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Differentiable Modelling for Cosmology

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Work mostly with Florian List, Cornelius Rampf, Natalia Porqueres, Lukas Winkler

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Precision Cosmology Post-CMB

era of large-scale structure has begun

key questions remain

law of gravity? any deviations from GR?

any hints beyond cosmological constant? $w(z)$?

initial conditions? what inflation?

dark matter nature?

neutrino masses?

huge model space (DM,DE,MG,inf)

multi-probe era

significantly more accurate modelling
will be needed than so far...

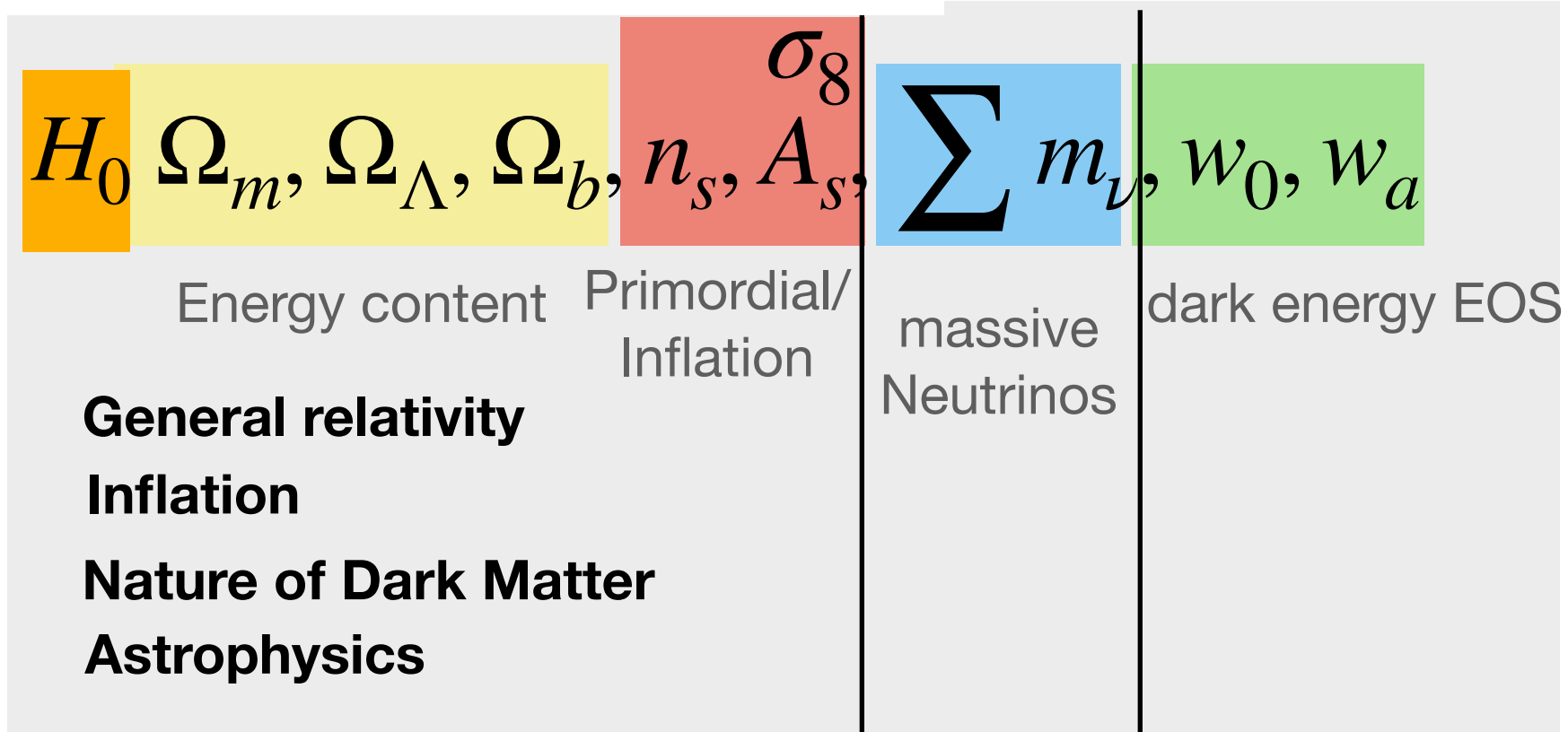


+LSST, Rubin,...

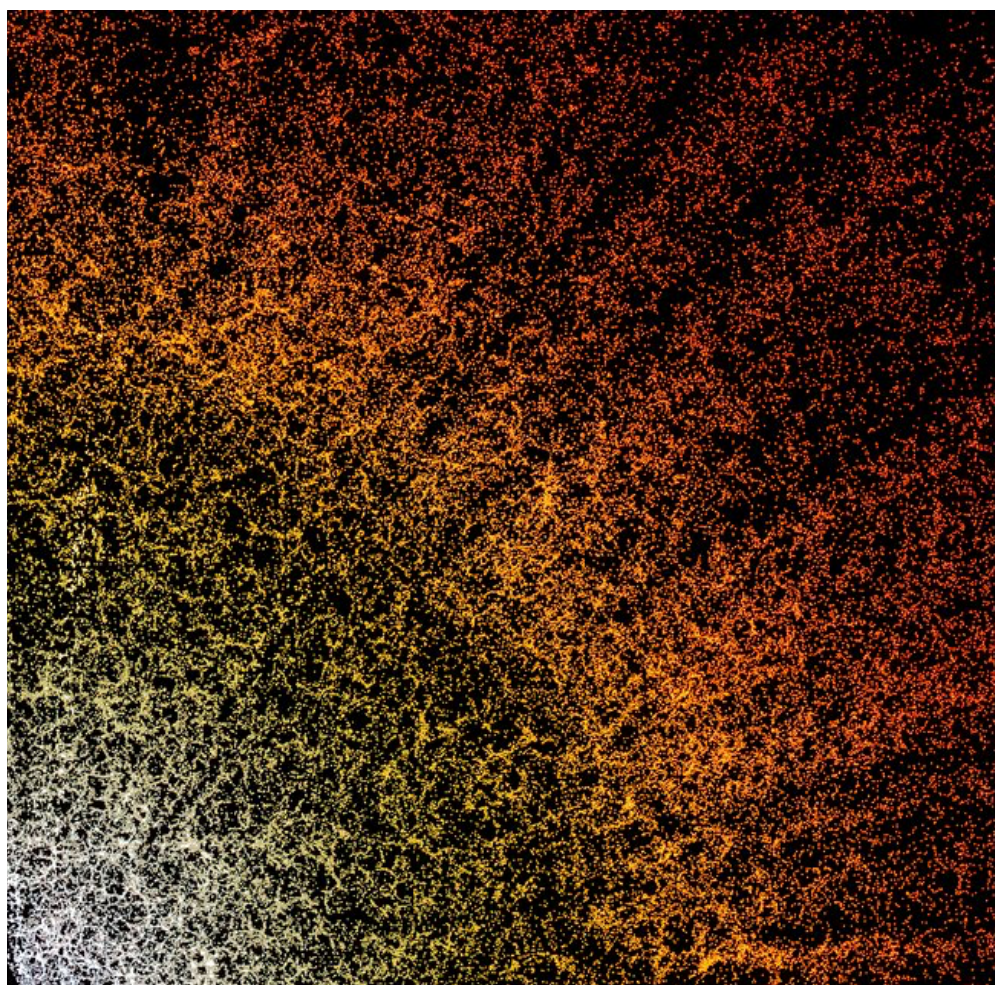
Classical approach

Model

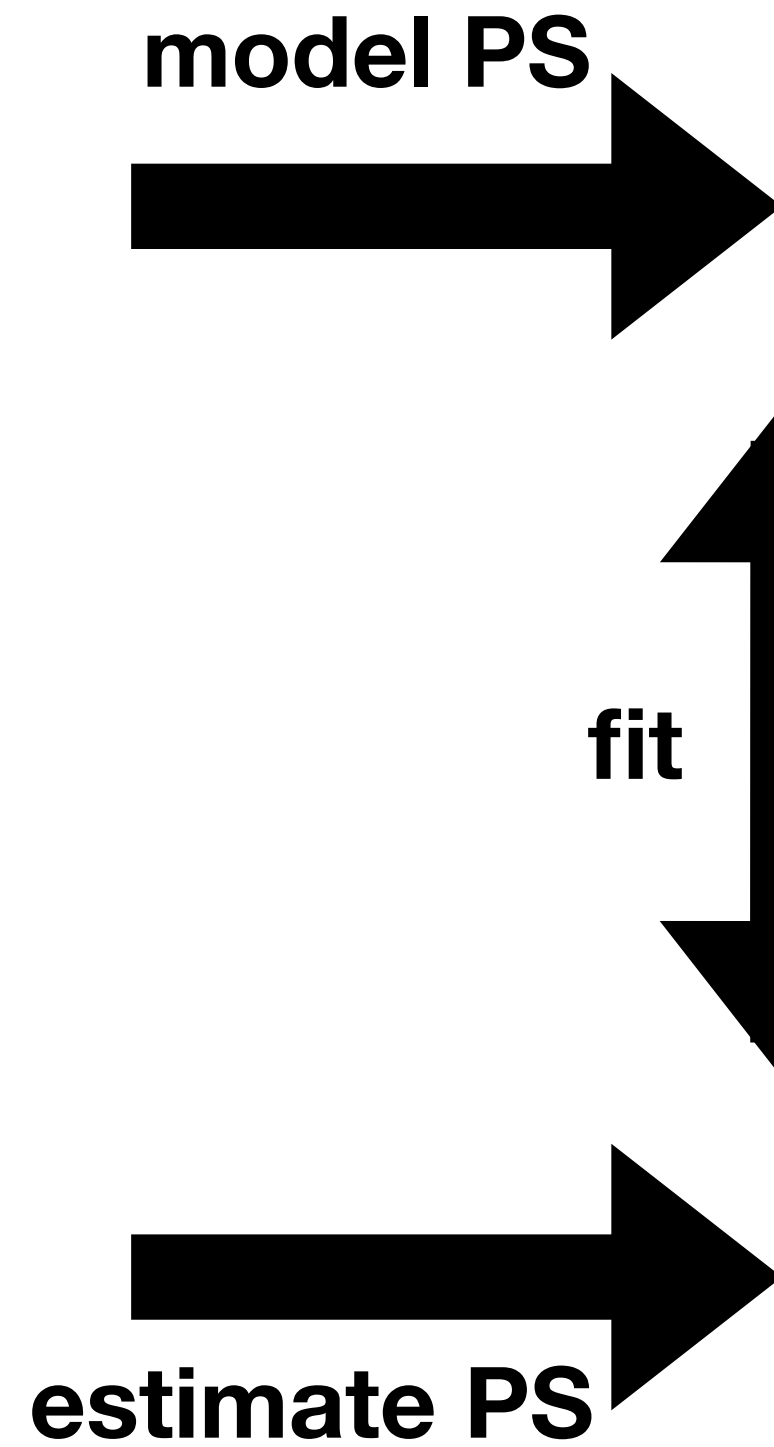
Cosmological parameters
 $\theta = \{\Omega_m, \Omega_b, H_0, \sigma_8, \dots\}$



Data

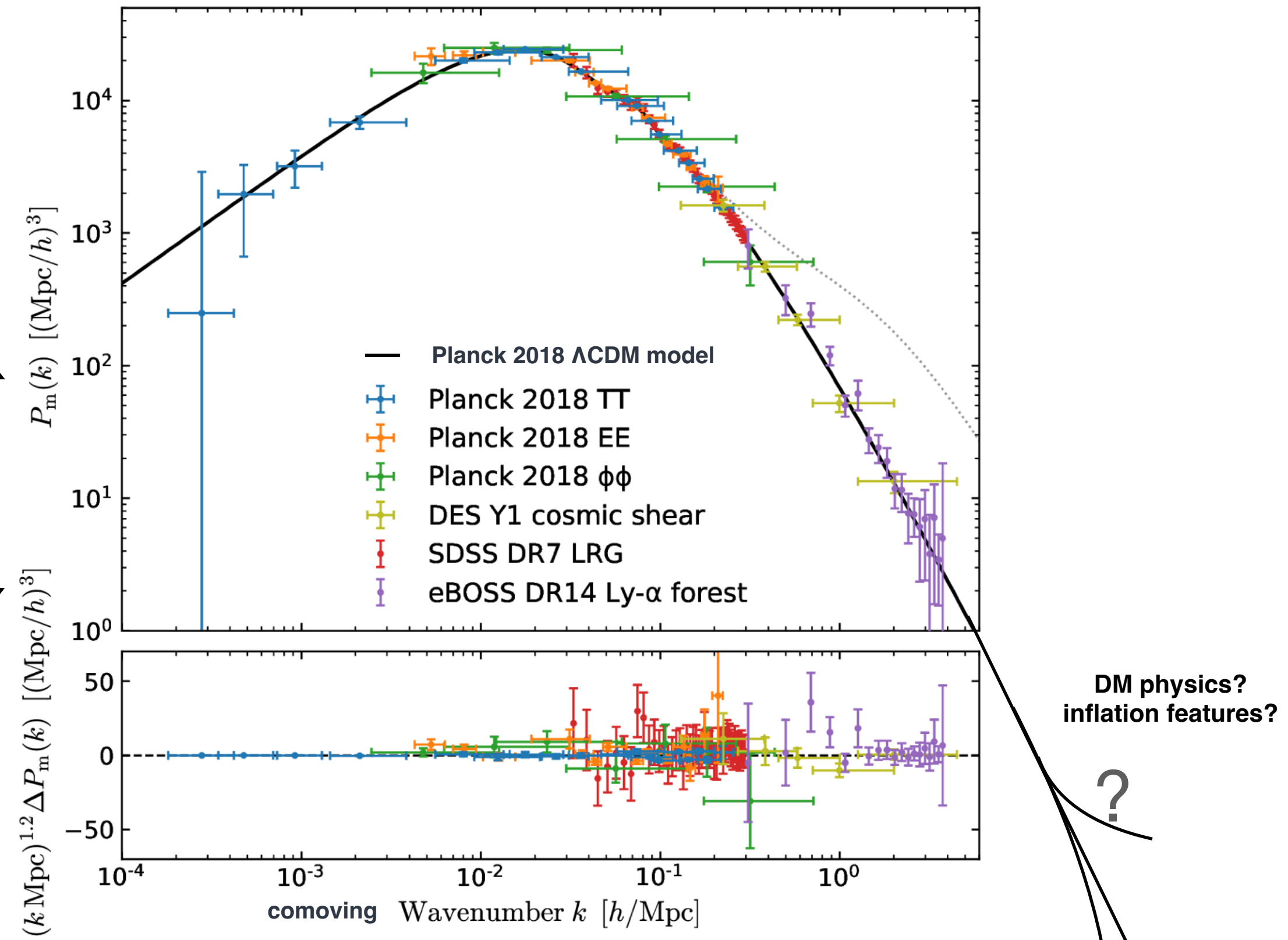


DESI collaboration



Summary Statistic (2pt, 3pt, ...)

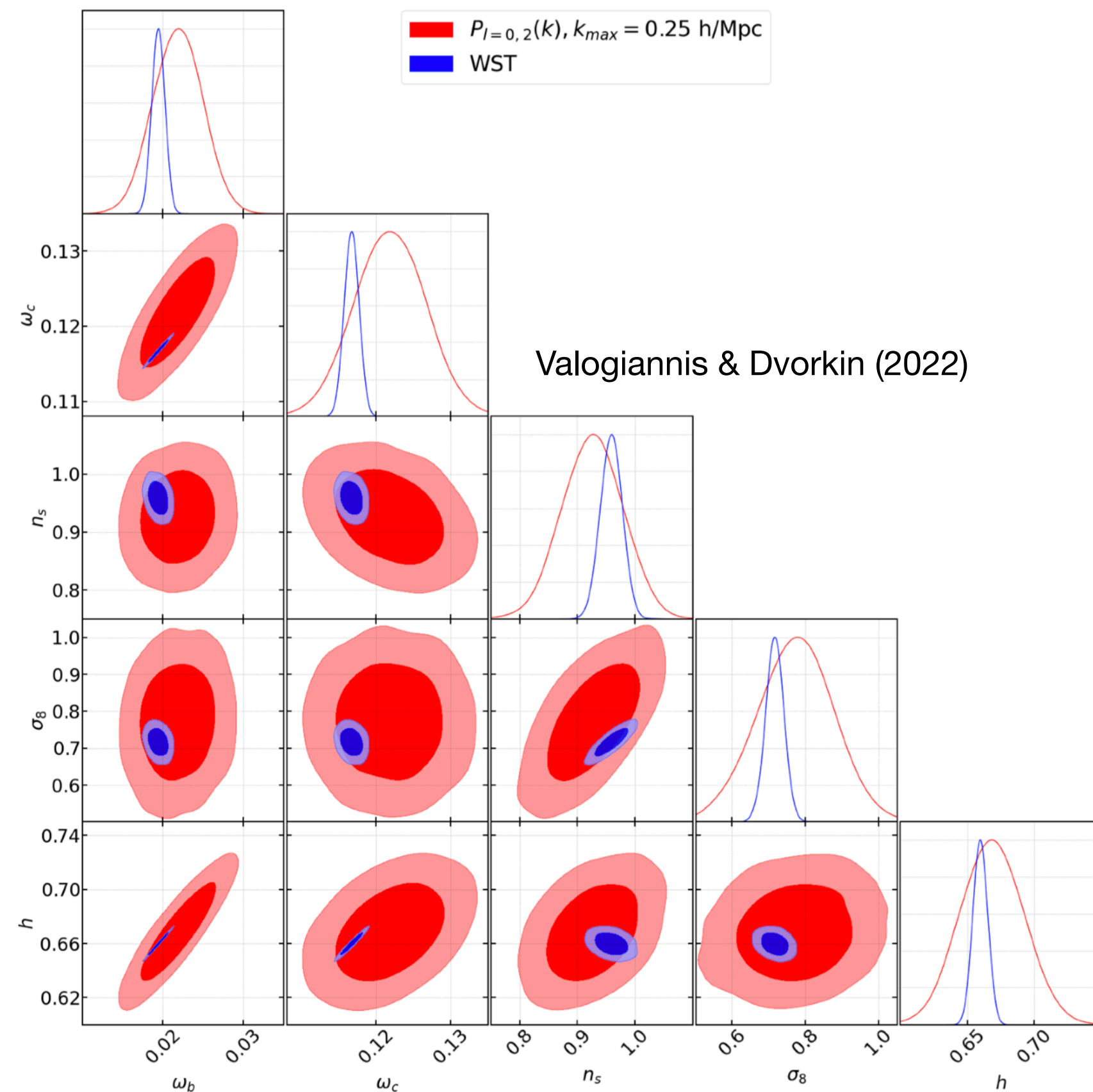
Chabanier et al. 2019



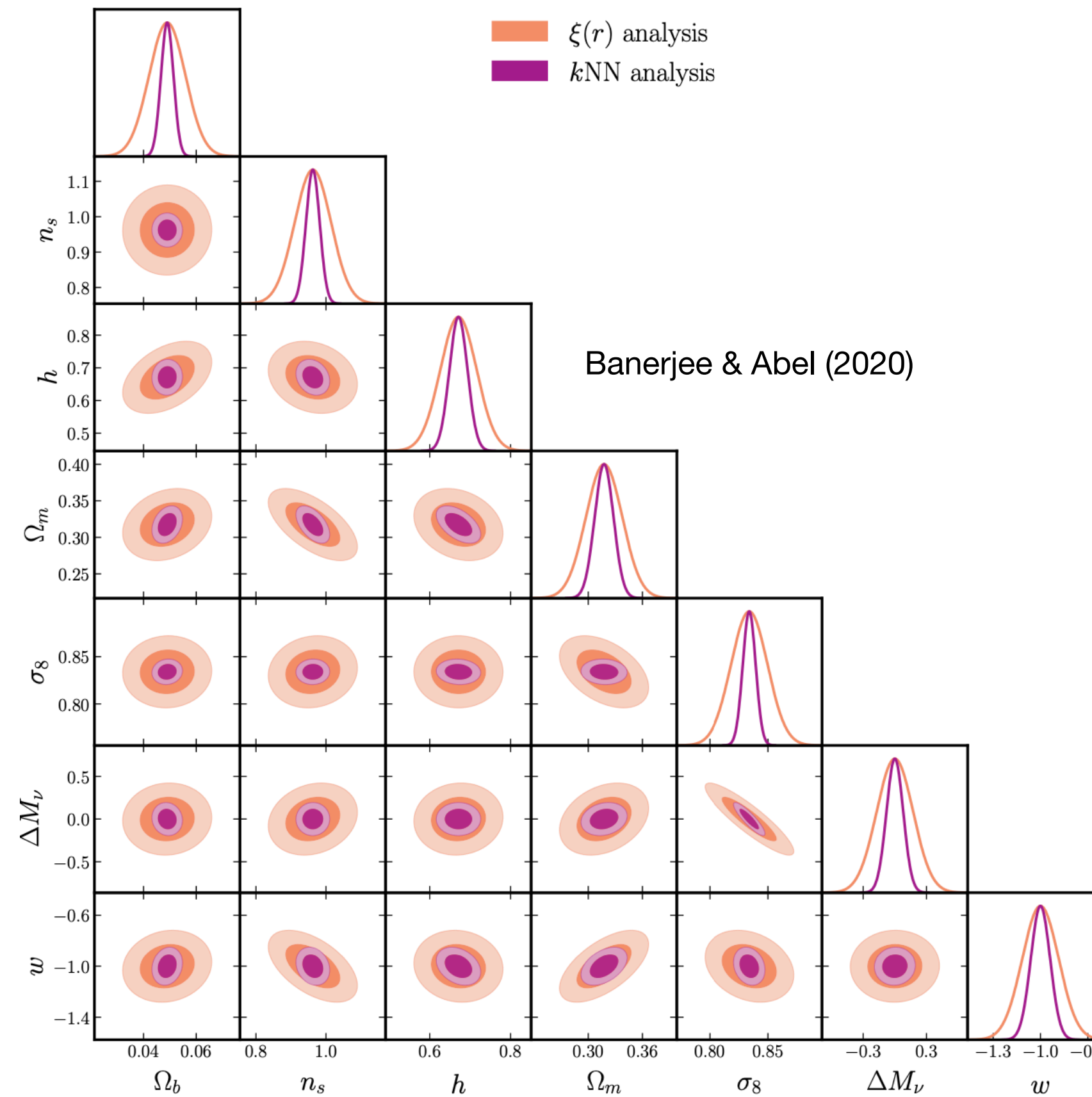
Move beyond simple statistics

- two-point statistics is complete description only for Gaussian fields
- n-point functions are useful in weakly non-Gaussian case, others exist:

Wavelet Scattering Transform Mallat 2012, Cheng+2020



kNN statistics Banerjee & Abel (2020)



- alternative: ‘field-level modelling’: use all data without a priori compression, model observables

The forward model

Modelling challenge:

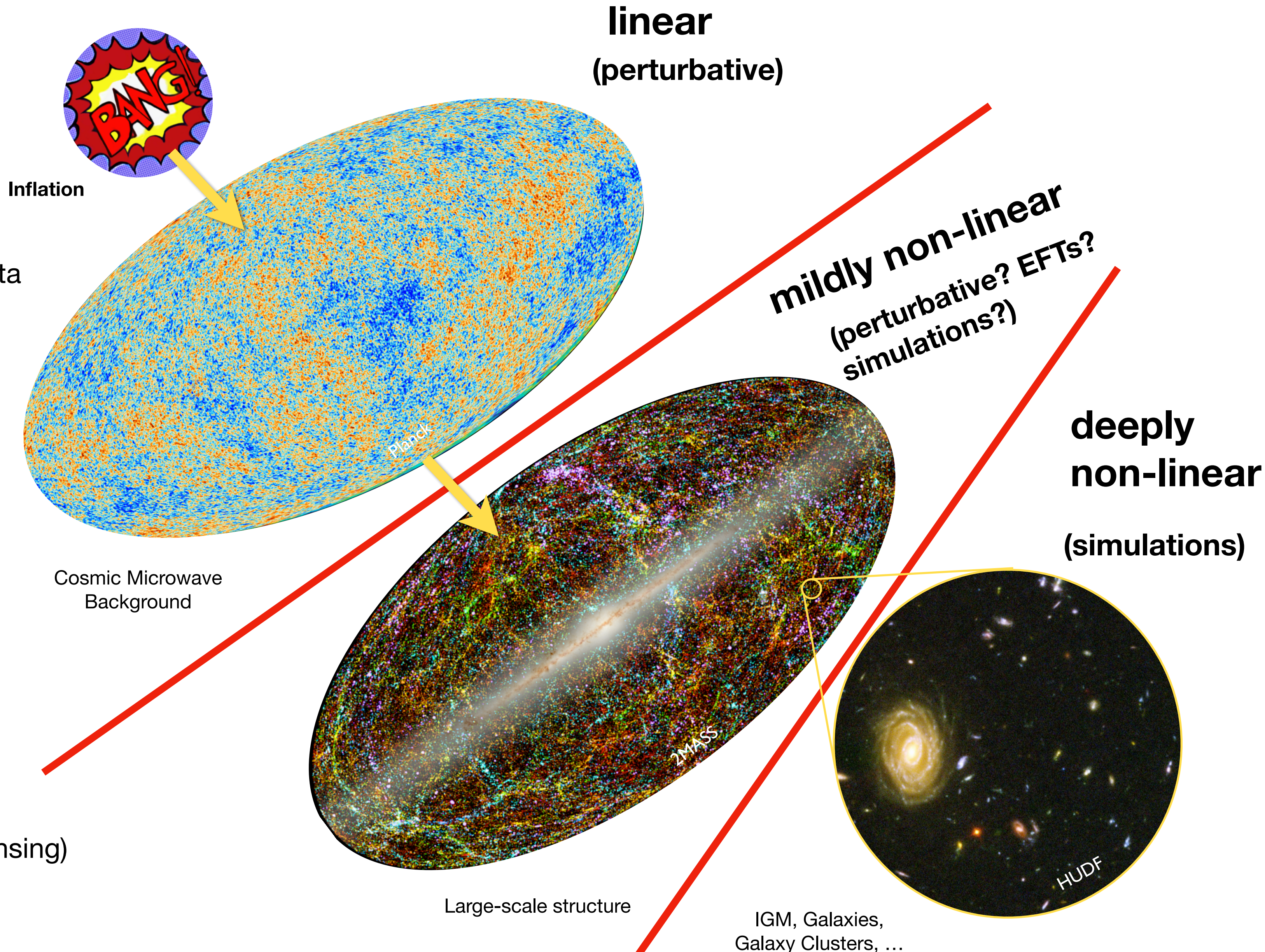
predict mapping between physical model and all observables

taking into account uncertainties, and all cross correlations

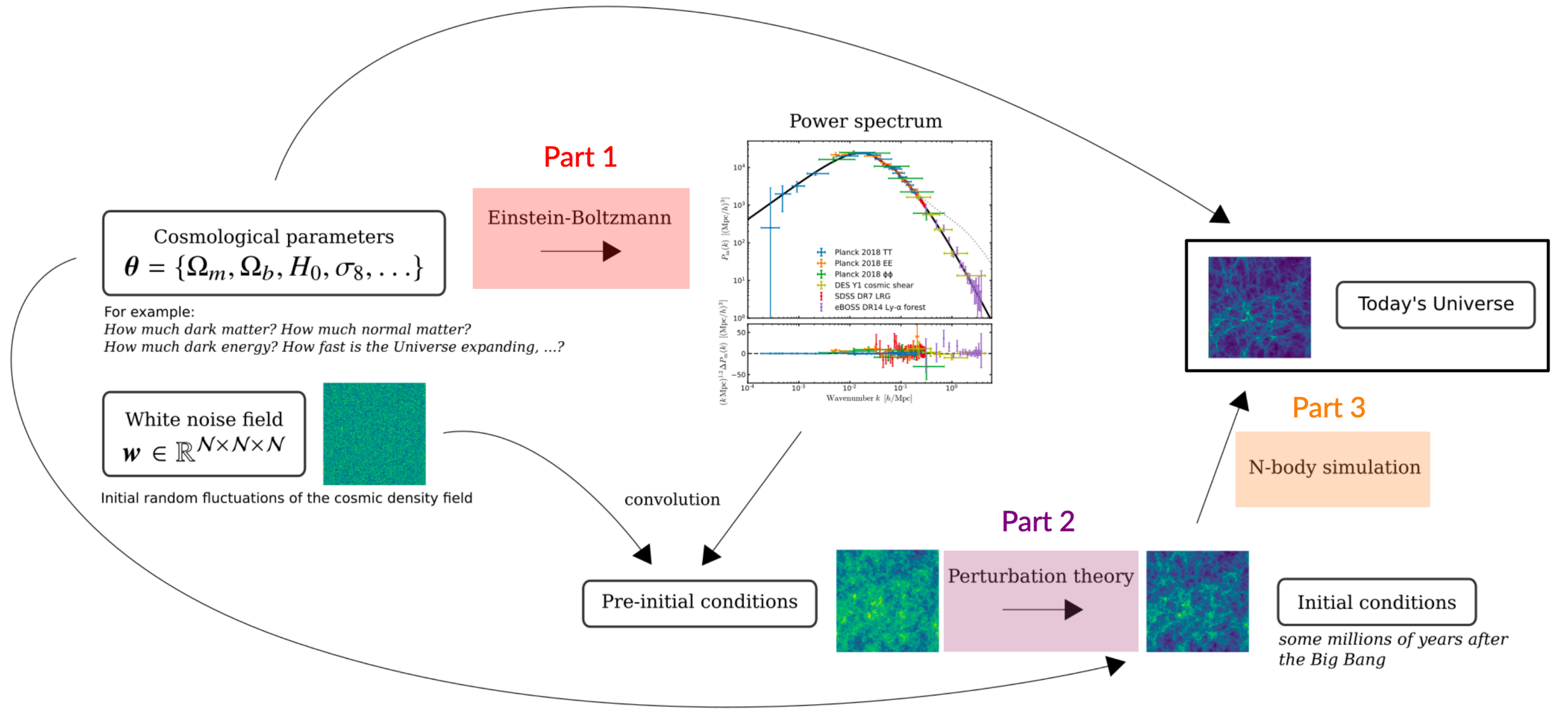
inference limitation is from modelling, not data already with current surveys!

Astronomical Survey Observables

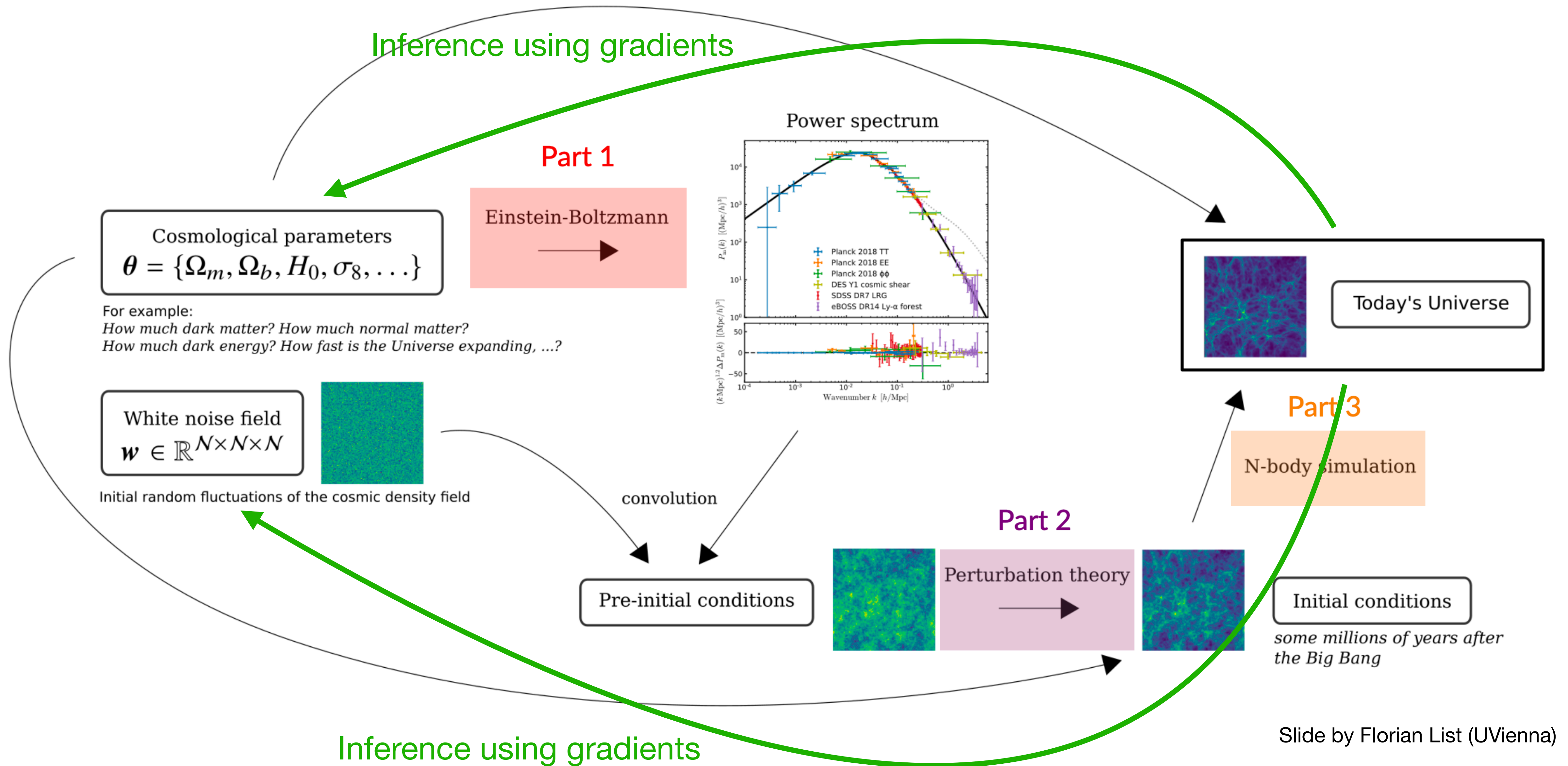
- Galaxy distribution (clustering, n-point, etc.)
- Gravitational Lensing (weak, strong, CMB lensing)
- Galaxy Clusters (optical, X-ray, tSZ)
- Ly-a, HI mapping



Field-level modelling



Field-level modelling



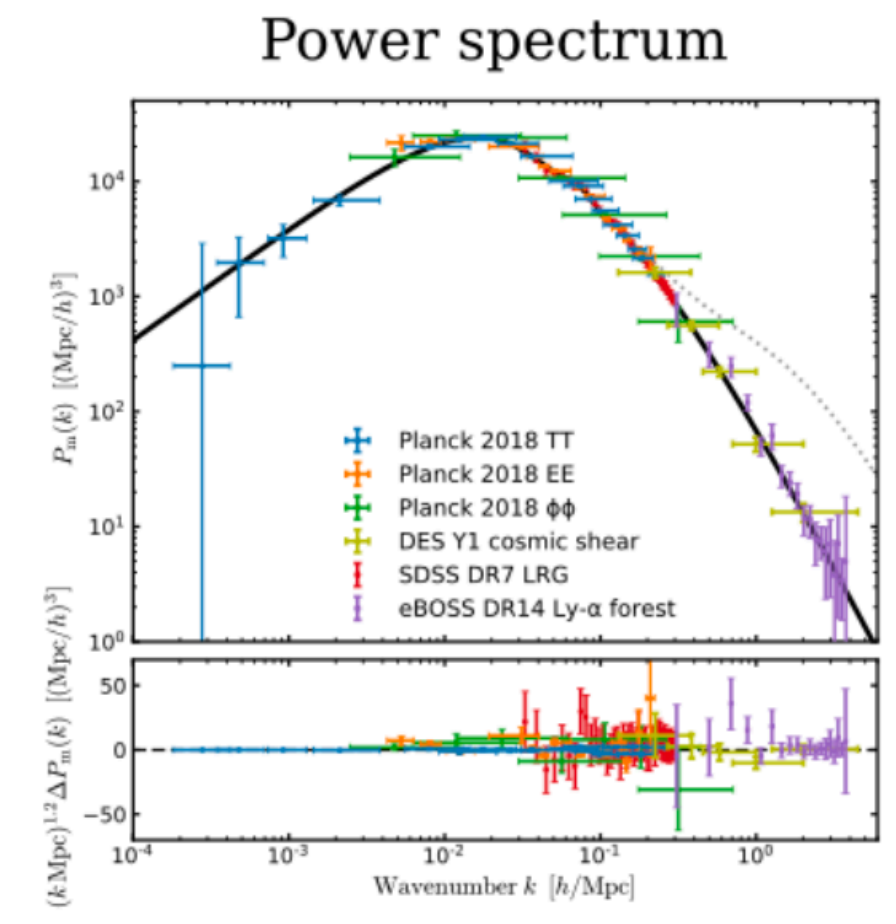
Field-level modelling



Inference using gradients

Part 1

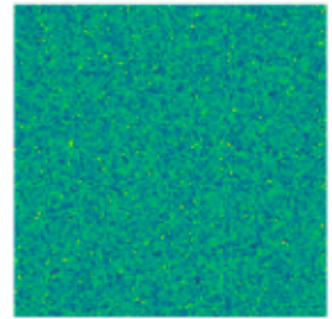
Einstein-Boltzmann



Cosmological parameters
 $\theta = \{\Omega_m, \Omega_b, H_0, \sigma_8, \dots\}$

For example:
How much dark matter? How much normal matter?
How much dark energy? How fast is the Universe expanding, ...?

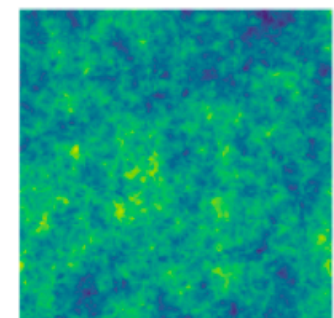
White noise field
 $w \in \mathbb{R}^{N \times N \times N}$



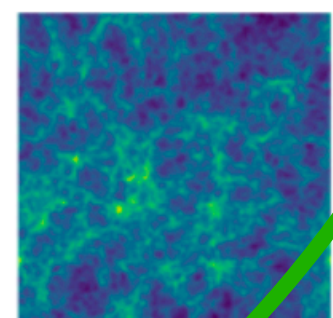
Initial random fluctuations of the cosmic density field

convolution

Pre-initial conditions



Perturbation theory



Initial conditions

some millions of years after the Big Bang

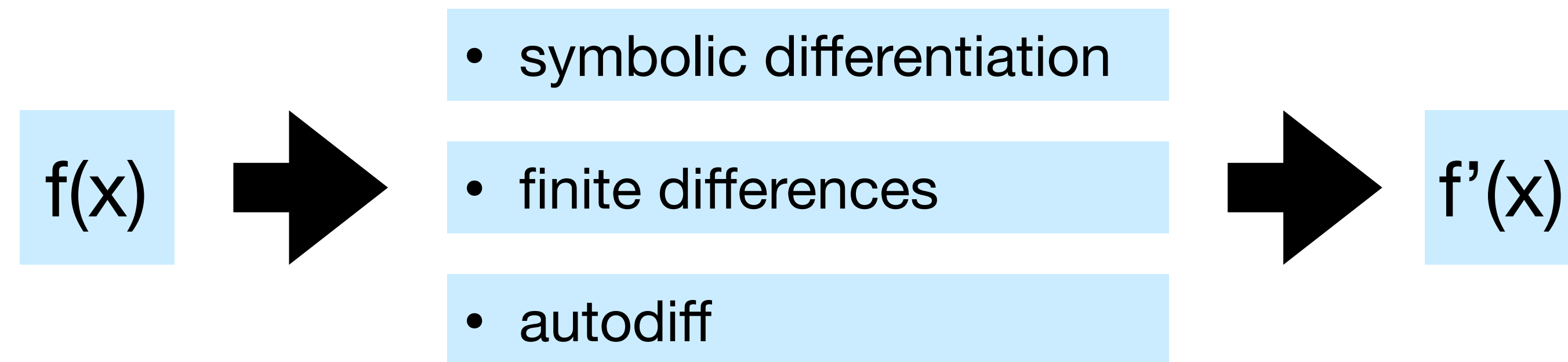
Part 3
N-body simulation



Today's Universe

Inference using gradients

Automatic differentiation/differentiable programming



- Computing gradients through long numerical expressions is a standard operation in machine learning (e.g. propagate gradient through NN)
- Two fundamental approaches: recursive application of chain rule
 - forward accumulation (tangent mode)
 - reverse accumulation (adjoint mode)
- Many high performance implementations exist through ML frameworks: pytorch, tensorflow, JAX, but also Julia has support
- Advantage: automatic, non-approximate, fast

Matching epochs in cosmological modelling

Early physics:

- GR effects (horizon+rel. species+aniso-stress)
- multi-species (CDM+baryon+photons+neutrinos)
- photon-baryon coupling + recombination
- perturbative quantity: δ and θ

Late physics:

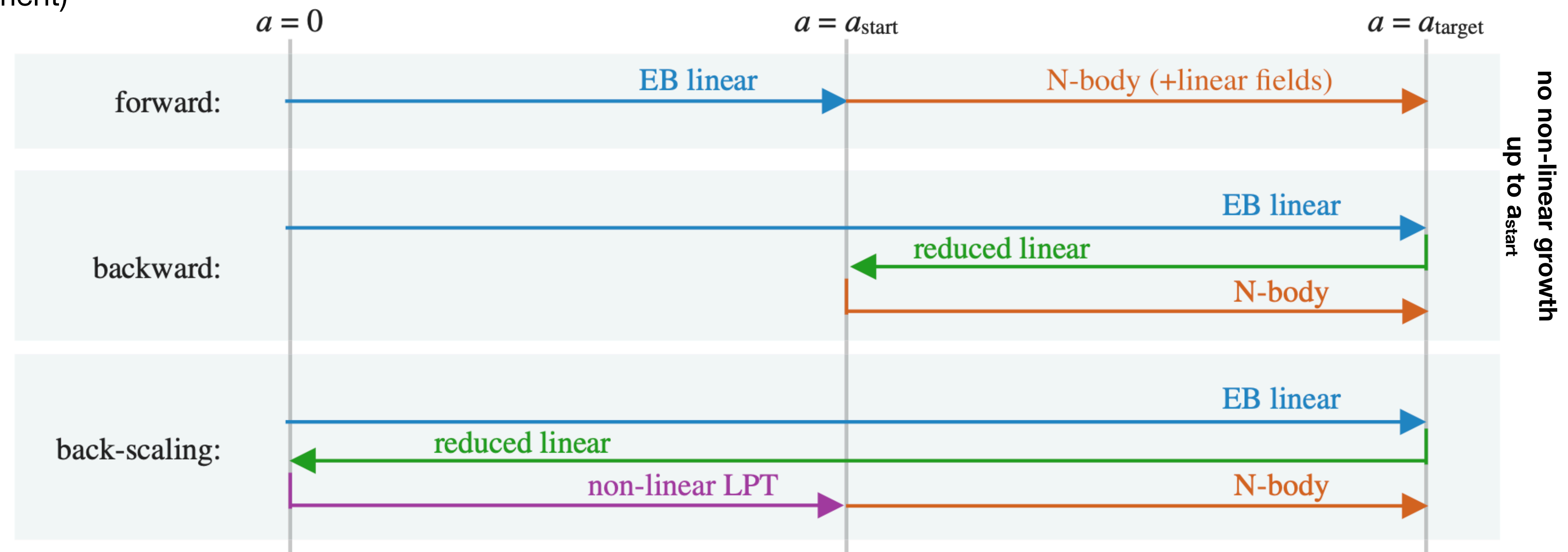
- Newtonian gravity + small corrections
- mostly interested in mass distribution, CDM+baryons
- non-linear growth
- perturbative quantity: ψ (displacement)

Matching problem!

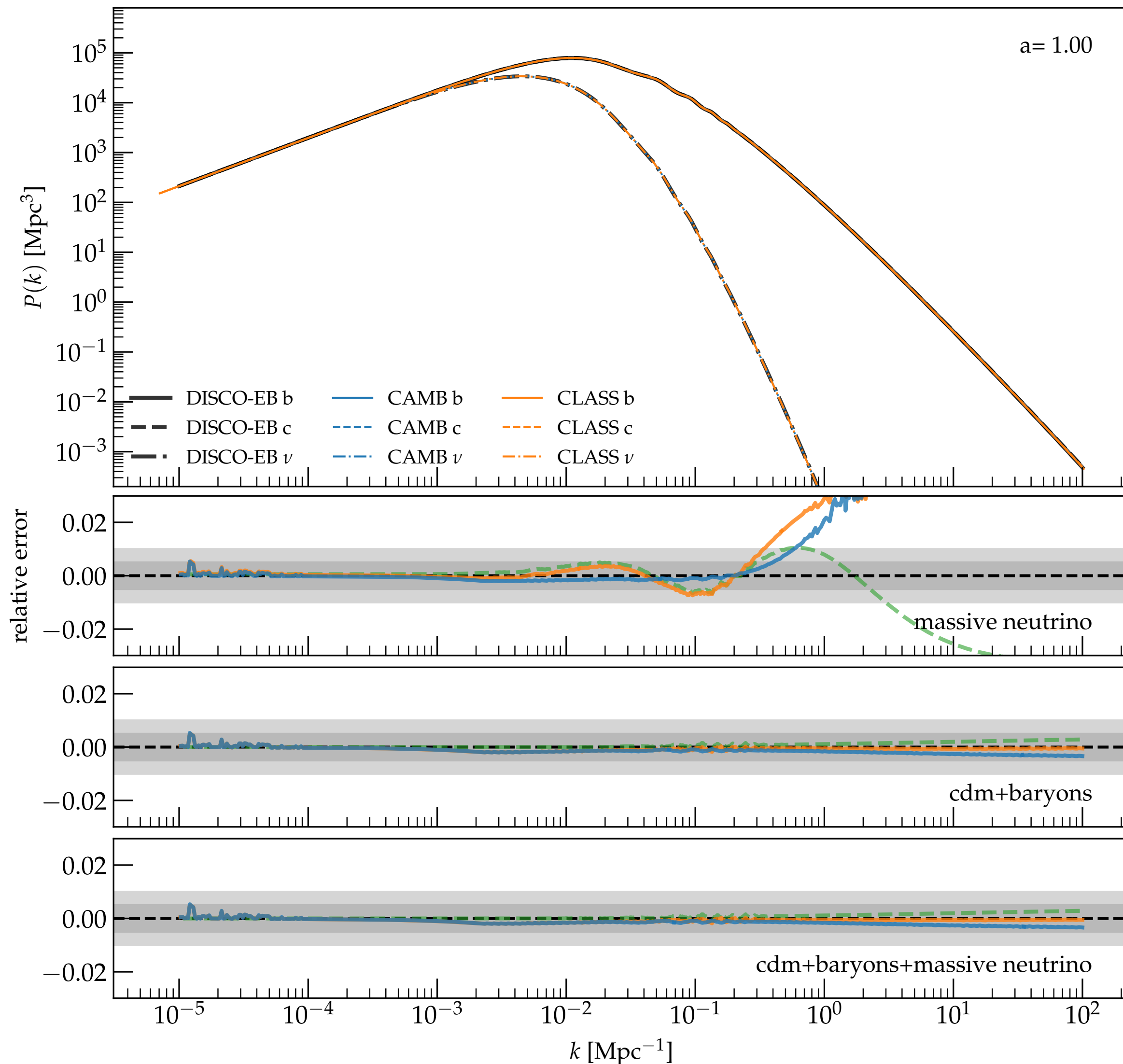
Eulerian

Lagrangian

choices in the literature:



Differentiable Einstein-Boltzmann Solver (DISCO-EB)



OH, List & Porqueres (2023, subm. to JCAP)

Multi-species fluid of DM+baryon+photon+(massive)neutrino+DE
→ **linear** Einstein-Boltzmann solver
(e.g. Ma & Bertschinger 1995, CLASS, CAMB)

~100 coupled ODEs (some stiff)

clean easily readable and extendable Python/JAX code

We use high order implicit solver from Diffrax library (Kidger 2022), supports forward and reverse mode differentiation

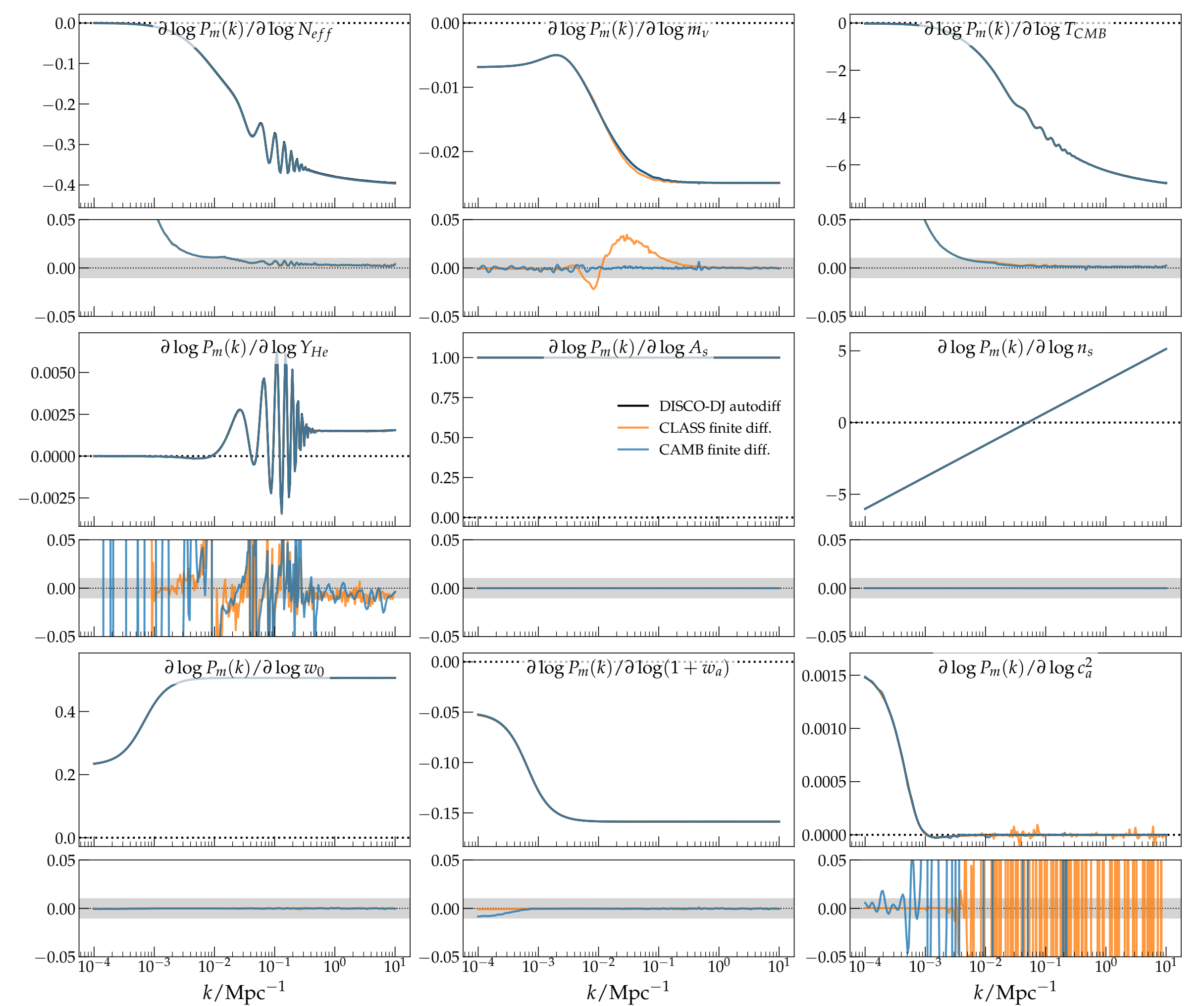
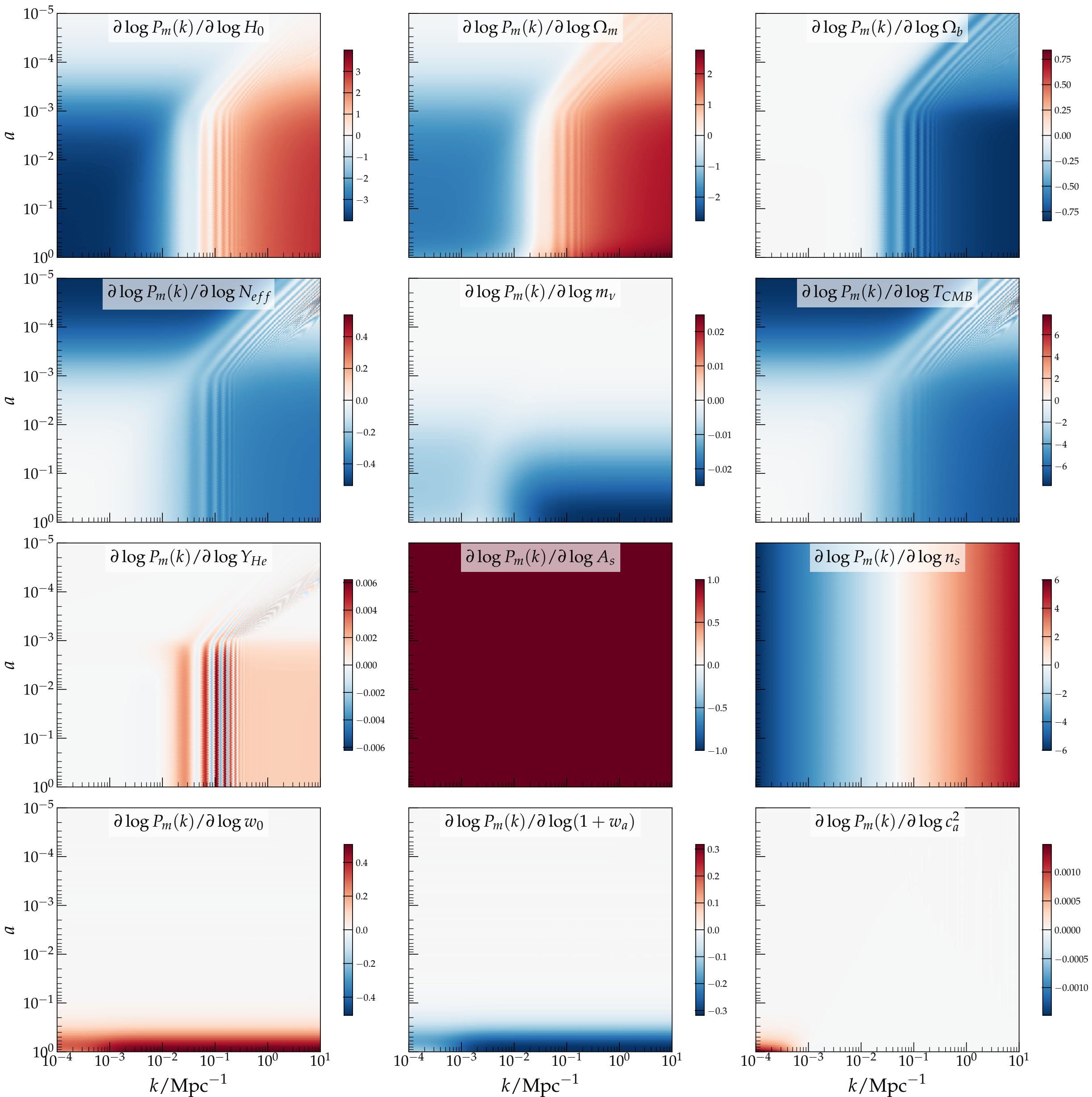
no need to specify Jacobian, due to autodiff

Current limitation: JAX does not support sparse matrices well

code publicly available in few weeks time, or on request:
oliver.hahn@univiea.ac.at



Differentiable Einstein-Boltzmann Solver (DISCO-EB)



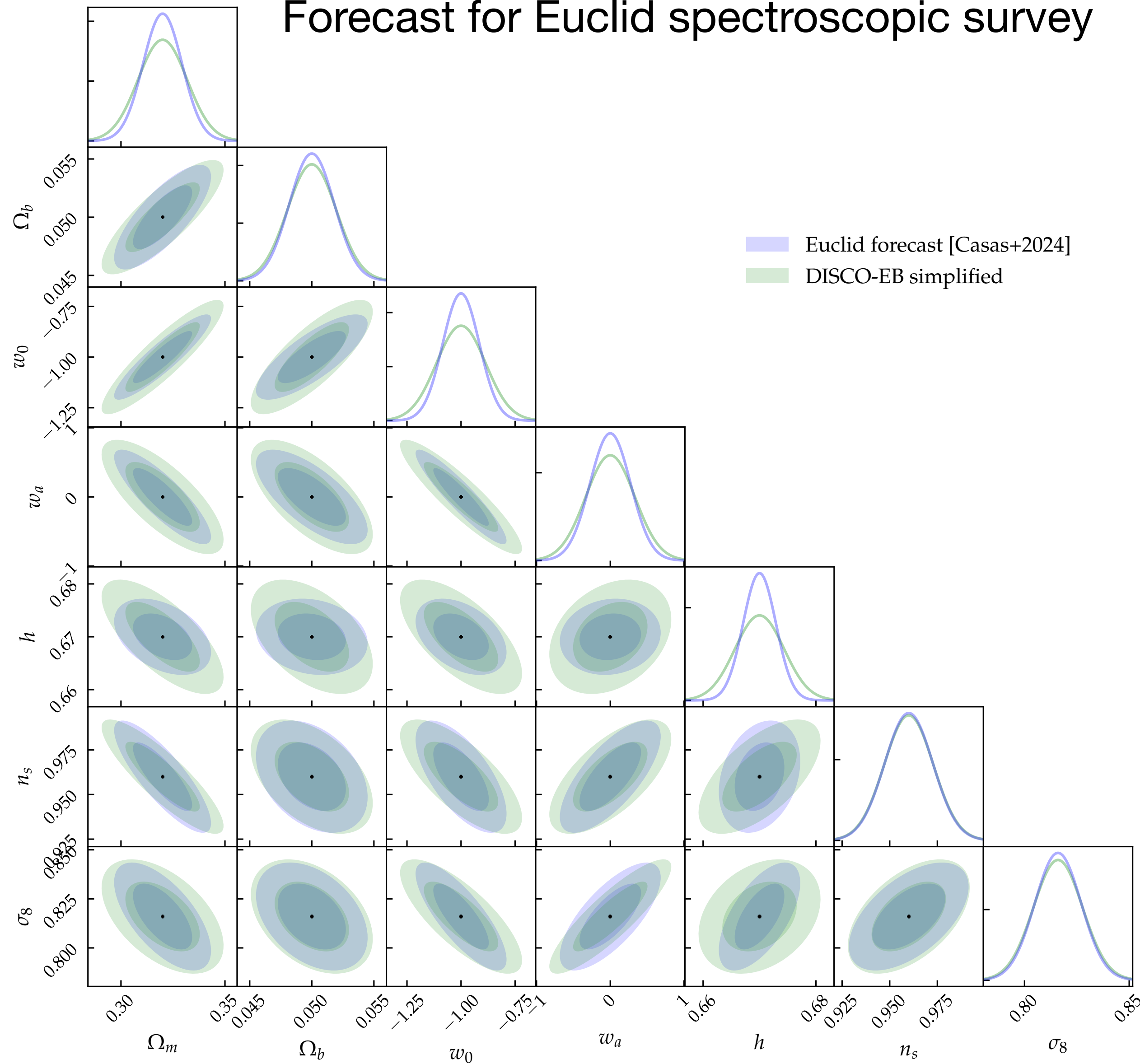
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Differentiable Einstein-Boltzmann Solver (DISCO-EB)

Forecast for Euclid spectroscopic survey



Fisher matrices are just calls to autodiff:

$$F_{ij} = \sum_{\ell} \frac{\partial y(\ell)^{\top}}{\partial \theta_i} \Sigma^{-1}(\ell) \frac{\partial y(\ell)}{\partial \theta_j}$$

Known/modelled *precision matrix* of the observables

Change of the *observable* w.r.t. the *i*-th *parameter*
 → **compute with autodiff**

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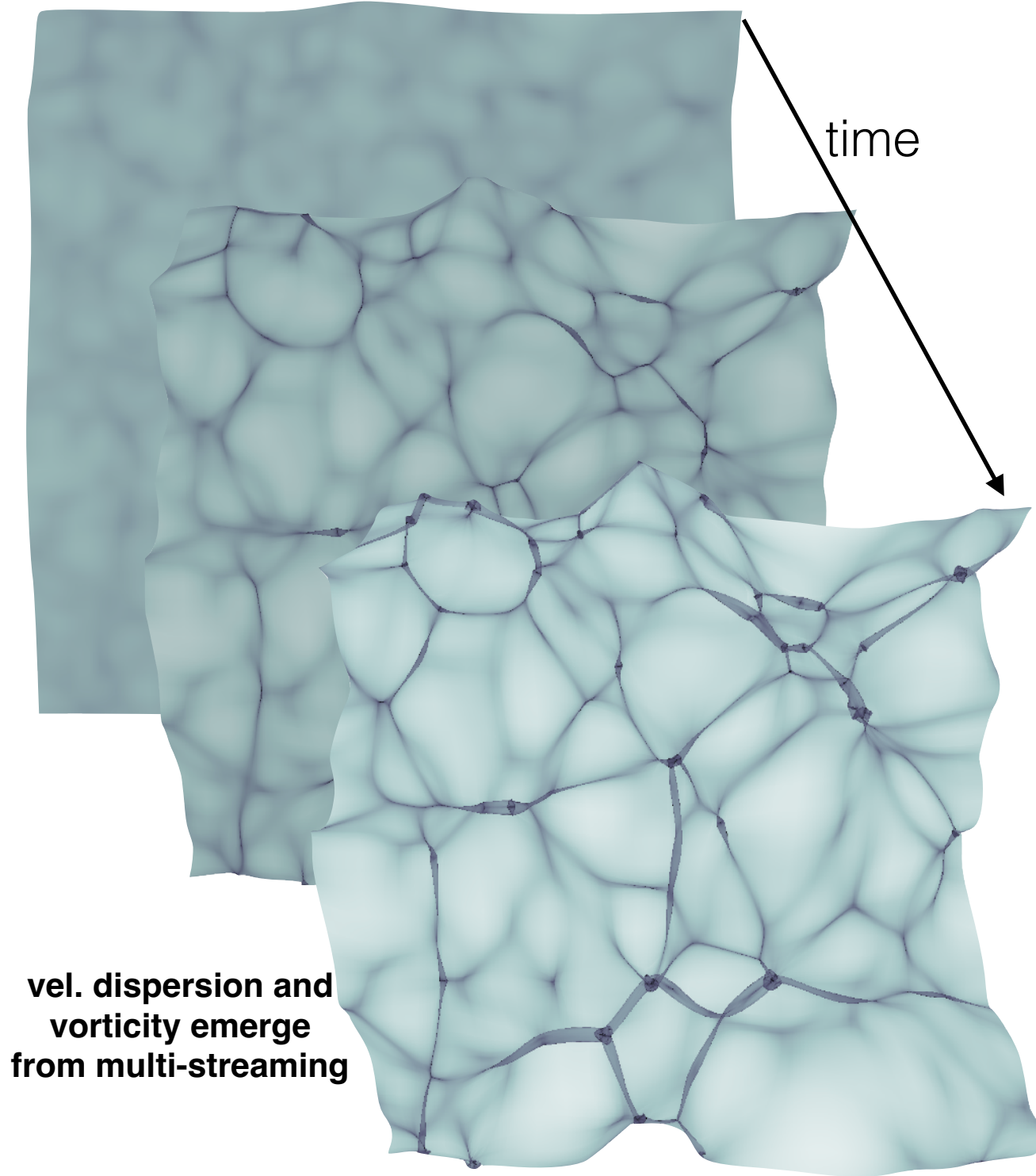


Non-Linear Evolution of Fluctuations

Cold Dark Matter lives on Lagrangian submanifold

Solve Vlasov-Poisson on submanifold characteristics $(\mathbf{q}, t) \mapsto (\mathbf{x}(\mathbf{q}, t), \mathbf{p}(\mathbf{q}, t))$

$$\frac{\partial f}{\partial t} + \frac{\mathbf{v}}{a^2} \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} \phi \cdot \nabla_{\mathbf{v}} f = 0 \quad \Leftrightarrow \quad \mathbf{x}'' + \mathcal{H} \mathbf{x}' = -\nabla \phi$$



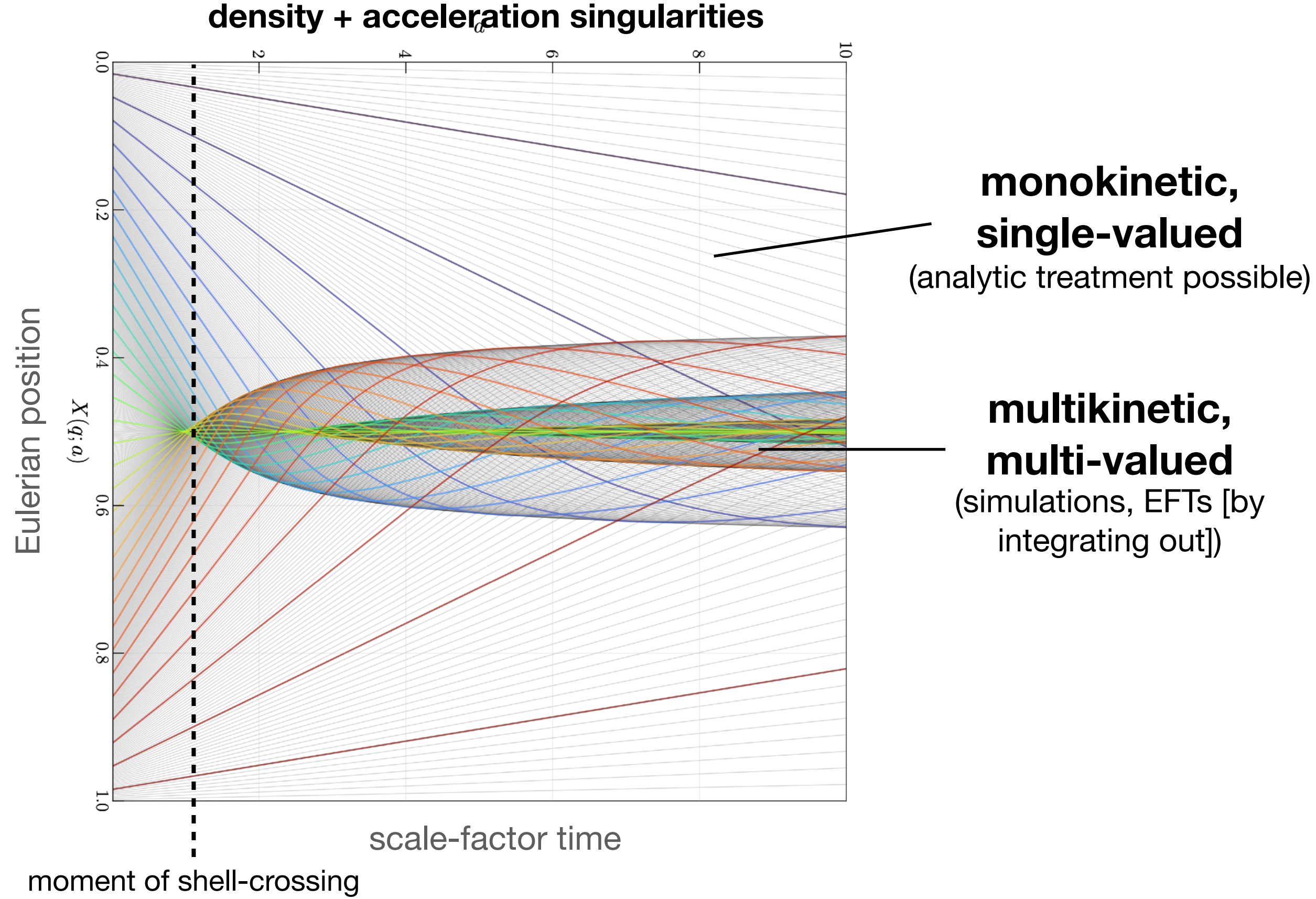
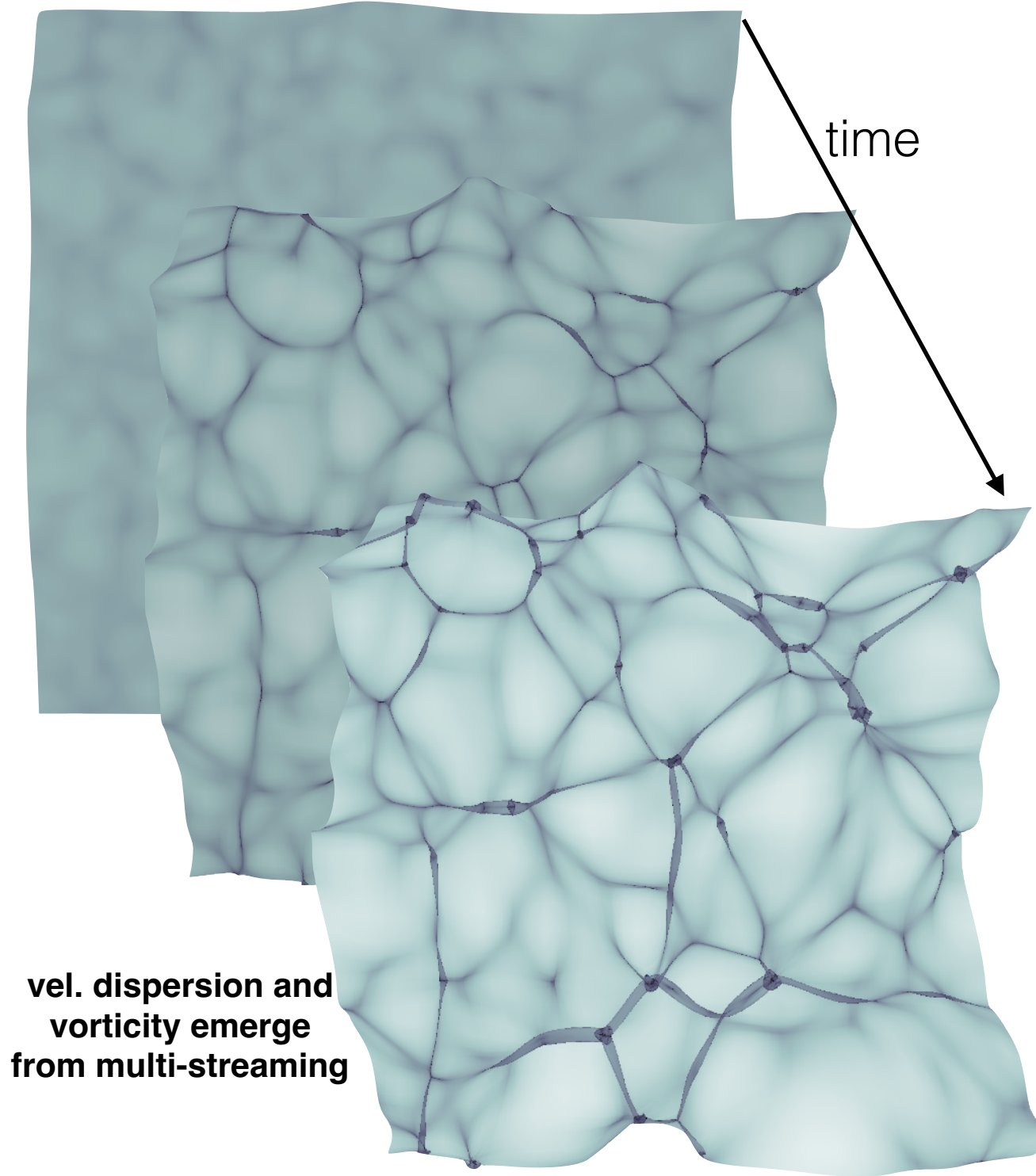
vel. dispersion and vorticity emerge from multi-streaming

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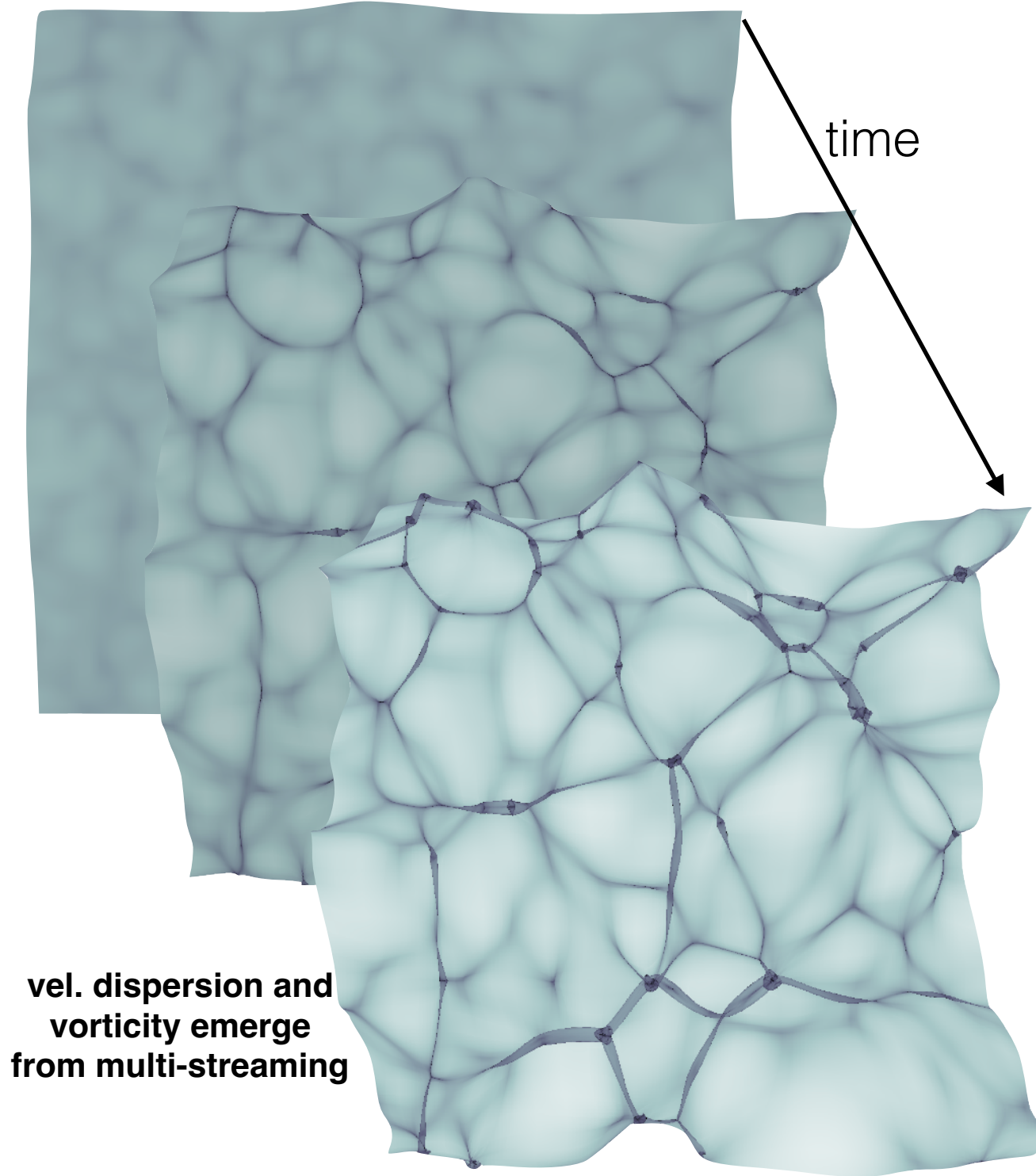


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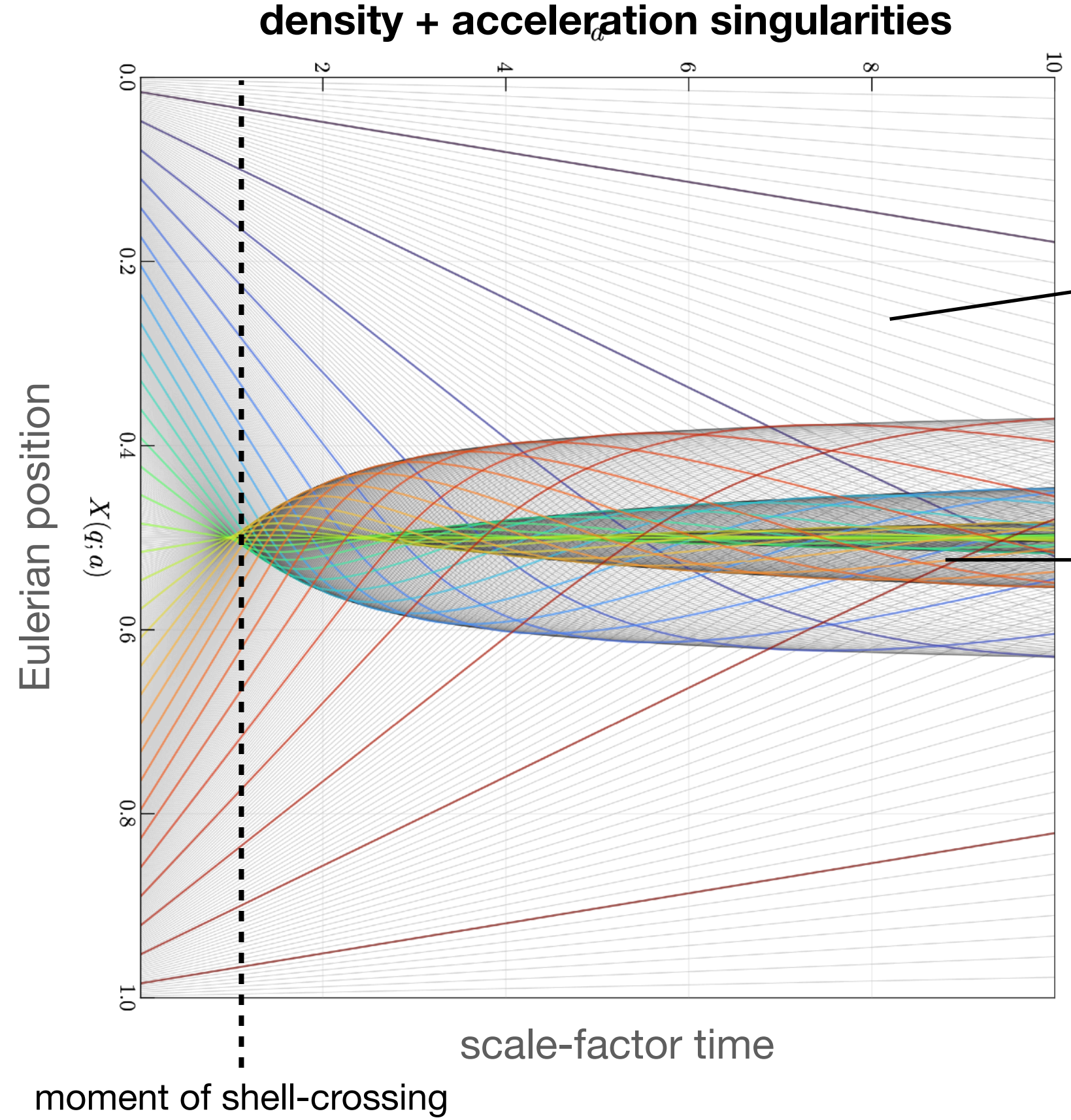
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vel. dispersion and vorticity emerge from multi-streaming



monokinetic, single-valued
(analytic treatment possible)

multikinetic, multi-valued
(simulations, EFTs [by integrating out])

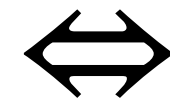
Zeldovich (1970) solution (straight lines) is exact prior to shell-crossing and outside shell-crossed regions

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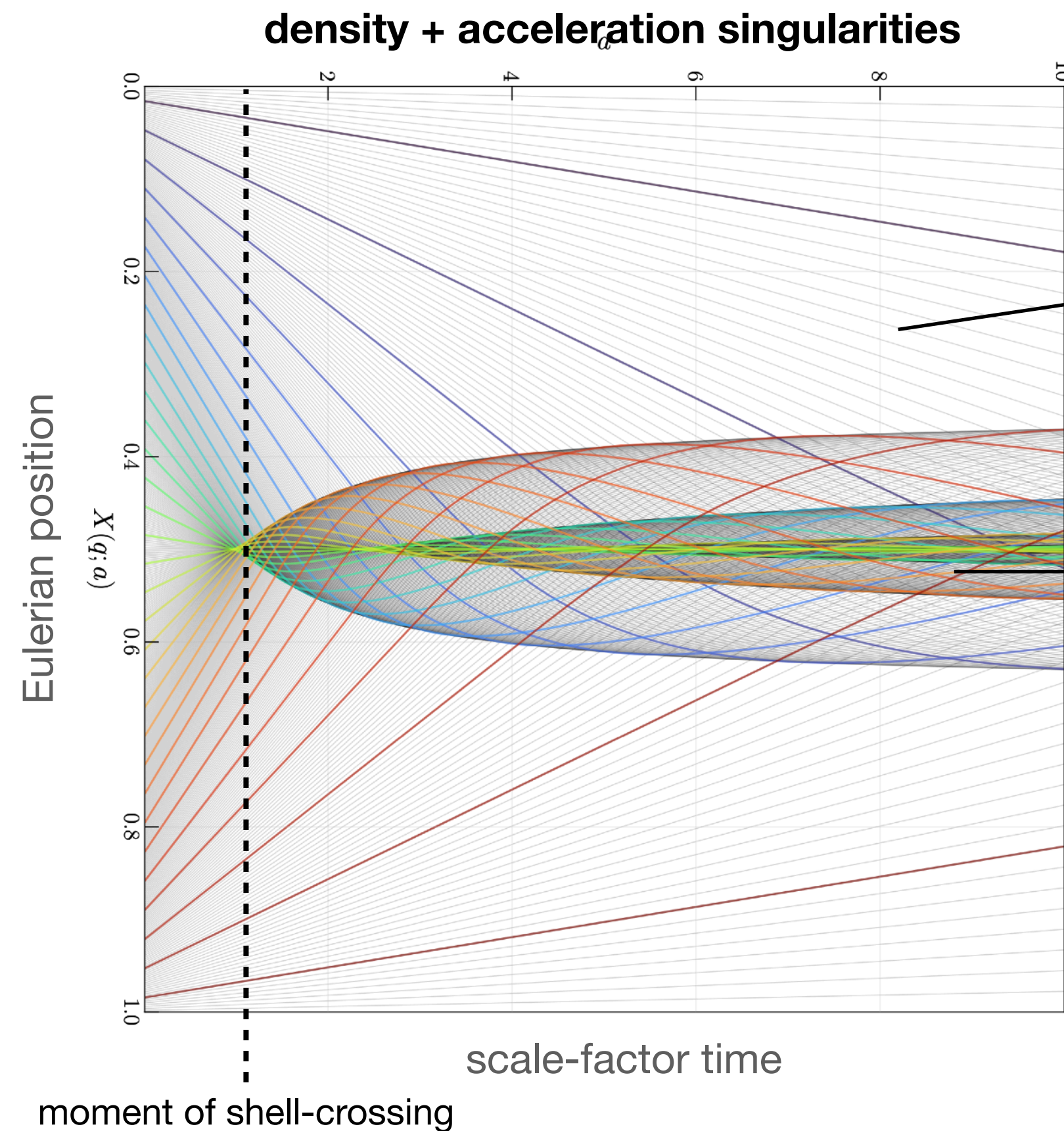
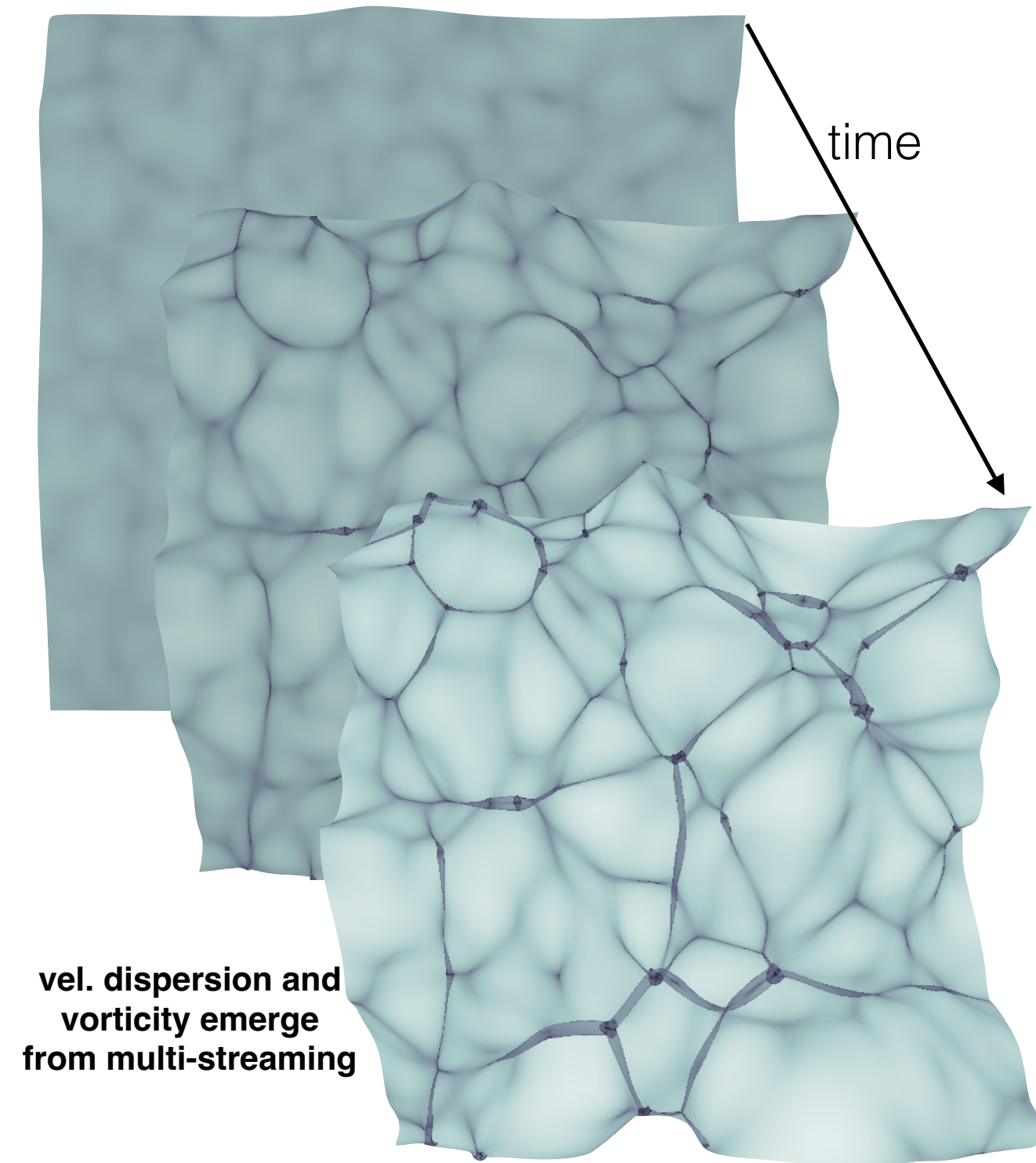
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$$\mathbf{x}'' + \mathcal{H}\mathbf{x}' = -\nabla\phi$$

entering the multi-stream region is non-analytic (only finitely many bounded derivatives)



monokinetic, single-valued
(analytic treatment possible)

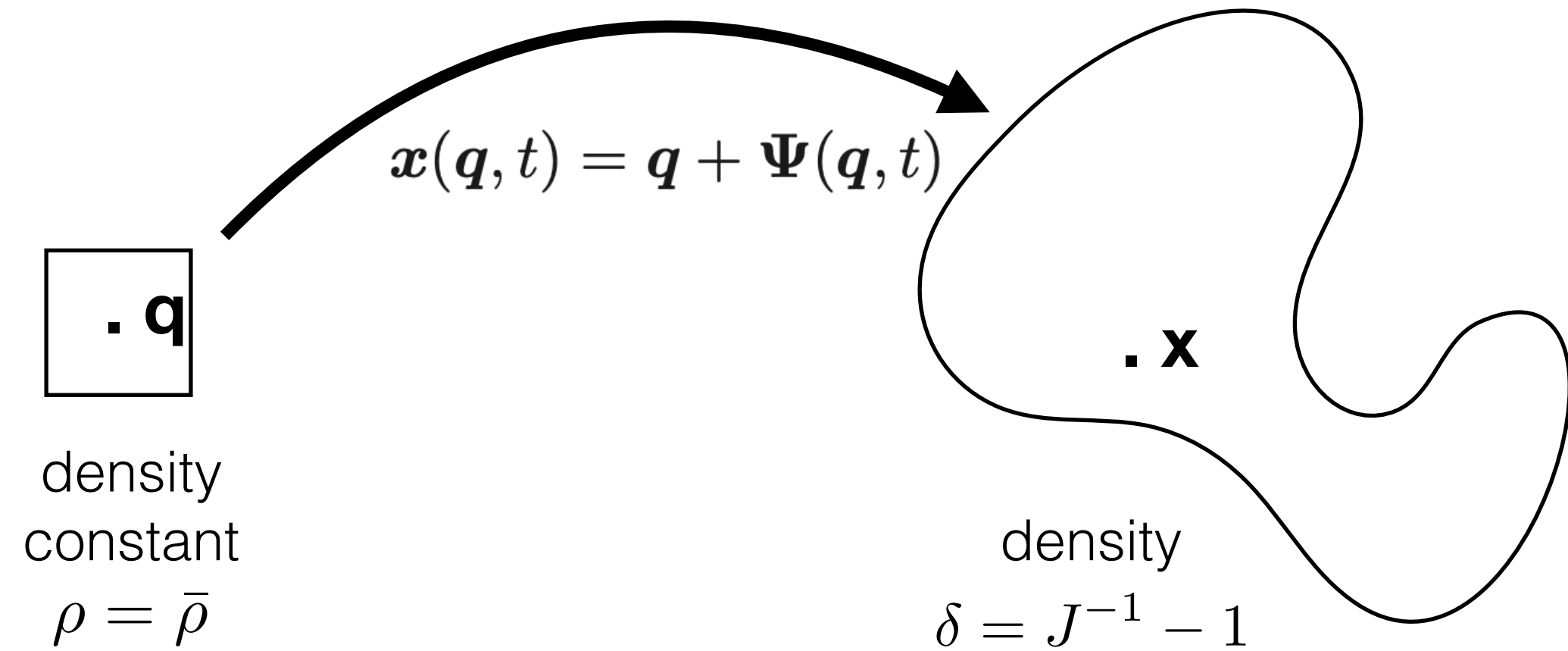
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Modelling LSS — Lagrangian perturbation theory

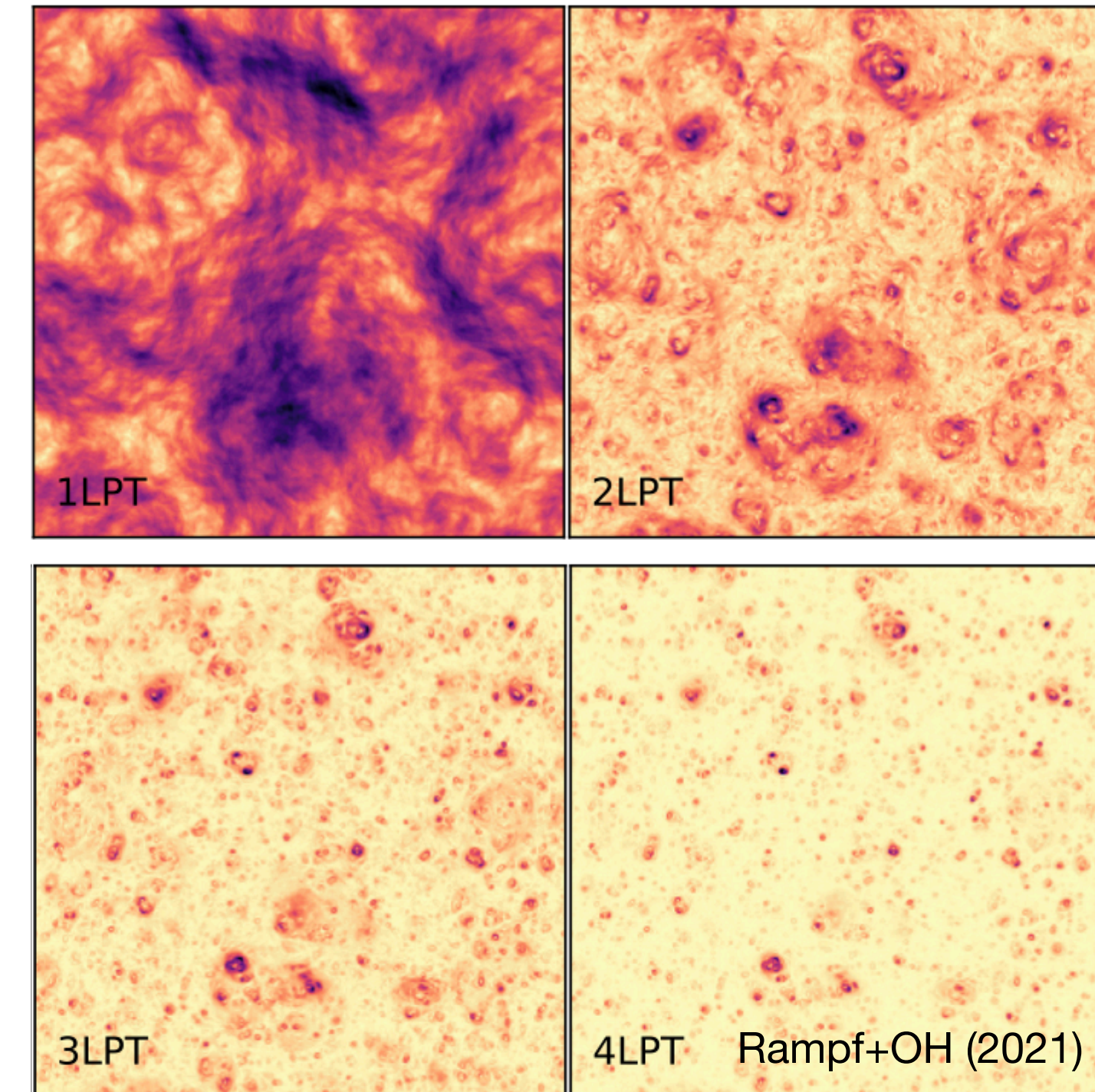
Non-linear evolution of perturbations

Solve Vlasov-Poisson on submanifold characteristics $(\mathbf{q}, t) \mapsto (\mathbf{x}(\mathbf{q}, t), \mathbf{p}(\mathbf{q}, t))$



**all-order recursion
relations first
implemented
in code**

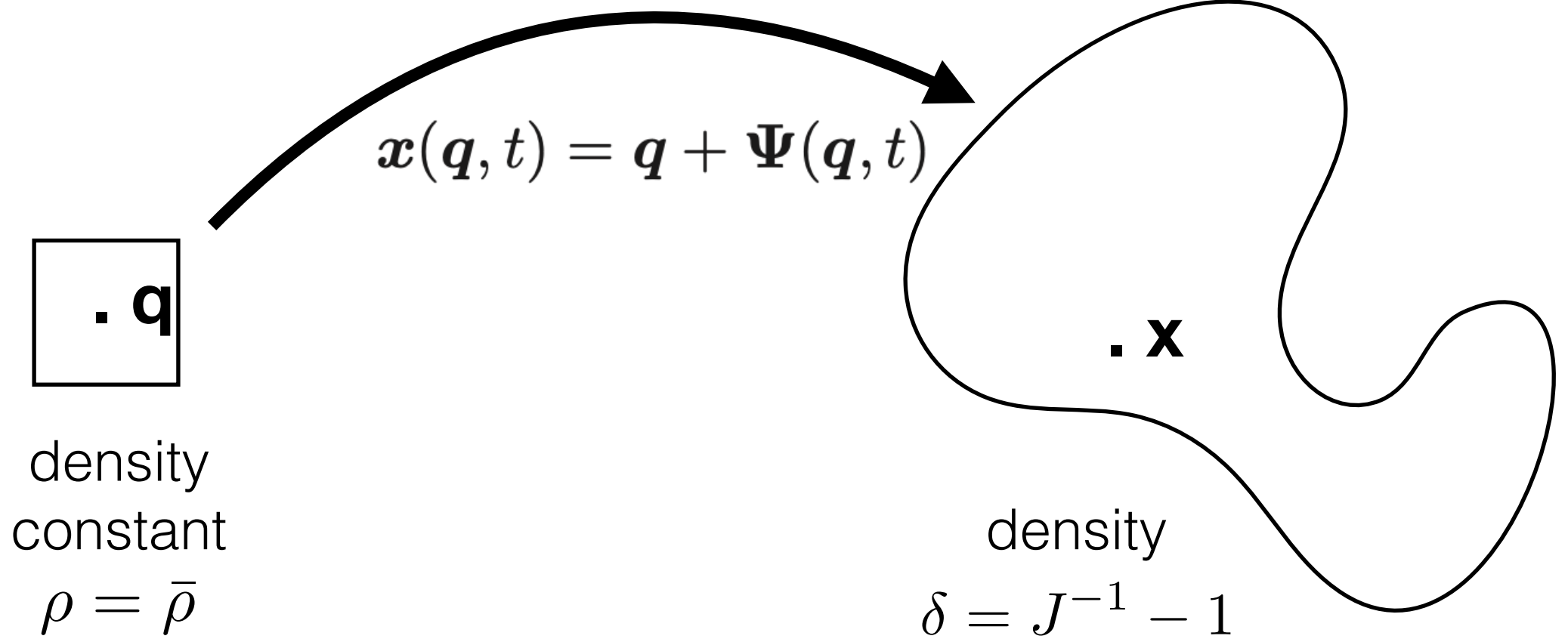
Rampf+OH (2021)
Schmidt (2021)



Modelling LSS – Lagrangian perturbation theory

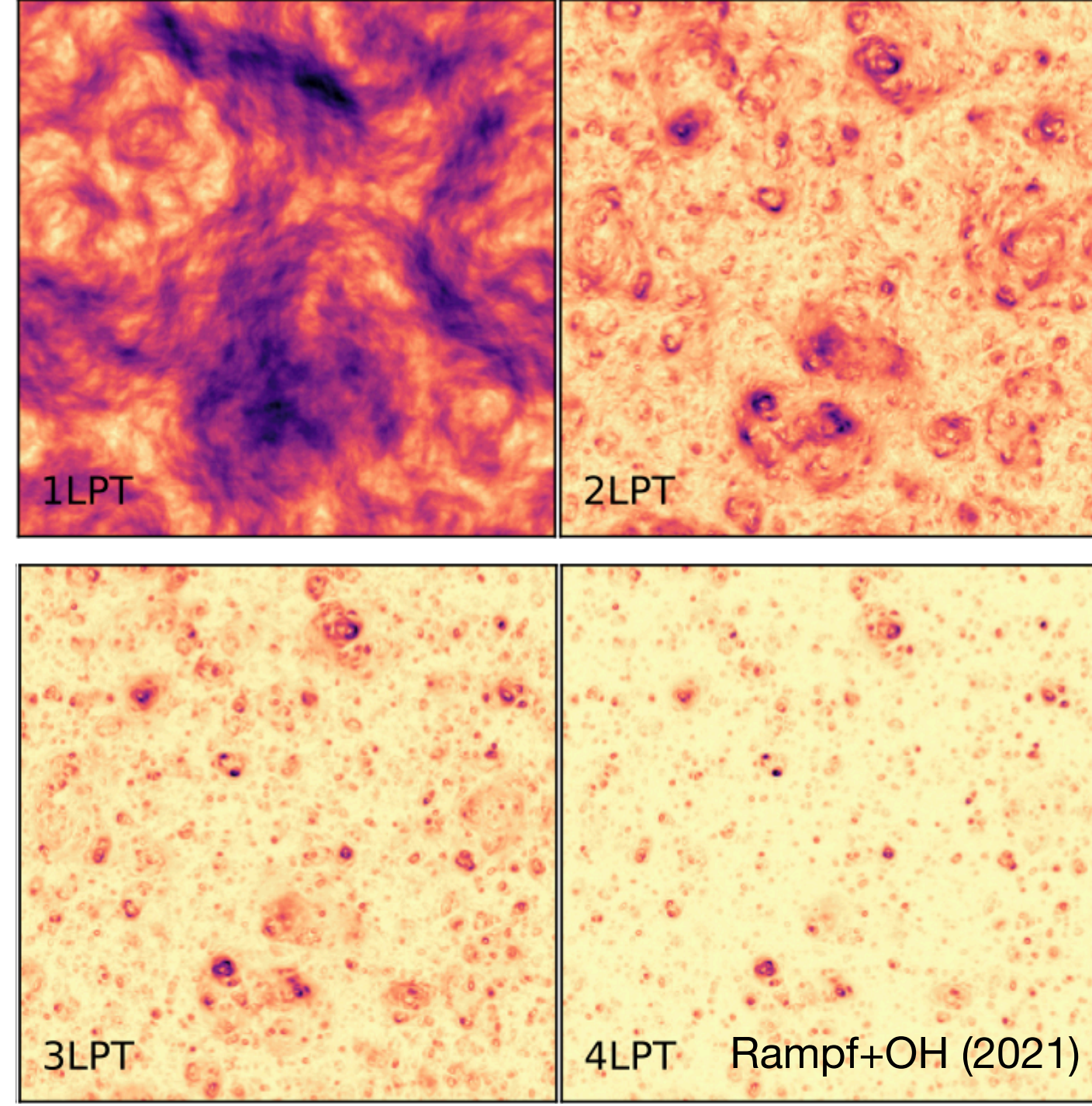
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all-order recursion relations first implemented in code

Rampf+OH (2021)
Schmidt (2021)



We want to solve this as a perturbative series (D is small parameter)

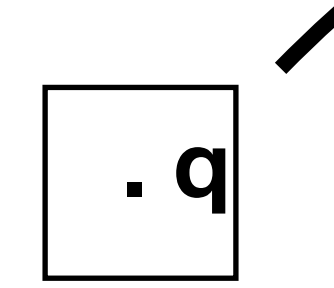
$$\Psi(\mathbf{q}, \tau) = \sum_{n=1}^{\infty} D(\tau)^n \Psi^{(n)}(\mathbf{q})$$

Buchert (1994), Catelan (1995), Bouchet+(1995), n=3
 Rampf (2012), Zheligovsky&Frisch (2014), Matsubara (2015), all order

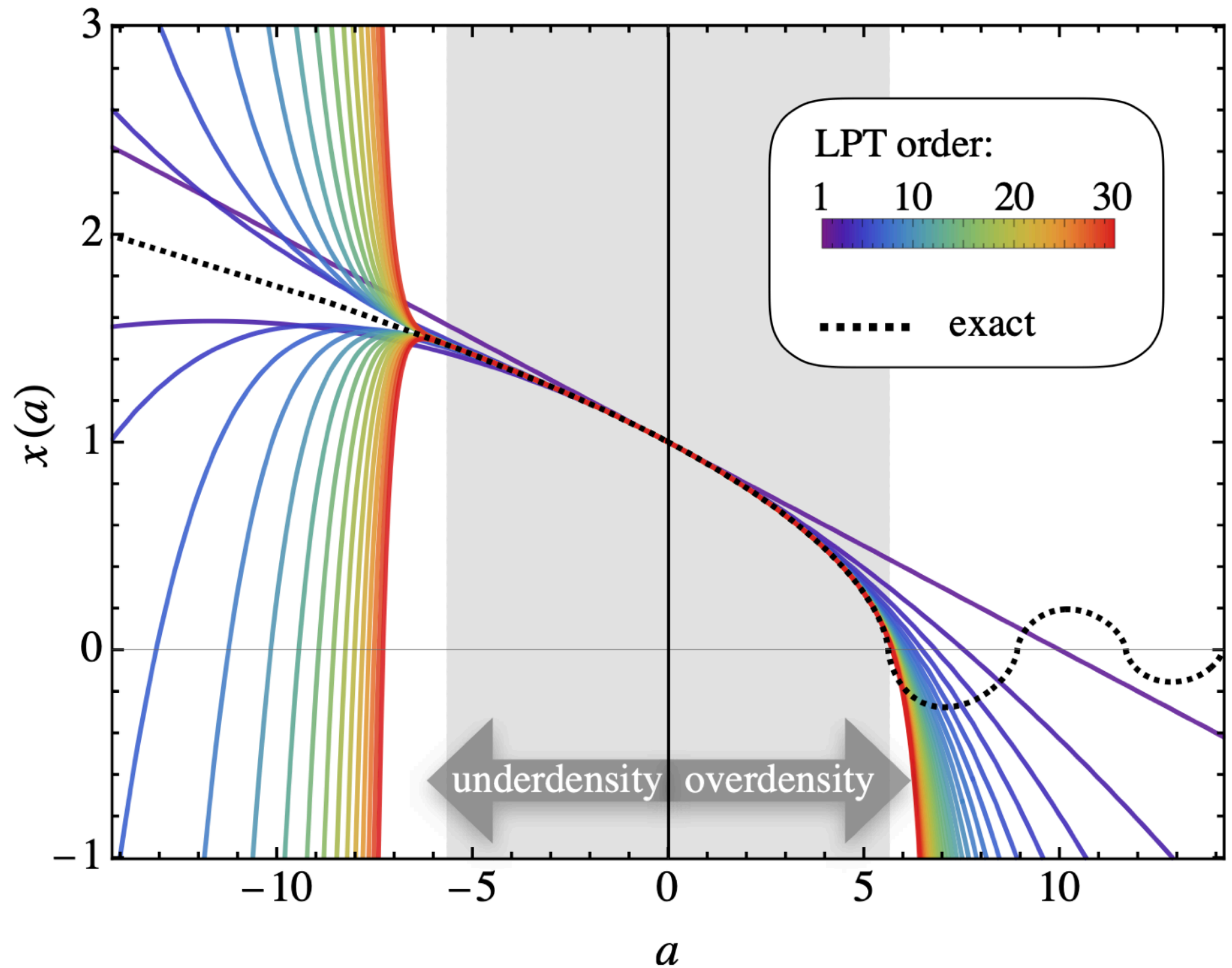
Modelling LSS – Lagrangian perturbation theory

Non-linear evolution of perturbations

Solve Vlasov



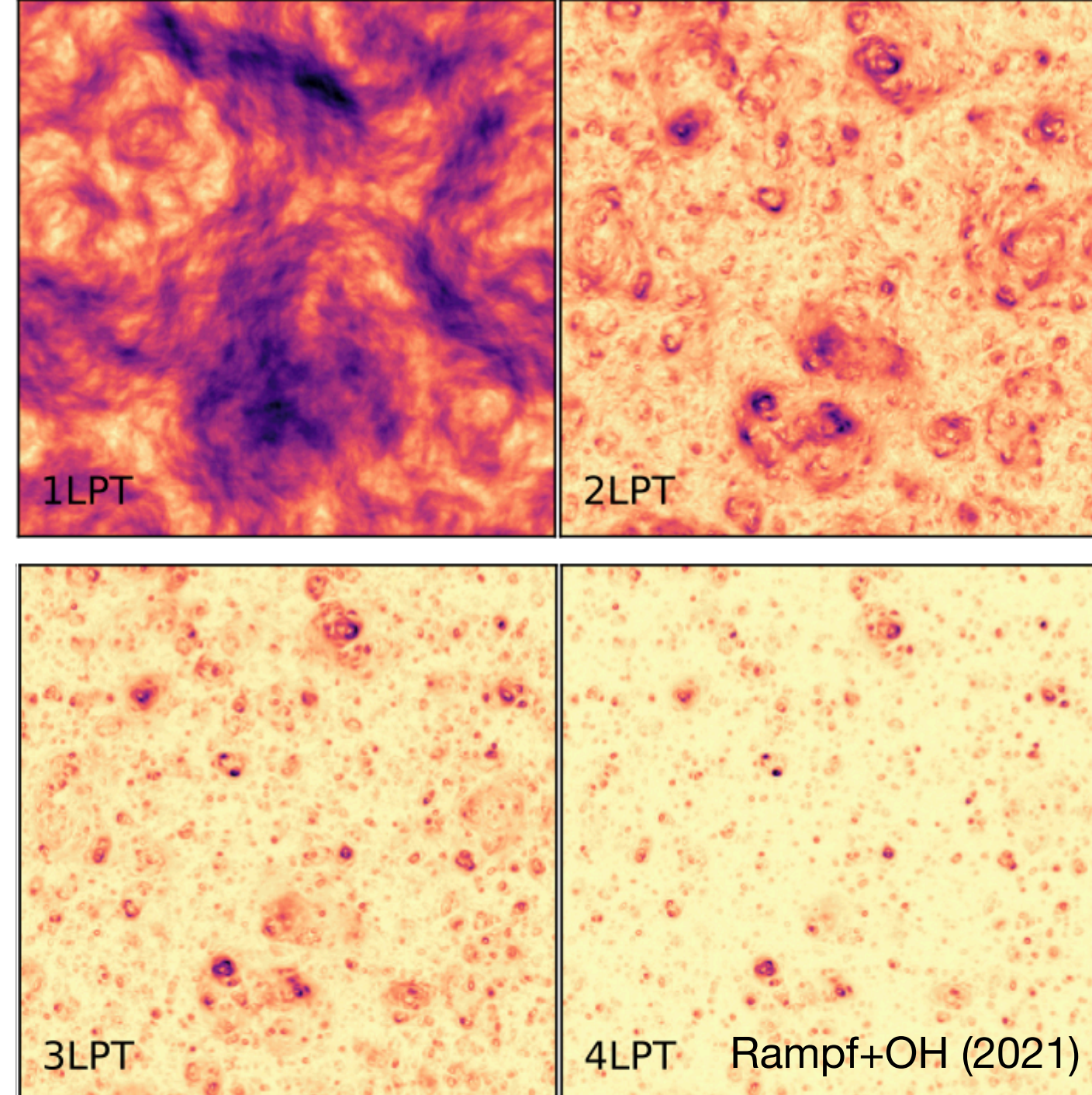
density constant
 $\rho = \bar{\rho}$



$l, t), p(\mathbf{q}, t)$

all-order recursion relations first implemented in code

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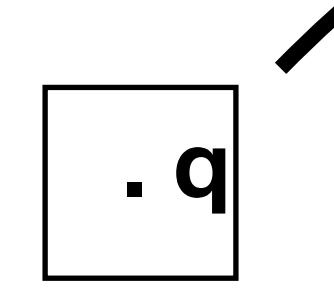
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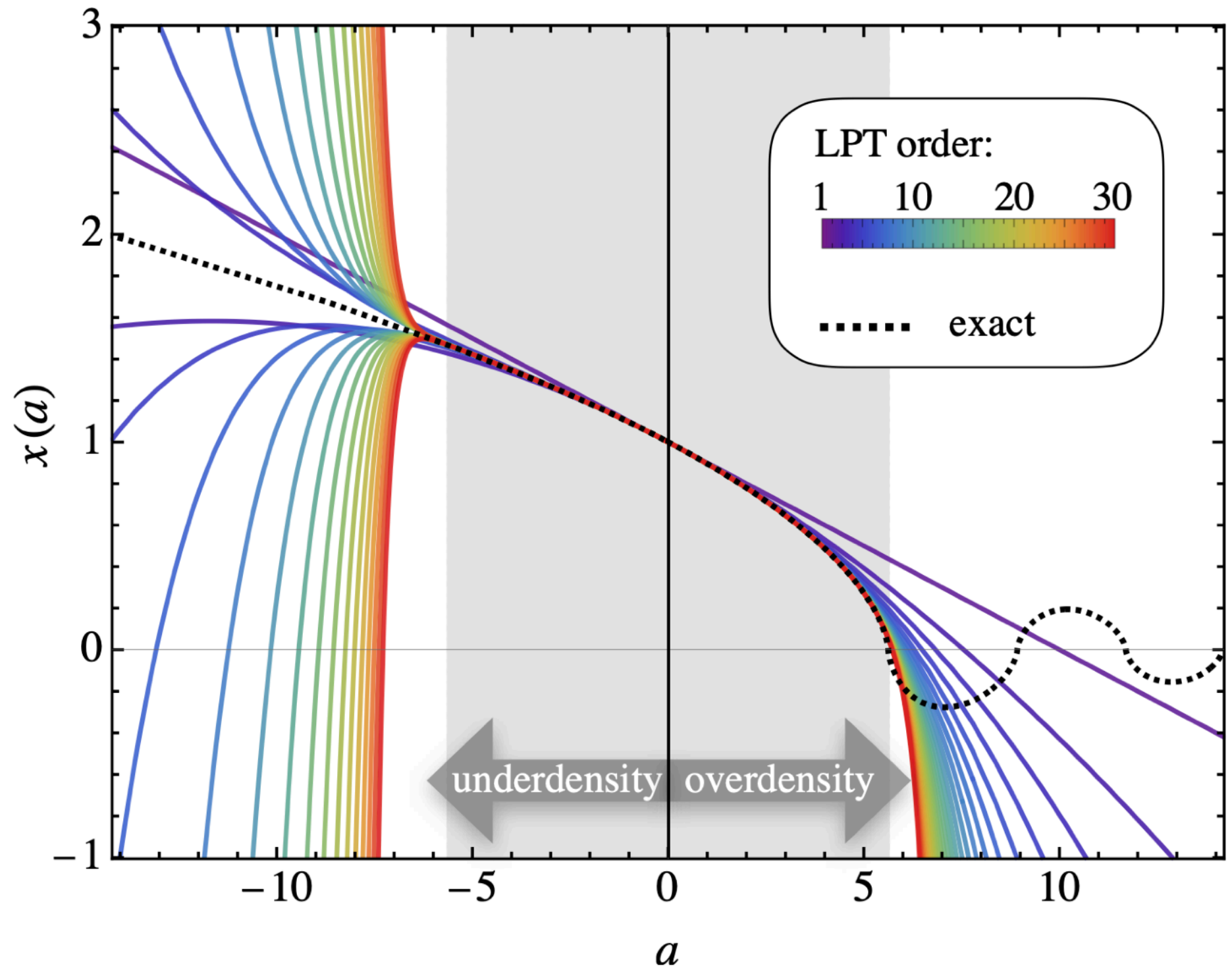
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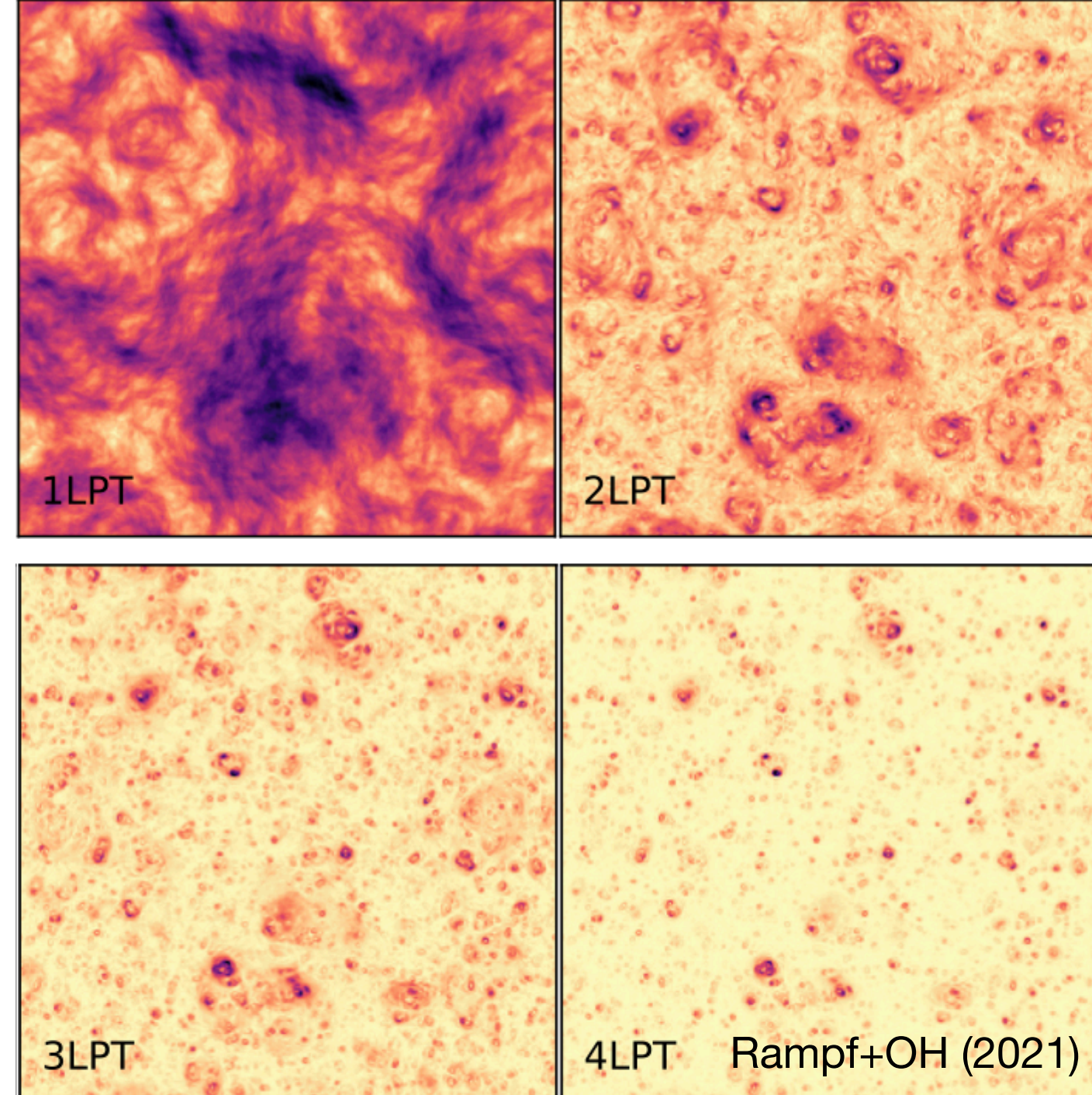
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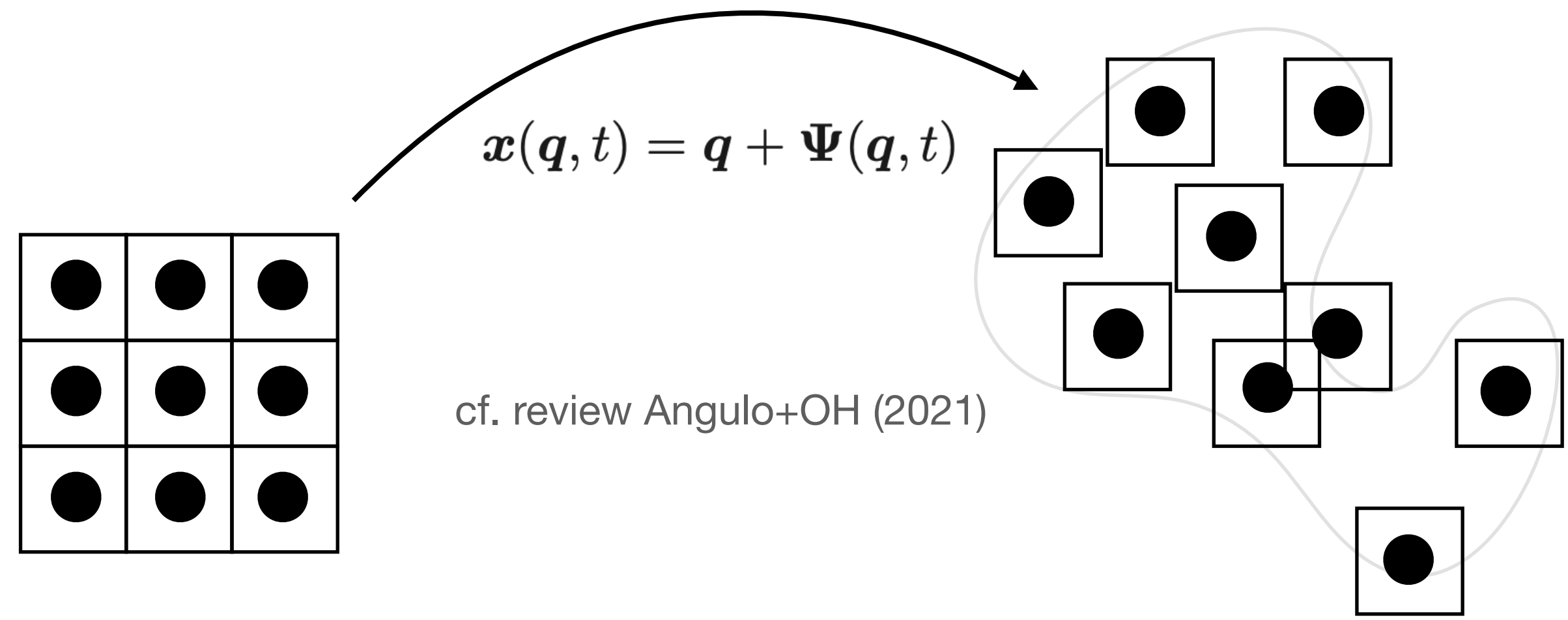
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All order recursion fully implemented in upcoming DISCO-DJ module (stay tuned! List, OH et al (2024, in prep)

Modelling LSS: Numerical N-body simulations

simulation maps discrete fluid elements from Lagrangian space to Eulerian space



the 10^{12} particle frontier:

(from Angulo+OH review)								
Year	Simulation	Code	Supercomputer	Cores [10 ³]	N_p [10 ¹²]	Box [h^{-1} Gpc]	Algorithm	ϵ [h^{-1} kpc]
2014	Dark Sky [916]	2HOT	Titan, USA	20	1.1	8	FMM	36.8
2017	TianNu [469]	CUBEP ³ M	Tianhe-2, China	331	2.97	1.2	PM-PM-PP	13
2017	Euclid Flagship [201]	PKDGRAV3	PizDaint, Switzerland	4	2.0	3.	Tree-FMM	4.8
2019	Outer Rim [917]	HACC	Mira, USA	524	1.07	3.0	Tree-PM	2.84
2019	Cosmo- π [613]	CUBE	π 2.0, China	20	4.39	3.2	PM-PM	195
2020	Ushuu [918]	GREEM	ATERUI-II, Japan	<40	2.0	2.0	Tree-PM	4.3
2020	Last Journey [919]	HACC	Mira, USA	524	1.24	3.4	Tree-PM	3.14

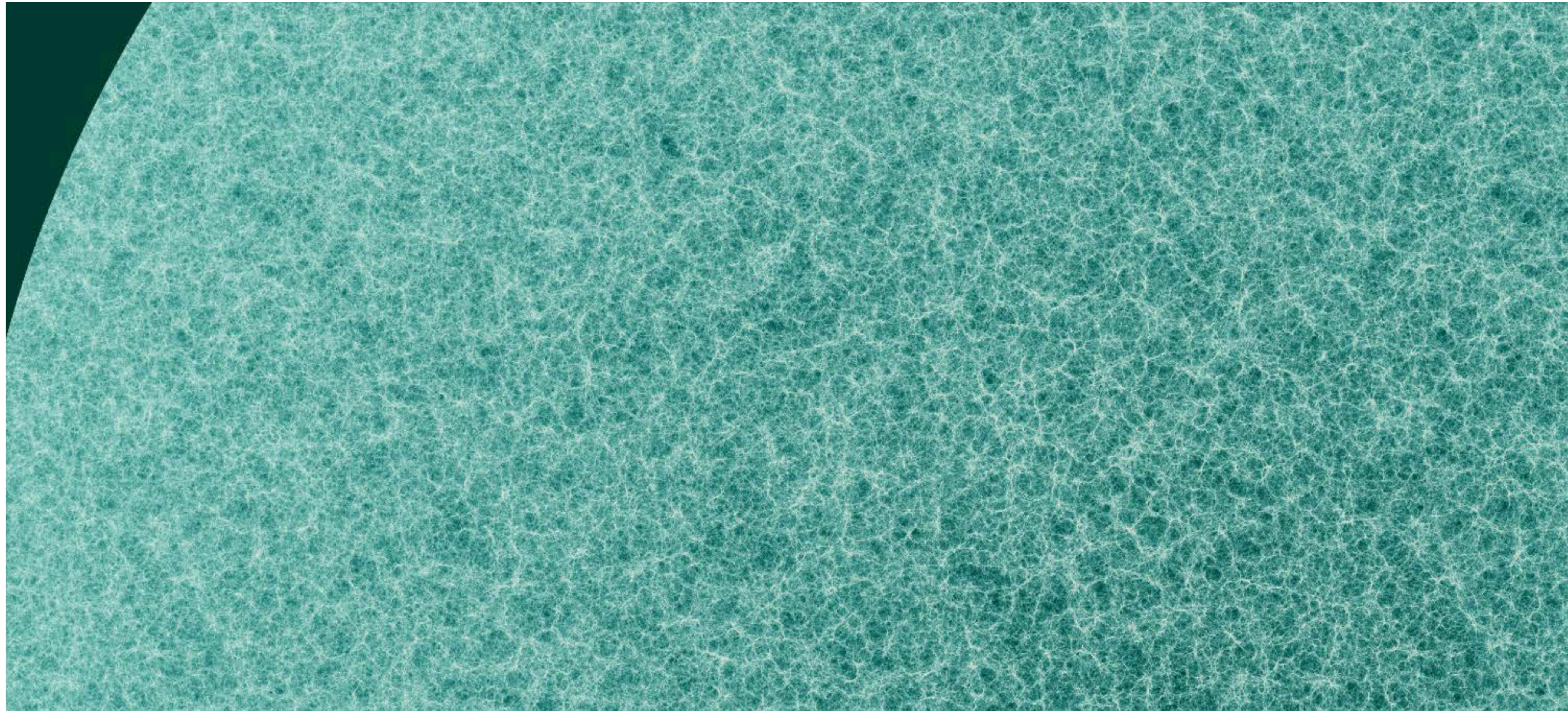
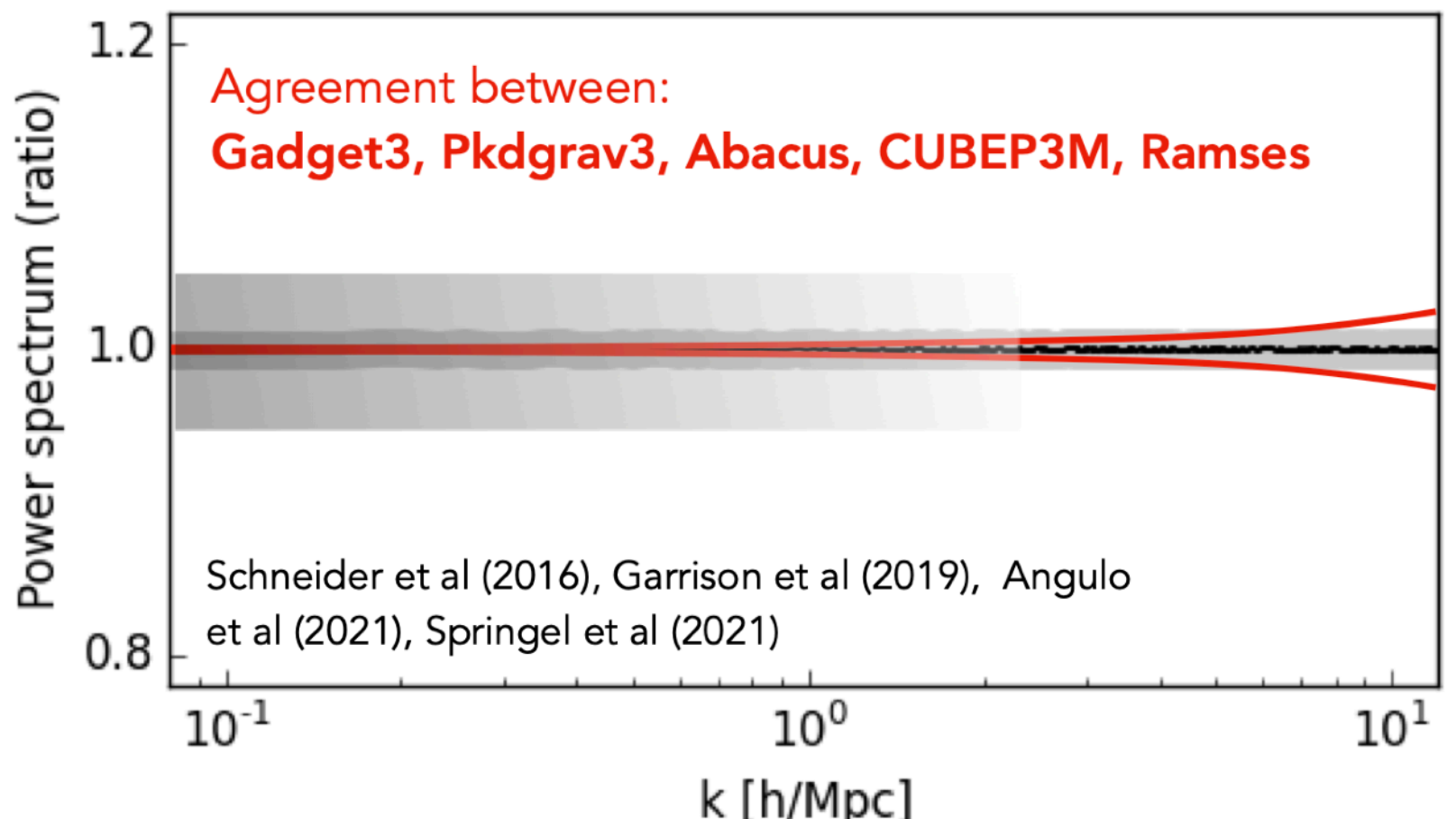
+ Farpoint (2021)

N-body simulations still the main work horse of LSS!

4 π Lightcone from the Euclid Flagship simulation (Potter et al. 2017)

Theory error in non-linear simulations under control (without including astrophysics effects)

Gravity only LCDM predictions for matter distribution in the Universe have essentially no theory error any more



Standard N-body simulations have difficulty reproducing nLPT

Feng+2016: FastPM idea: modify time integrator to get 1LPT agreement

Can do better: second order LPT (2LPT) can be written

$$X_i(D) = X_i^n + [D - D_n] \psi_i^{n,(1)} + [D - D_n]^2 \psi_i^{n,(2)}$$

$$d_D X_i(D) = \psi_i^{n,(1)} + 2[D - D_n] \psi_i^{n,(2)},$$

$$d_D^2 X_i(D) = 2\psi_i^{n,(2)} = \text{const.}$$

i.e. acceleration can be made constant

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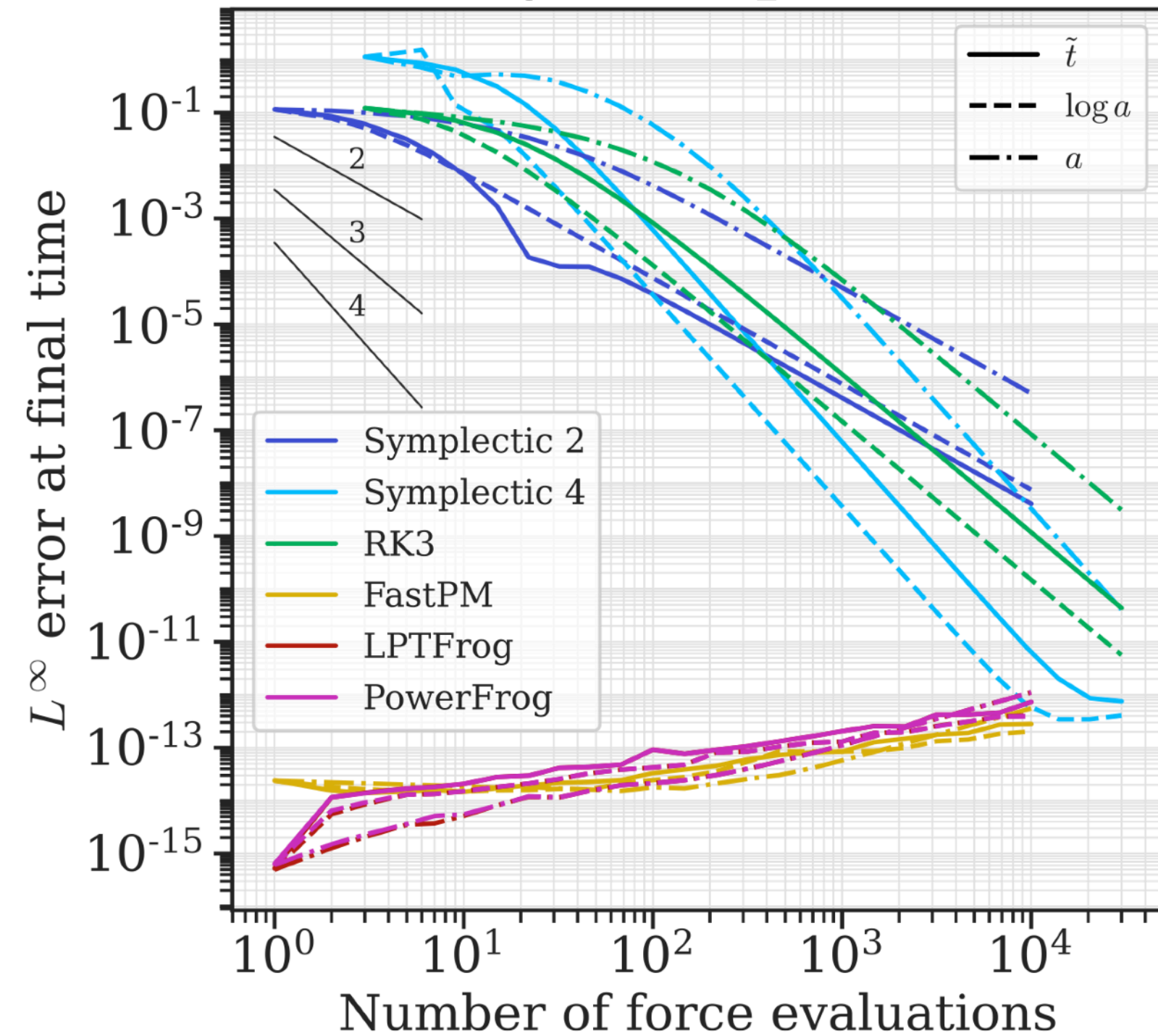
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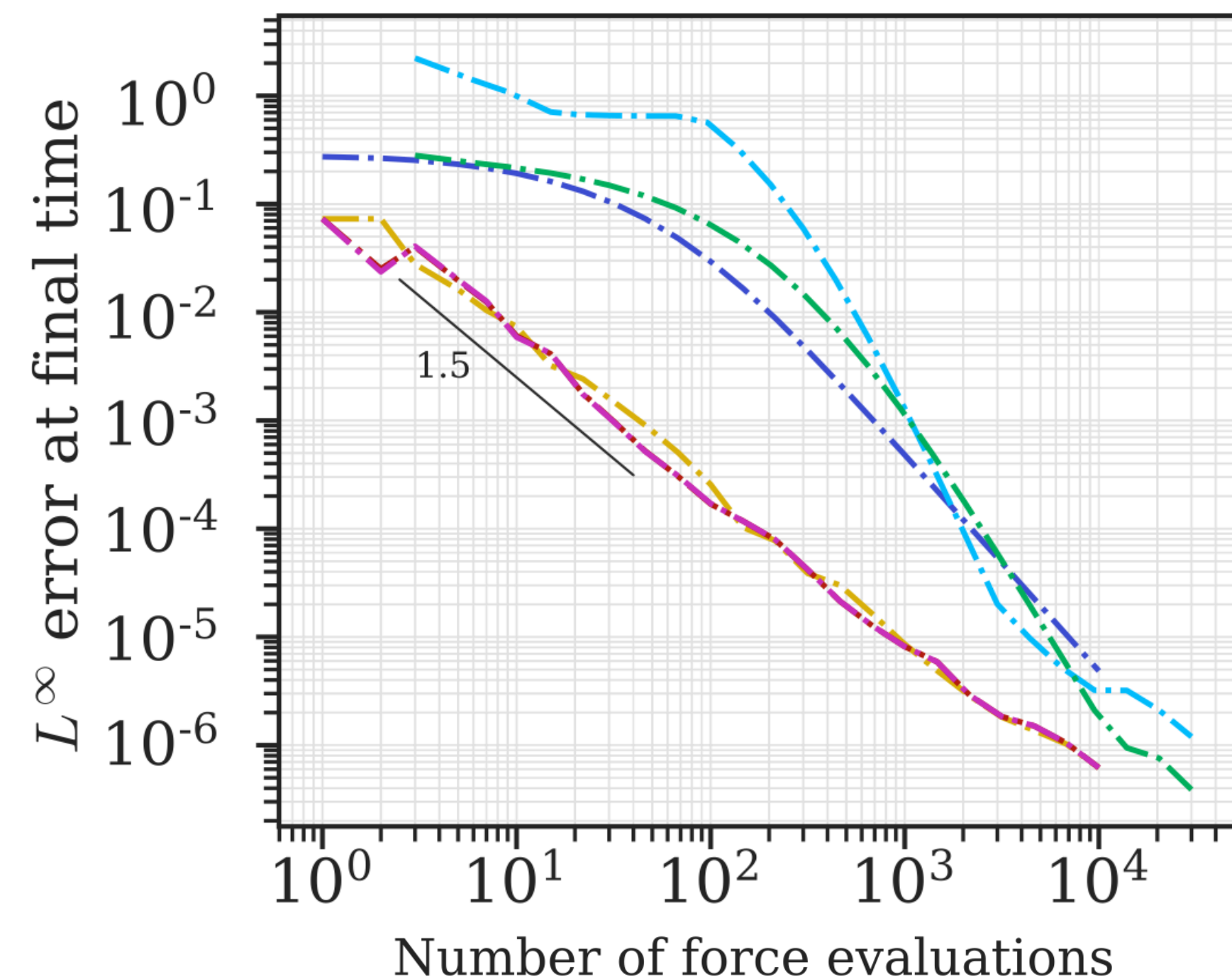
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Tests for 1D collapse

Growing mode plane wave



post shell-crossing:



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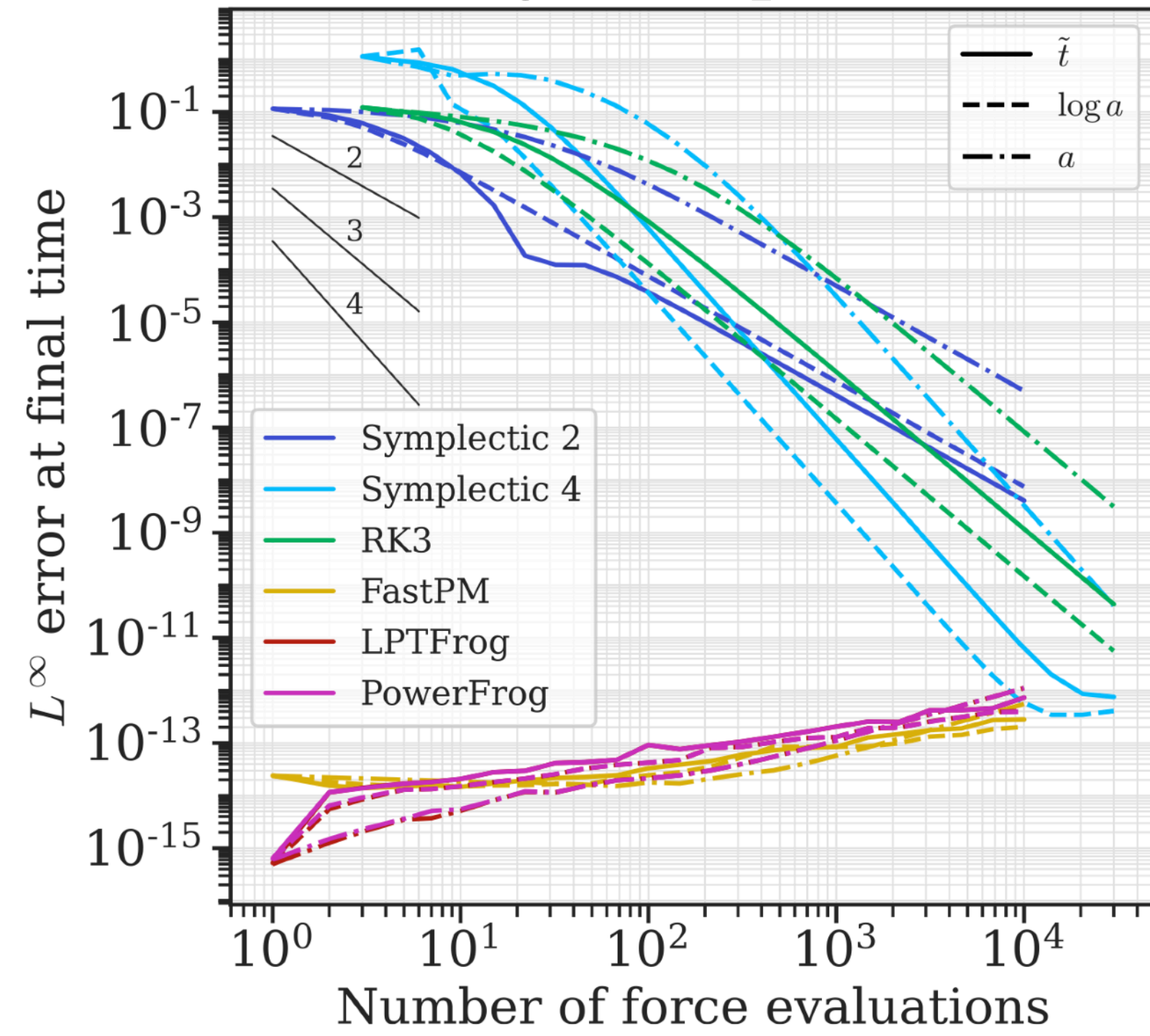
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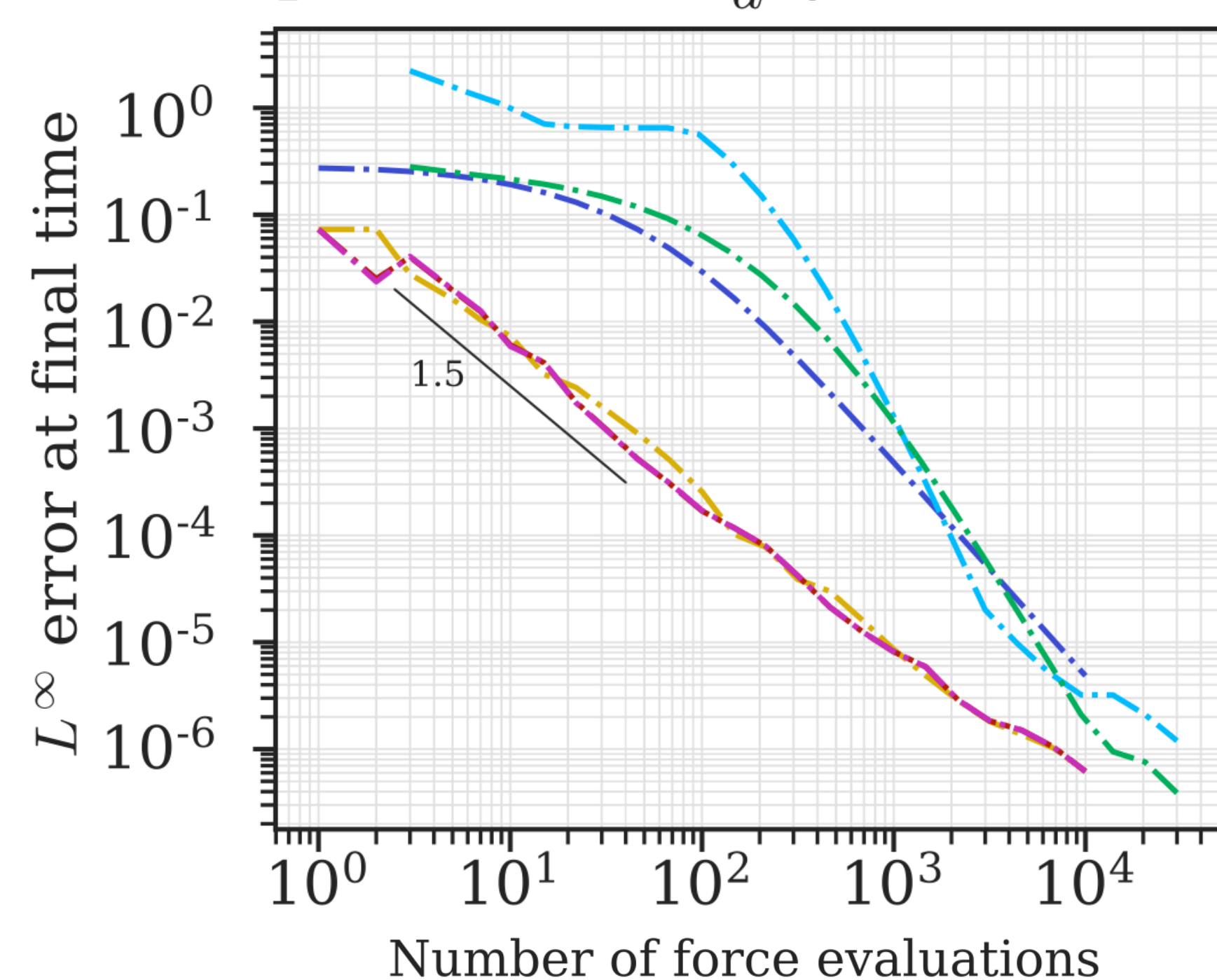
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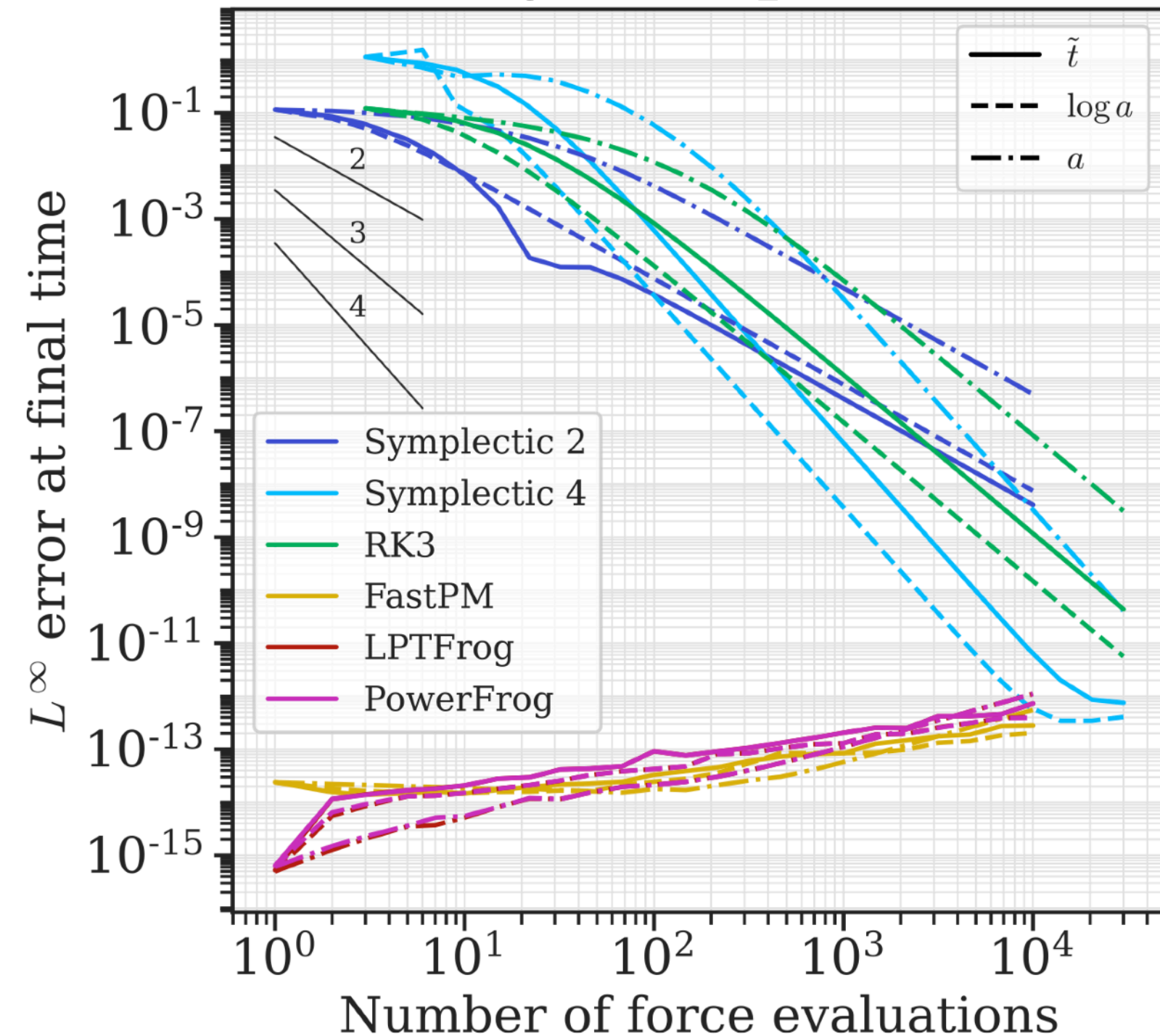
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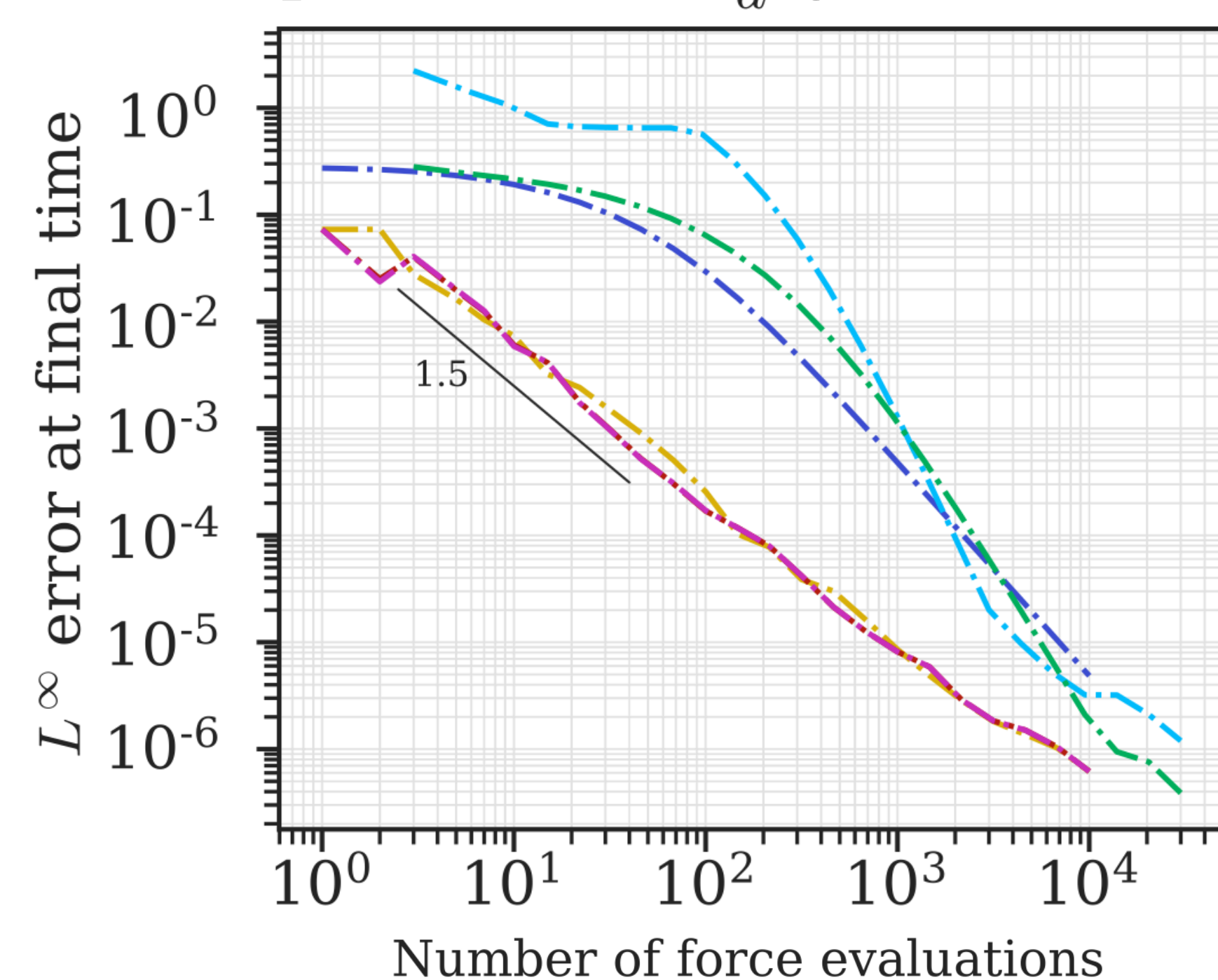
Tests for 1D collapse

Rampf, List & OH 2024, in prep.

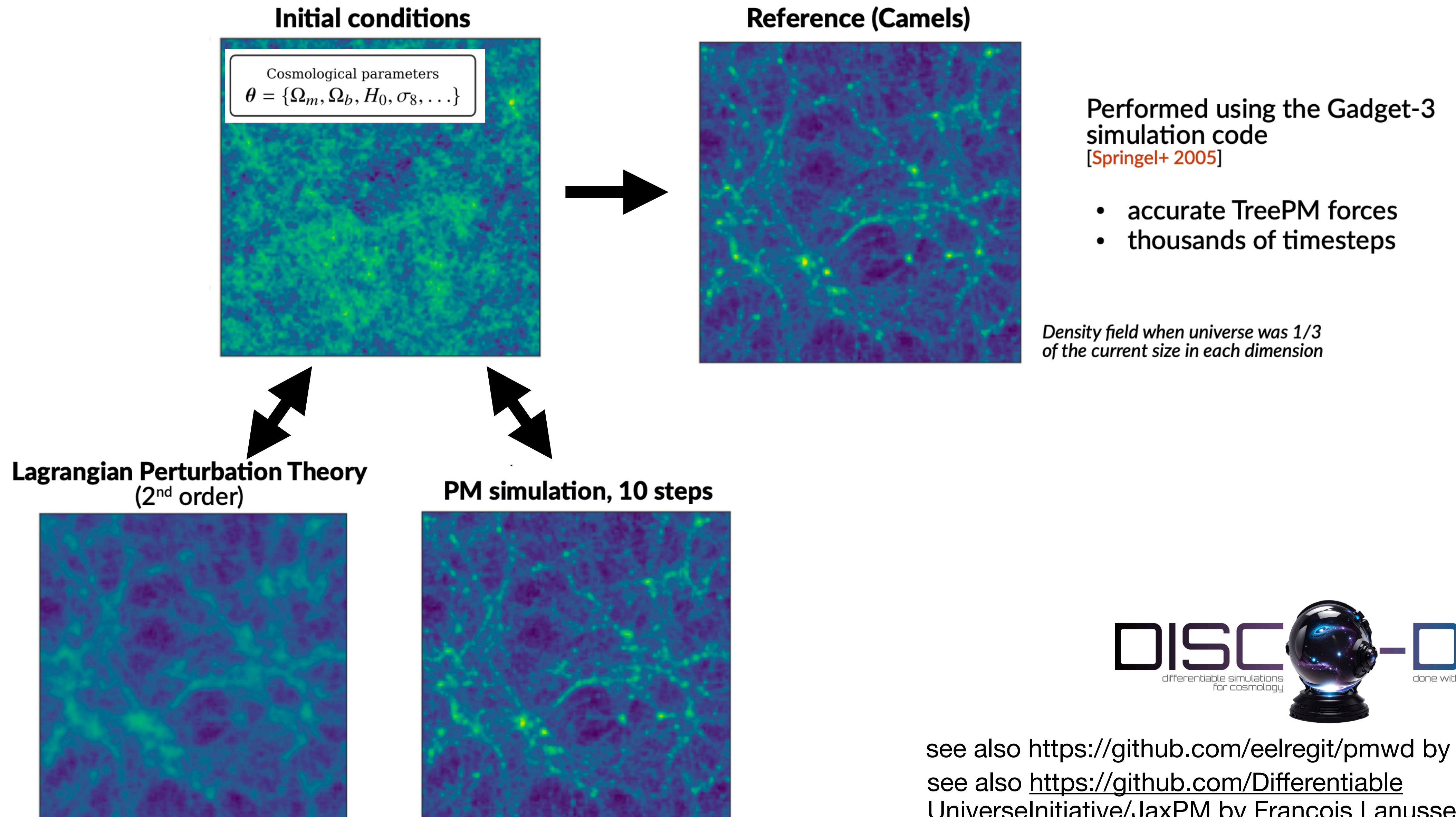
Growing mode plane wave



post shell-crossing:



Comparison of methods

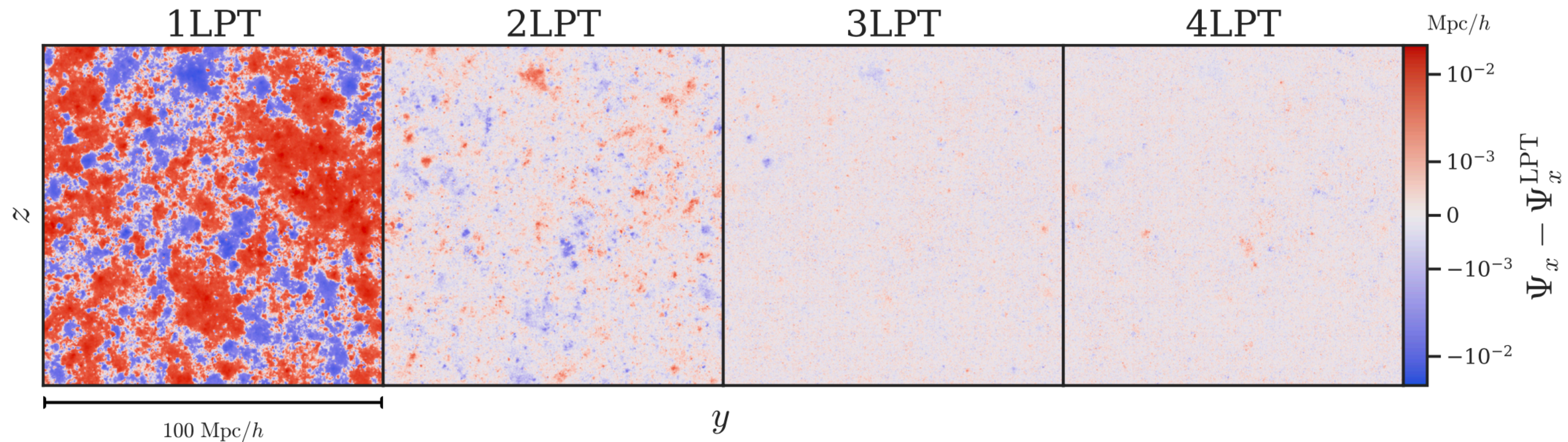


see also <https://github.com/eelregit/pmwd> by Yin Li
see also <https://github.com/DifferentiableUniverseInitiative/JaxPM> by François Lanusse et al
see also FlowPM by Seljak & collaborators

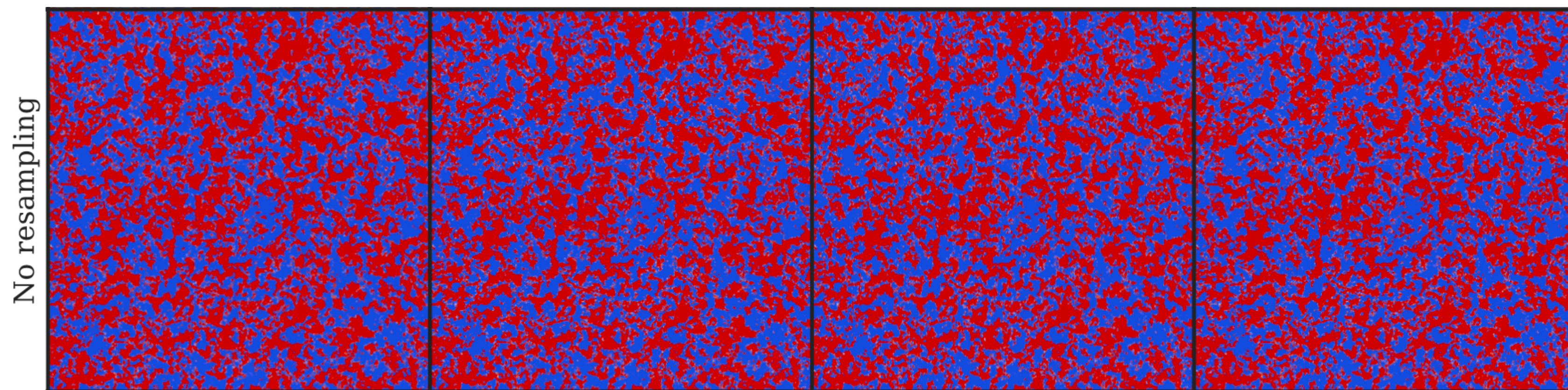
Unifying LPT and N-body...(but UV-complete!)

PowerFrog integrator is asymptotically consistent with 2LPT for $a \rightarrow 0$, so can start at $a=0$ as we do in LPT

Residual of single PowerFrog step from $a=\infty$ to $a=0.05$, wrt. nLPT:



This is only possible after controlling **all** discreteness effects in the N-body simulation, otherwise:

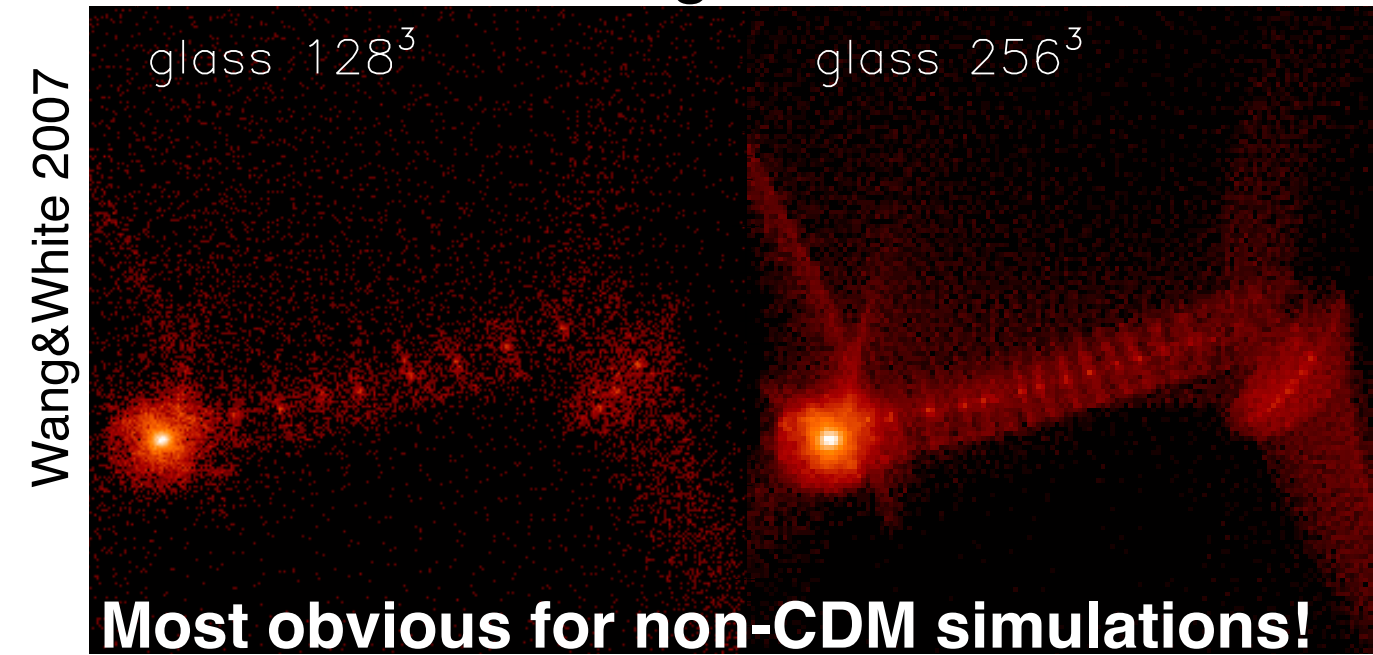


Towards the fluid limit for dark matter modelling

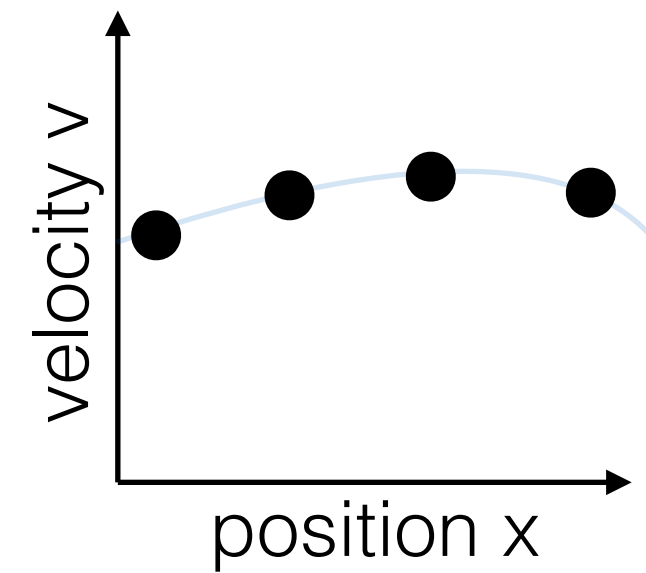
Curing Discreteness Noise in N-body and Fragmentation

spurious fragmentation is well-known phenomenon in N-body sims with cut-off

“Beads-on-a-string” in WDM simulations



N-body just have particles

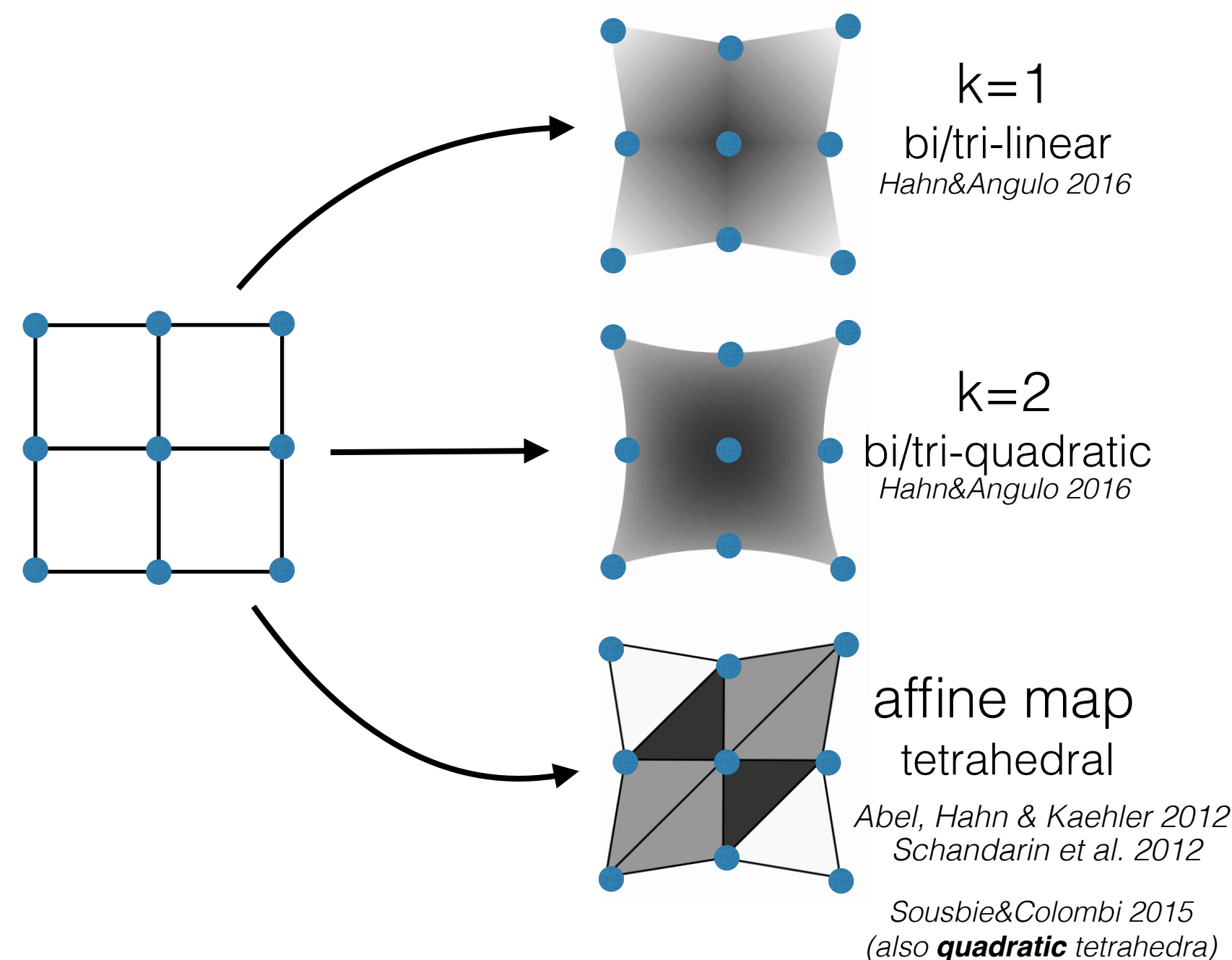
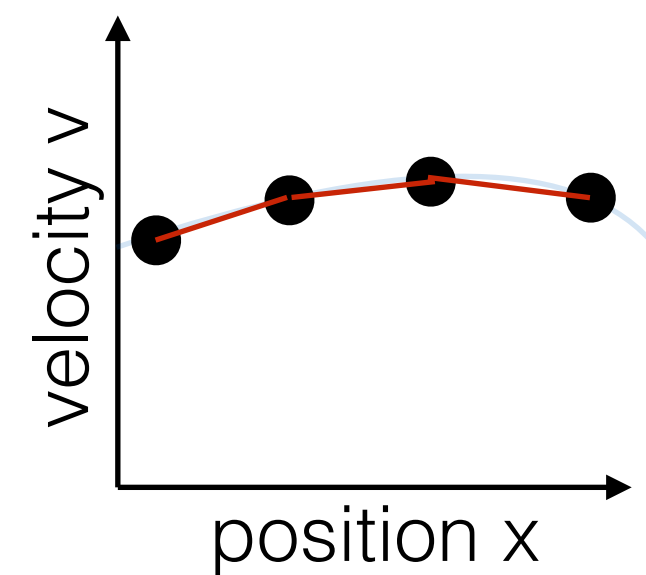


In >1 dim: multivariate maps

Abel, Hahn & Kaehler 2012

Schandarin et al. 2012

now: connect particles
by interpolating functions

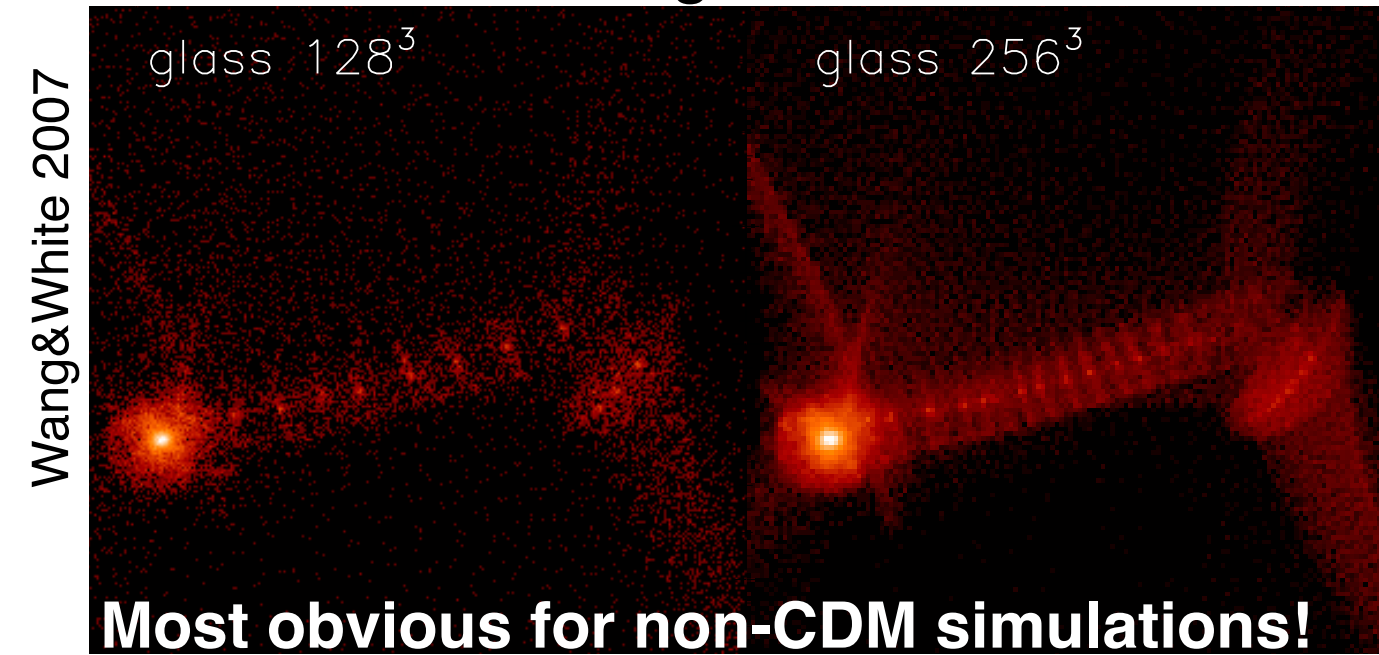


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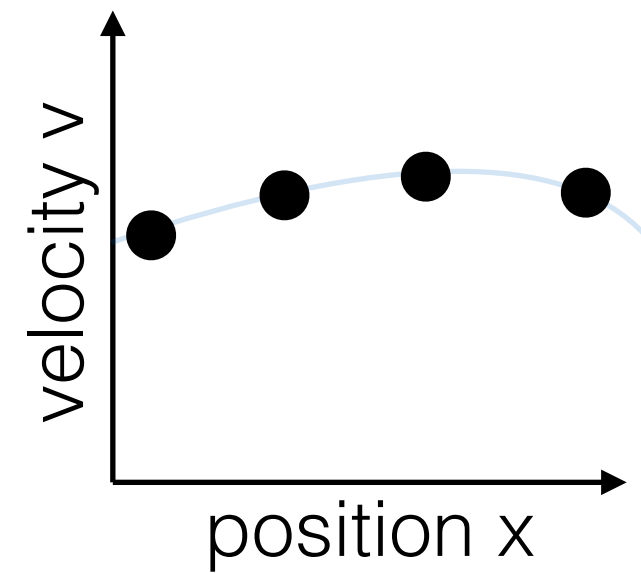
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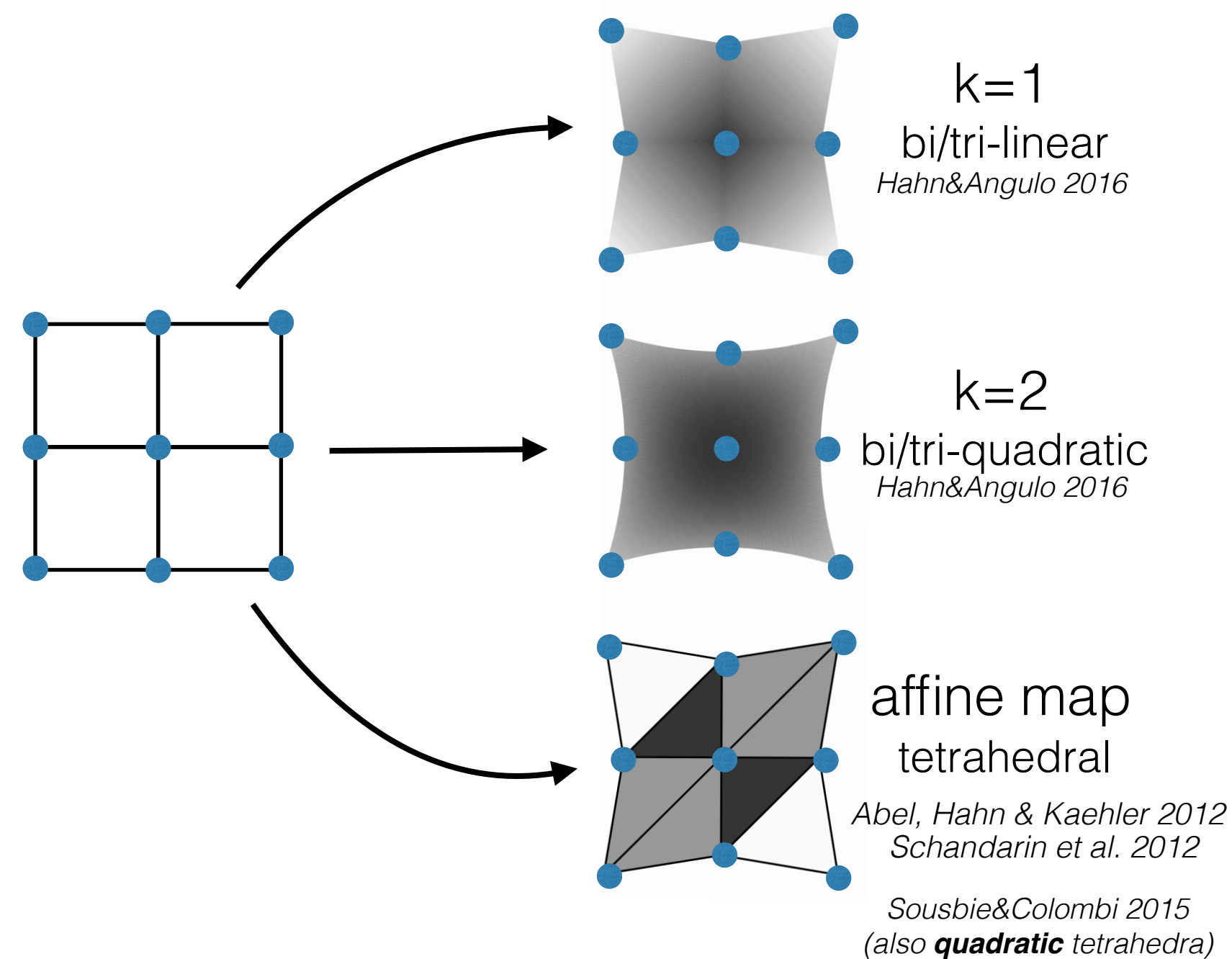
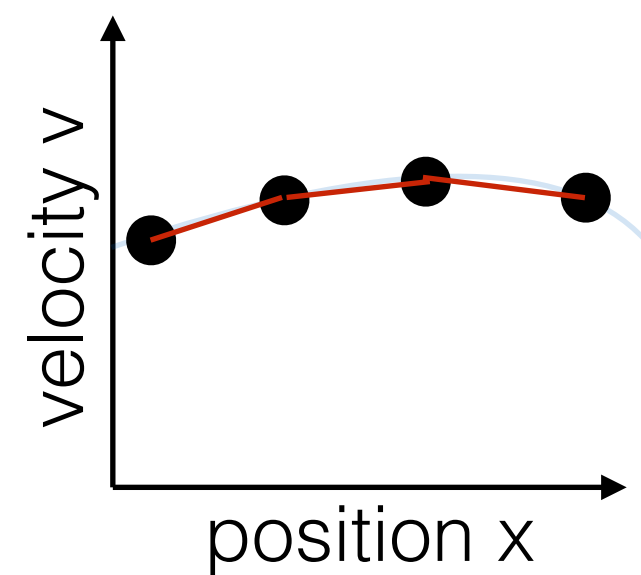
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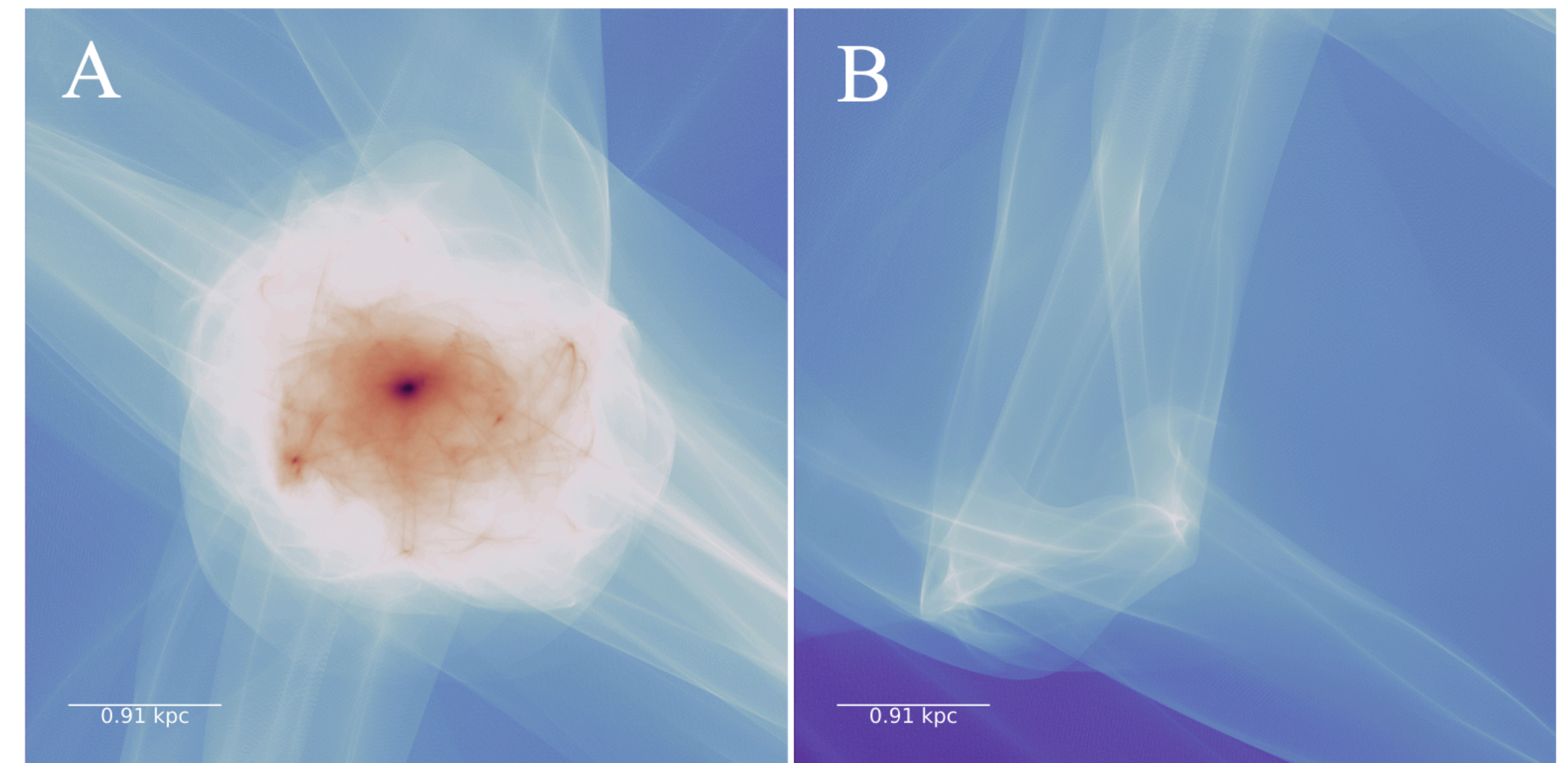
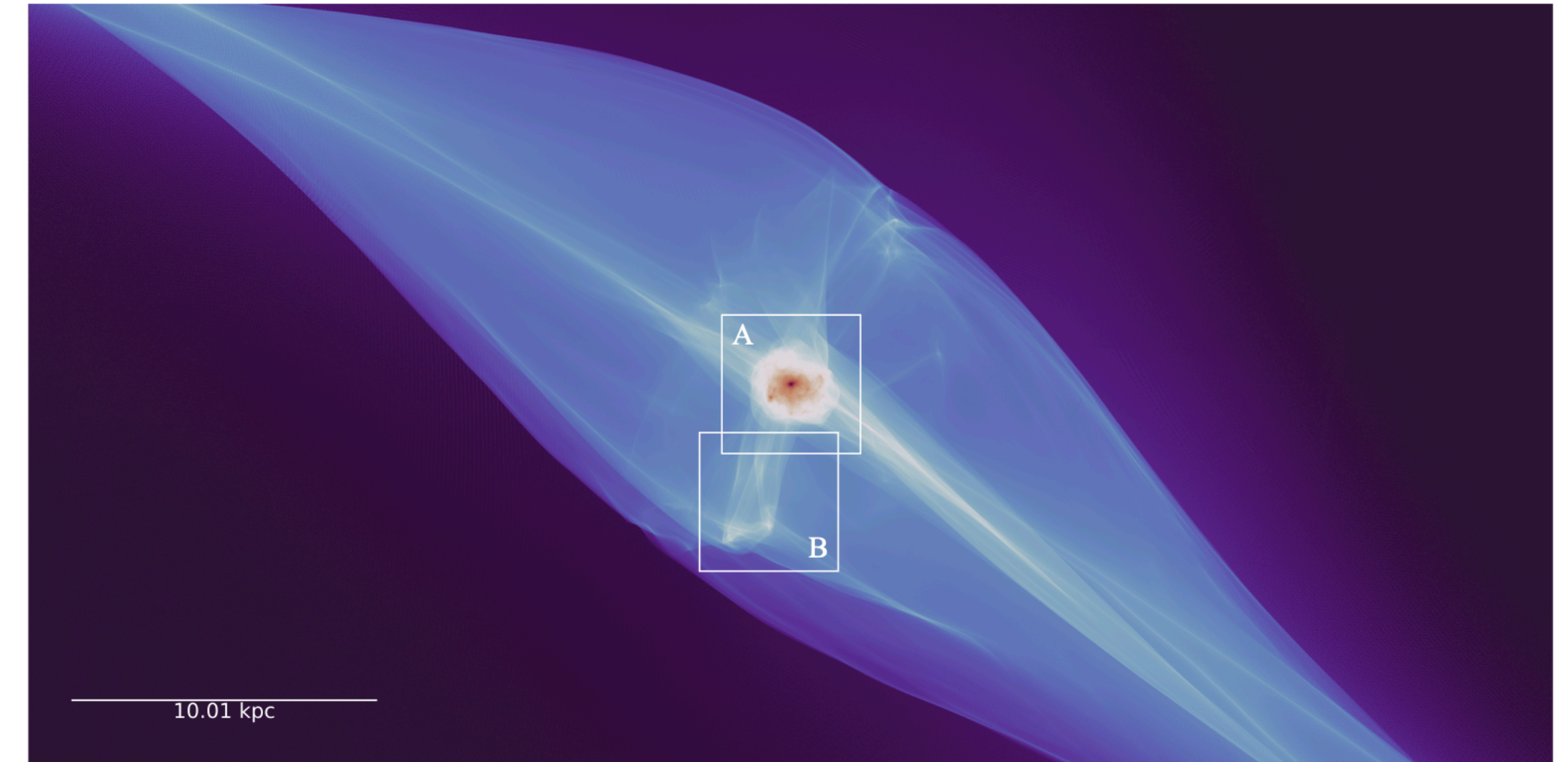
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Latest incarnation of sheet-based simulations of prompt CDM cusps (deviations from NFW of first gen. haloes)



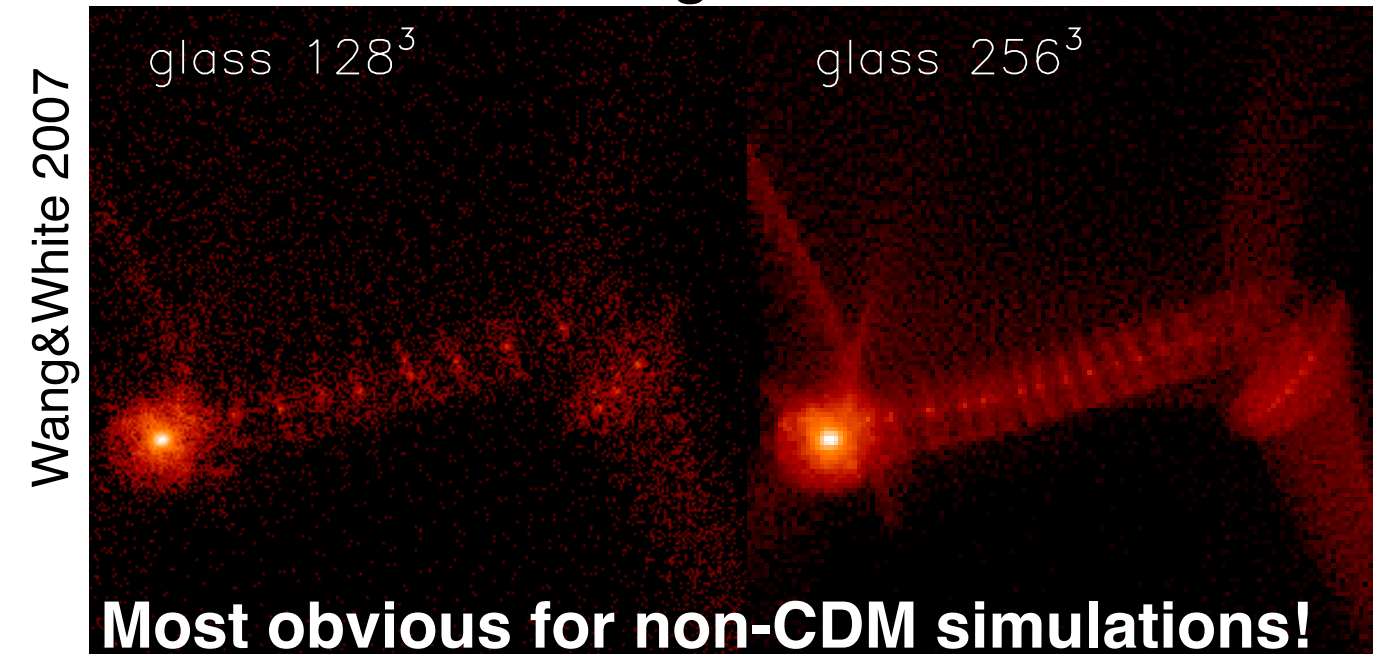
Ondaro-Mallea et al. 2023

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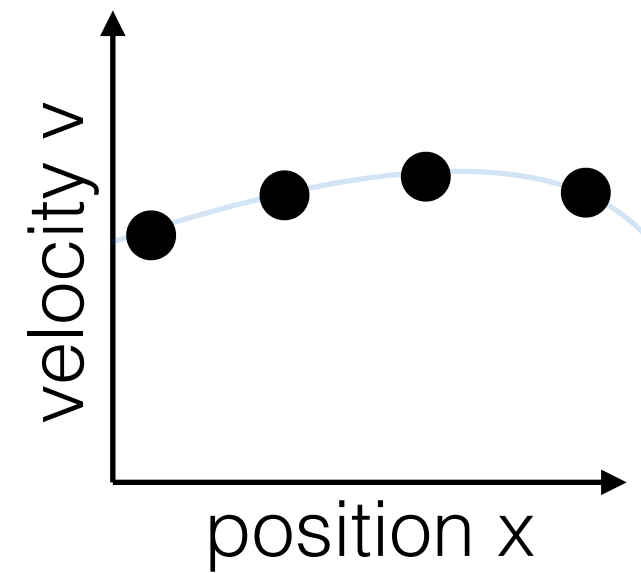
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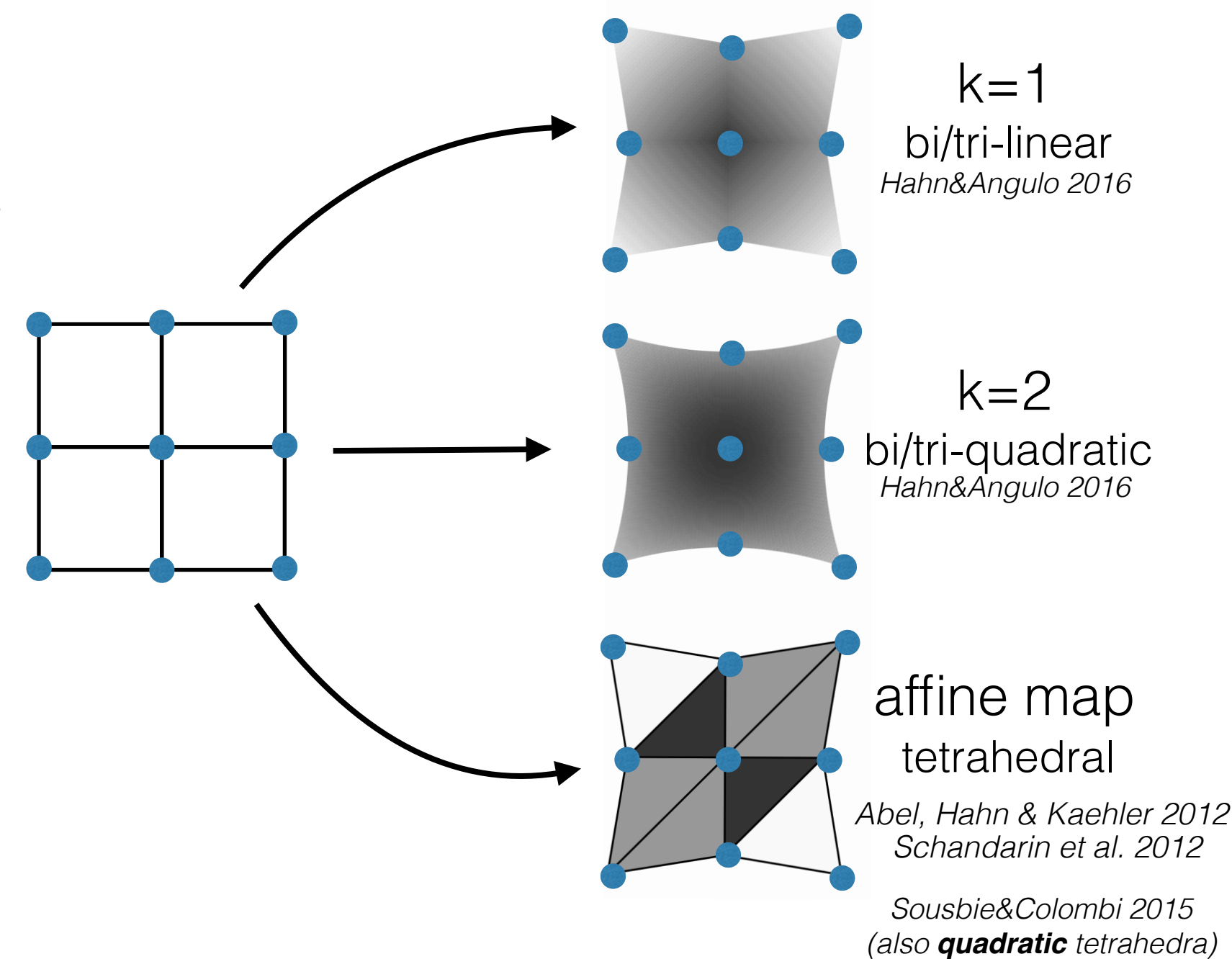
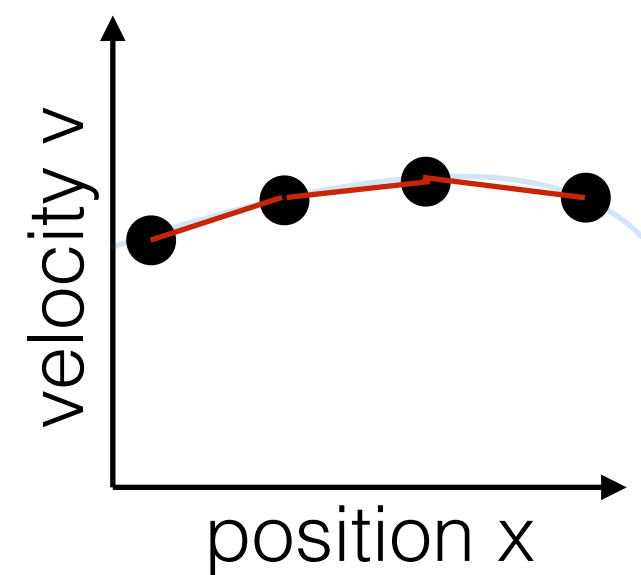
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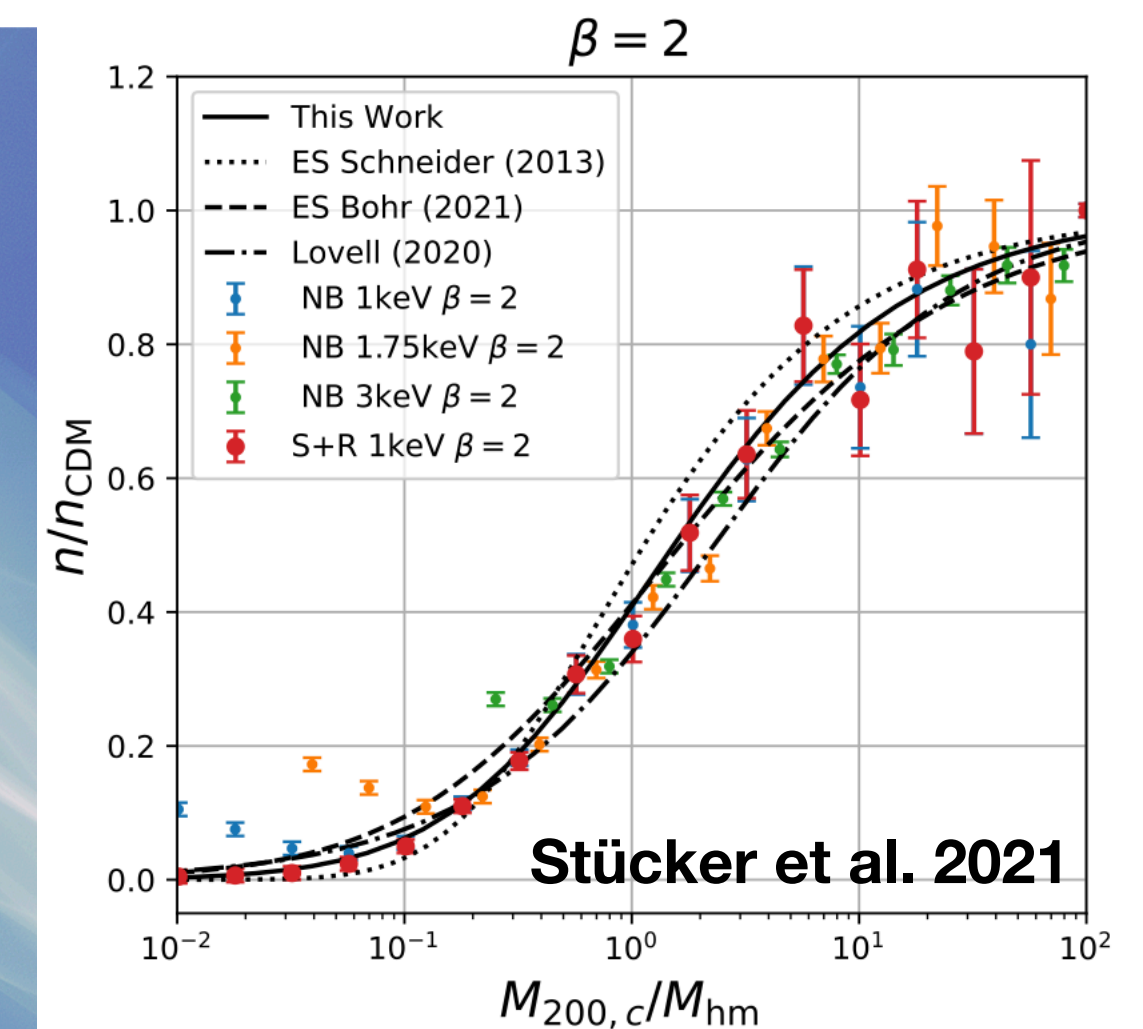
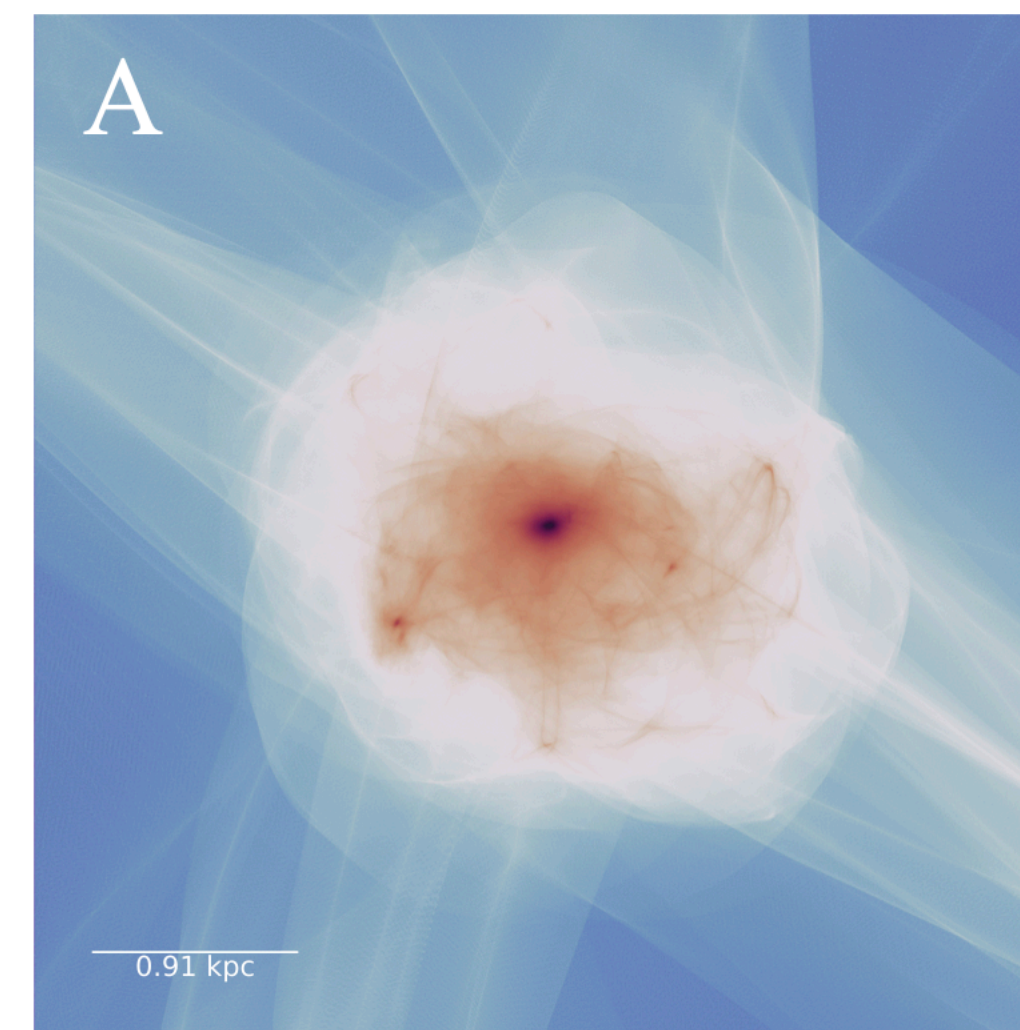
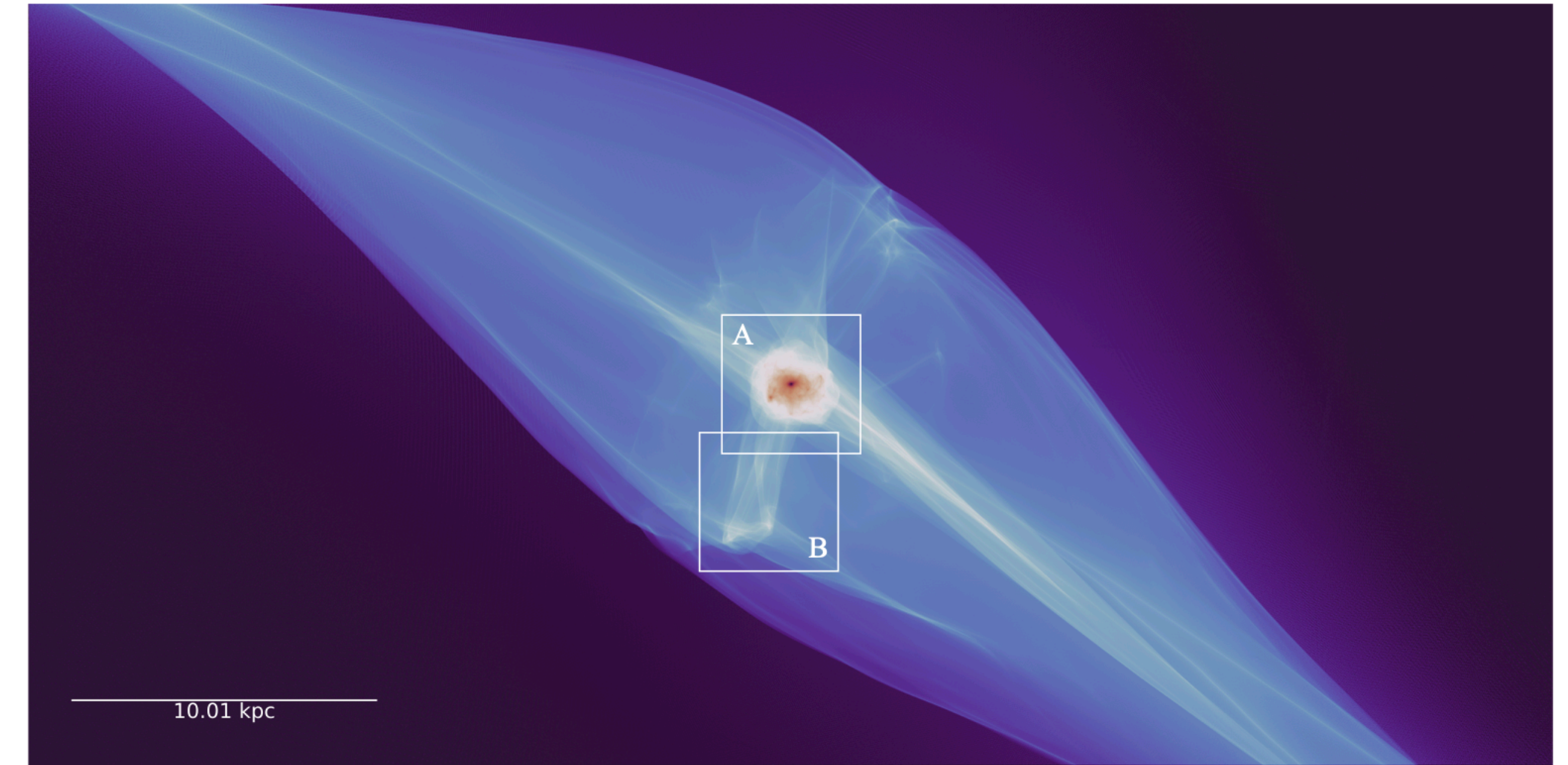
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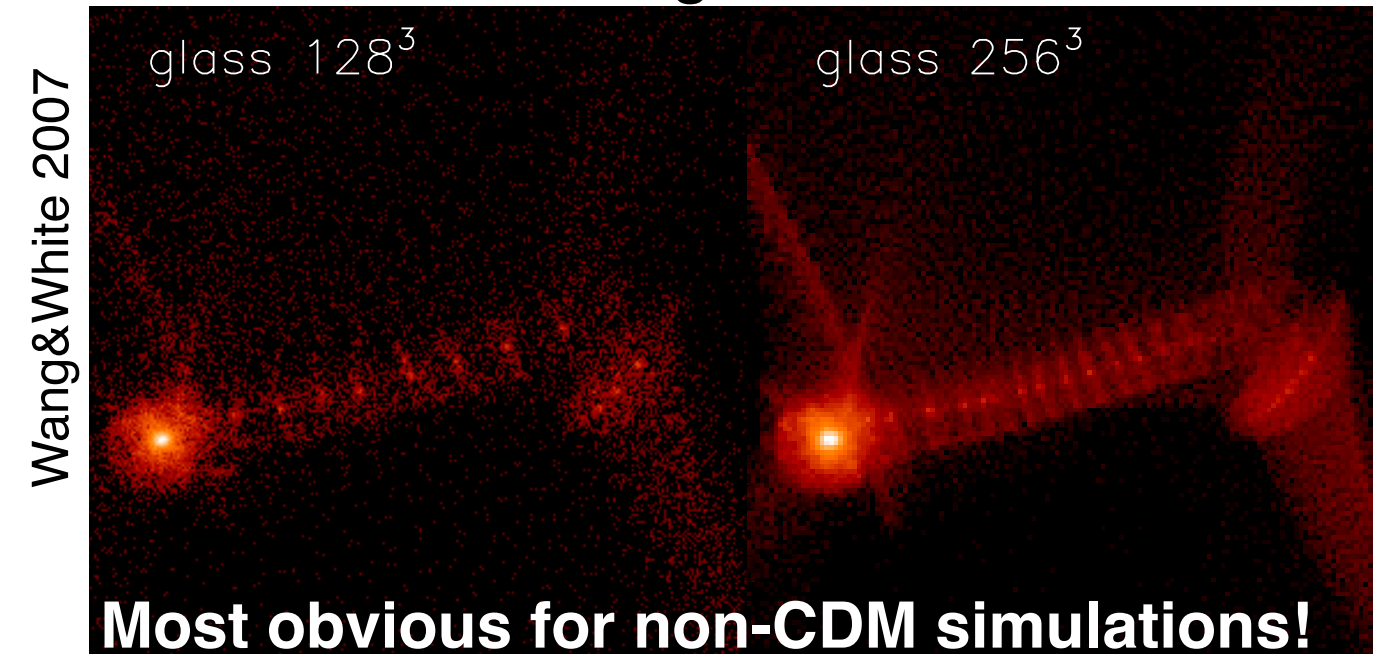
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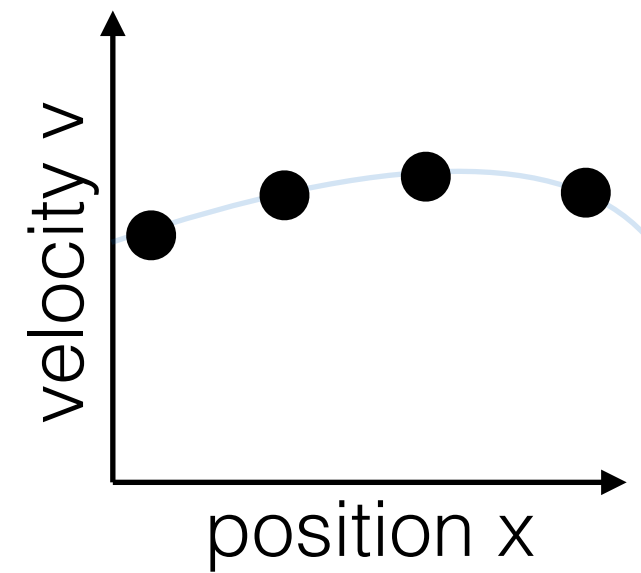
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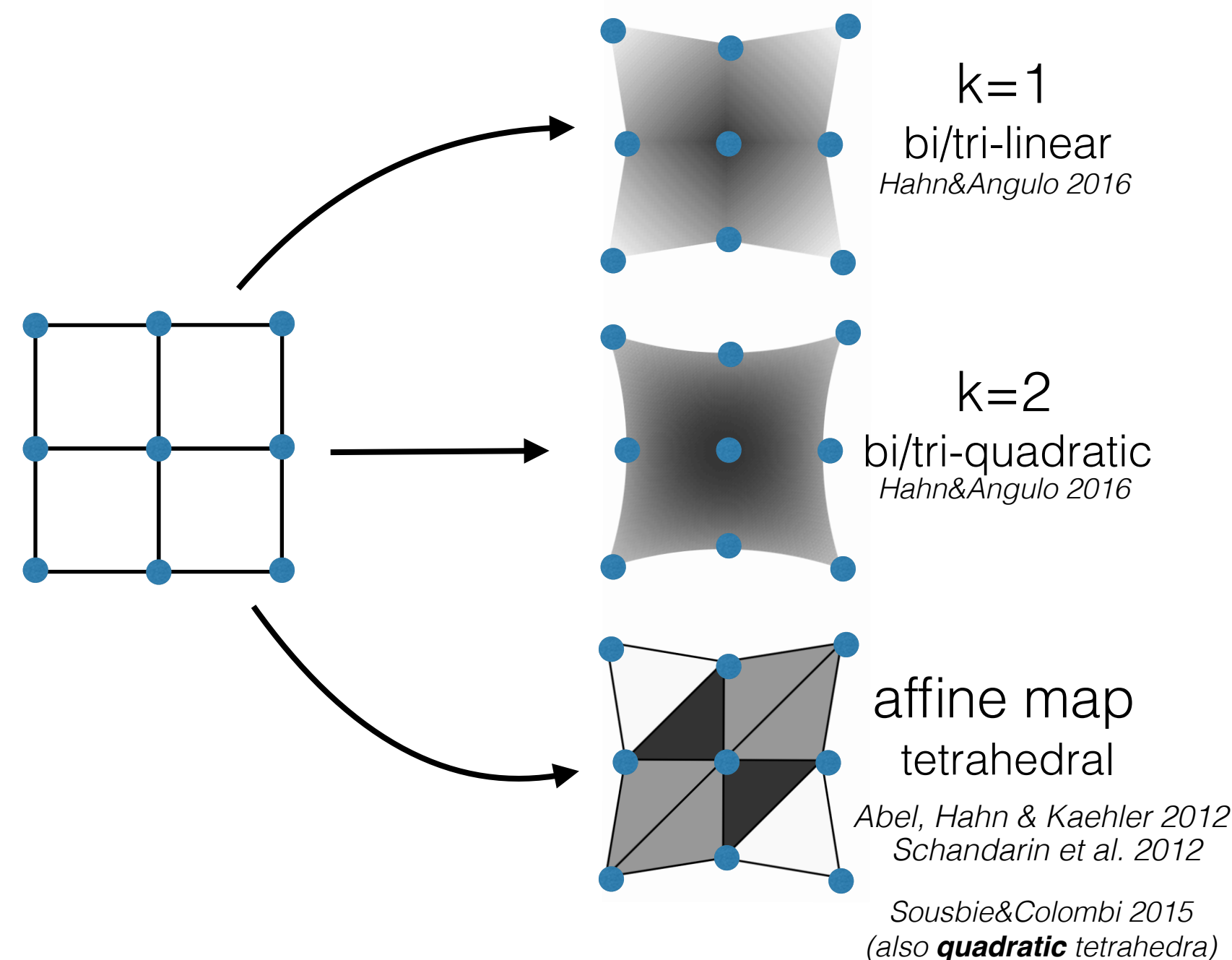
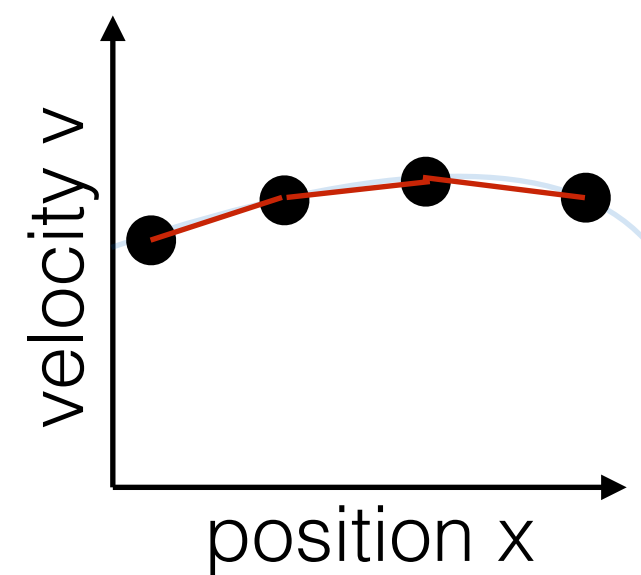
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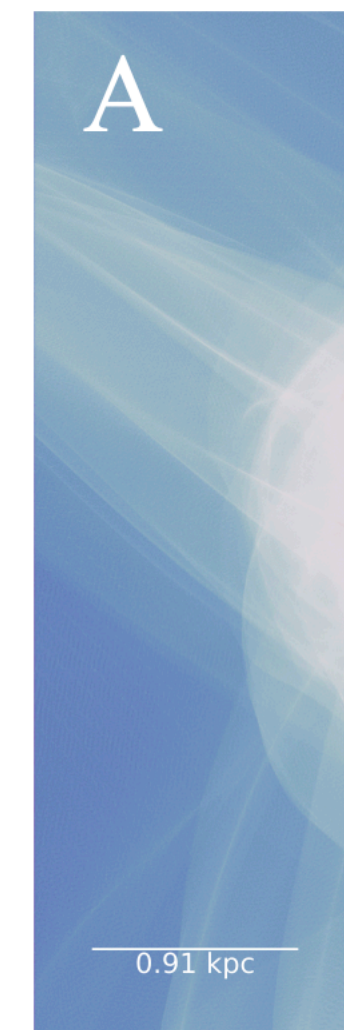
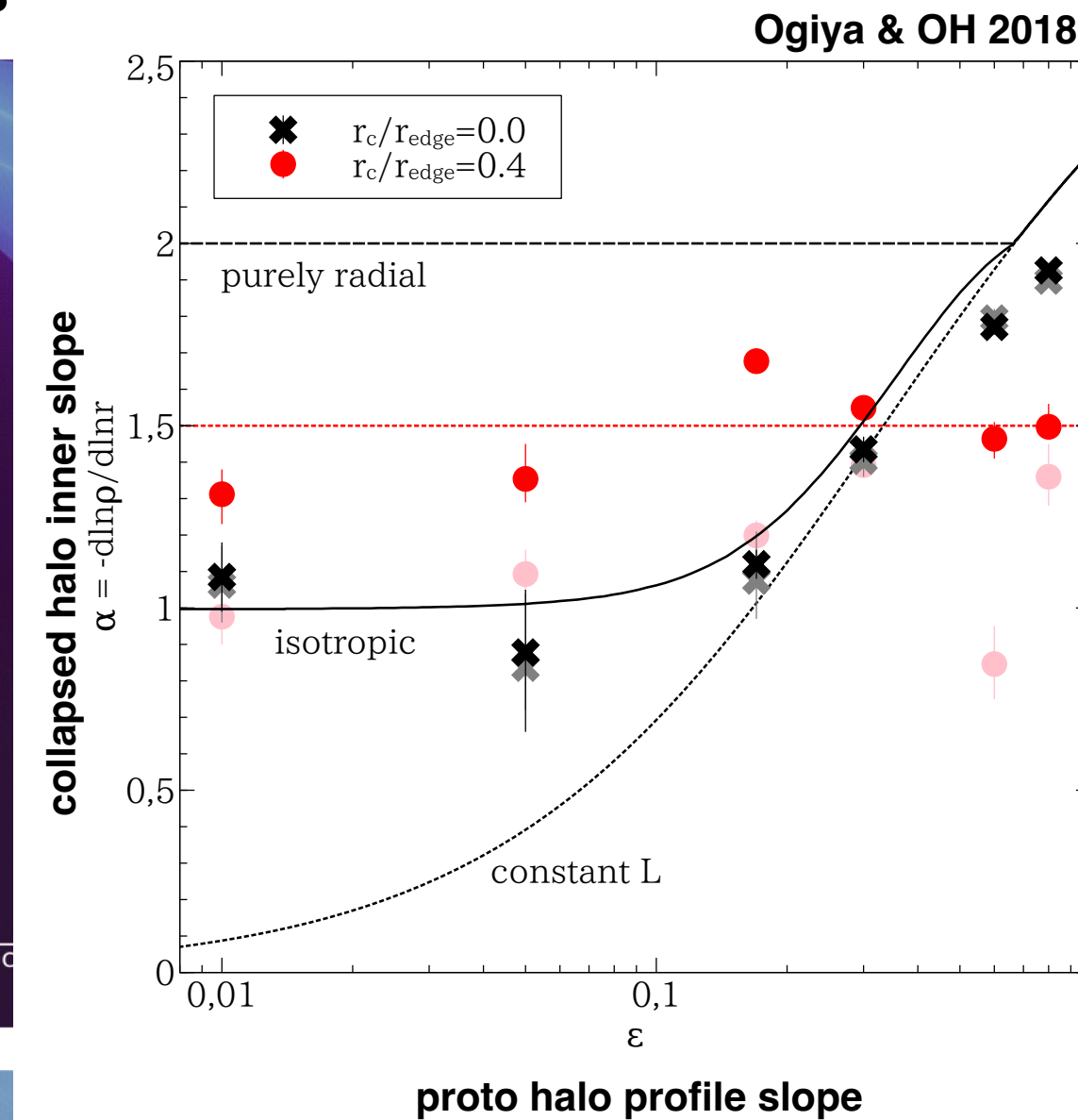
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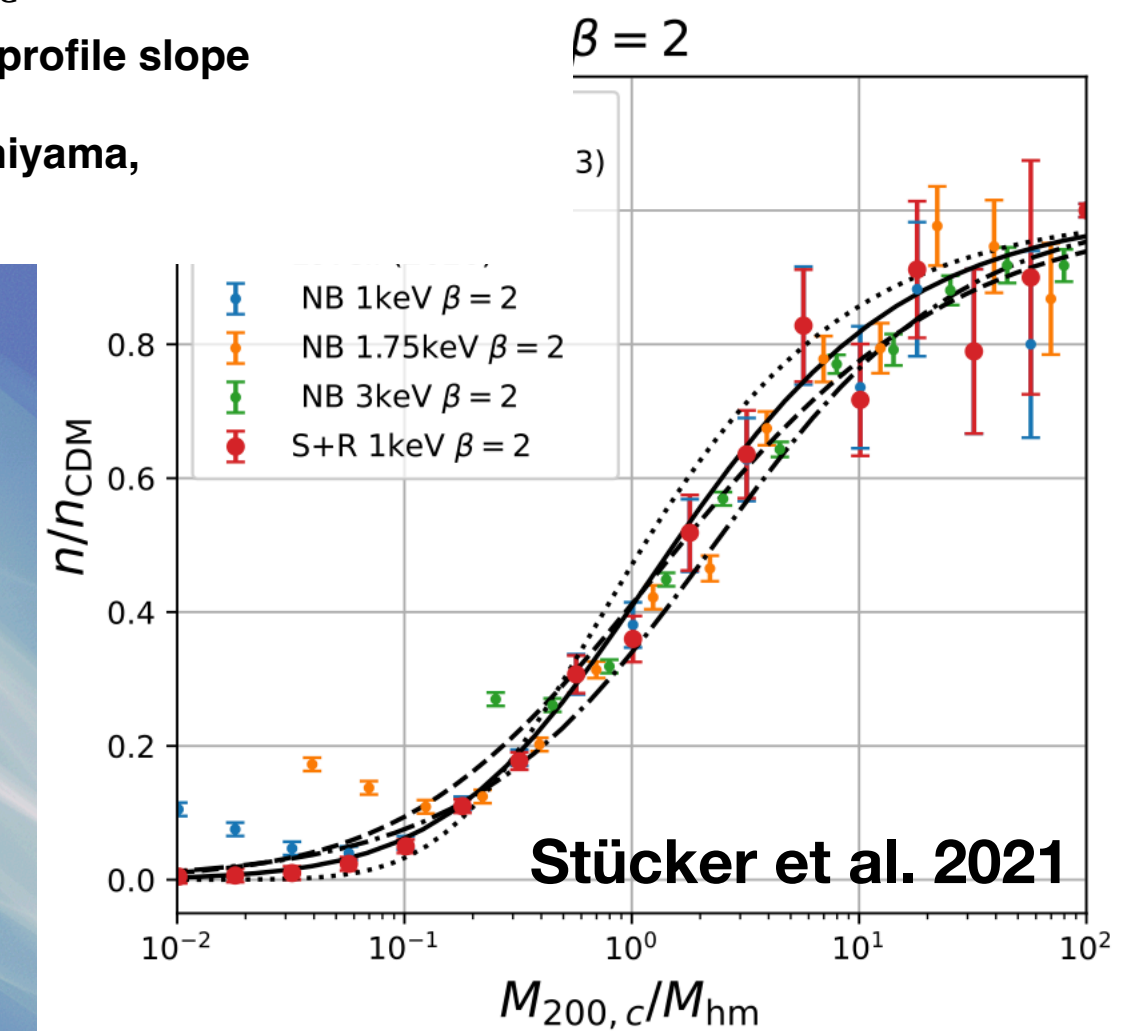
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Latest incarnation of sheet-based simulations of prompt CDM cusps (deviations)



see also work by Tomoaki Ishiyama, Sten Delos, Simon White



Stücker et al. 2021

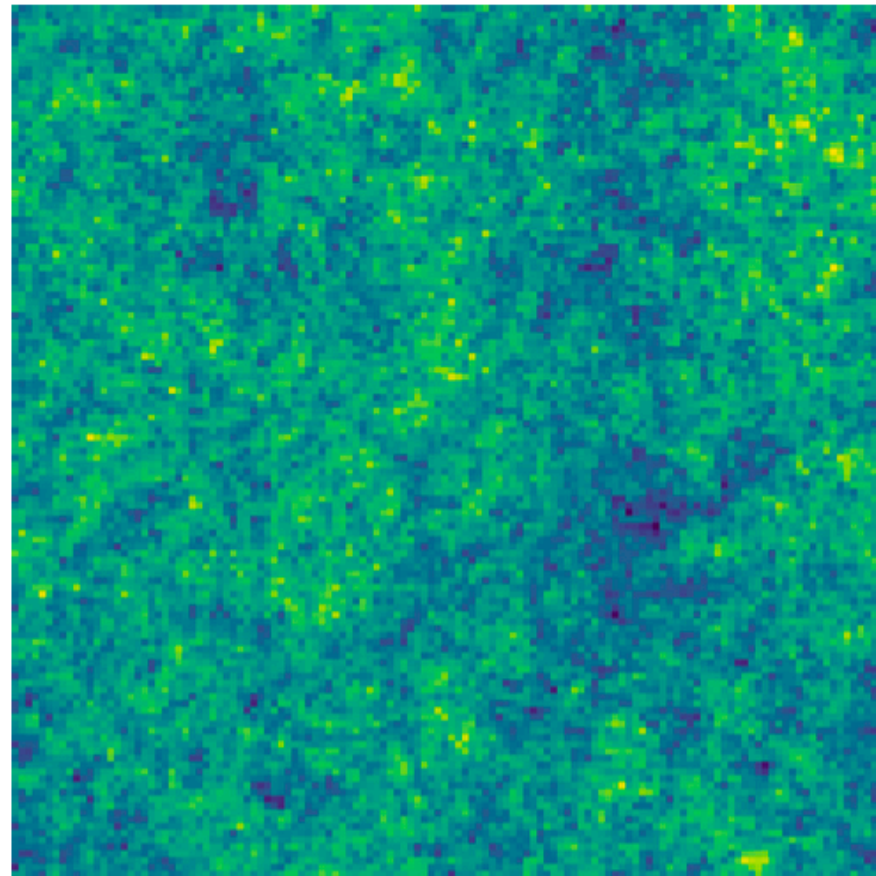
Ondaro-Mallea et al. 2023

Field-level inference: reconstruction

Task: given a (simulated) late-time density field, reconstruct initial conditions

$$\mathbb{P}(\Phi \mid \delta) \propto \mathbb{P}(\delta \mid \Phi) \mathbb{P}(\Phi)$$

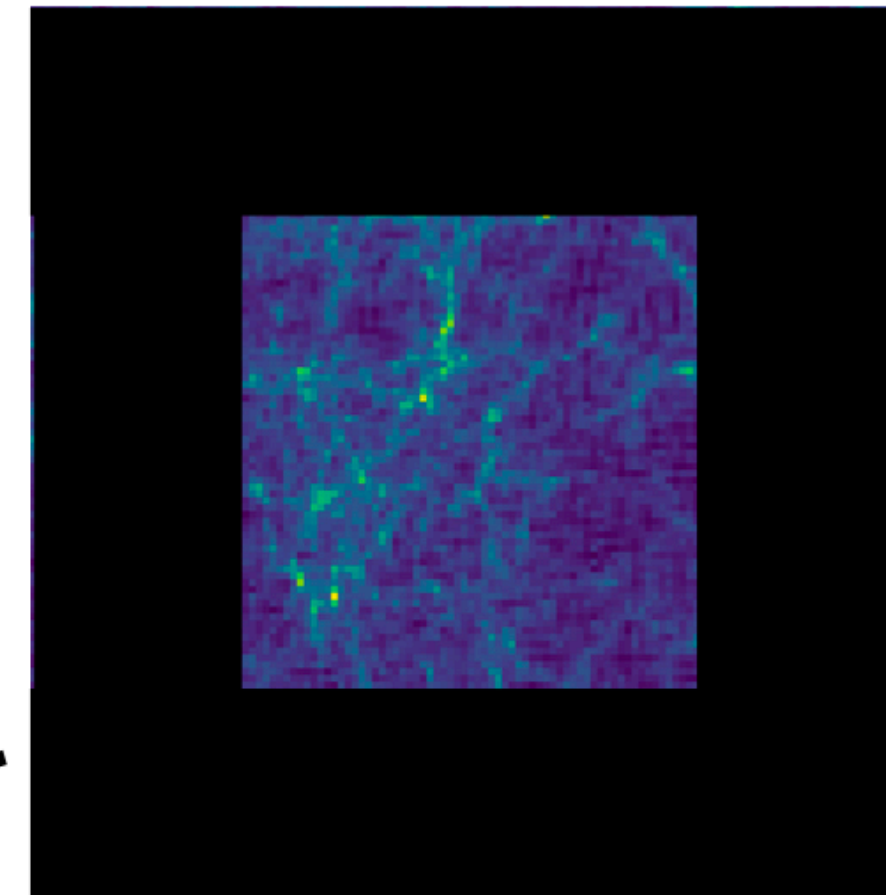
True label
(initial conditions)



forward model
(Lagrangian perturbation theory)

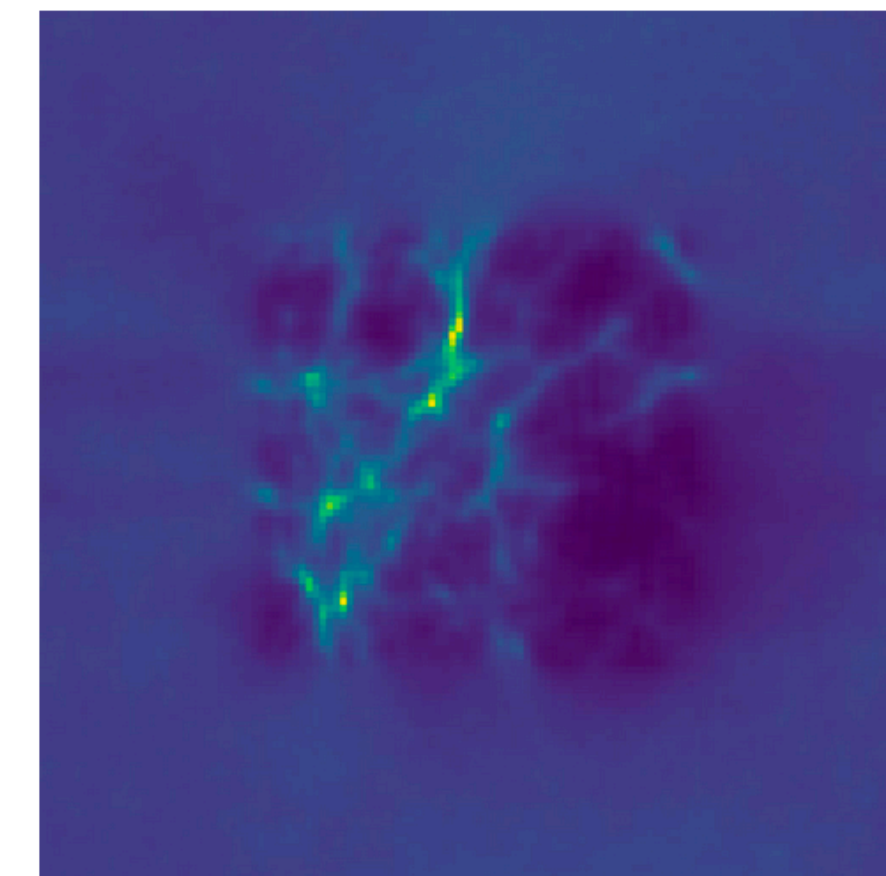
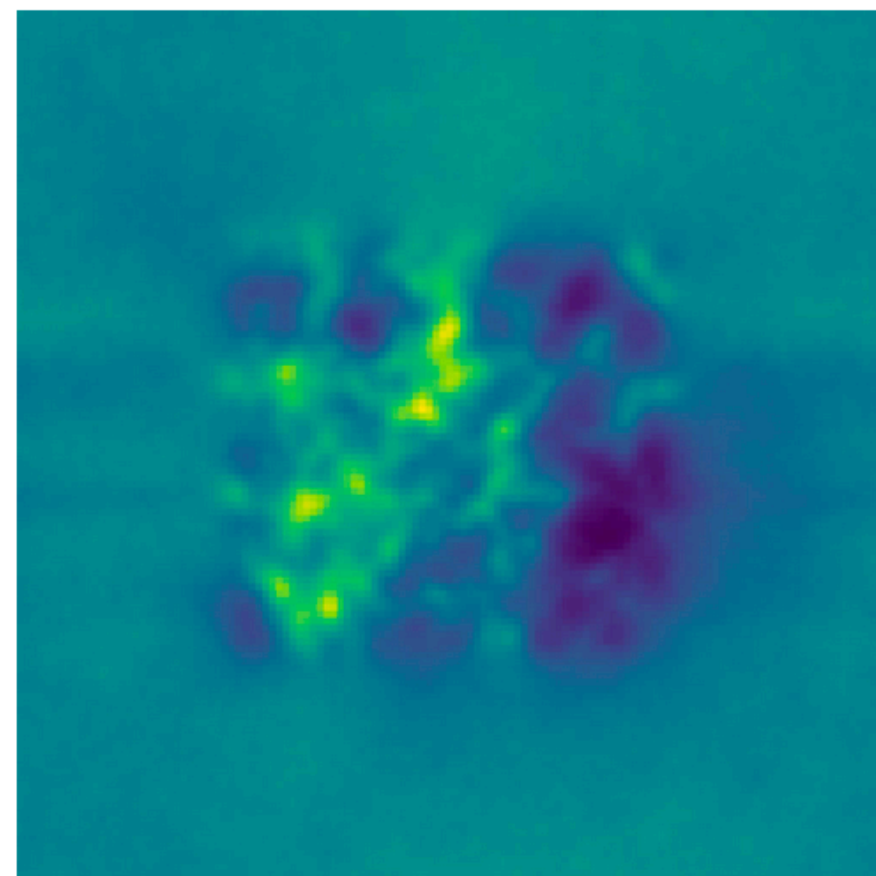


Resulting observation
(late-time density field)



survey mask

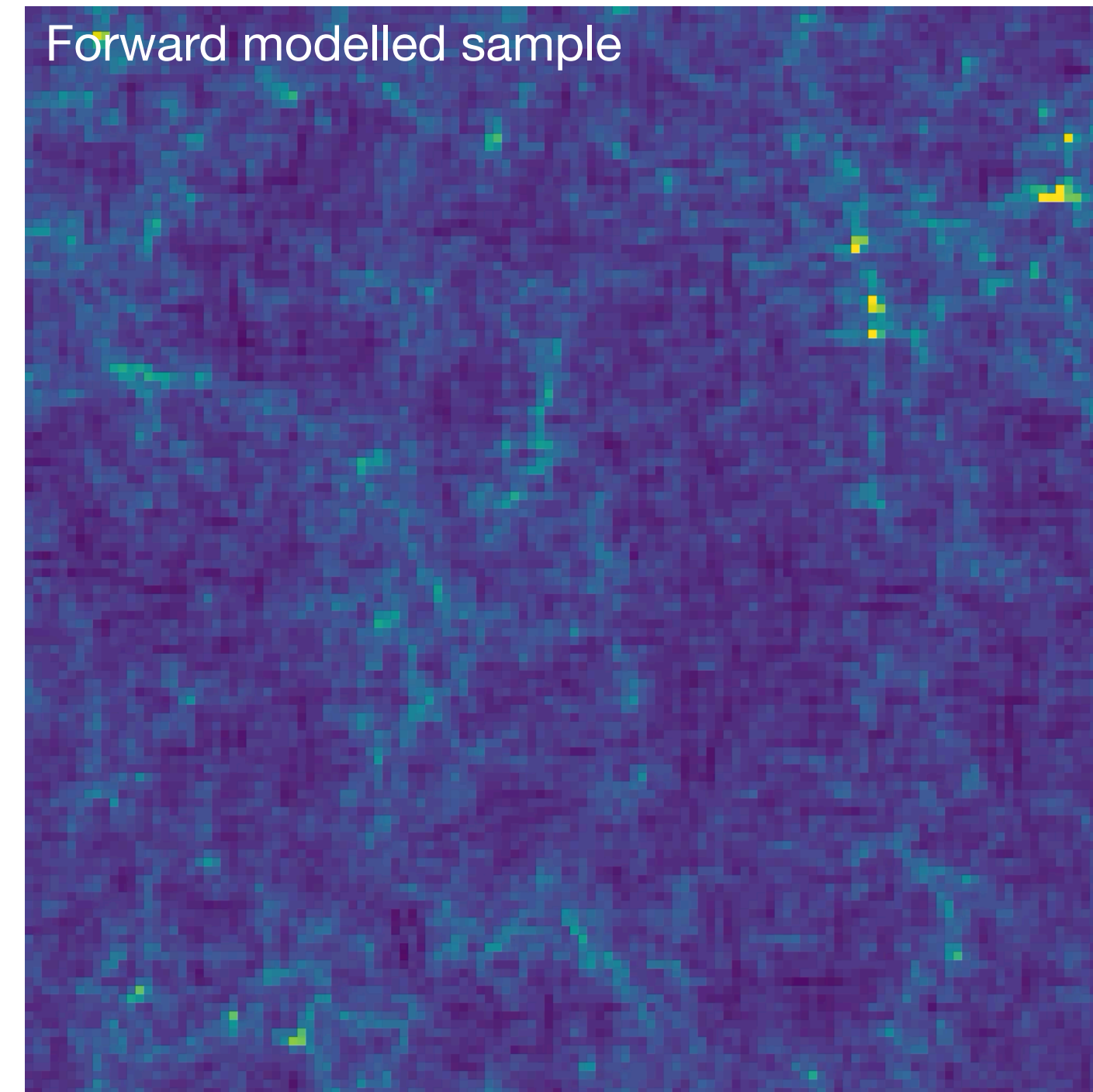
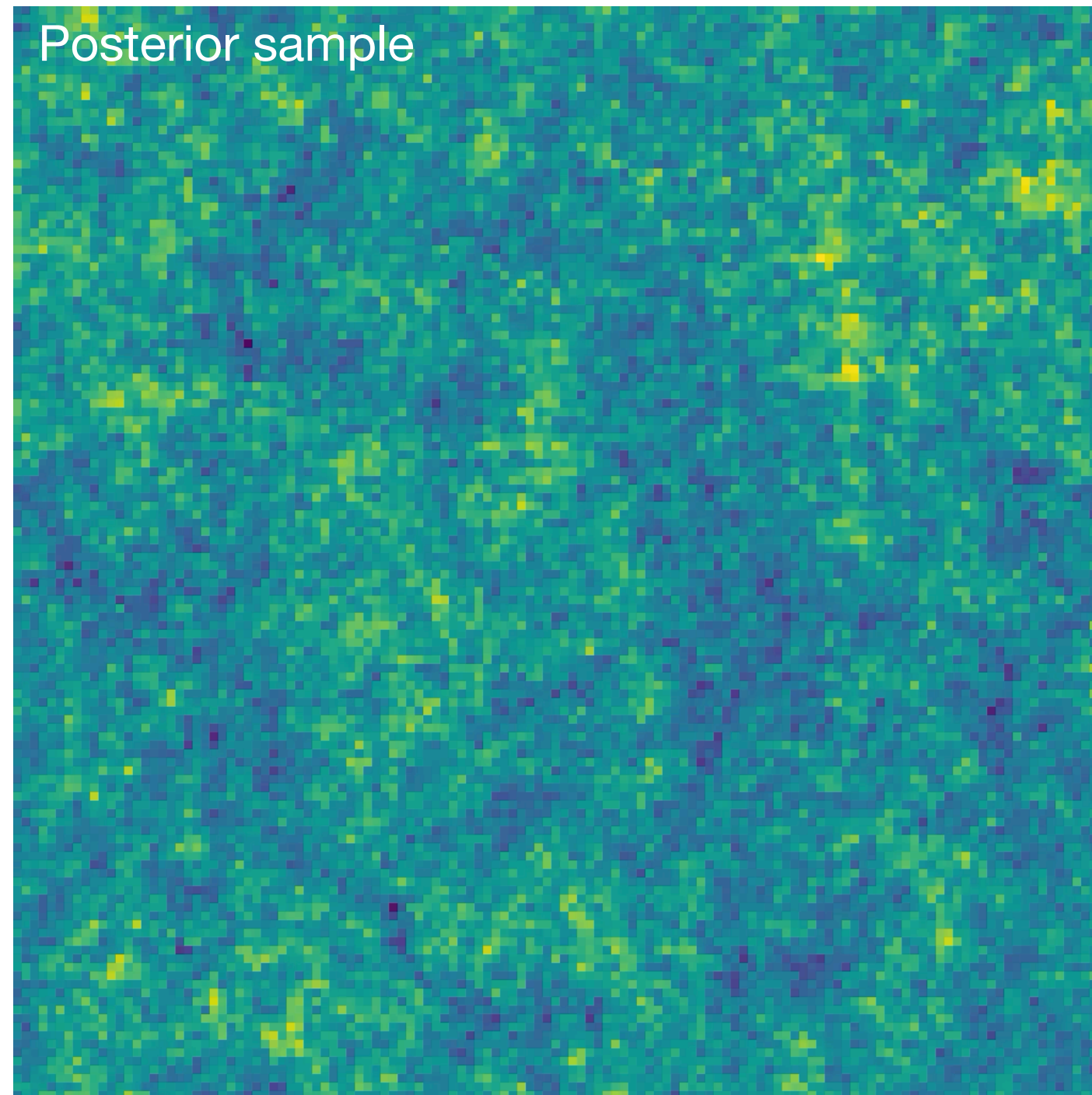
Mean reconstruction



Field-level inference: reconstruction

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Example: drawing posterior samples (PhD thesis of Lukas Winkler)

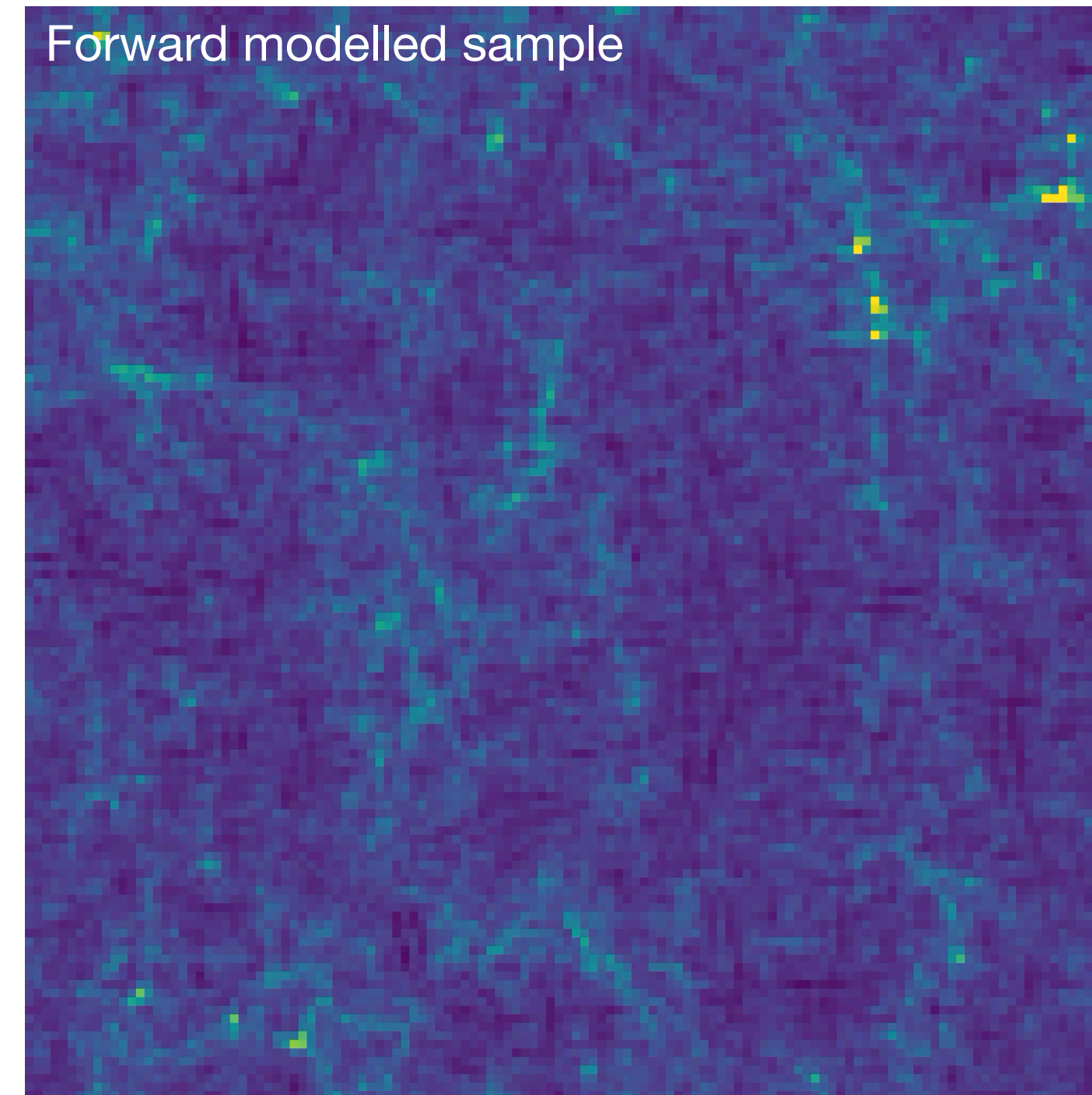
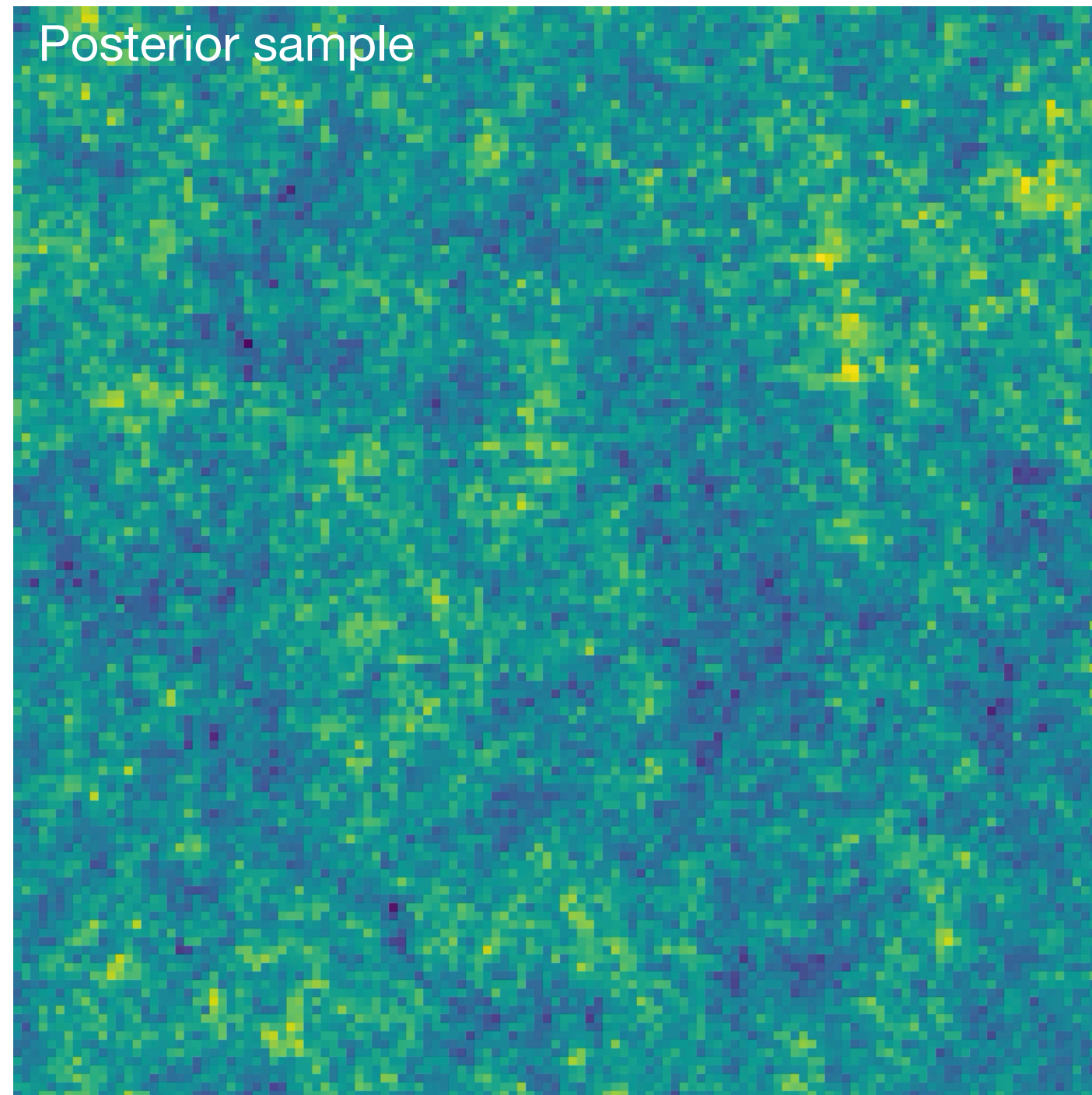


Here, we use a **No U-Turn Sampler (NUTS)** – a variant of Hamiltonian Monte Carlo – provided by the BlackJax library <https://blackjax-devs.github.io/blackjax/>.

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Summary

- Diff'able model = prediction + dprediction/d{parameters,ICs,...}
- Differentiable models allow new ways of confronting data -> beyond simple summary statistics
- DISCO-DJ new contender:
 - DISCO-EB Einstein-Boltzmann solver
 - “easy” forecasting, add your models
 - currently still too slow for MCMC analysis (work in progress...)
 - DISCO-DJ LSS model (optimized PM solver, see also JaxPM, pmwd, FlowPM)
 - will directly integrate with EB module (differentiate through both)
 - nLPT recursion
 - new PT-informed time integrators+discreteness suppression
 - currently only single GPU, multi-GPU is WIP

- <http://cosmology.univie.ac.at>
- oliver.hahn@univie.ac.at