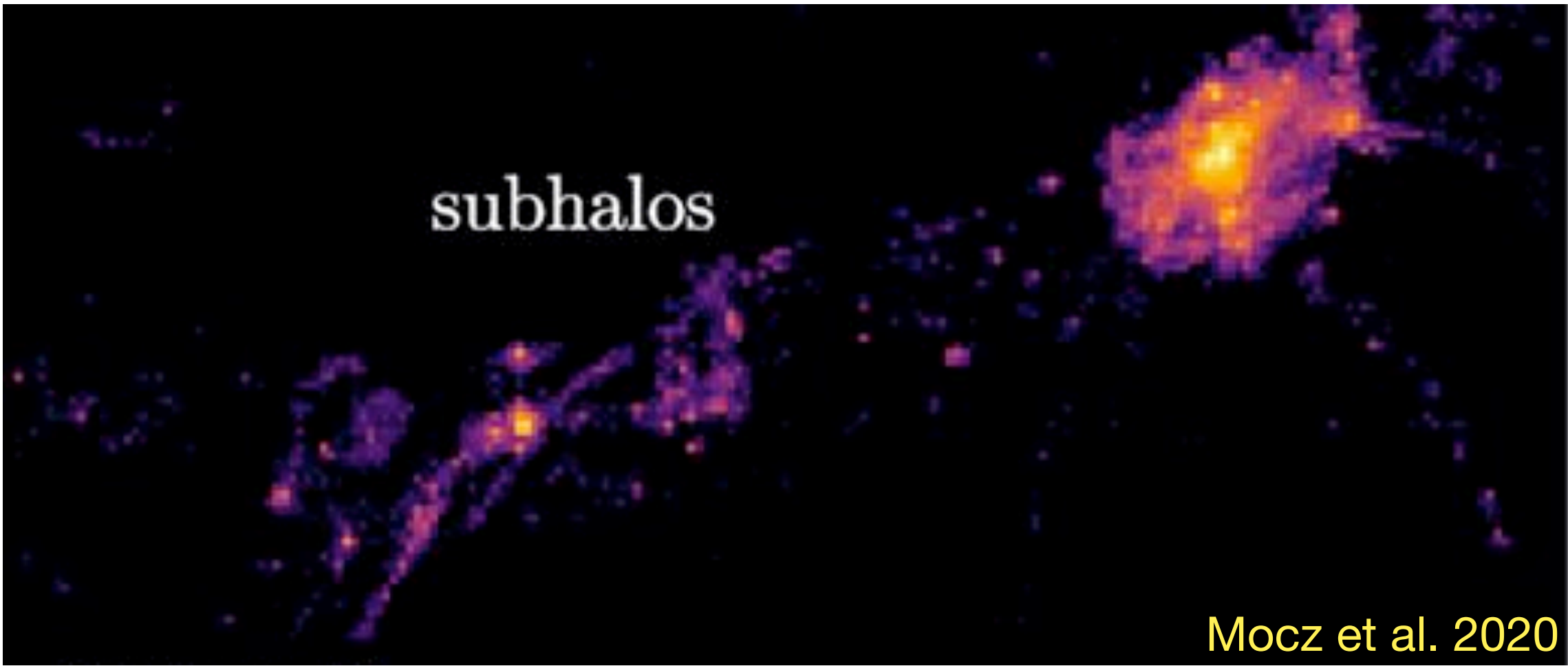
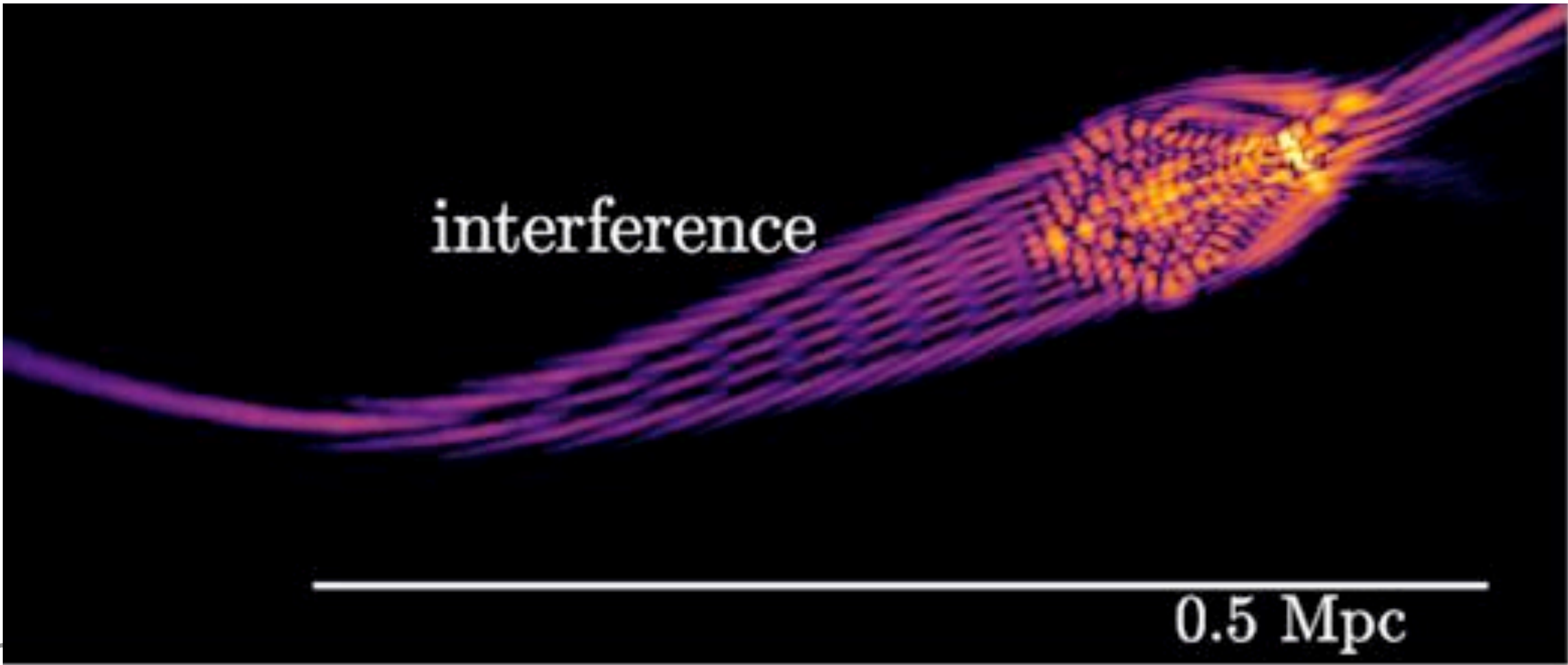
Dwarf galaxy which does not match simulation with baryonic feedback included

FUZZY VS COLD DARK MATTER



Fuzzy Dark Matter (FDM): dark matter is a quantum wave with a kpc-scale deBroglie wavelength

Cold Dark Matter (CDM): dark matter is a cold, collisionless fluid



Mocz et al. 2020

FUZZY VS COLD DARK MATTER

FDM obeys the
Shroedinger-Poisson Equations

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + mV\psi,$$

$$\nabla^2 V = 4\pi G(\rho - \bar{\rho}),$$

$$\rho \equiv |\psi|^2$$

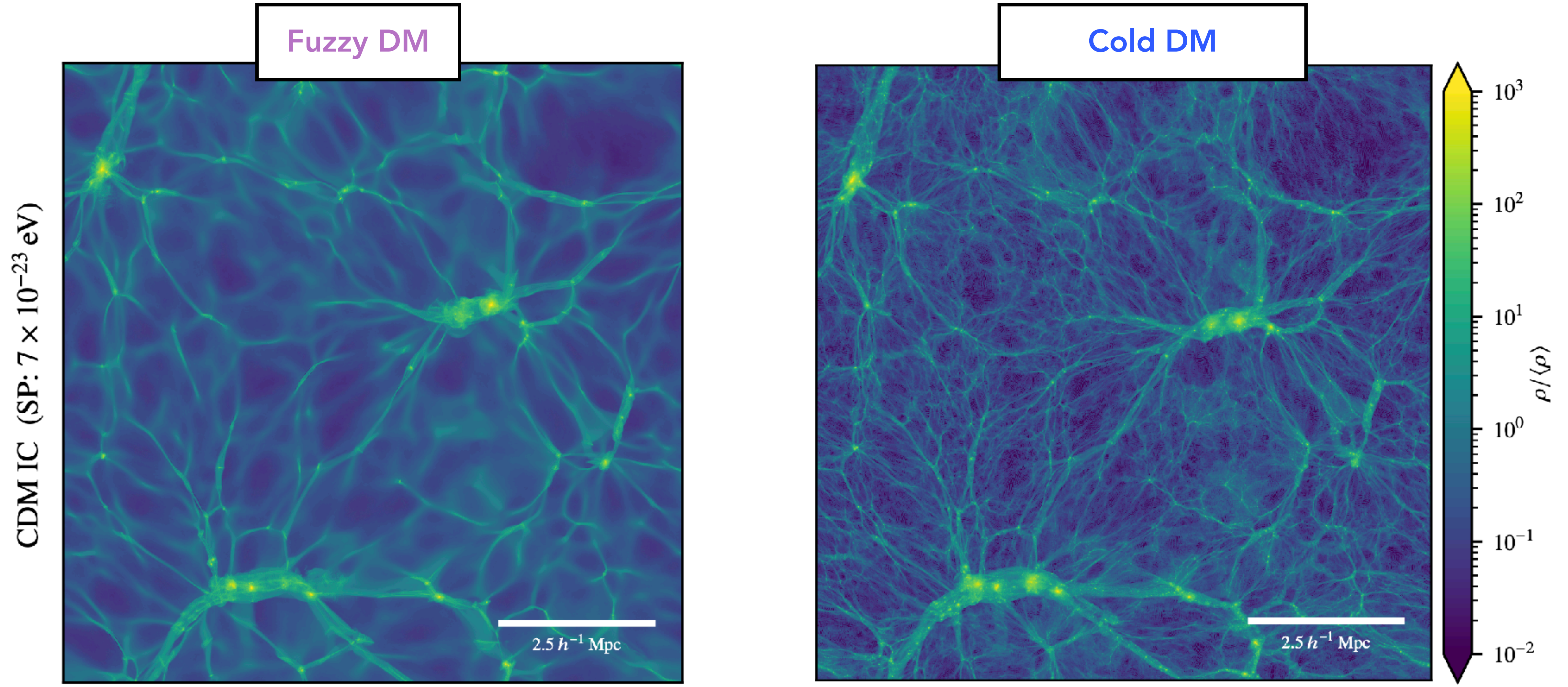
CDM obeys the
Vlasov-Poisson Equations

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} - \nabla V \cdot \frac{\partial f}{\partial \mathbf{v}} = 0,$$

$$\nabla^2 V = 4\pi G(\rho - \bar{\rho}),$$

$$\rho = \int f d^3v$$

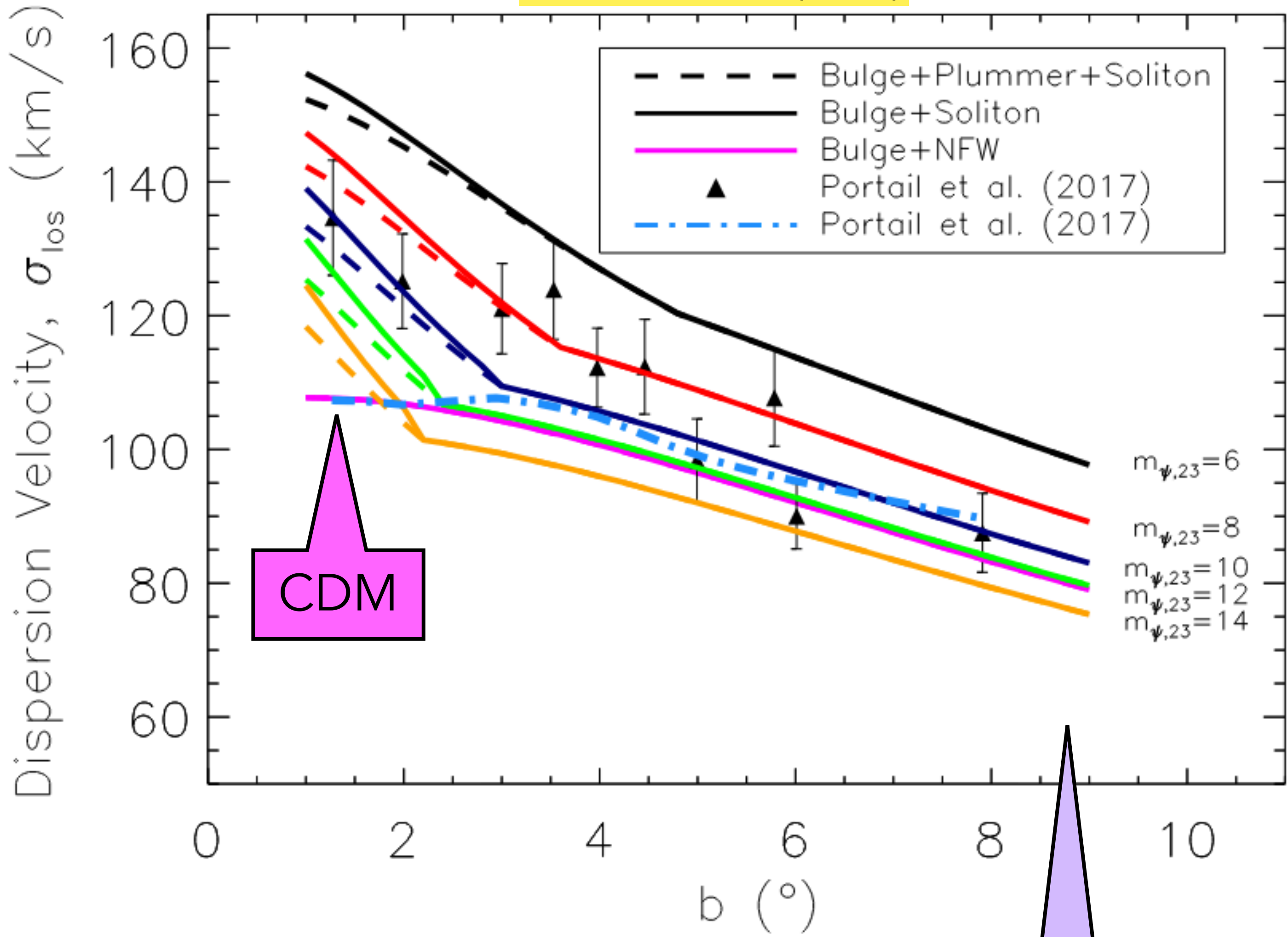
FUZZY VS COLD DARK MATTER



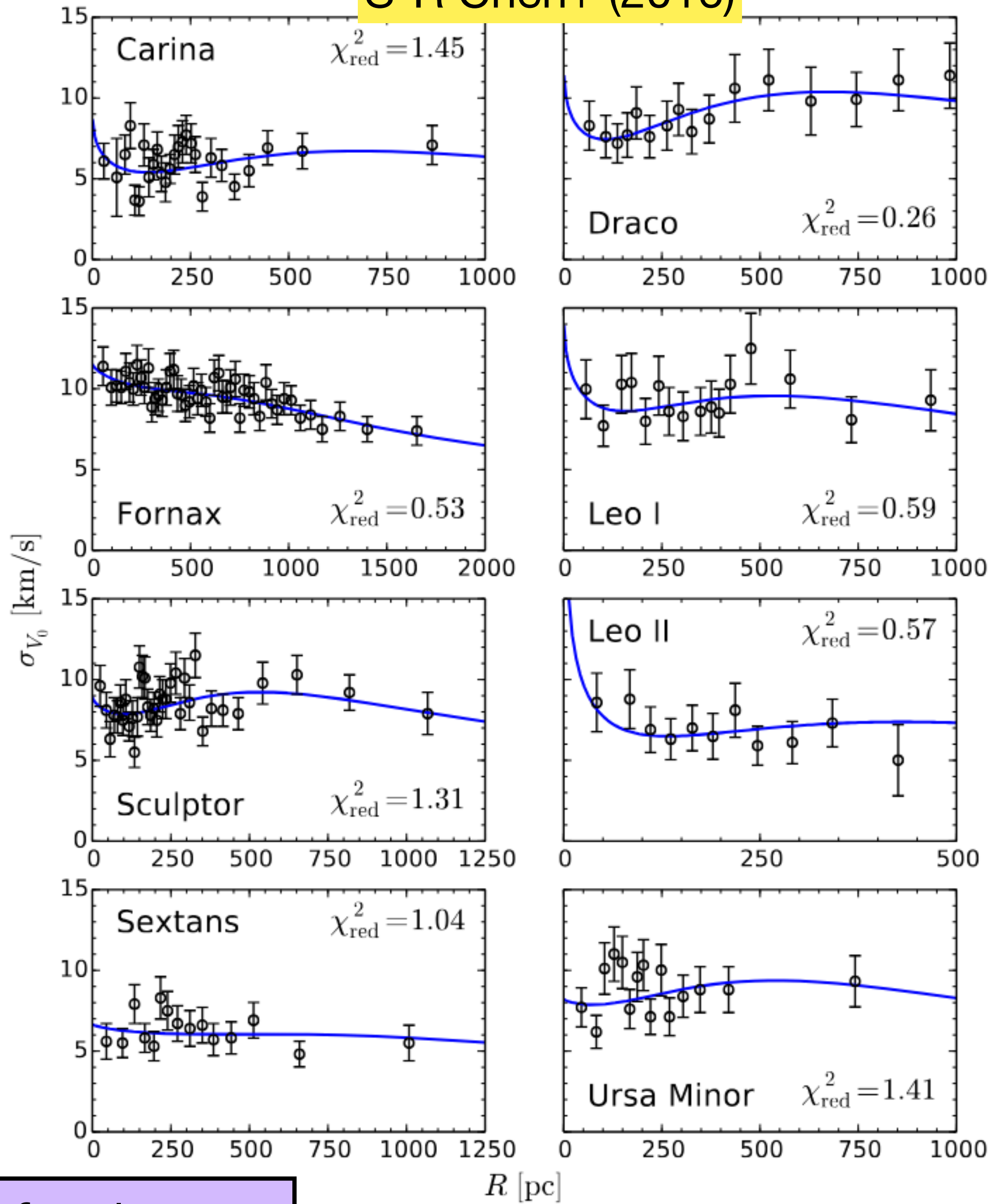
May & Springel (2022), arXiv:2209.14886

FUZZY DARK MATTER

I. De Martino+ (2020)



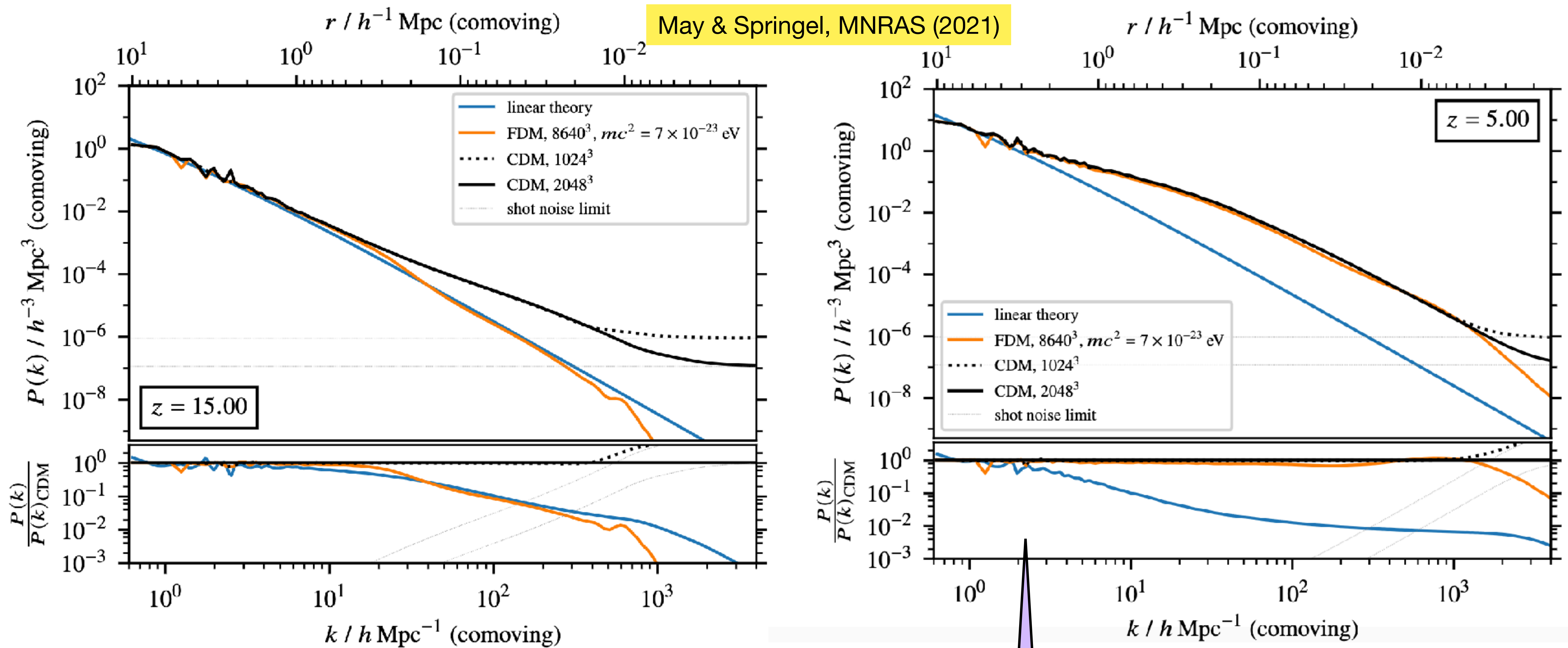
S-R Chen+ (2016)



FDM can explain halo profiles of our galaxy & many dwarf galaxies

FUZZY DARK MATTER

May & Springel, MNRAS (2021)



Existing simulations very limited in size (**computationally expensive**)

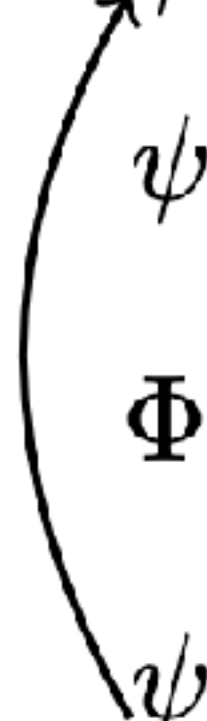
FUZZY DARK MATTER

Schroedinger-Poisson Equations

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + mV\psi,$$

$$\nabla^2 V = 4\pi G(\rho - \bar{\rho}),$$

Very **computationally expensive** due to requirement of small step size & fine resolution (need to resolve wave phenomena)


$$\begin{array}{ll} \psi \leftarrow e^{-i \frac{m}{\hbar} \frac{\Delta t}{2} \Phi} \psi & \text{kick} \\ \psi \leftarrow \text{IFFT} \left(e^{-i \frac{\hbar}{m} \frac{\Delta t}{2} k^2} \text{FFT}(\psi) \right) & \text{drift} \\ \Phi \leftarrow \text{IFFT} \left(-\frac{1}{k^2} \text{FFT}(4\pi Gm(|\psi|^2 - \langle |\psi|^2 \rangle)) \right) & \text{update potential} \\ \psi \leftarrow e^{-i \frac{m}{\hbar} \frac{\Delta t}{2} \Phi} \psi & \text{kick} \end{array}$$

$$\text{Choice of time step: } \Delta t < \min \left(\frac{4}{9\pi} \frac{m}{\hbar} a^2 \Delta x^2, 2\pi \frac{\hbar}{m} a \frac{1}{|\Phi_{\max}|} \right)$$

PHYSICS INFORMED MACHINE LEARNING

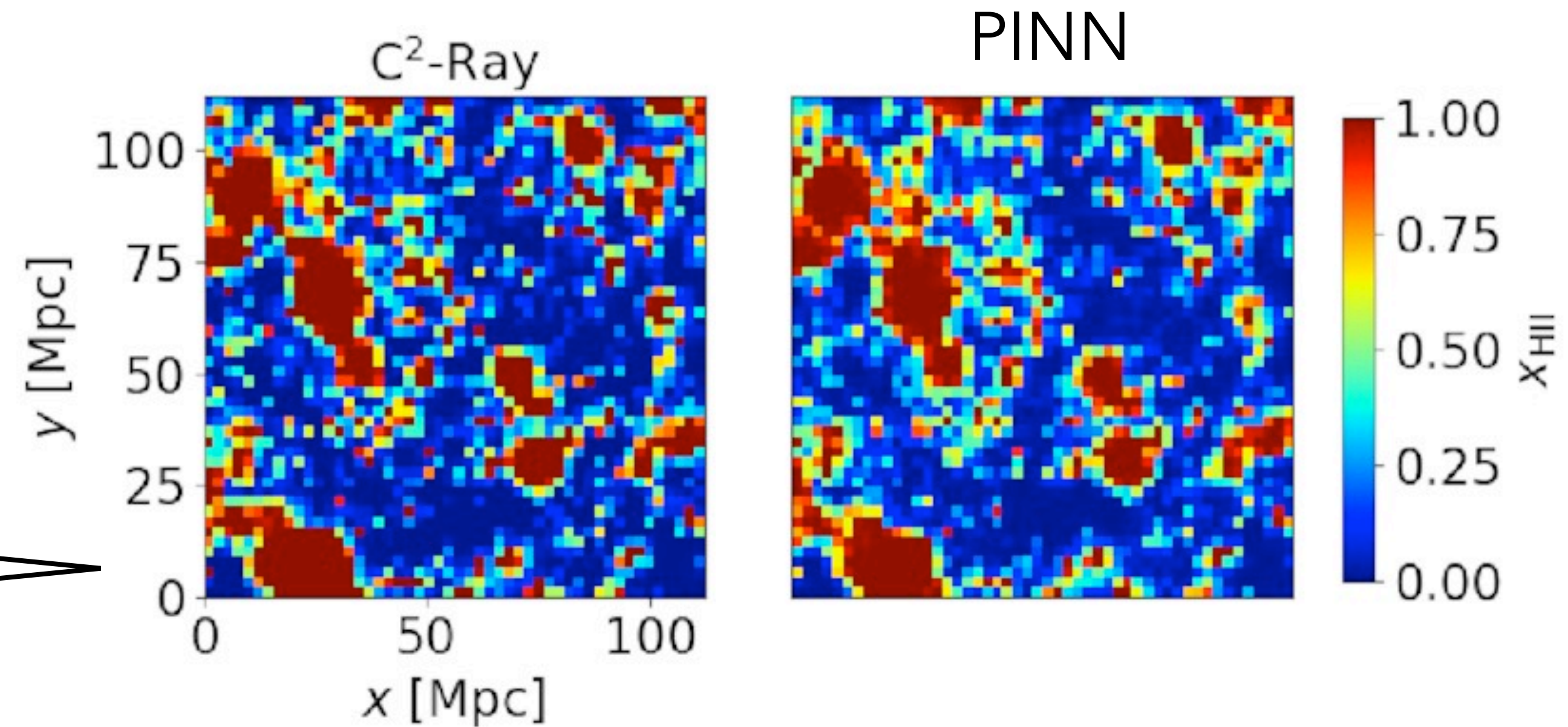
Physics-informed neural networks (PINNs) incorporate physical laws to efficiently solve PDEs

- Can be semi-supervised or **unsupervised** (no training data)
- Can take advantage of **AI hardware** like GPUs, tensor cores, etc
- Can easily **validate** network outputs using the PDE loss

Semi-supervised PINN can predict entire 4D reionization history with only 5 snapshots from true simulation and the constraint:

$$\frac{dx_{\text{HII}}}{dt} = (1 - x_{\text{HII}})\Gamma - C\alpha_B n_{\text{H}} x_{\text{HII}}^2$$

Training time: **1.5 hours** on one NVIDIA Tesla P100 16GB GPU



Korber, Bianco, Tolley, Kneib. MNRAS (2023) DOI: [10.1093/mnras/stad615](https://doi.org/10.1093/mnras/stad615)

PHYSICS INFORMED MACHINE LEARNING

Schroedinger-Poisson Equations

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + mV\psi,$$

$$\nabla^2 V = 4\pi G(\rho - \bar{\rho}),$$

$$\rho \equiv |\psi|^2$$

Can we develop a PINN to solve for ψ ?

PHYSICS INFORMED MACHINE LEARNING

Schroedinger-Poisson Equations

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + mV\psi,$$

$$\nabla^2 V = 4\pi G(\rho - \bar{\rho}),$$

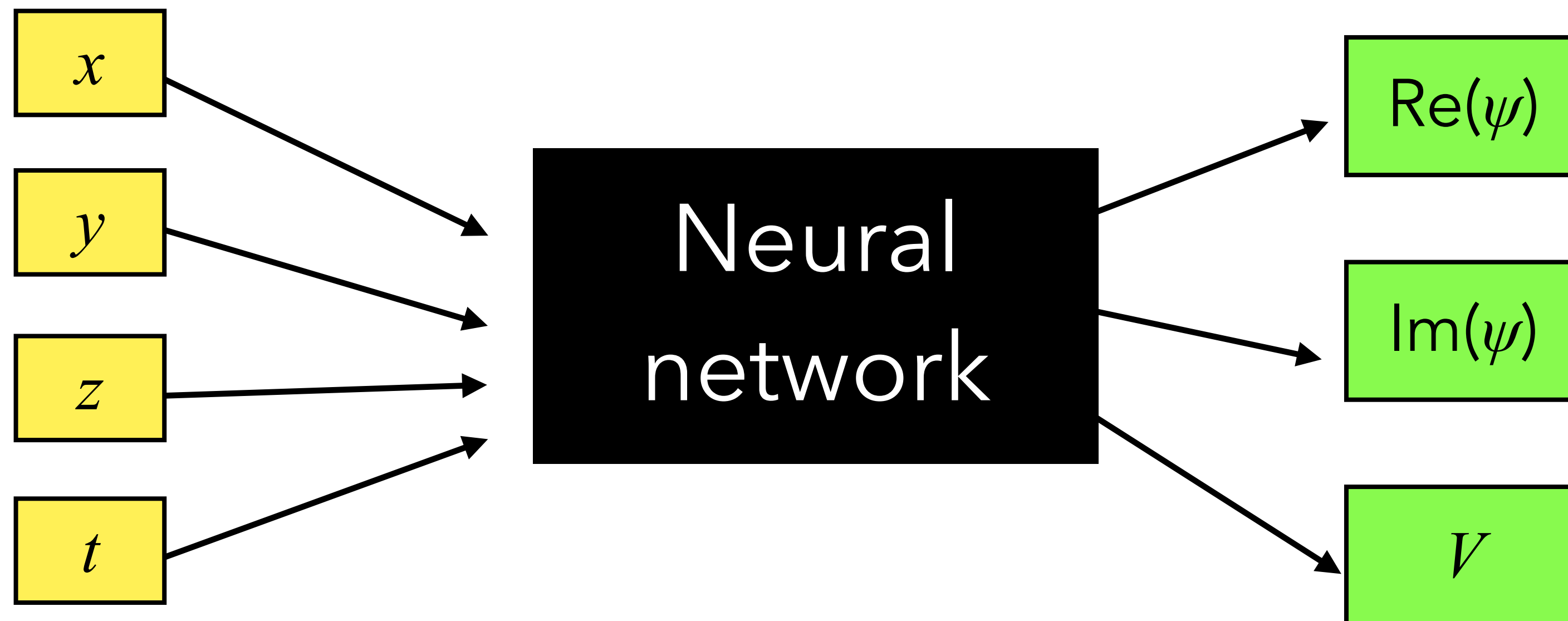
$$\rho \equiv |\psi|^2$$

Theorem (Cybenko, 1989)

Let σ be any continuous sigmoidal function. Then, the finite sums of the form

$$g(x) = \sum_{j=1}^N w_j^2 \sigma((w_j^1)^T x + b_j^1)$$

are dense in $C(I_d)$.



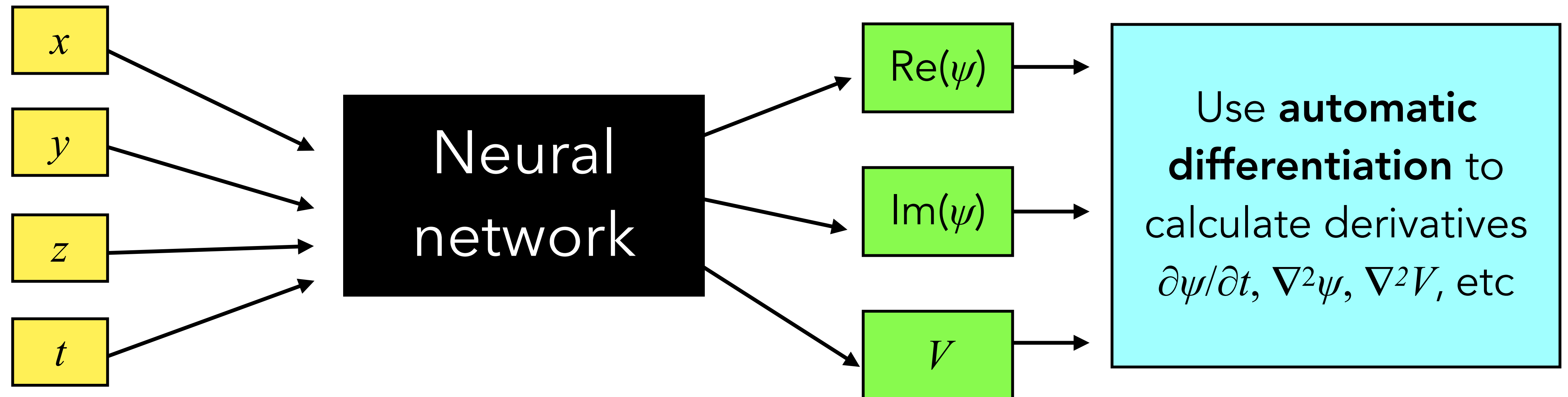
PHYSICS INFORMED MACHINE LEARNING

Schroedinger-Poisson Equations

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + mV\psi,$$

$$\nabla^2 V = 4\pi G(\rho - \bar{\rho}),$$

$$\rho \equiv |\psi|^2$$



PHYSICS INFORMED MACHINE LEARNING

Schroedinger-Poisson Equations

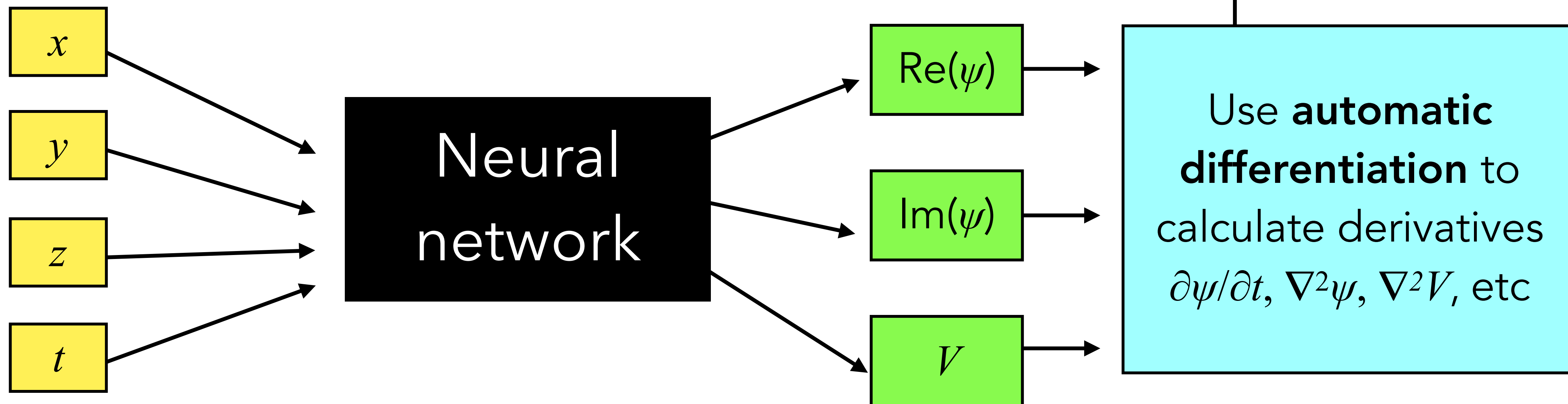
$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + mV\psi,$$

$$\nabla^2 V = 4\pi G(\rho - \bar{\rho}),$$

$$\rho \equiv |\psi|^2$$

Construct physics-informed loss:

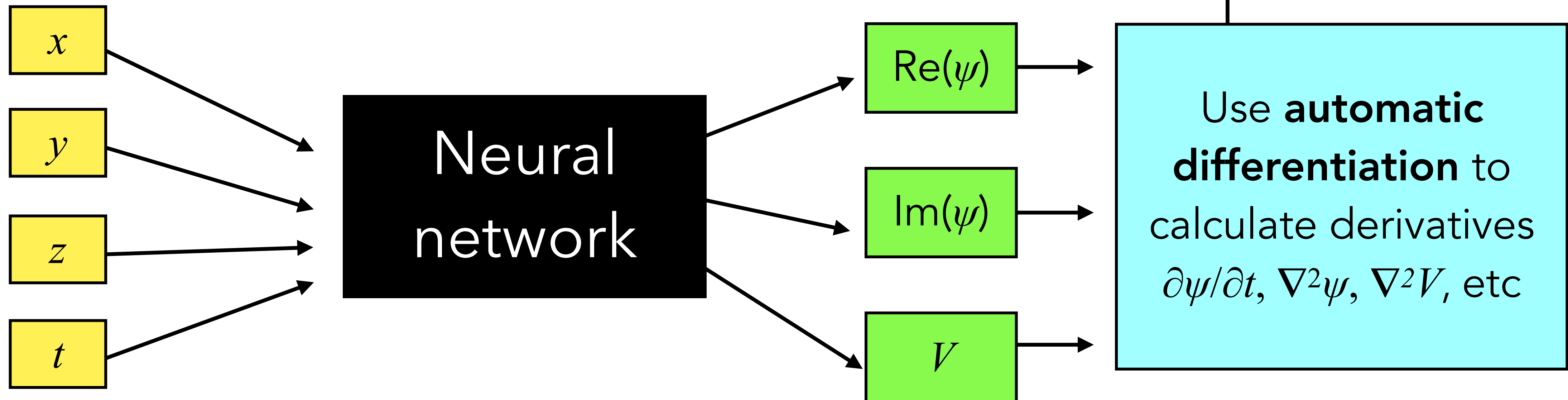
$$L = |(i\partial\psi/\partial t + \nabla^2\psi/2 - mV\psi) + (\nabla^2V - 4G|\psi|^2 + 1)|^2$$



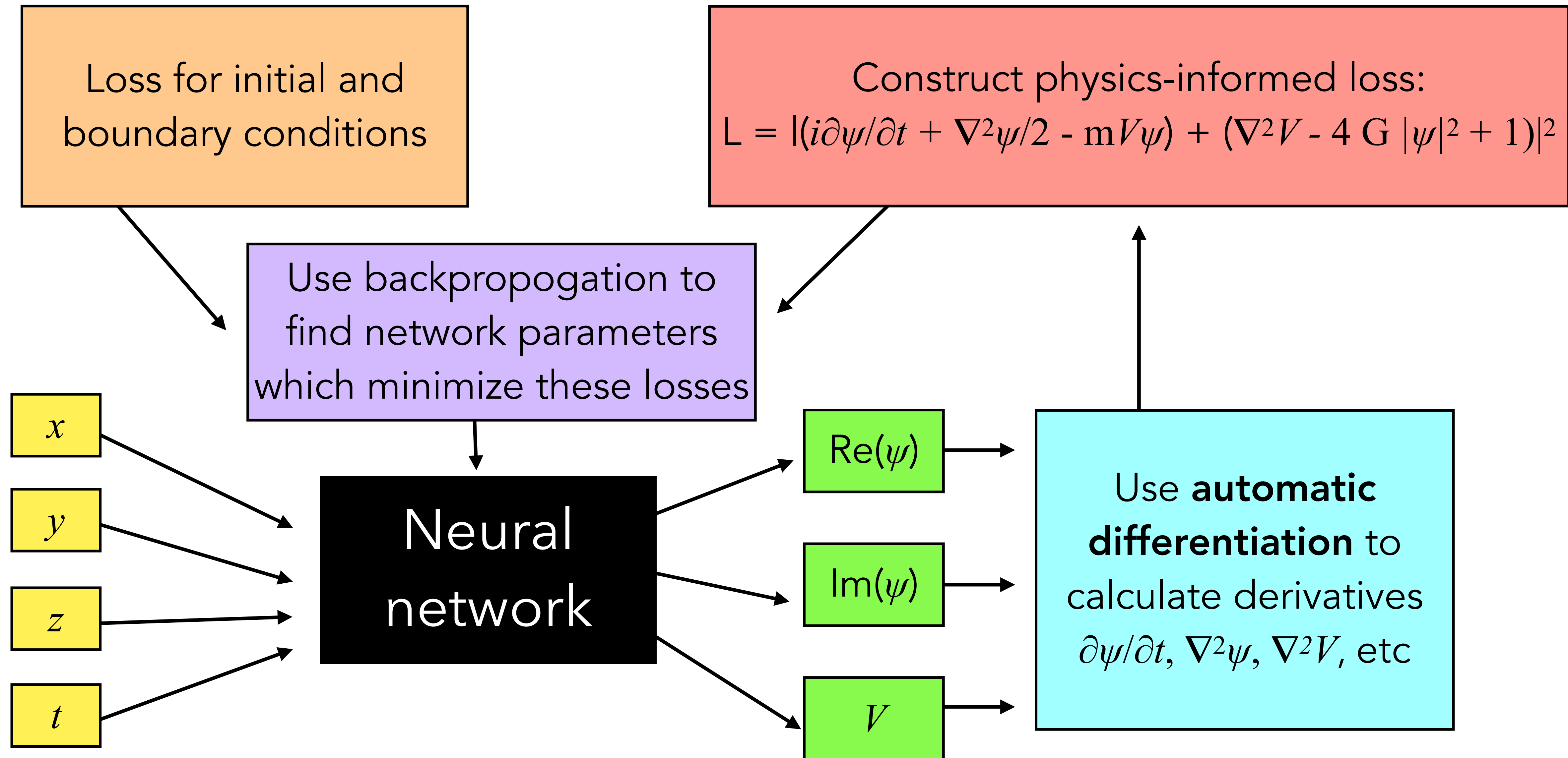
PHYSICS INFORMED MACHINE LEARNING

Loss for initial and boundary conditions

Construct physics-informed loss:
$$L = |i\partial\psi/\partial t + \nabla^2\psi/2 - mV\psi| + (\nabla^2V - 4G|\psi|^2 + 1)|^2$$



PHYSICS INFORMED MACHINE LEARNING

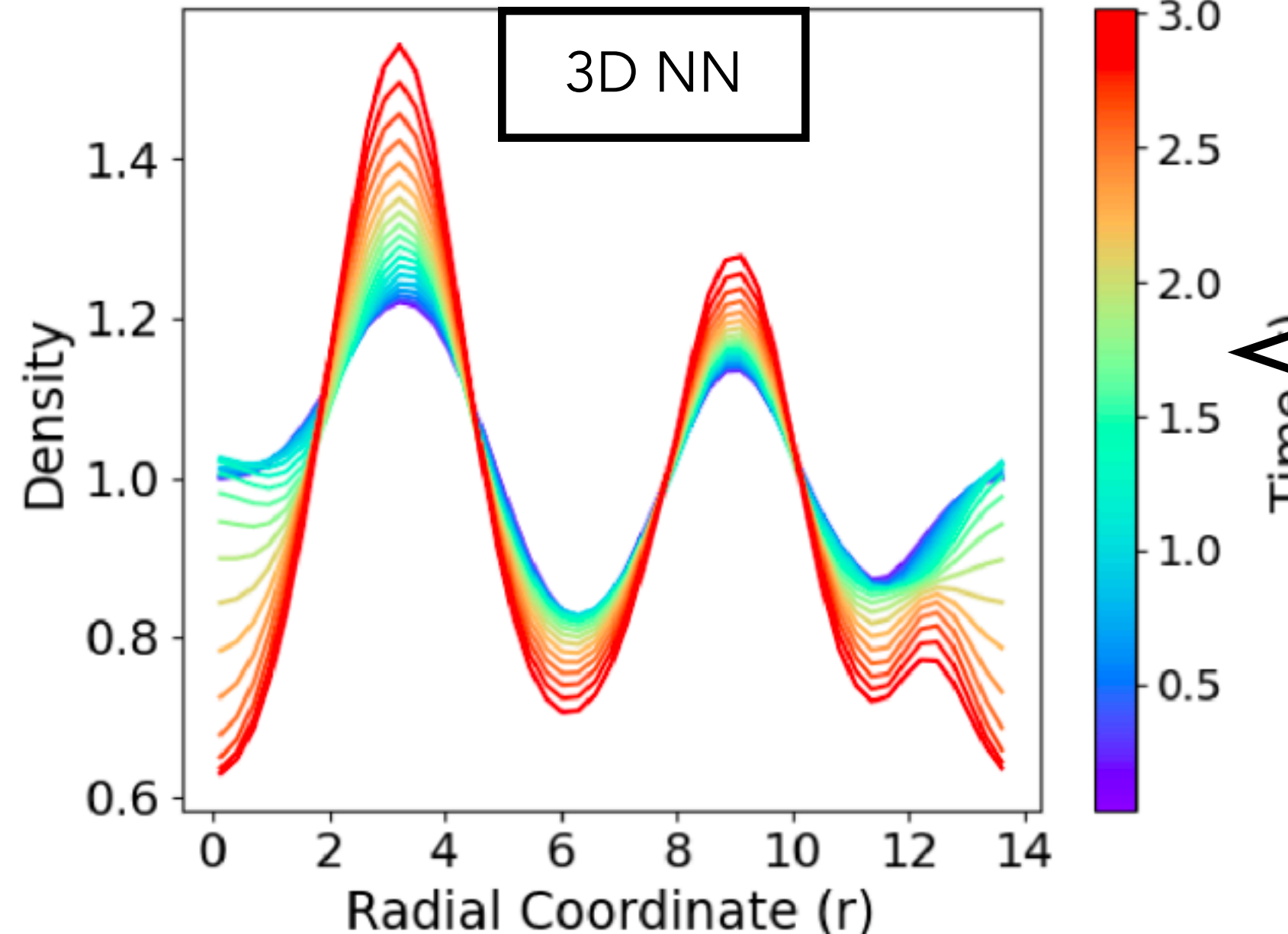
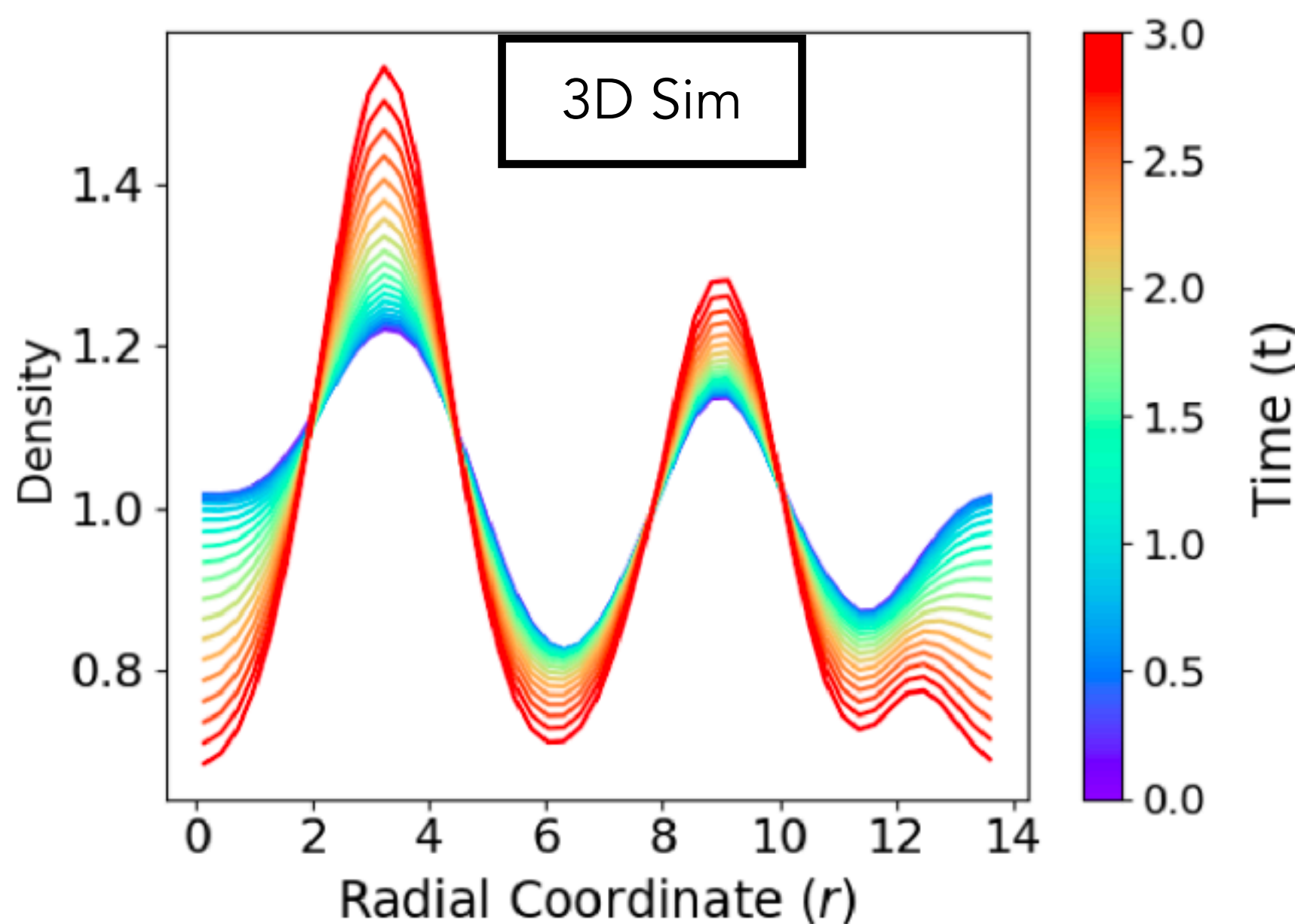
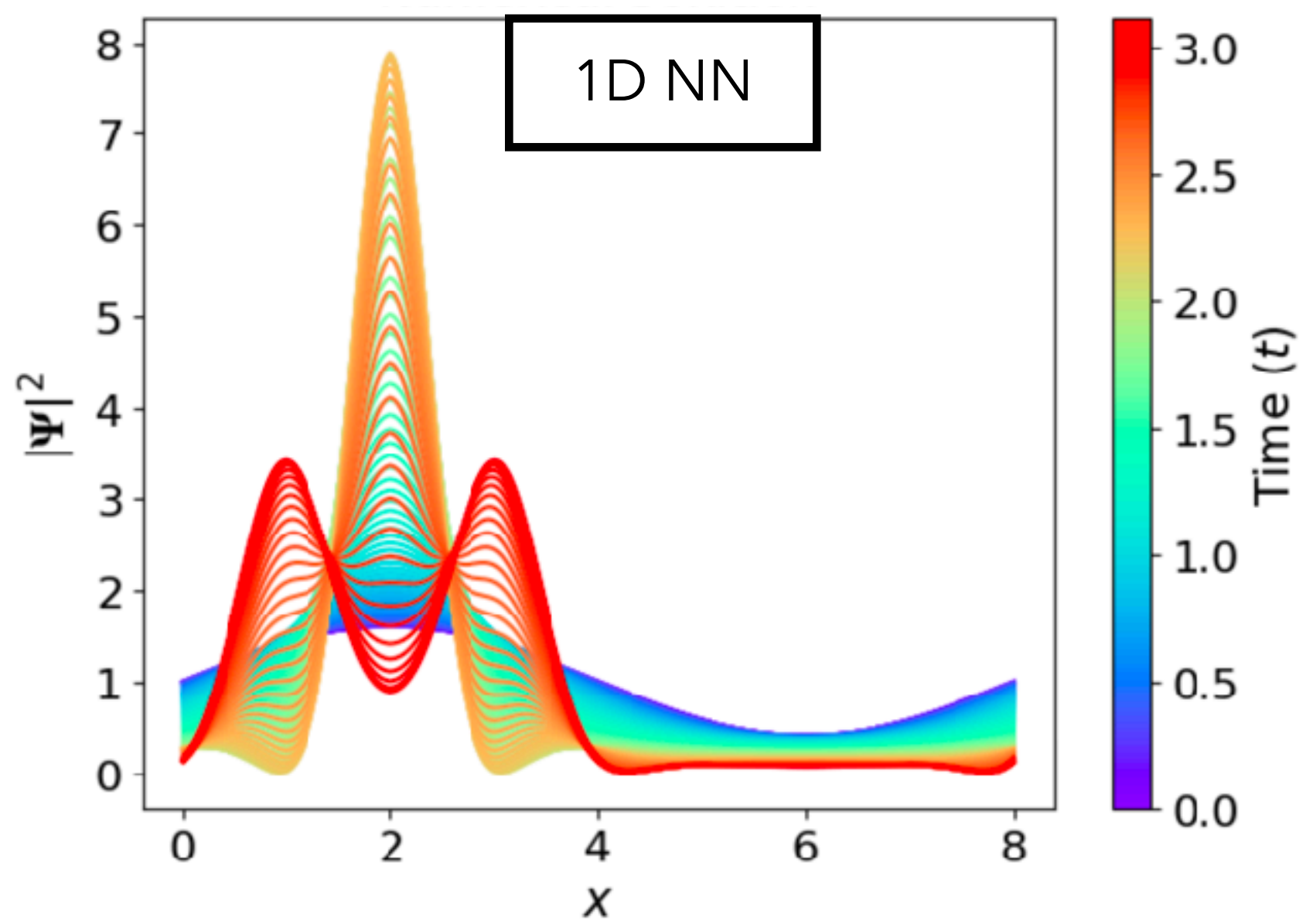
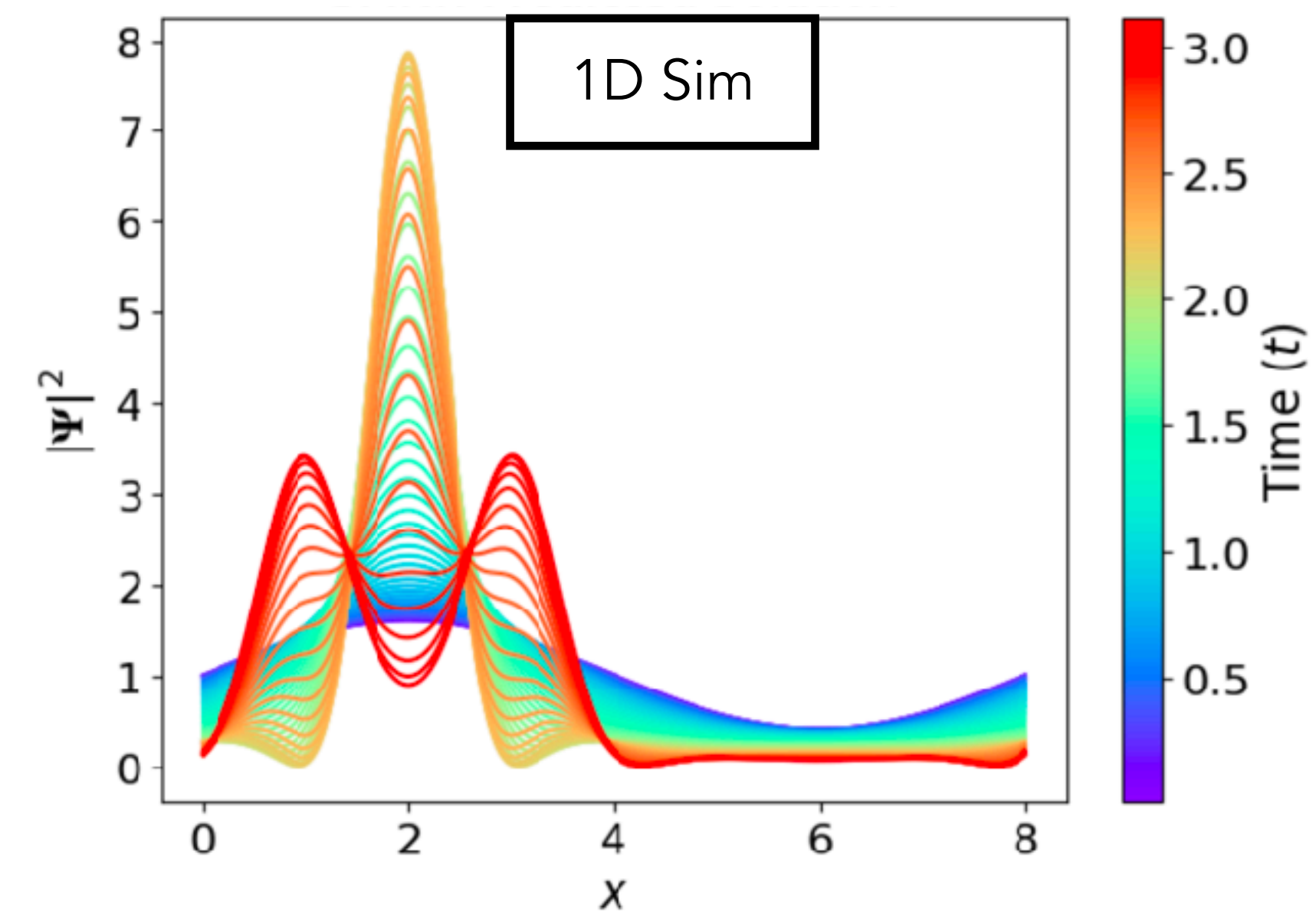


SOLVING FUZZY DARK MATTER



Ashutosh Mishra

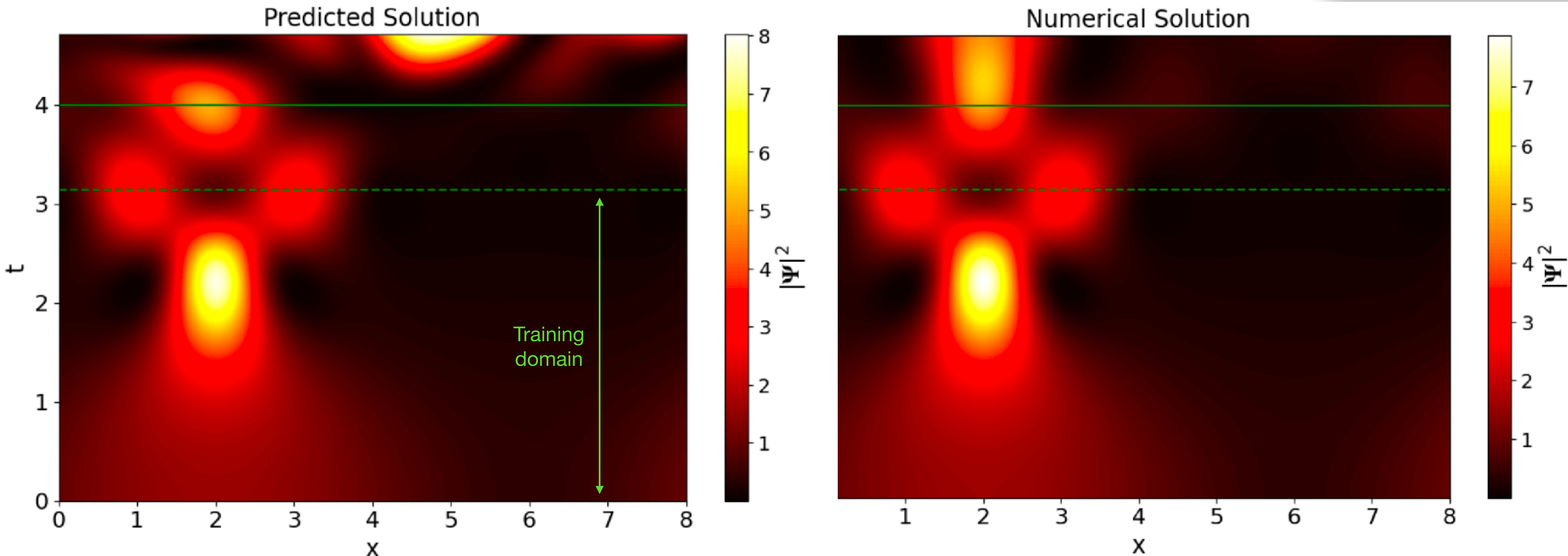
Mishra & Tolley 2025,
ApJ **988** 114



Unsupervised neural network predicting Fuzzy DM dynamics using only physics constraints and initial conditions

SOLVING FUZZY DARK MATTER

Mishra & Tolley 2025,
ApJ **988** 114



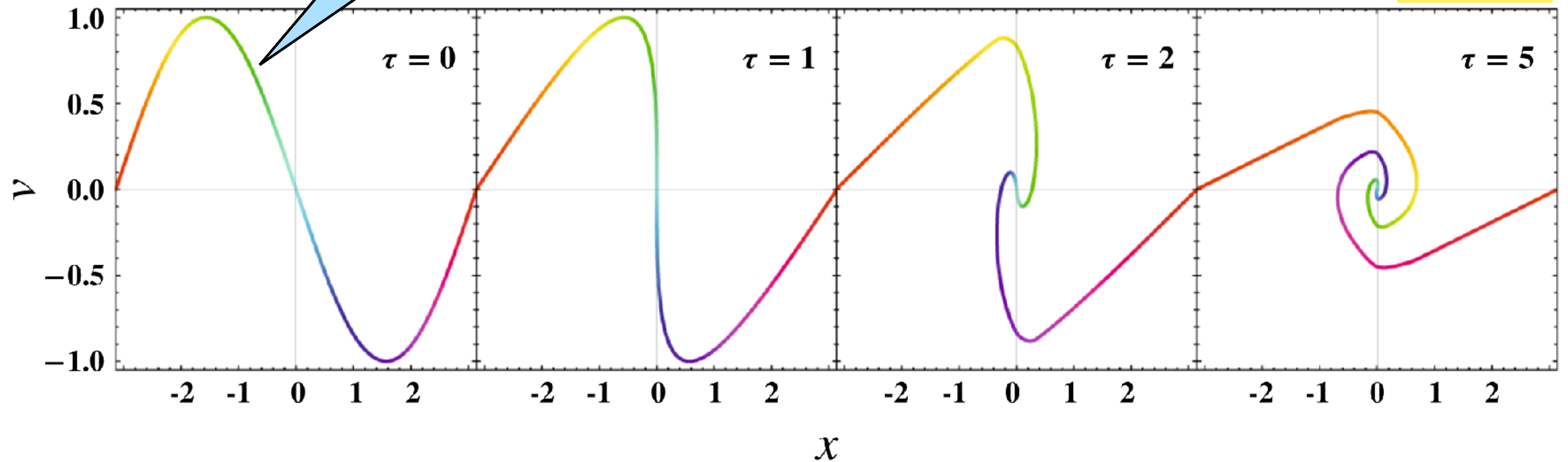
WHAT ABOUT CDM?



COLD DARK MATTER

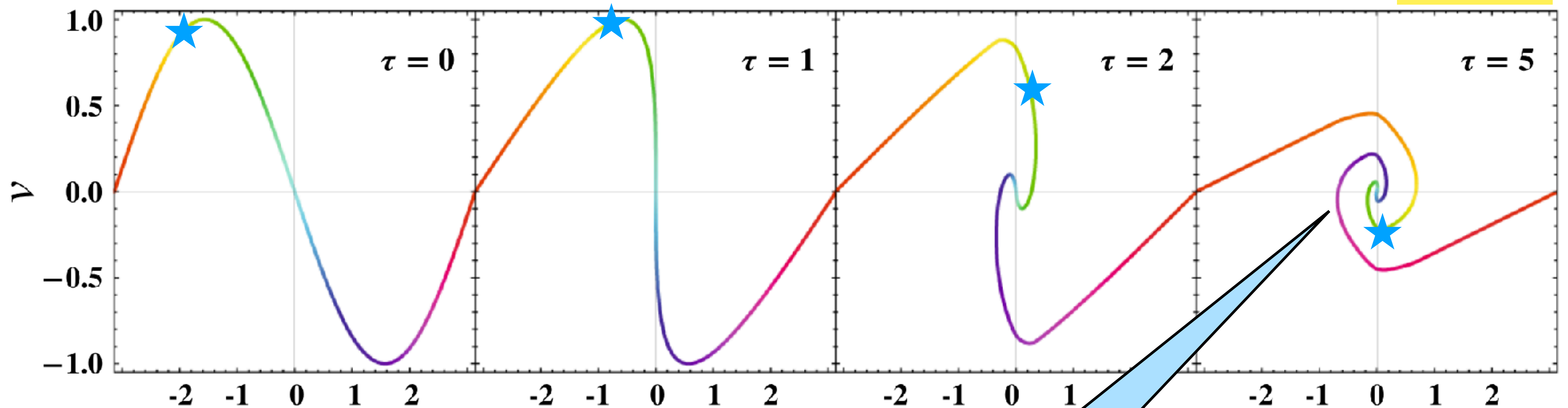
Cold: vanishing velocity dispersion

Rampf 2021



COLD DARK MATTER

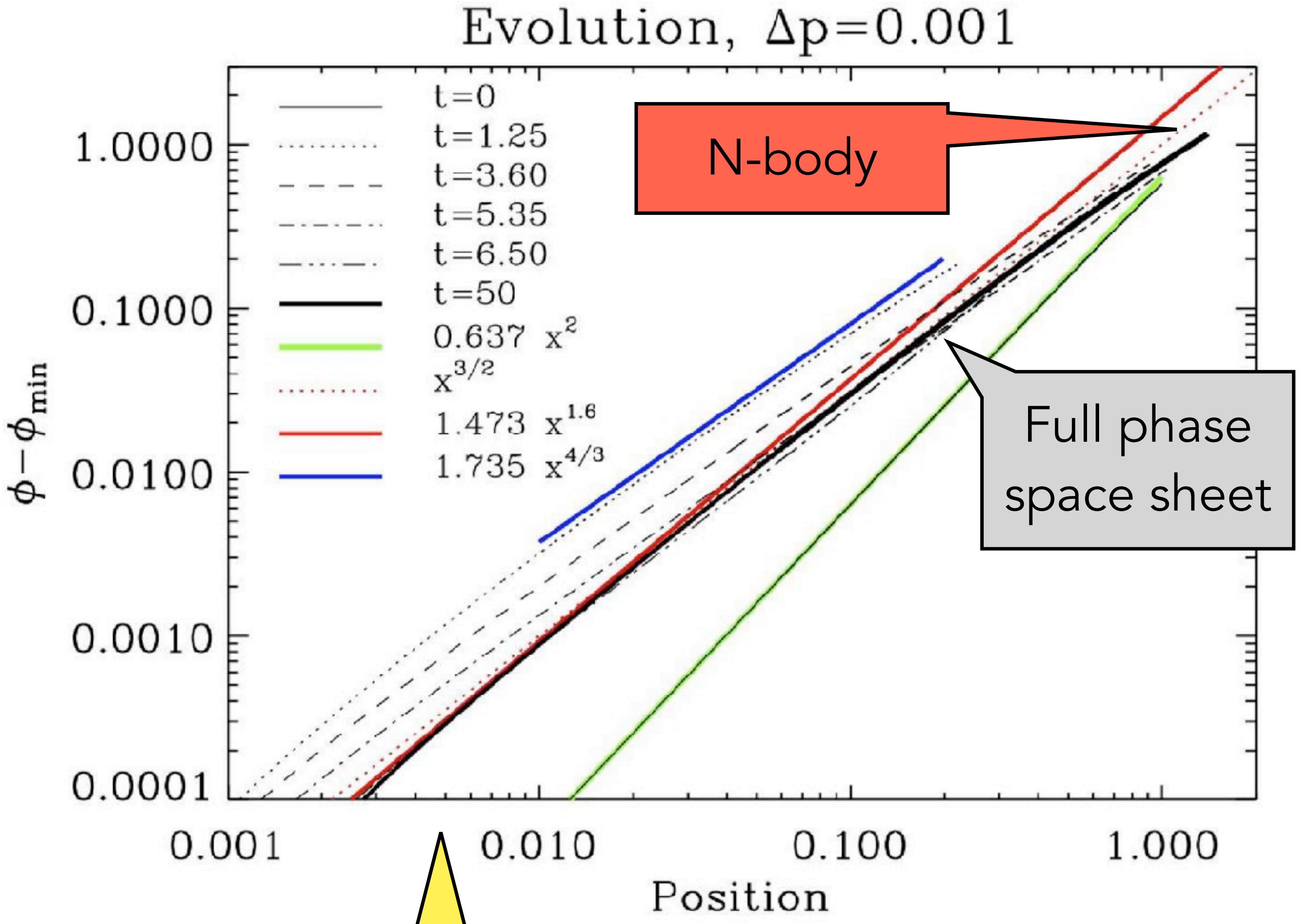
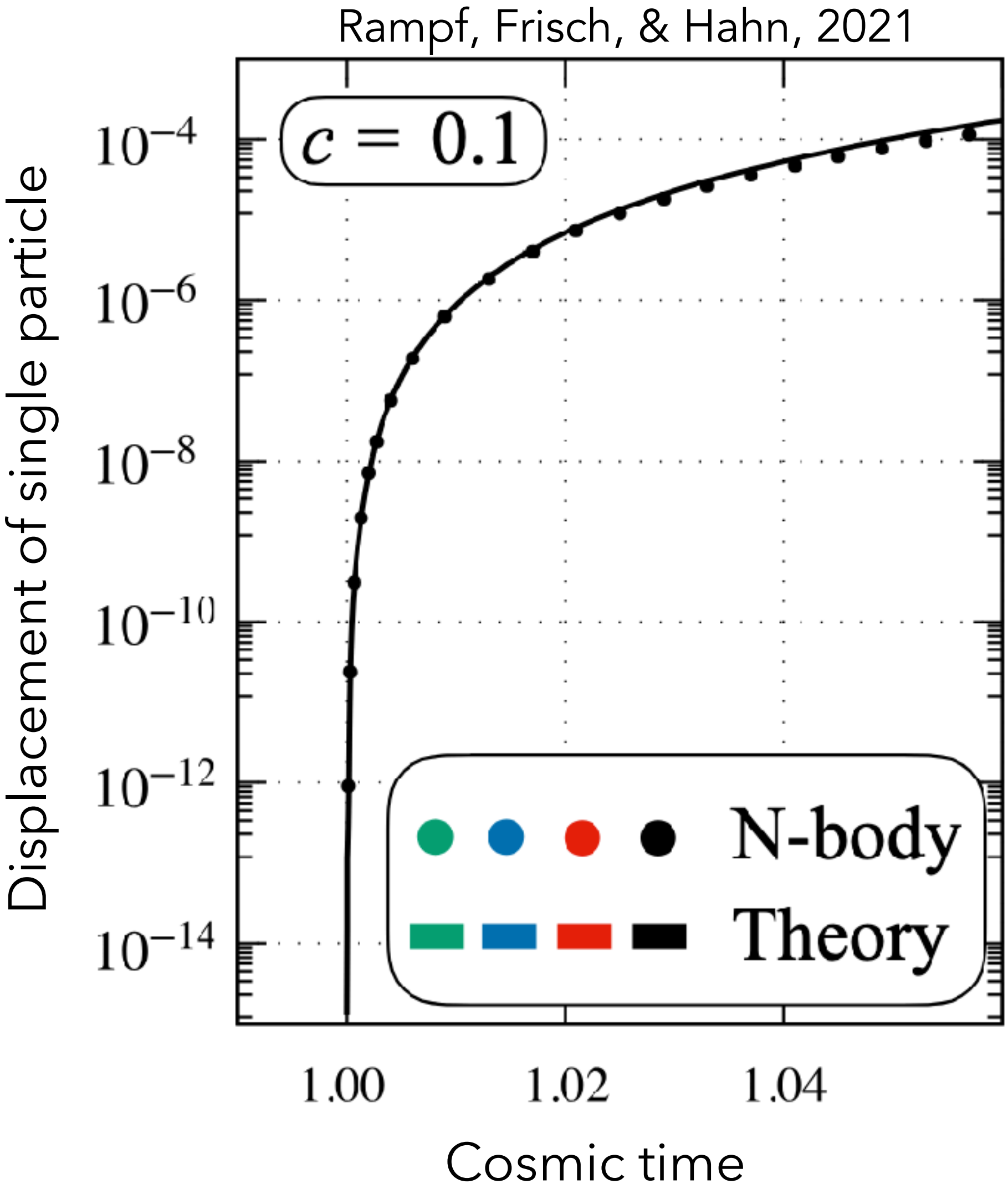
Rampf 2021



N-body simulation evolves points along this sheet in phase space

COLD DARK MATTER

Colombi & Touma 2014

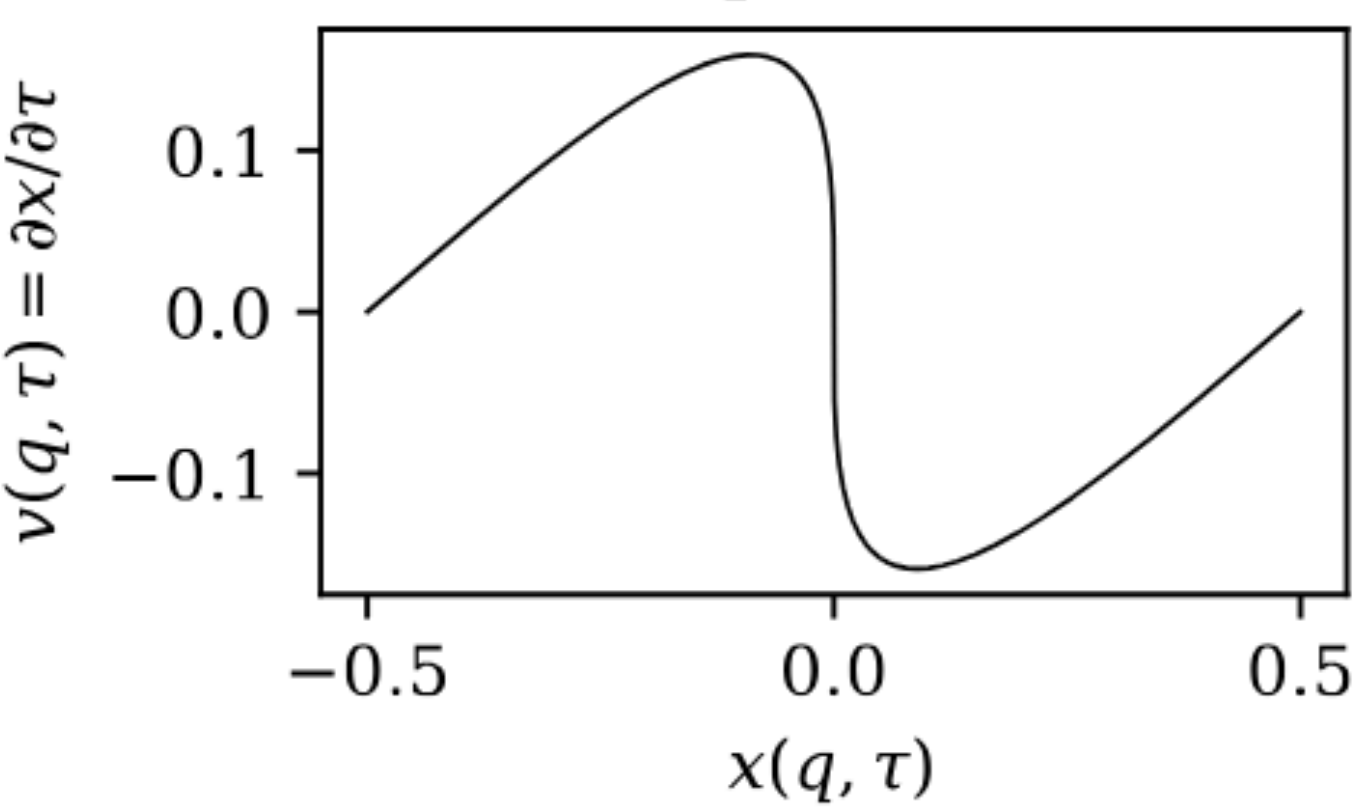


Deep learning...?

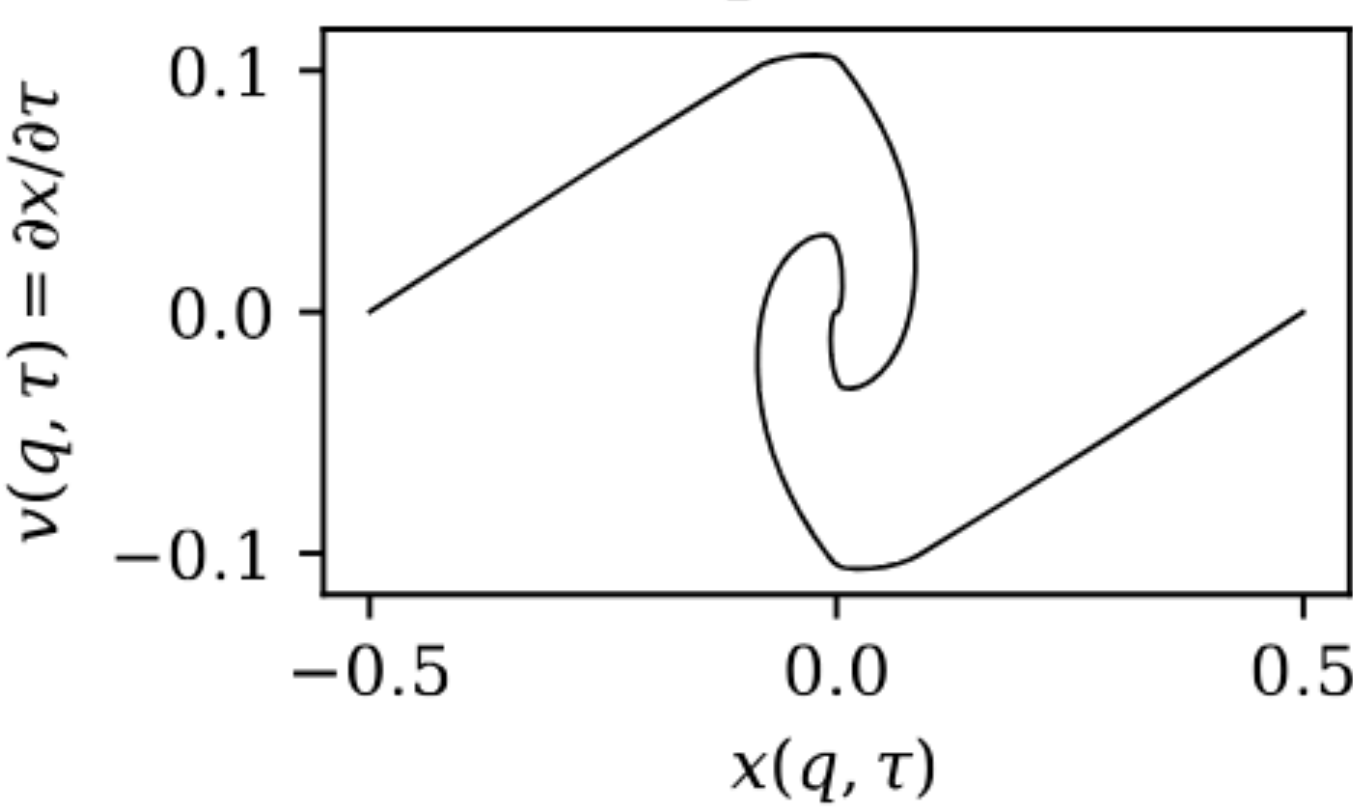
COLD DARK MATTER

Cerardi, Tolley, Mishra, submitted to MNRAS

Phase Space $\tau = 1.01$

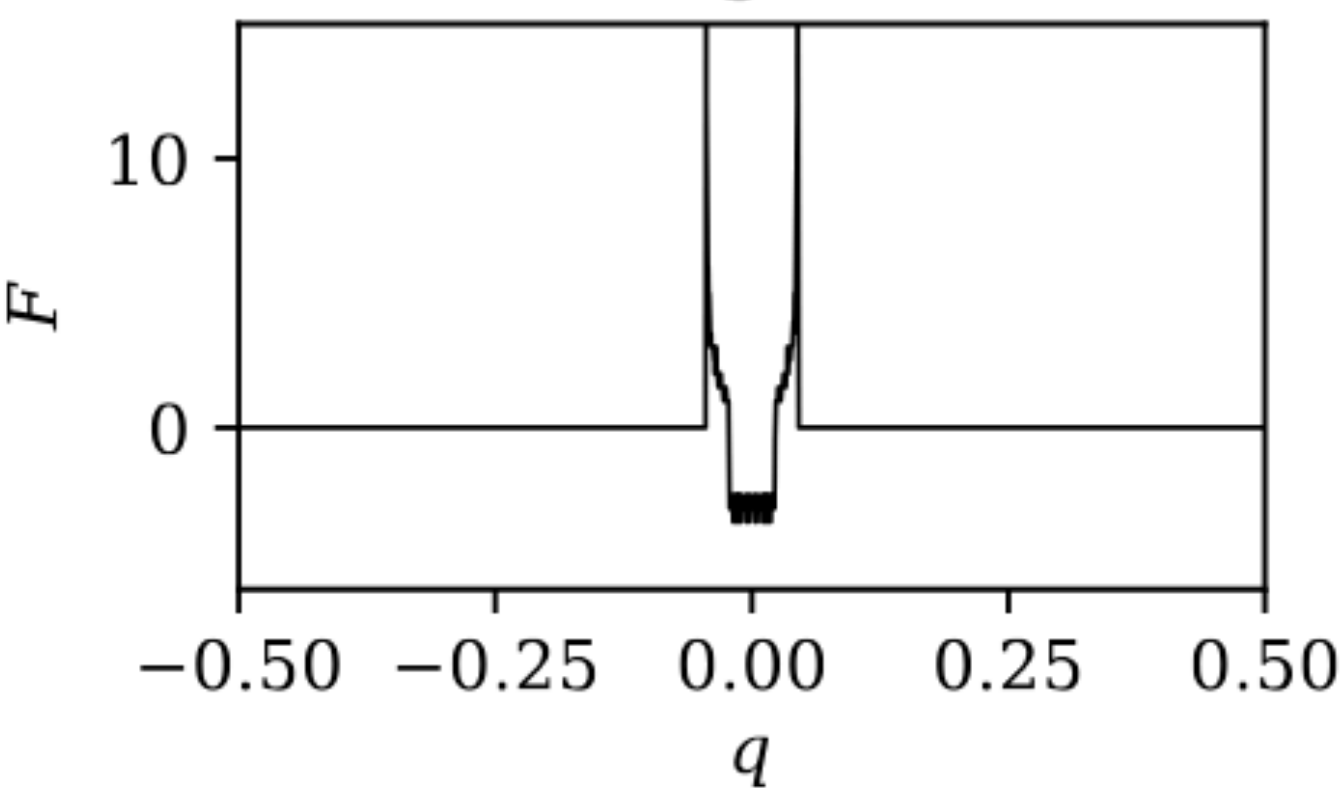


Phase Space $\tau = 3.01$

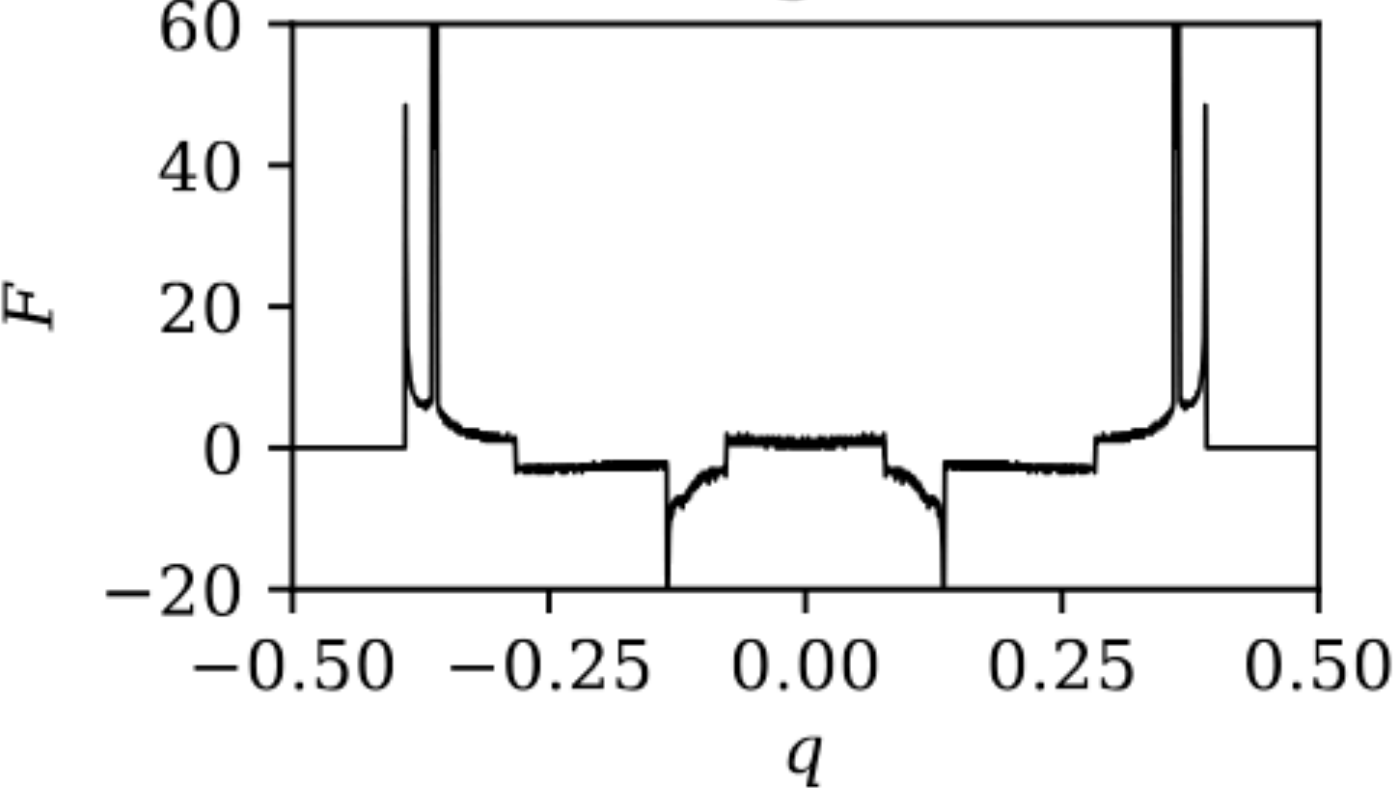


Discontinuous force ->
discontinuous acceleration, very
difficult to model with traditional
neural network

Free-Streaming Force $\tau = 1.01$



Free-Streaming Force $\tau = 3.01$



~~Theorem (Cybenko, 1989)~~

~~Let σ be any continuous sigmoidal function. Then, the finite sums of the form~~

$$g(x) = \sum_{j=1}^N w_j^2 \sigma((w_j)^T x + b_j^1)$$

~~are dense in $C(I_d)$.~~

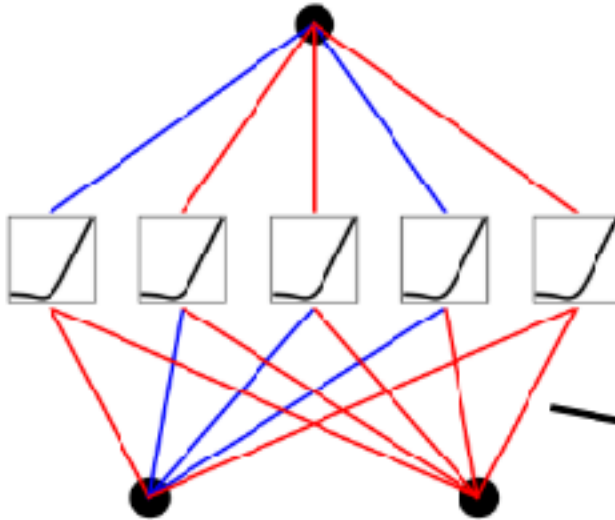
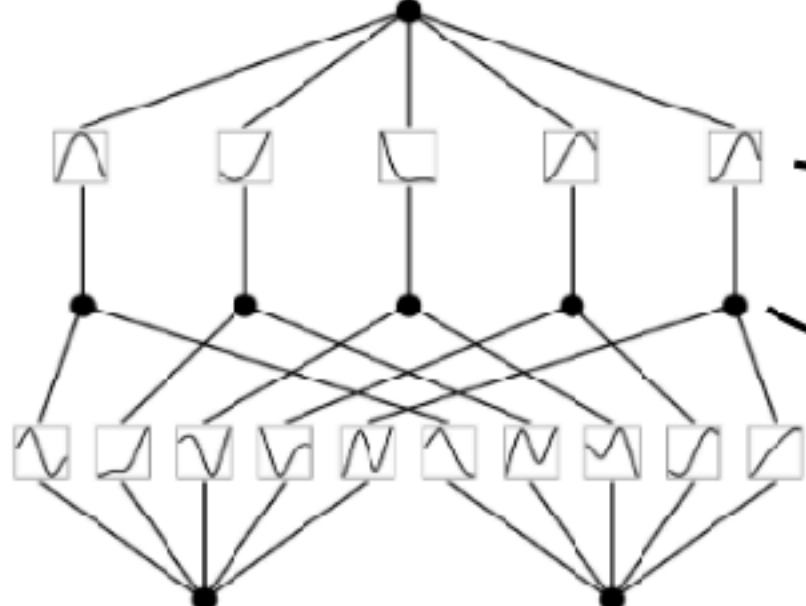
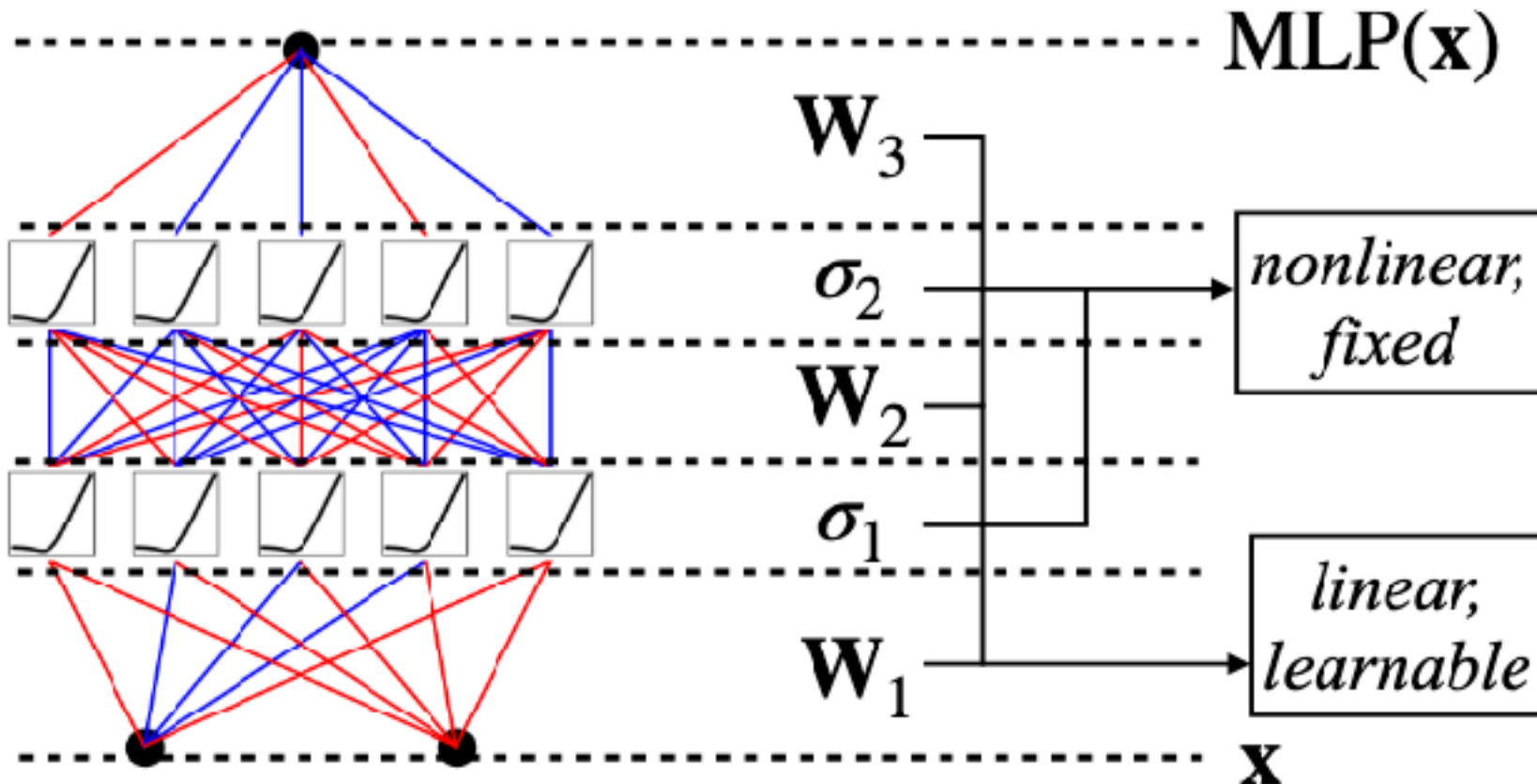
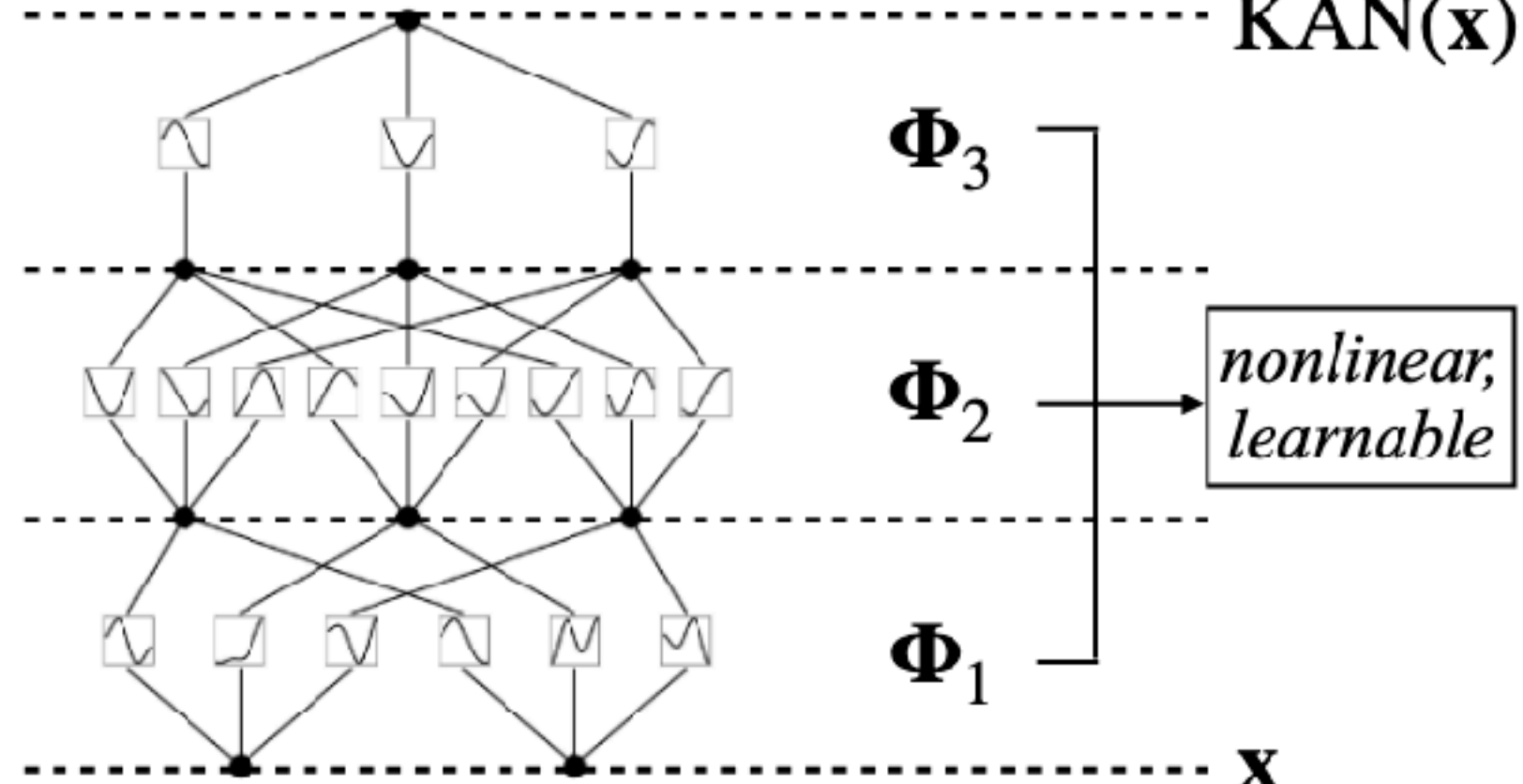
Model	Multi-Layer Perceptron (MLP)	Kolmogorov-Arnold Network (KAN)
Theorem	Universal Approximation Theorem	Kolmogorov-Arnold Representation Theorem
Formula (Shallow)	$f(\mathbf{x}) \approx \sum_{i=1}^{N(\epsilon)} a_i \sigma(\mathbf{w}_i \cdot \mathbf{x} + b_i)$	$f(\mathbf{x}) = \sum_{q=1}^{2n+1} \Phi_q \left(\sum_{p=1}^n \phi_{qp}(x_p) \right)$
Model (Shallow)	<p>(a)</p>  <p><i>fixed</i> activation functions on <i>nodes</i></p> <p><i>learnable</i> weights on <i>edges</i></p>	<p>(b)</p>  <p><i>learnable</i> activation functions on <i>edges</i></p> <p>sum operation on <i>nodes</i></p>
Formula (Deep)	$\text{MLP}(\mathbf{x}) = (\mathbf{W}_3 \circ \sigma_2 \circ \mathbf{W}_2 \circ \sigma_1 \circ \mathbf{W}_1)(\mathbf{x})$	$\text{KAN}(\mathbf{x}) = (\Phi_3 \circ \Phi_2 \circ \Phi_1)(\mathbf{x})$
Model (Deep)	<p>(c)</p>  <p>\mathbf{W}_3</p> <p>σ_2</p> <p>\mathbf{W}_2</p> <p>σ_1</p> <p>\mathbf{W}_1</p> <p>\mathbf{x}</p> <p>linear, learnable</p> <p>nonlinear, fixed</p> <p>MLP(x)</p>	<p>(d)</p>  <p>Φ_3</p> <p>Φ_2</p> <p>Φ_1</p> <p>\mathbf{x}</p> <p>nonlinear, learnable</p> <p>KAN(x)</p>

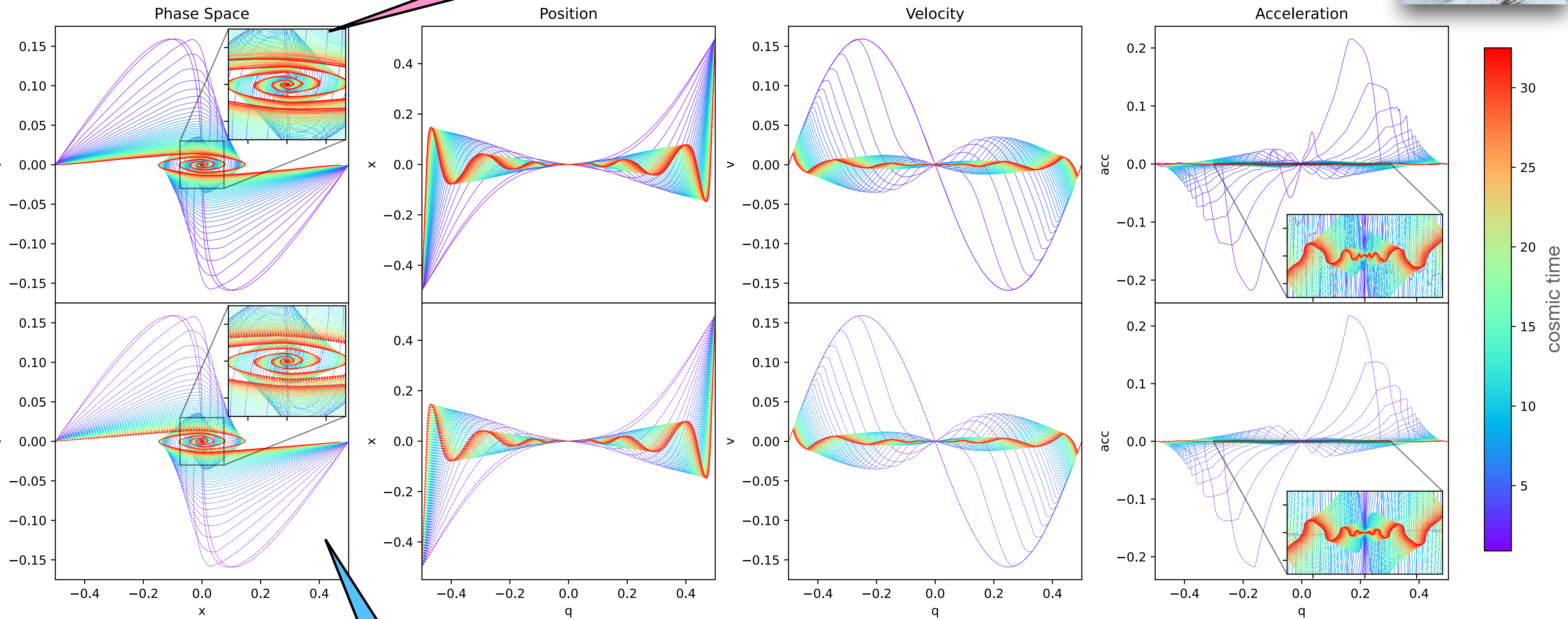
Figure from Liu et al (2024), arXiv:2404.19756

CDM PINN

Cerardi, Tolley, Mishra, submitted to MNRAS



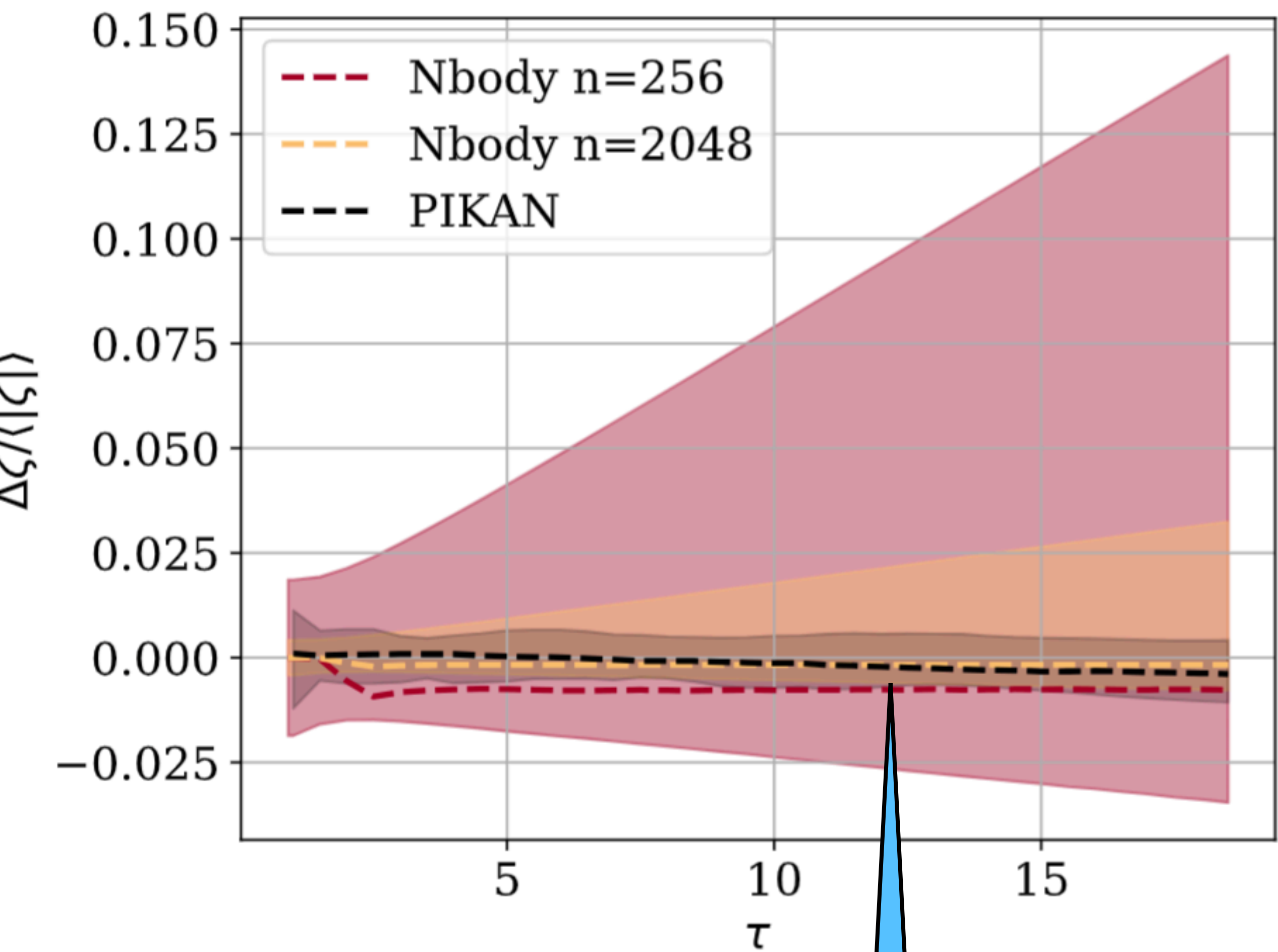
Unsupervised neural network



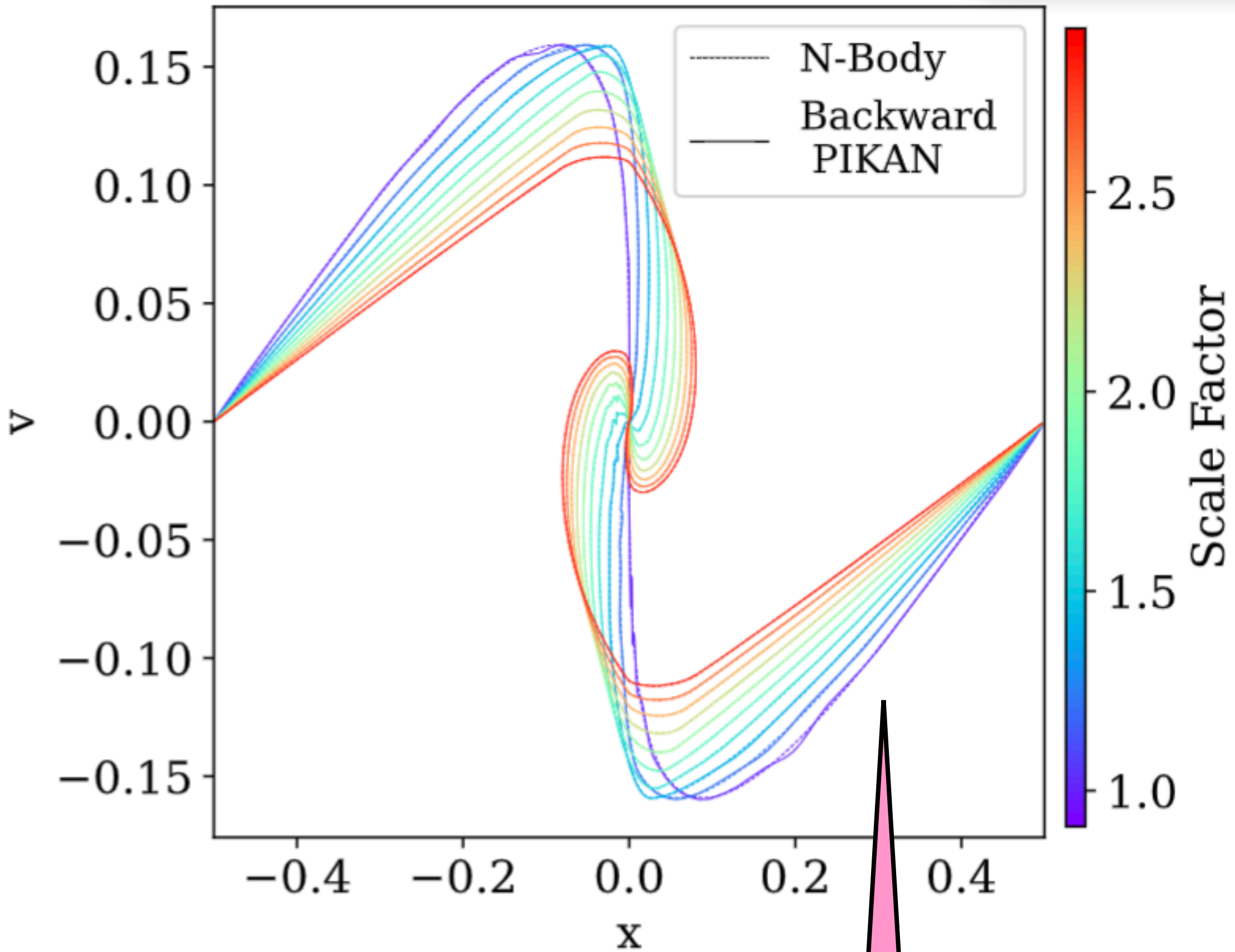
NBody simulation

CDM PINN

Cerardi, Tolley, Mishra, submitted to MNRAS



Much smaller errors in PINN



Can also evolve simulation backwards in time

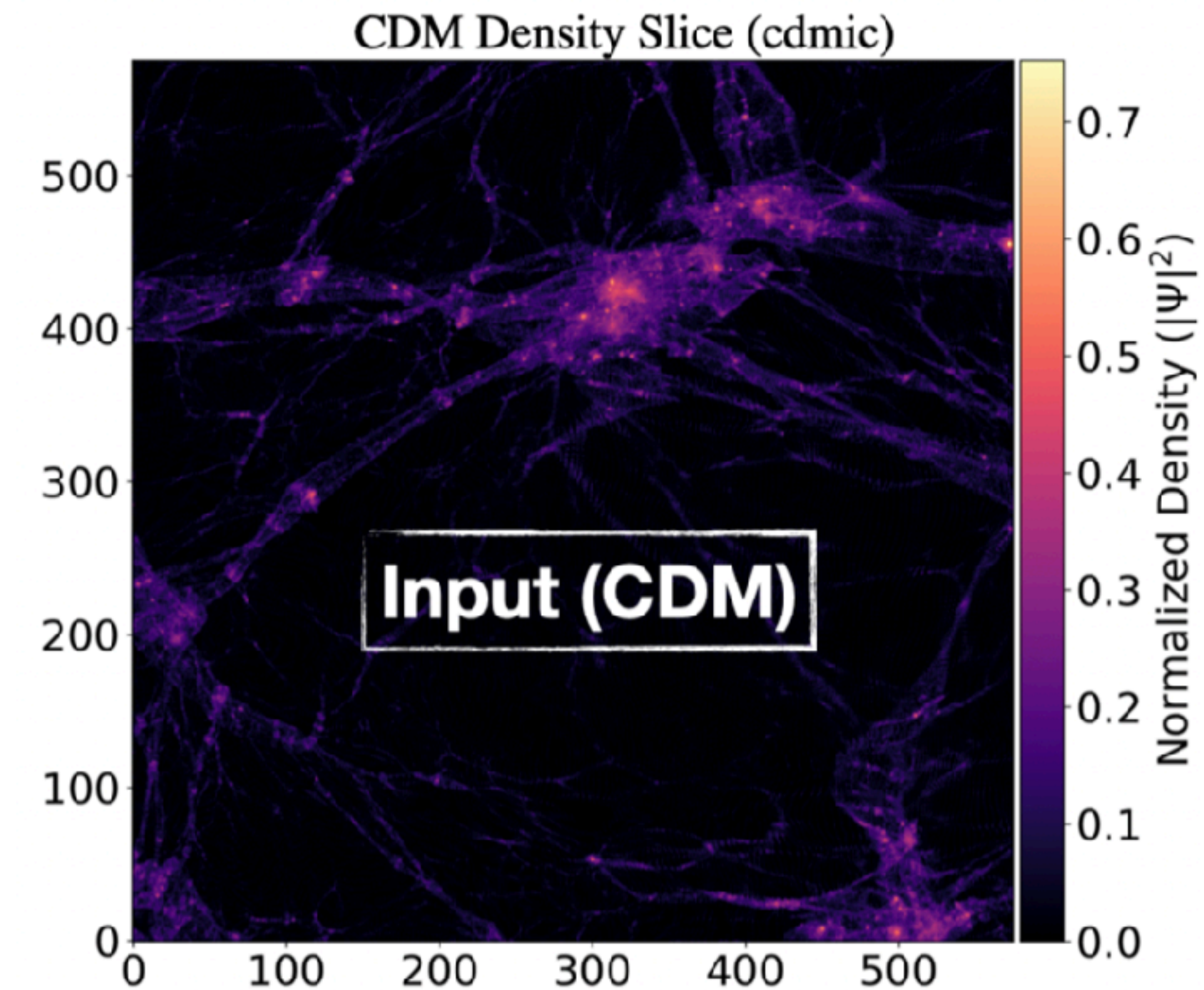
...IN SUMMARY

- **Physics-informed neural networks as PDE solvers for cosmology**
 - **Challenges**: Extremely **large space/time domains** needed for cosmology, and long-ranged **gravitational force** needs to be calculated across entire spatial domain
- Exploring physics informed neural networks to solve PDEs for **CDM** (1D only) and **FDM** (1D & 3D)
 - Initial results show excellent results, including **better error accumulation** compared to numerical solvers
 - But so far **not computationally cheaper** compared to traditional methods
 - Exploring implementations with NVIDIA PhysicsNeMo to improve performance

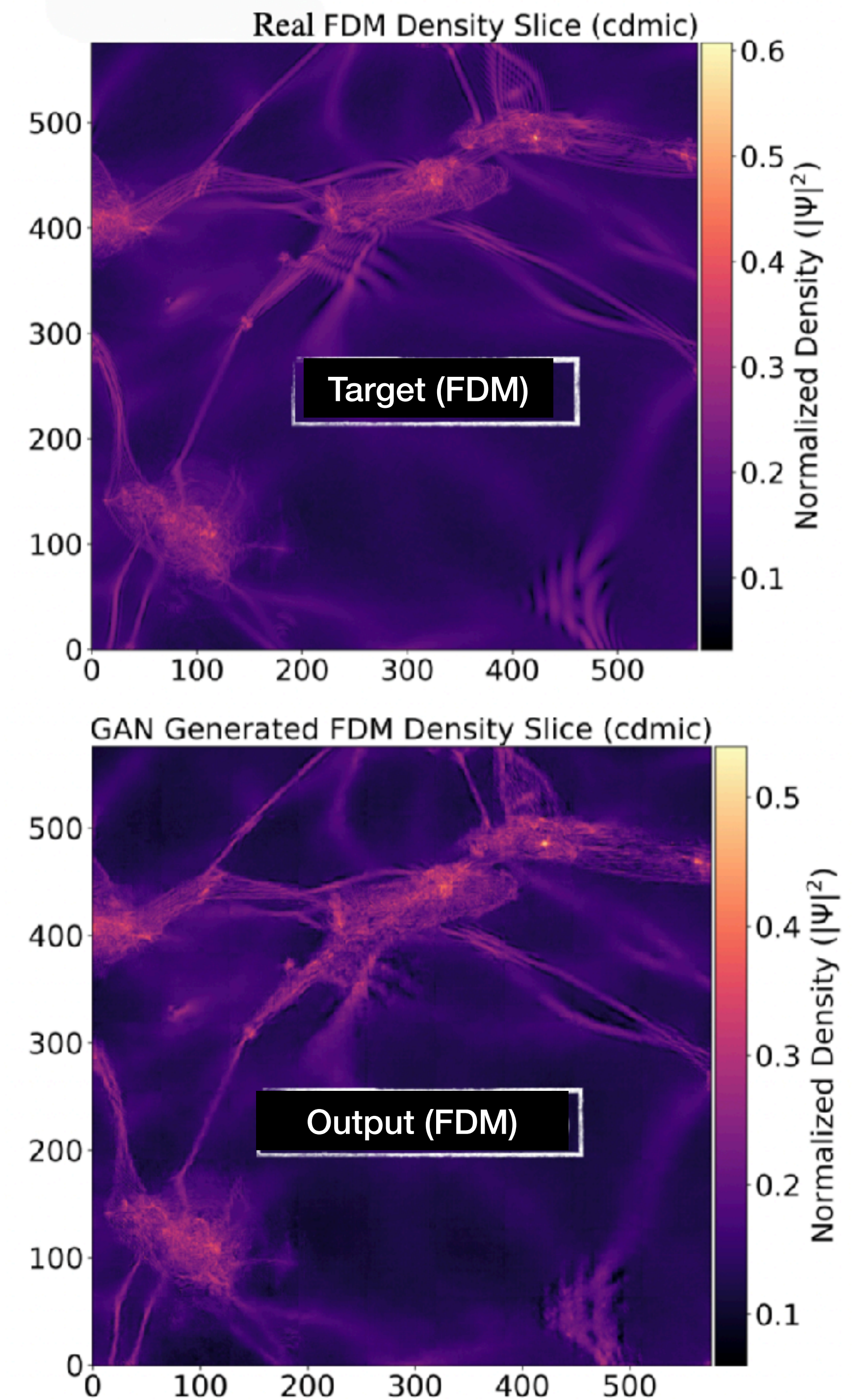
...NEXT STEPS

Now exploring **hybrid methods**, conditional generative models with physics constraints

Plots by A. Mishra



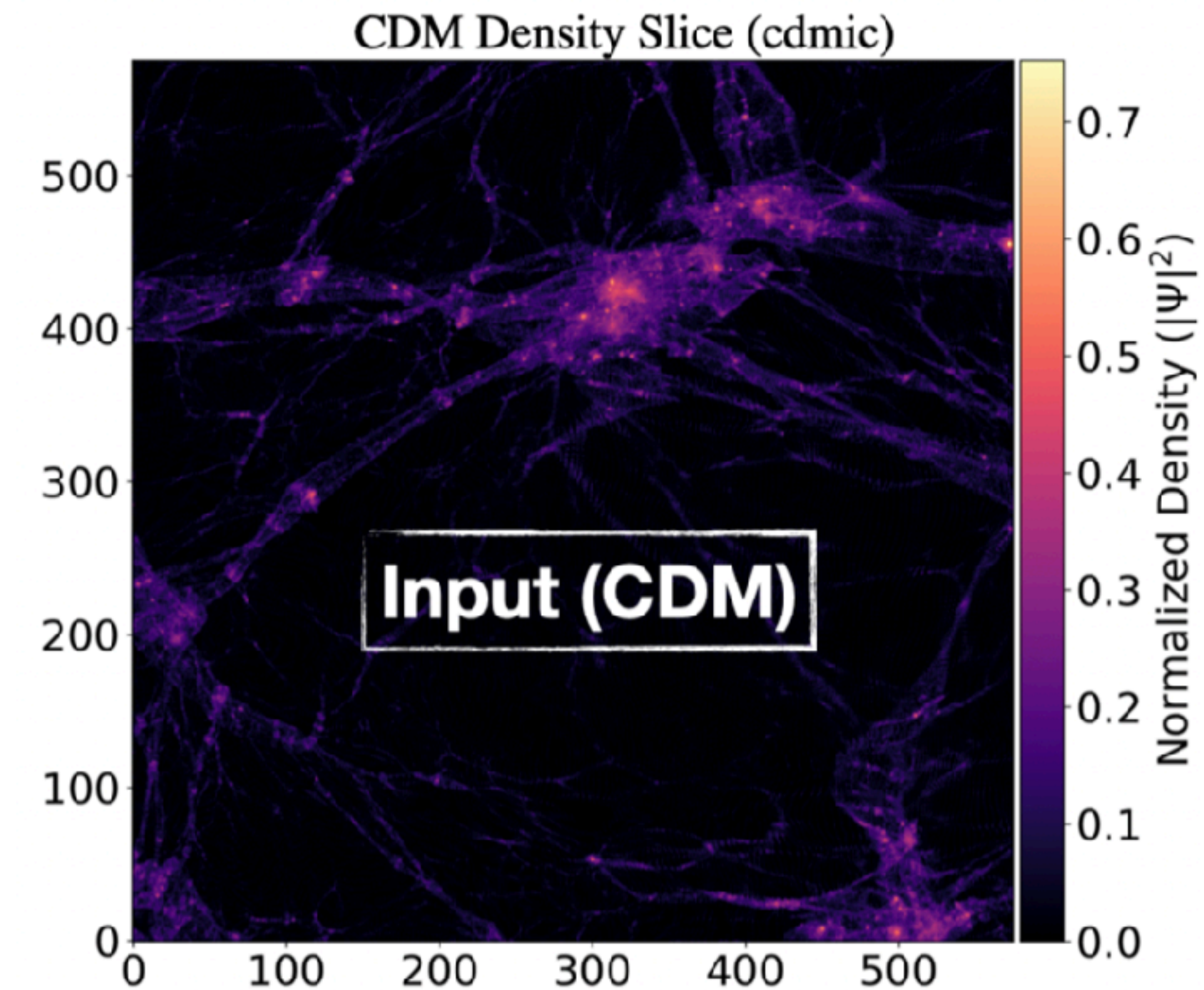
→ GAN →



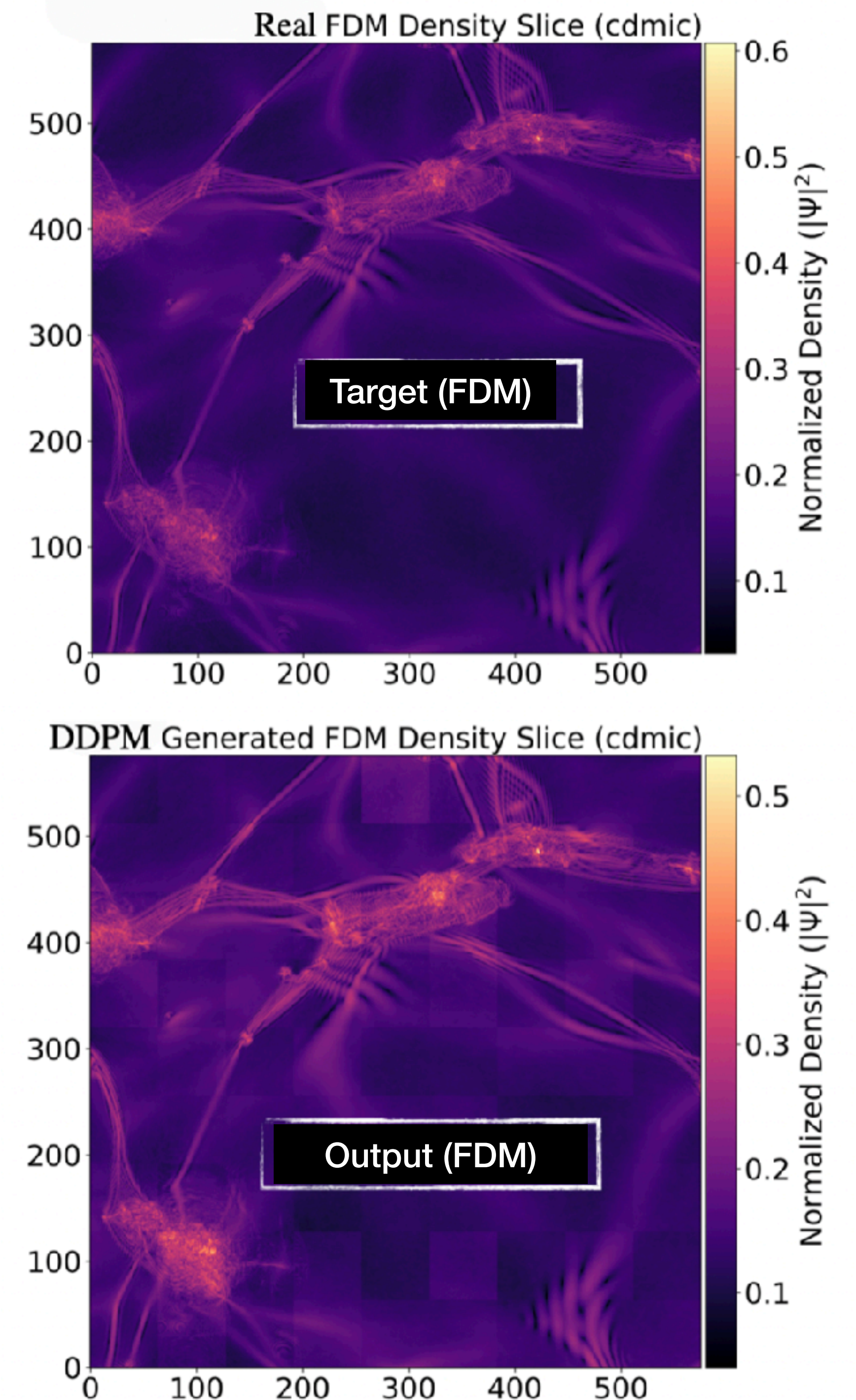
...NEXT STEPS

Now exploring **hybrid methods**, conditional generative models with physics constraints

Plots by A. Mishra



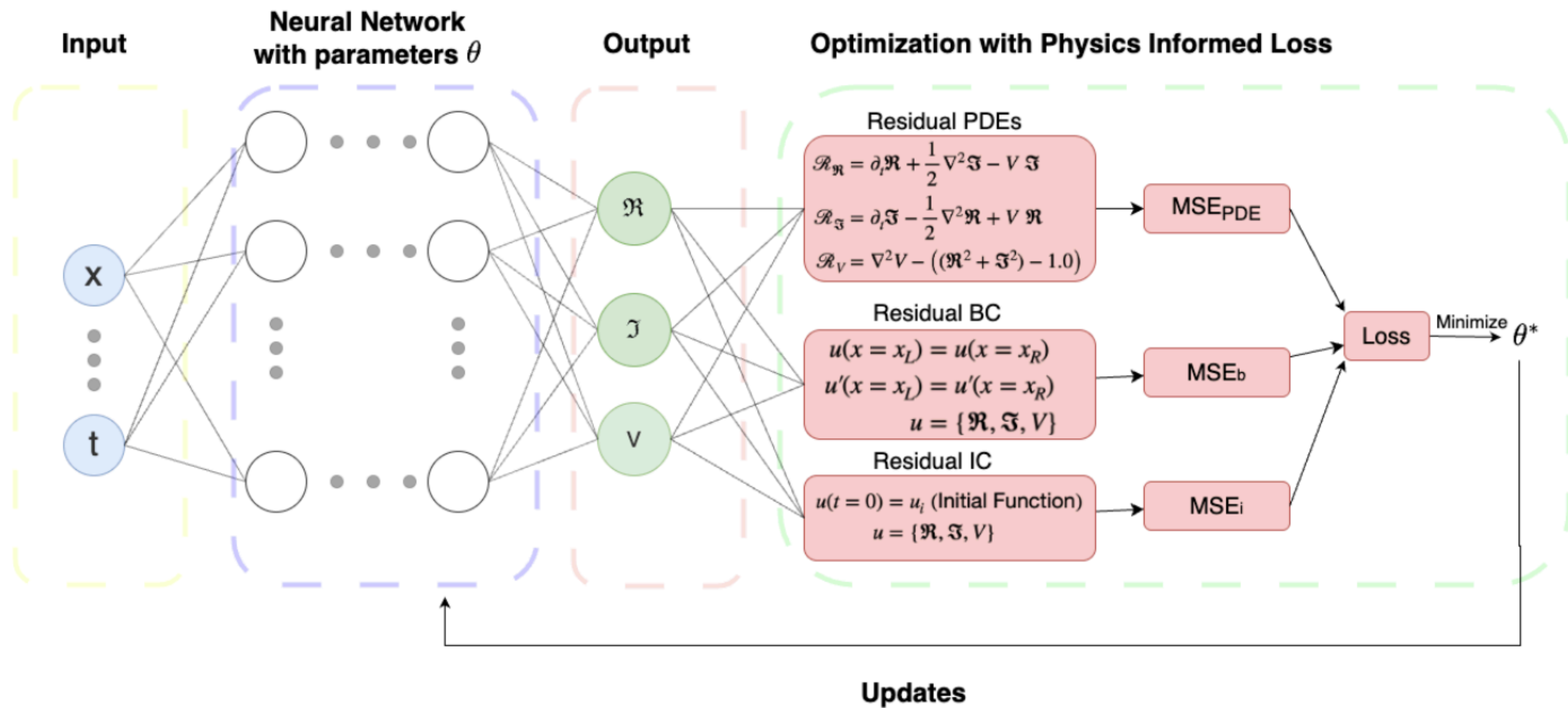
→ **DDPM** →



THANK YOU!

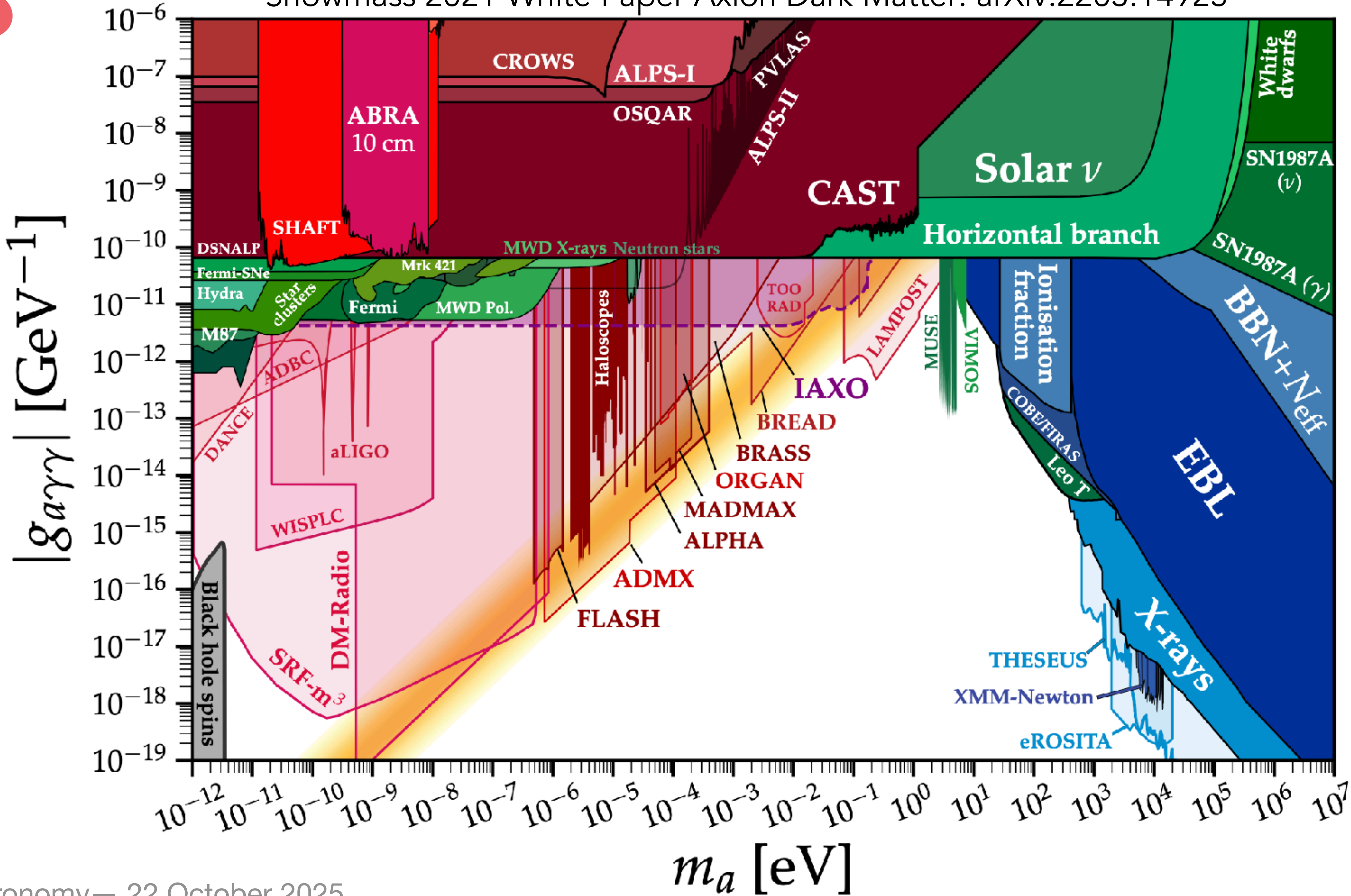


PHYSICS-INFORMED DEEP LEARNING



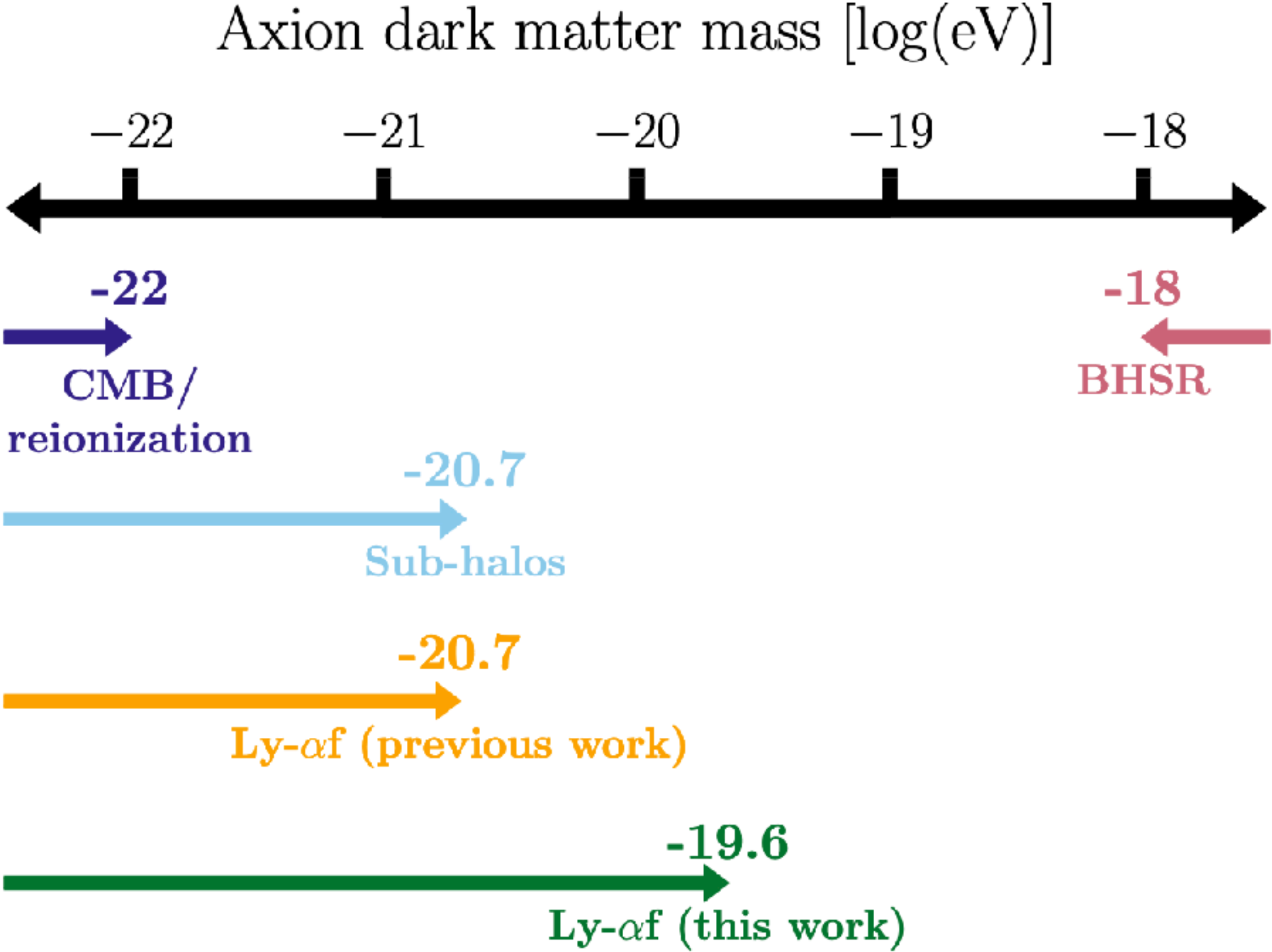
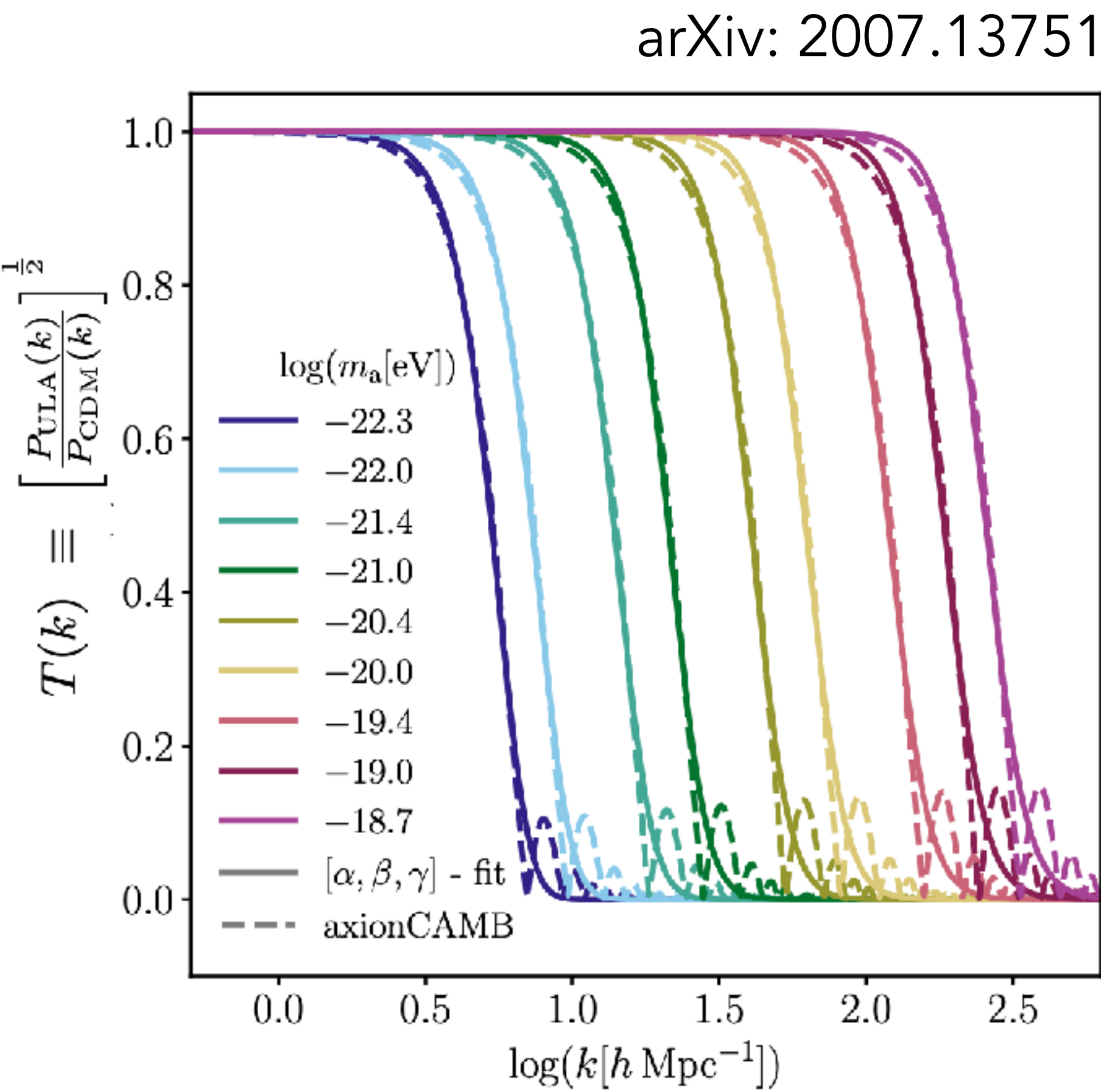
AXIONS & ALPS

Snowmass 2021 White Paper Axion Dark Matter: arXiv:2203.14923



FUZZY DARK MATTER

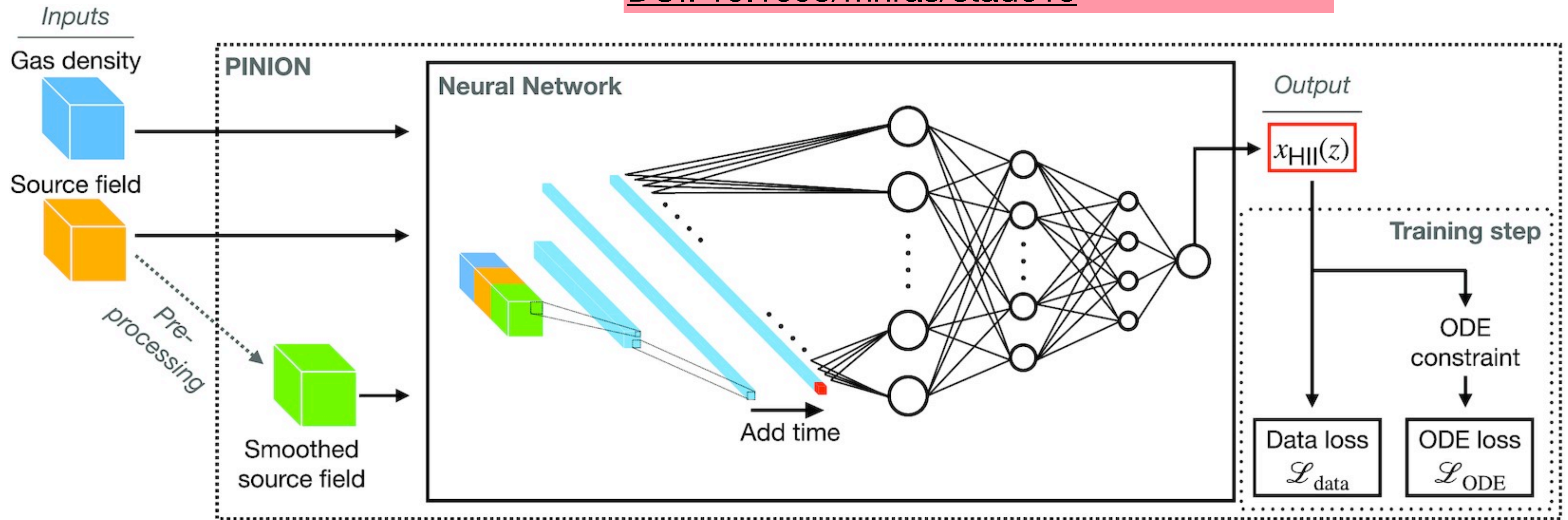
Linear theory predicts sharp cutoff in power spectrum due to quantum pressure



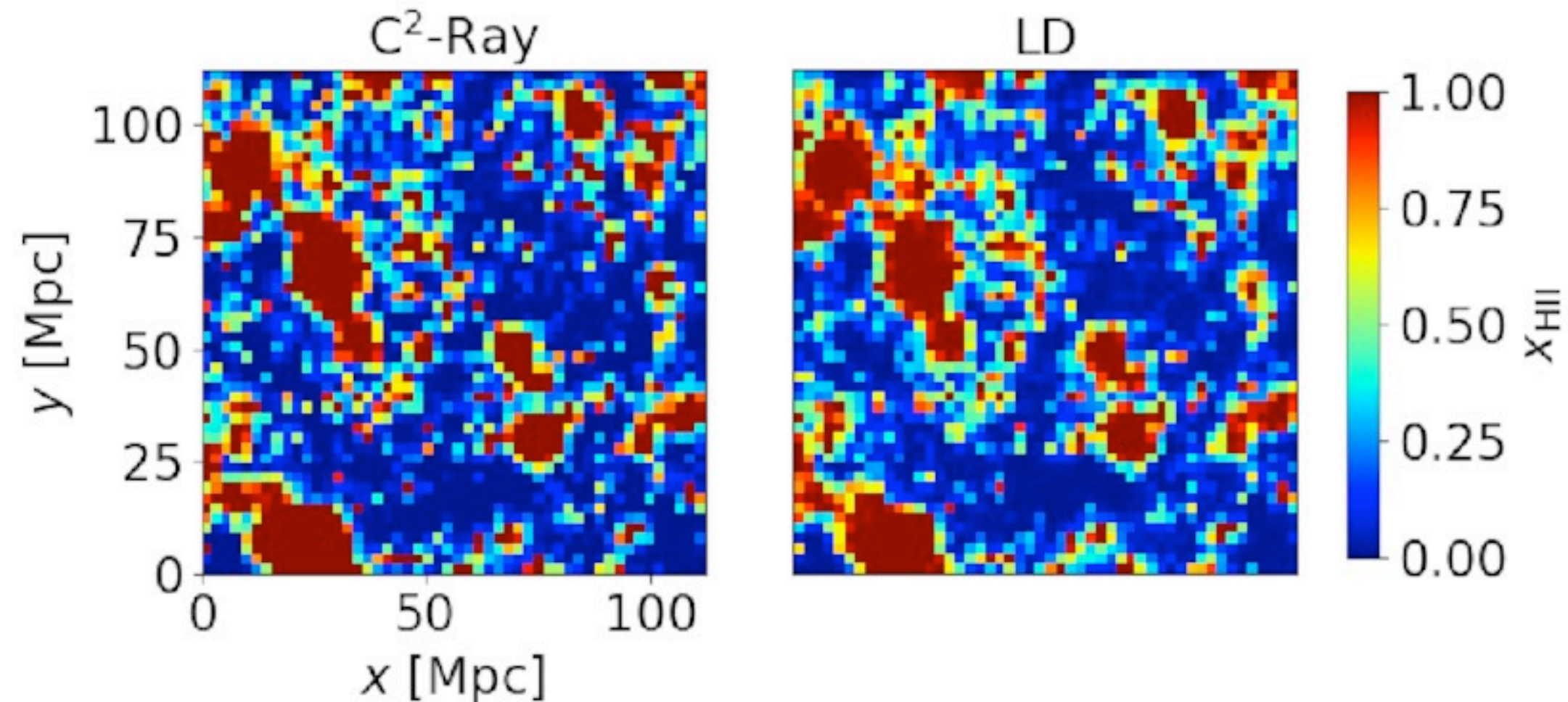
arXiv: 2007.12705

REIONIZATION

Korber, Bianco, Tolley, Kneib. MNRAS (2023)
DOI: [10.1093/mnras/stad615](https://doi.org/10.1093/mnras/stad615)



$$\frac{dx_{\text{HII}}}{dt} = (1 - x_{\text{HII}})\Gamma - C\alpha_{\text{B}}n_{\text{H}}x_{\text{HII}}^2$$



DEEP LEARNING

**Neural networks are
universal function
approximators**

$$f(x) = y$$

$$\text{NN}(x, \theta) = \tilde{y}$$

With enough neurons and an appropriate set of network weights and biases θ :

$$|y - \tilde{y}| < \epsilon$$

Model parameters θ minimized
using loss function

$$\mathcal{L}_{\text{MSE}} = \frac{1}{n} \sum_i^n (\tilde{y}_i - y_i)^2$$

LEARNING BIAS

Let's go back to the classic MSE loss

$$f(x) = y$$

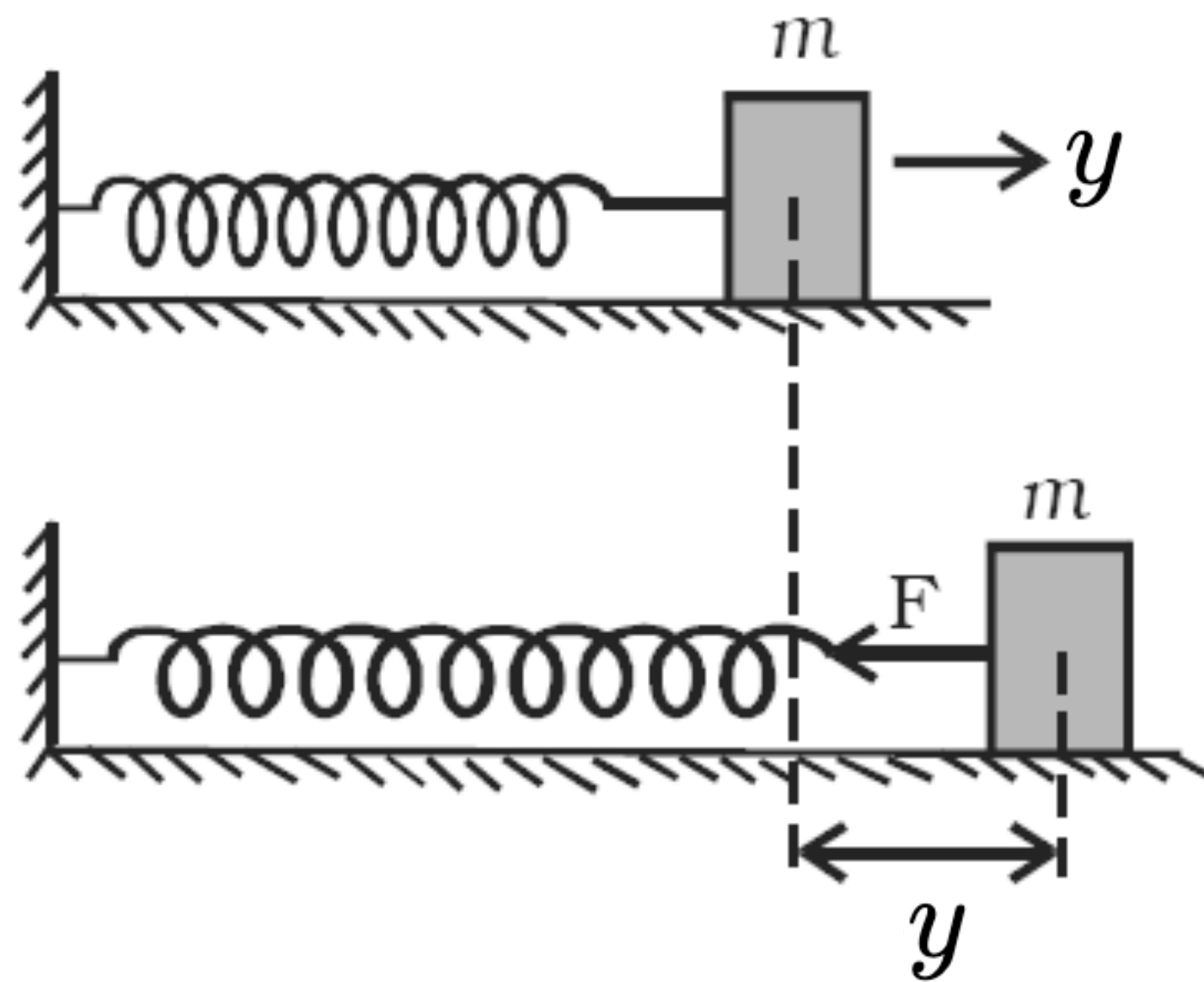
$$\text{NN}(x, \theta) = \tilde{y}$$

$$\mathcal{L}_{\text{MSE}} = \frac{1}{n} \sum_i^n (\tilde{y}_i - y_i)^2 = \frac{1}{n} \sum_i^n (\text{NN}(x_i, \theta) - y_i)^2$$

Limited by sampling of x and y

LEARNING BIAS

A simple physics example



Harmonic oscillator if x is time and y is displacement

$$m \frac{\partial^2 y}{\partial x^2} + ky = 0$$

$f(x) = y$ obeys this dynamical equation, can use this to constrain the NN

LEARNING BIAS

A simple physics example

$$m \frac{\partial^2 y}{\partial x^2} + ky = 0$$

Does not need samples of y !
 \Rightarrow unsupervised learning

$$\mathcal{L}_{\text{ODE}} = \frac{1}{n} \sum_i^n \left(m \frac{\partial^2 \tilde{y}_i}{\partial x^2} + k \tilde{y}_i \right)^2 = \frac{1}{n} \sum_i^n \left(m \frac{\partial^2}{\partial x^2} \text{NN}(x_i, \theta) + k \text{NN}(x_i, \theta) \right)^2$$

If Loss=0 then network solves PDE (neural solver)

PHYSICS-INFORMED NEURAL NETWORK

<https://www.brown.edu/research/projects/crunch/home>

Use physics-based constraints from PDEs to make network training more efficient and generalizable

