

A new way to Learn the Universe:

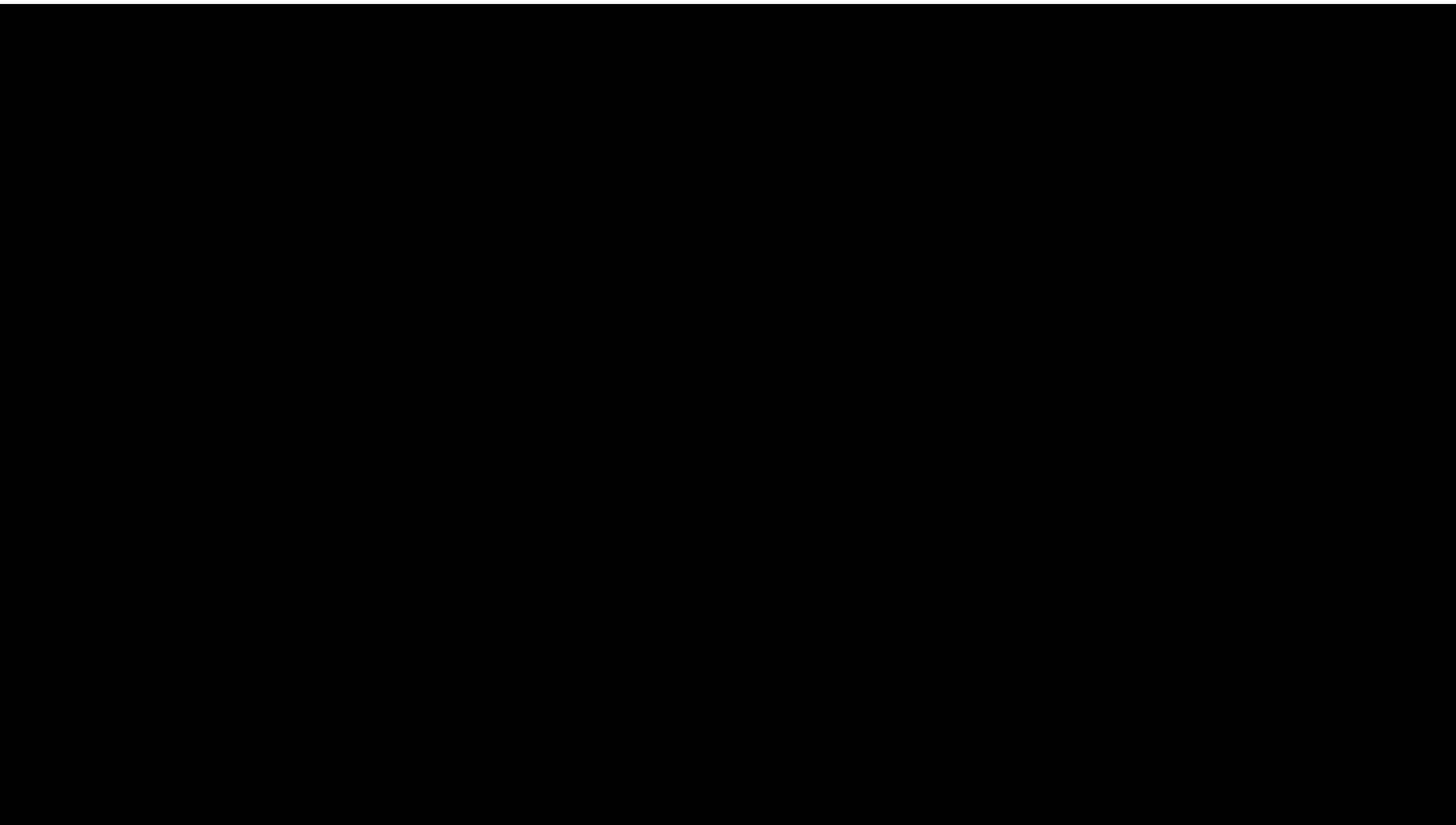
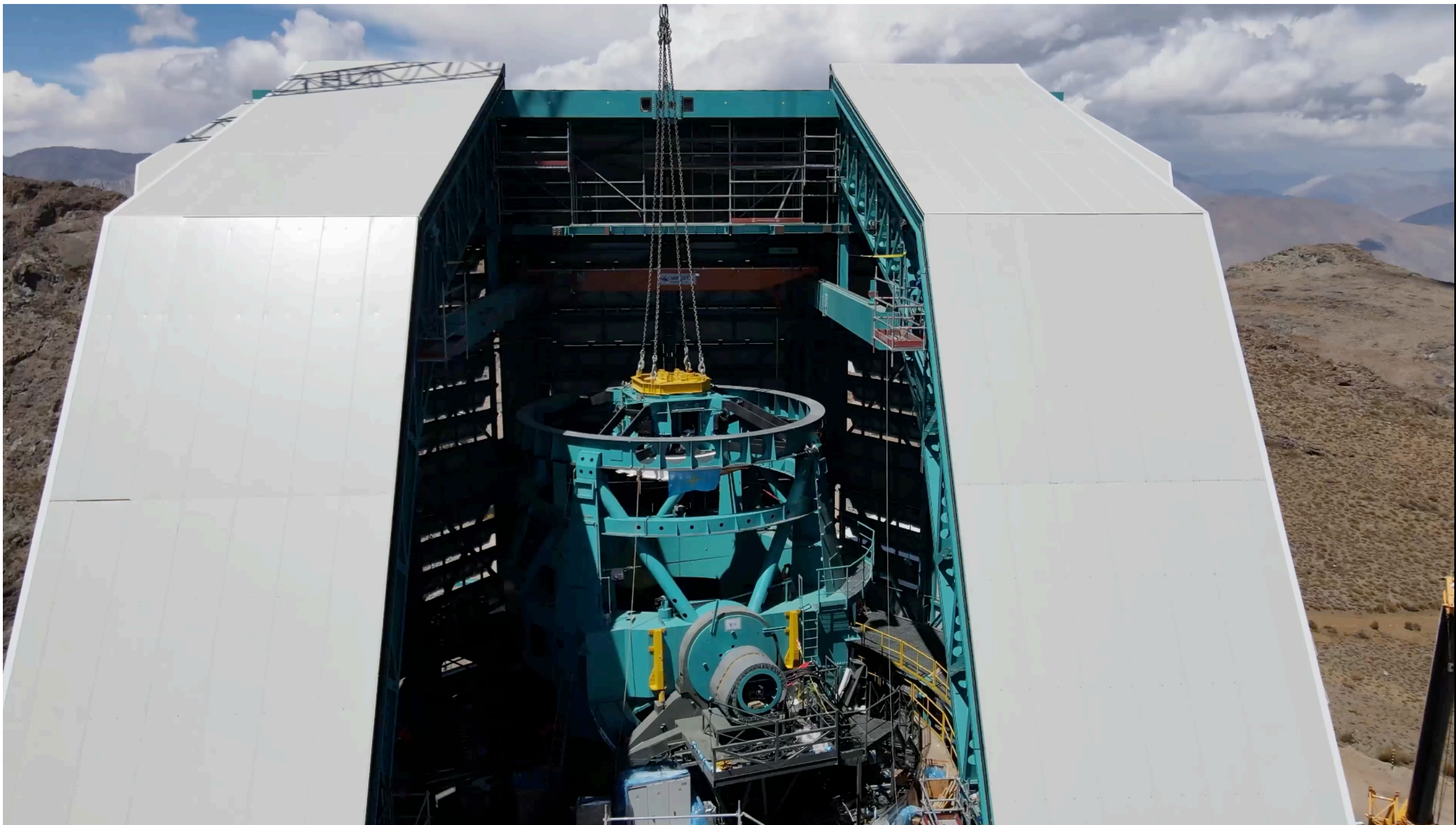
Deep Learning Accelerated Simulation Based Inference

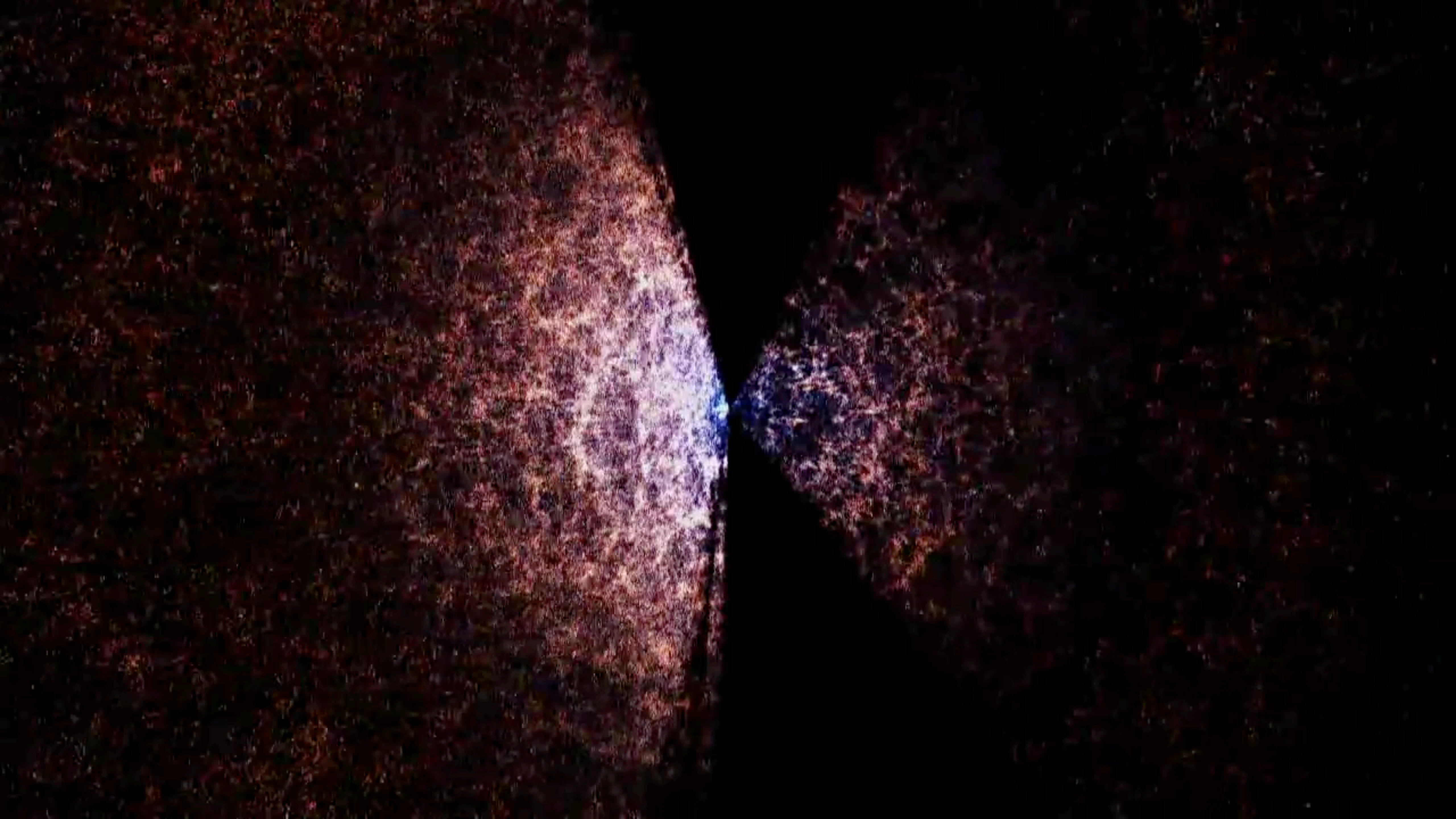
Shirley Ho (Flatiron Institute/NYU/Princeton/CMU)

Siyu He (CMU/PlusAI), Yin Li (Flatiron), Miles Cranmer (Princeton), Pablo Lemos (UCL/ Sussex), Jay Wadekar (NYU), Gabriella Contardo (Flatiron), Siamak Ravanbakhsh (McGill), Barnabas Poczos (CMU/DE Shaw), Peter Battaglia (Deepmind), Wei Zhang (NYU), Yueqiu Sun (NYU), Wei Chen (FaceBook), Yu Feng (Berkeley/Google), Seda Bilaloglu (NYU), Asena Derin-Cengiz (NYU), Laurence Levasseur (McGill), Jeff Schneider (CMU), Jeremy Tinker (NYU)

The mysteries of the Universe as seen by mortals

With help of large scale astronomical observatories





Many Mysteries about the Universe

How did it all begin?

A faint afterglow of the sky tells of a universe that came into being 13.8 billion years ago. But we haven't got the story of the Big Bang nailed yet

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Will we find other “earths” that make our own not so special? Is our particular solar system special?

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What makes supermassive blackholes?

There isn't enough time for these very massive blackholes to form if they form through normal “channels”, how did they come about?

.....

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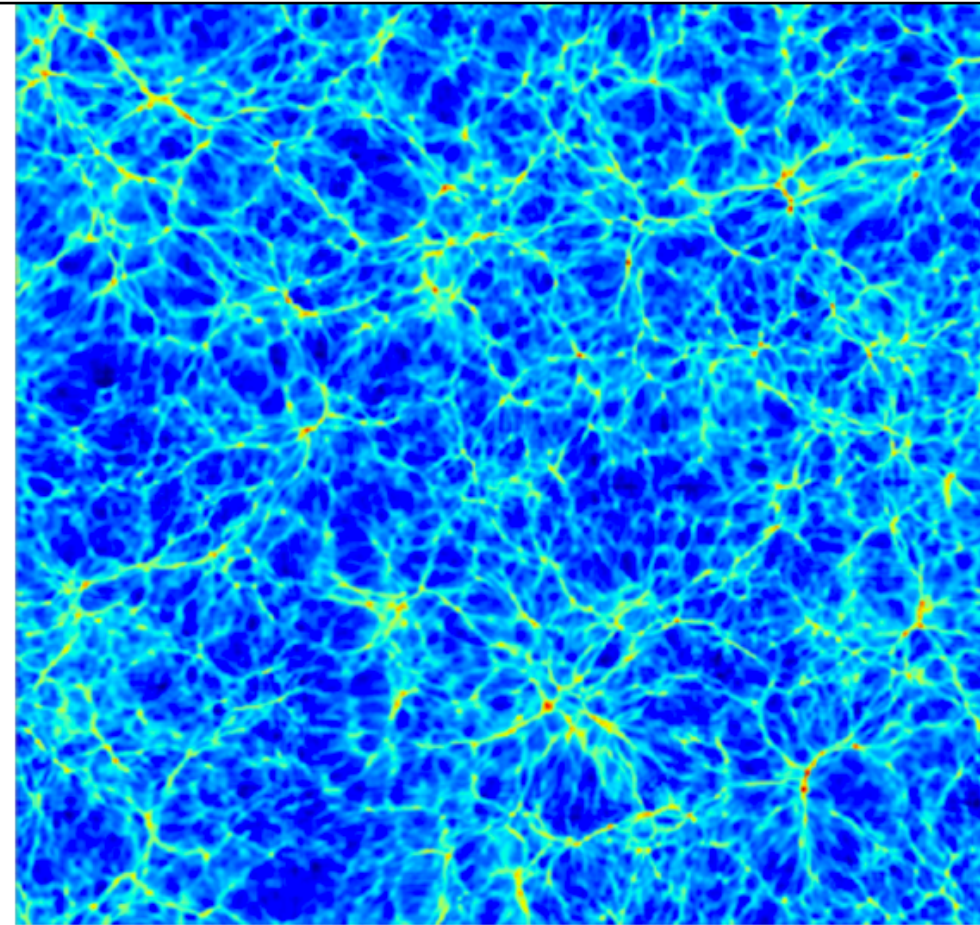
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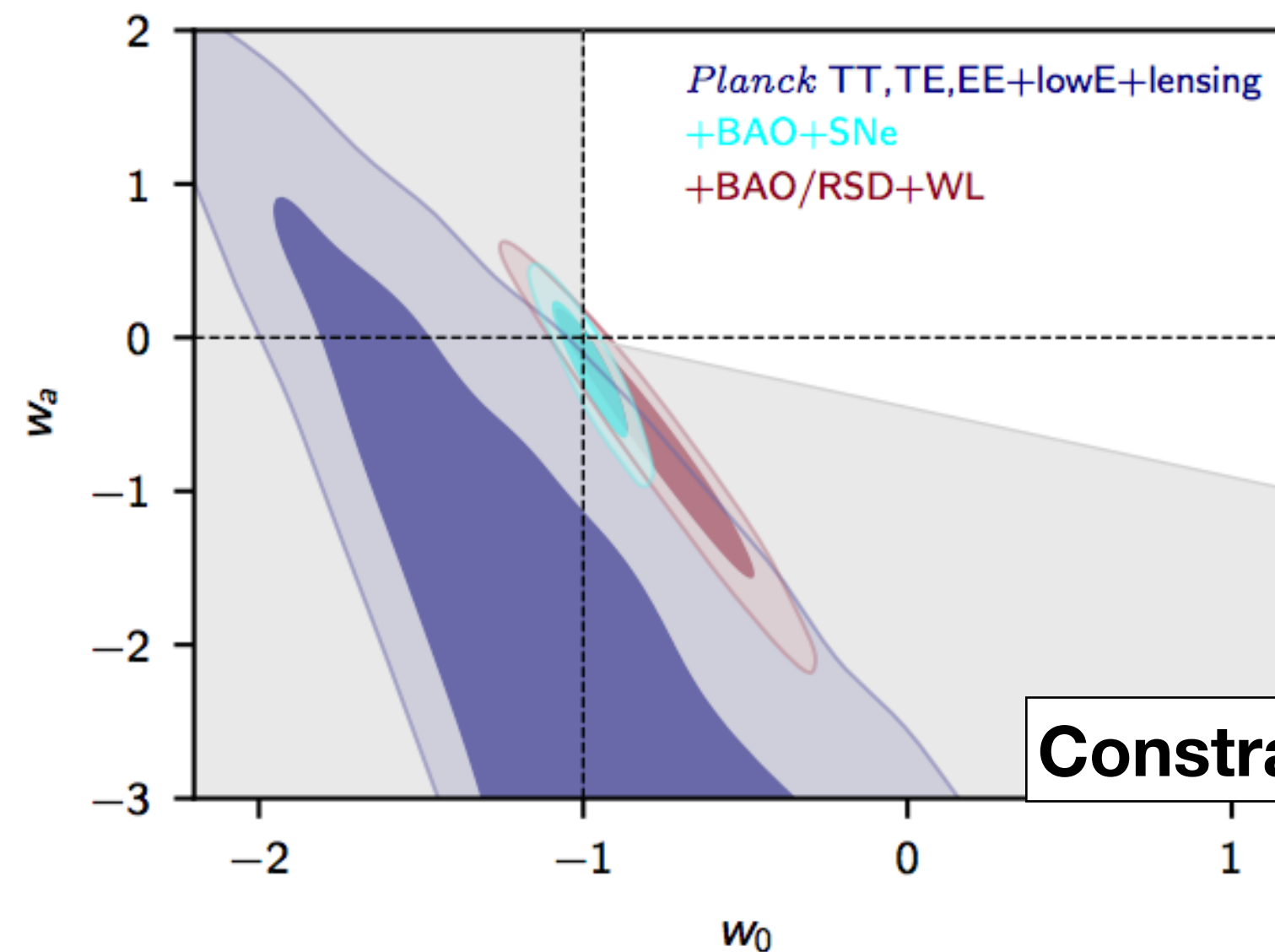
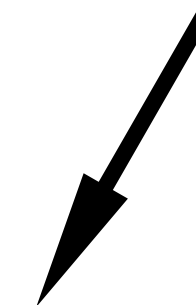
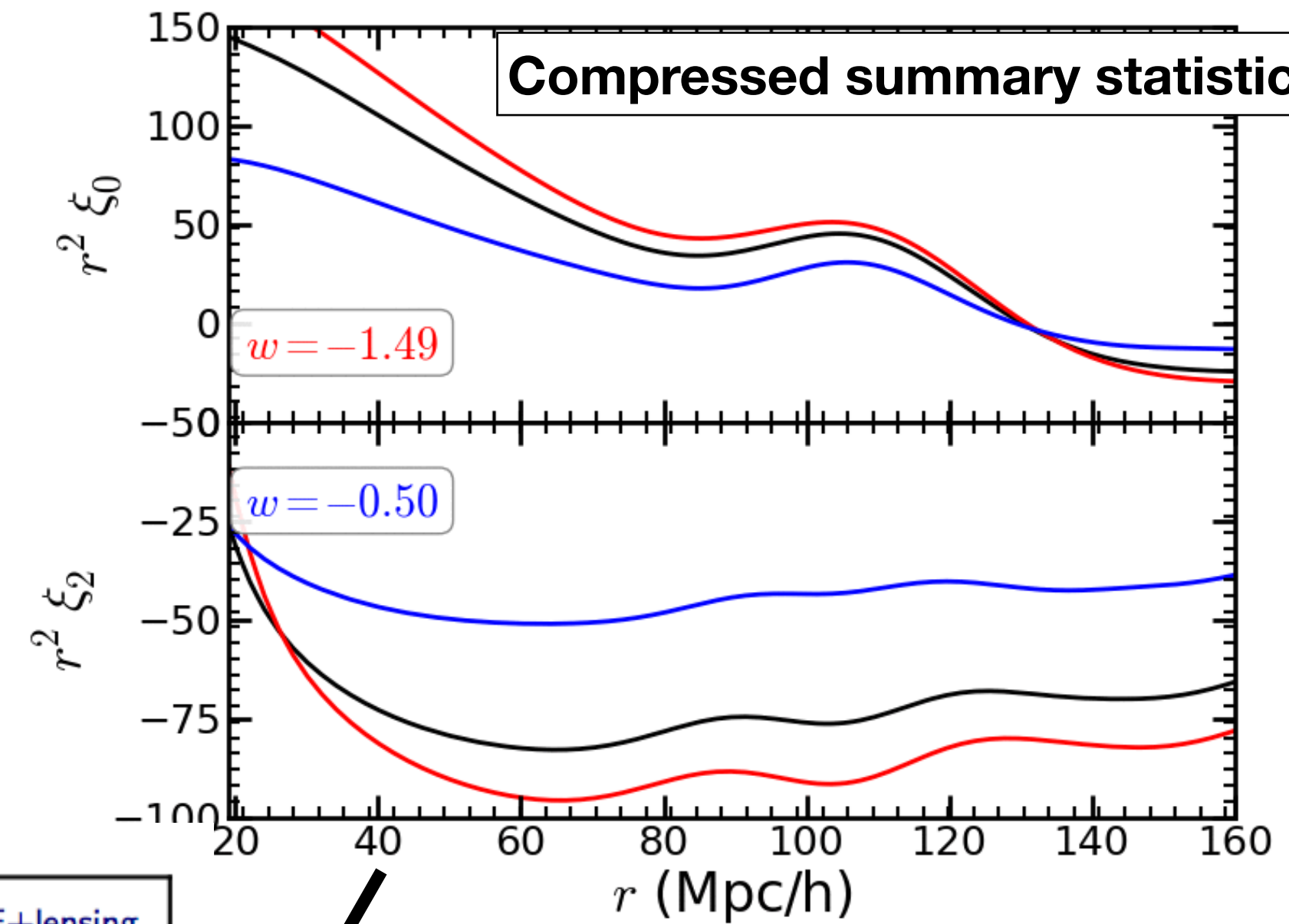
We will concentrate today on the above three questions
(though what I propose here will potentially work for the other questions as well)

Here is what we usually do right now

Distribution of matter in the Universe



Compressed summary statistics



Constraints on Dark Energy

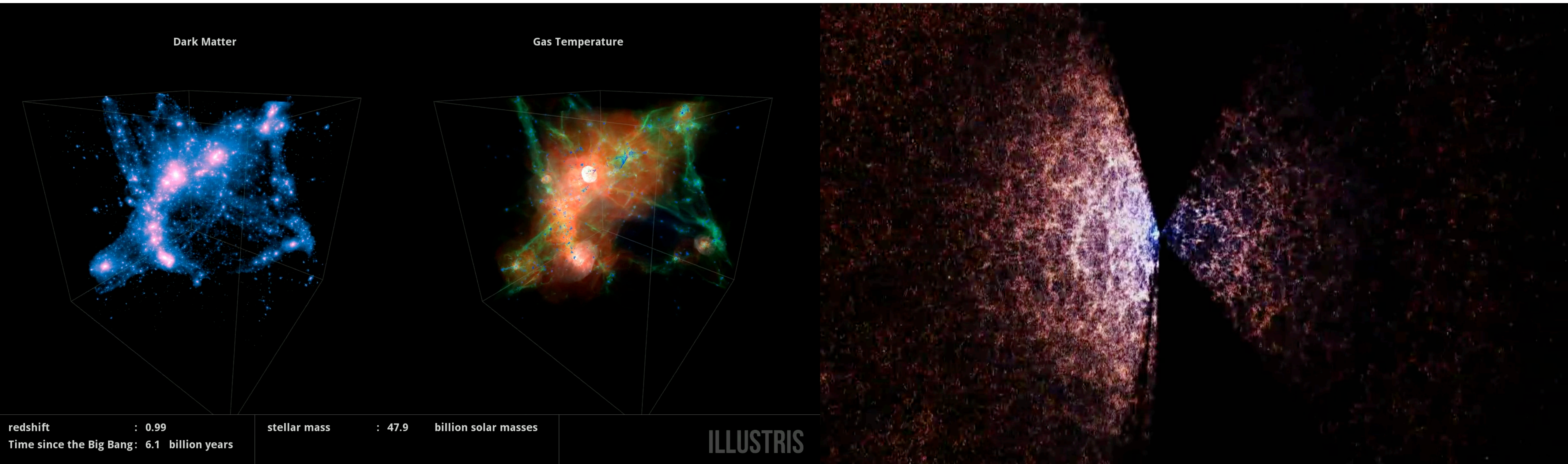
Why compress all the observed Universe into 40 numbers?
Is there more information that we can gleam?

Why compress all the observed Universe into 40 numbers?
Is there more information that we can glean?

Yes, there is more information!
IF we can compare the **observed Universe against Theory**
at the field level

Theory (Simulated Universe) VS Observed Universe

Credit: SDSS Collaboration



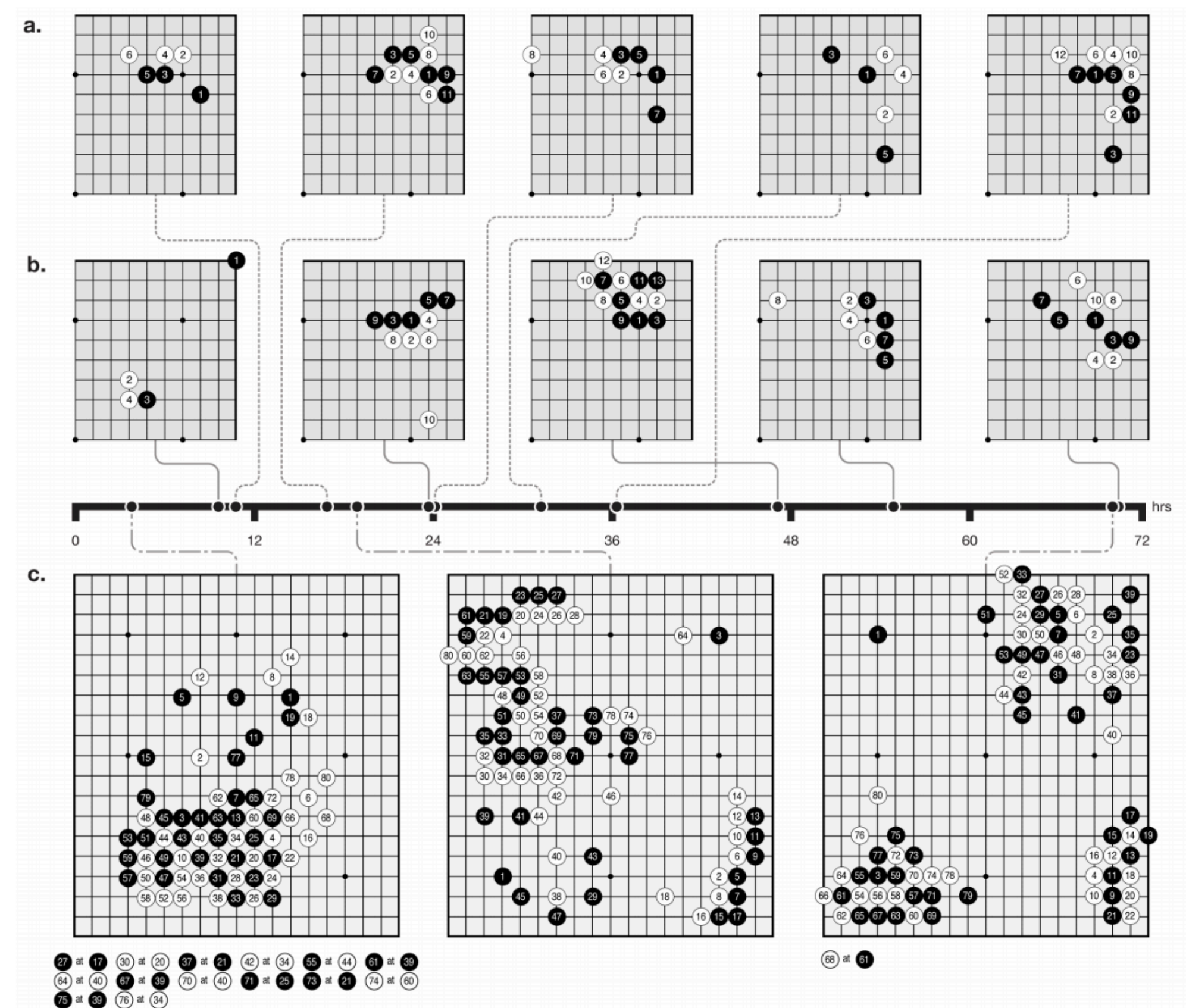
Credit: Illustris Project

Simulation based inference: Hard...

- Universe is *big*. And the *range of scales* to model is vast.
- We want to **simulate many Universes** in a *large parameter space*
- And we like to compare many *theoretical universes* against the **Observed one**
- And we need to do it **fast**.

Deep Learning to rescue?

Mastering the Game of Go without Human Knowledge



Five human joseki (common corner sequences)
discovered by AlphaZero during training.

Silver, Schrittwieser, Simonyan Nature 2016

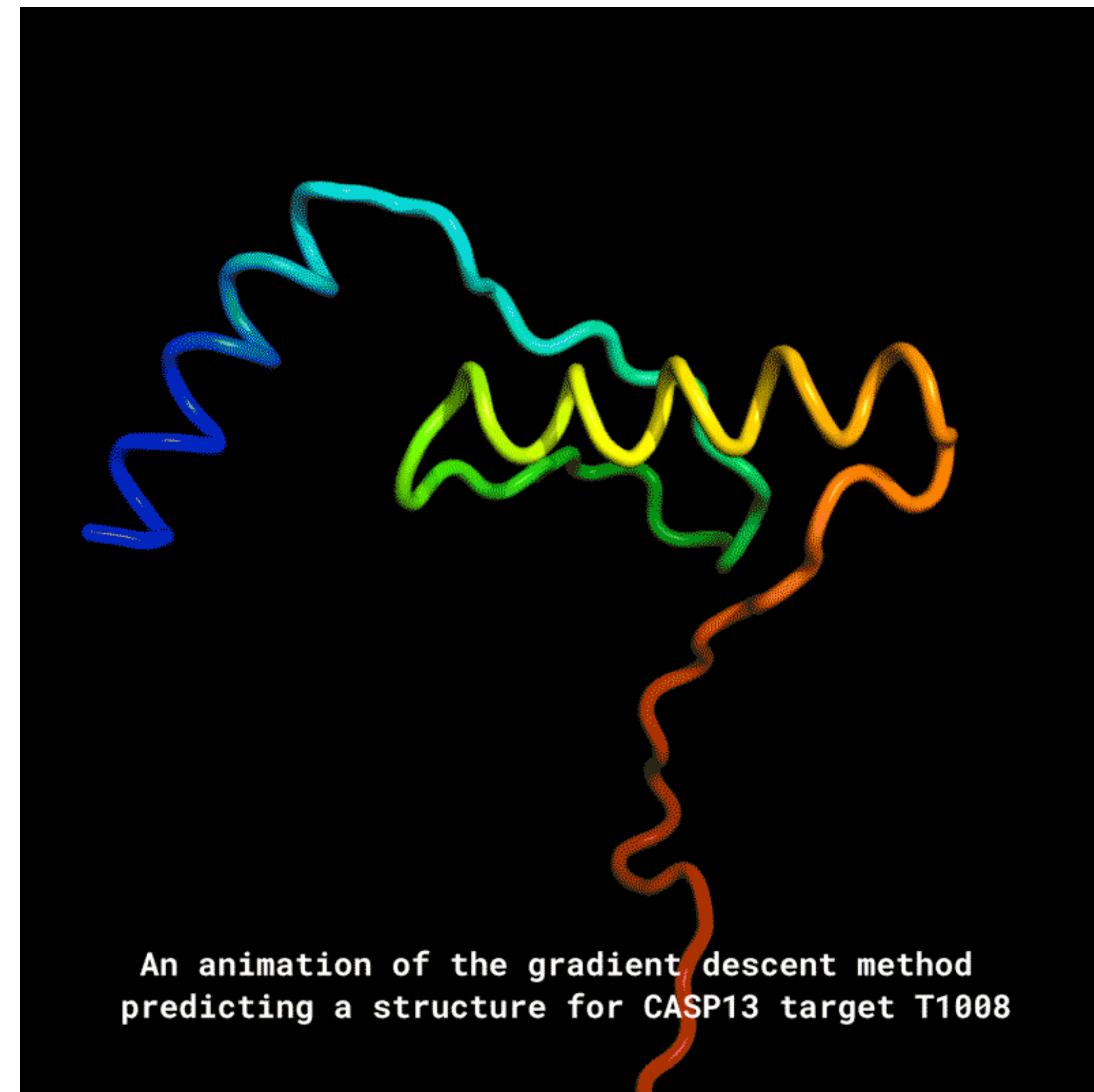
Deep learning and Protein Folding

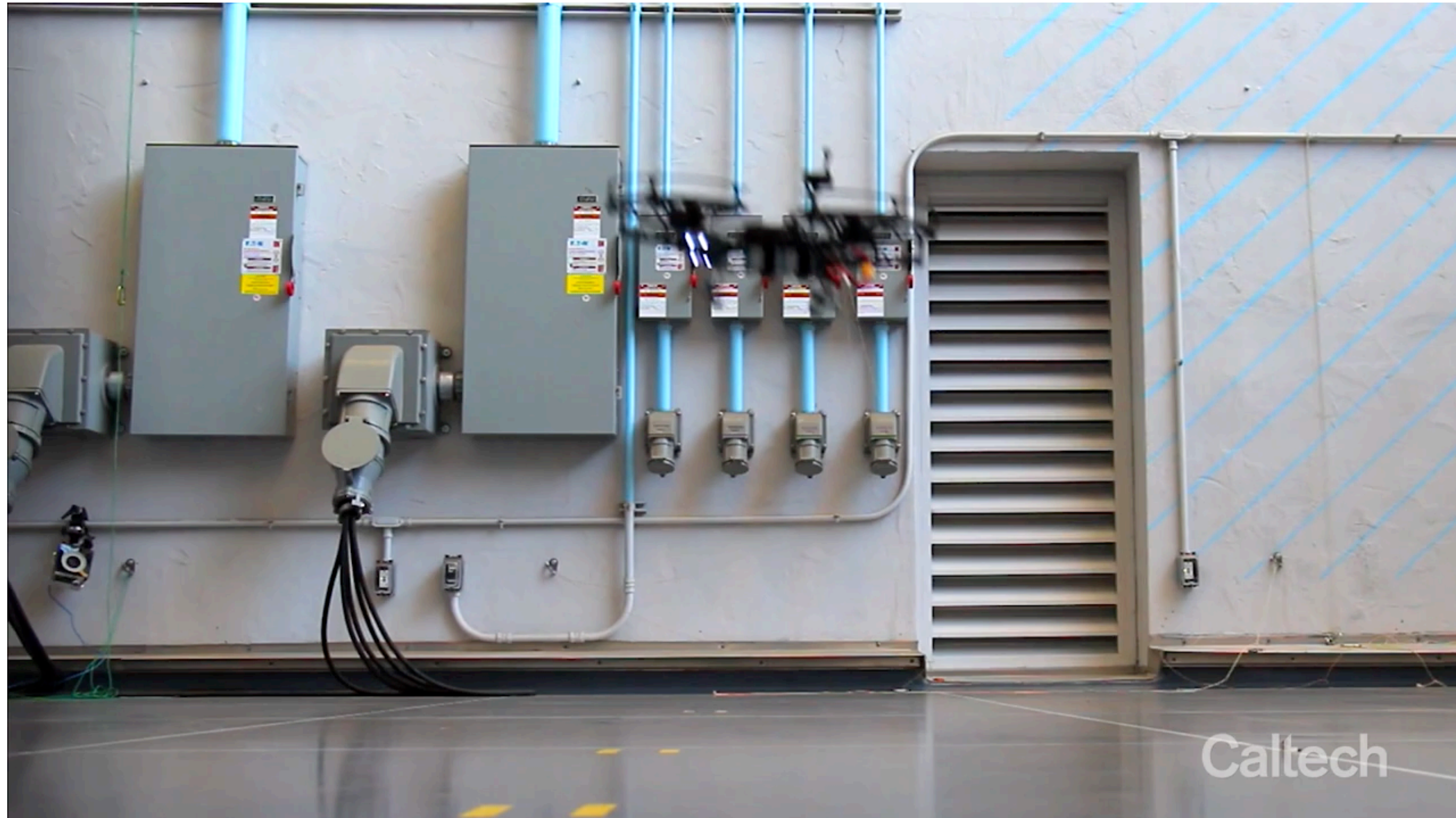
The ability to predict a protein's shape is useful to scientists because it is fundamental to understanding its role within the body, as well as diagnosing and treating diseases believed to be caused by misfolded proteins, such as **Alzheimer's**, **Parkinson's**, and **cystic fibrosis**.

The problem is as follows: people are given sequences of amino acid, and they are to predict the shape of the protein that were not published before.

Out of 43 proteins, the second best competitor got 3 right; while the best team from Google Deepmind uses deep learning got 25 out of 43 right.

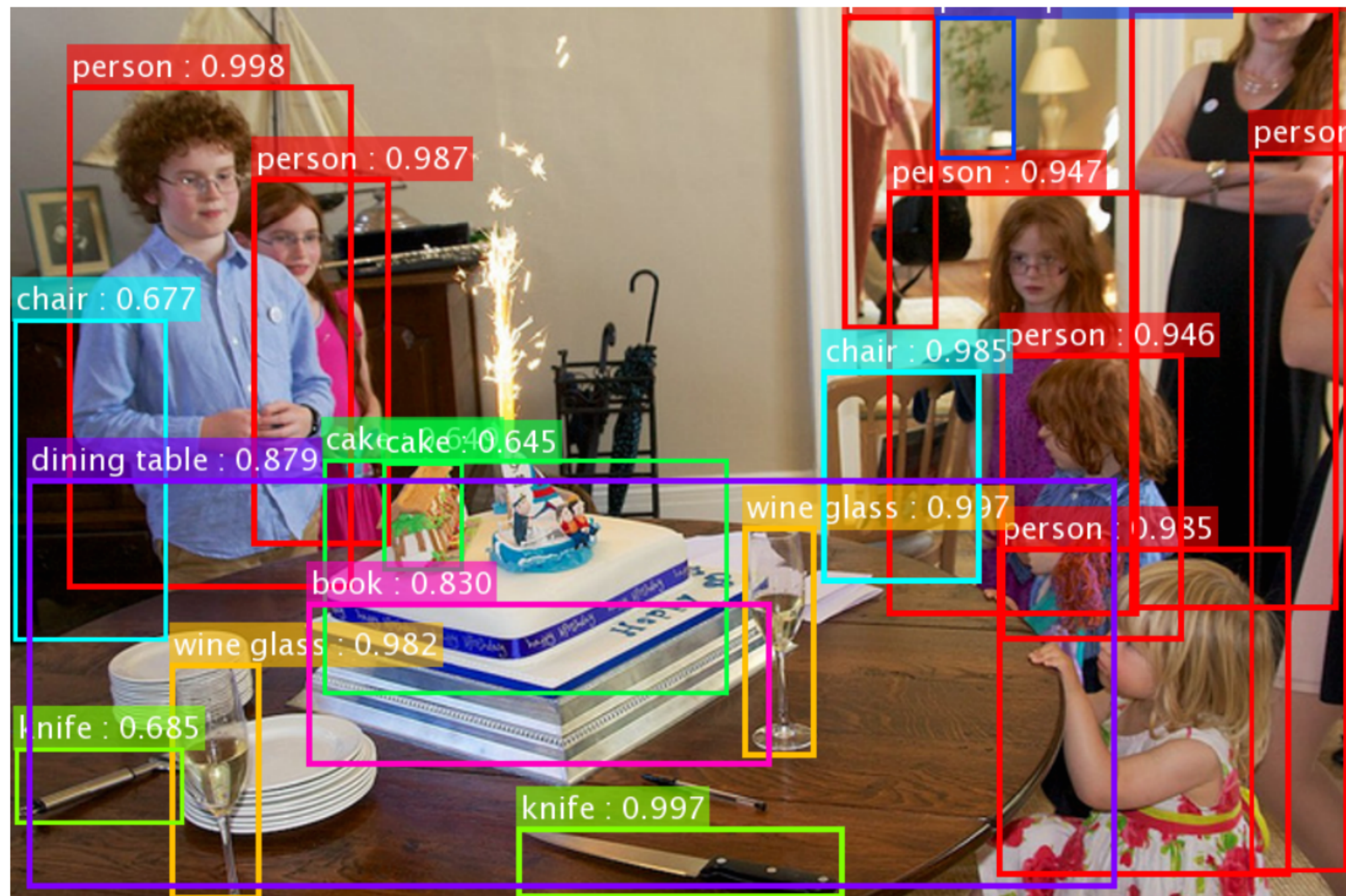
CASP13, 2019





Credit : Anima Anandkumar (Caltech)

Machine learning in image recognition



ResNet's object detection result on Common Object in Context

Deep Learning Accelerated Simulation Based Inference: Attack Plans

1/ Create large scale theory predictions of the Universe

with state of the art multi-scale physical models and deep learning

2/ Create full scale predictions of the Universe with observational and hardware-dependent systematics.

3/ Compare large scale predictions of the Universe and observations with high fidelity

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Deep Learning Accelerated Simulation Based Inference: Attack Plans (1)

**Create large scale theory predictions of the Universe
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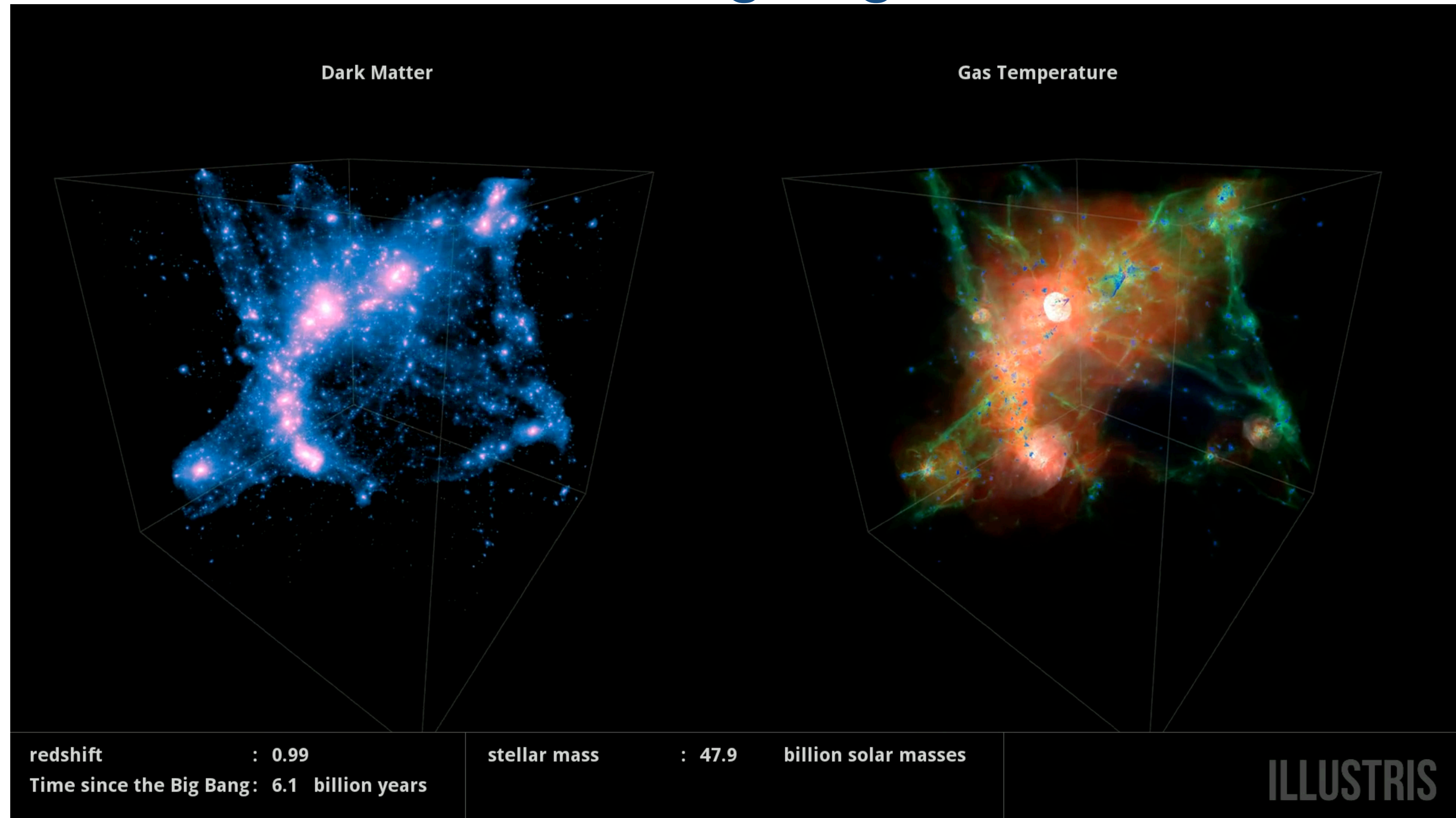
- Can deep learning help build a fast N-body simulator?
- Can deep learning help build a fast hydrodynamic simulator of galaxies?
 - Galaxy number density
 - Stellar masses of each galaxies
 - HI content of the Universe
 - Star formation rate of each galaxies
 - ...

Deep Learning Accelerated Simulation Based Inference: Attack Plans (1)

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Deep Learning to simulate the Universe: So what are we going to do first?



Using Machine Learning to simulate the Universe: The Setup of the Experiment

Inputs

Machine Learning model

Outputs

Analytical approximation of the
non-linear evolution of the Universe

Using Machine Learning to simulate the Universe: The Setup of the Experiment

Inputs

Machine Learning model

Outputs

Positions and velocities of all particles,
evolved under **gravity** after X years

Using Machine Learning to simulate the Universe: The Setup of the Experiment

Inputs

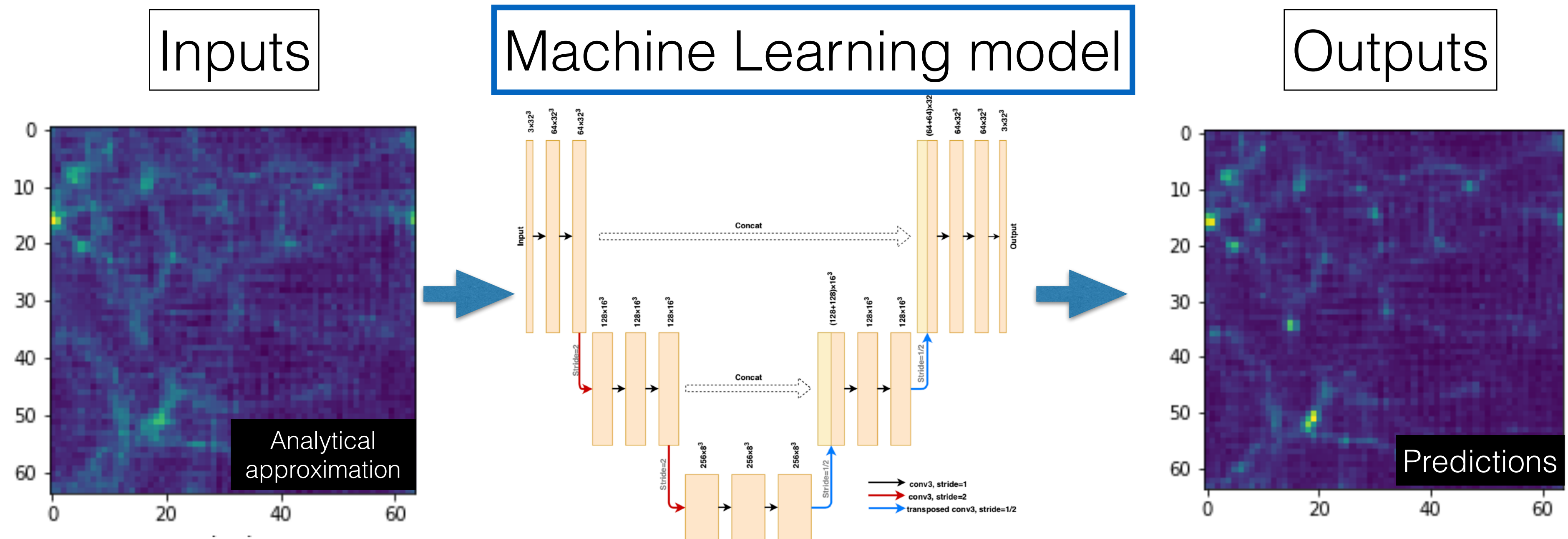
Machine Learning model

Outputs

Instead of using **numerical simulations** of newton's laws for all the particles,
with smart algorithms to run really fast.

We will attempt to use machine learning to
“learn”/ interpolate from a large number of pre-run simulations.

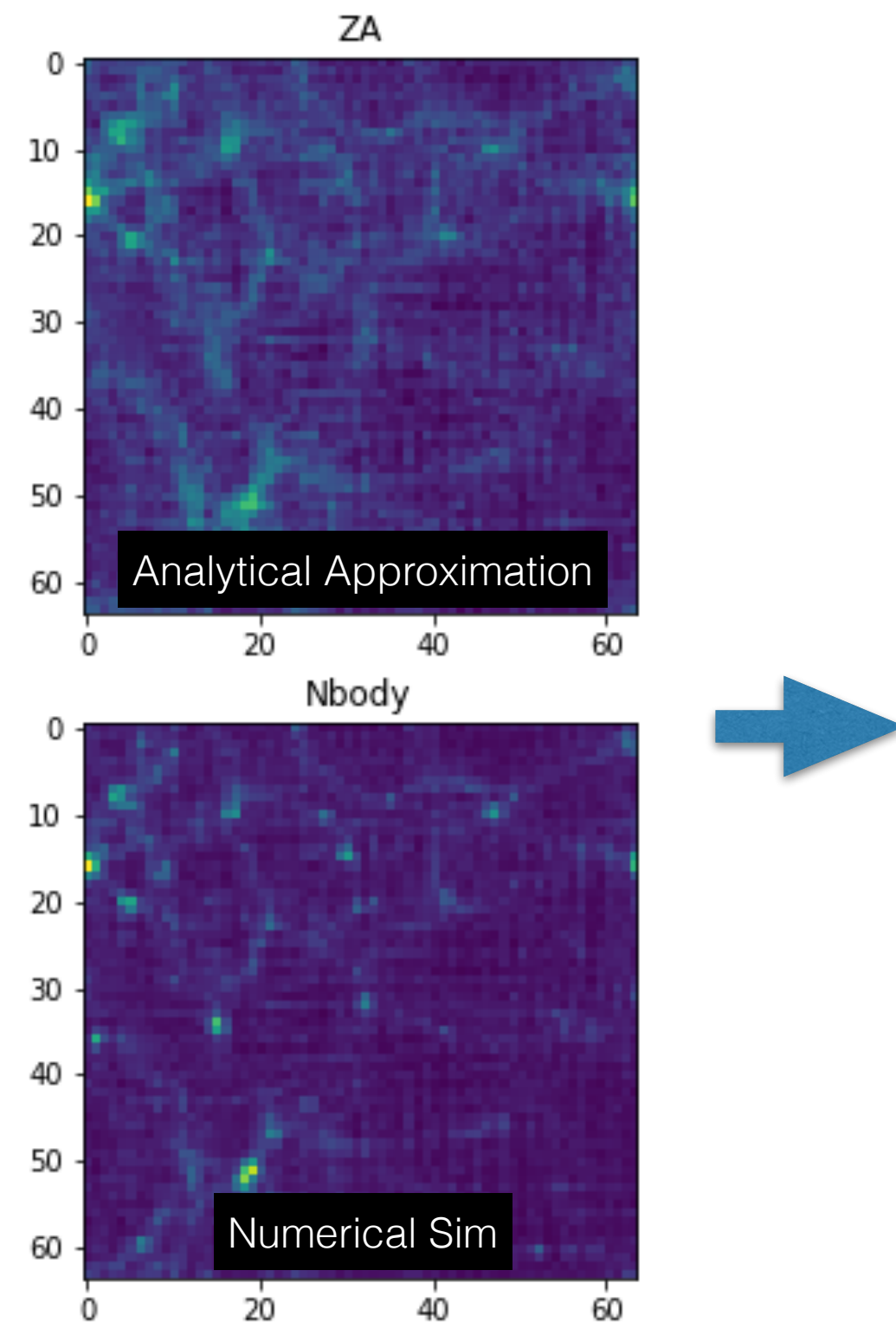
From Analytical approximated fields to numerically simulated fields



Siyu He, Yin Li, Yu Feng, **S.H.**, Siamak Ravanbaksh, Barnabas Póczos,
Proceedings of National Academy of Sciences 2019

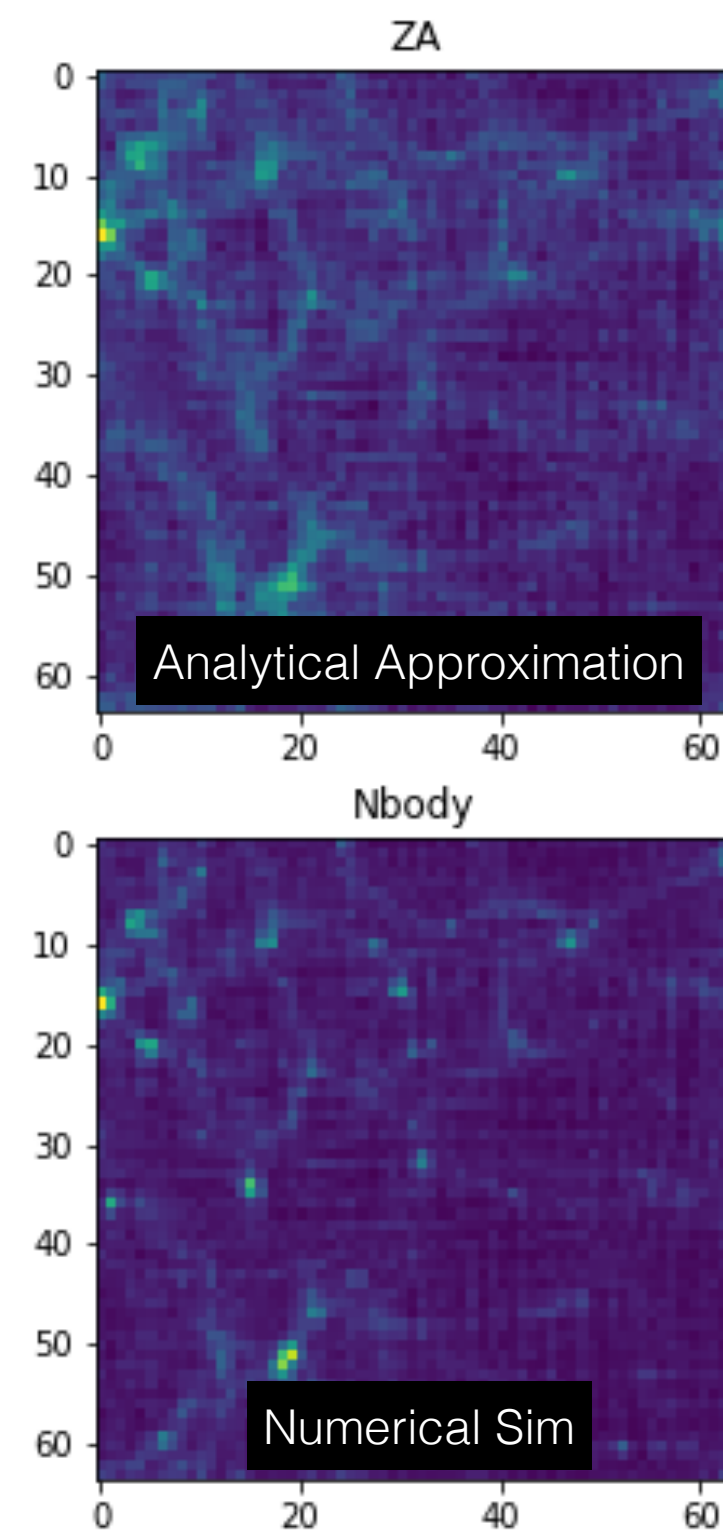
From Analytical approximated fields to numerically simulated fields: Training

Training



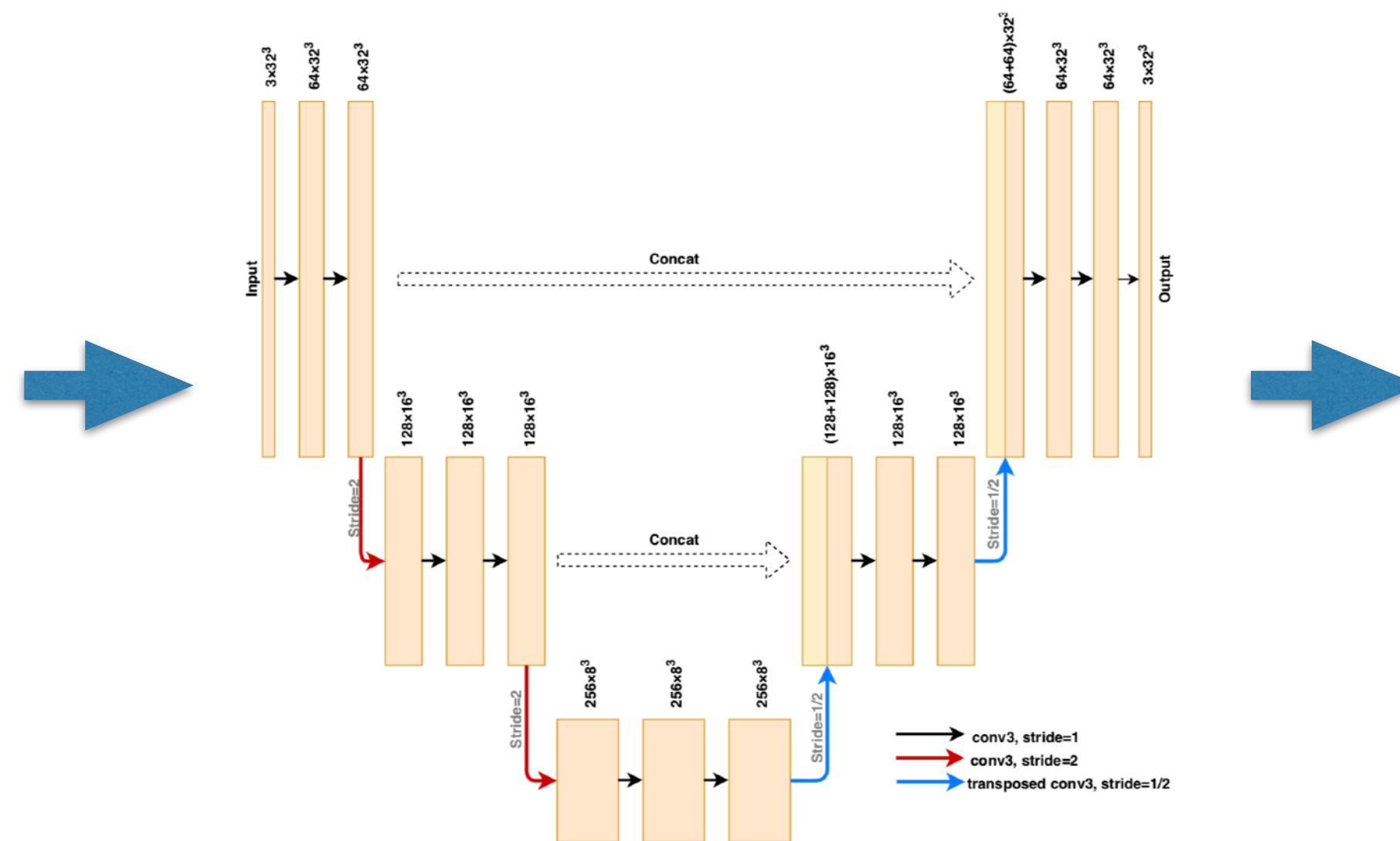
8,000 pairs of
[Analytical, Sim] 3D boxes
For training

From Analytical approximated fields to numerically simulated fields: Model



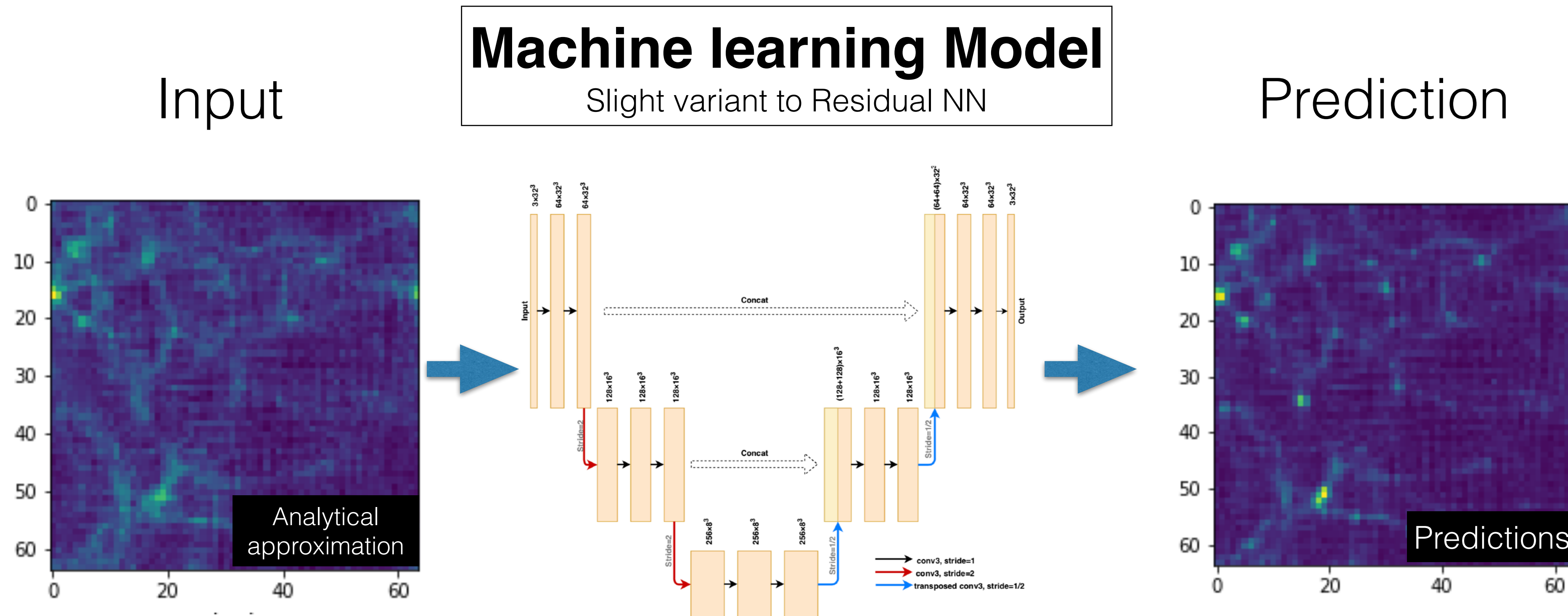
Machine learning Model

Slight variant to Residual NN

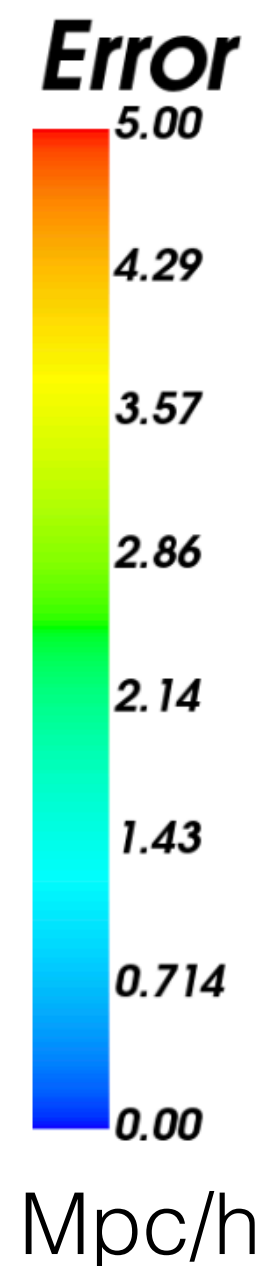


8,000 pairs of
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From Analytical approximated fields to numerically simulated fields: Final setup



Using Machine learning to simulate the Universe: How well do we do ?

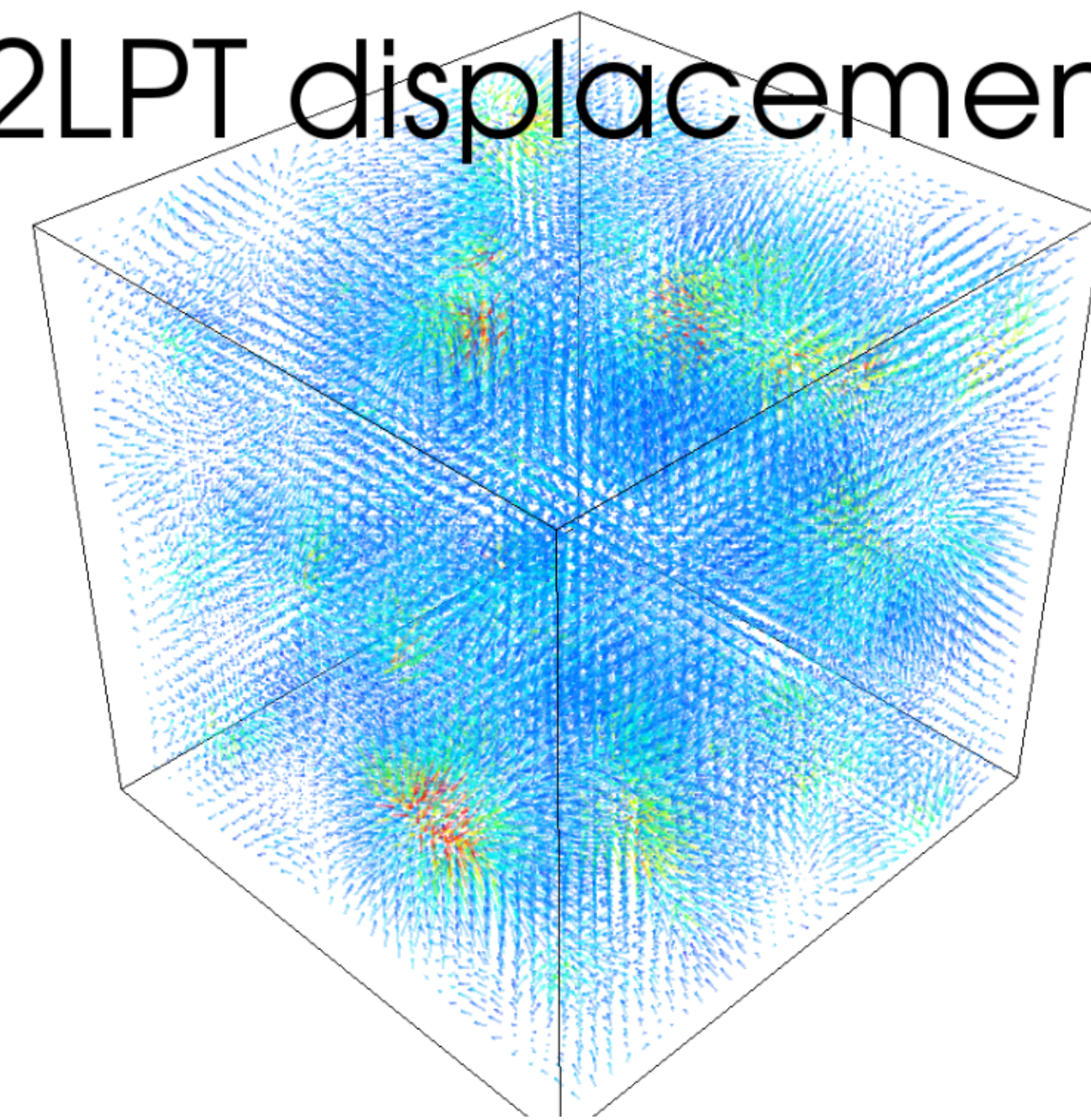
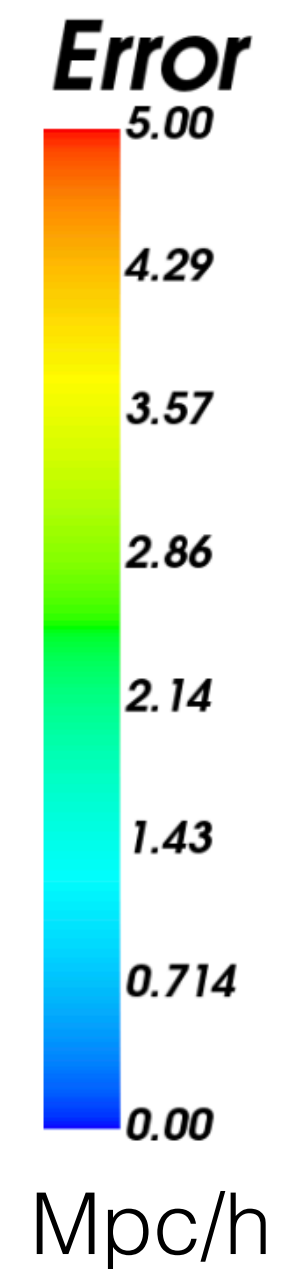


We will show the errors in displacement field, predicted by
Our benchmark model (2LPT), and our ML model
Displacement field is the difference
between current position to the initial position of the particles

Using Machine learning to simulate the Universe: How well do we do ?

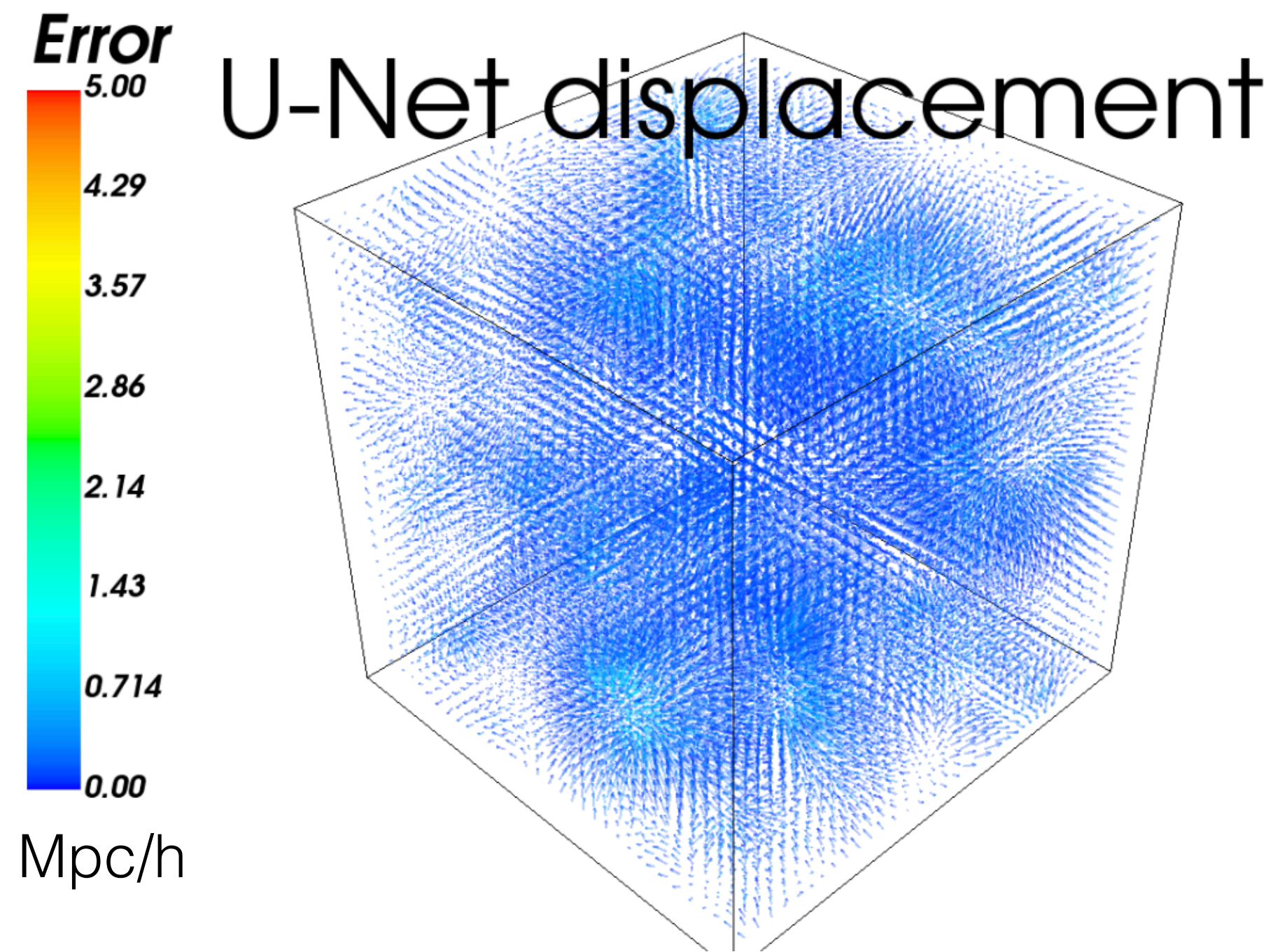
Benchmark (2LPT)
prediction errors

2LPT displacement

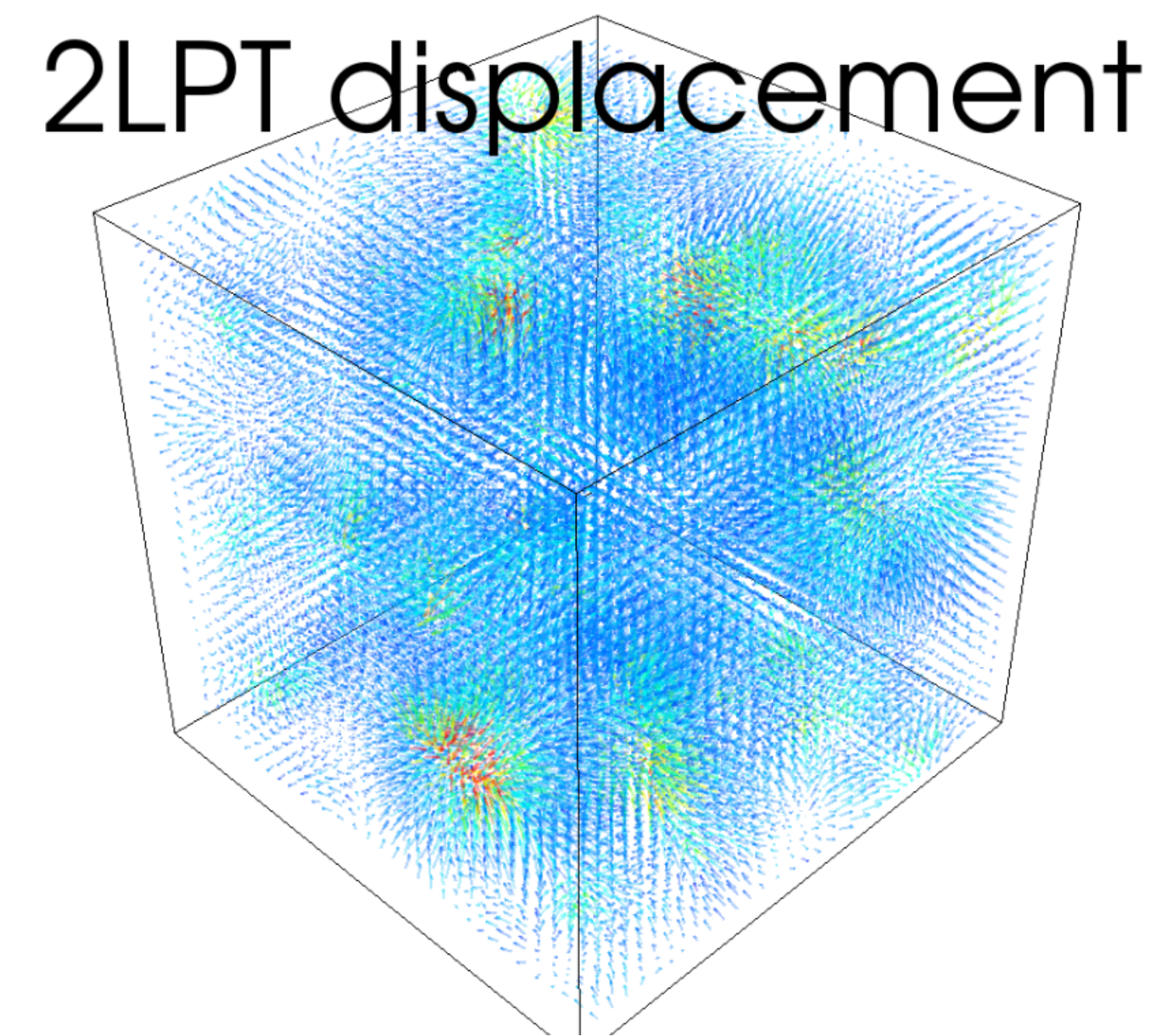


Using Machine learning to simulate the Universe: How well do we do ?

Machine Learning Model
prediction errors



Benchmark (2LPT)
prediction errors



Using Machine learning to simulate the Universe: How well do we do?

Checking the following:

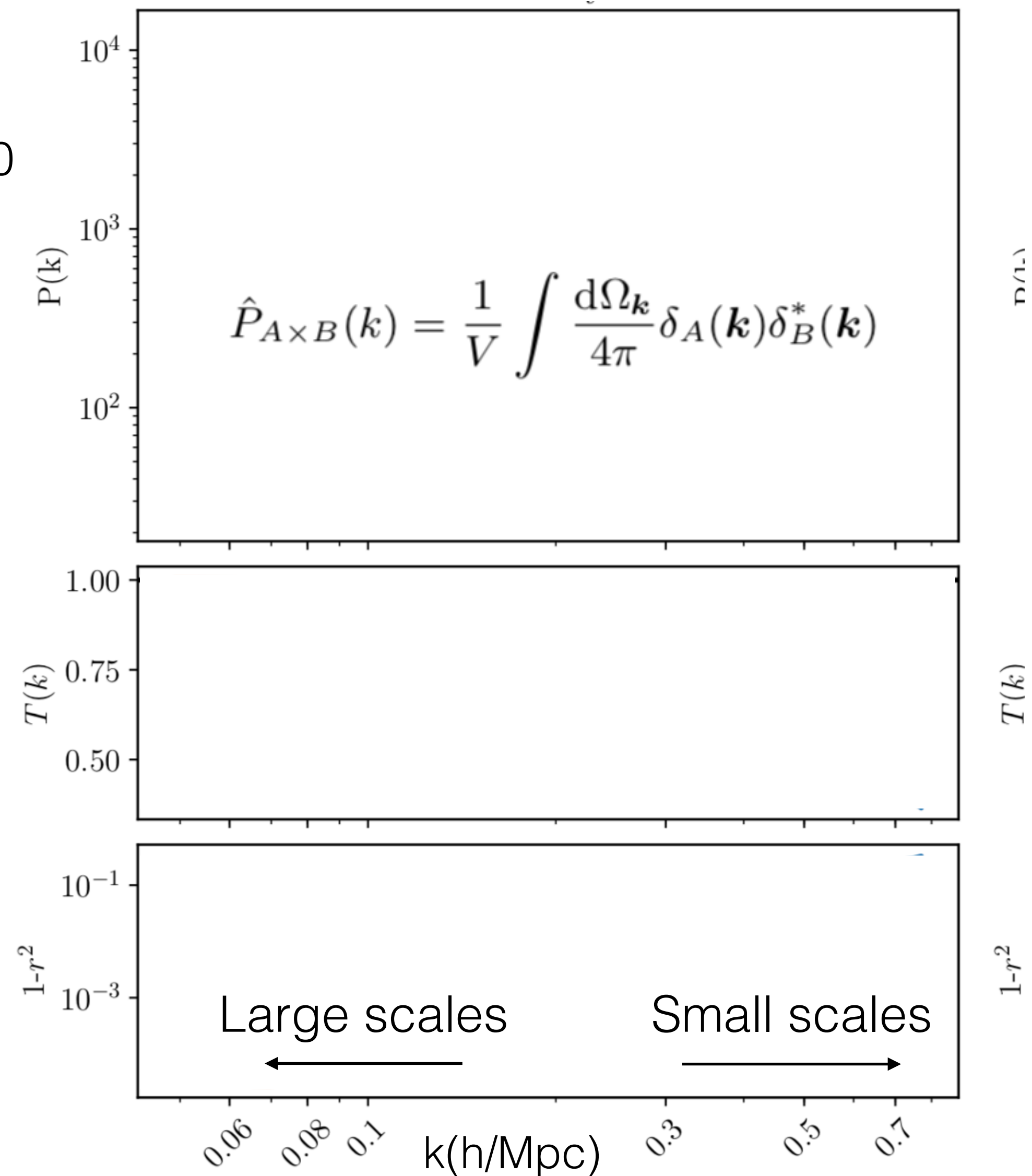
- 1) the average **power-spectrum** of 1000 sims, and
- 2) **ratios** to the true power-spectrum ($T(k)$), and
- 3) The **cross-correlation coefficient**

1000 simulations predicted in **30 sec.**

1 training simulation takes **1.8 million sec**

$$T(k) = \frac{P_{\text{pred}}(k)}{P_{\text{true}}(k)}$$

$$r(k) = \frac{P_{\text{pred} \times \text{true}}(k)}{\sqrt{P_{\text{pred}}(k)P_{\text{true}}(k)}}$$



(a) Results from the density field

Distance (1 Mpc/h = 4.5×10^6 light years)

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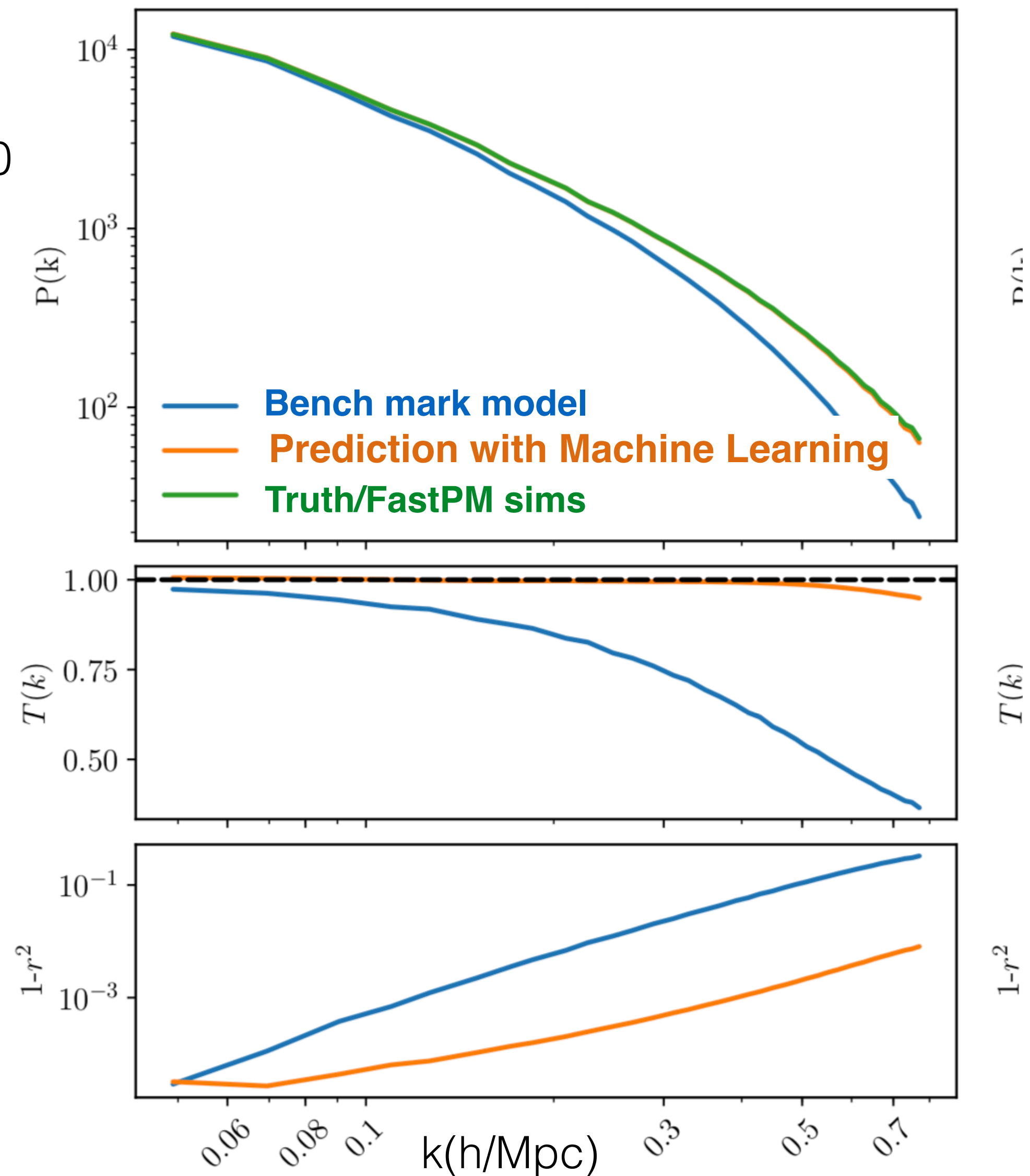
1000 simulations predicted in 30 sec.

1 training simulation takes 1.8 million sec

~60 million times faster

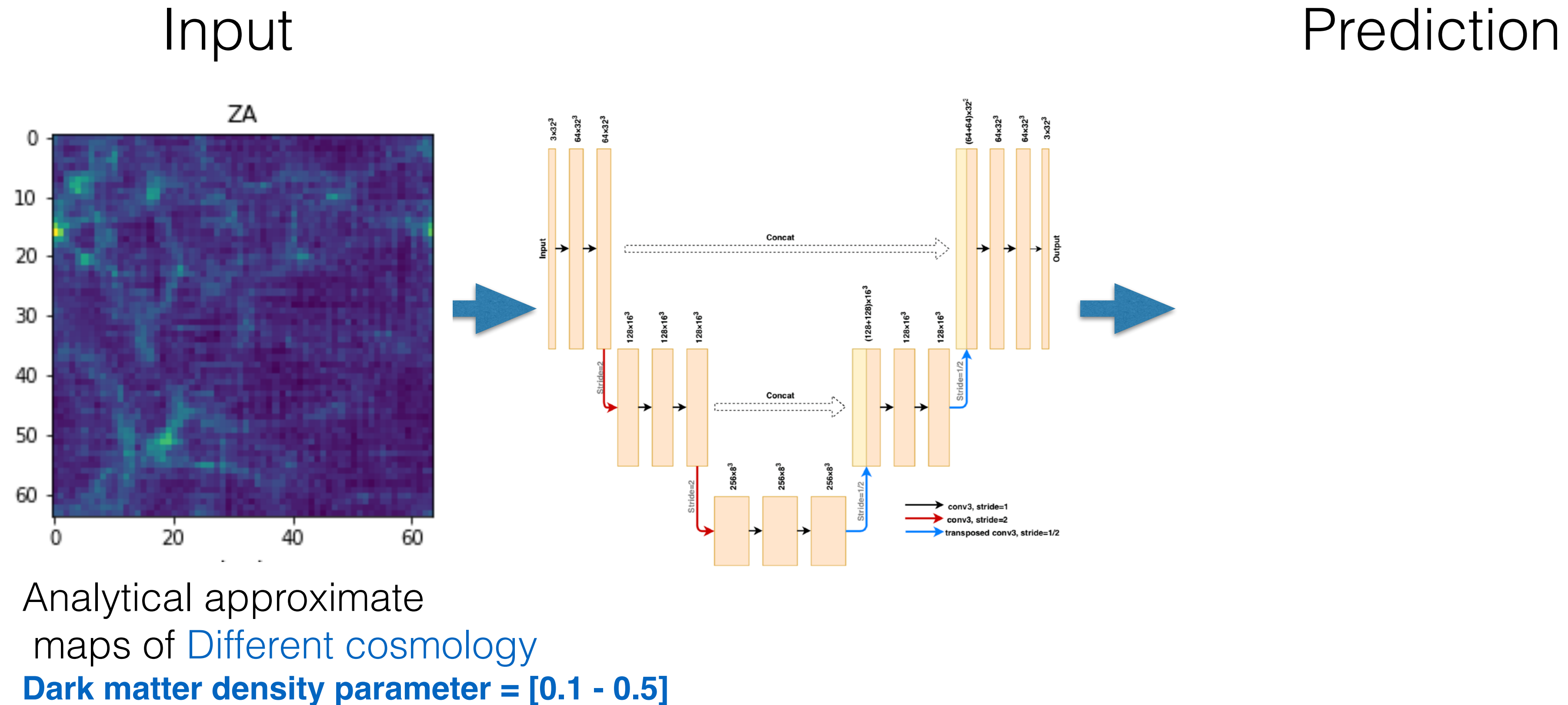
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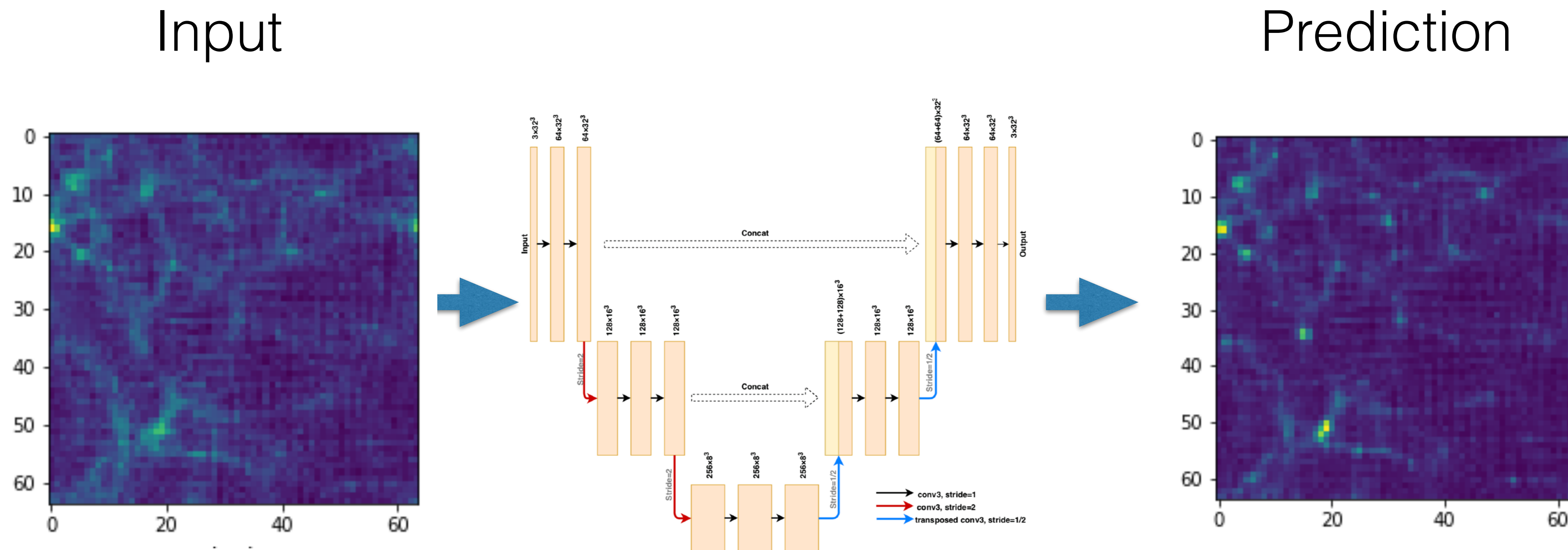


(a) Results from the density field

Making simulations that are different from our training set: Extrapolating instead of interpolating?



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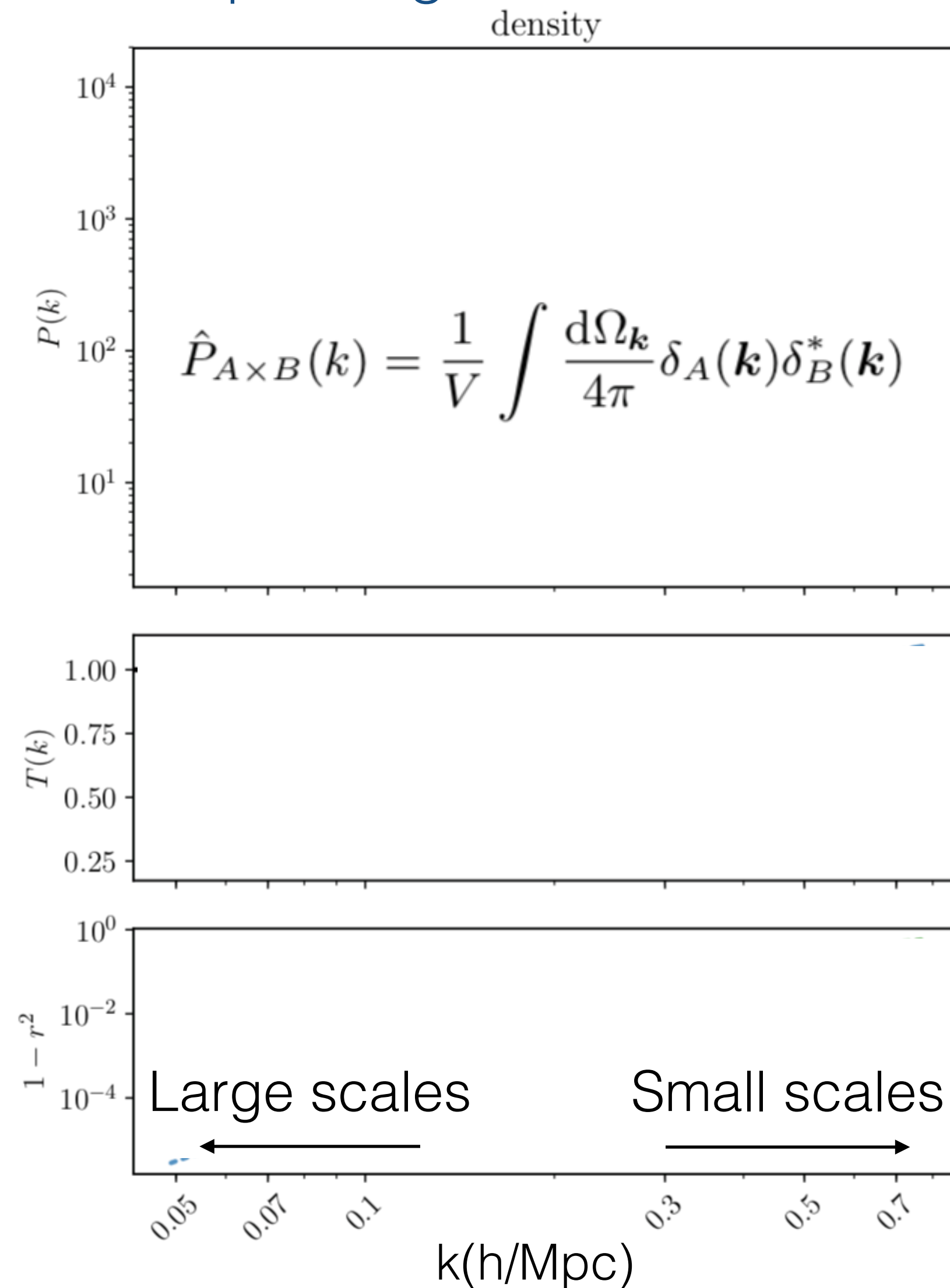
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Solid Line: Simulation /Truth

Long Dashed line: Prediction using ML

Short Dashed Line: Analytical approximation (2LPT)



(b) Two point analysis for density field

Making simulations that are different from our training set:

Extrapolating instead of interpolating? YES!

Checking the following:

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- 2) ratios to the true power-spectrum ($T(k)$), and
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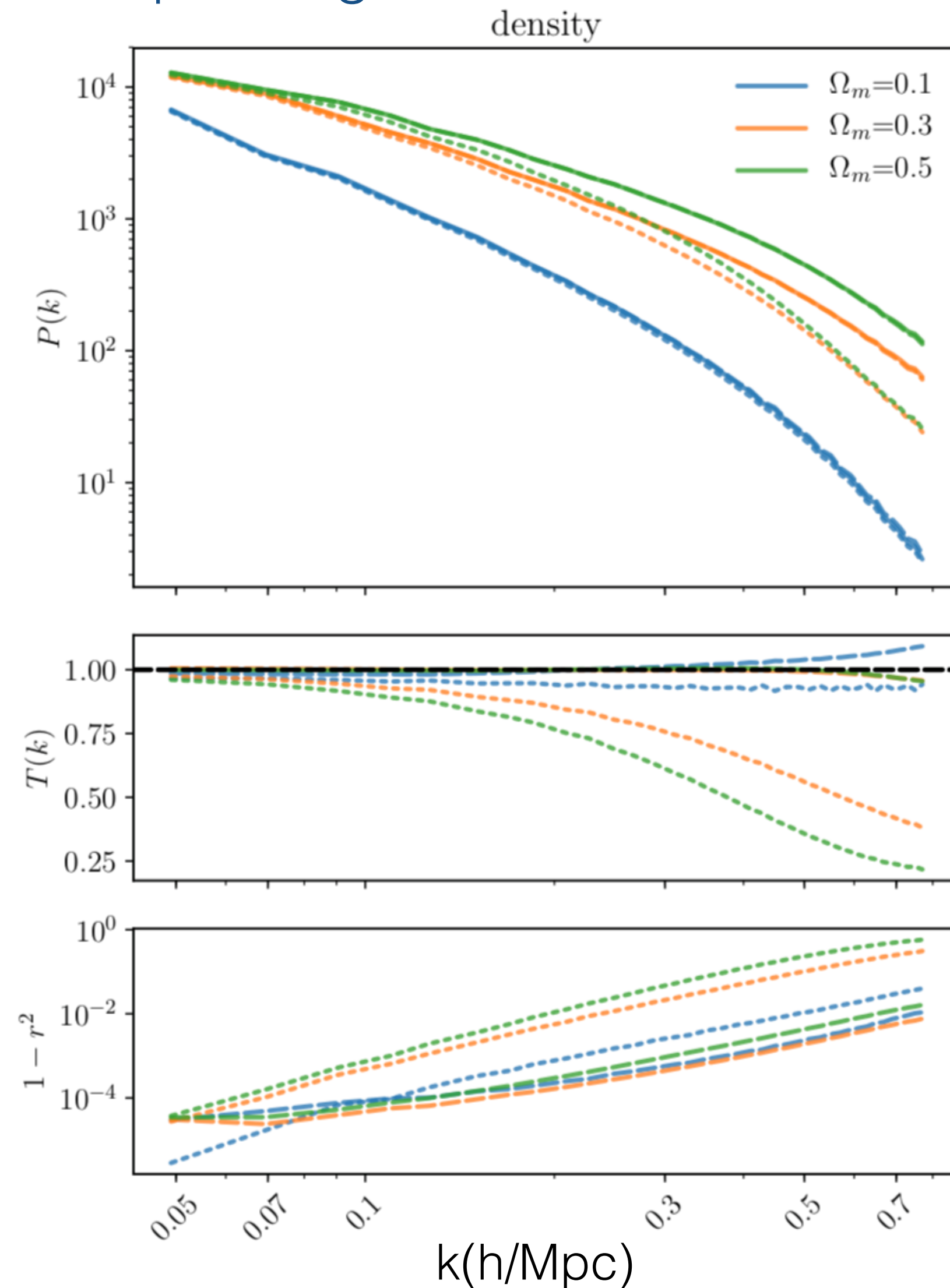
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Solid Line: Simulation /Truth

Long Dashed line: Prediction using ML

Short Dashed Line: Benchmark Model (2LPT)

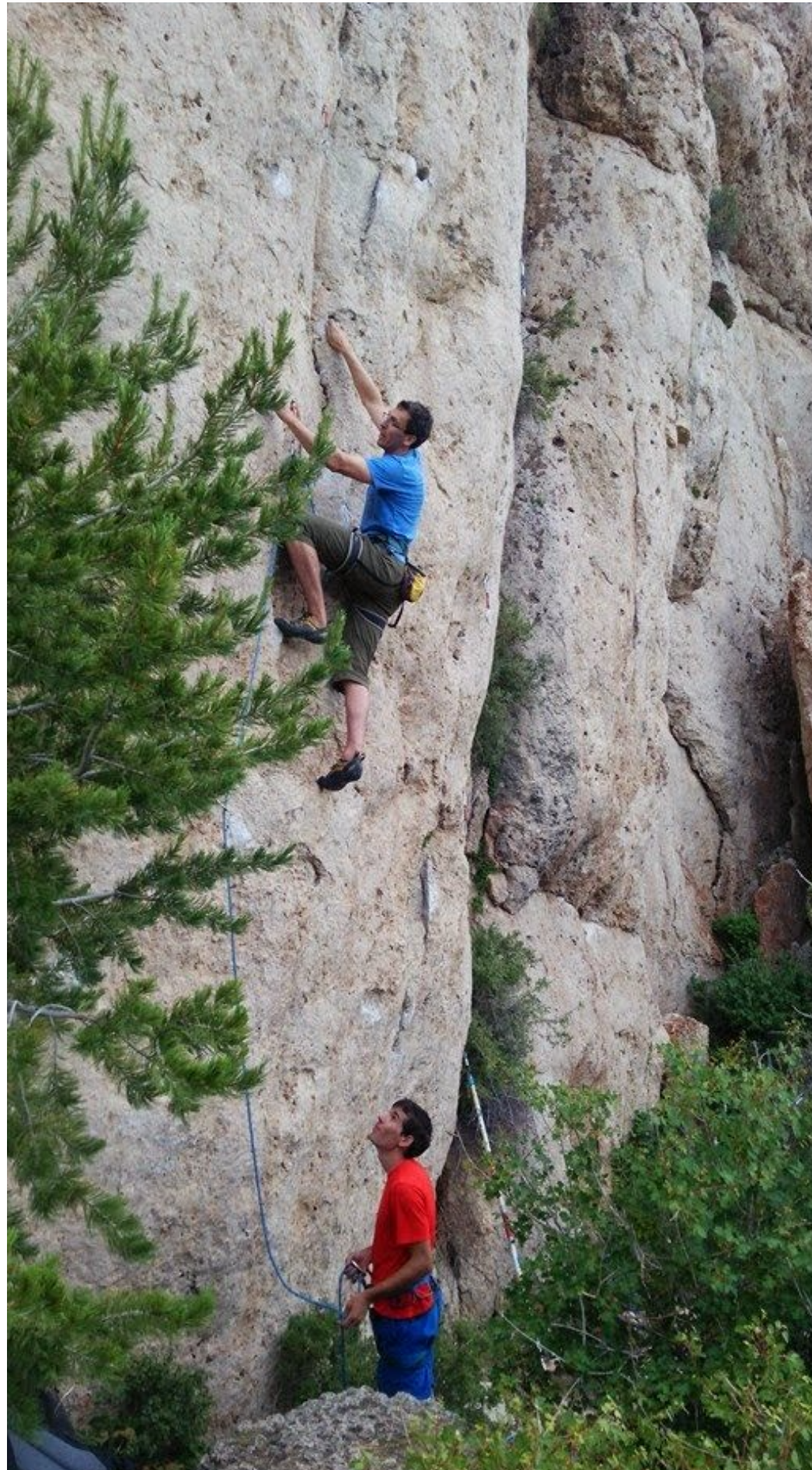


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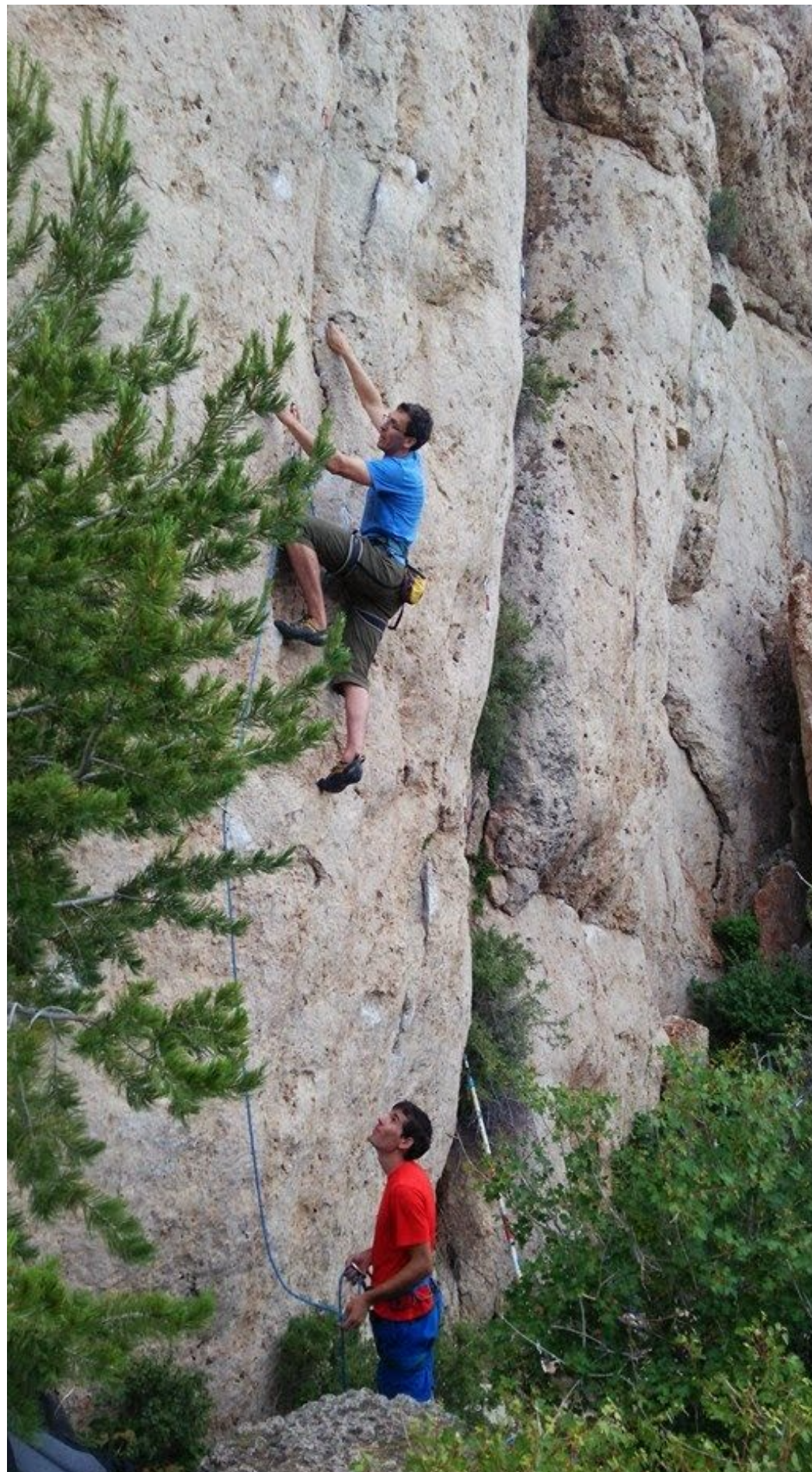
What happened?

- The model generalized significantly outside the training set!
- We did not explicitly use any transfer learning or meta-learning
- Maybe there is overlap in information somewhere between these universes?
- Maybe the Universe is fairly simple, so that the generalization and extrapolation by the network is 'easy'?
- Can we explain/interpret this generalization?

My possible climb to fame?



My possible climb to fame?



- Understanding Machine Learning?
- Compressing the learned model into physical laws
 - See work led by Miles Cranmer (Princeton), NeurIPS 2020
- Discover laws of nature?
 - See work led by Pablo Lemos (UCL/Sussex) & Miles Cranmer (Princeton), submitted to PNAS 2021