Simons Collaboration on Learning the Universe:

AI-Driven Inference of Galaxy Formation and Cosmology

Greg Bryan
Columbia University

SIMONS

Learning the Initial Conditions of the Universe

A Simons Collaboration

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Laurence Levasseur (Université de Montréal)
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Ben Wandelt (IAP/CCA)
Rachel Somerville (CCA)
Simone Ferraro (Berkeley)
Shy Genel (CCA)
Francisco Villaescusa-Navarro (CCA)

www.learning-the-universe.org

COLLABORATION MEMBERS

Last	First	Institution
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Alsing	Justin	Stockholm University
Andrews	Adam	INAF OAS Bologna
Anglés-Alcázar	Daniel	University of Connecticut
Ata	Metin	Stockholm University
Bairagi	Anirban	Institut d'Astrophysique de Paris (IAP)
Bartlett	Deaglan	Institut d'Astrophysique de Paris
Bayer	Adrian	Princeton University
Bennett	Jake	Harvard University
Bhowmick	Aklant	University of Virginia
Blecha	Laura	University of Florida
Bonab	Ariyana	CUNY
Borodina	Olga	Harvard University
Bourdin	Antoine	McGill University
Bryan	Greg	Columbia University
Burger	Jan David	Max Planck Institute for Astrophysics
Chartier	Nicolas	Seoul National University
Choi	Ena	University of Seoul
Choi	Hyunseop (Joseph)	Université de Montréal
Cochrane	Rachel	University of Edinburgh
Costa	Tiago	Newcastle University
Cuesta-Lazaro	Carolina	Harvard University
Darlinger	Rachel	University de Montreal
Delgado	Ana Maria	Harvard University
Ding	Simon	Institut d'Astrophysique de Paris (IAP)
Doeser	Ludvig	Stockholm University
Dong	Jameson	Johns Hopkins University
Farcy	Marion	École polytechnique fédérale de Lausanne (EPFL)
Ferraro	Simone	Lawrence Berkeley Lab
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Gabrielpillai	Austen	CUNY Graduate Center
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Genel	Shy	Flatiron Institute
Genina	Anna	Max Planck Institute for Astrophysics
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Hezaveh	Yashar	Université de Montréal
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Hlavacek-Larrondo	Julie	Université de Montréal
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Holma	Pontus	Stockholm University
Iyer	Kartheik	Columbia University
Jasche	Jens	Stockholm University
Jeffreson	Sarah	Harvard University
Jeffrey	Niall	University College London
Jespersen	Christian	Princeton University
Jo	Yongseok	Columbia University
Kim	Chang-Goo	Princeton University
Koudmani	Sophie	University of Cambridge
Lapel	Axel	Institut d'Astrophysique de Paris
Lavaux	Guilhem	Institut d’Astrophysique de Paris
Leclercq	Florent	Institut d'Astrophysique de Paris
Lee	Max	Columbia University
Legin	Ronan	Université de Montréal
Lovell	Chris	University of Portsmouth
Lue	Amanda	Columbia University
Makinen	Lucas	Imperial College London
Malandrino	Rosa	IAP
McAlpine	Stuart	Stockholm University
Messere	Michael	Columbia University
Modi	Chirag	Flatiron Institute
Ni	Yeuying	Harvard University
Oh	Boon Kiat	University of Connecticut
Ostriker	Eve	Princeton University
Pakmor	Ruediger	MPA
Pandey	Shivam	University of Pennsylvania
Pandya	Viraj	Columbia University
Payot	Nicolas	Université de Montreal
Perez	Lucia	Princeton University
Perreault-Levasseur	Laurence	Université de Montréal
Poczos	Barnabas	Carnegie Mellon University
Prunier	Marine	University de Montreal
Quataert	Eliot	Princeton University
Scoggins	Matthew	Columbia Unviersity
Sharief	Sammy	University de Montreal
Singh	Aarti	Carnegie Mellon University
Smith	Matthew	Max-Planck-Institute for Astrophysics
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Sotoudeh	Hadi	University of Cambridge
Spergel	David	Simons Foundation
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Steinwandel	Ulrich	Max-Planck-Institute for Astrophysics
Stiskalek	Richard	Oxford University
Stone	Jim	IAS
Su	Kung-Yi	Northeast University
Sui	Ce	Johns Hopkins University
Talbot	Rosemary	Max-Planck-Institute for Astrophysics
Terrazas	Bryan	Oberlin College
Thiele	Leander	IPMU, University of Tokyo
Torrey	Paul	University of Virginia
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Wandelt	Ben	Johns Hopkins University
Weinberger	Rainer	Leibniz Institute Potsdam (AIP)
Wilkins	Steve	Sussex
Yung	Aaron	Space Telescope Science Institute
Zhao	Xiaosheng	Johns Hopkins University
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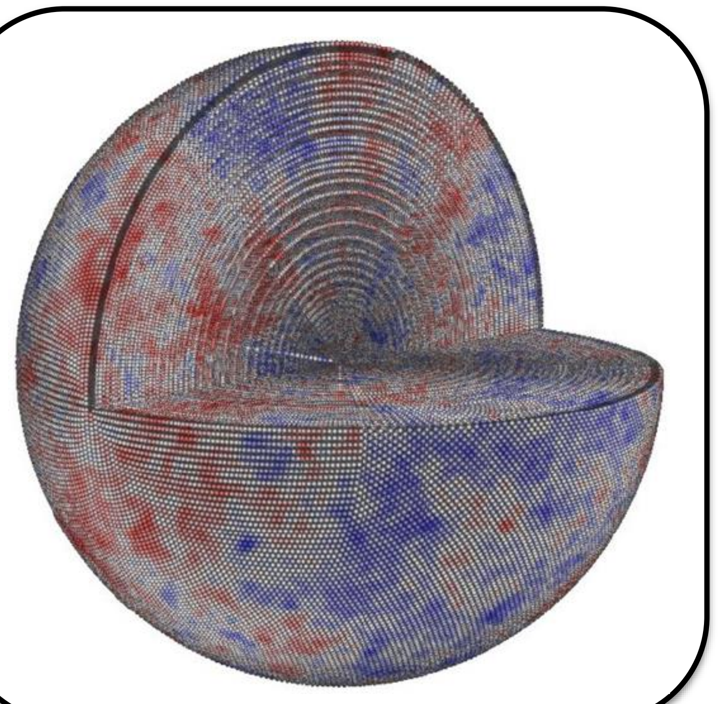
Project Goals

Use cosmological observations to infer:

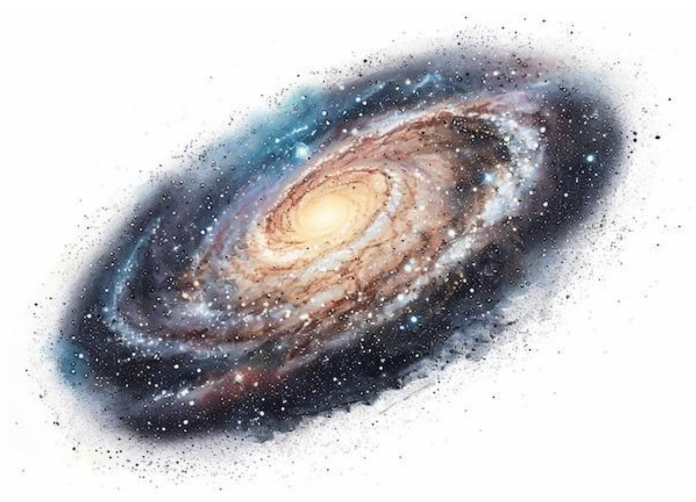
Initial conditions of the universe



Cosmological parameters

$$\Omega_m, \Omega_b, m_\nu, \ldots$$
$$\Omega_\Lambda, w_0, w_a, \ldots$$

Galaxy Physics



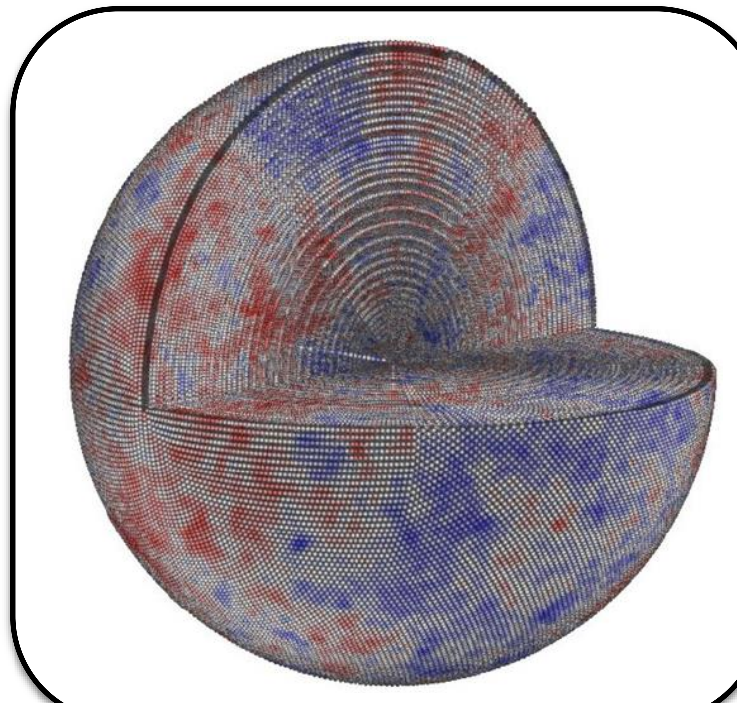
How Can We Do This?

Galaxy Physics

Cosmological parameters

$$\Omega_m, \Omega_b, m_\nu, \ldots$$
$$\Omega_\Lambda, w_0, w_a, \ldots$$

Initial conditions of the universe



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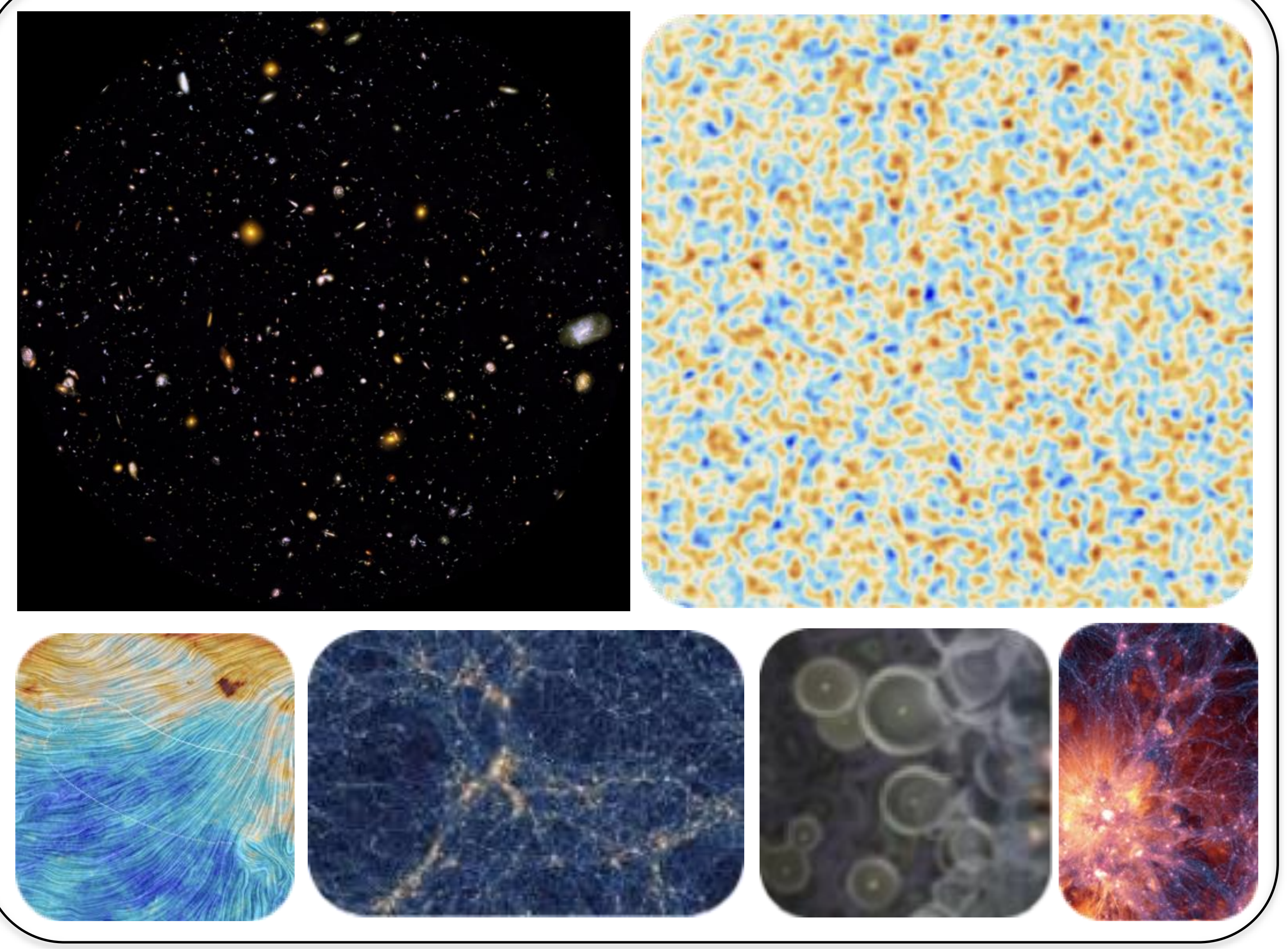
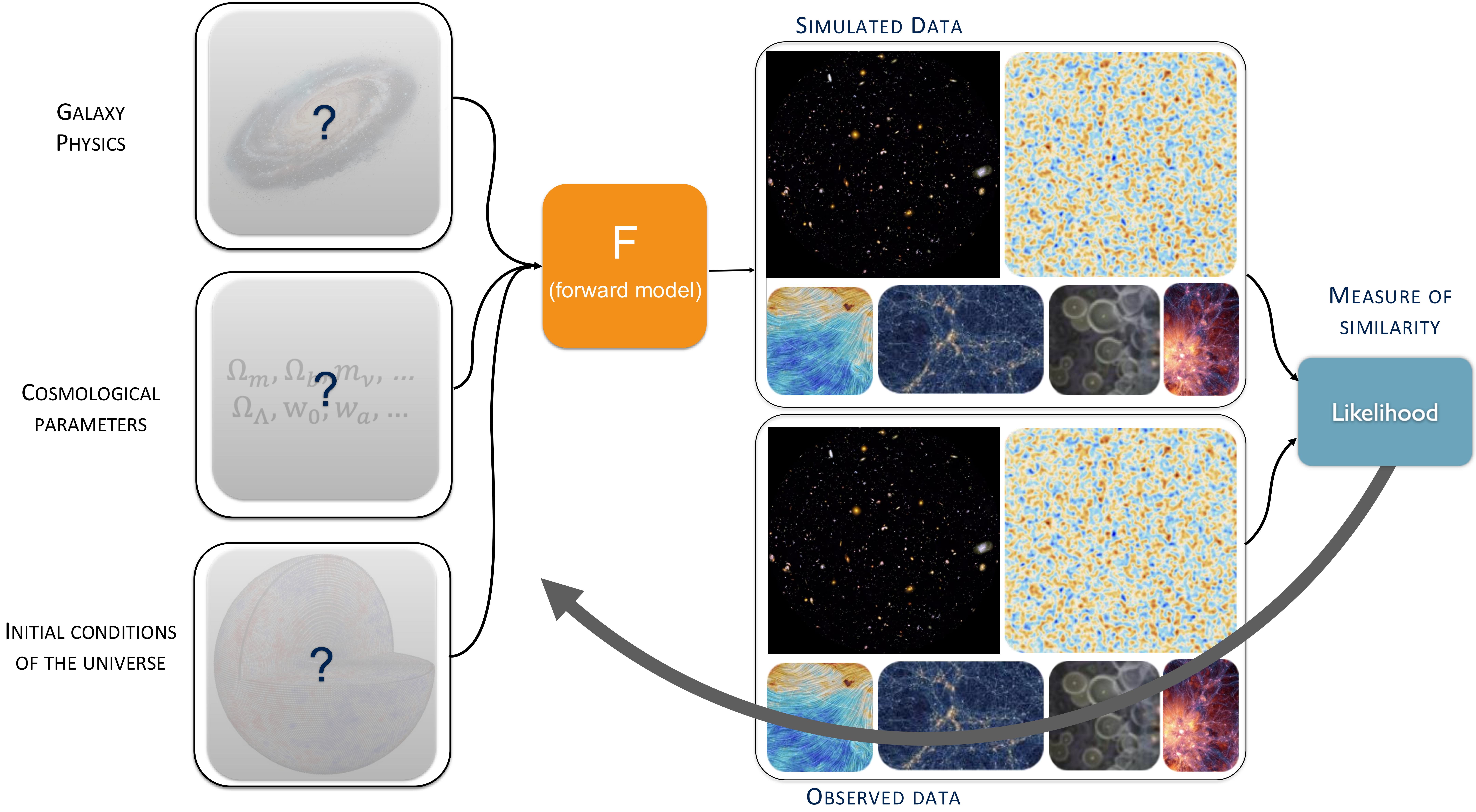


Observed data

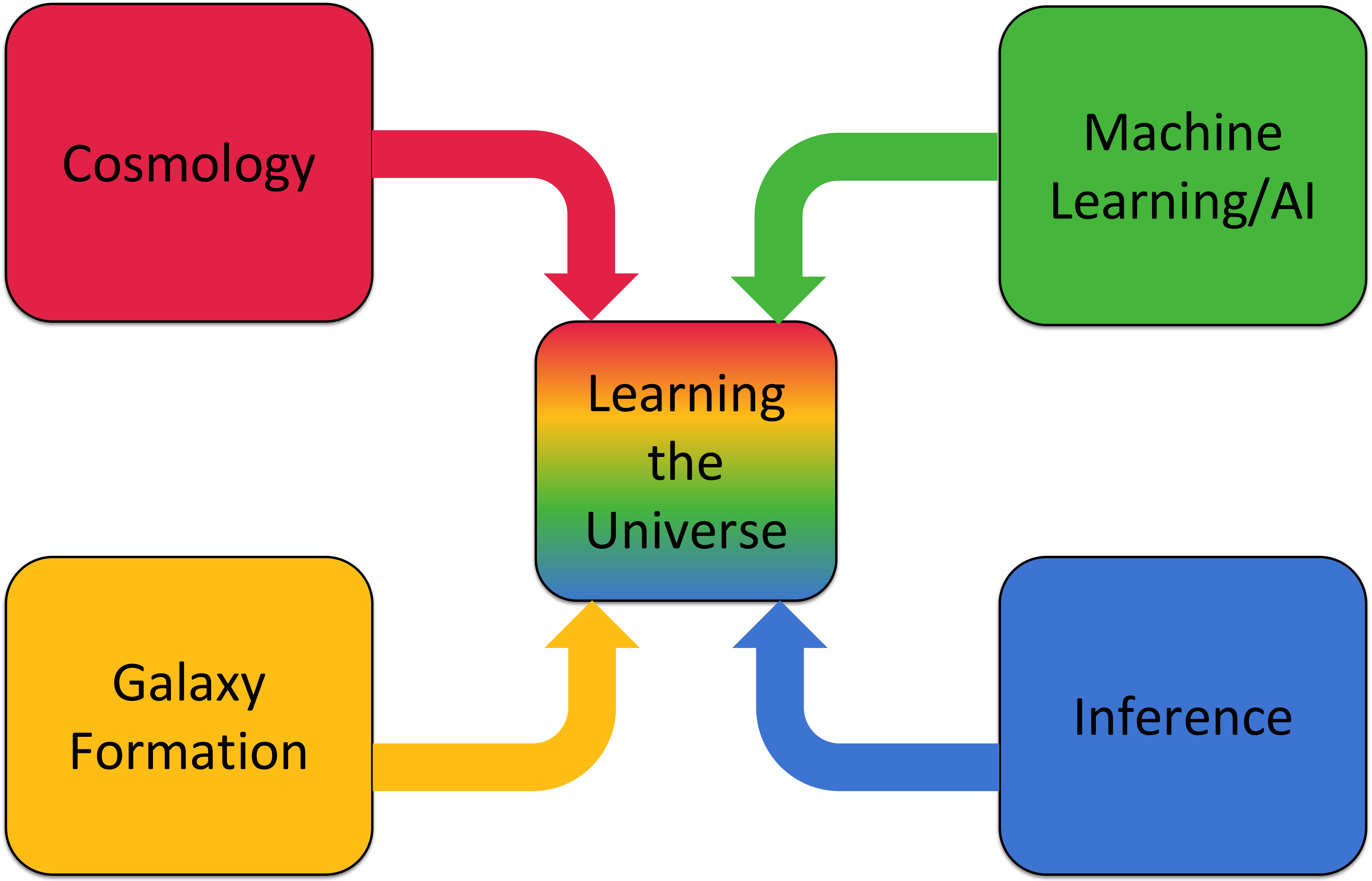
INFERRING THE INITIAL CONDITIONS THROUGH BAYESIAN MODELING



However…

- This approach works well for small inference problems with simple likelihoods and a handful of parameters. For this problem it is *intractable in multiple ways*:
  - The forward model is expensive (millions of CPU hours)
  - Even if we had the simulations, the exact likelihood for a galaxy survey is too complex to write down in closed form.
  - Inferring the initial conditions means inferring billions of parameters.
  - Our forward models are imperfect.

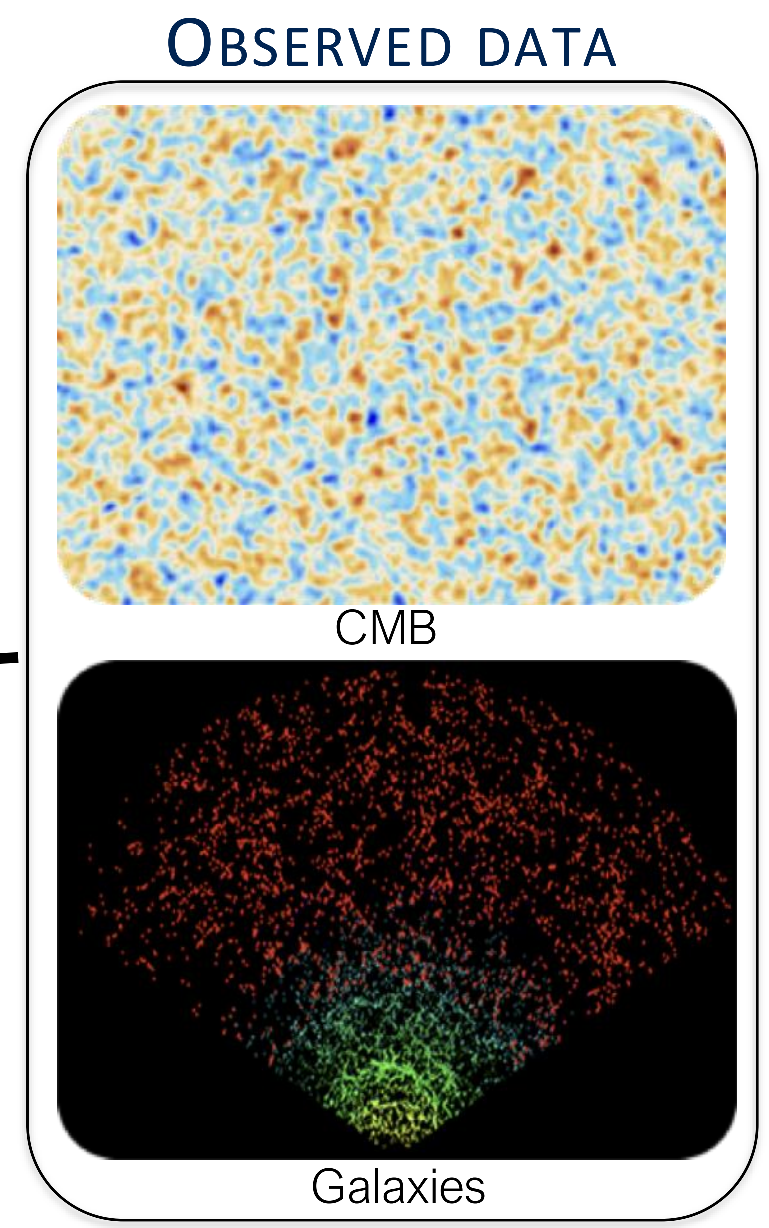
LtU: Bringing Together Domain Experts From Four Fields

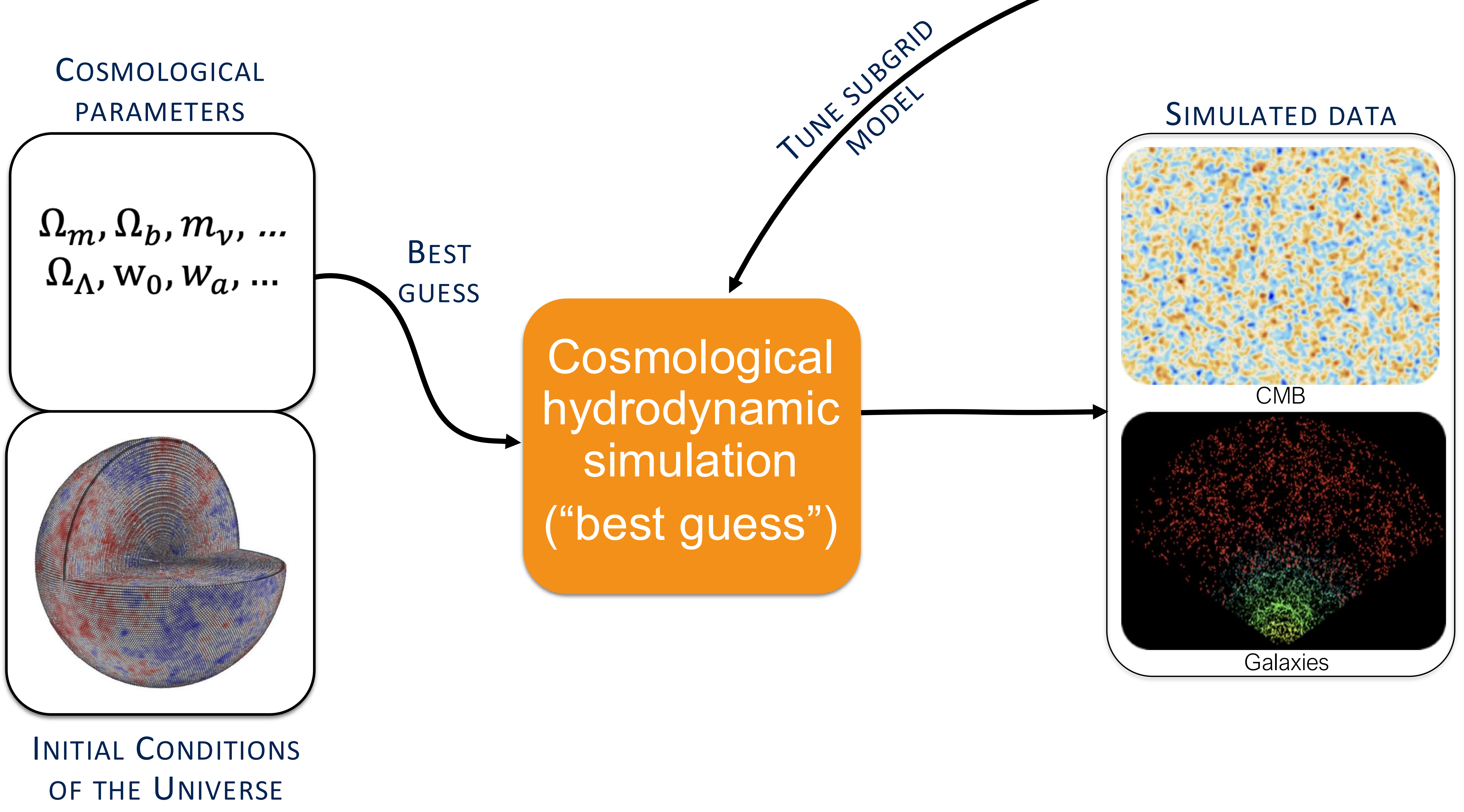


PREVIOUS APPROACH

1. Galaxy formation simulations

- Most galaxy simulations use single “best guess” sub-grid model (no exploration of uncertainty)
- Sub-grid models for star formation/winds and black holes/AGN+jets tuned to fit observations



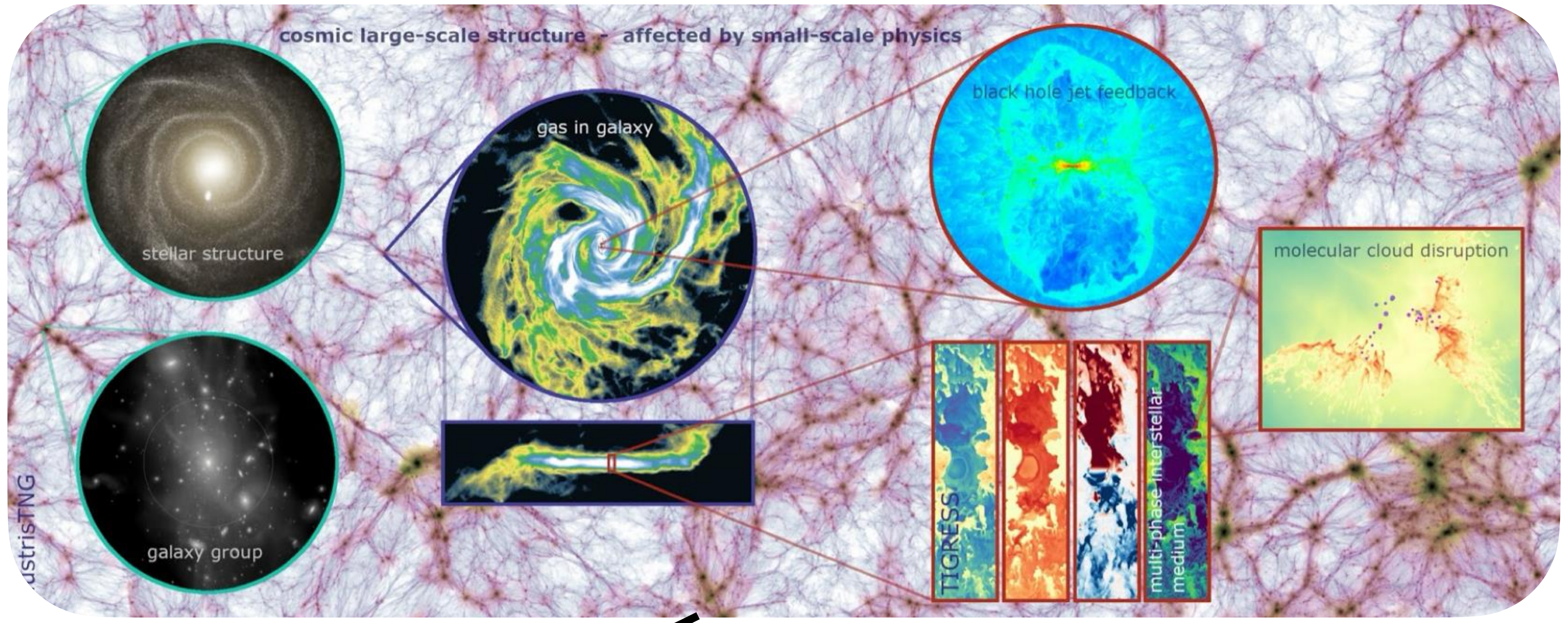


OUR APPROACH

1. Develop next-generation galaxy formation simulations

- Calibrated sub-grid model for star formation and galactic winds *from resolved (small-scale) simulations*
- Comprehensive set of sub-grid models for black hole accretion/feedback *from resolved simulations*

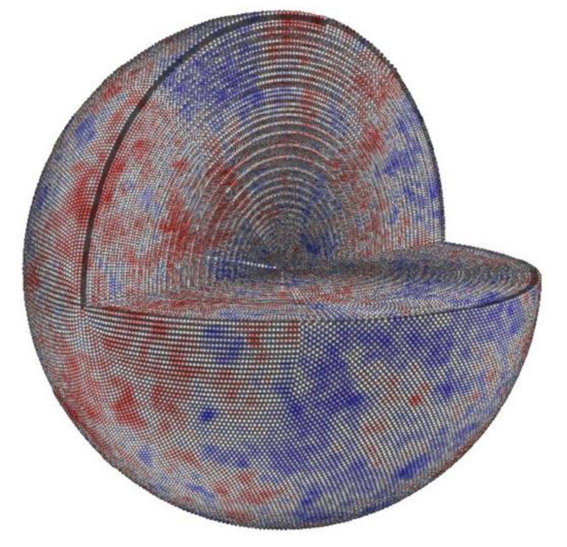
Subgrid models for cosmological simulations



From small-scale simulations

Cosmological parameters

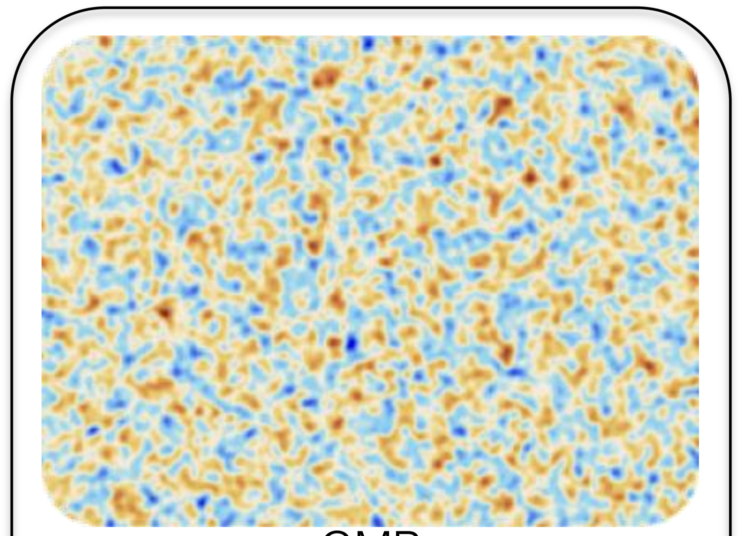
$\Omega_m, \Omega_b, m_\nu, \ldots$
$\Omega_\Lambda, w_0, w_a, \ldots$



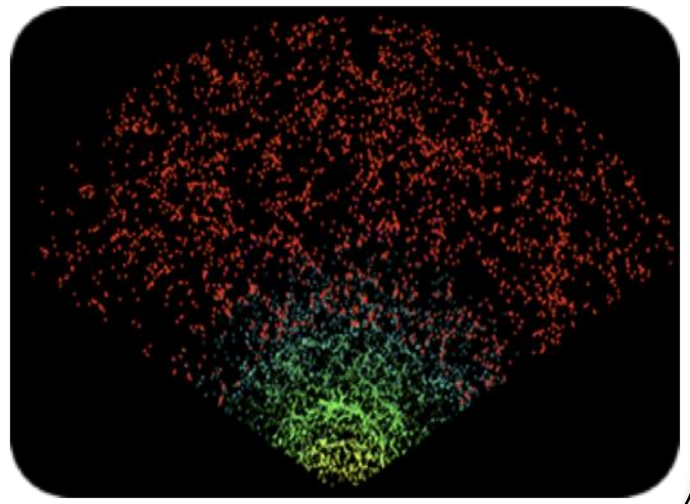
Initial Conditions of the Universe

Cosmological hydrodynamic simulation (resolved models)

Simulated data



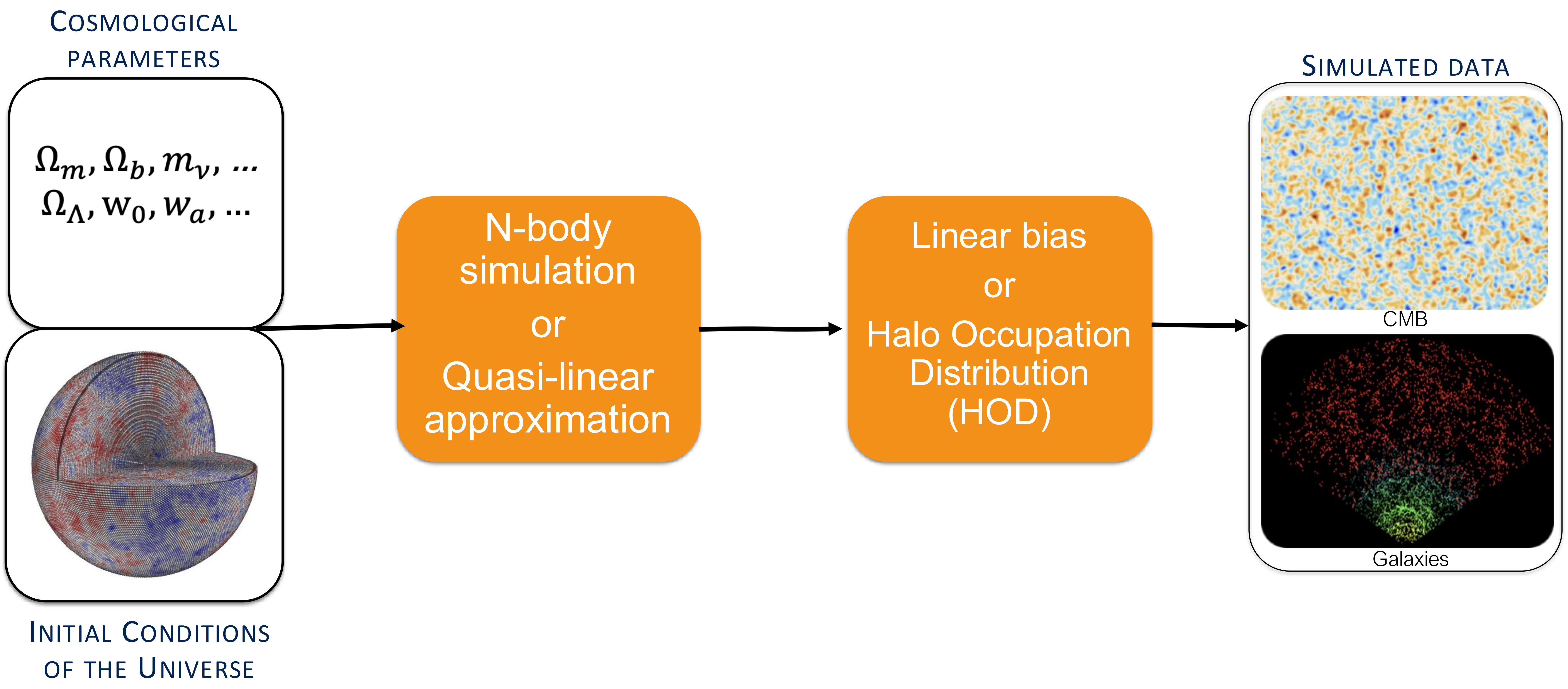
CMB



Galaxies

2. Forward modeling

- Dark matter distribution from either (i) limited set of N-body simulations or (ii) approximate quasi-linear approximation
- Connection from dark matter to halos based on simple bias or Halo Occupation (HOD) model
- Cannot predict small-scales, so limited to large-scales, often two-point functions

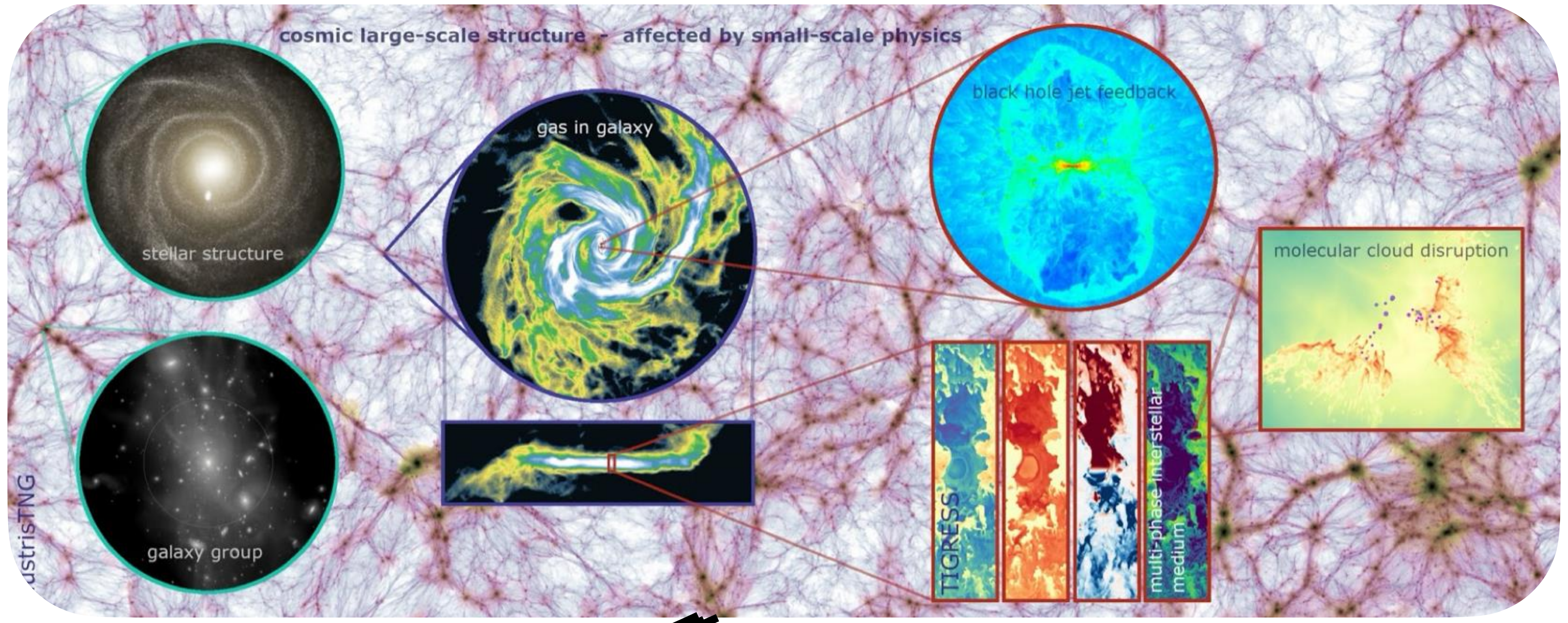


OUR APPROACH

2. FORWARD MODELING

- Carry out a large suite of cosmological simulations, varying parameters

SUBGRID MODELS FOR COSMOLOGICAL SIMULATIONS



COSMOLOGICAL PARAMETERS

$\Omega_m, \Omega_b, m_\nu, \ldots$
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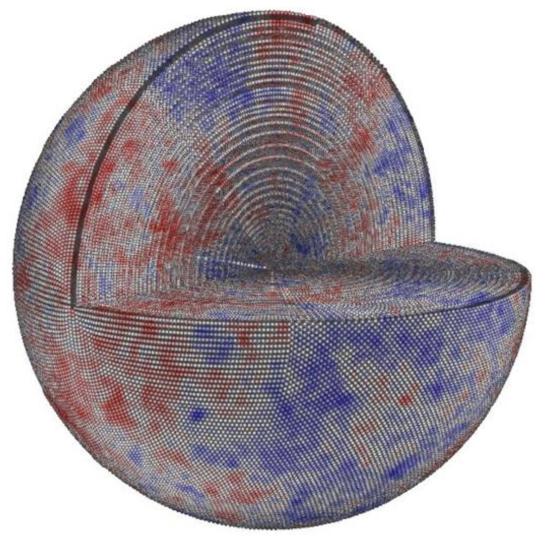


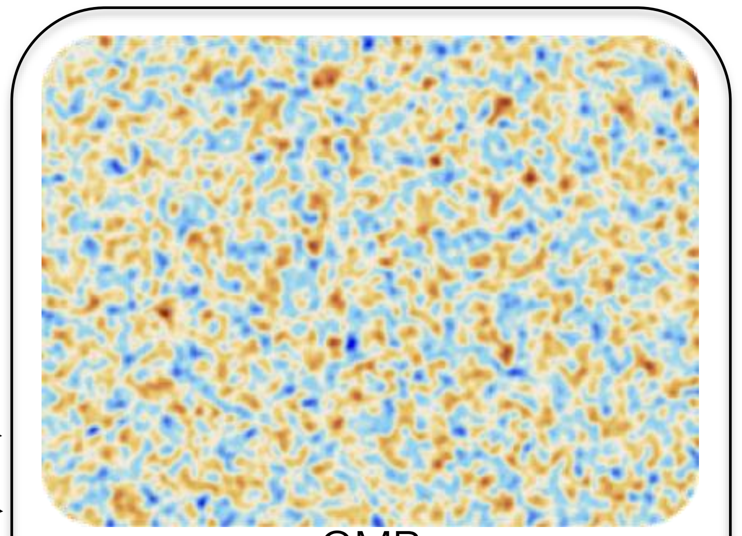
INITIAL CONDITIONS OF THE UNIVERSE

~~BEST GUESS~~

Cosmological simulation (“best guess”)

Ensemble of hydrodynamic cosmological simulations

SIMULATED DATA



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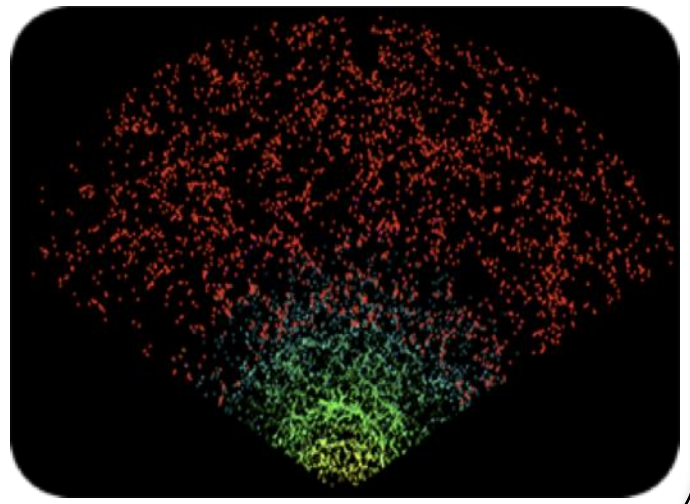
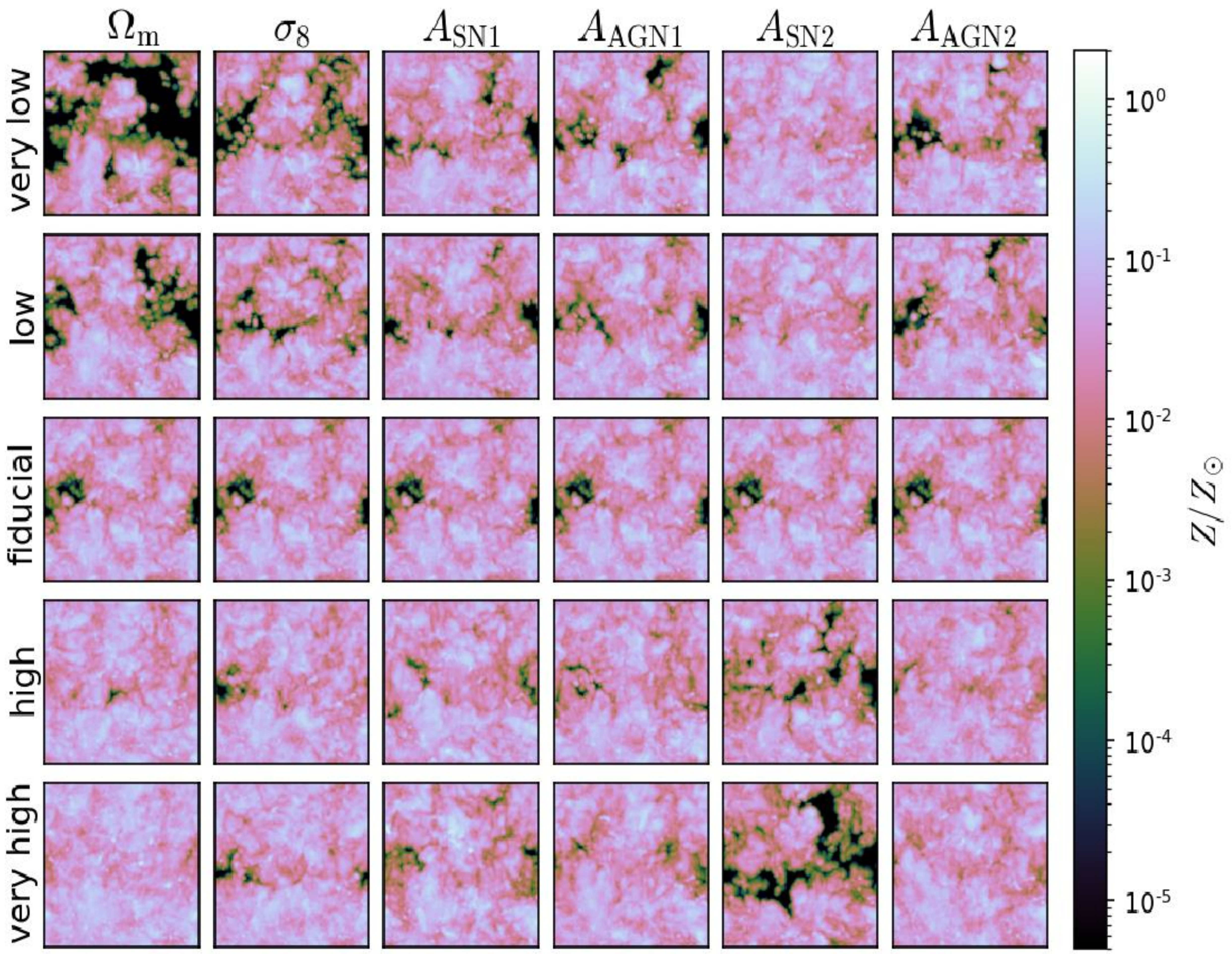


Galaxies

ENSEMBLE OF COSMOLOGICAL SIMULATIONS
(WITH CAMELS COLLABORATION - NAVARRO-VILLAESCUSA/GENEL/ANGLES-ALCAZAR)

- Simulations run with many cosmological hydrodynamics codes.
  - Well-tested, widely used, scales well
- Large suite of cosmological simulations required for emulator training
  - Vary cosmological parameters
  - Vary initial conditions
  - Vary astrophysics parameters
- Training sets:
  - "small boxes" (~25 Mpc) for galaxy properties
  - *larger volumes just released (Genel et al. 2026)*

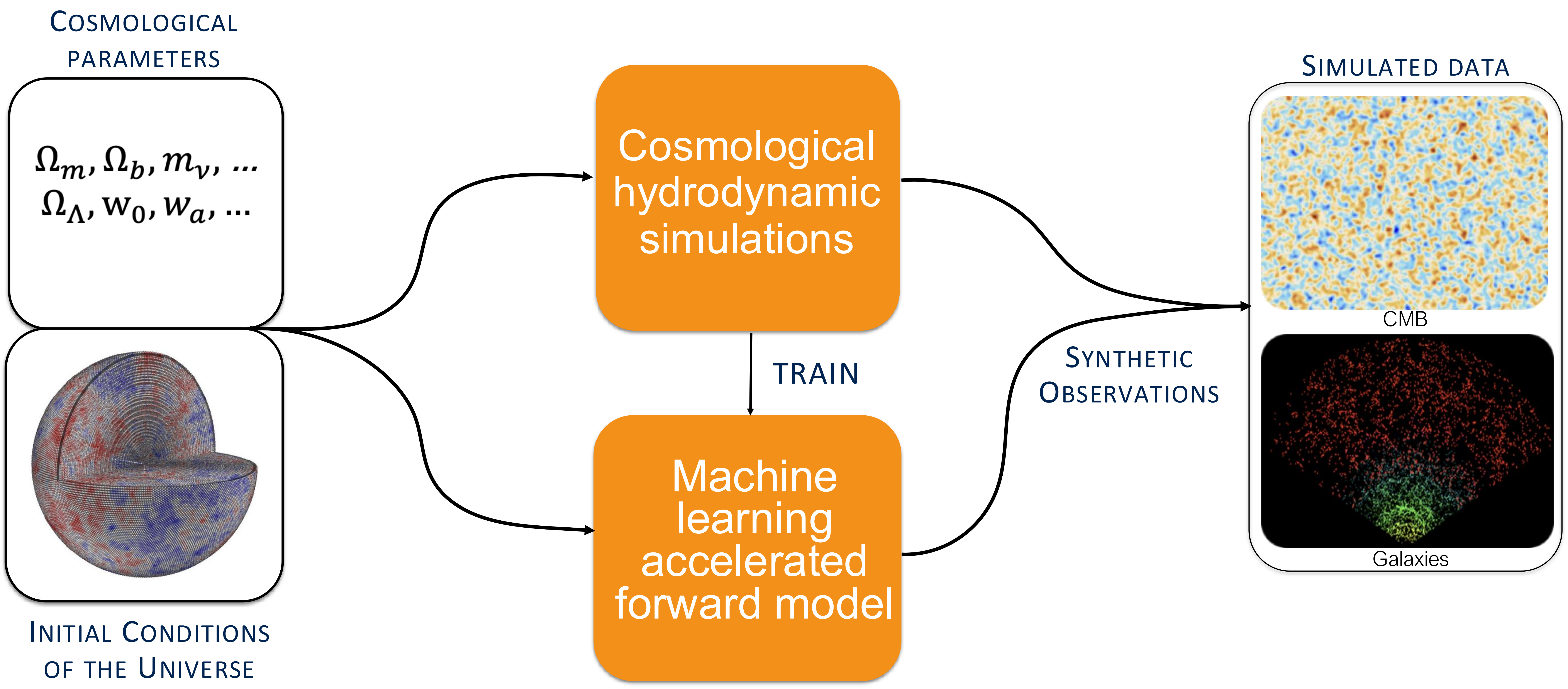


CAMELS

Navarro-Villaescusa et al. (2021)

2. Forward modeling

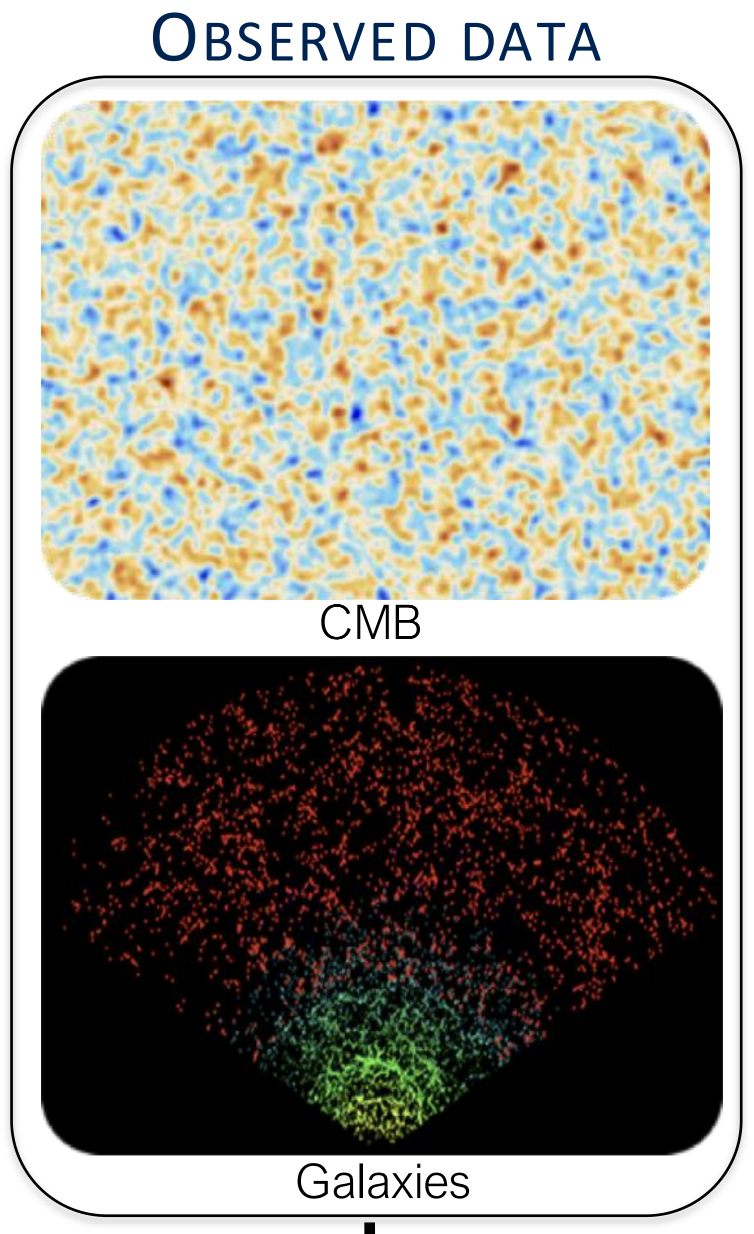
- Use large suite of N-body simulations to train neural network to predict dark matter distribution
- Use cosmological simulation suite to train machine to predict galaxy properties from dark matter
- Develop rapid emulators to predict galaxy and SZ mock observations

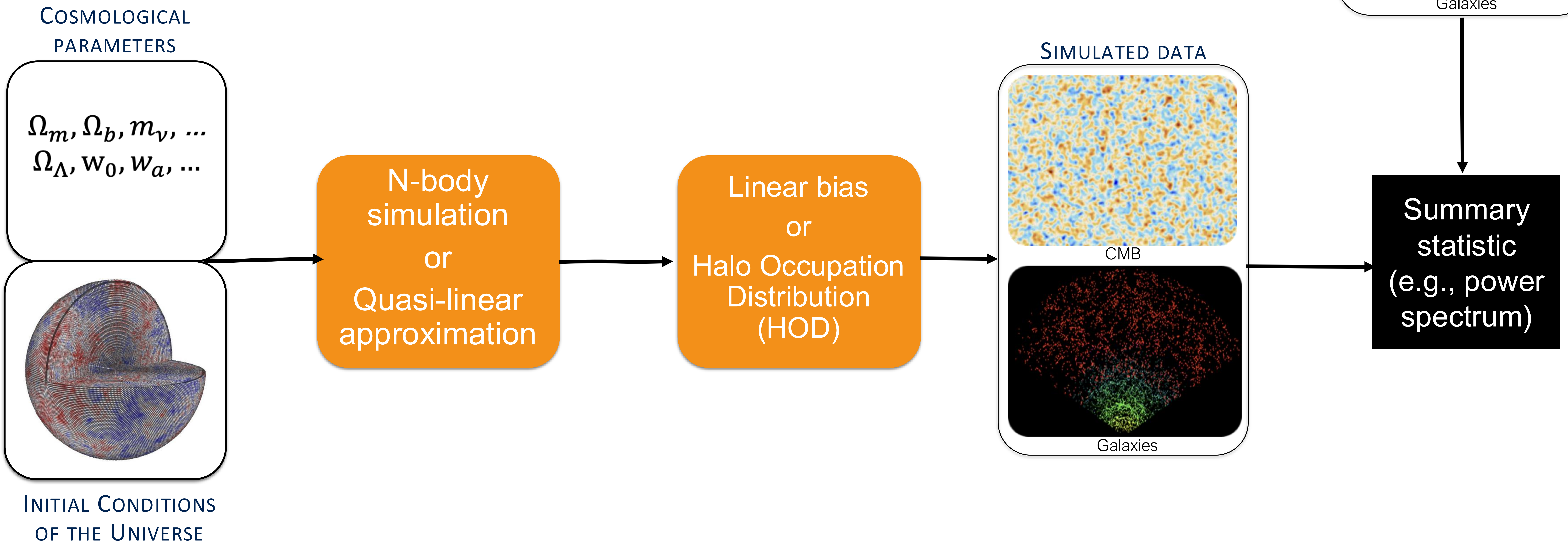


PREVIOUS APPROACH

3. Infer initial conditions (parameters)

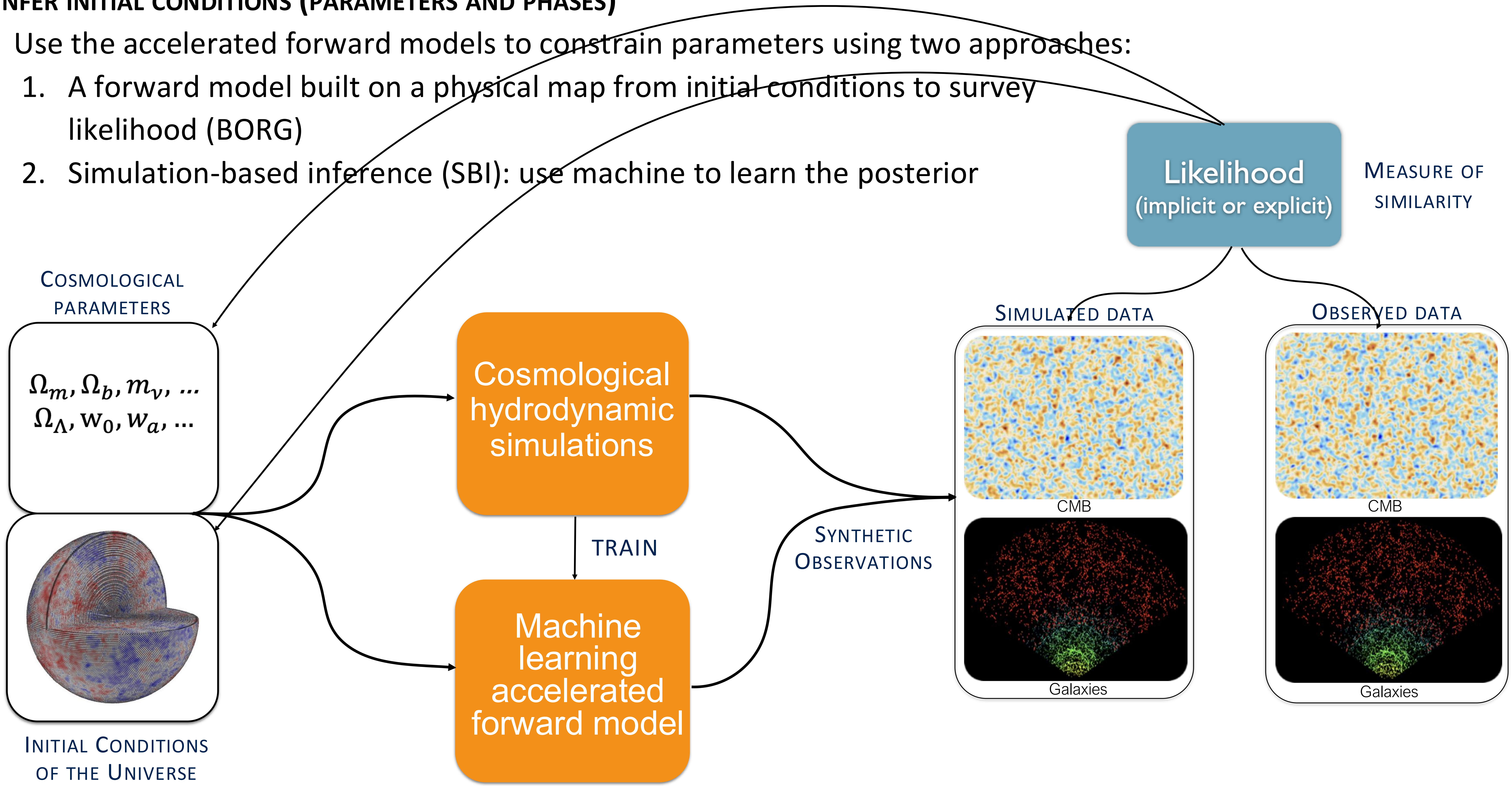
- Likelihood computed with summary statistics (e.g. n-point correlations or power spectrum)
- Form of likelihood is approximate, often assumed Gaussian.
- Summary statistics lose a lot of information (small-scales)

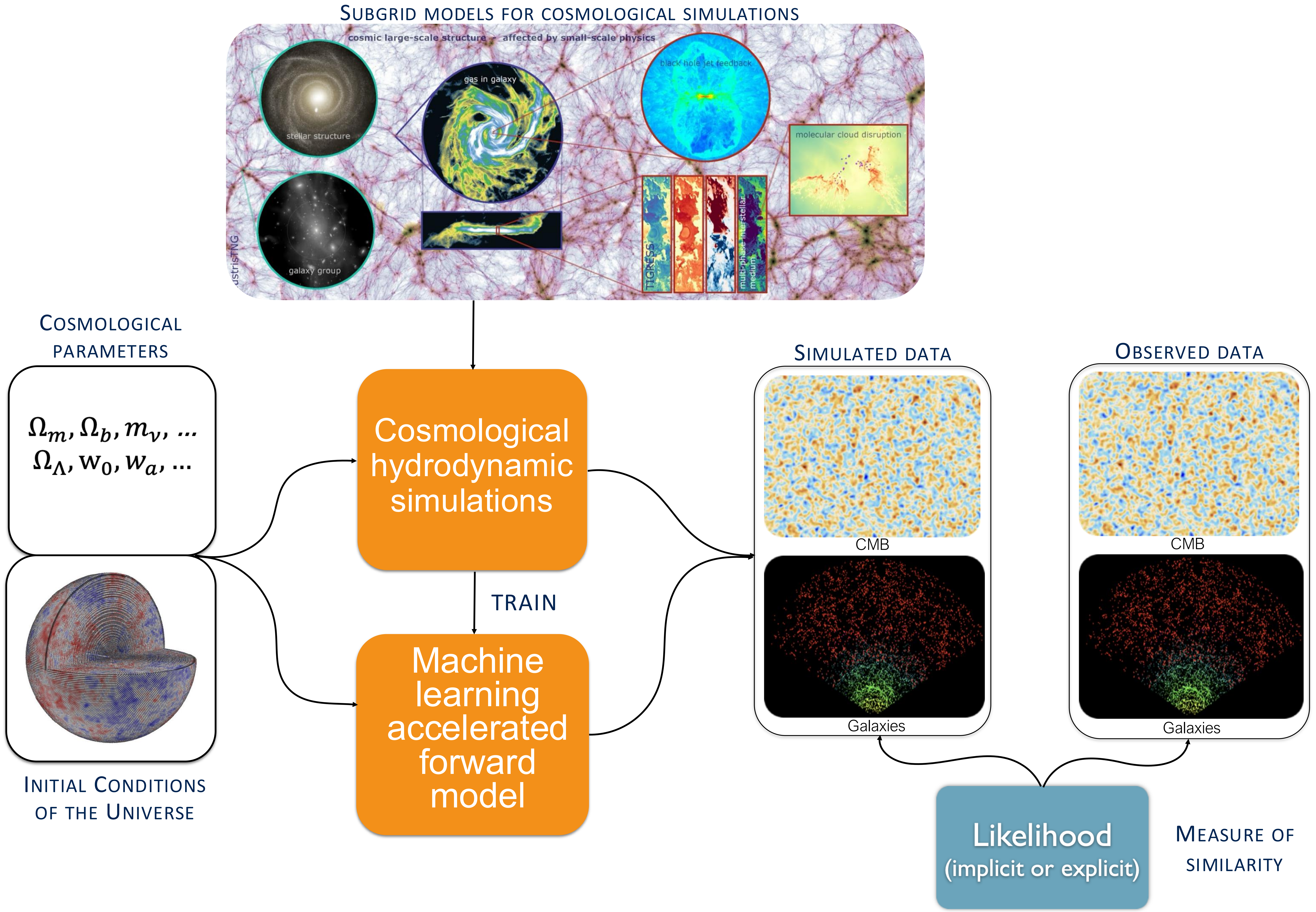




3. Infer initial conditions (parameters and phases)

- Use the accelerated forward models to constrain parameters using two approaches:
  1. A forward model built on a physical map from initial conditions to survey likelihood (BORG)
  2. Simulation-based inference (SBI): use machine to learn the posterior





Subgrid models for cosmological simulations
cosmic large-scale structure → affected by small-scale physics
stellar structure
galaxy group
gas in galaxy
black hole jet feedback
molecular cloud disruption
TIGRESS
multi-phase interstellar medium
Cosmological parameters
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$\Omega_\Lambda, w_0, w_a, \ldots$
Initial conditions of the Universe
Cosmological hydrodynamic simulations
TRAIN
Machine learning accelerated forward model
Simulated data
CMB
Galaxies
Observed data
CMB
Galaxies
Likelihood (implicit or explicit)
Measure of similarity

Subgrid models for cosmological simulations
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gas in galaxy
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ArkenstoneWinds
ArkenstoneBH
BH ML Accretion
Mistral
BH seeding (Bhowmick)
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GO BIG
CAMELS50
DREAMS (Torrey)
Cosmological hydrodynamic simulations
CMB tSZ+kSZ
Simulated data
Observed data
PQMass & Mira
IOB (Ho)
TARP
CMB
CMB
Synthesizer
MIEST
Dust Model
TRAIN
Sapphire
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Manticore
BORG
Charm
COCA
GOTHAM+ (Zhang)
PM++
BIND
Initial Conditions of the Universe
Field level inference (Bayer)
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LtU-ILI (Matt Ho)
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SUBGRID MODELS FOR COSMOLOGICAL SIMULATIONS
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MEASURE OF SIMILARITY
PineTree

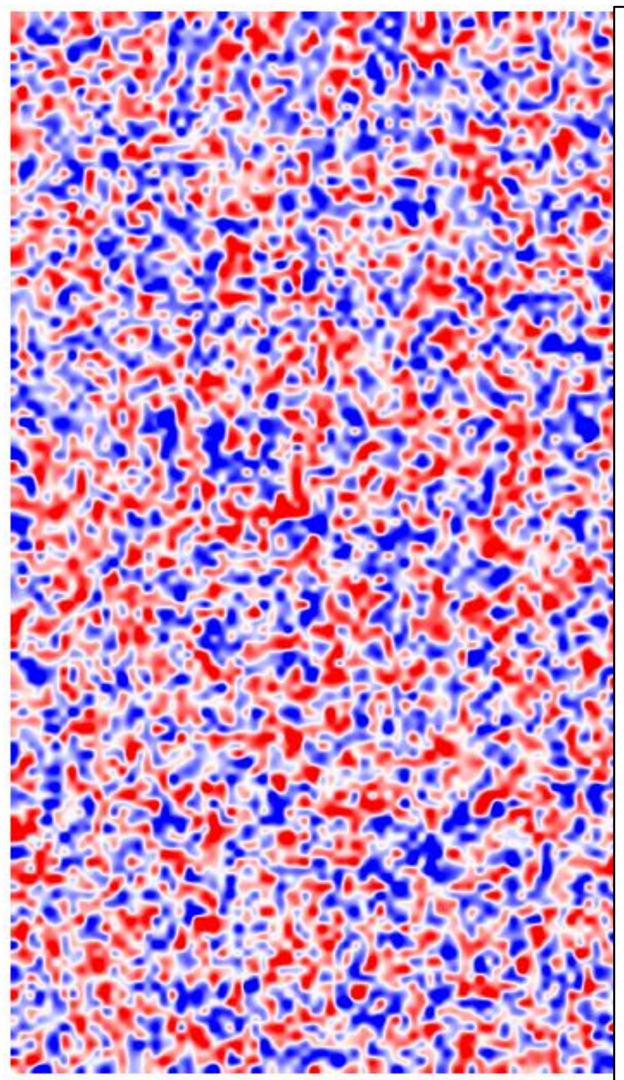
GO BIG:
AI POWERED COSMOLOGICAL INFERENCE

Ho et al (in prep)

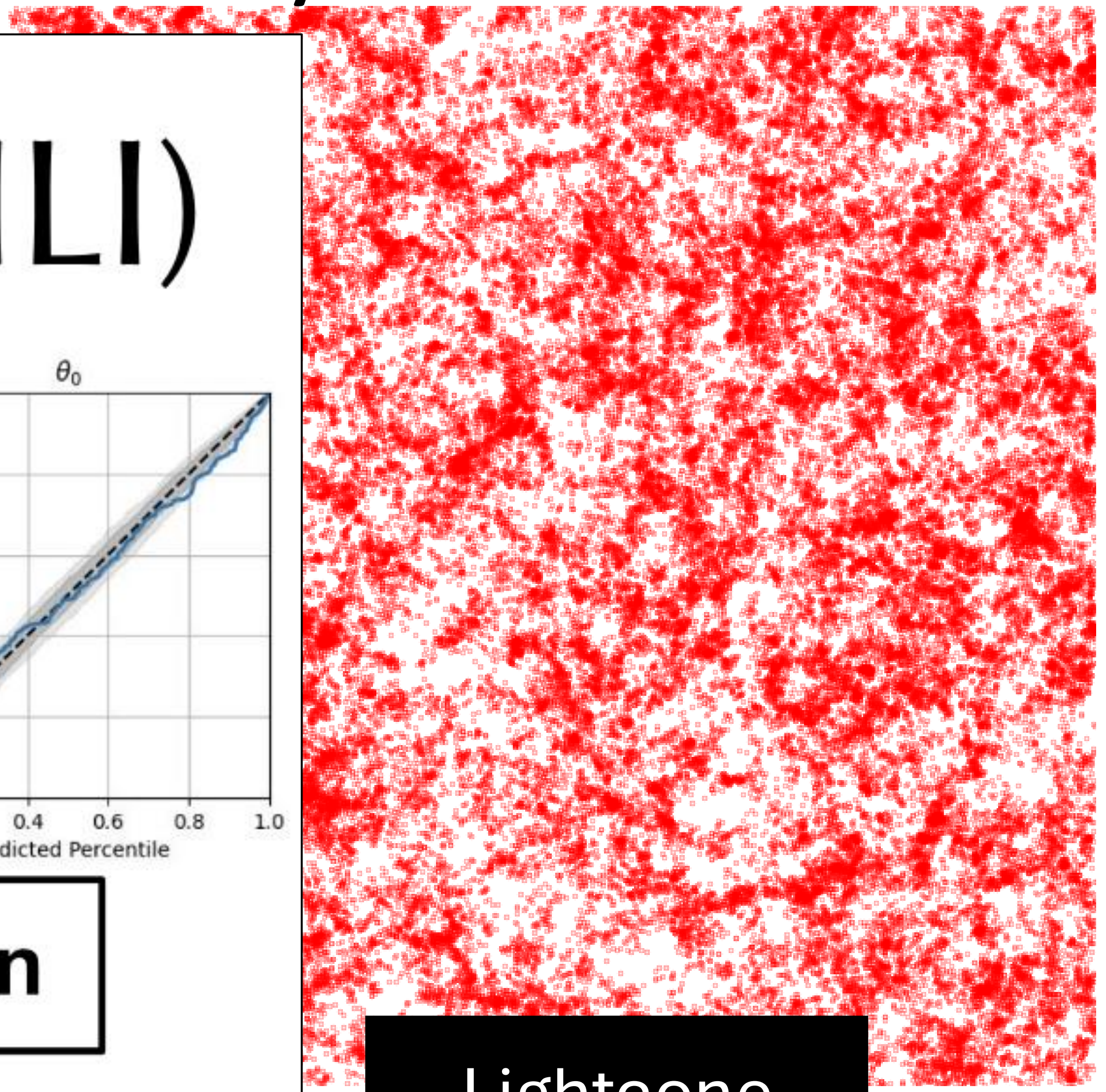
Matthew Ho

Cosmology Parameters

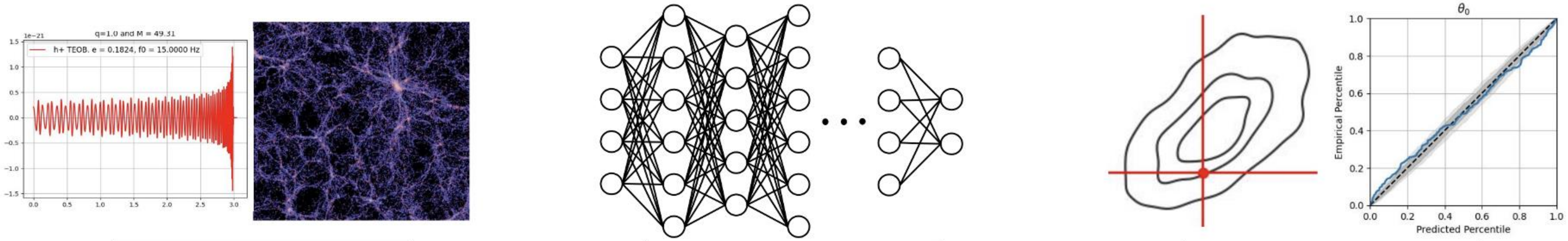
Initial conditions



Galaxy distribution



LtU Implicit Likelihood Inference (LtU-ILI)



I: Data → II: Inference → III: Validation

An **all-in-one** framework for implicit inference in astronomy.

Includes: SOTA architectures, training procedures, best practices, embedding networks, tutorials, documentation, preprocessing, etc.

Ho et al. 2024,
arxiv:2402.05137
https://github.com/maho3/ltu-ili

A full inference pipeline in 5 lines!

```
X, Y = load_data()
loader = ili.dataloaders.NumpyLoader(X, Y)

trainer = ili.inference.InferenceRunner.load(
  backend = 'lampe', engine = 'NPE',
  prior = ili.utils.Uniform(low=-1, high=1),
  nets = [ili.utils.load_nde_lampe(model='maf')]
)

posterior, _ = trainer(loader)

samples = posterior.sample(x[0], (1000,))
```

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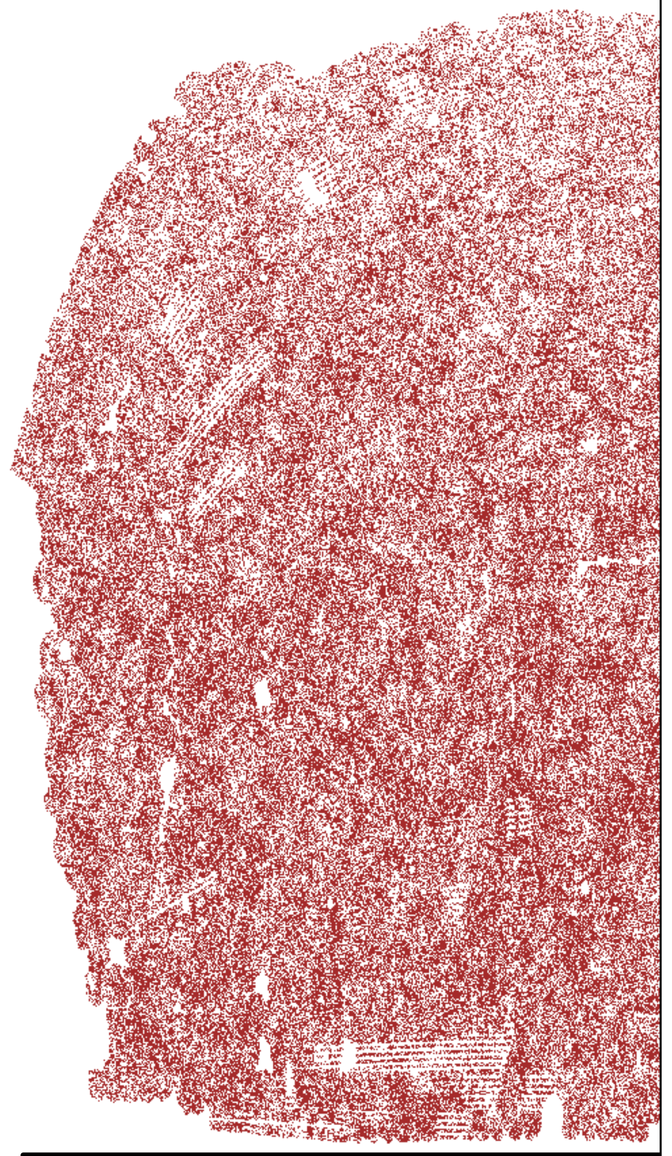
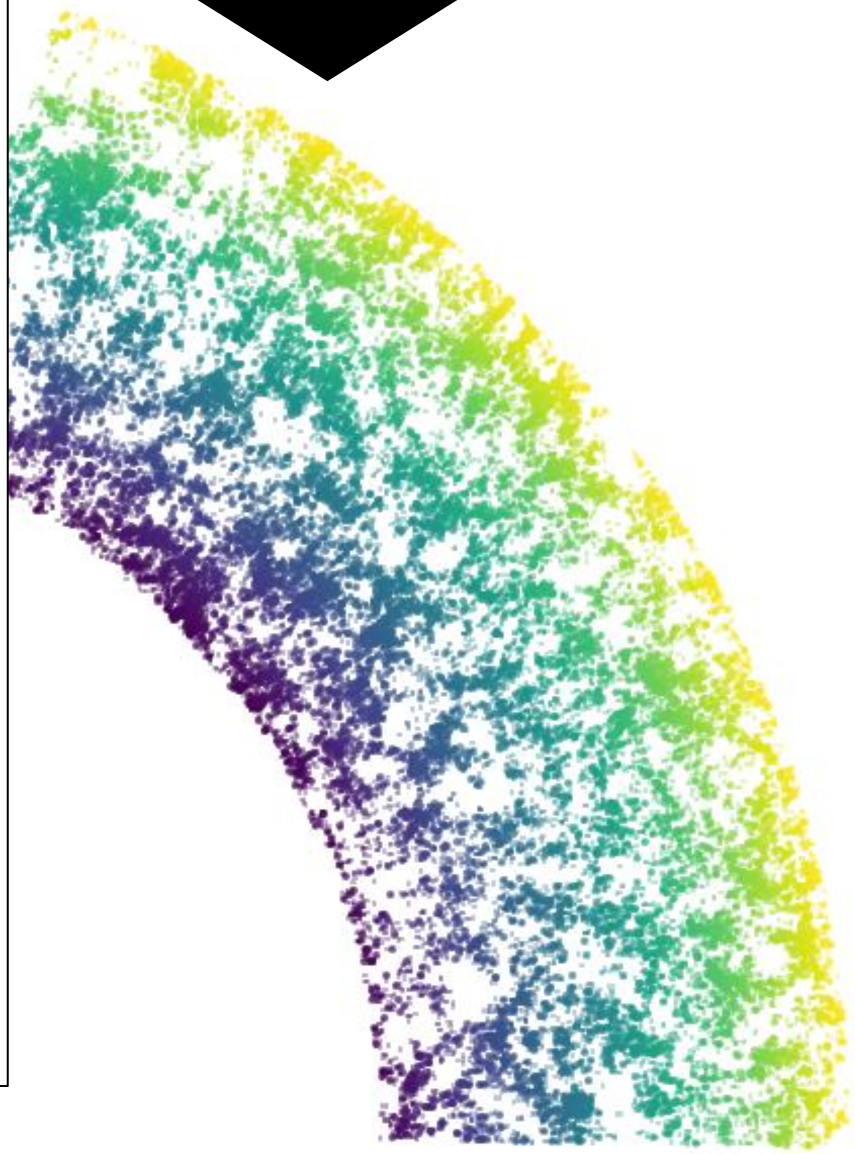


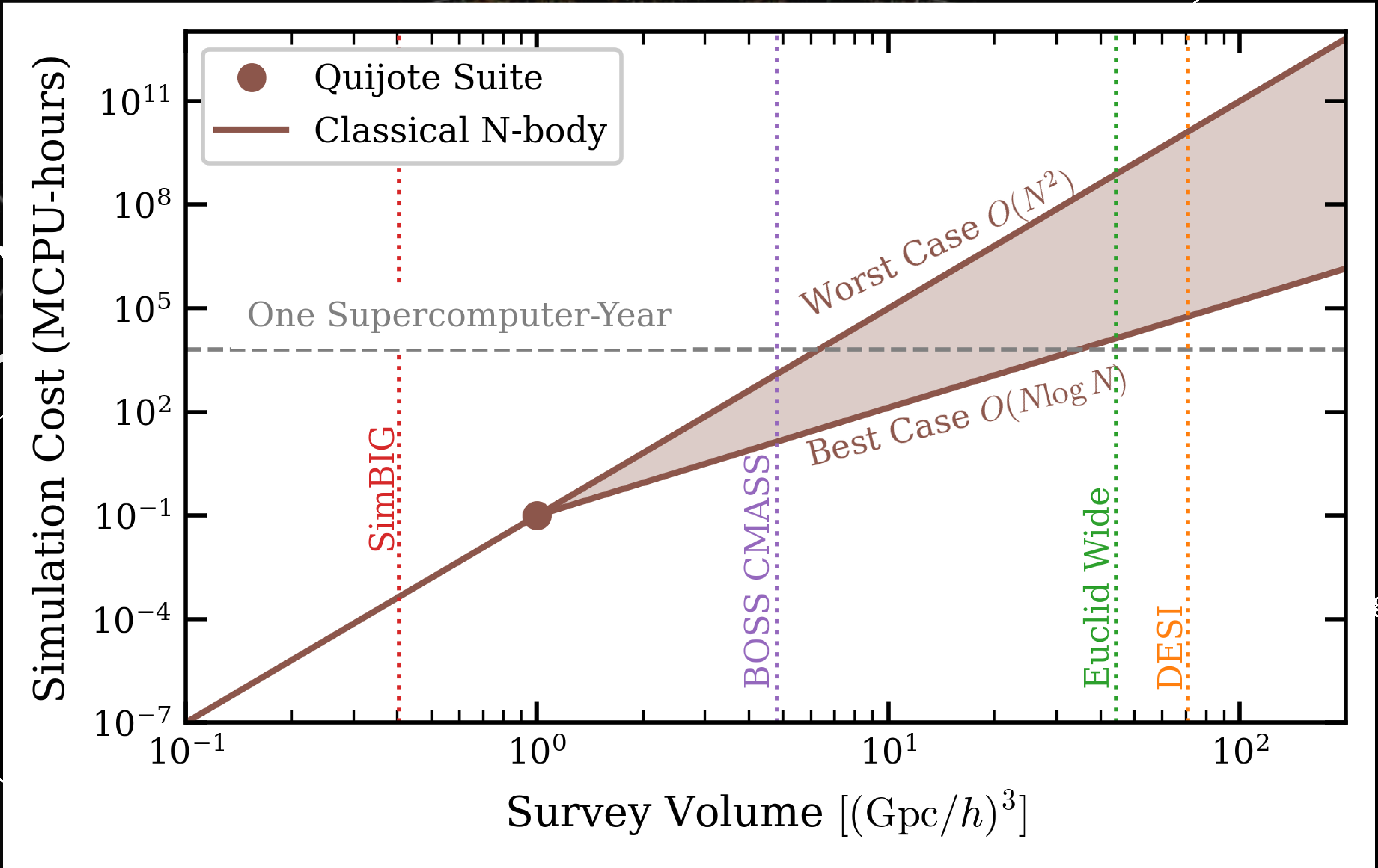
REAL GALAXIES

Lightcone Extrapolation



FAKE GALAXIES

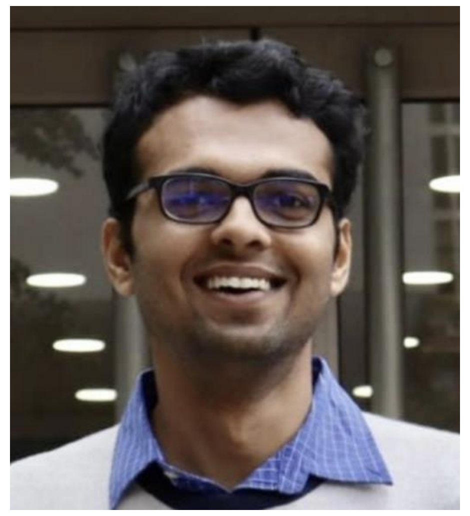
Sim

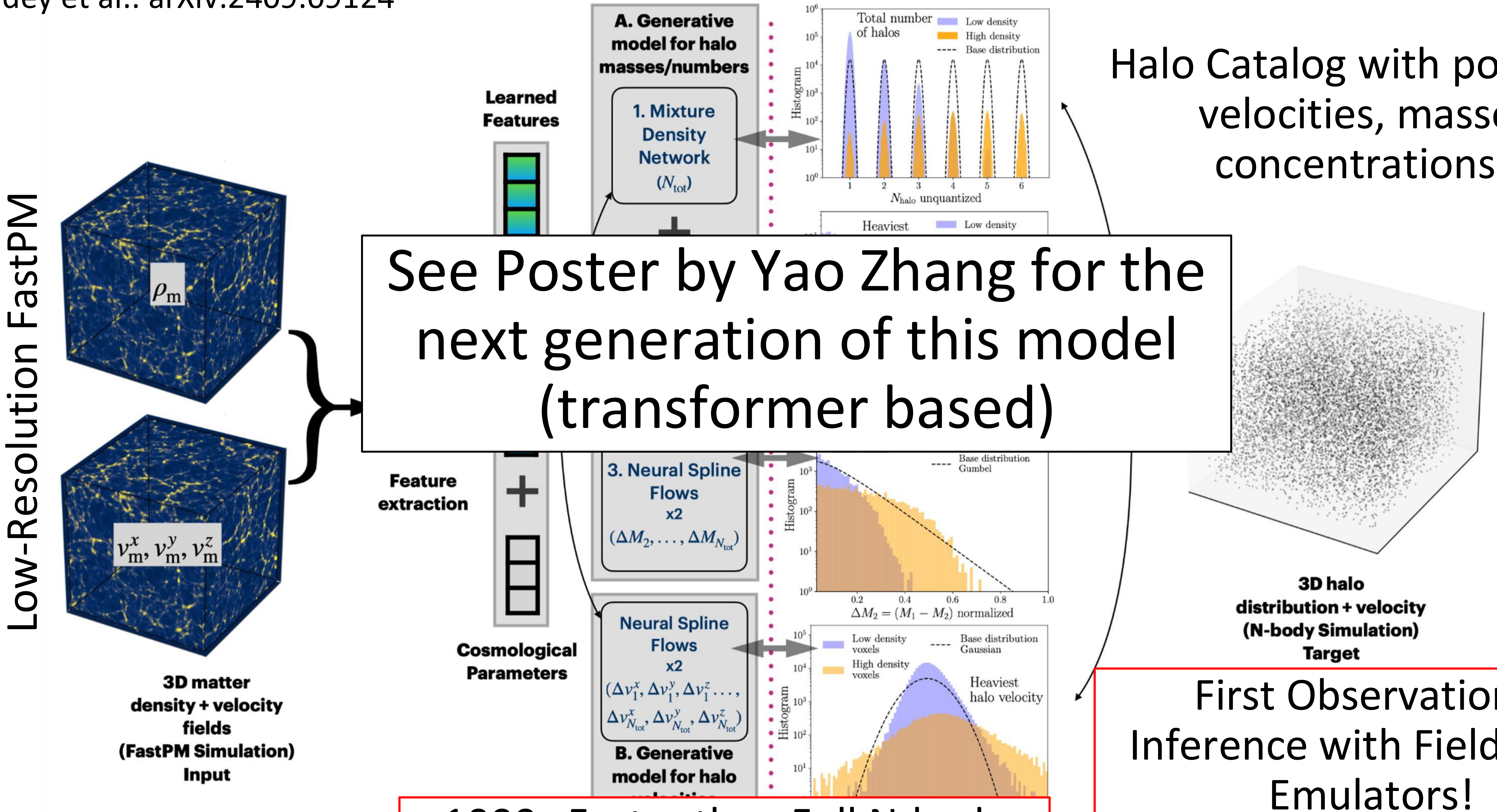


SimBIG
CMASS
$(1\ \mathrm{Gpc}^3)$

CHARM (Creating Halos with Auto-Regressive Multi-stage Networks)

Shivam Pandey et al.: arXiv:2409.09124





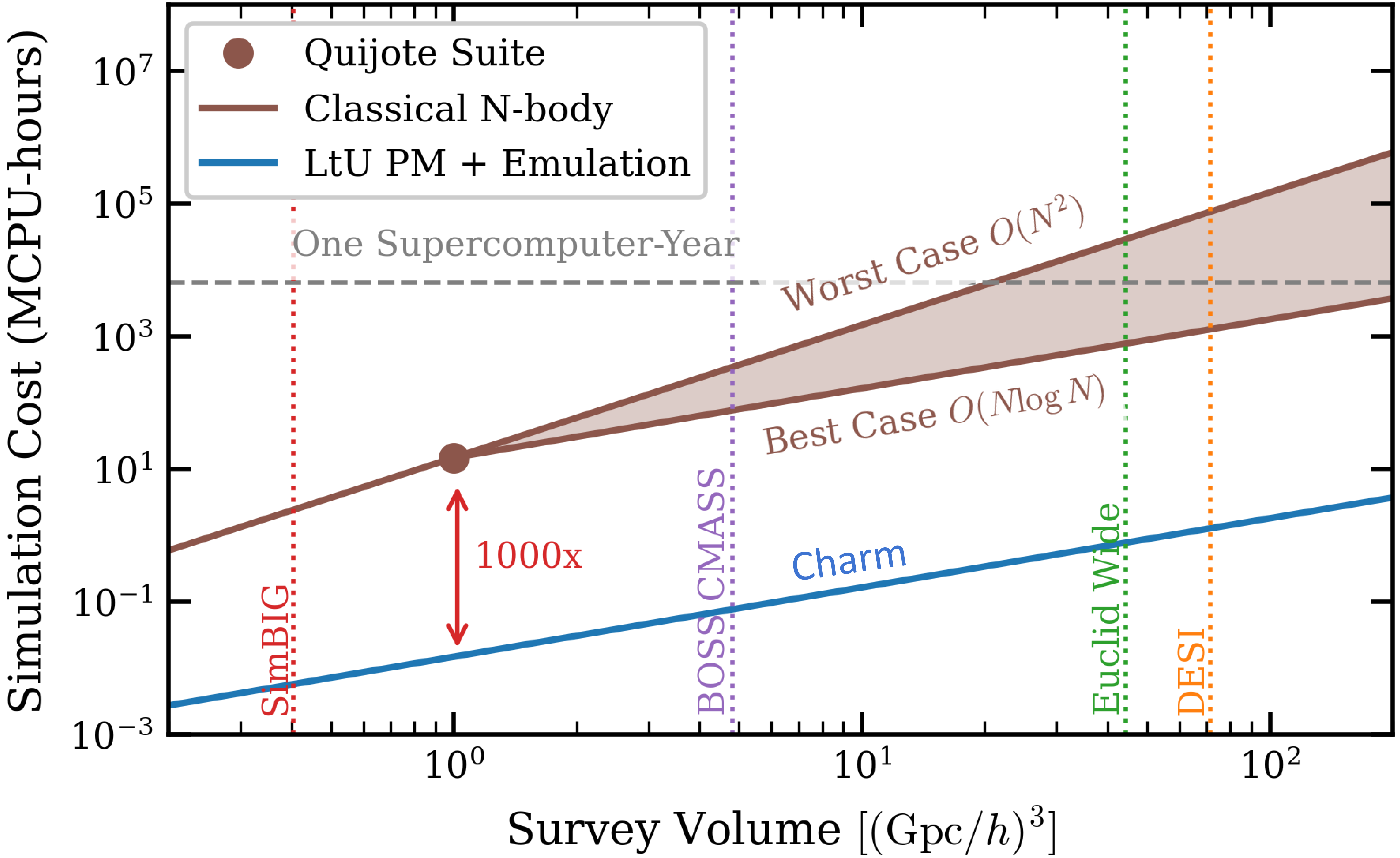
Halo Catalog with positions, velocities, masses, concentrations…

See Poster by Yao Zhang for the next generation of this model (transformer based)

First Observational Inference with Field-Level Emulators!

1000x Faster than Full N-body

CHARM is at least 1000x faster than N-body



Replace full simulations with Charm/GOTHAM

PQMass & MIRA: How Good is Your Generative Model?

Lemos et al (2025), Sharif et al. (2026)

Sammy
Sharief

PQMass is a Likelihood-free Test:
Are model samples drawn from the data distribution?

Given samples $(x_i) \sim p$ (data) and $(y_i) \sim q$ (generative model), test the hypothesis $p = q$ using only the samples.

PQMass returns a **p-value** from counts of samples in regions of sample space: no density estimation, no auxiliary model training, no feature extraction. Sensitive to **fidelity, diversity, and novelty** at once.

github.com/Ciela-Institute/PQM

Lemos et al (2025)

The algorithm: tessellate, count samples, test

1. Tessellate

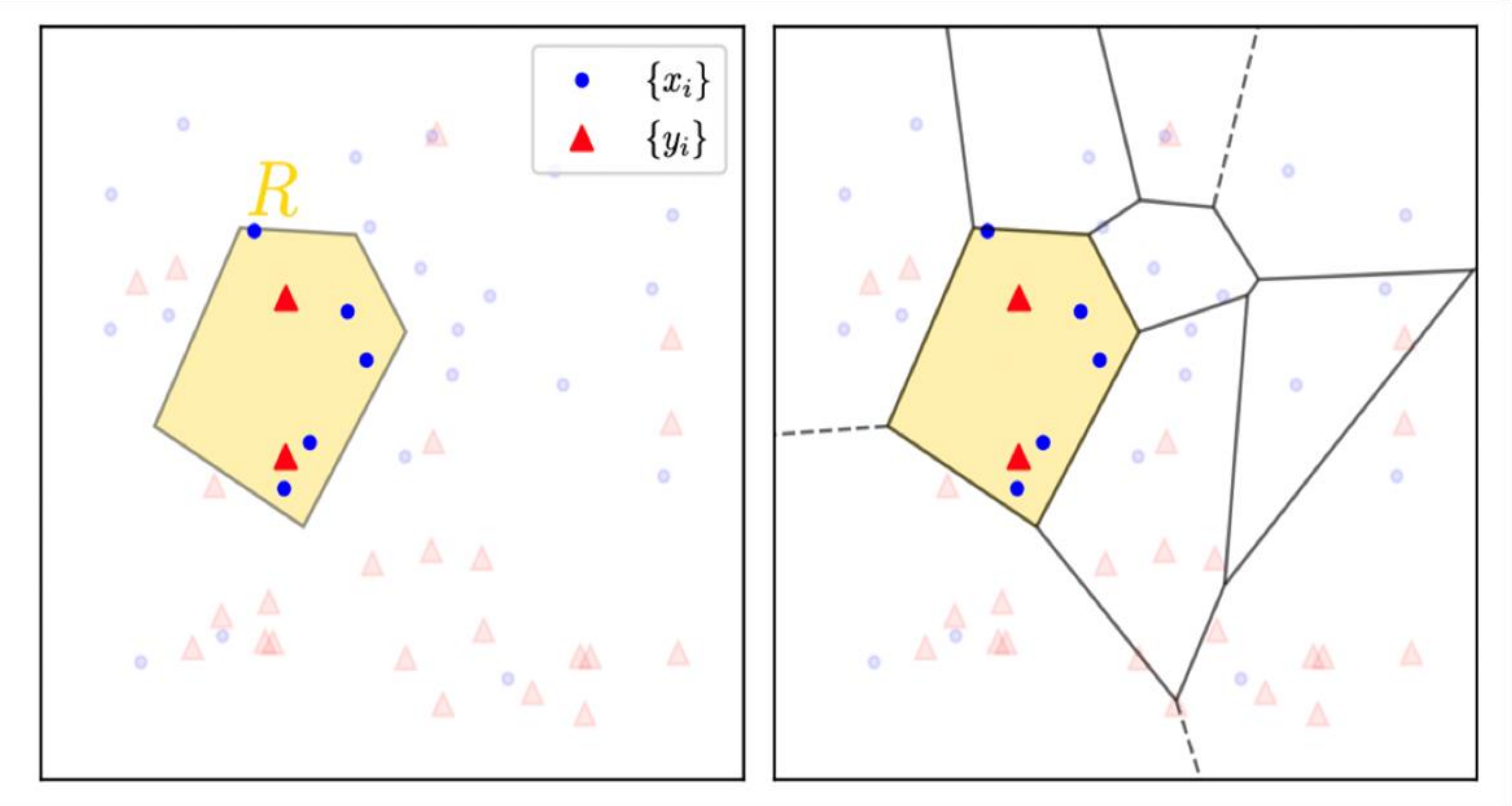
Draw n_k reference points from the pooled samples (half from each set); their Voronoi cells partition $\mathbb{R}^d$. Any distance metric works: L1, L2, or feature-space.

2. Count

Assign each remaining sample to its nearest reference point. The two count vectors are multinomial with parameters $p(R_j)$ and $q(R_j)$ — and $p = q$ only if these match on every region.

3. Test

Pearson χ^2 test on equality of the two multinomials. Under the null, the statistic follows χ^2 with $n_k - 1$ dof; the tail integral is the p-value. Re-tessellate and repeat to reduce variance.



$$k(\mathbf{x}, R) \sim \mathcal{B}\left(n, \mathbb{P}_p(R)\right)$$

$$\{k(\mathbf{x}, R_i)\}_{i=1\ldots n_R} \sim \mathcal{M}\left(n, \{\mathbb{P}_p(R_i)\}_{i=1\ldots n}\right.$$

$$\chi^2_{\mathrm{PQM}} \equiv \sum_{i=1}^{n_R} \left[\frac{\left(k(\mathbf{x}, R_i) - \hat{N}_{x,i}\right)^2}{\hat{N}_{x,i}} + \frac{\left(k(\mathbf{y}, R_i) - \hat{N}_{y,i}\right)^2}{\hat{N}_{y,i}} \right]$$

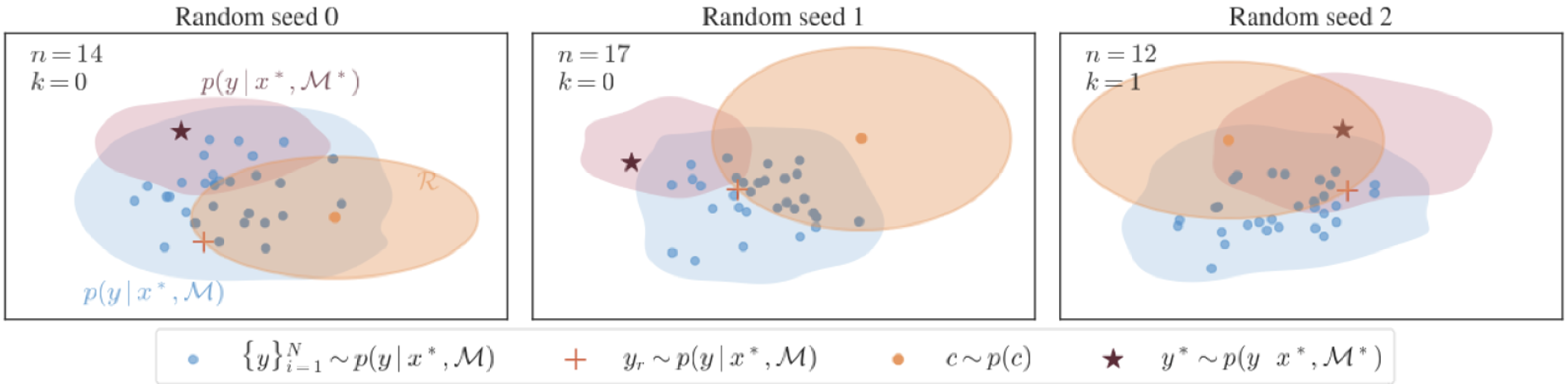
Lemos et al (2025)

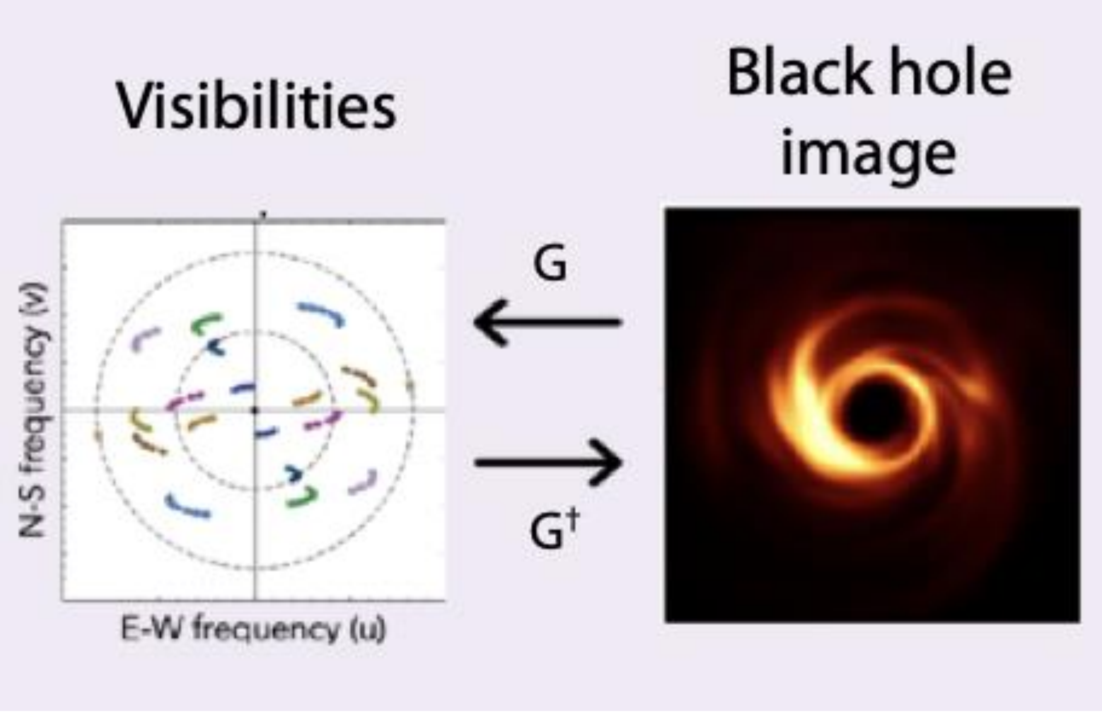
MIRA (Mass In Random Areas): An extension to Conditional Distribution Accuracy and Model Comparison

Justine Zeghal

Sammy Sharief

Mira quantifies the fidelity of a candidate conditional distribution p(y | x, M) against the true, unknown one p(y | x, M*)
where M is the candidate model for M*



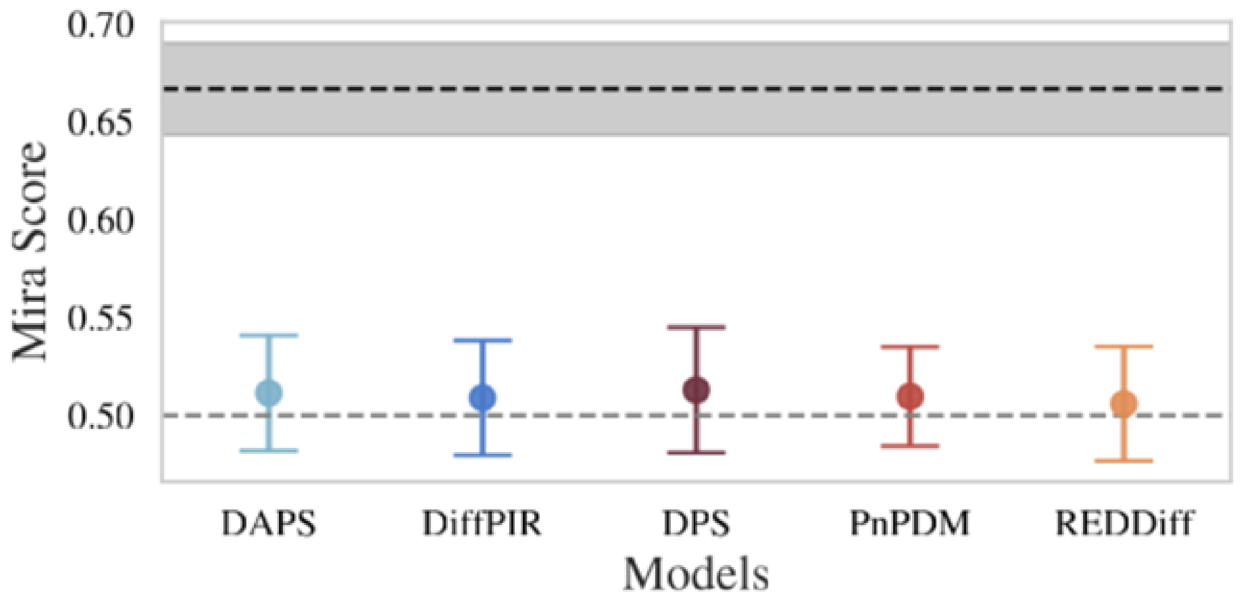


$$\mu_{\mathrm{Mira}}(\mathcal{M}) = \mathbb{E}_{p(Z)}\left[\mathbb{E}_{p(k,n|Z)}\left[p(k \mid n)\right]\right]$$

$$\mathbb{E}_{p(k,n)}\left[P_N\right] \to \frac{2}{3} \quad as\ N \to \infty$$

$$p(k \mid n) = \frac{n+1}{N+2}\mathbb{1}(k=1) + \frac{N-n+1}{N+2}\mathbb{1}(k=0)$$

Mira Score provides an absolute measure of conditional model accuracy

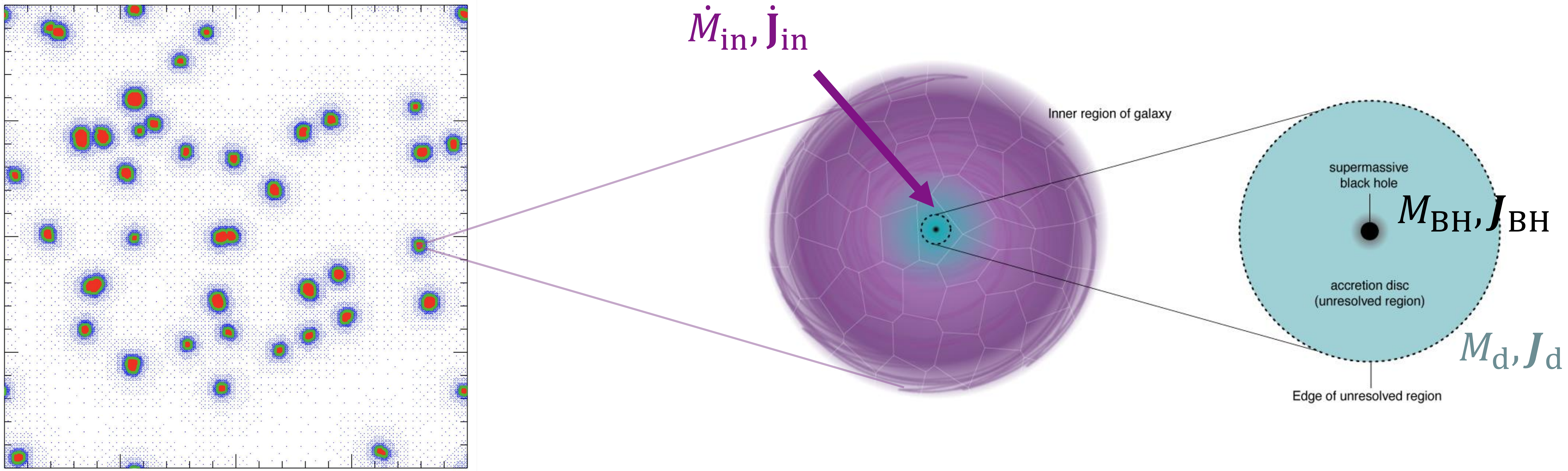


BH ACCRETION: NN-BASED SUBGRID MODEL

Koudmani et al (in prep)

Sophie
Koudmani

Bridging the scales: the connection between black holes, galaxies, and the cosmos



For selected galaxies: additional/super-Lagrangian refinement

Inflow rate

Cosmological simulation → **Inner region around black hole** → **Black hole subgrid model**

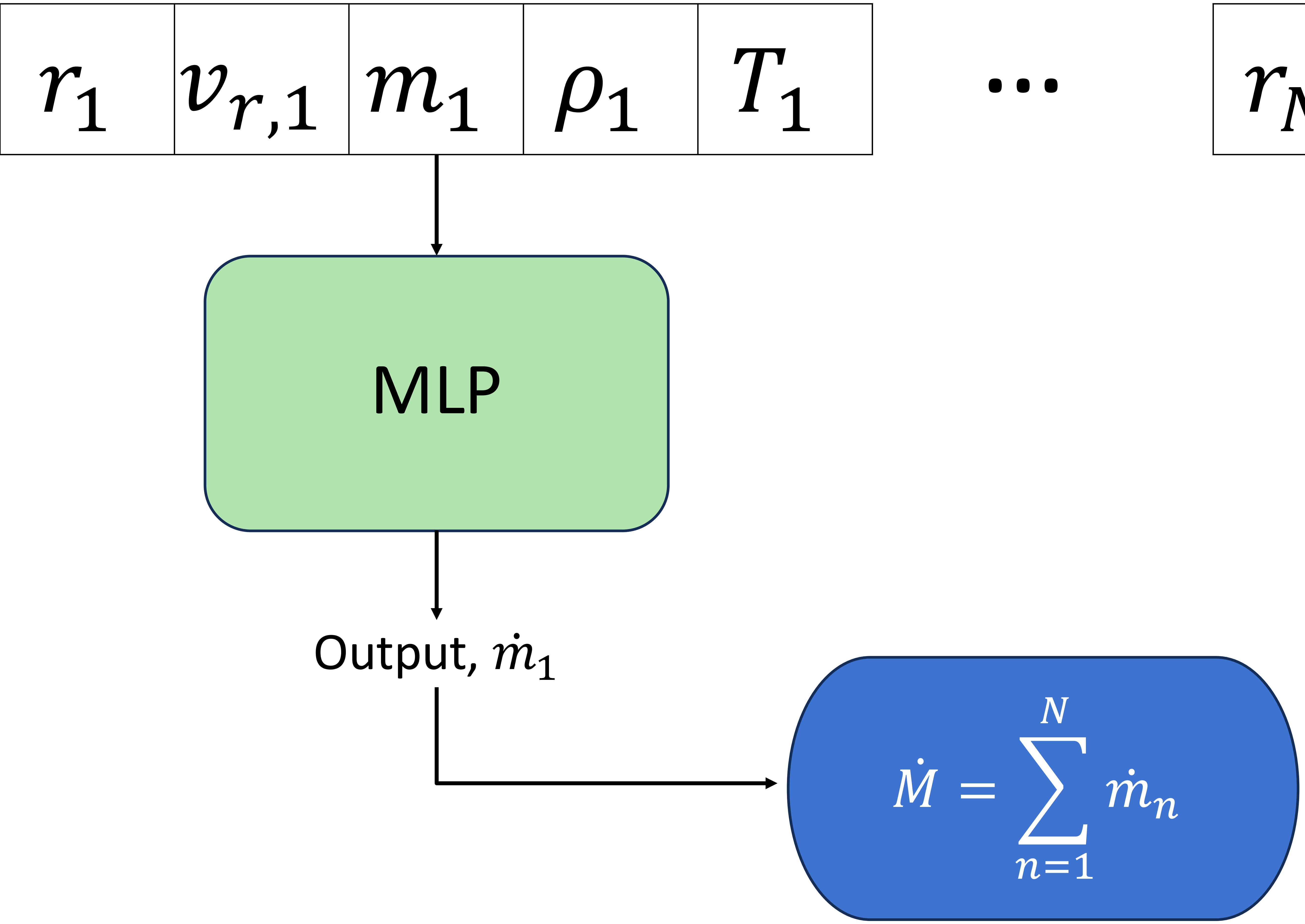
Learned coarse model based on e.g. GNN + MLP

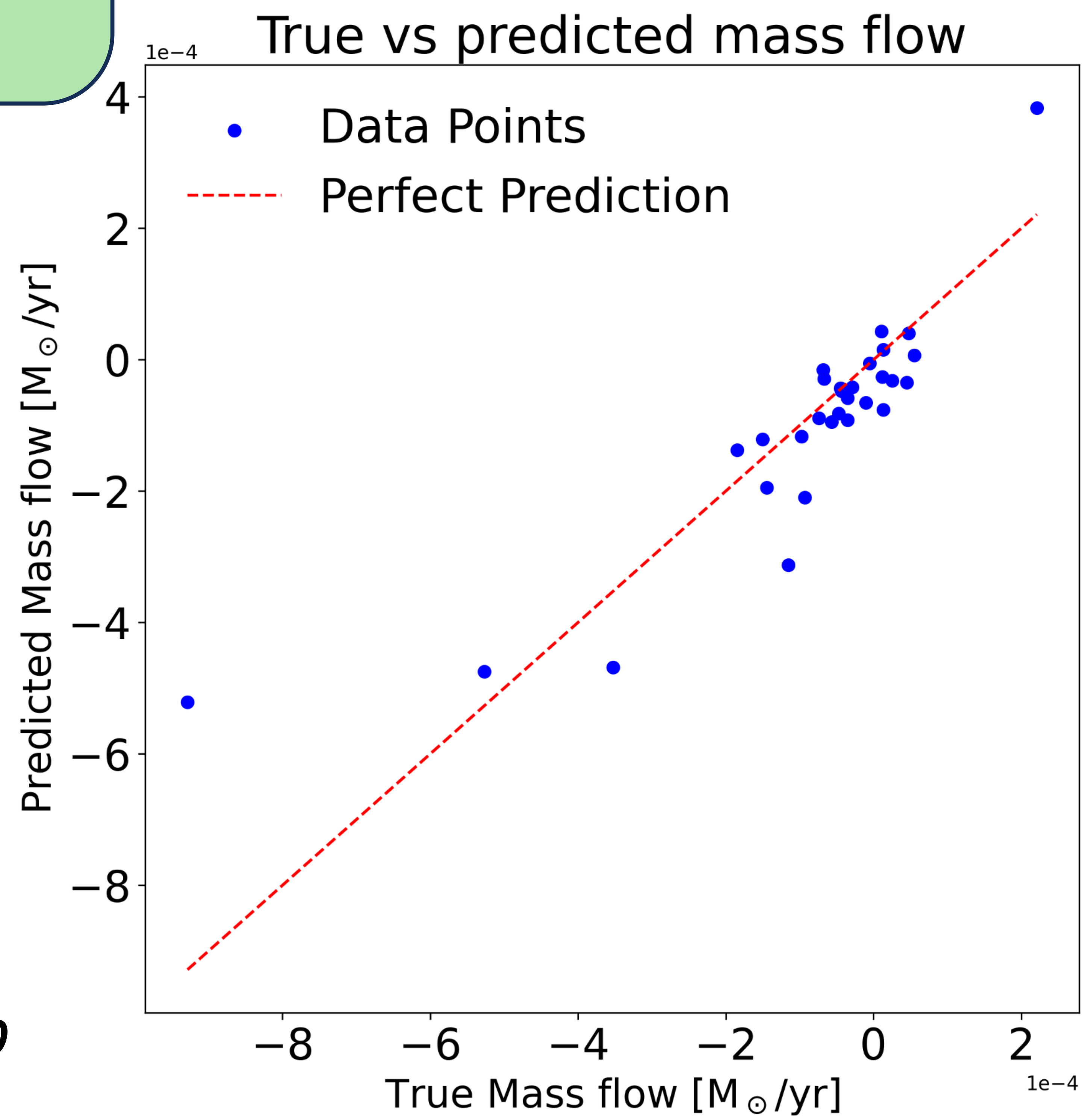
Pioneer **machine-learning-accelerated supermassive black hole models** in cosmological volumes

→ build on ML-accelerated models in planet (*e.g. Pfeil+22*) and star formation (*e.g. Wells&Norman,21*)

→ make **survey predictions**, including luminosity functions and scaling relations

Pilot project: summed MLP framework for estimating small-scale mass inflow rates in large cosmological volumes

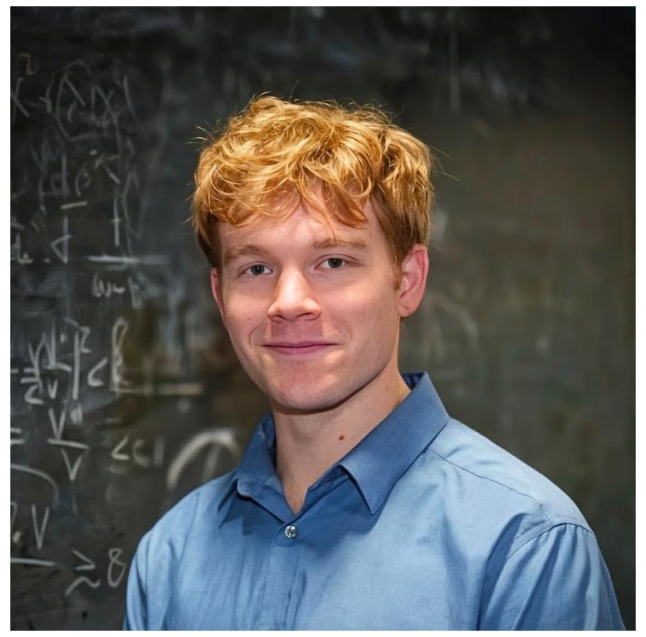




Arango+ in prep

DEGENERACY DISTILLERY: CURING DEGENERACIES IN SIMULATION BASED INFERENCE

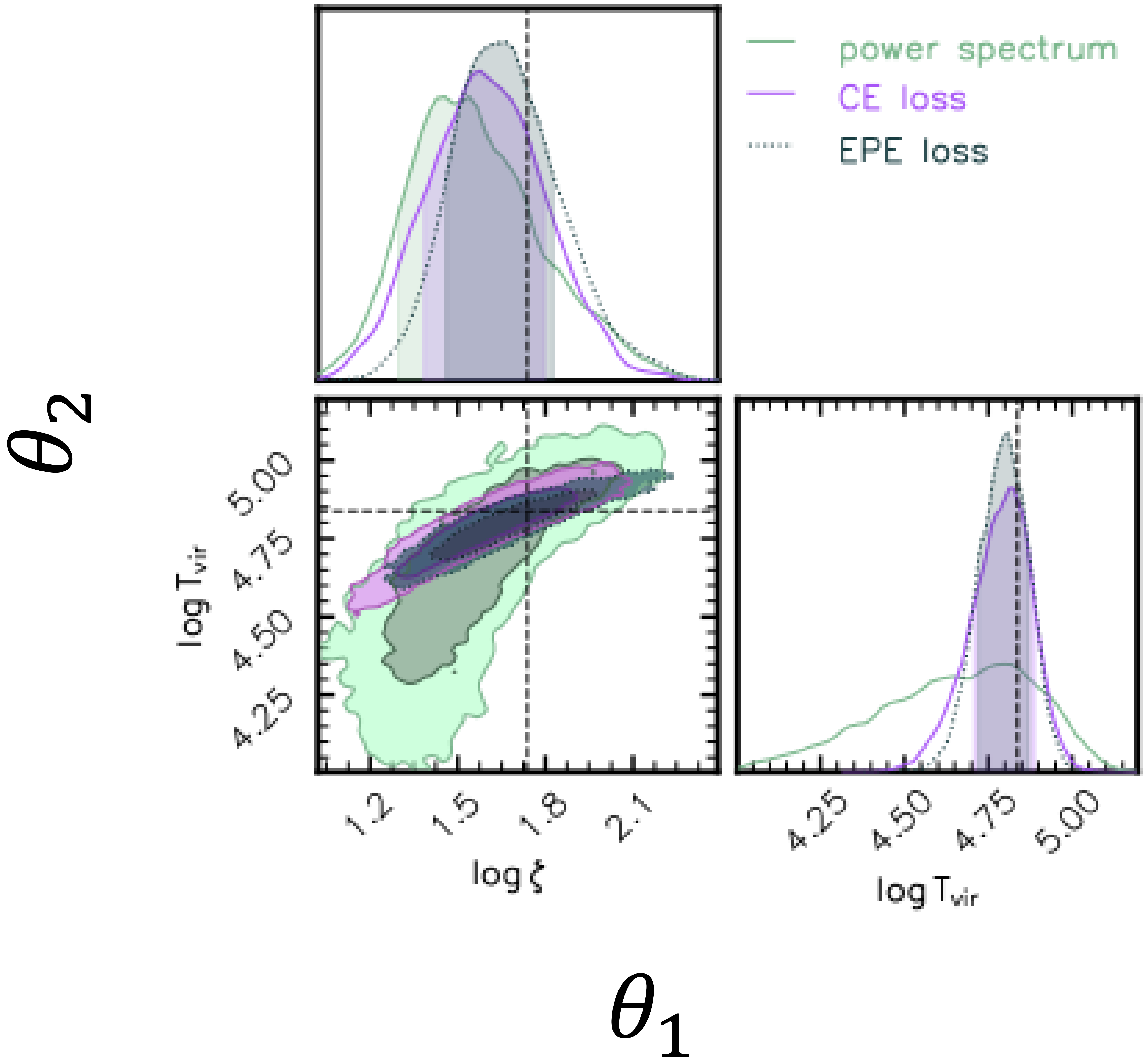
Makinen et al. (2026)



Lucas Makinen

For SBI Practitioners…

you have a (degenerate) posterior… now what ?



Information Geometry

Information geometry is measured via the Fisher Information Metric

$$F_{ab}(\theta) = -\int d\mathbf{x}\, p(\mathbf{x}|\,\theta)\, \frac{\partial}{\partial\theta^a}\frac{\partial}{\partial\theta^b}\log p(\mathbf{x}|\theta)$$

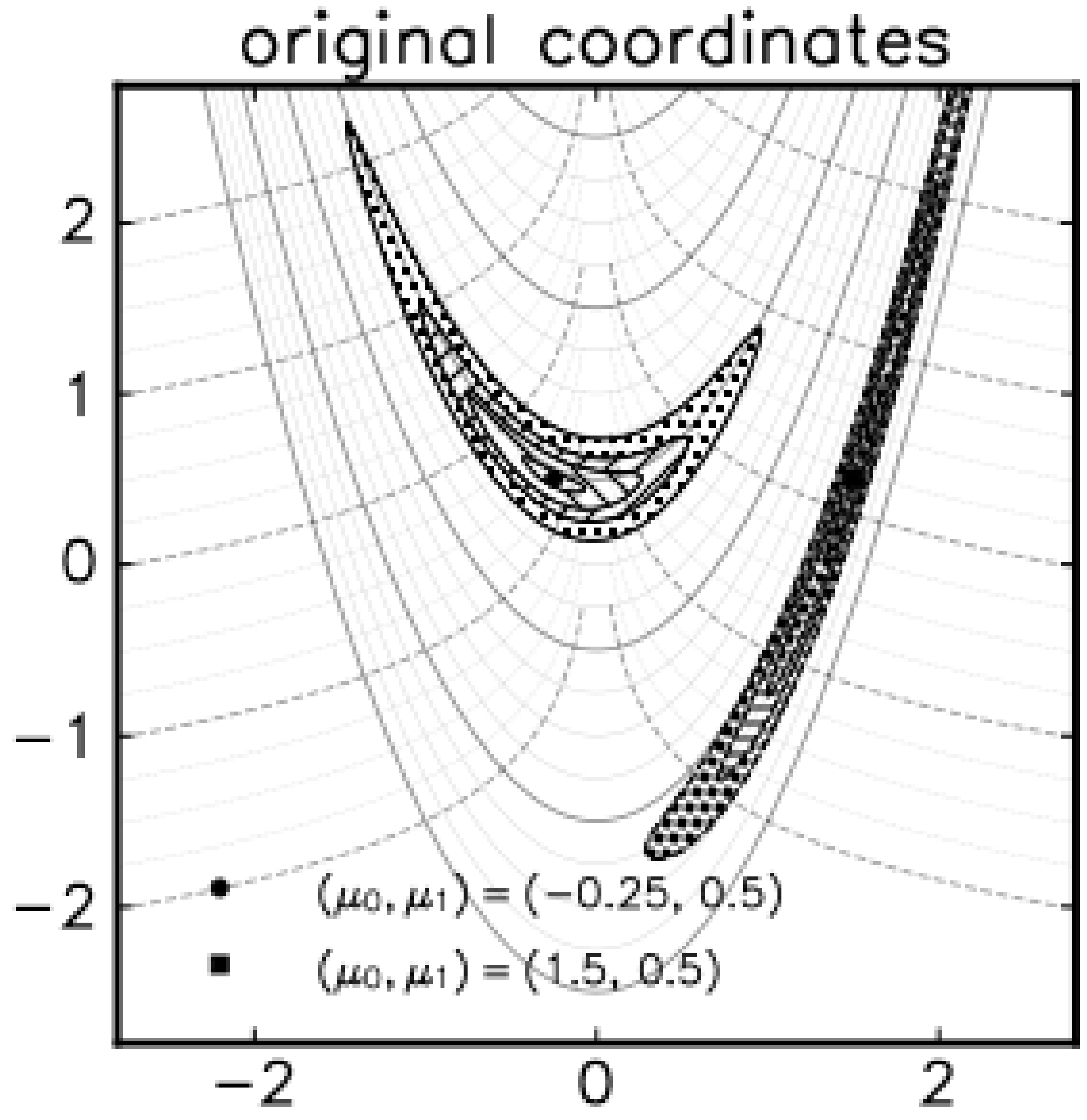
For flat regions, the ellipse looks circular (no preferred direction). For a "peak" or a "valley", we see the ellipse stretched in one preferred direction, indicating a slope or gradient in information space.

low information　　high information　　moderately degenerate　　highly degenerate

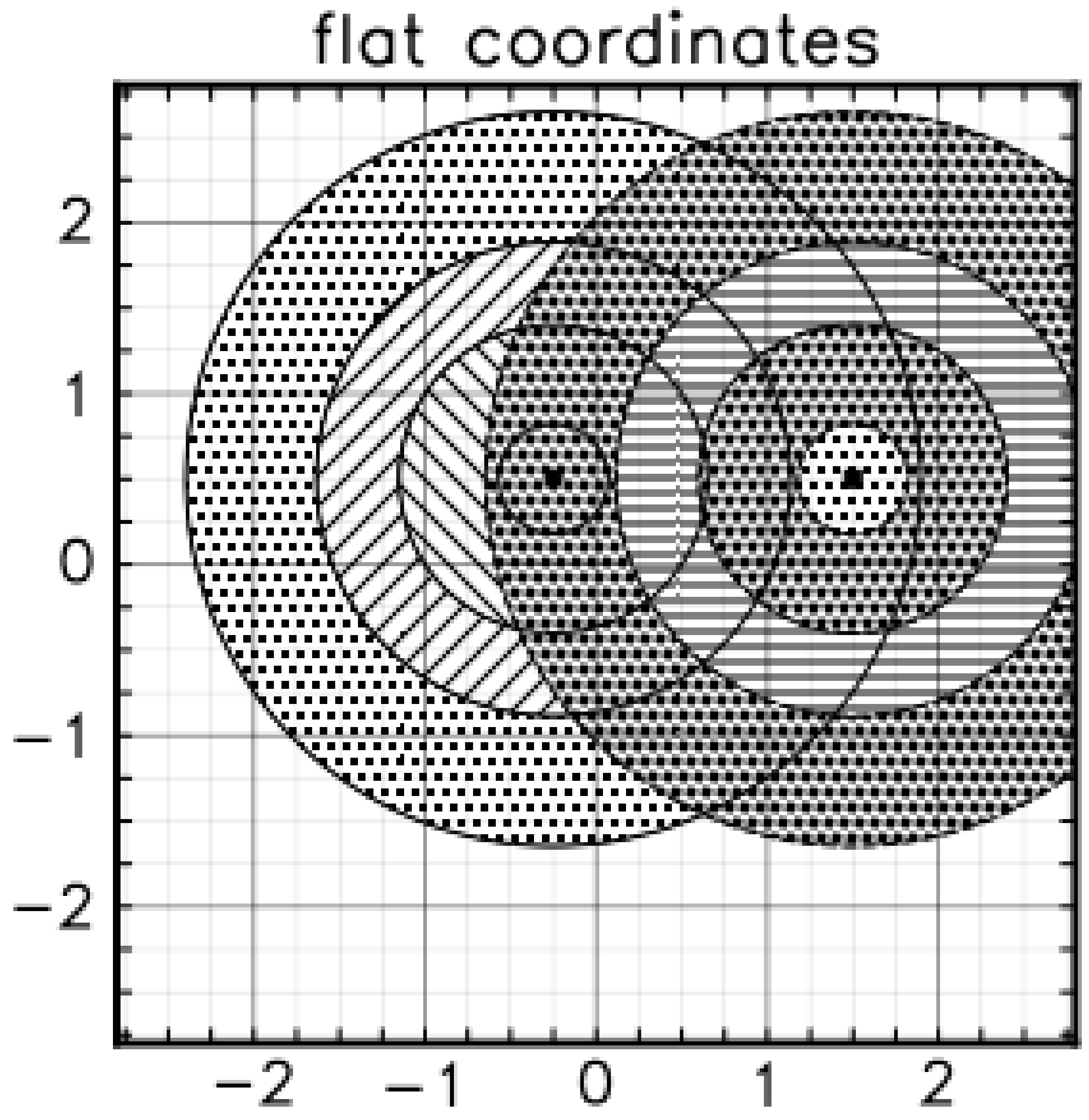
Can we learn better coordinates from data ?

model labels / parameters / coordinates

latent, physical coordinates that control the data



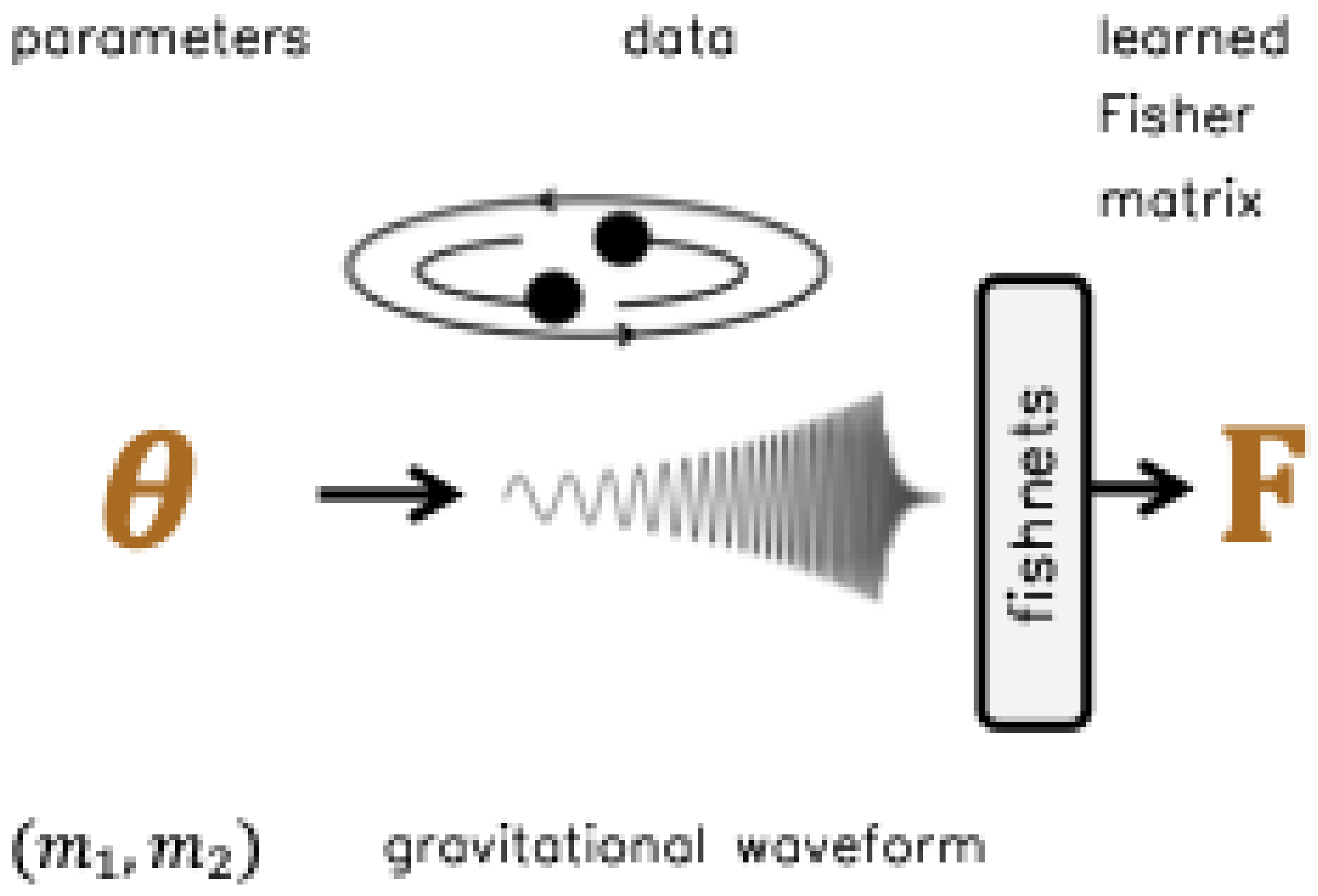
$$\theta \xrightarrow{f} \eta$$



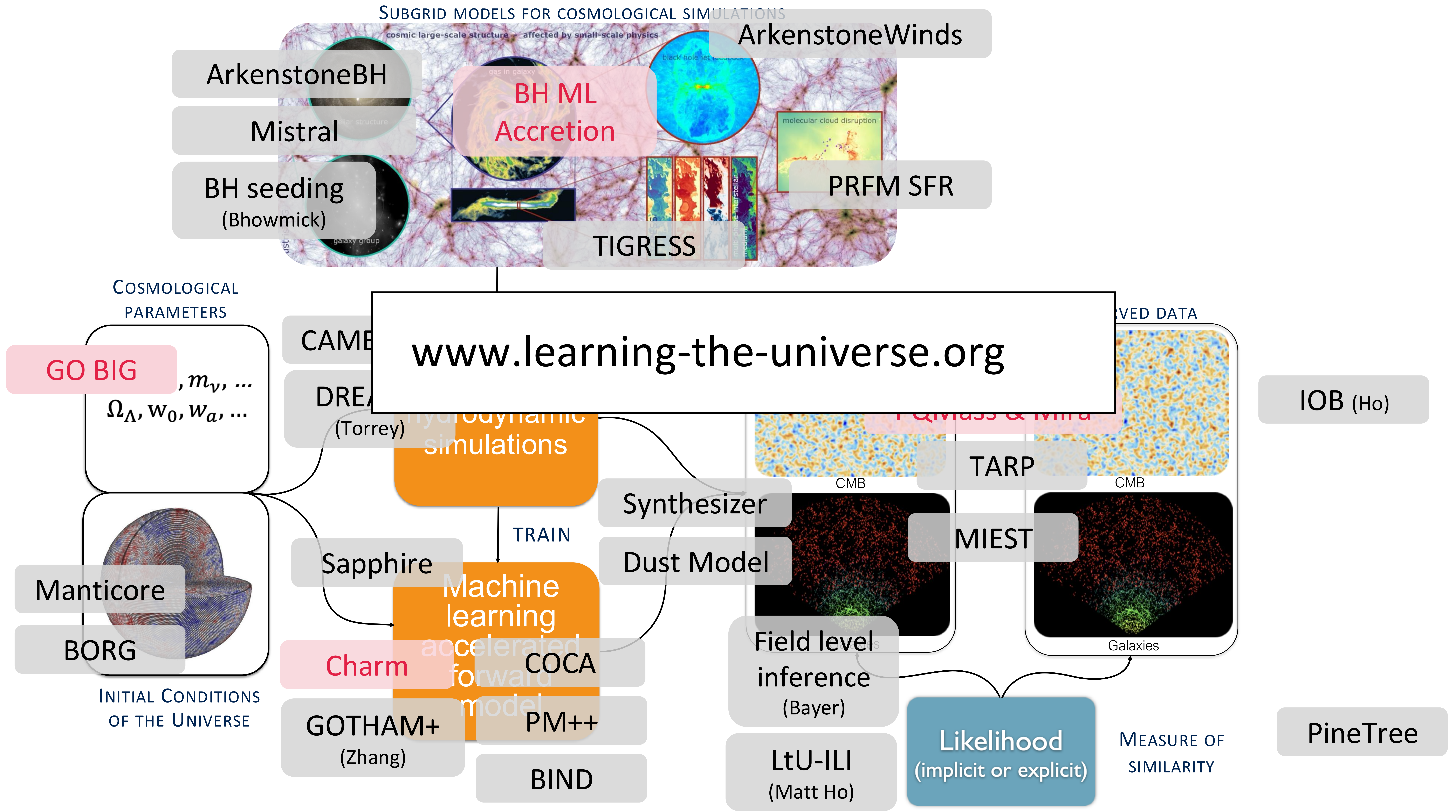
θ

η

The Degeneracy Distillery in 3 steps



1. compress data to labels and learn information geometry



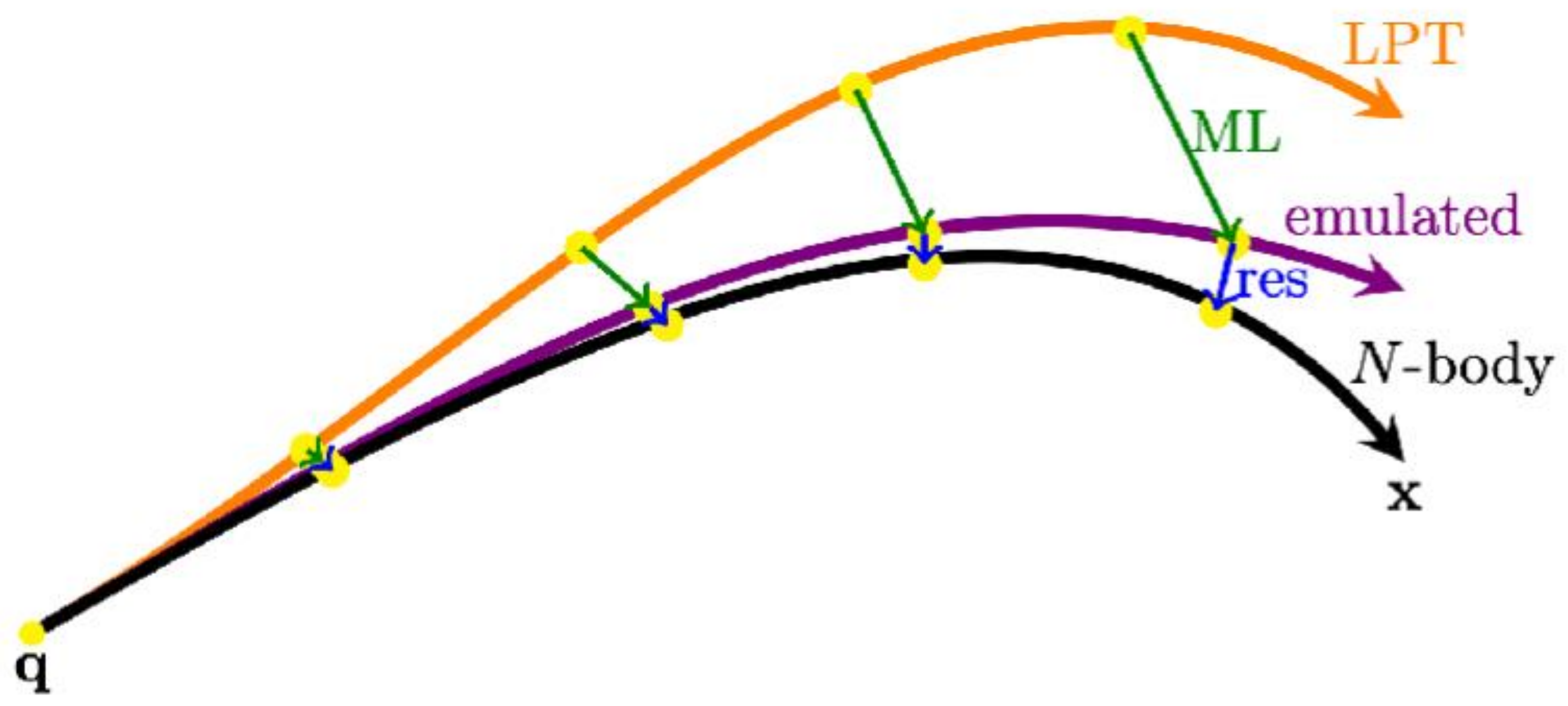
Subgrid models for cosmological simulations
cosmic large-scale structure
affected by small-scale physics
ArkenstoneWinds
ArkenstoneBH
Mistral
BH ML
Accretion
black hole jet feedback
molecular cloud disruption
BH seeding
(Bhowmick)
PRFM SFR
galaxy group
TIGRESS
Cosmological
parameters
CAME
GO BIG
$, m_\nu, \ldots$
$\Omega_\Lambda, w_0, w_a, \ldots$
DREA
(Torrey)
www.learning-the-universe.org
simulations
VED DATA
IOB (Ho)
TARP
CMB
CMB
Synthesizer
TRAIN
Sapphire
Dust Model
MIEST
Manticore
Machine
learning
BORG
Charm
COCA
Field level
inference
(Bayer)
Galaxies
Initial conditions
of the Universe
GOTHAM+
(Zhang)
PM++
Likelihood
(implicit or explicit)
Measure of
similarity
PineTree
BIND
LtU-ILI
(Matt Ho)

EXTRA SLIDES

Correcting Emulation Errors

COmoving Computer Acceleration (COCA)
Bartlett et al. 2024 (2409.02154)

- Neural networks can emulate expensive N-body simulations.
- These have (until now) **un-correctable emulation errors**.
- By learning a frame of reference rather than the output, we can **correct for emulation errors** by adding a few force evaluations.



Deaglan Bartlett

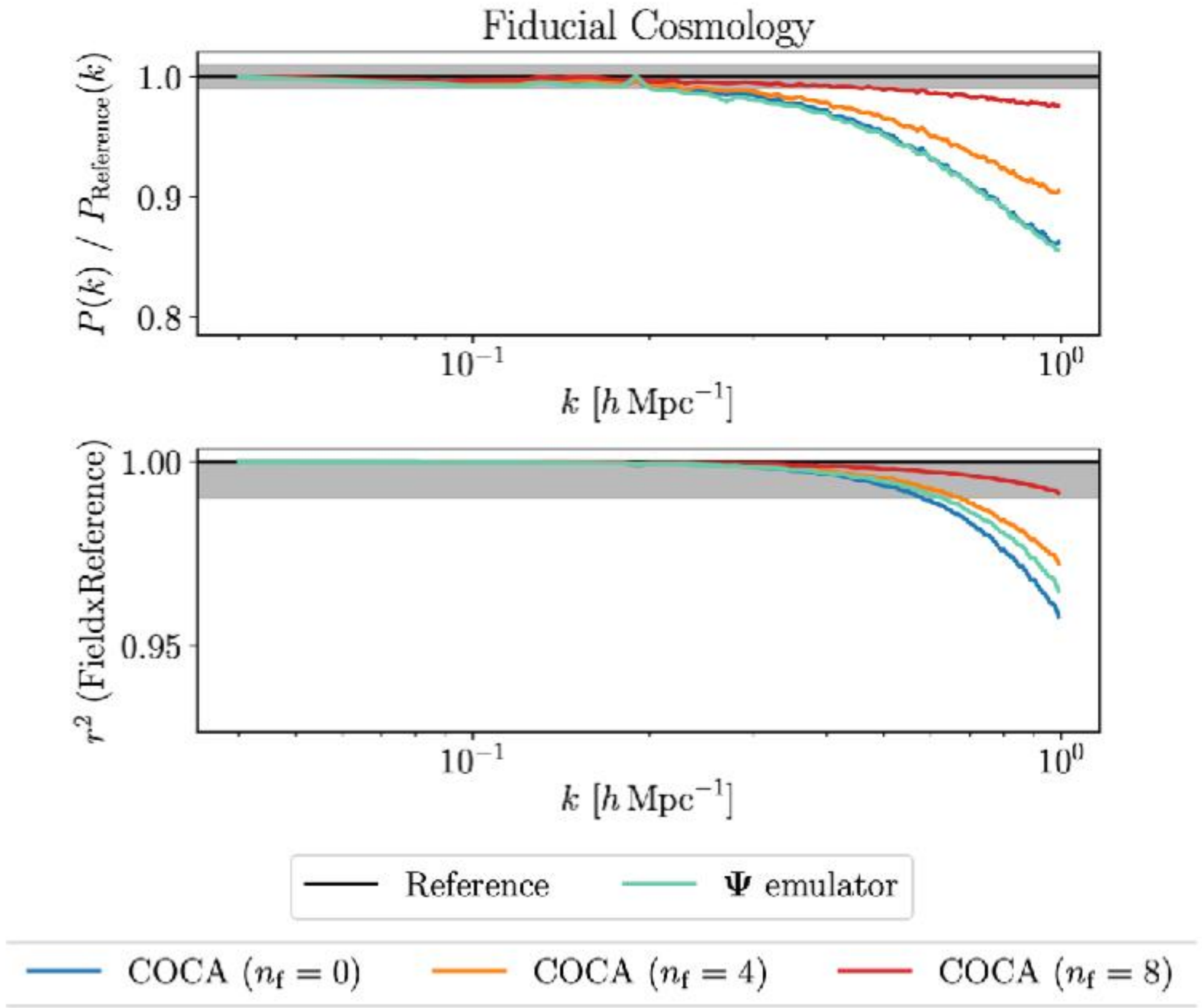
Solve trajectory around ML solution

Express displacement field as emulator prediction plus an error

$$\boldsymbol{\Psi}(\boldsymbol{q}, a) \equiv \boldsymbol{\Psi}_{\mathrm{LPT}}(\boldsymbol{q}, a) + \boldsymbol{\Psi}_{\mathrm{ML}}(\boldsymbol{q}, a) + \boldsymbol{\Psi}_{\mathrm{res}}(\boldsymbol{q}, a)$$

Now solve for this residual in a simulation

$$\partial_a^2 \boldsymbol{\Psi}_{\mathrm{res}}(\boldsymbol{q}, a) = \nabla \Phi(\boldsymbol{x}, a) - \partial_a^2 \boldsymbol{\Psi}_{\mathrm{LPT}}(\boldsymbol{q}, a) - \partial_a^2 \boldsymbol{\Psi}_{\mathrm{ML}}(\boldsymbol{q}, a)$$



Force evaluations correct emulation errors

- Only need 8 force evaluations to practically **eliminate emulation errors**.
- **4 to 5 times more accurate** than a Lagrangian displacement emulator when the frame of reference emulator is trained with the **same resources** as the Lagrangian displacement emulator.
- Can correct for **extrapolation** errors.