Fast numerical methods for cosmological inference from LSS

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w/ **Florian List, Cornelius Rampf**

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universität wien

Matching early to late in simulations…

Early physics:

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

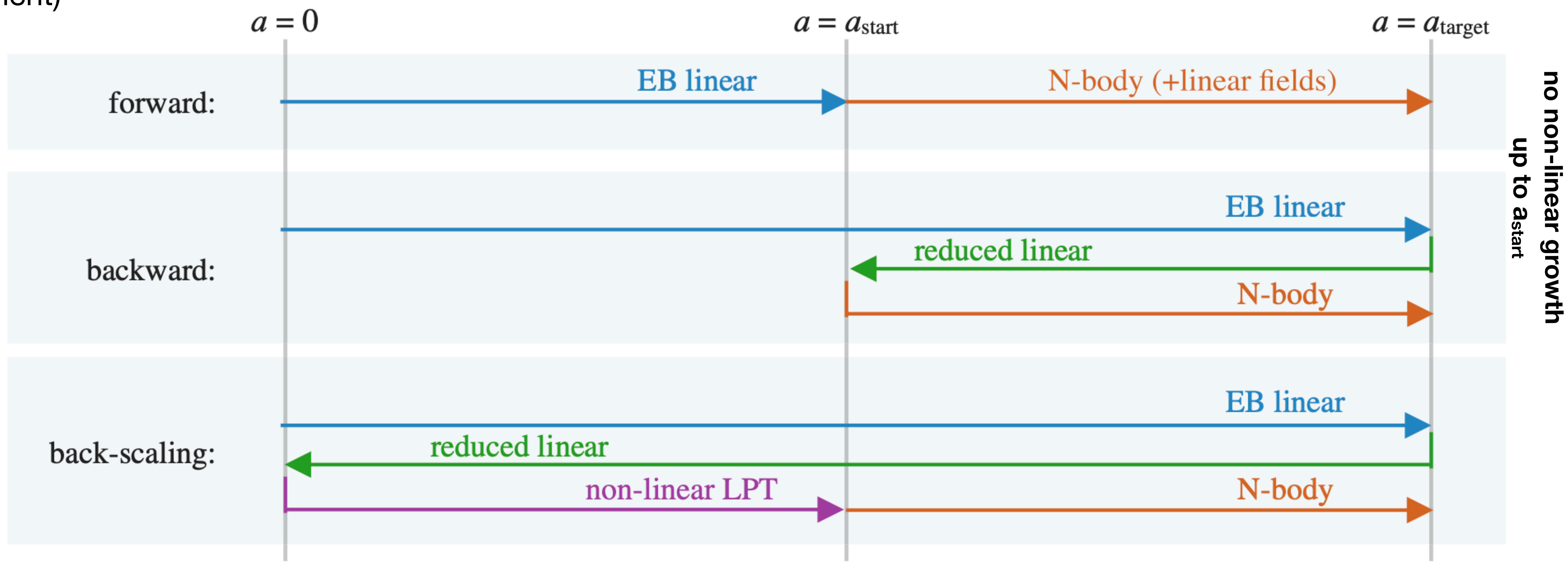
Eulerian

Late physics:

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

Lagrangian

choices in the literature:



Angulo & Hahn 2022 review

Newtonian Gravitational Evolution: Vlasov-Poisson

Consider the (on-shell) phase-space density of non-interacting massive particles $f(\boldsymbol{x}, \boldsymbol{v}, t)$

Evolution given by non-relativistic limit of the relativistic Liouville equation = **Vlasov-Poisson**, assume config space $\mathscr{C} = \mathbb{T}^3$

$$\mathrm{d}_t f = \partial_t f + \frac{\boldsymbol{v}}{a^2} \cdot \boldsymbol{\nabla}_{\boldsymbol{x}} f + \frac{\boldsymbol{g}}{a} \cdot \boldsymbol{\nabla}_{\boldsymbol{p}} f = 0$$

$$\boldsymbol{g} := -\frac{3\Omega_m}{2} \boldsymbol{\nabla}_{\boldsymbol{x}} \nabla_{\boldsymbol{x}}^{-2} (n-1)$$

$$n = \int_{\mathbb{R}^3} \mathrm{d}^3 p \; f \qquad \int_{\mathscr{C}} \mathrm{d}^3 x \; n = 1$$

can be solved by **method of characteristics**:

Consider 1-parameter families of curves $\boldsymbol{X}(t),\ \boldsymbol{V}(t)$ (the characteristics)

Study evolution of f along the characteristics

$$f_c : \; t \mapsto f(\boldsymbol{X}(t), \boldsymbol{V}(t), t) \qquad \text{given} \qquad \boldsymbol{X}(t = t_0) =: \boldsymbol{X}_0, \quad \boldsymbol{V}(t = t_0) =: \boldsymbol{V}_0$$

by chain rule

$$\frac{\mathrm{d} f_c}{\mathrm{d} t} = \frac{\partial f_c}{\partial t} + \boldsymbol{\nabla}_x f_c \big|_{\boldsymbol{x}=\boldsymbol{X}(t)} \cdot \frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} + \boldsymbol{\nabla}_v f_c \big|_{\boldsymbol{v}=\boldsymbol{V}(t)} \cdot \frac{\mathrm{d}\boldsymbol{V}}{\mathrm{d}t}.$$

comparing with VP

$$\frac{\mathrm{d} f_c}{\mathrm{d} t} = 0 \qquad \text{iff} \qquad \begin{cases} \dot{\boldsymbol{X}}(t) &= a^{-2}\, \boldsymbol{V}(t) \\ \dot{\boldsymbol{V}}(t) &= -\, \boldsymbol{\nabla}_x \phi \big|_{\boldsymbol{x}=\boldsymbol{X}(t)} \end{cases}$$

has Hamiltonian

$$\mathscr{H} = \frac{1}{2} \frac{V^2}{a^2} + \phi$$

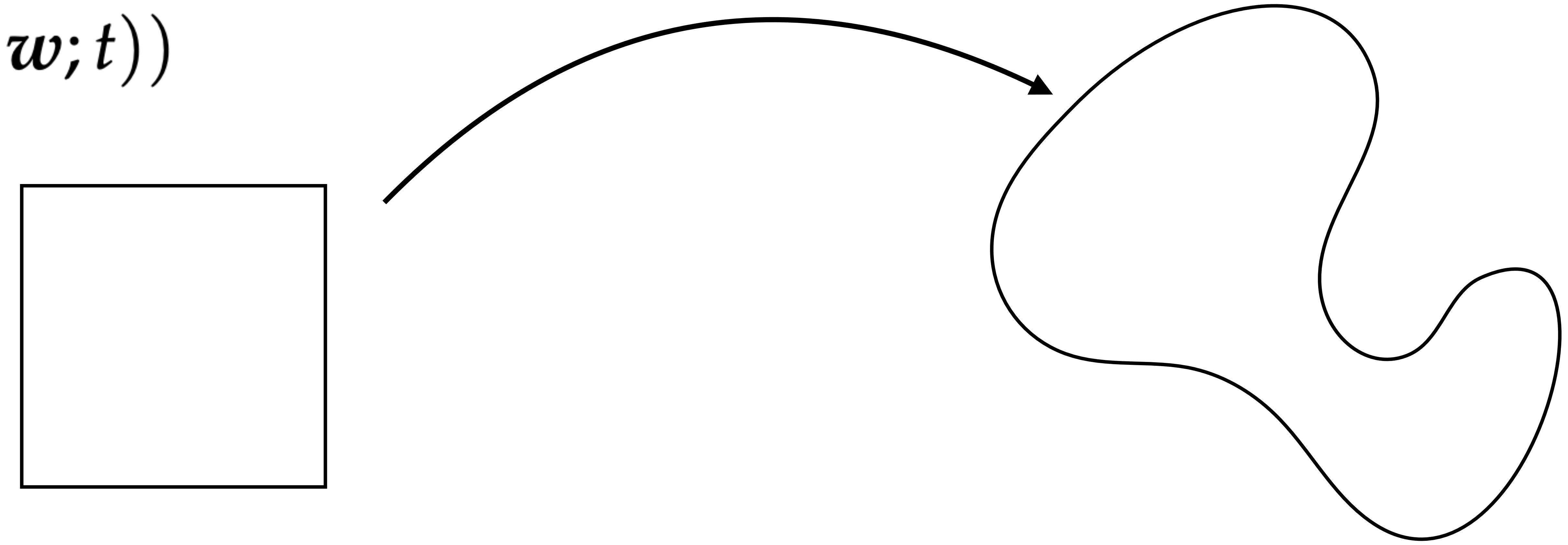
$$\boldsymbol{\nabla}_x \phi = -\frac{\boldsymbol{g}}{a}$$

The fluid and the N-body model

Lagrangian description, evolution of fluid element

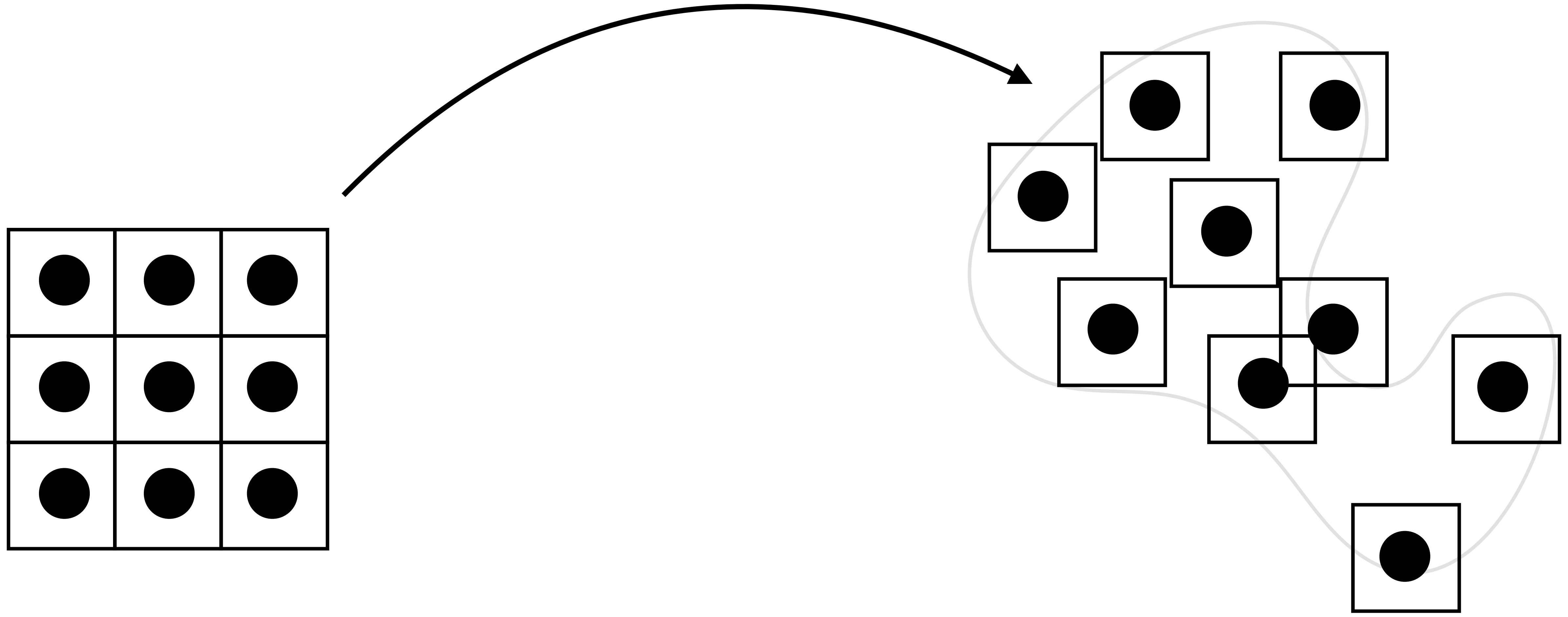
Lagrangian map of the $\mathbb{R}^{2d}$ phase space onto itself

$$\mathbb{R}^{2d} \to \mathbb{R}^{2d}: \quad (\boldsymbol{q}, \boldsymbol{w}) \mapsto (\boldsymbol{x}(\boldsymbol{q}, \boldsymbol{w}; t), \boldsymbol{v}(\boldsymbol{q}, \boldsymbol{w}; t))$$



The N-body approximation:
follow only *N* characteristics, use them to reconstruct the density field that sources the Poisson equation

$$\mathbb{R}^{N2d} \to \mathbb{R}^{N2d}: \quad (\boldsymbol{Q}_i, \boldsymbol{W}_i) \mapsto (\boldsymbol{X}_i(t), \boldsymbol{V}_i(t)), \qquad i = 1, \ldots, N$$



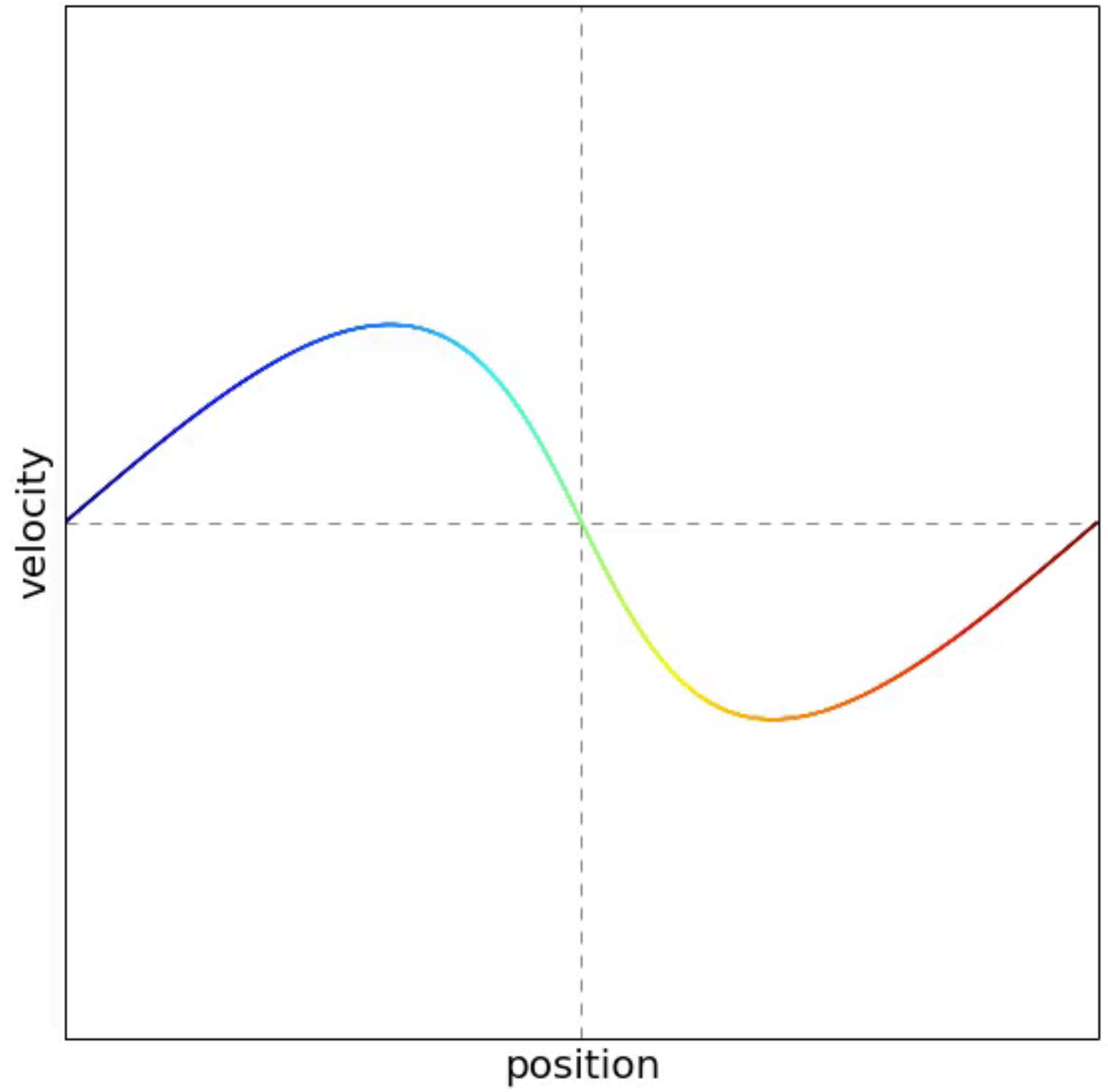
Non-Linear Evolution of Fluctuations

Cold Dark Matter lives on Lagrangian submanifold

Solve Vlasov-Poisson on submanifold characteristics $(\boldsymbol{q}, t) \mapsto (\boldsymbol{X}_{\boldsymbol{q}}(t), \boldsymbol{V}_{\boldsymbol{q}}(t)),$

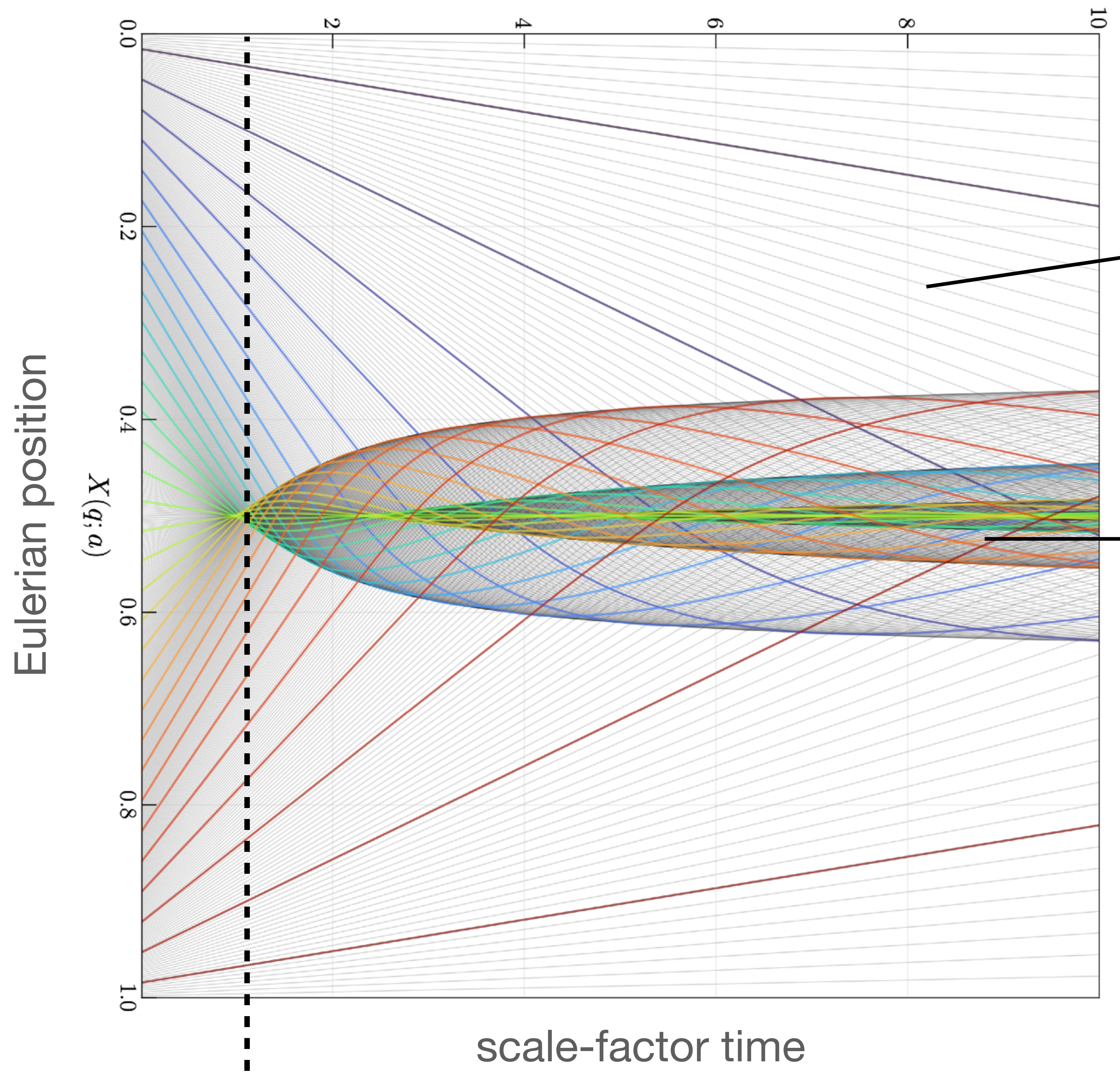
$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{v}}{a^2} \cdot \boldsymbol{\nabla}_x f - \boldsymbol{\nabla}_x \phi \cdot \boldsymbol{\nabla}_v f = 0 \quad \Leftrightarrow \quad \boldsymbol{X}_{\boldsymbol{q}}'' + \mathcal{H} \boldsymbol{X}_{\boldsymbol{q}}' = -\boldsymbol{\nabla}\phi(\boldsymbol{X}_{\boldsymbol{q}})$$

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



1D singularities: Rampf, Frisch & OH (2021)

density + acceleration singularities



moment of shell-crossing

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

Lagrangian Perturbation Theory
(for single fluid with cold initial data)

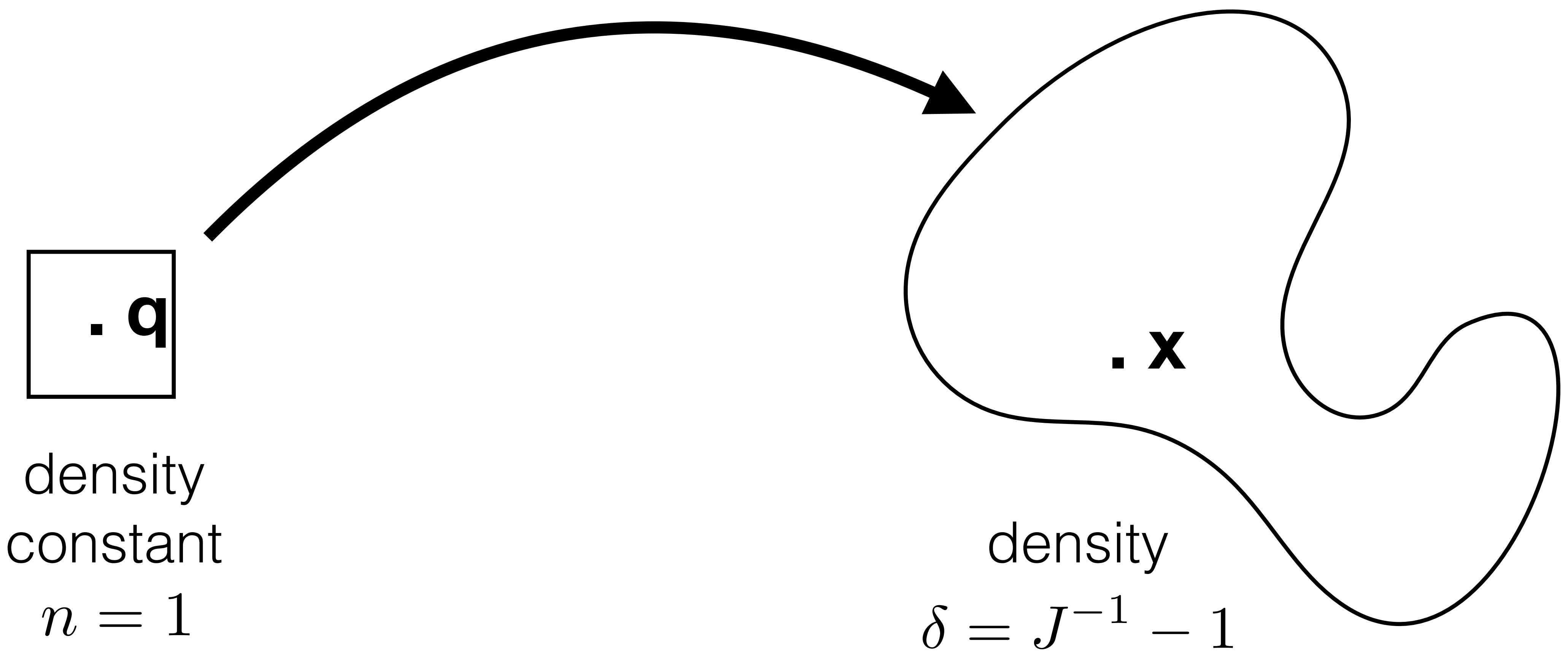
Lagrangian map

$$\boldsymbol{X}_{\boldsymbol{q}}(t) = \boldsymbol{q} + \boldsymbol{\Psi}(\boldsymbol{q}, t)$$

Overdensity given by Jacobian

$$\delta(\boldsymbol{x}, t) = \frac{1}{J(\boldsymbol{q}, t)} - 1$$

$$J := \det \boldsymbol{\nabla}_{\boldsymbol{q}} \otimes \boldsymbol{X}_{\boldsymbol{q}}$$



LPT eq: $\mathrm{J}\, \left(\delta_{ij} + \Psi_{i,j}\right)^{-1} \left(\Psi''_{i,j} + \mathcal{H}\Psi'_{i,j}\right) = \frac{3}{2}\mathcal{H}^2\Omega_m(\mathrm{J} - 1)$

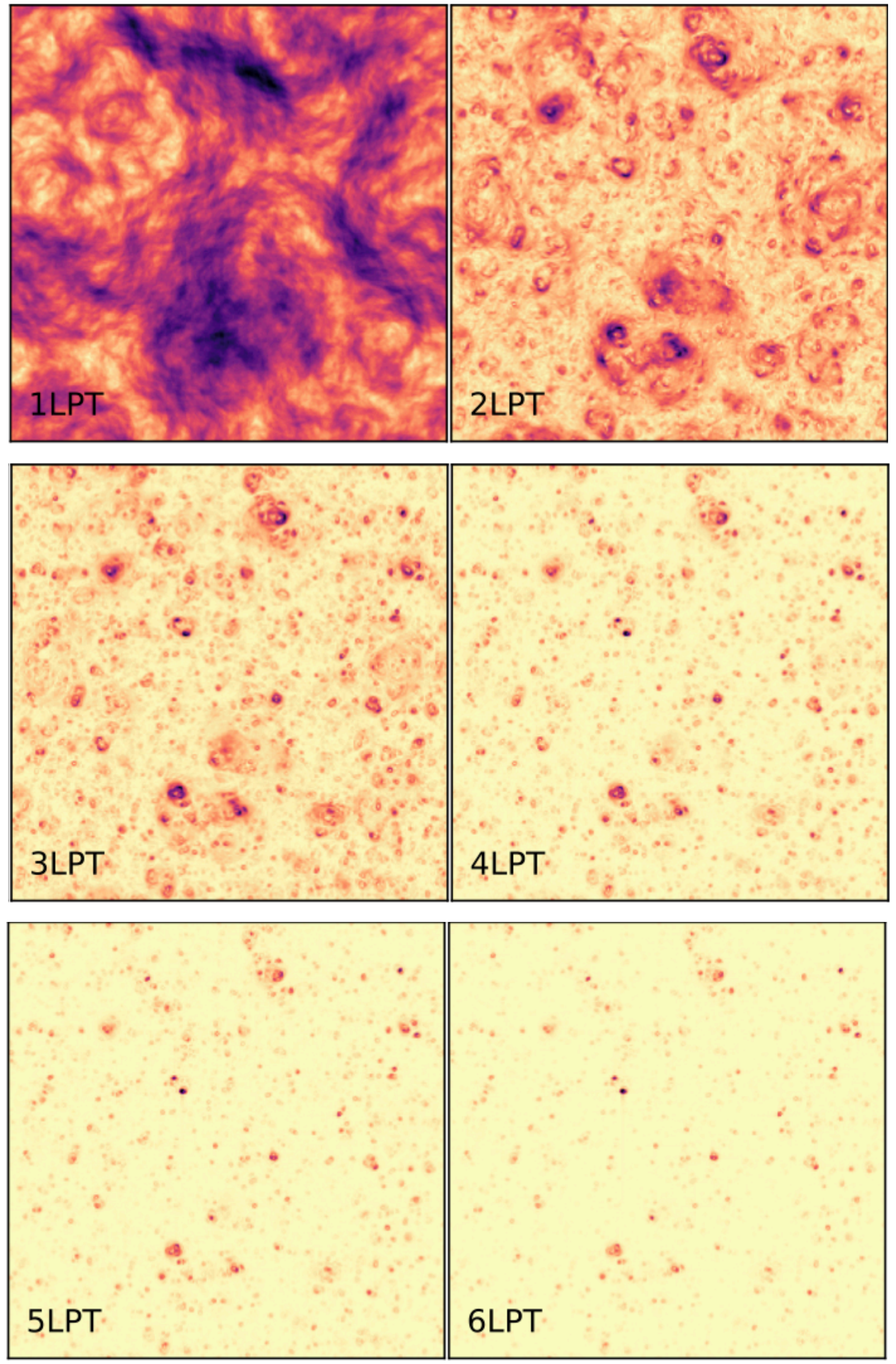
We want to solve this as a perturbative series (D is small parameter)

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

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

yields recursion relations to all orders.

For LCDM, actually $D^{(n)}(\tau) \neq D^n(\tau)$ **,** see Rampf, Schobesberger & OH(2022), Fasiello, Fujita, Vlah (2022)



Rampf+OH (2021)

What is the range of applicability of such a theory (aka the ‘radius of convergence’)?

Perturbative forward model

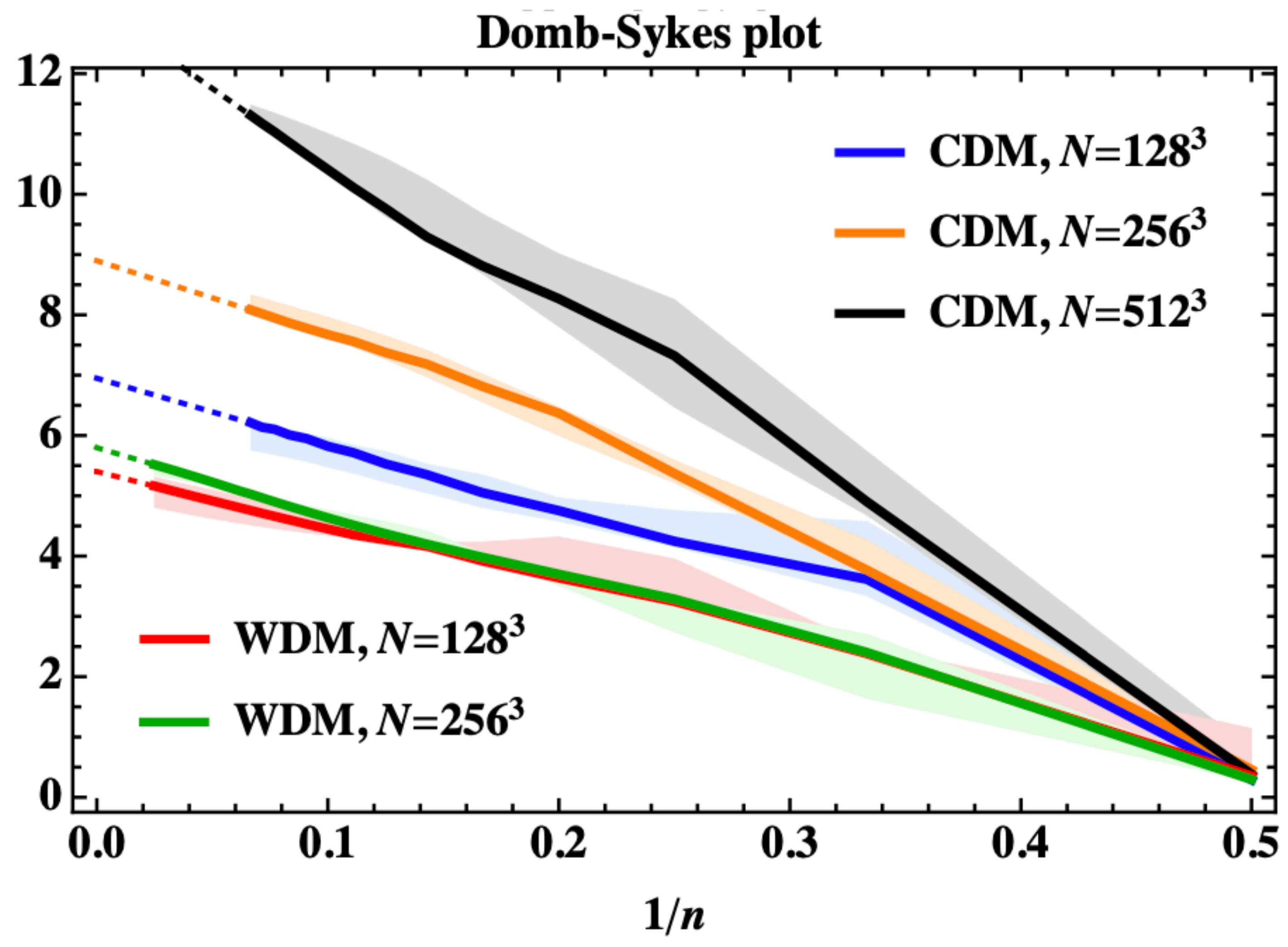
- Advantage: analytical insight
- Lagrangian PT: Extend the asymptotic case to a full Taylor-series

$$\boldsymbol{\Psi}(\boldsymbol{q},a) := \boldsymbol{X}(\boldsymbol{q},a) - \boldsymbol{q} = \sum_{n=1}^{\infty} \boldsymbol{\psi}^{(n)}(\boldsymbol{q})\, a^n$$

  truncate at order N

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

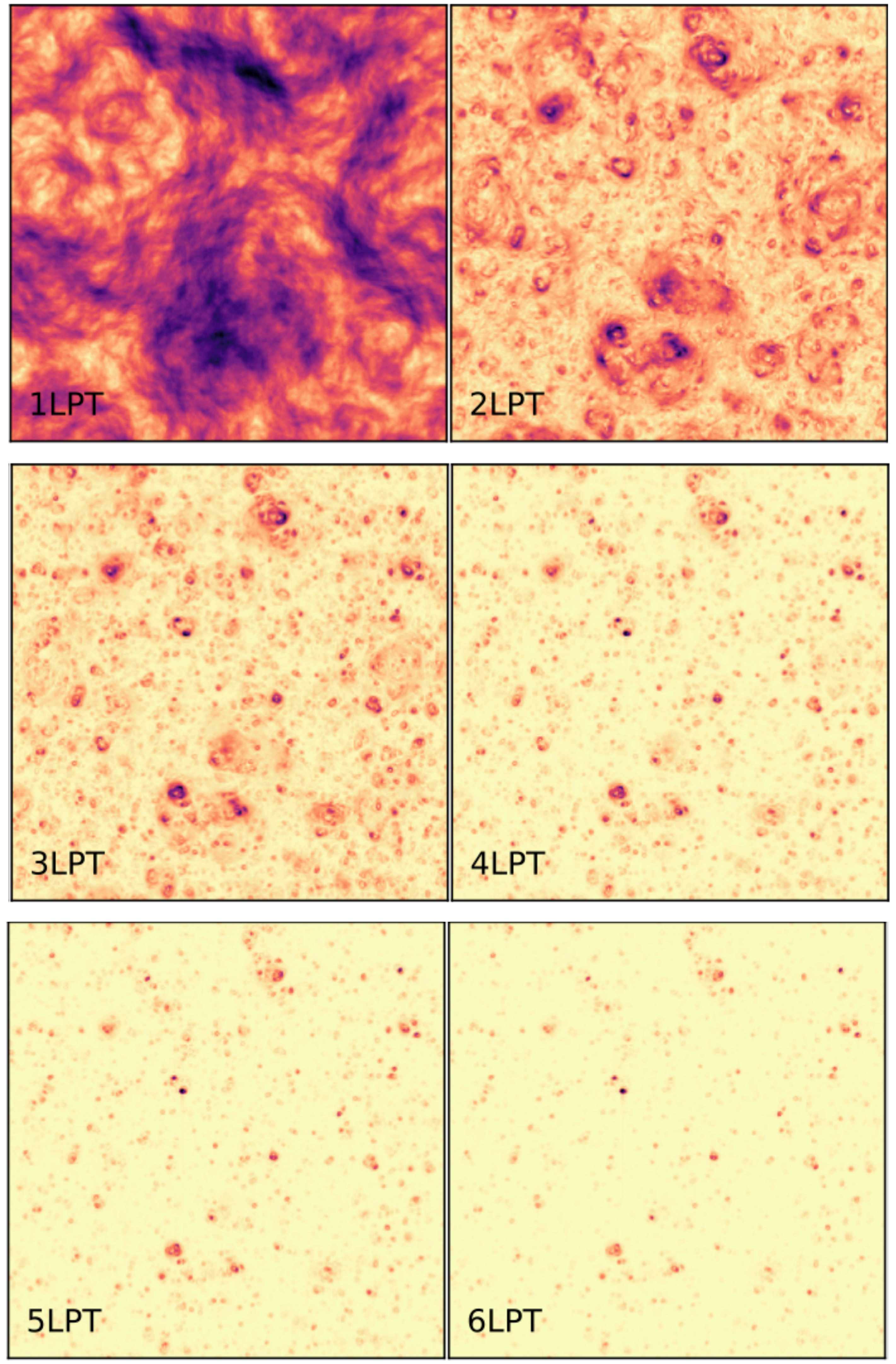
- Strong numerical evidence for convergence prior to shell-crossing:



$$\lim_{n\to\infty} \|\boldsymbol{\psi}^{(n)}\| / \|\boldsymbol{\psi}^{(n-1)}\| = \frac{1}{D_\star}$$

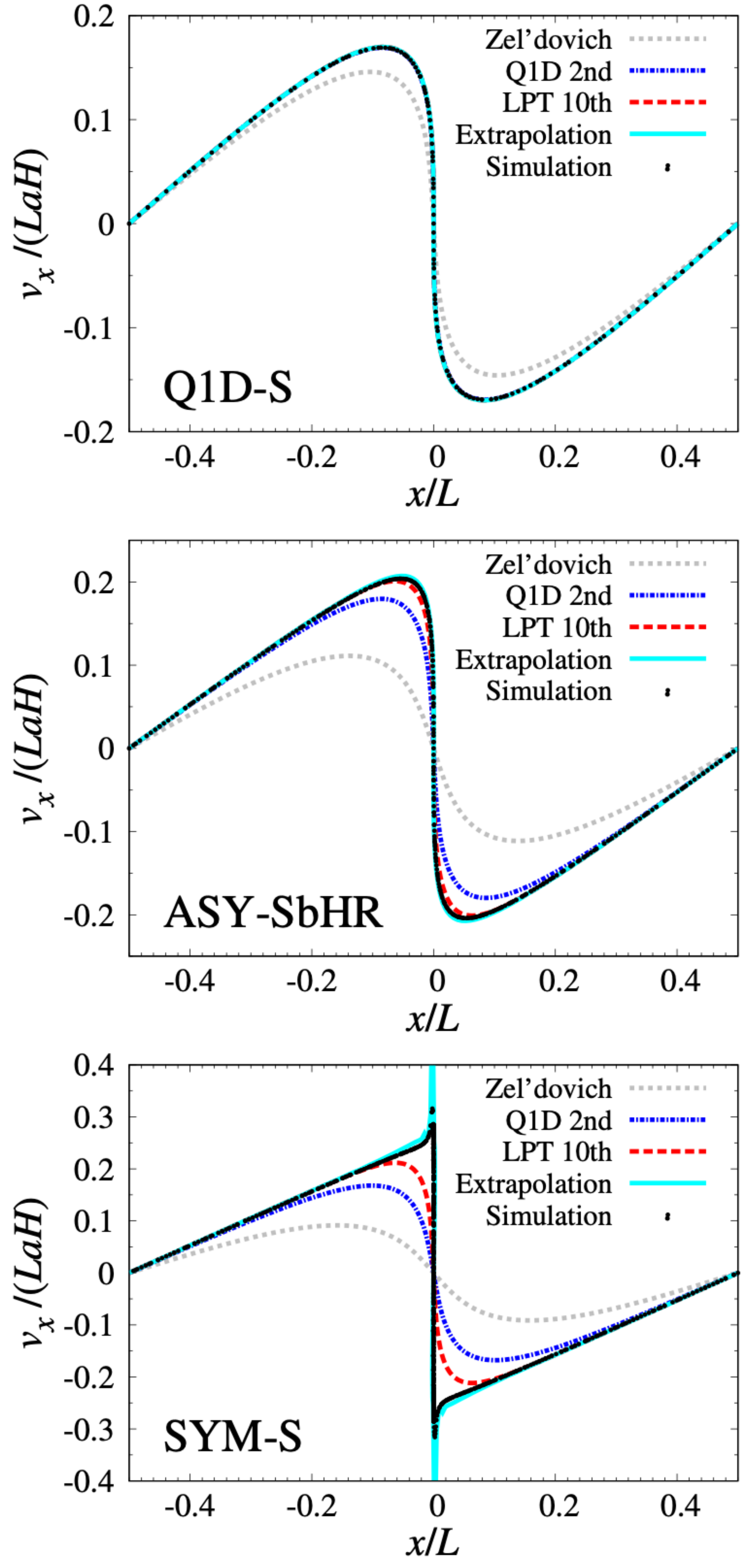
Numerically $D_* \geq a_*$

(Except for measure 0 set)



Rampf+OH (2021)

Convergence limiting singularities



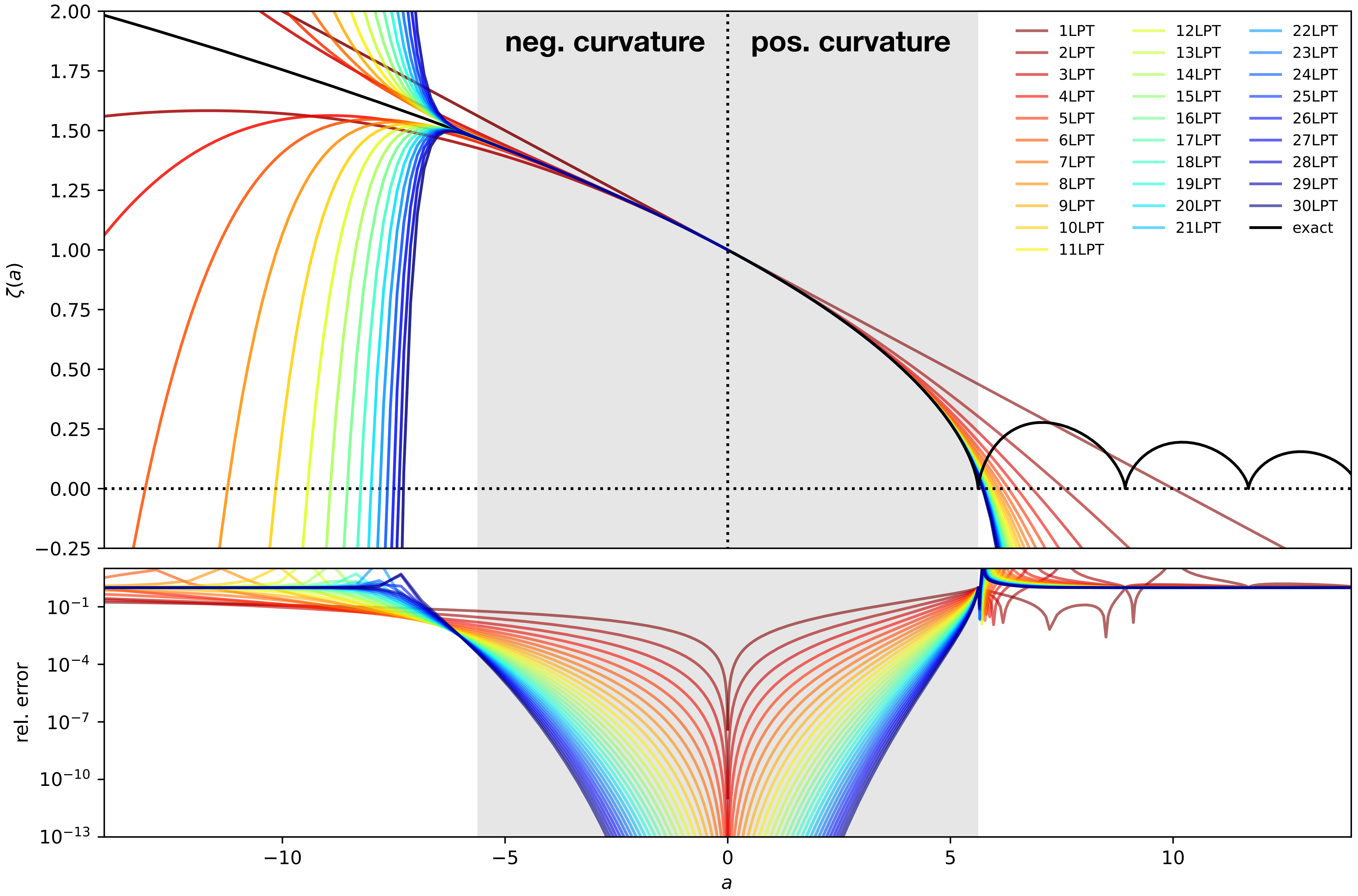
Saga, Colombi, Taruya 2019

Rampf, Frisch, OH '21: For 1D planar initial data, generic non-analyticity appears in the displacement

$$\boldsymbol{\Psi}(\boldsymbol{q}, a) \propto (a - a_*(\boldsymbol{q}))^{\frac{5}{2}}$$

for 1D spherically symmetric initial data, this is hardened to (Rampf & OH '23)

$$\boldsymbol{\Psi}(\boldsymbol{q}, a) \propto (a - a_*(\boldsymbol{q}))^{\frac{2}{3}}$$



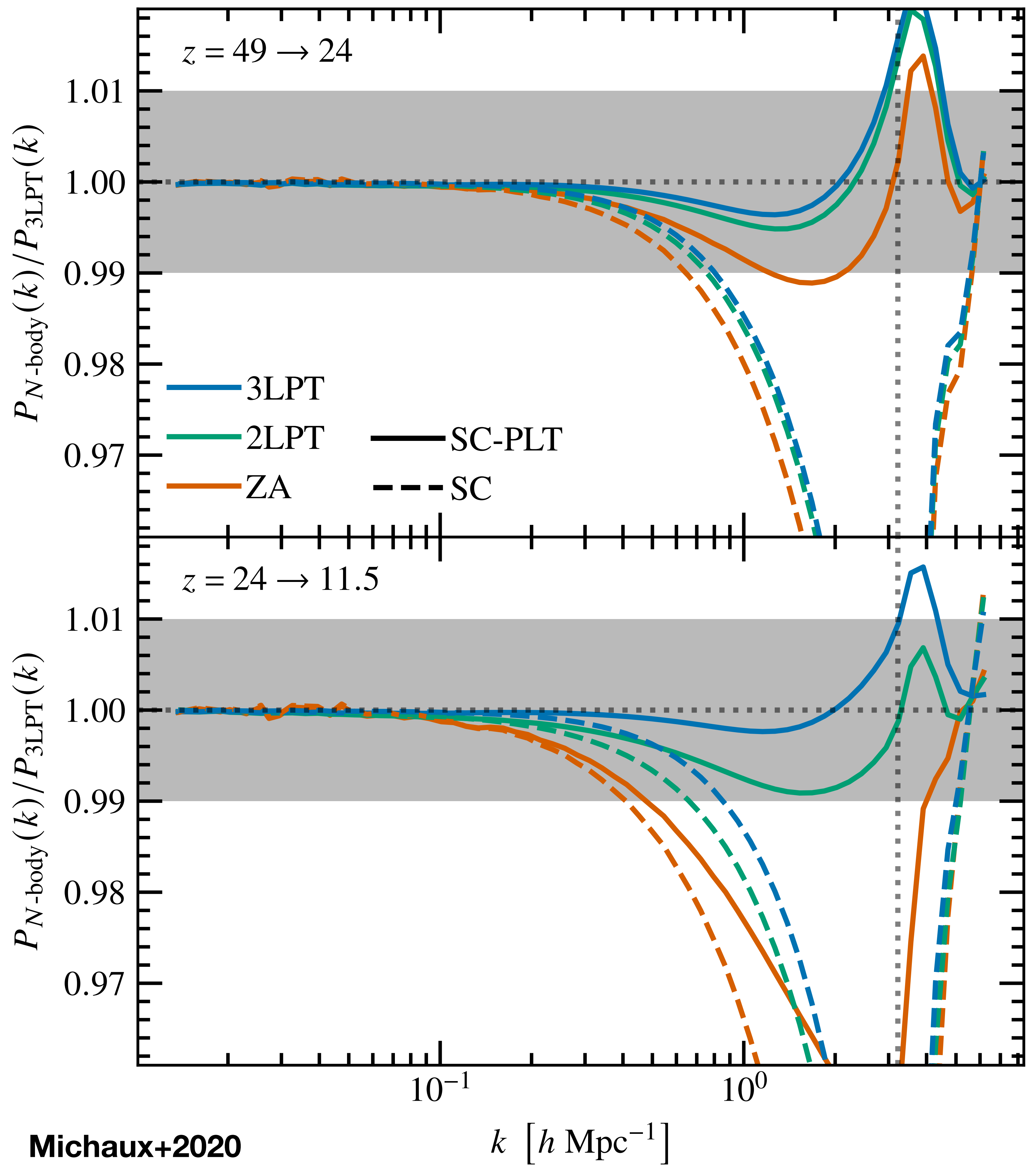
Rampf & OH 2022

Using N-body to go further:

use finite order, discretised LPT to set up an N-body simulation, then run it

Agreement between N-body and LPT?

Comparison of weakly evolved power spectra:

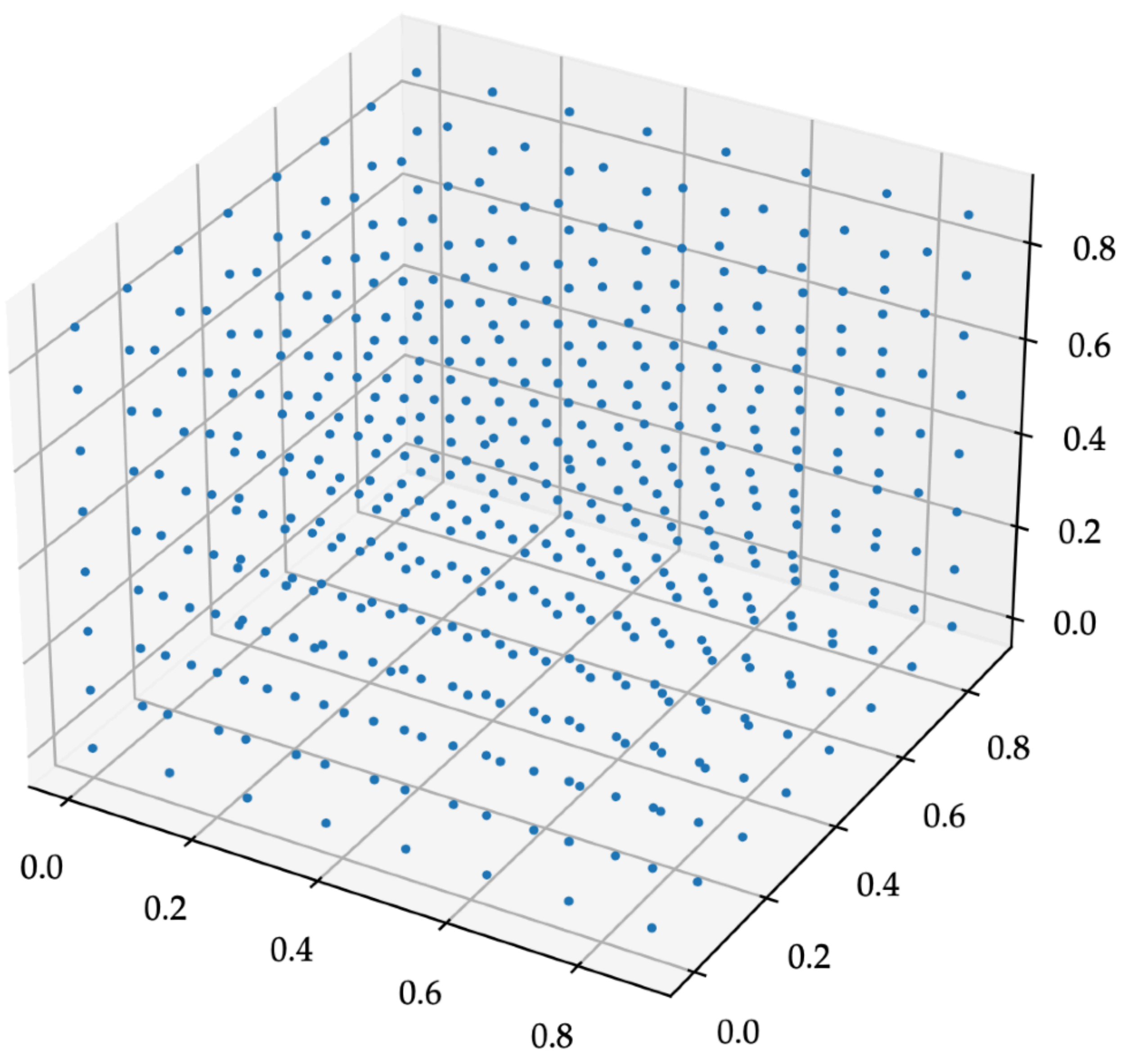


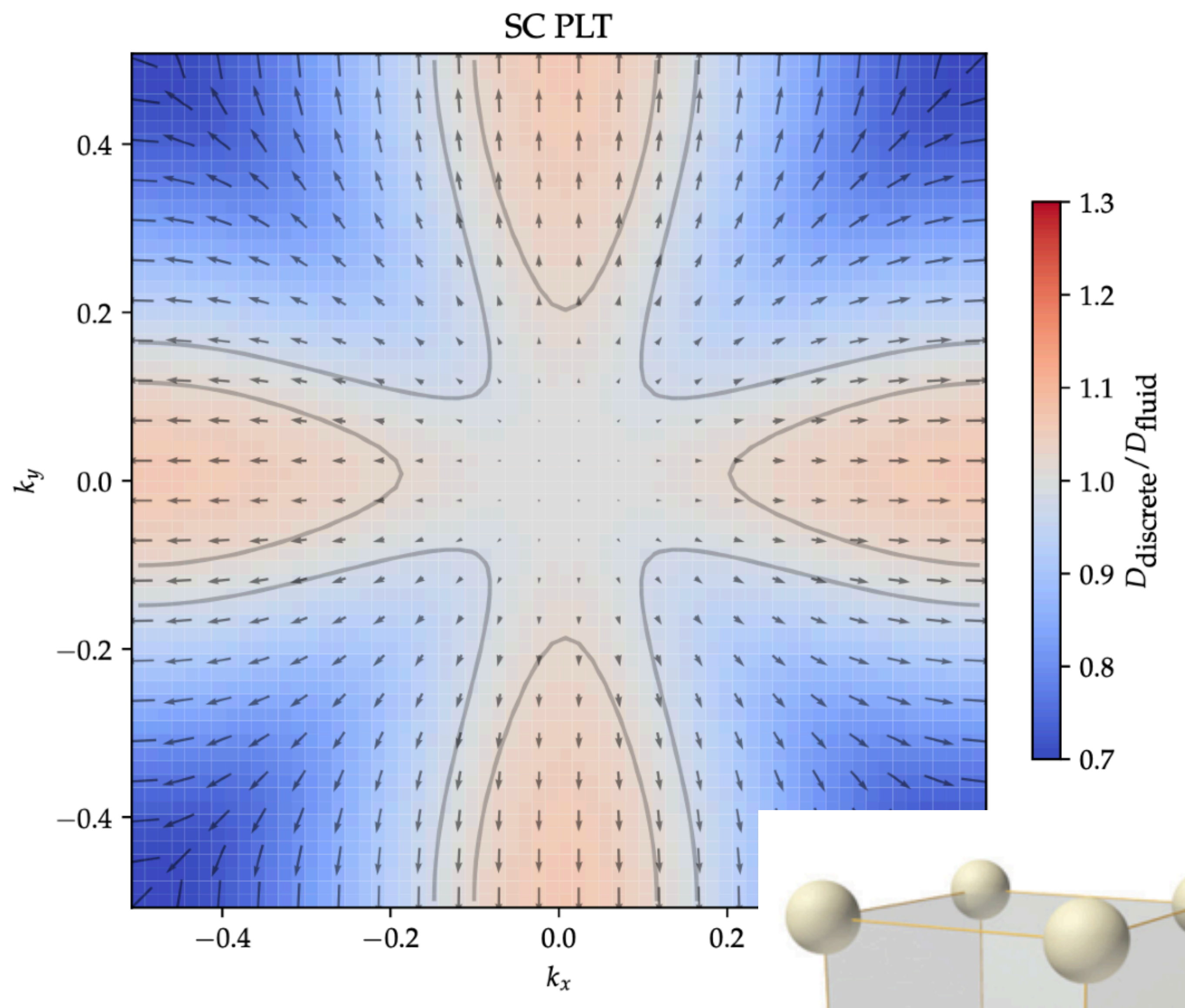
Michaux+2020

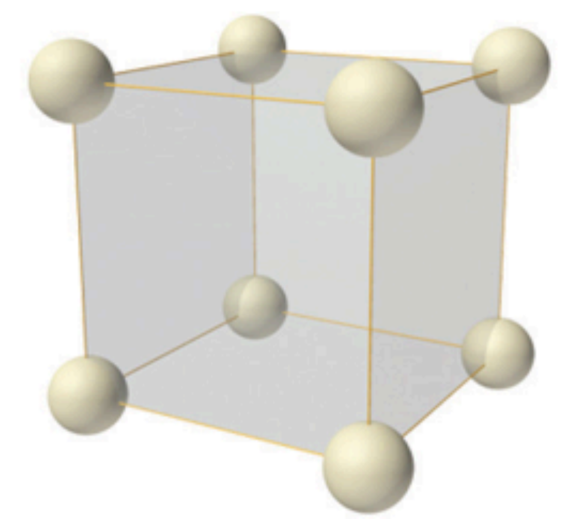
How is this possible? They model the same discrete set of modes

Two sources of error:

1) the nLPT truncation error (Scoccimarro 1998, Crocce+2006) aka 'transients'
2) the N-body discreteness (and force) errors:







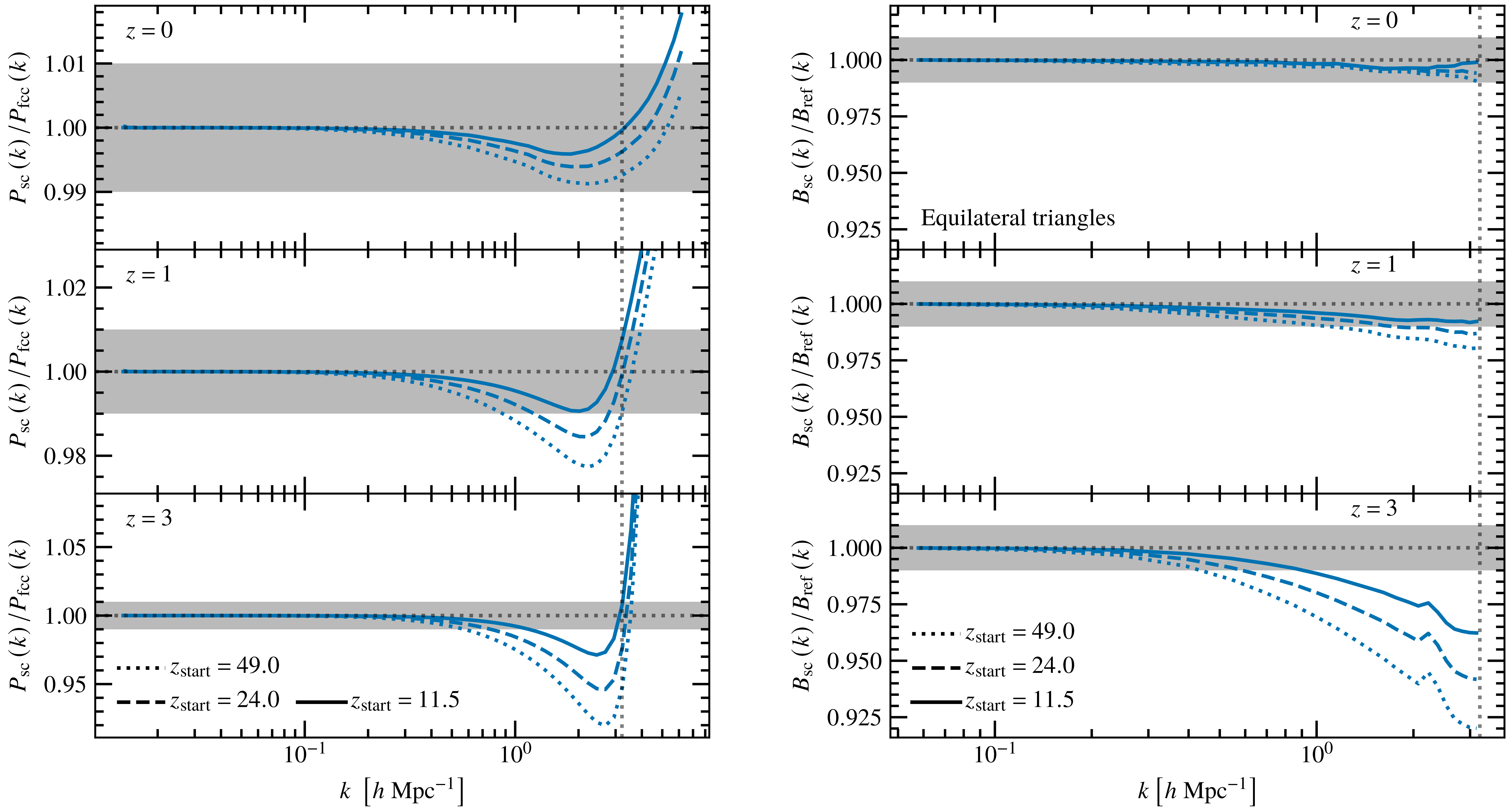
SC
(simple cubic)

cf. PLT of Joyce+2005, Joyce&Marcos 2007, Marcos 2008, but also Garrison+2016

Discreteness — impact on low-z spectra

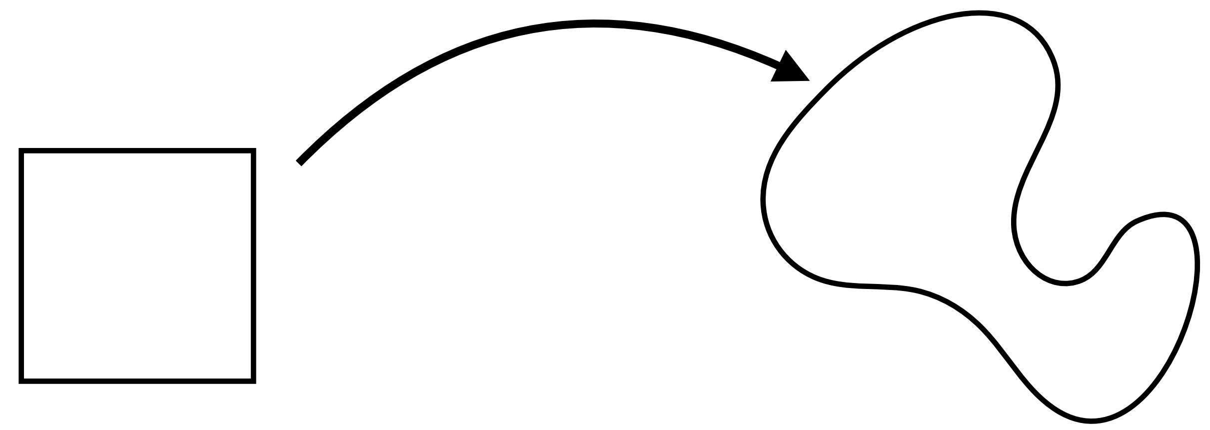
effect at low z wiped out by non-linearity (scale-mixing, asymptotic halo profiles), but not at higher z

Michaux+2020



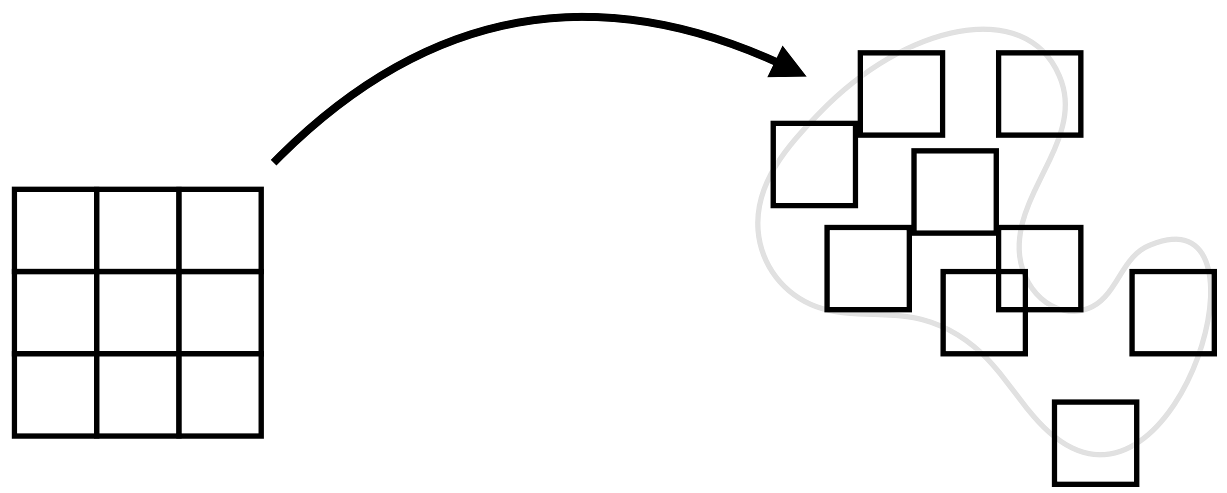
fluid-limit

$\mathbb{Q} \subset \mathbb{R}^3 \to \mathbb{R}^6\ :\ \mathbf{q} \mapsto (\mathbf{x}_\mathbf{q}(t), \mathbf{v}_\mathbf{q}(t))$



discrete case

$i \in \{1 \dots N\} \mapsto (\mathbf{x}_i, \mathbf{v}_i)$



should start late for smaller errors (LPT more correct than N-body while valid)

(cf. also Marcos 2008)

So nLPT wins? use N-body only to go where nLPT cannot?

Time integrators, what do they do

Lump all phase space coordinates together $\boldsymbol{\xi}_j := (\boldsymbol{X}, \boldsymbol{P})_j$

Then Hamiltonian EoMs are a first order operator equation

$$\dot{\boldsymbol{\xi}}_j = \hat{\mathscr{H}}(t)\,\boldsymbol{\xi}_j \qquad \text{with} \qquad \hat{\mathscr{H}}(t) := \{\cdot, \mathscr{H}(t)\} = \{\cdot, \alpha T\} + \{\cdot, \beta V\} =: \hat{D}(t) + \hat{K}(t).$$

With formal solution

$$\boldsymbol{\xi}_j(t) = \mathcal{T}\exp\left[\int_0^t \mathrm{d}t'\,\hat{\mathscr{H}}(t')\right]\boldsymbol{\xi}_j(0)$$

Now apply Strang operator splitting to find coefficients consistent with an expansion to order m

$$\mathcal{T}\exp\left[\int_t^{t+\epsilon} \mathrm{d}t'\,\hat{\mathscr{H}}(t')\right] \simeq \exp\left[\epsilon_n \hat{K}\right]\cdots\exp\left[\epsilon_3 \hat{D}\right]\,\exp\left[\epsilon_2 \hat{K}\right]\,\exp\left[\epsilon_1 \hat{D}\right] + \mathcal{O}(\epsilon^m).$$

Finally expand operator exponentials into generators

$$\boldsymbol{\xi}_j(\tilde{t}+\epsilon) = \left(I + \frac{\epsilon}{2}\hat{D}\right)\left(I + \epsilon\hat{K}\right)\left(I + \frac{\epsilon}{2}\hat{D}\right)\boldsymbol{\xi}_j(\tilde{t})$$

Better time integrators for LSS studies

Definition 1 (Canonical DKD integrator)**.**

$$\boldsymbol{X}_i^{n+1/2} = \boldsymbol{X}_i^n + \alpha(\tau_n, \tau_{n+1})\boldsymbol{P}_i^n,$$
$$\boldsymbol{P}_i^{n+1} = \boldsymbol{P}_i^n + \beta(\tau_n, \tau_{n+1})\boldsymbol{A}\left(\boldsymbol{X}_i^{n+1/2}\right),$$
$$\boldsymbol{X}_i^{n+1} = \boldsymbol{X}_i^{n+1/2} + \gamma(\tau_n, \tau_{n+1})\boldsymbol{P}_i^{n+1},$$

Given some conditions on the coefficients, the integrator is globally 2nd order, if $\boldsymbol{A}$ is sufficiently smooth

Consider also more restrictive form (List&OH 23):

Definition 2 (Π-integrator)**.**

$$\boldsymbol{X}_i^{n+1/2} = \boldsymbol{X}_i^n + \frac{\Delta D}{2}\boldsymbol{\Pi}_i^n,$$
$$\boldsymbol{\Pi}_i^{n+1} = p(\Delta D, D_n)\boldsymbol{\Pi}_i^n + q(\Delta D, D_n)\boldsymbol{A}(\boldsymbol{X}_i^{n+1/2}),$$
$$\boldsymbol{X}_i^{n+1} = \boldsymbol{X}_i^{n+1/2} + \frac{\Delta D}{2}\boldsymbol{\Pi}_i^{n+1},$$

Do N-body integrators reproduce LPT?

Should be able to get Zeldovich in **one** time step

Proposition 4 (Characterisation of Zel'dovich consistency). *A* Π*-integrator is Zel'dovich consistent if and only if* $p(\Delta D, D_n)$ *and* $q(\Delta D, D_n)$ *satisfy the following relation:*

$$\frac{1 - p(\Delta D, D_n)}{q(\Delta D, D_n)} = \frac{3}{2}\Omega_m D_{n+1/2} \overset{\text{EdS}}{\asymp} \frac{3}{2} a_{n+1/2} \, .$$

Example (FastPM). FastPM method of Feng et al. (2016), but this is the DKD version, while they used KDK

$$\begin{aligned}
\boldsymbol{X}_i^{n+1/2} &= \boldsymbol{X}_i^n + \frac{D_{n+1/2} - D_n}{F(D_n)} \boldsymbol{P}_i^n && \overset{\text{EdS}}{\asymp} \boldsymbol{X}_i^n + \frac{\Delta a}{2a_n^{3/2}}, \\
\boldsymbol{P}_i^{n+1} &= \boldsymbol{P}_i^n + \frac{F(D_{n+1}) - F(D_n)}{G(D_{n+1/2})} \boldsymbol{A}(\boldsymbol{X}^{n+1/2}) && \overset{\text{EdS}}{\asymp} \boldsymbol{P}_i^n + \frac{2}{3} \frac{a_{n+1}^{3/2} - a_n^{3/2}}{a_{n+1/2}} \boldsymbol{A}(\boldsymbol{X}^{n+1/2}), \\
\boldsymbol{X}_i^{n+1} &= \boldsymbol{X}_i^{n+1/2} + \frac{D_{n+1} - D_{n+1/2}}{F(D_{n+1})} \boldsymbol{P}_i^{n+1} && \overset{\text{EdS}}{\asymp} \boldsymbol{X}_i^{n+1/2} + \frac{\Delta a}{2a_{n+1}^{3/2}},
\end{aligned}$$

FastPM is the unique Π*-integrator that is both Zel'dovich consistent and symplectic.*

Proof of symplecticity, consistency, and convergence order see List&OH 23 (not done in Feng+12)

Counterexample. All integrators typically used for N-body simulations are not Zel'dovich consistent.

Can we do even better?

Spoiler: yes, but have to give up symplecticity

Second order LPT (2LPT) can be written

$$\boldsymbol{X}_i(D) = \boldsymbol{X}_i^n + [D - D_n]\boldsymbol{\psi}_i^{n,(1)} + [D - D_n]^2\boldsymbol{\psi}_i^{n,(2)}$$

$$\mathrm{d}_D \boldsymbol{X}_i(D) = \boldsymbol{\psi}_i^{n,(1)} + 2[D - D_n]\boldsymbol{\psi}_i^{n,(2)},$$

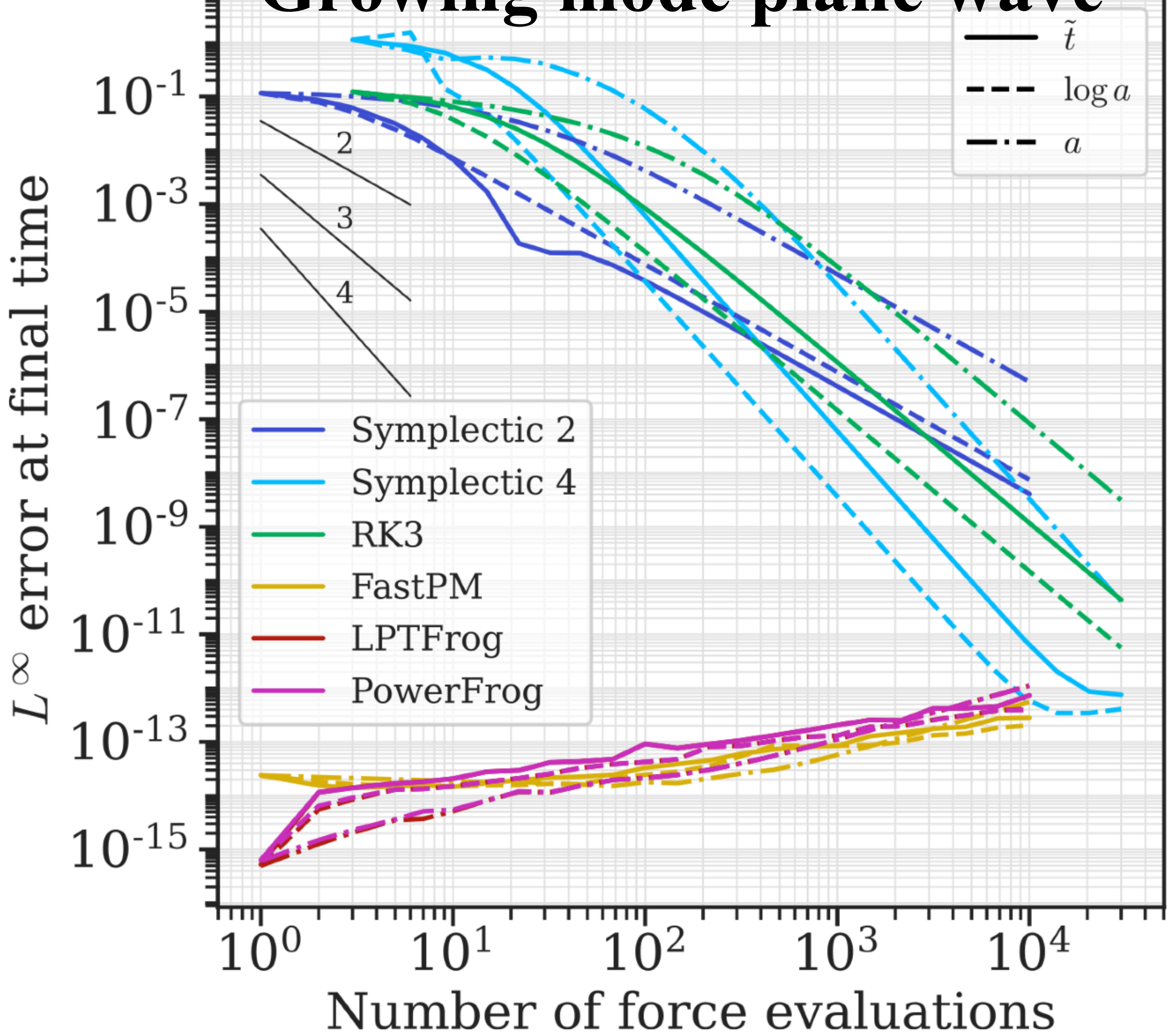
$$\mathrm{d}_D^2 \boldsymbol{X}_i(D) = 2\boldsymbol{\psi}_i^{n,(2)} = \text{const.}$$

i.e. acceleration is constant

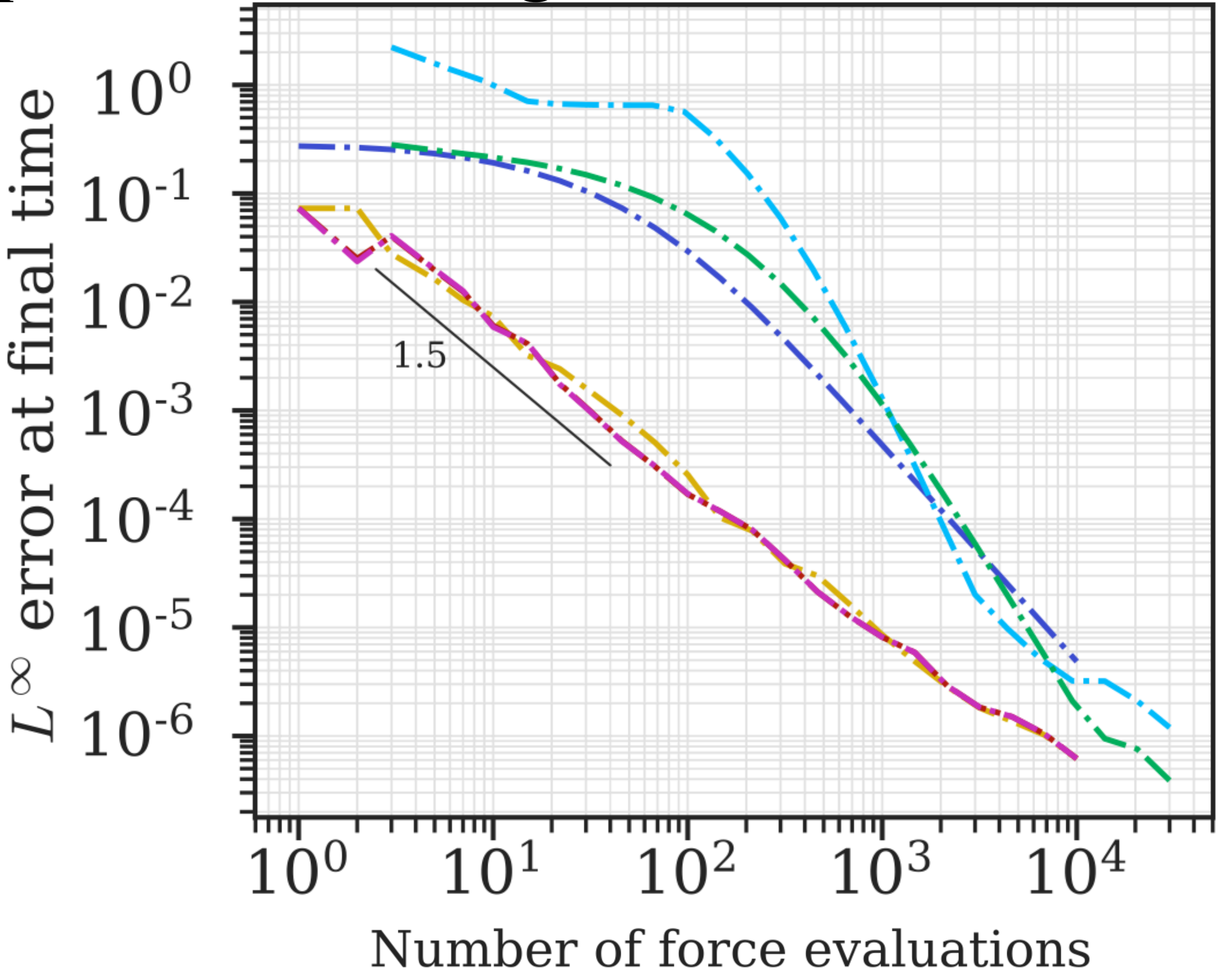
This can be matched in various ways to yield new integrators that should reproduce 2LPT, not only Zeldovich.

Tests for 1D collapse

Growing mode plane wave

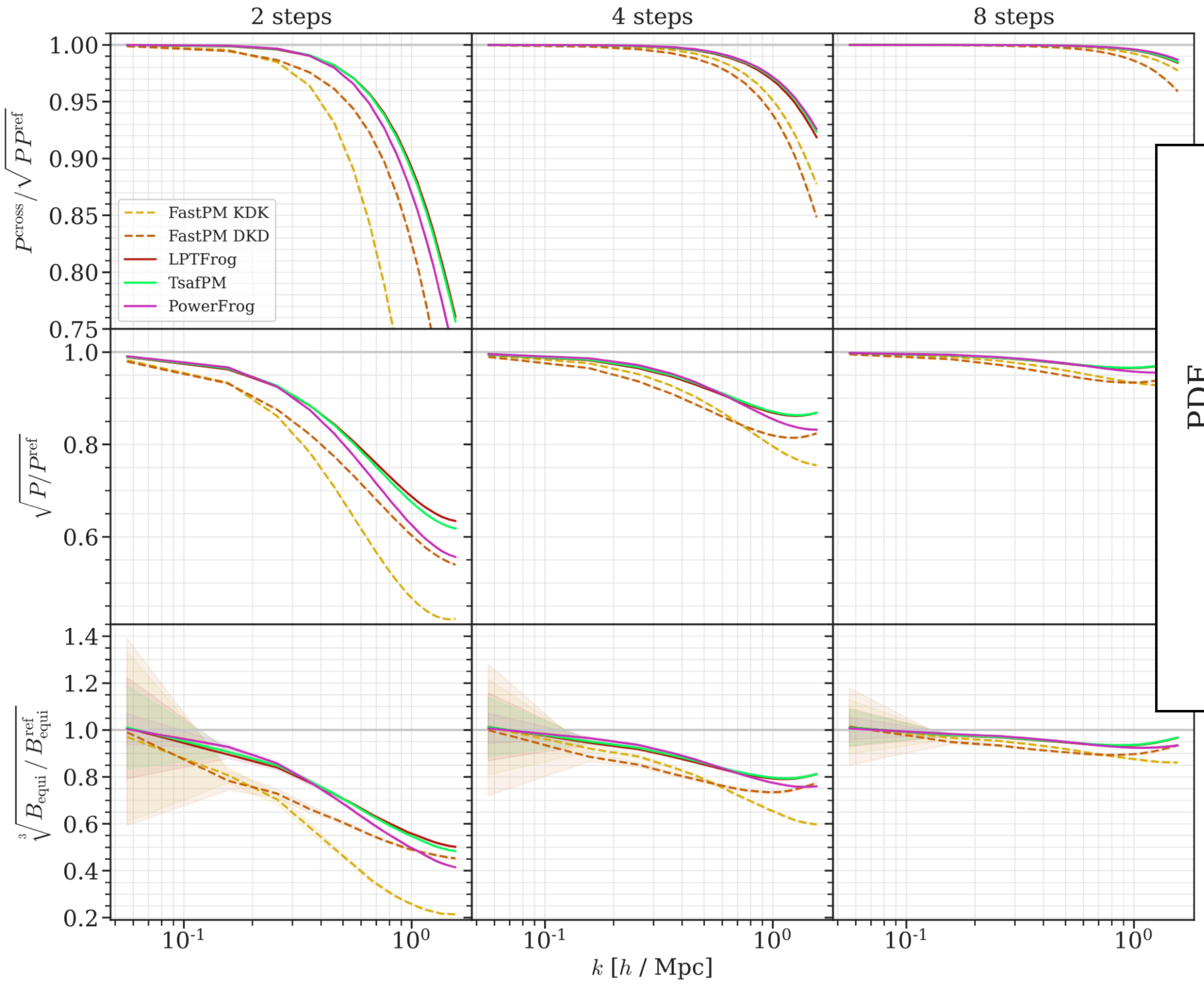


post shell-crossing: a

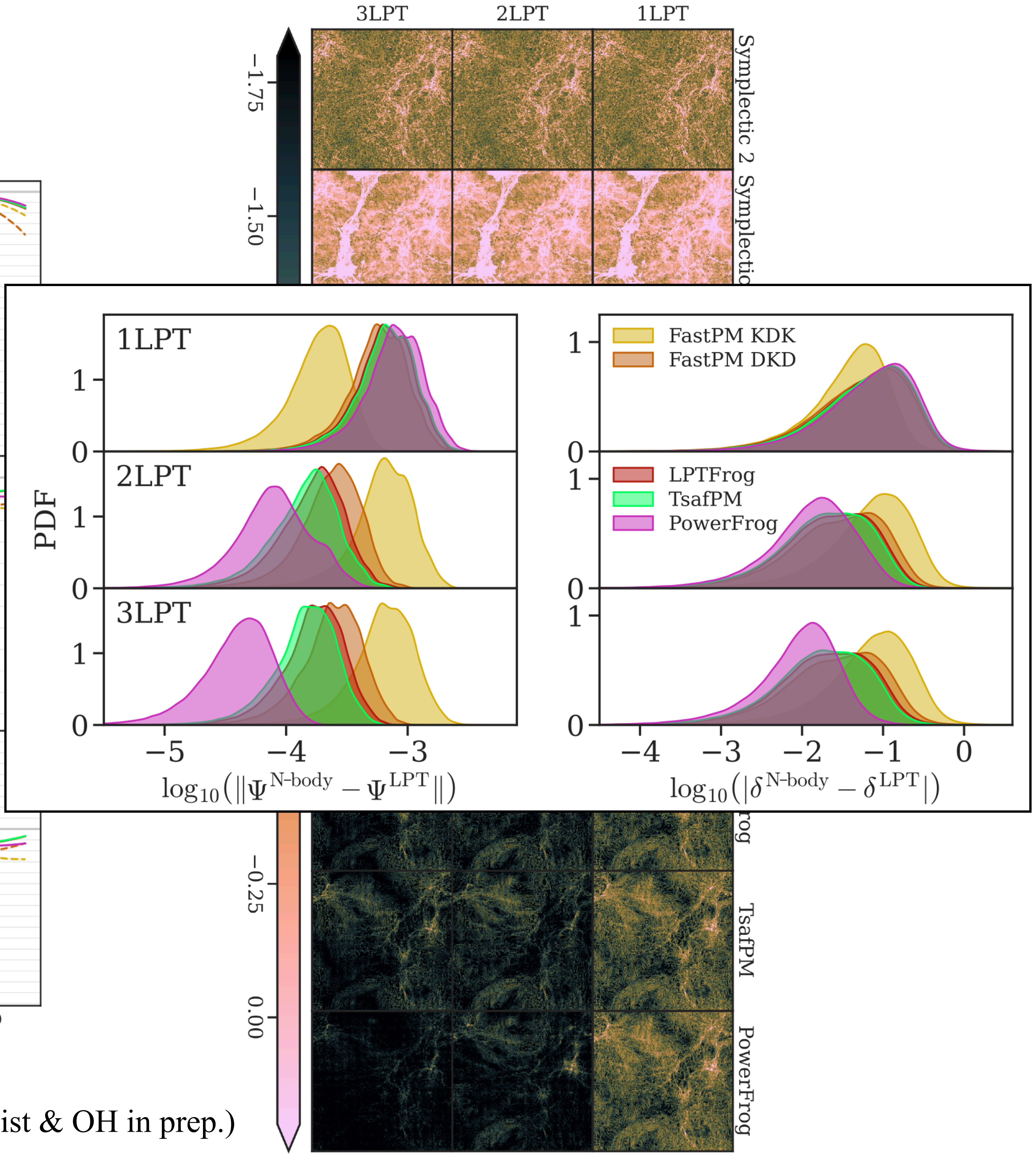


Tests in 2D and 3D

Quijote simulation at z=0



Comparison to nLPT



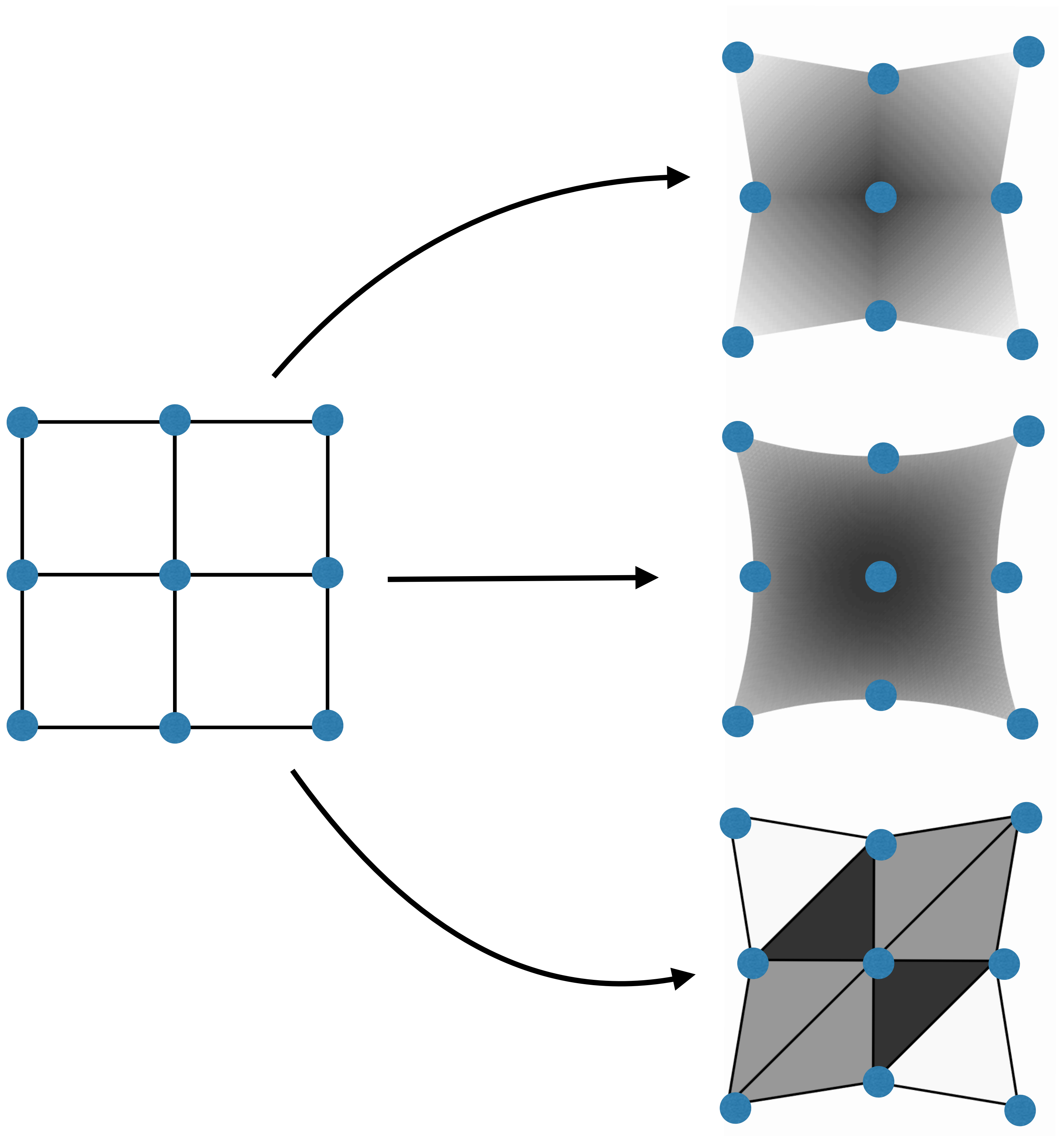
List&Hahn23

(+another new integrator Rampf, List & OH in prep.)

What do we need nLPT for now?

integrator is 2.5LPT,
but can we beat discreteness?

Beyond N-body - tessellation/resampling methods



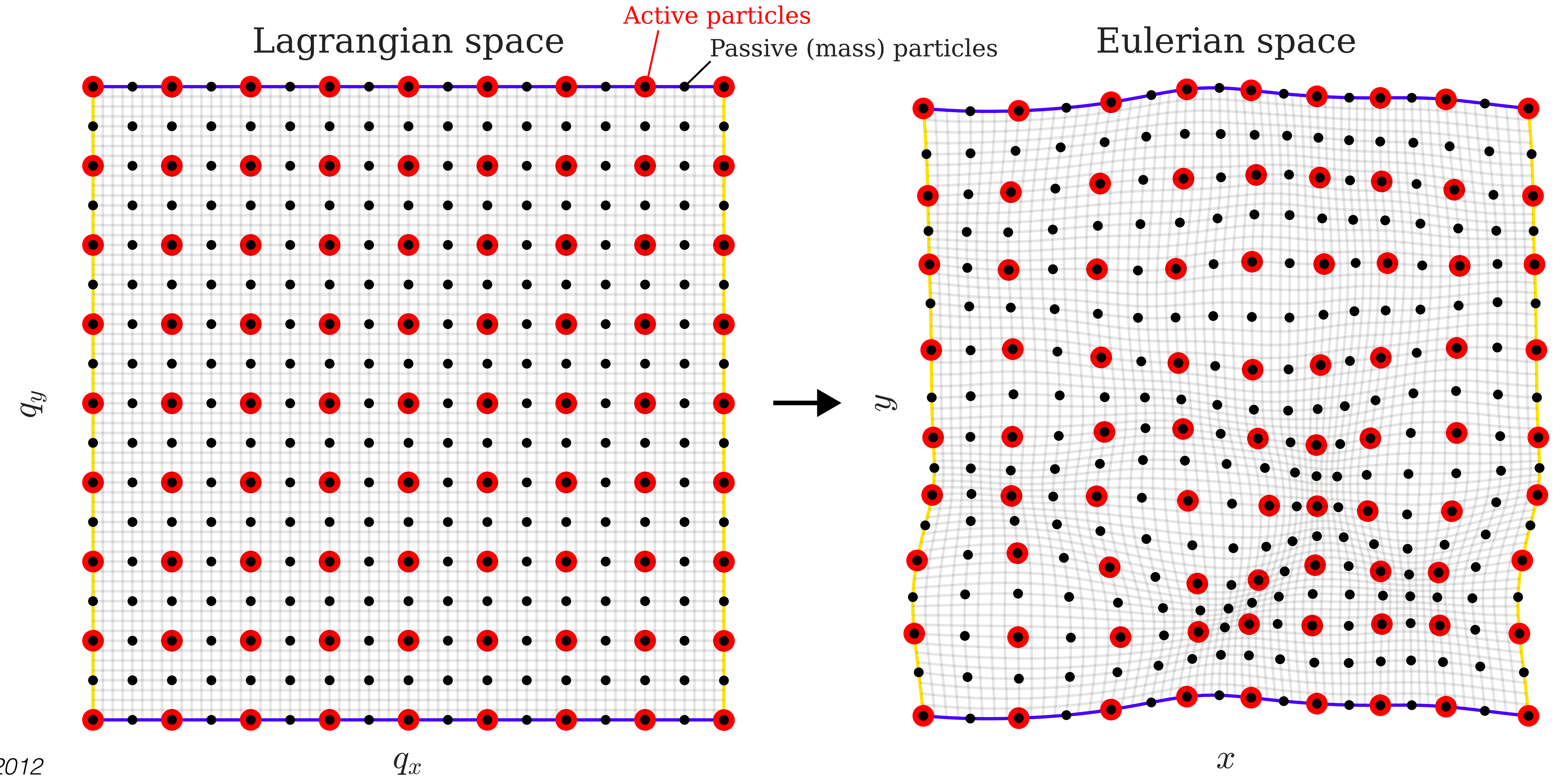
k=1
bi/tri-linear
Hahn&Angulo 2016

k=2
bi/tri-quadratic
Hahn&Angulo 2016

affine map/
simplicial complex

tetrahedral
Abel, Hahn & Kaehler 2012
Schandarin et al. 2012

Sousbie&Colombi 2015
*(also **quadratic** tetrahedra)*



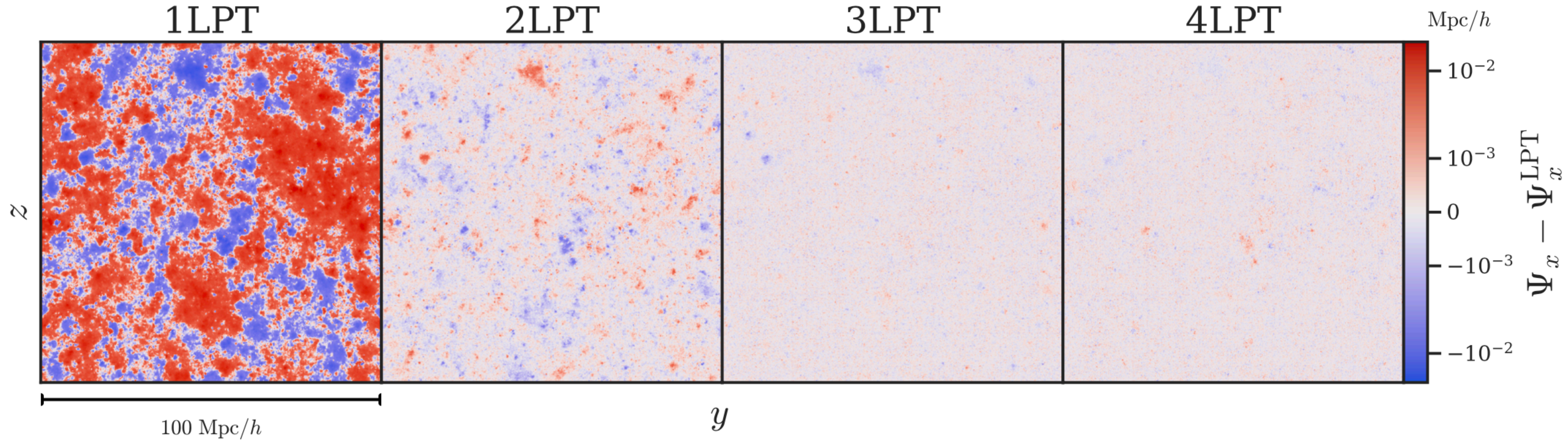
or spectral interpolation (Stücker+2020; List, OH, Rampf 2024)

Unifying LPT and N-body: ICs without "LPT"

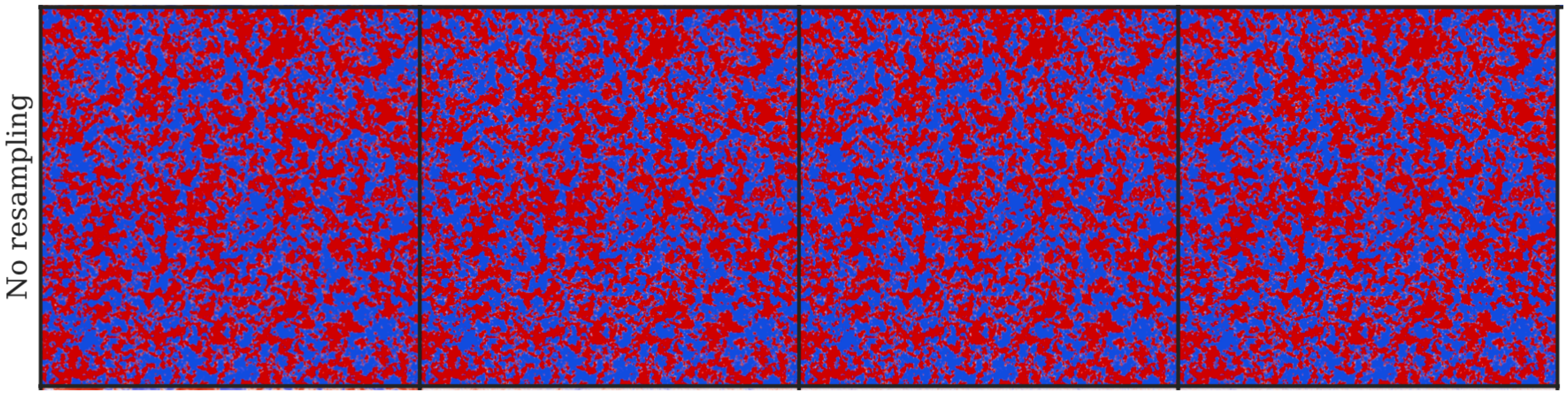
List, OH & Rampf, PRD 2024

PowerFrog integrator is asymptotically consistent with 2LPT for a→0, **can start at a=0** as we do in LPT

Residual of **single PowerFrog step** from a=∞ to a=0.05, wrt. nLPT:

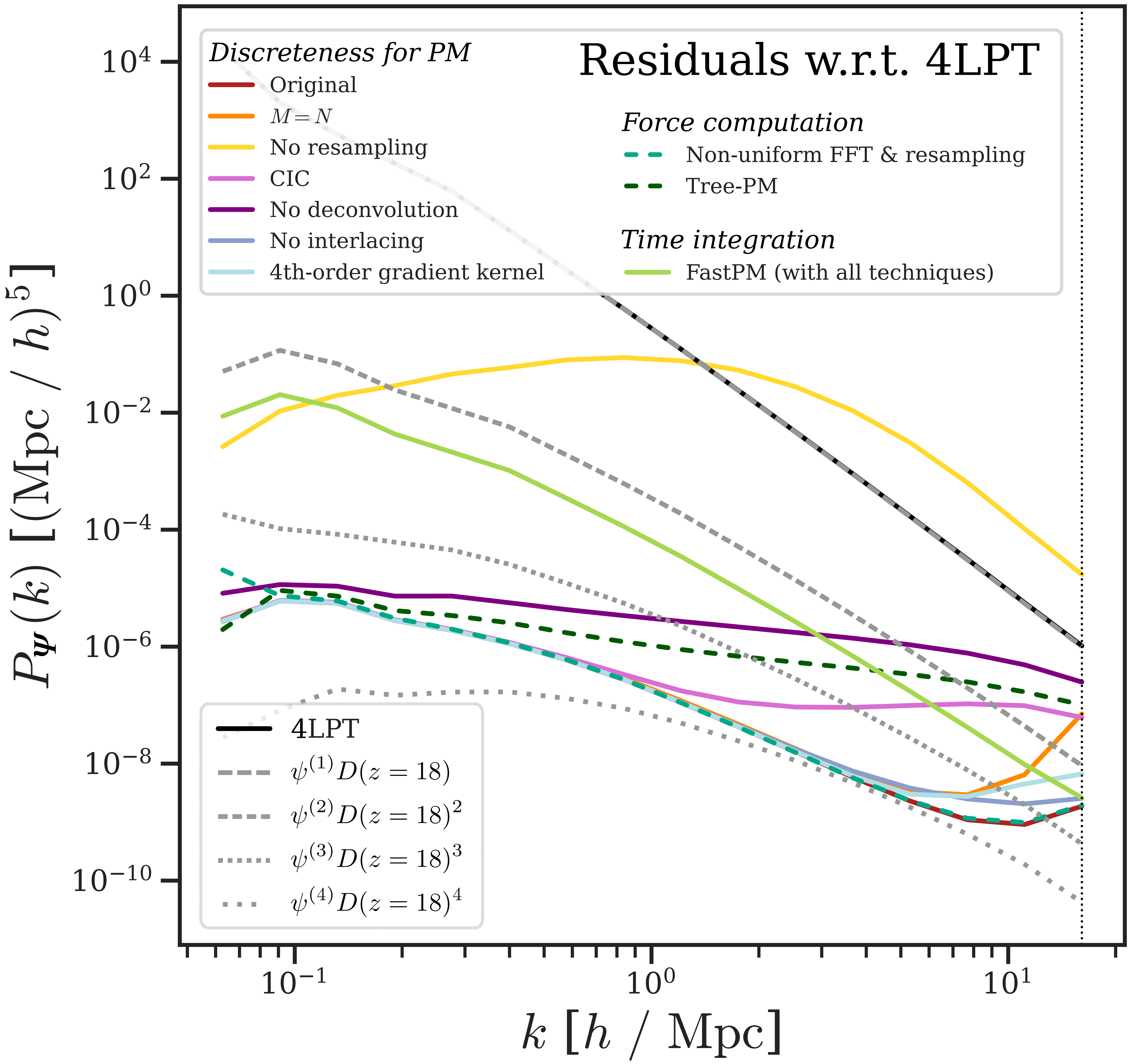


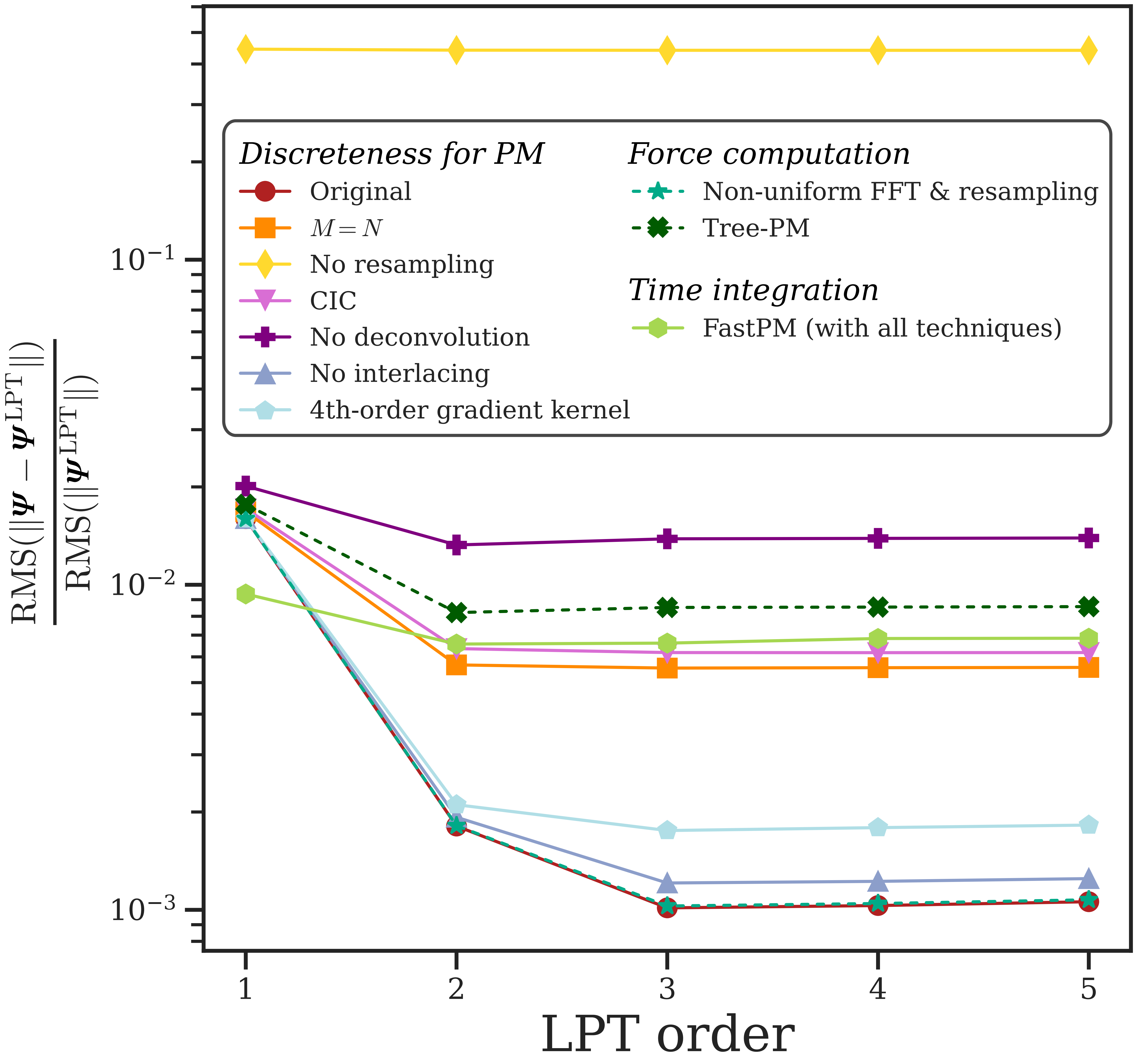
This is only possible after controlling **all** discreteness effects and approx. errors in the N-body simulation, otherwise:



Unifying LPT and N-body: ICs without “LPT”

Errors at “IC” time (a=0.05)

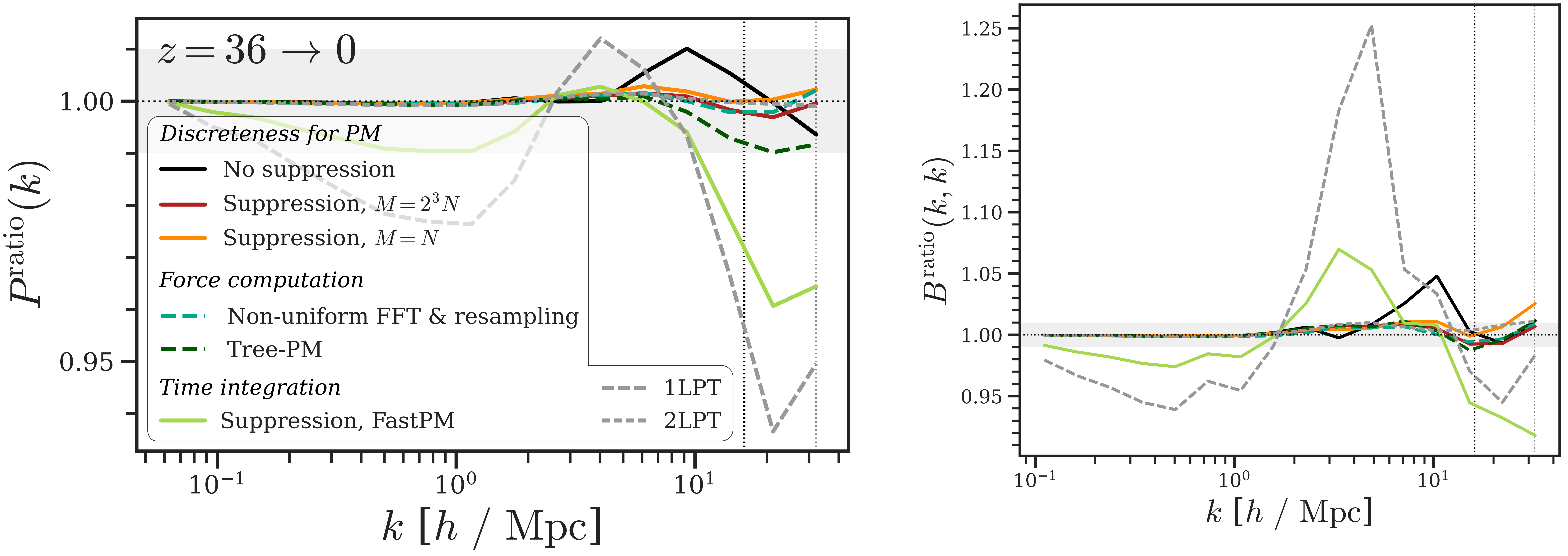




List, OH & Rampf, PRD 2024

Unifying LPT and N-body: ICs without “LPT”

Errors at final time (powerfrog step to z=36, then standard Gadget-4 N-body run)



List, OH & Rampf, PRD 2024

SUMMARY

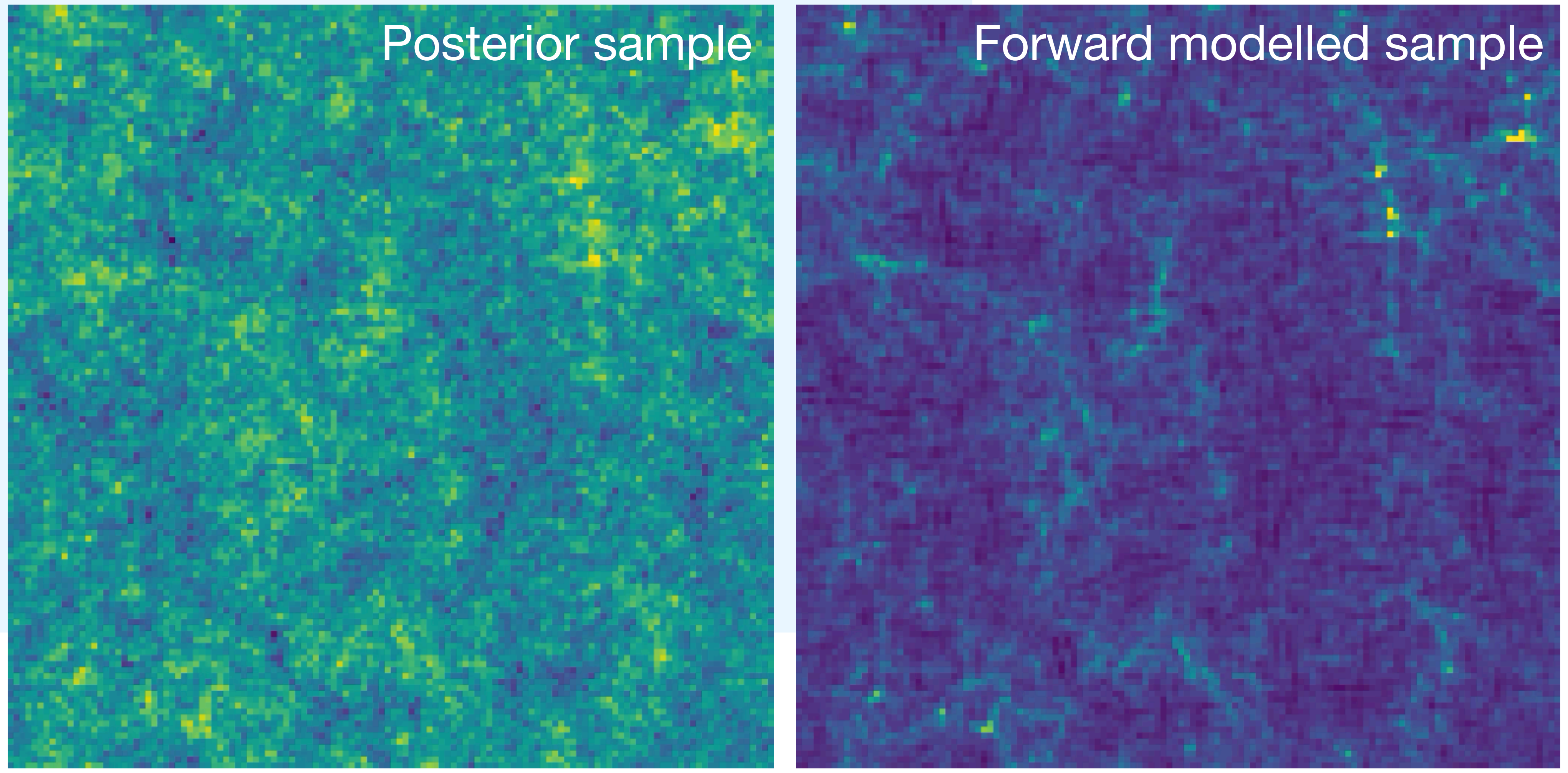
- LPT has key role in ICs for cosmological simulations, or as a field-level forward model
- Demonstrated convergence of LPT beyond shell-crossing, slow convergence due to SC singularities
- 3LPT needed for precision era N-body simulations, push to late starts to reduce errors
- new LPT inspired integrators (beyond ‘FastPM’) for fast simulations
- can now replace LPT initial conditions with N-body

SUMMARY

- LPT has key role in ICs for cosmological simulations, or as a field-level forward model
- Demonstrated convergence of LPT before shell-crossing, slow convergence due to SC singularities
- 3LPT needed for highest precision N-body simulations, push to late starts to reduce errors
- many new LPT inspired integrators (beyond ‘FastPM’) possible for fast simulations
- now possible to replace nLPT initial conditions with N-body, particularly interesting for inference

DISCO-DJ
differentiable simulations for cosmology
done with jax

- n-LPT recursion
- all fast time integration methods (‘ultimate’ Rampf, List, OH, in prep.)
- discreteness suppression/sheet interpolation, NUFFT,…
- GPU based (run 512^3 in seconds)
- forward and backward differentiable
- has Einstein-Boltzmann module included (OH, List & Porqueres 2024)
- easy interface to inference
- **stay tuned…**



Inversion movie by Lukas Winkler