



universität  
wien

# Large-scale structure at the interface of numerical and analytical techniques

**Oliver Hahn**

Institute for Astrophysics & Institute for Mathematics  
University of Vienna, Austria

with **Cornelius Rampf, Florian List, Cora Uhlemann, Michaël Michaux, Natalia Porqueres,  
Sonja Schobesberger, Raul Angulo, Mateja Gosenca**



universität  
wien

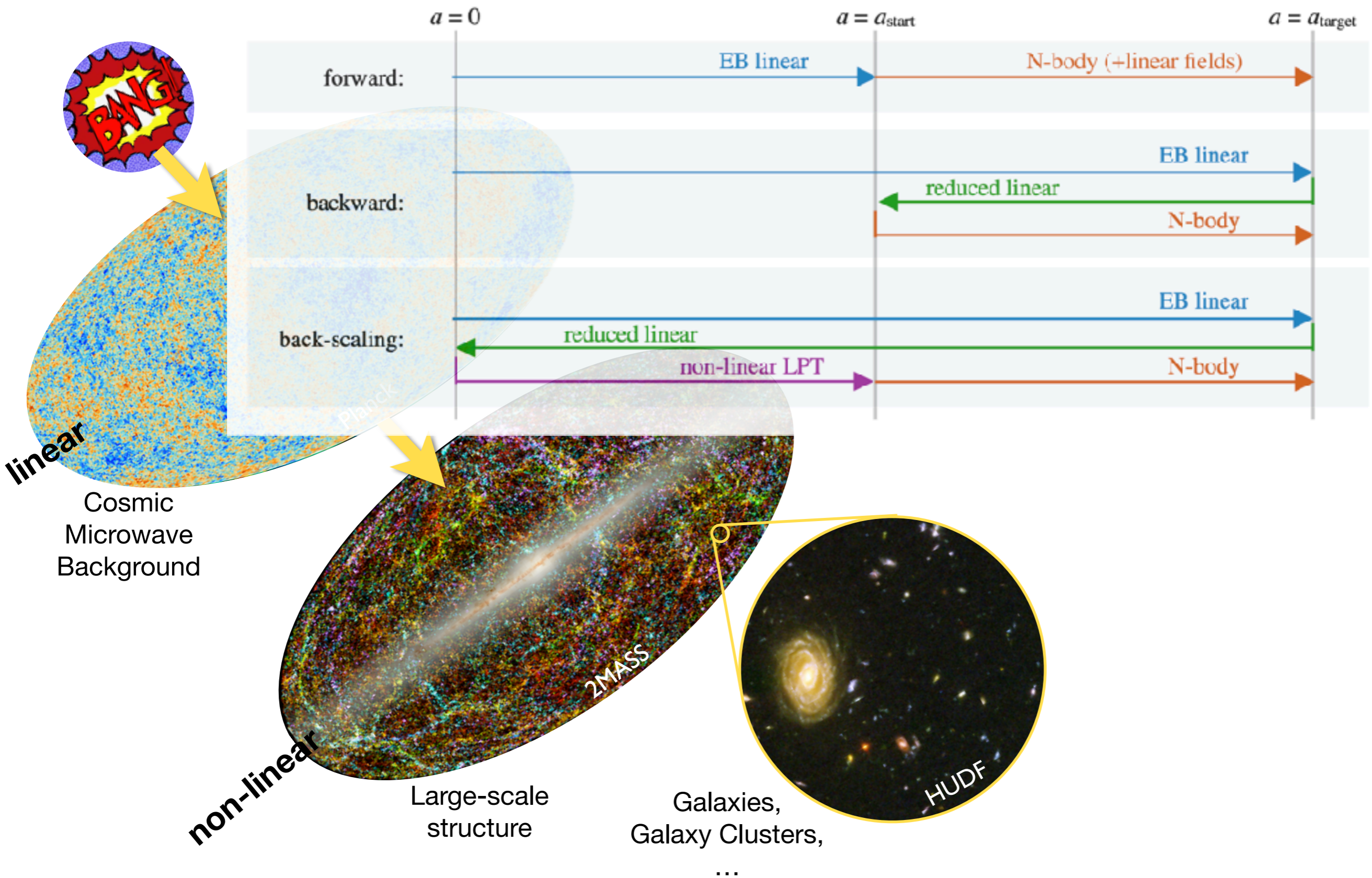
# Large-scale structure at the interface of numerical and analytical techniques

**Oliver Hahn**

Institute for Astrophysics & Institute for Mathematics  
University of Vienna, Austria

with **Cornelius Rampf, Florian List, Cora Uhlemann, Michaël Michaux, Natalia Porqueres,  
Sonja Schobesberger, Raul Angulo, Mateja Gosenca**

# The Inhomogeneous Universe: evolution

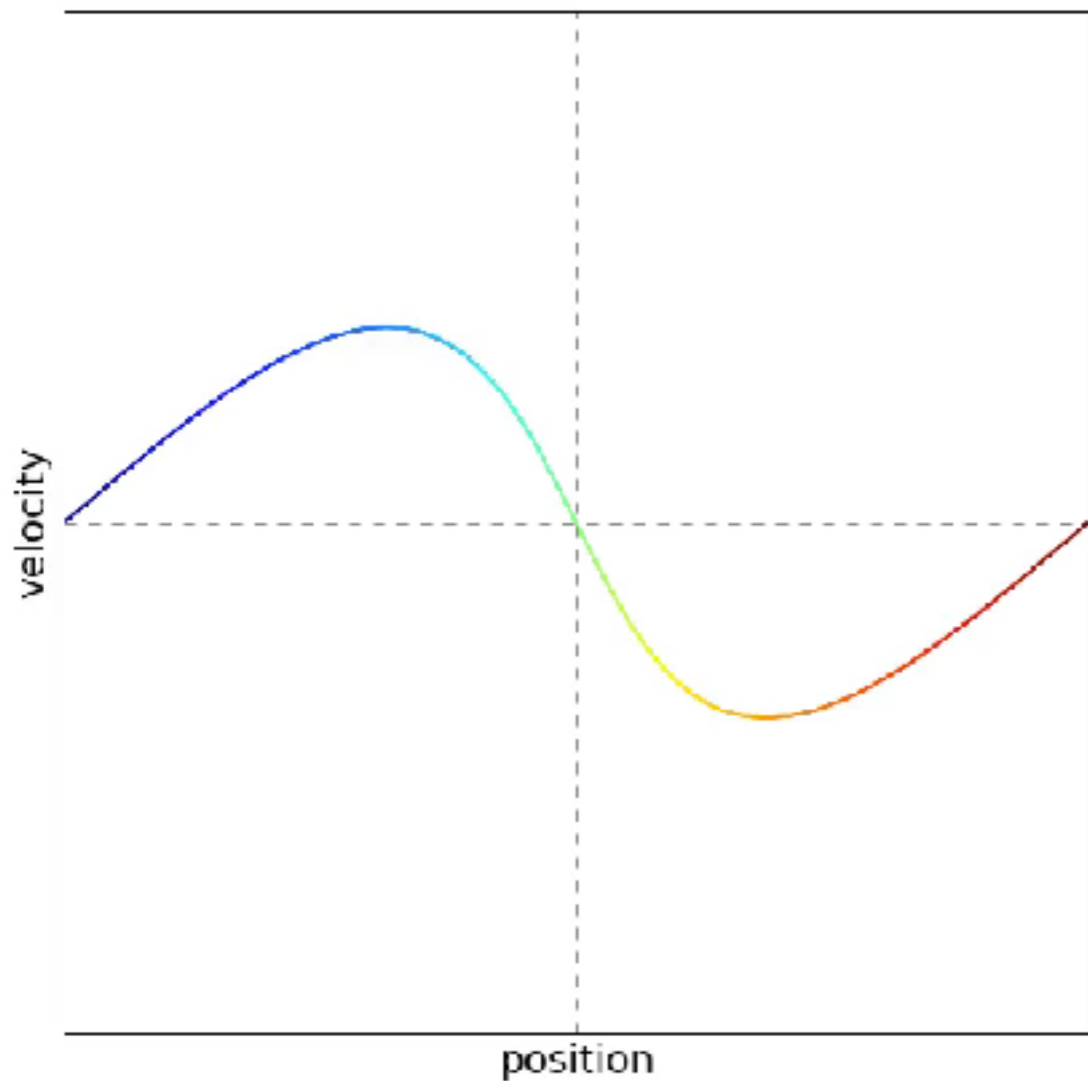


# Evolution of Fluctuations

## Cold Dark Matter lives on Lagrangian submanifold

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

$$\frac{\partial f_m}{\partial t} + \frac{p_i}{ma^2} \frac{\partial f_m}{\partial x^i} - m \frac{\partial \phi}{\partial x^i} \frac{\partial f_m}{\partial p_i} = 0 \quad \Leftrightarrow \quad \mathbf{x}'' + \mathcal{H}\mathbf{x}' = -\nabla\phi$$



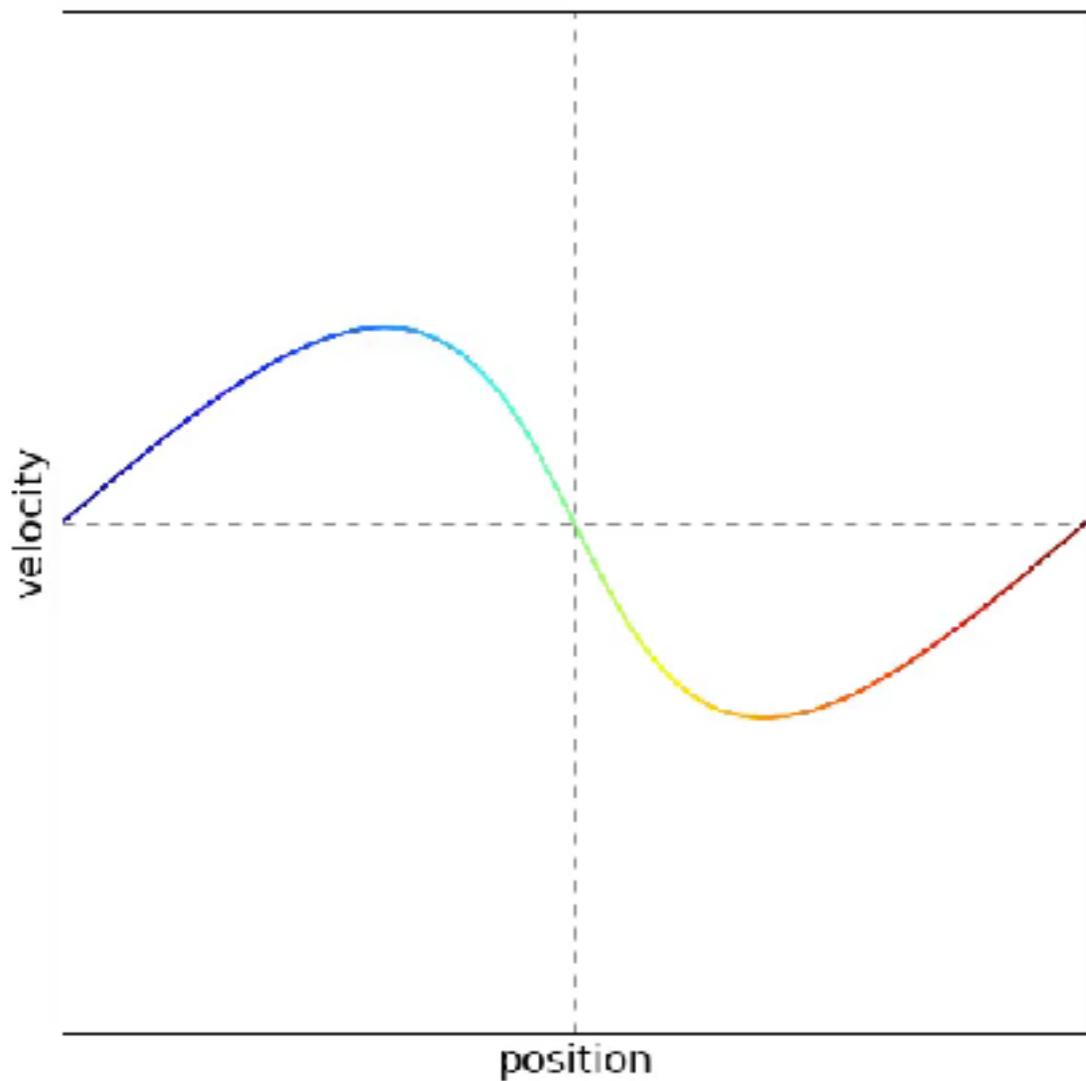
1D singularities: Rampf, Frisch & OH (2021)

# Evolution of Fluctuations

## Cold Dark Matter lives on Lagrangian submanifold

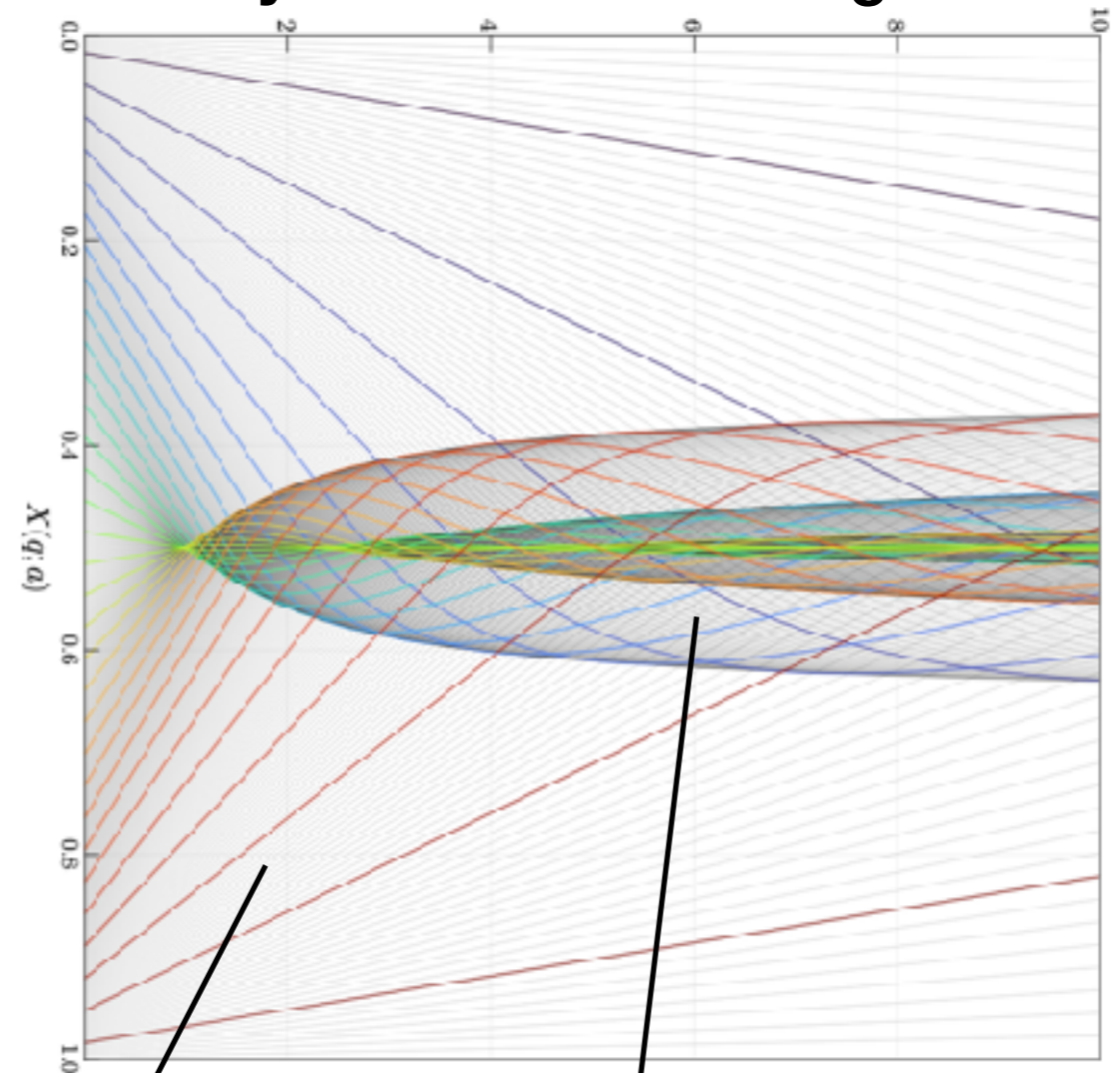
Solve Vlasov-Poisson on submanifold characteristics  $(q, t) \mapsto (x(q, t), p(q, t))$

$$\frac{\partial f_m}{\partial t} + \frac{p_i}{ma^2} \frac{\partial f_m}{\partial x^i} - m \frac{\partial \phi}{\partial x^i} \frac{\partial f_m}{\partial p_i} = 0 \quad \Leftrightarrow \quad \mathbf{x}'' + \mathcal{H}\mathbf{x}' = -\nabla\phi$$



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

## density + acceleration singularities



**monokinetic,  
single-valued**  
(analytic treatment possible)

**multikinetic,  
multi-valued**  
(due to collisionless nature)

# Lagrangian Perturbation Theory

(for single fluid with cold initial data)

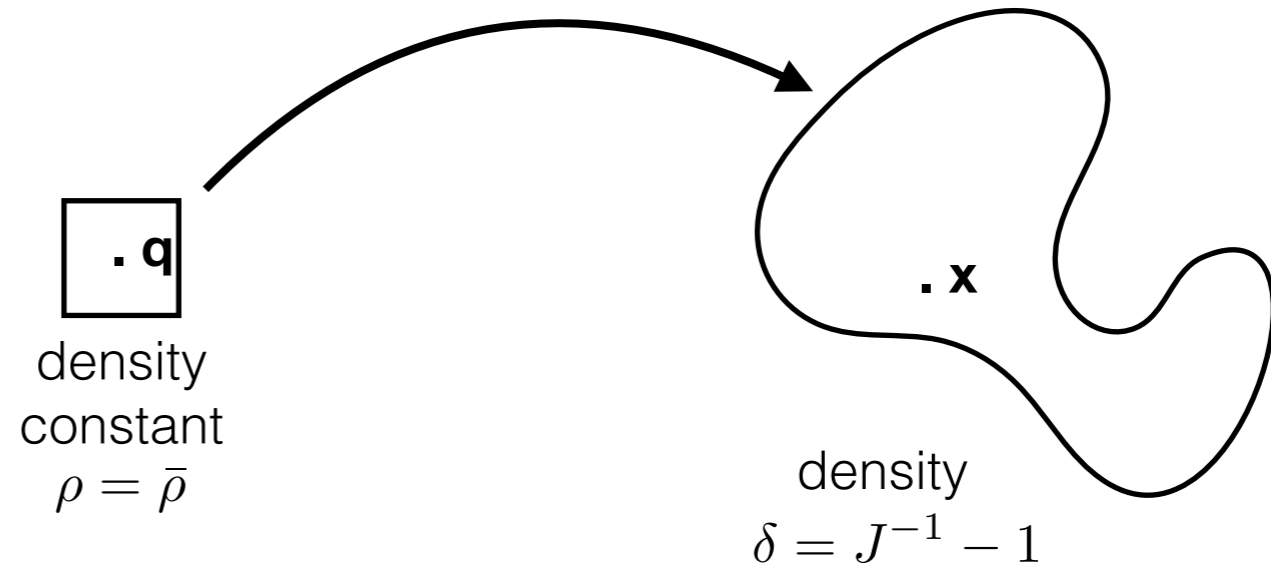
Lagrangian map

$$\mathbf{x}(\mathbf{q}, t) = \mathbf{q} + \mathbf{\Psi}(\mathbf{q}, t)$$

Overdensity given by Jacobian

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

$$J := \det \frac{\partial \mathbf{x}}{\partial \mathbf{q}}$$



# Lagrangian Perturbation Theory

(for single fluid with cold initial data)

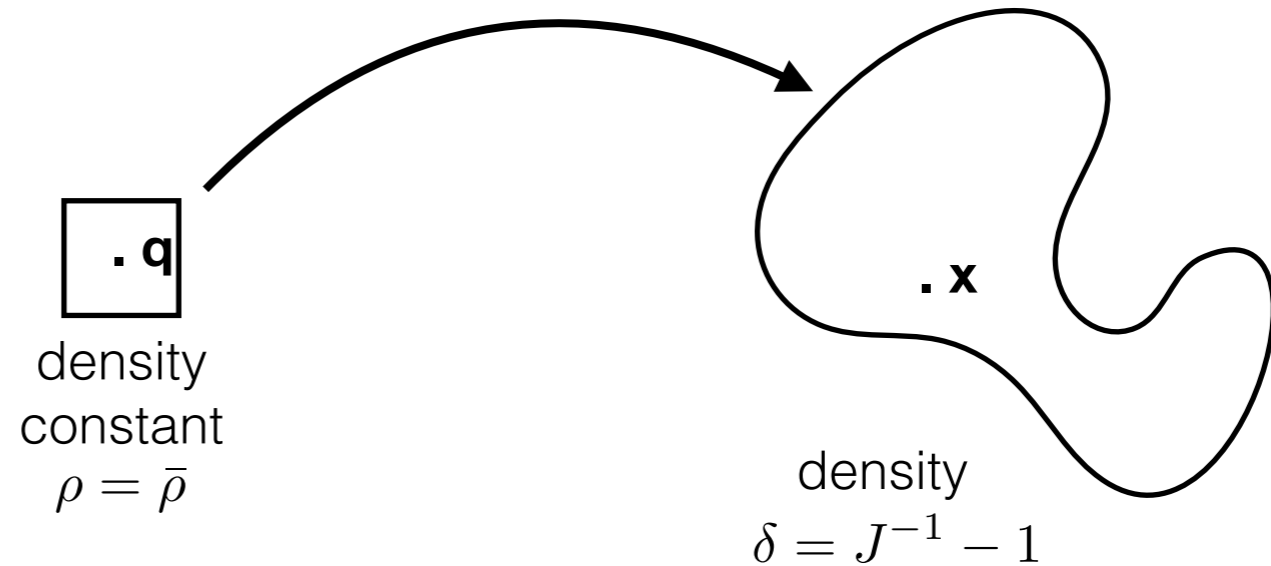
Lagrangian map

$$\mathbf{x}(\mathbf{q}, t) = \mathbf{q} + \mathbf{\Psi}(\mathbf{q}, t)$$

Overdensity given by Jacobian

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

$$J := \det \frac{\partial \mathbf{x}}{\partial \mathbf{q}}$$



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

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

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

**We will go to  $n=3$  (3LPT), Michaux et al. (2021), and  $n$  very large, Rampf & Hahn (2021)**

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

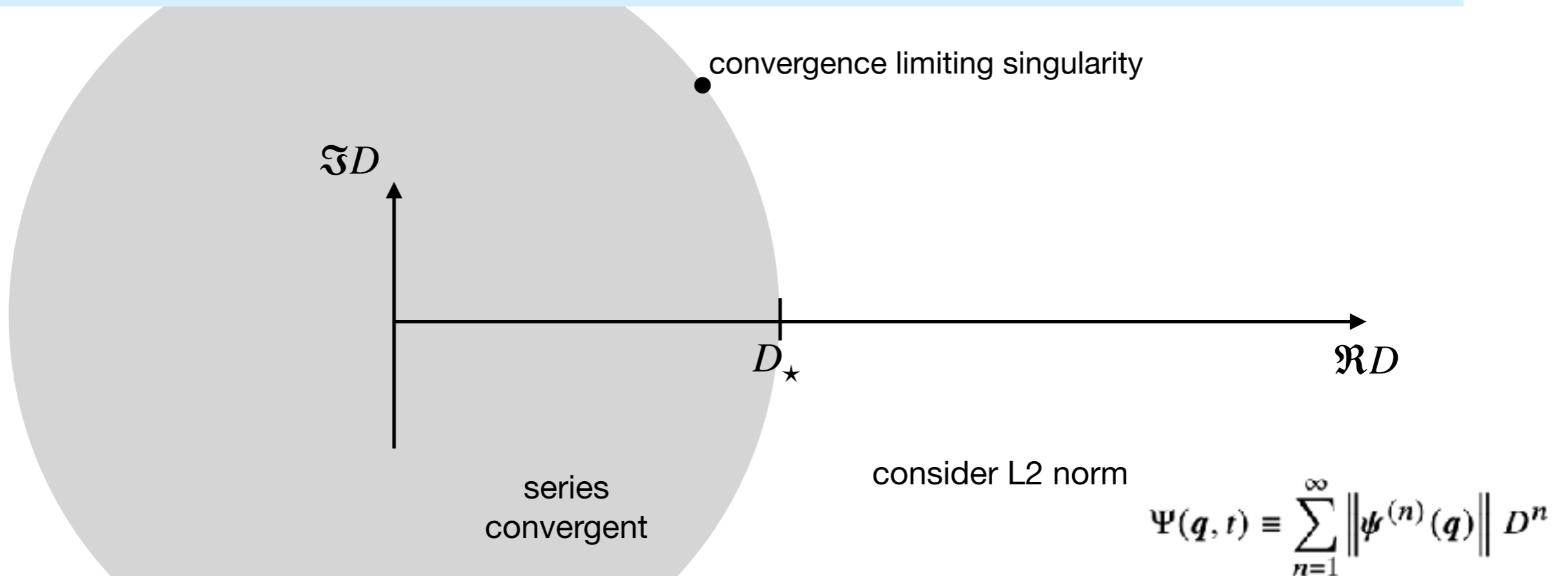
# Shell-crossing – the limit of LPT?

gives rise to cosmic structure, and marks the breakdown of cold limit

**BUT: Does LPT provide a convergent expansion until equations break down?**

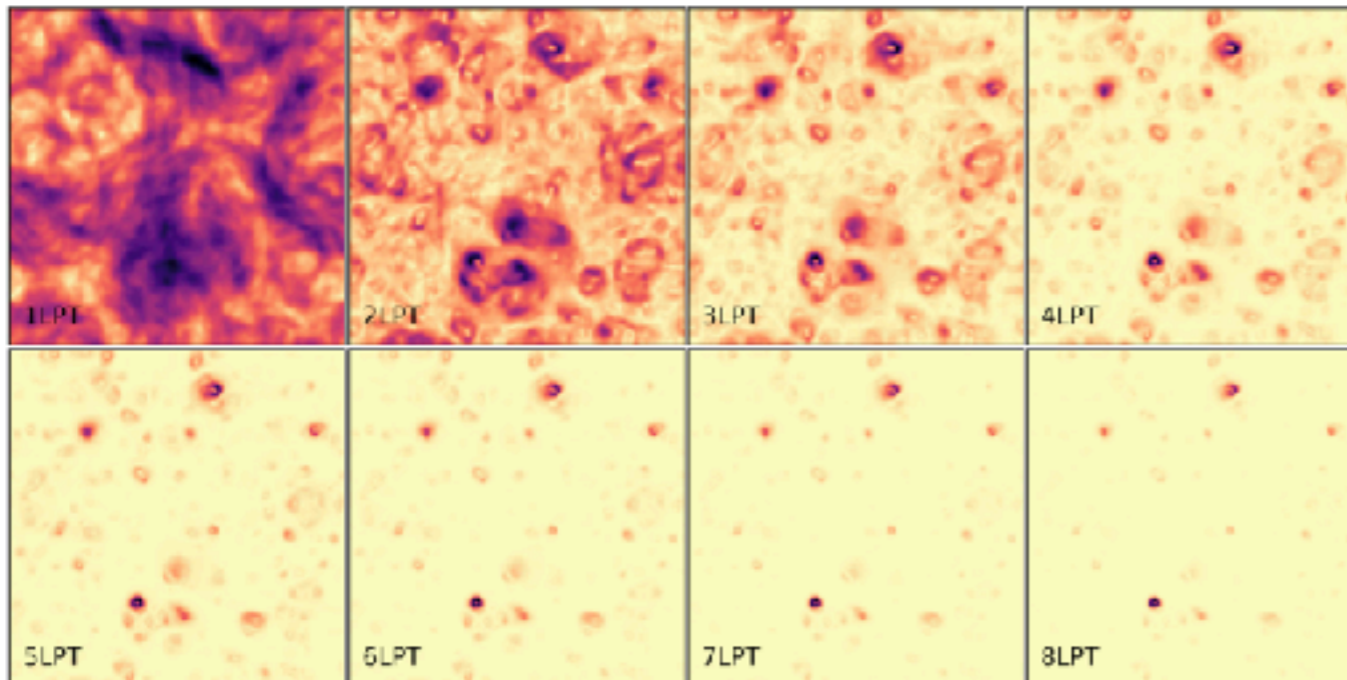
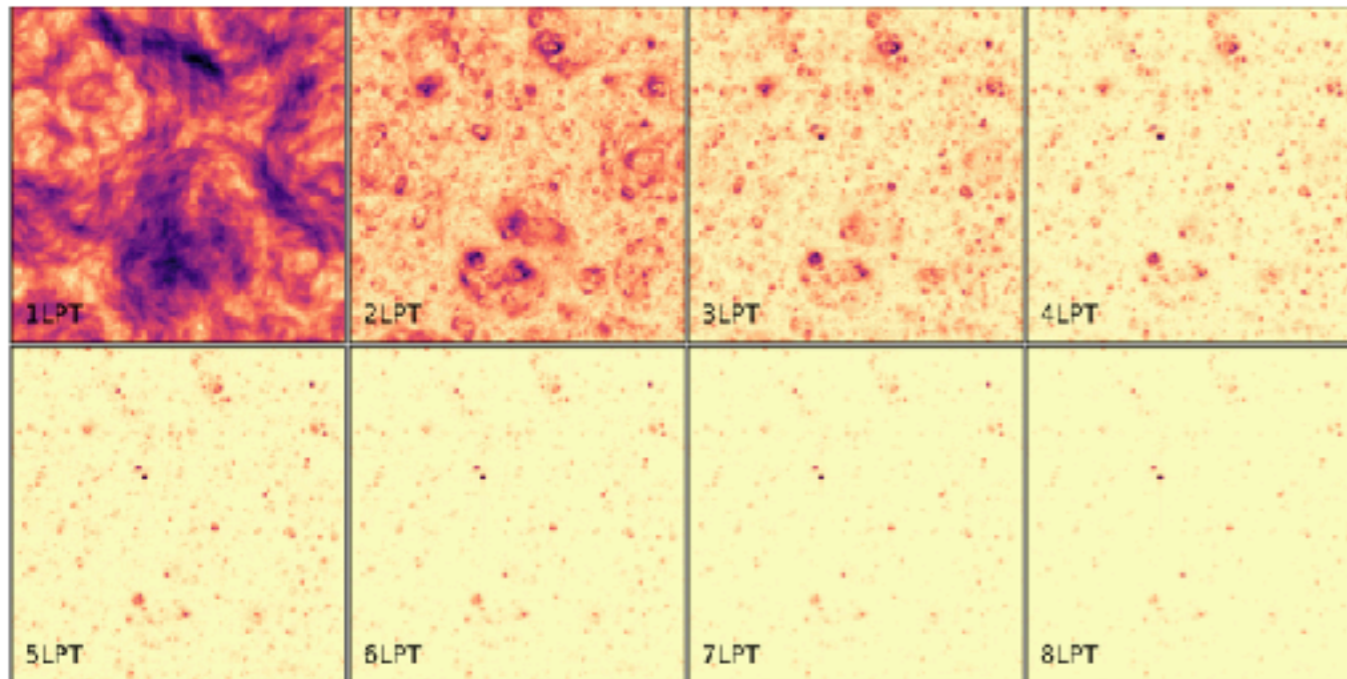
**LPT expansion:** 
$$\Psi(\mathbf{q}, \tau) = \sum_{n=1}^{\infty} D(\tau)^n \Psi^{(n)}(\mathbf{q})$$

It has never been shown if LPT is convergent and if so what is its radius of convergence for realistic (random) ICs





# To go where no-one has gone before...



until recently: 2LPT was state of art

Have now implementation of  
all-order recursion relations  
of LPT!

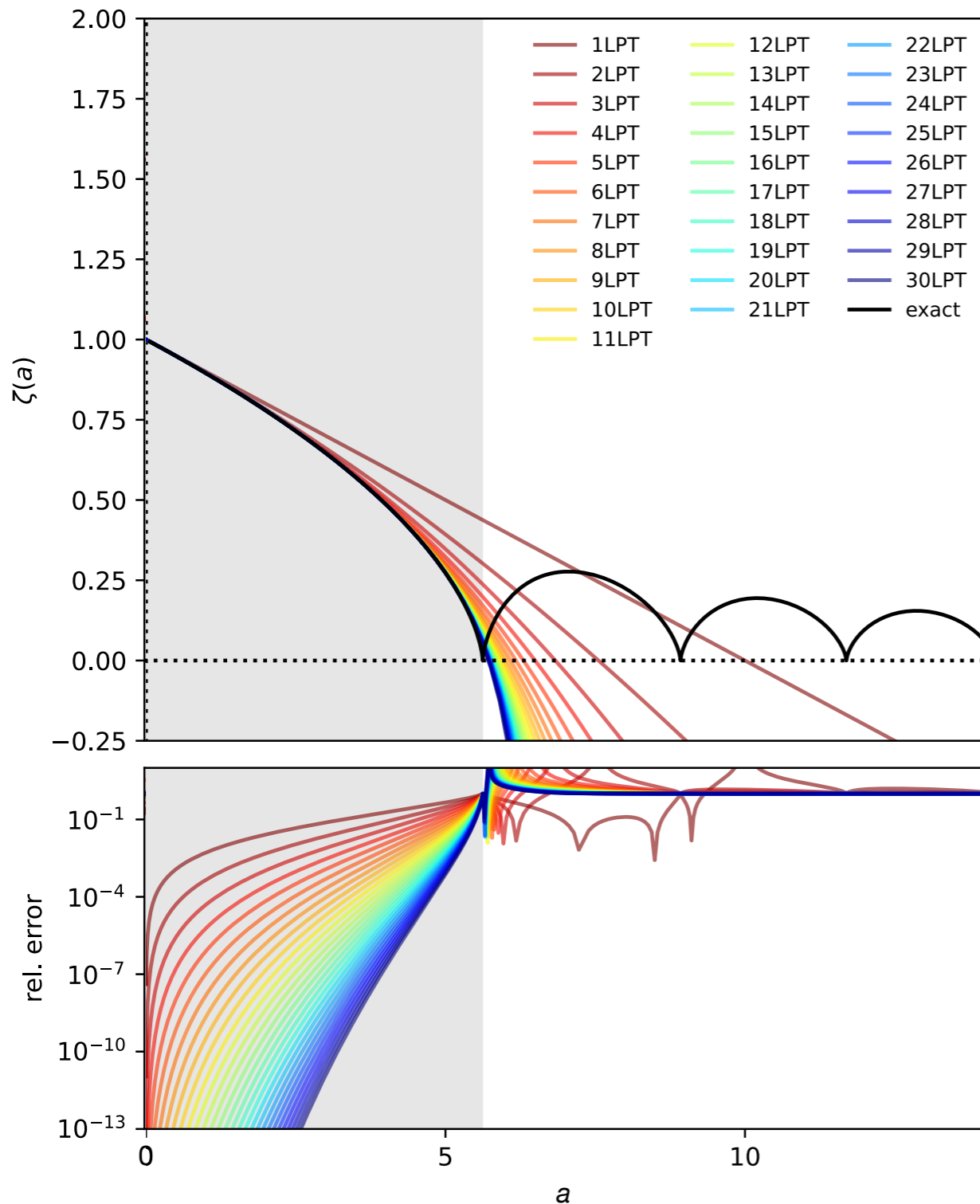
LPT converges everywhere  
even after first shell-crossing in field

But: For late times, converges very  
slowly for isolated set of points  
(see also Nadkarni-Ghosh & Chernoff 2011)

Rampf+OH (2021)

on request: all order **monofonIC** code

# Convergence limiting singularities

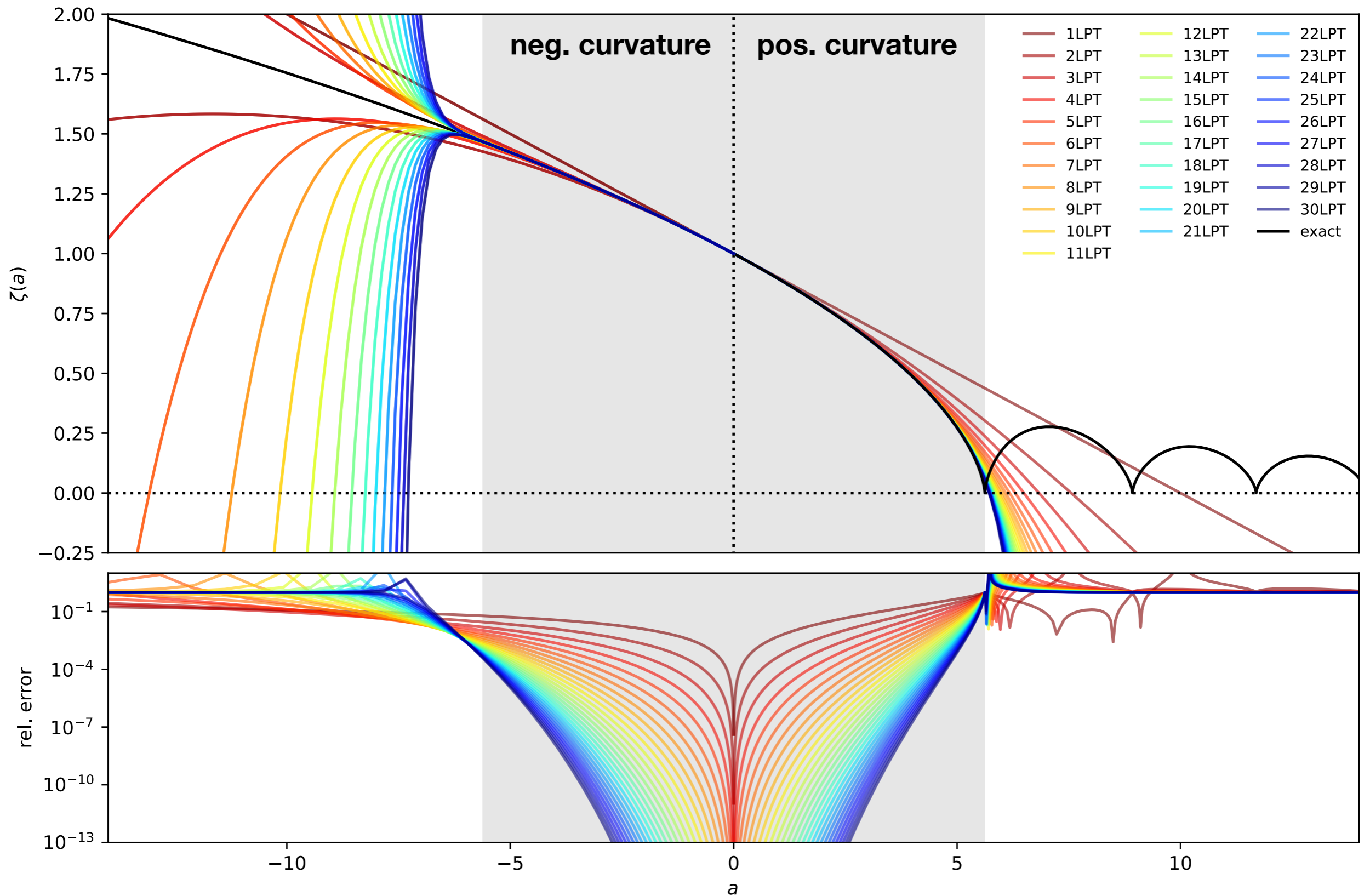


**Spherical collapse has a physical singularity, acceleration is infinite**

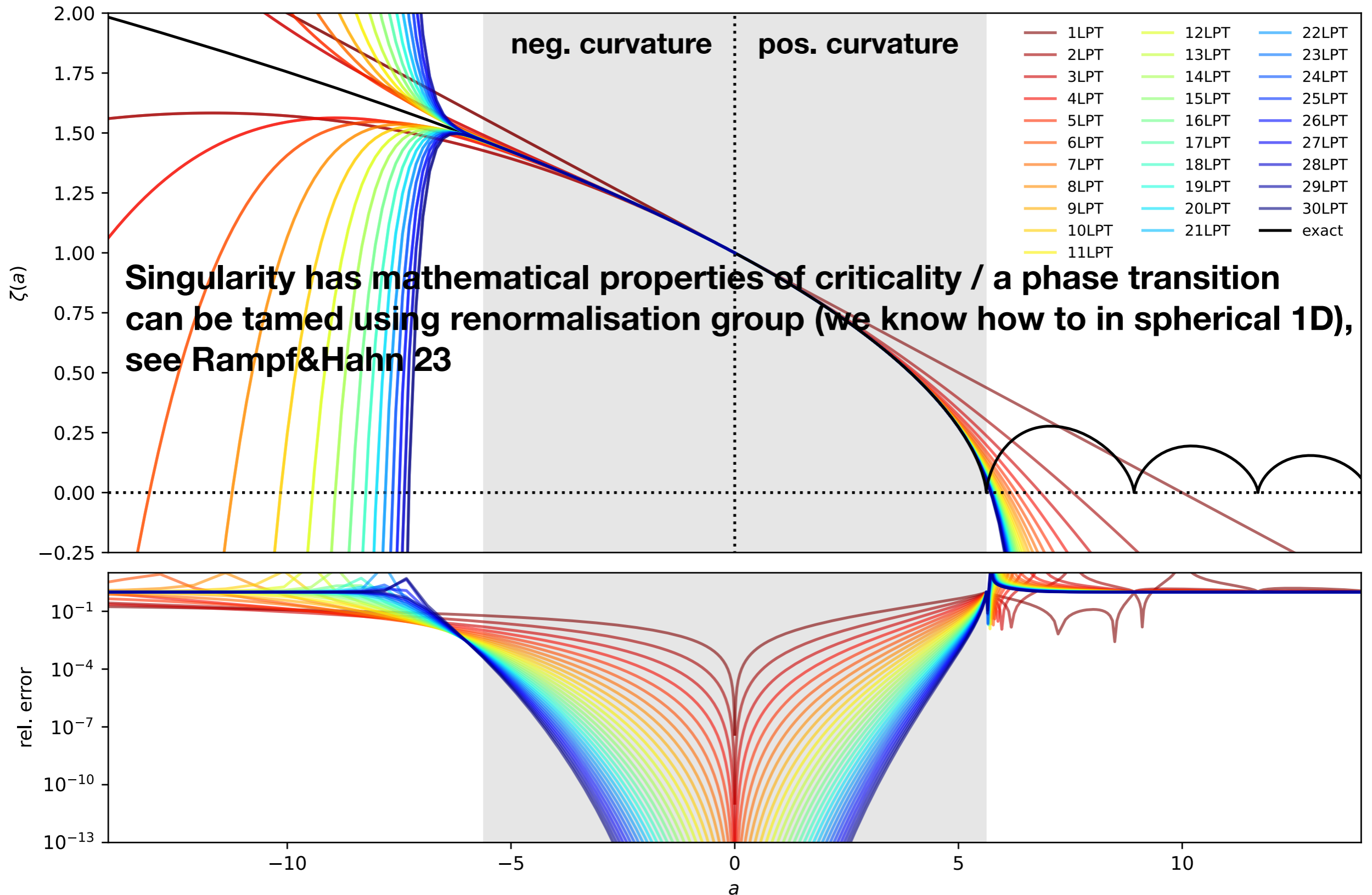
**This leads to slow convergence of LPT, also no transition to bound states**

**numerous ad hoc UV completions in the literature**  
e.g. ALPT (Kitauro&Hess 2013),  
MUSCLE (Neyrinck 2016),...

# Convergence limiting singularities



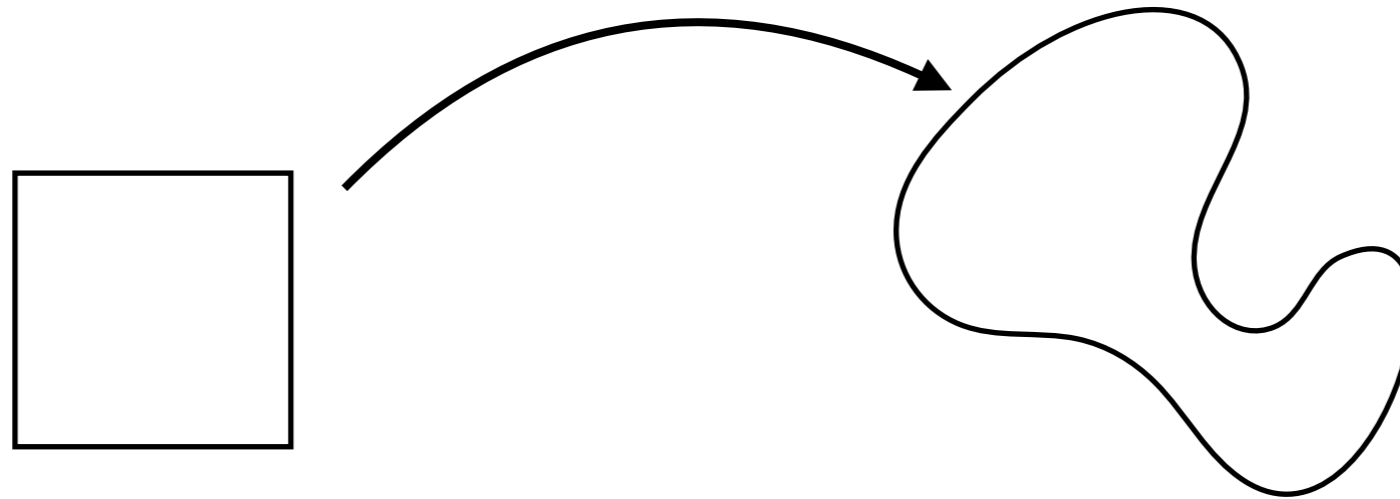
# Convergence limiting singularities



# Discrete evolution vs. fluid evolution

Lagrangian description, evolution of fluid element

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

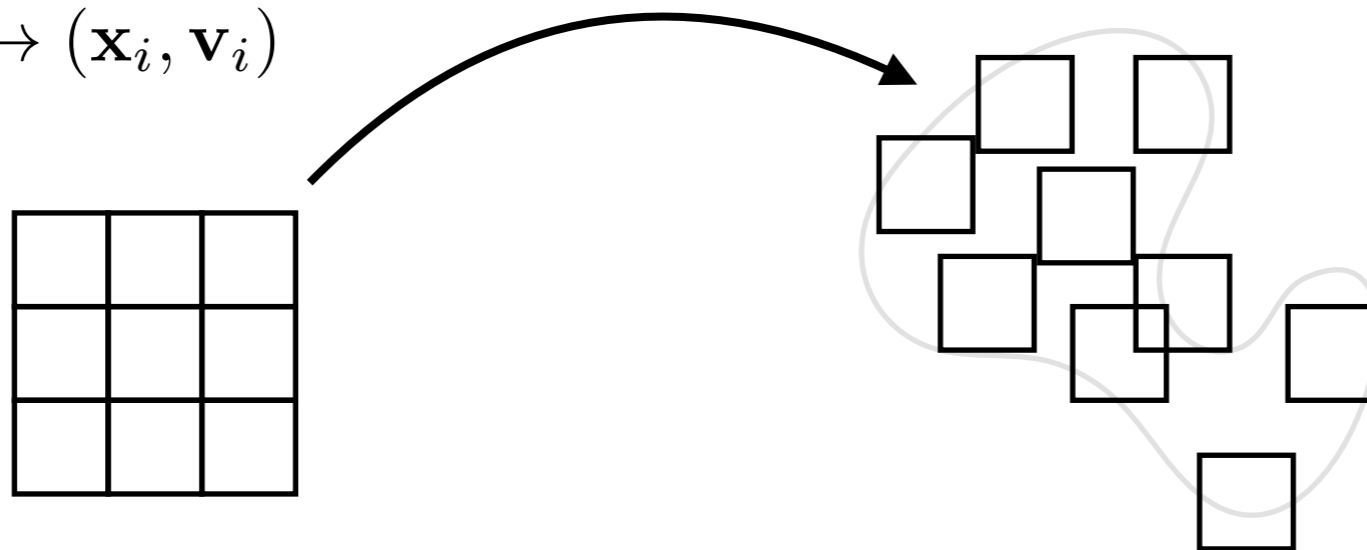


$$\frac{Df_m}{Dt} = 0$$

## The N-body approximation:

cover distribution function with N characteristics, estimate  $f_m$  from them

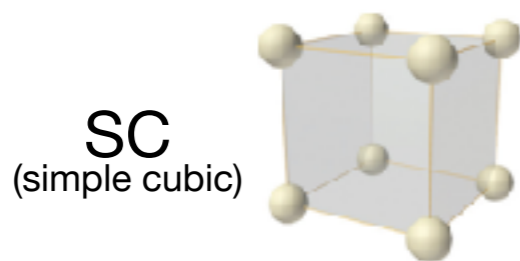
$$i \in \{1 \dots N\} \mapsto (\mathbf{x}_i, \mathbf{v}_i)$$



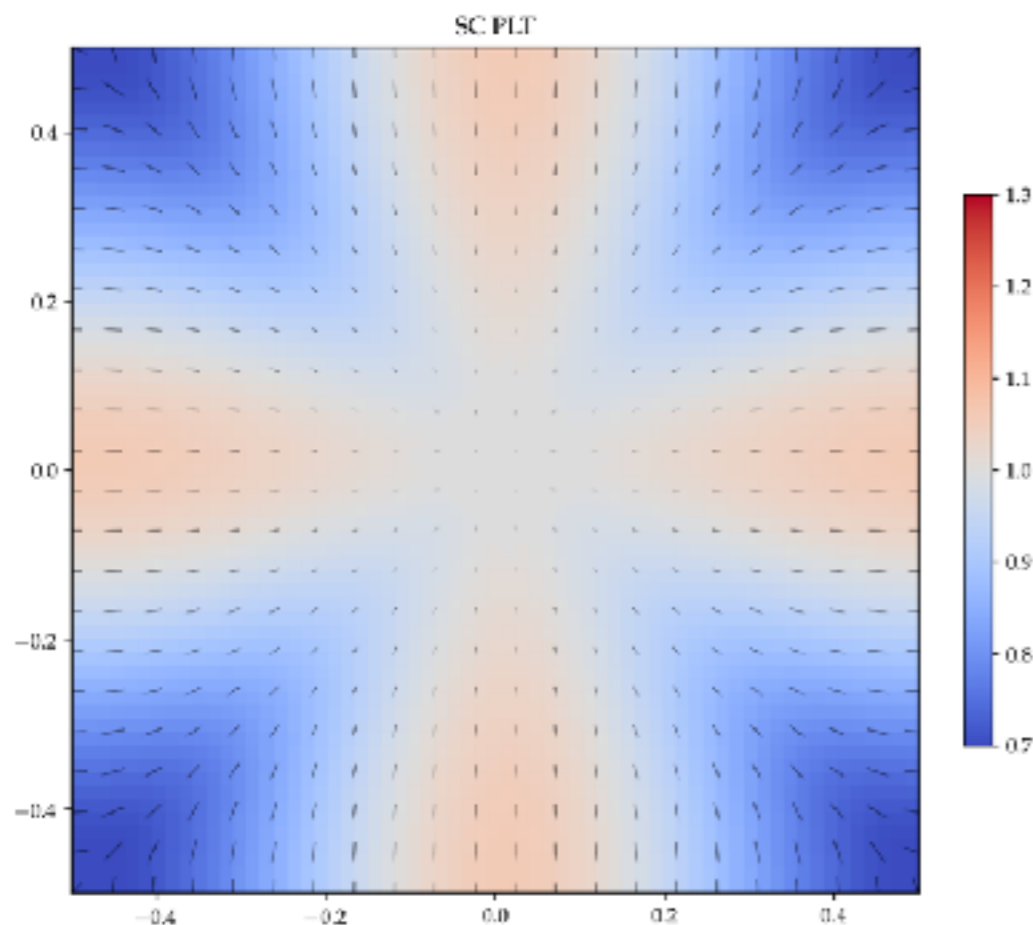
**This can re-introduce short-range interactions -> softening...**

# Convergence of LPT and N-body...

I've talked a lot about discreteness and Vlasov in the past. Here is a new take:

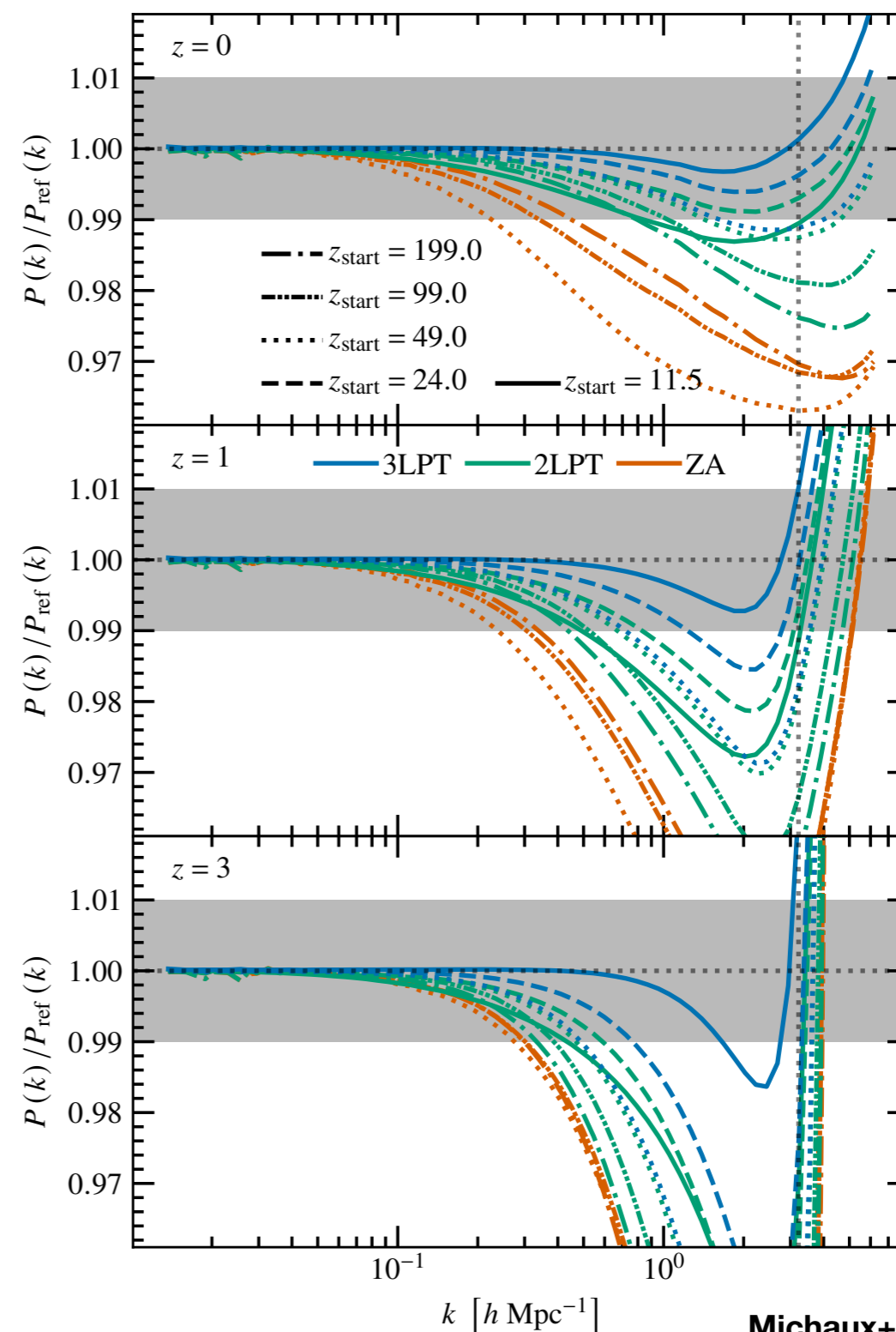


Particle motion on small scales not isotropic.  
Can be calculated for Bravais lattices:



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

same line style = same  $z_{\text{start}}$ , same color = same order LPT



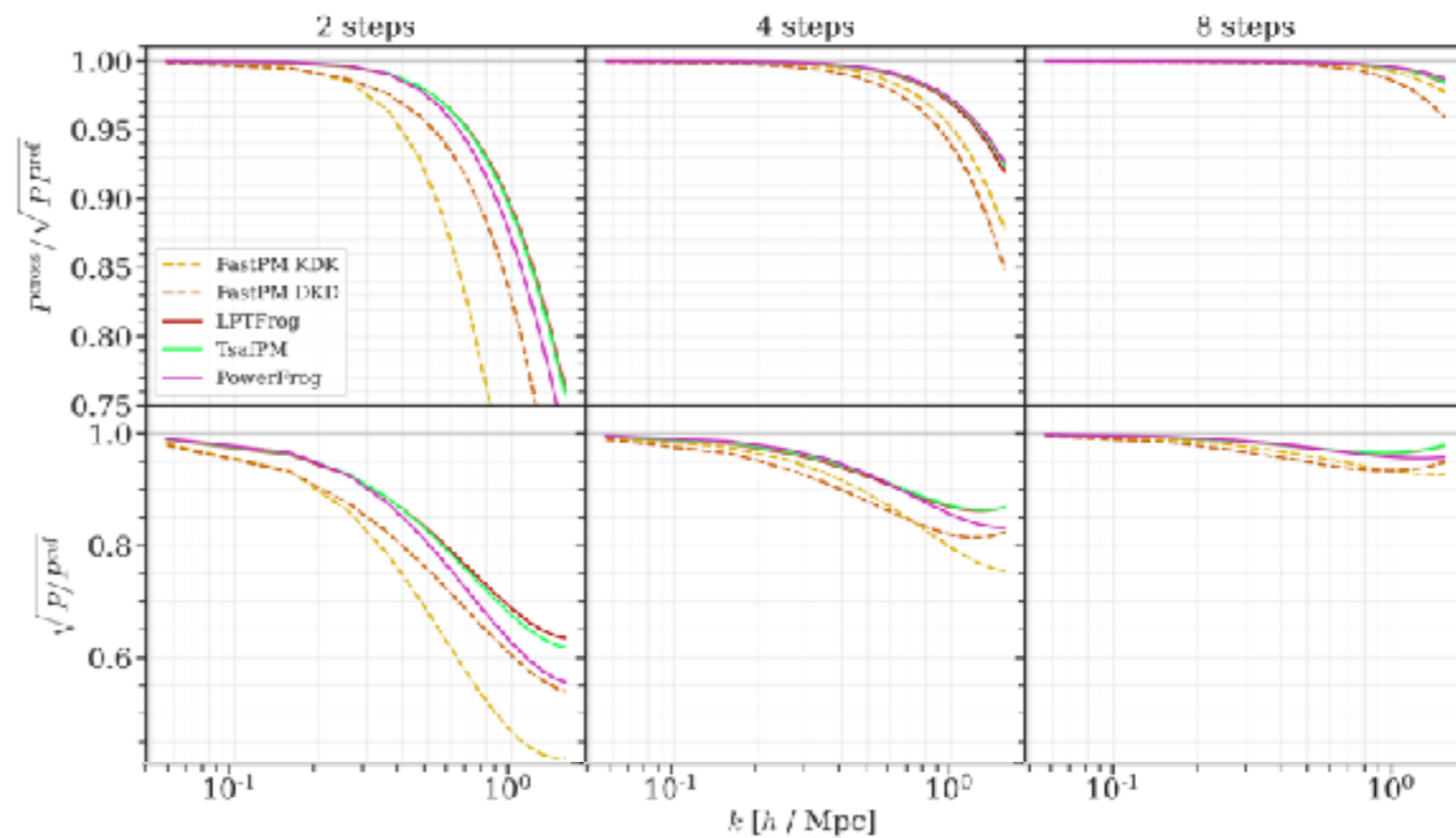
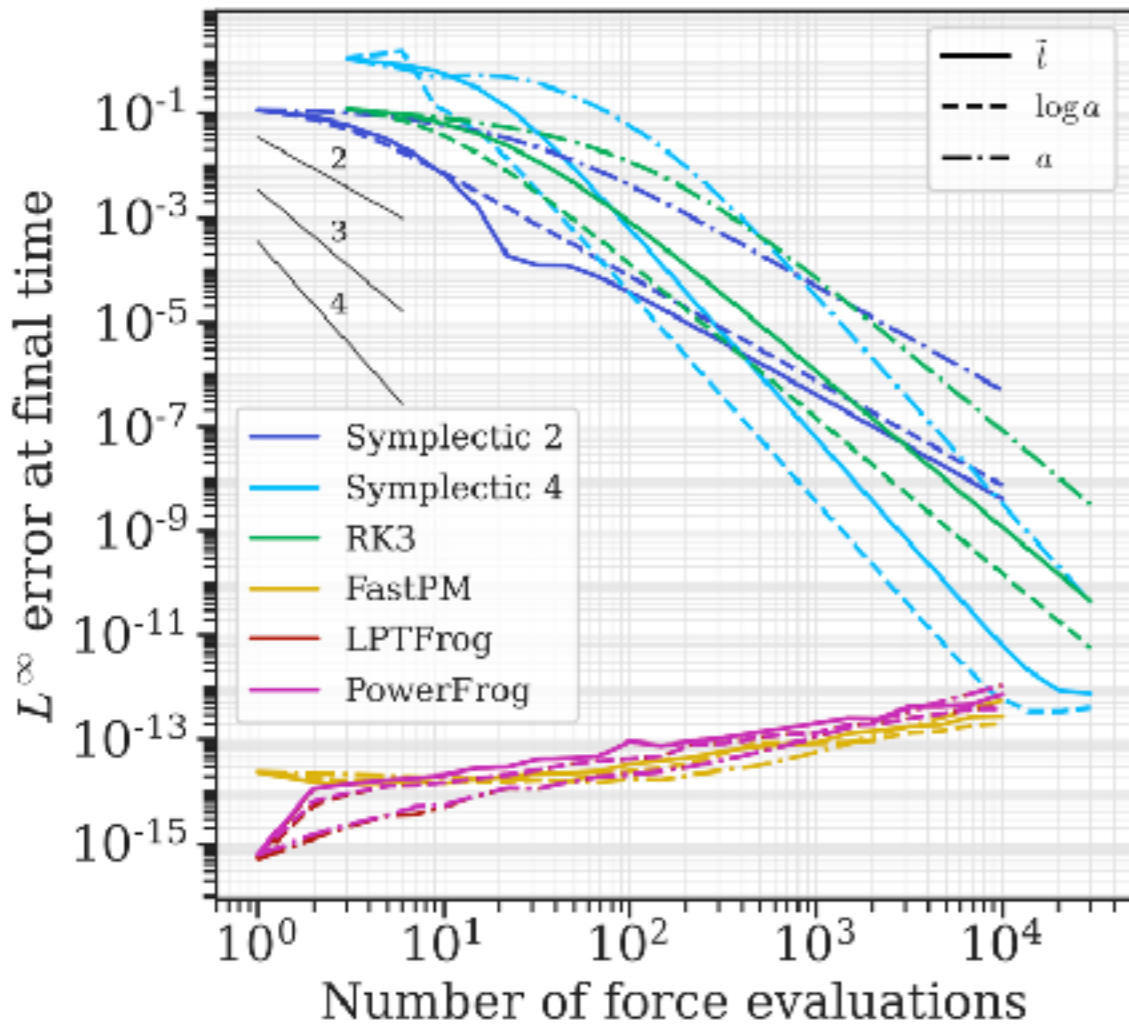
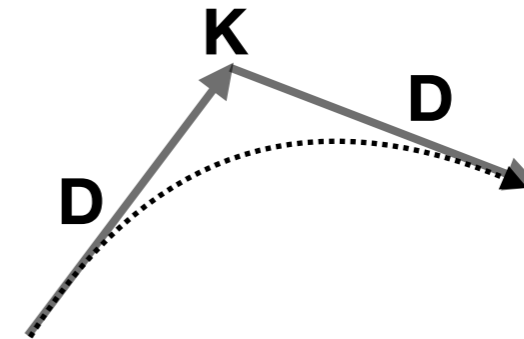
Michaux+2020

... discreteness effects large at early times. better to start as late as possible...

# Perturbation-theory informed integrators

Integrators for N-body simulations are agnostic about perturbation theory (derived naively from Hamiltonian)

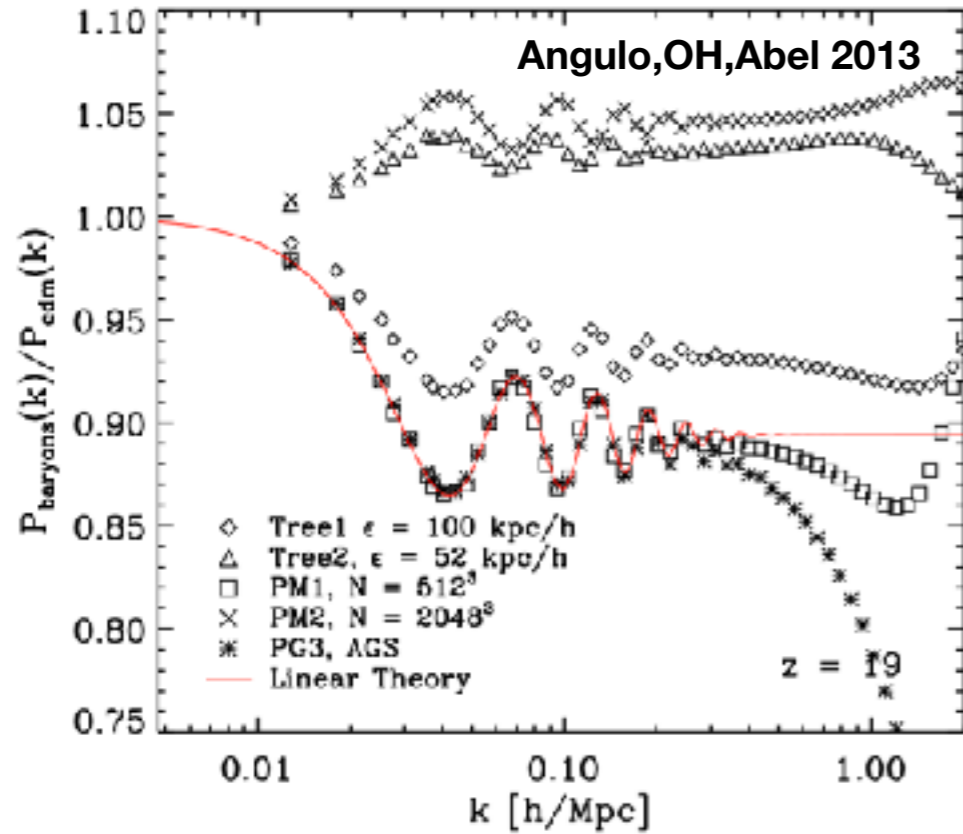
Exception: FastPM (Feng+16 - match Zel'dovich)  
 BUT: Can make them agree to 2nd order!



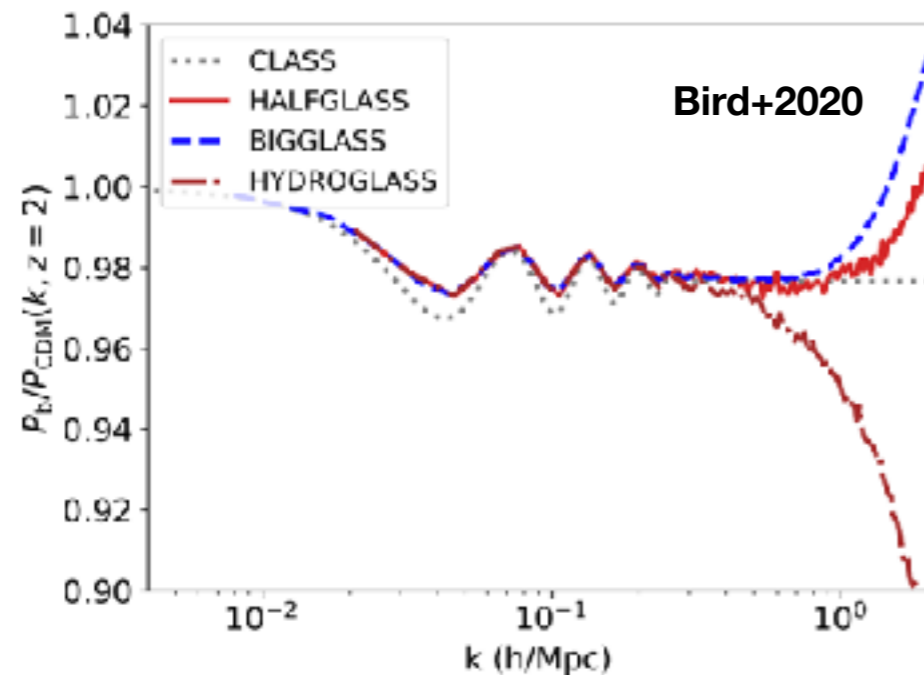
List&Hahn 23

# Adding baryons: two fluid baryon+CDM simulations

N-body two-fluid sims have completely dominant discreteness errors



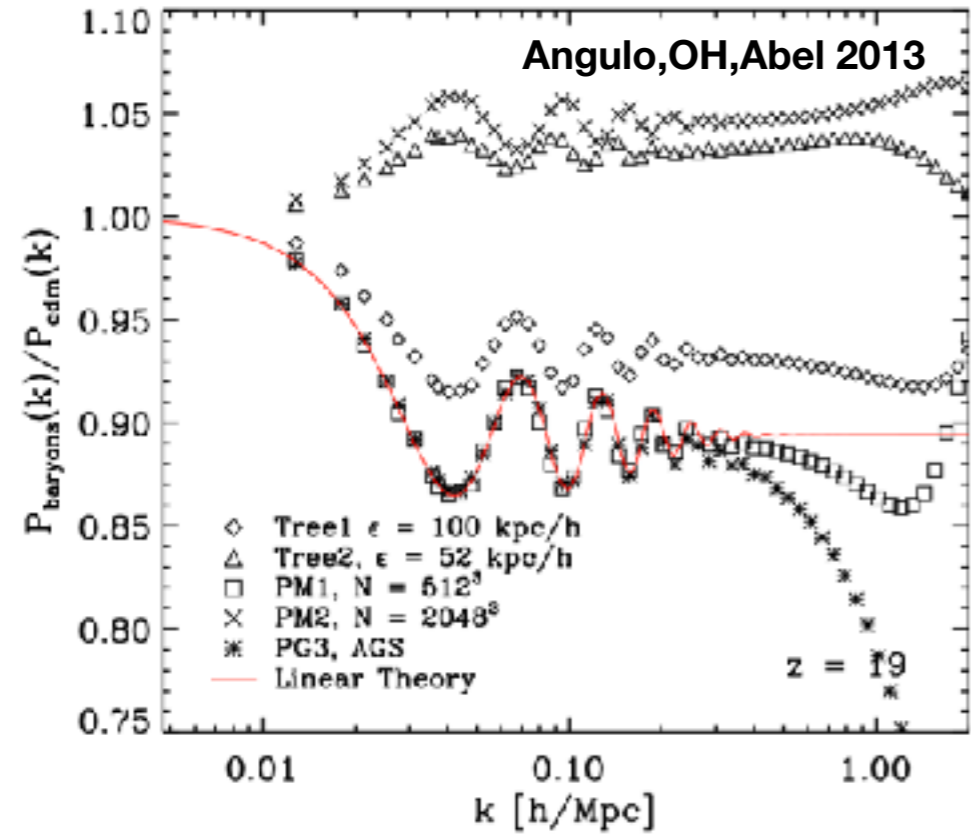
we thought it requires large softening,  
or decorrelated particle arrangements...



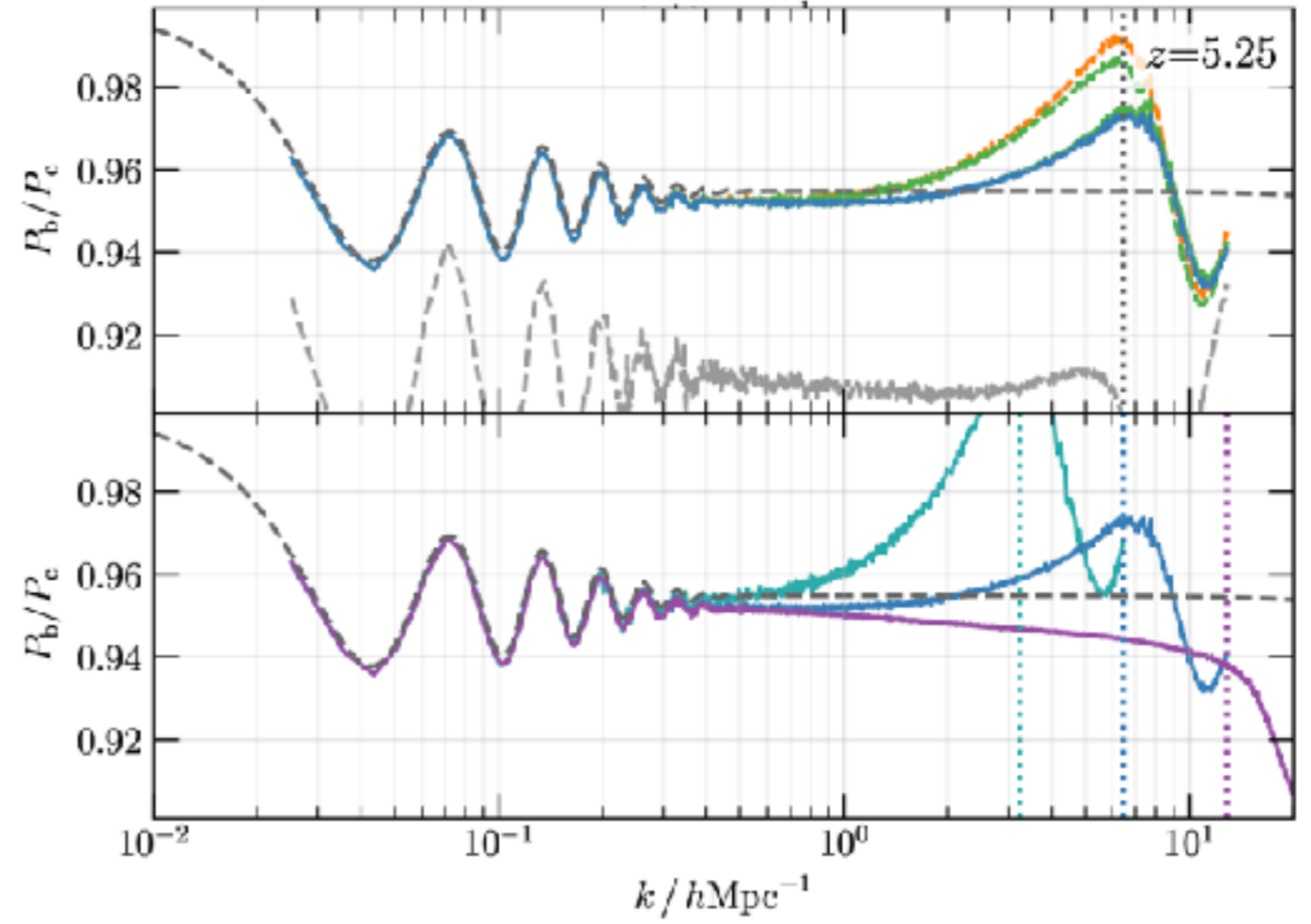


# Adding baryons: two fluid baryon+CDM simulations

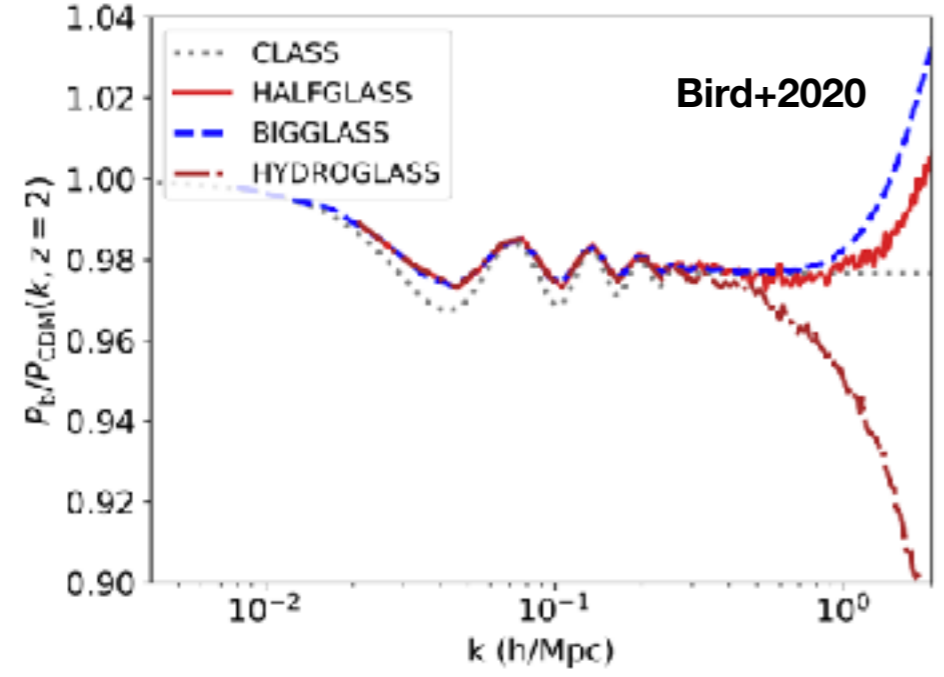
N-body two-fluid sims have completely dominant discreteness errors



correct solution is to incorporate isocurvature perturbations correctly:



we thought it requires large softening, or decorrelated particle arrangements.



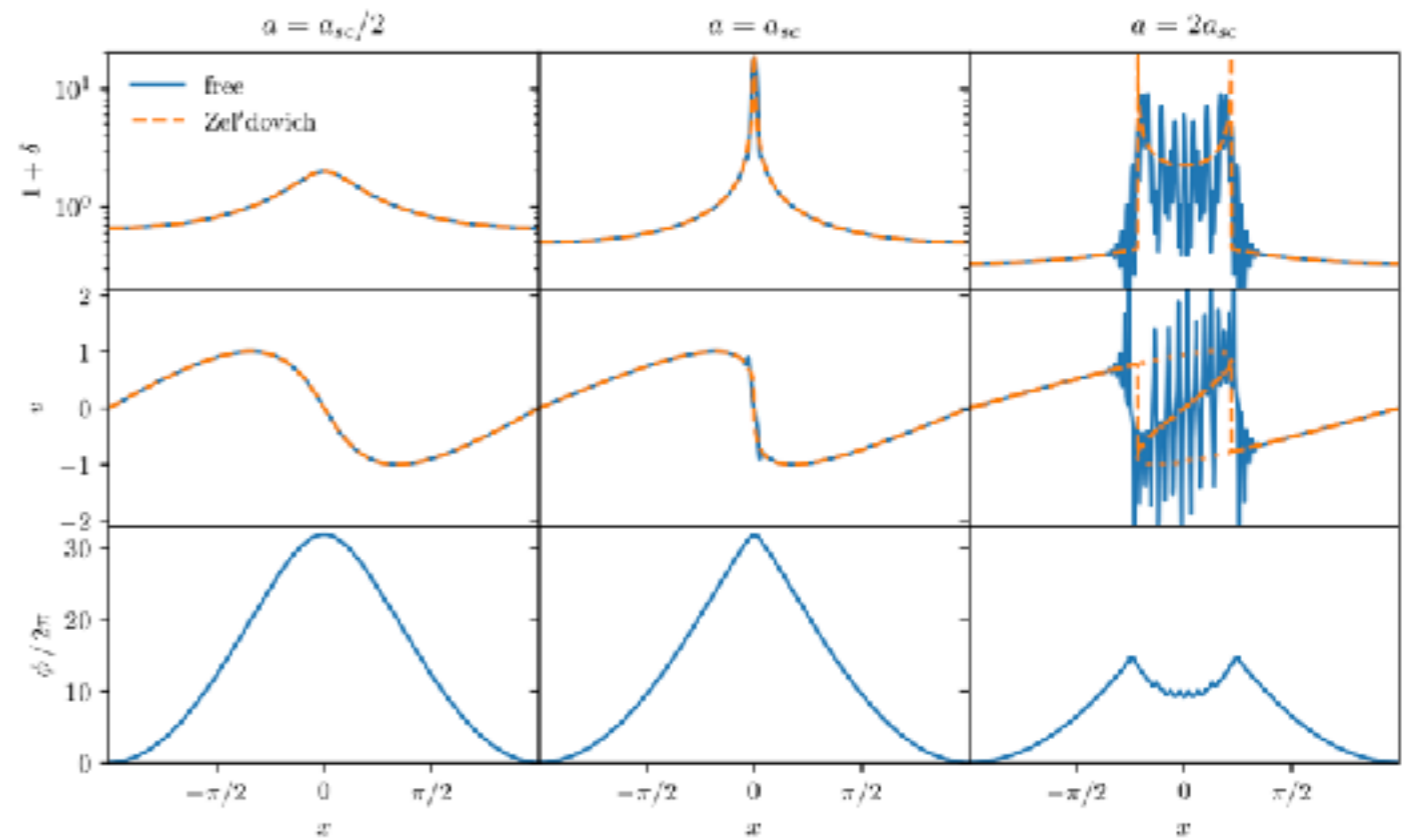
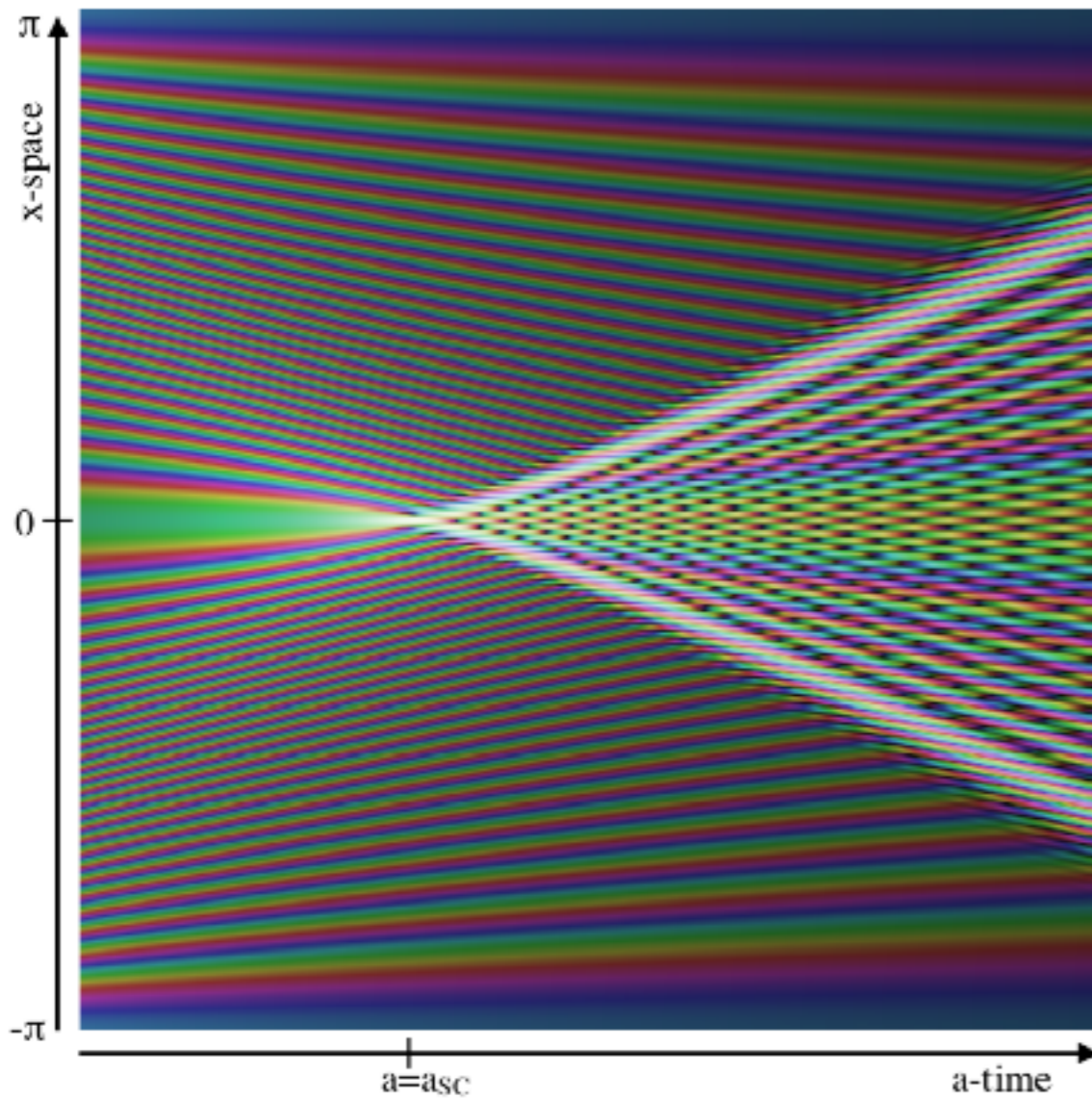
by perturbing not only particle pos+vel but also particle masses

(see Hahn,Rampf,Uhlemann 2021, Rampf,Uhlemann,Hahn 2021)

# Lagrangian Perturbative Dynamics in a Field Framework I

Use QM inspired transition matrix  $q \rightarrow x$  to predict transition probabilities to go from Lagrangian to Eulerian space

Obtain a field version of Zeldovich trajectories:



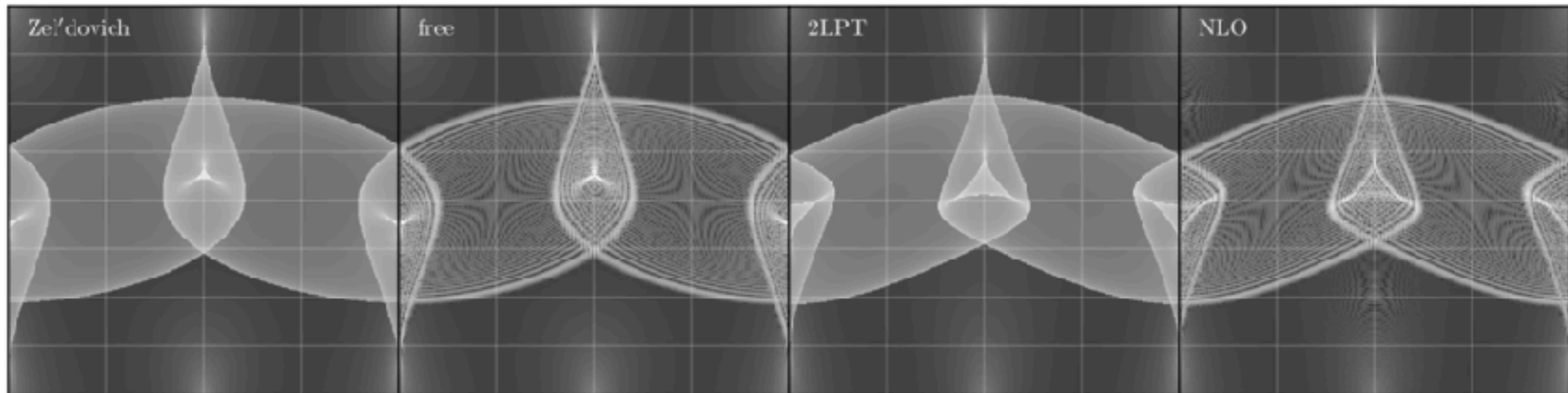
dynamics 'smoothed' by  $\hbar$  scale

Interference = multi-streaming

# Lagrangian Perturbative Dynamics in a Field Framework II

This can be expanded to n-th order LPT

Comparison 1LPT, 2LPT with 1PPT, 2PPT for phased wave ICs



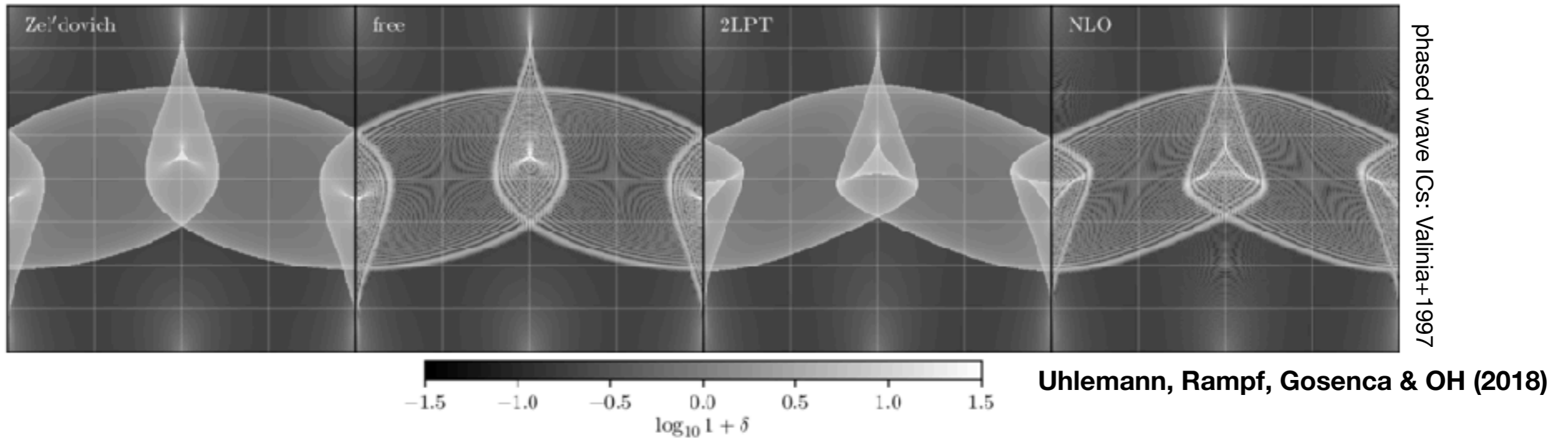
phased wave ICs: Valinia+1997

Uhlemann, Rampf, Gosenca & OH (2018)

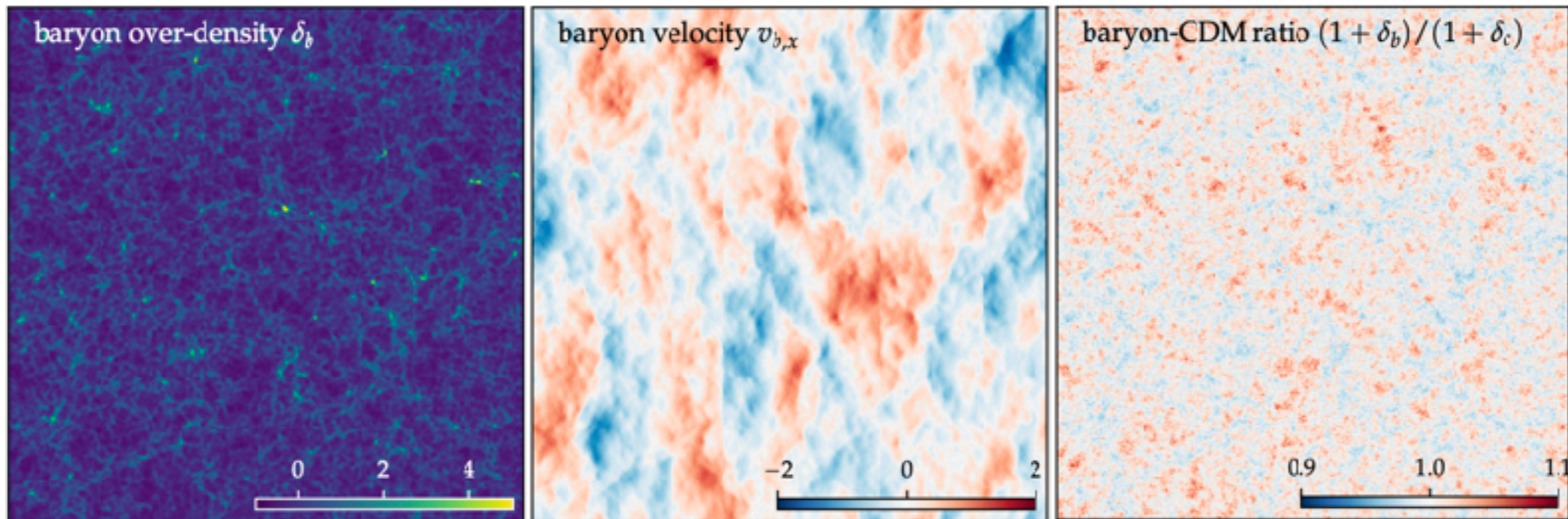
# Lagrangian Perturbative Dynamics in a Field Framework II

This can be expanded to n-th order LPT

Comparison 1LPT, 2LPT with 1PPT, 2PPT for phased wave ICs

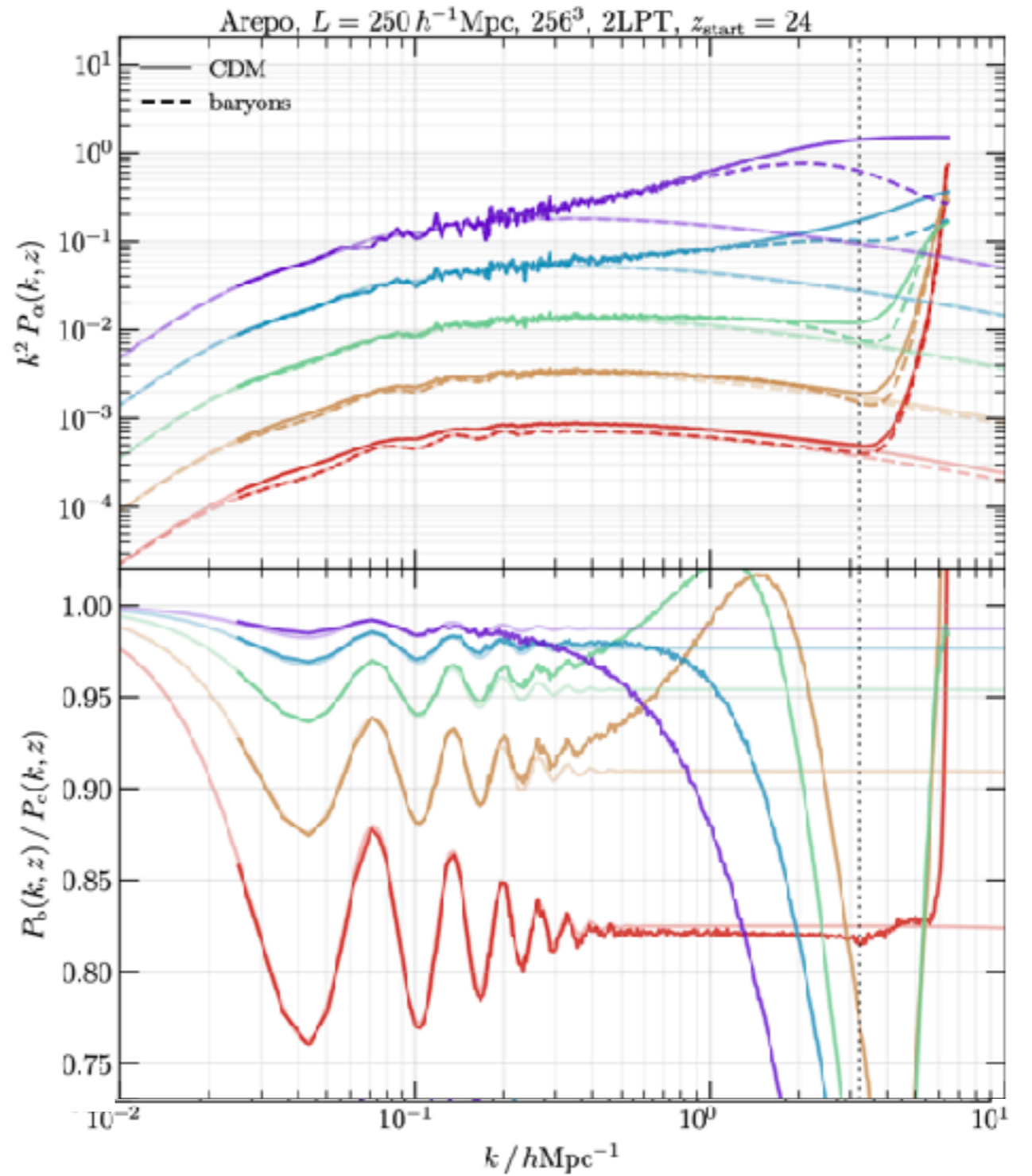
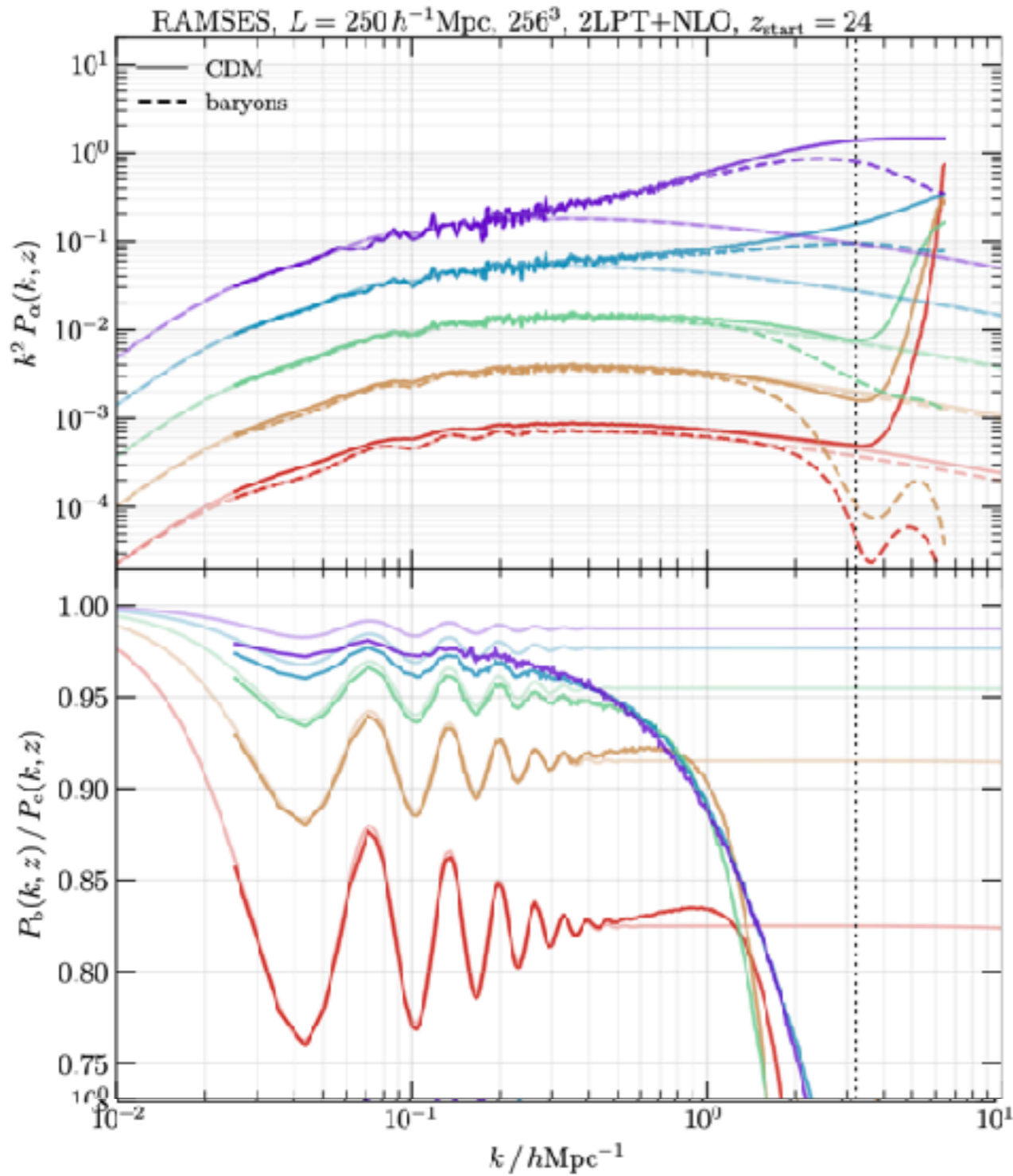


Can upgrade also to 2-fluid baryon+CDM version, use as ICs for Eulerian codes



built into monofonIC, see OH et al. 2021, Rampf et al. 2021

# A fairer comparison of Eulerian and Lagrangian codes for precision cosmology...



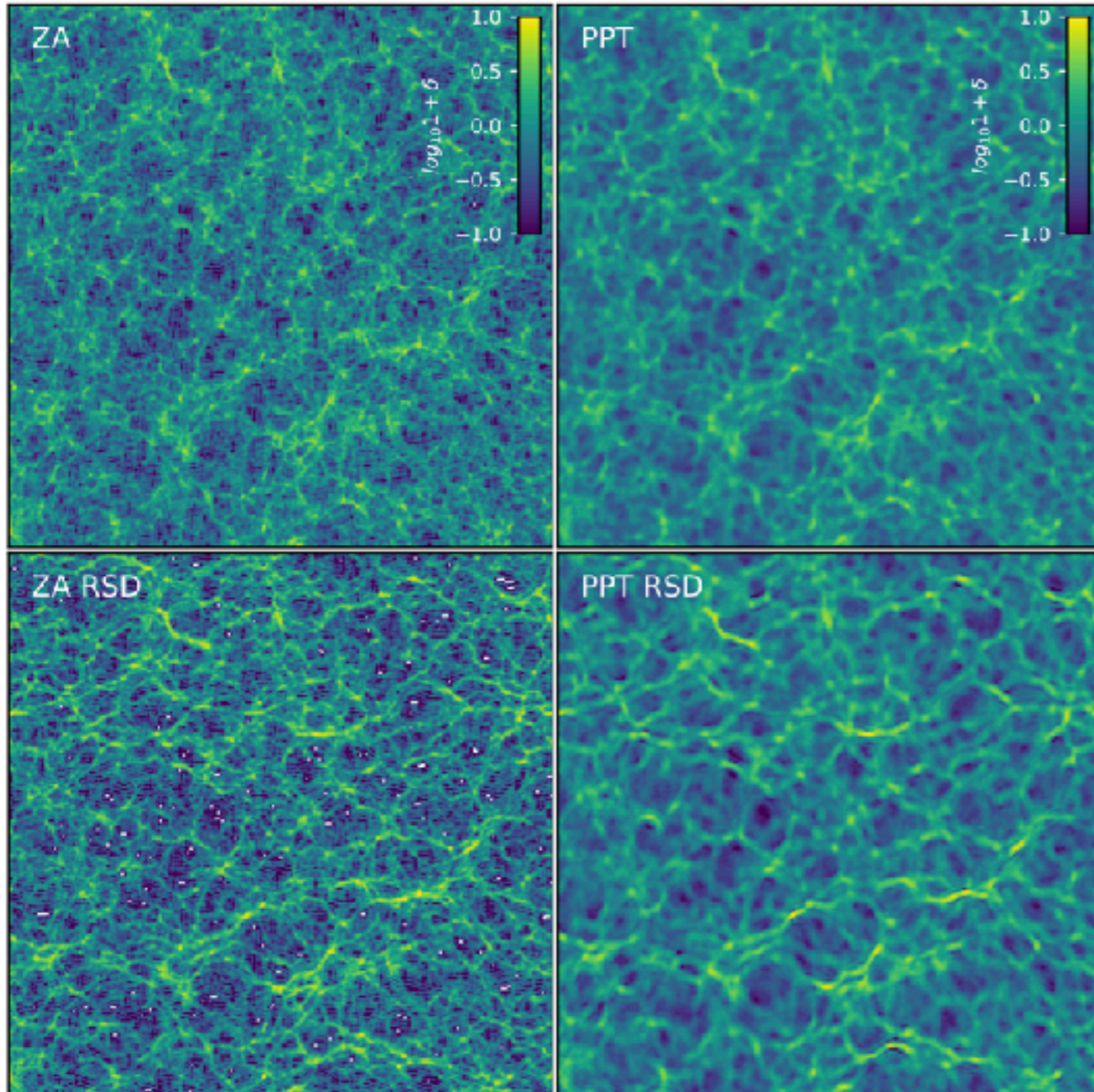
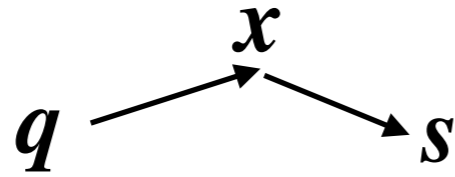
OH et al. 2021, Rampf et al. 2021

# PPT as forward model for IGM

In LPT:

$$s := x + f(a) (\Psi \cdot \hat{e}_{\text{LOS}}) \hat{e}_{\text{LOS}}$$

As propagator:



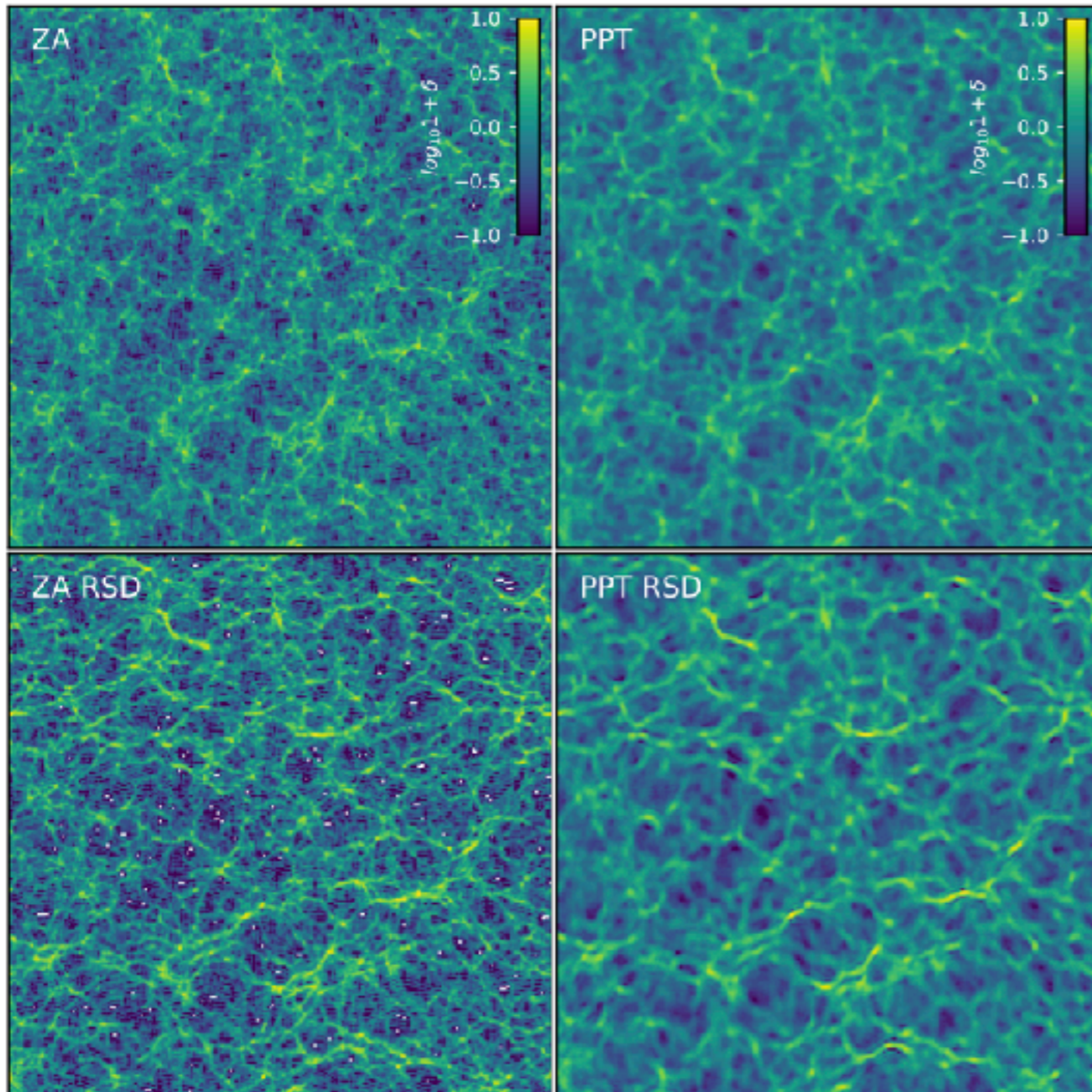
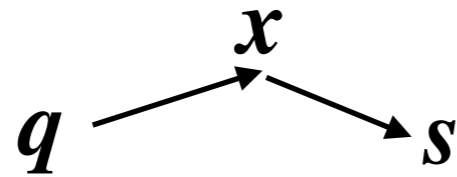
Porqueres+2020

# PPT as forward model for IGM

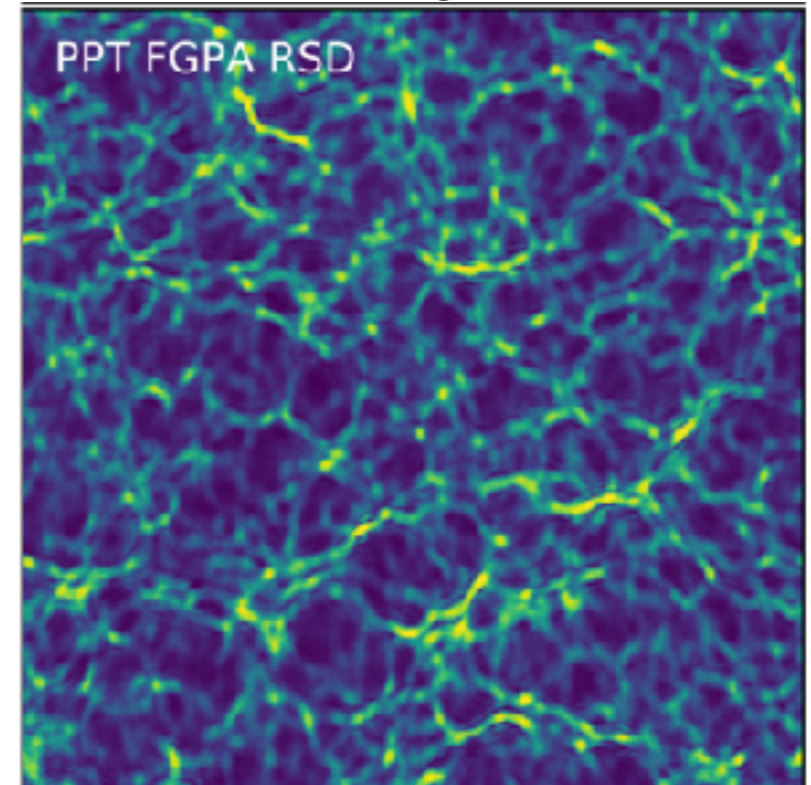
In LPT:

$$s := x + f(a) (\Psi \cdot \hat{e}_{\text{LOS}}) \hat{e}_{\text{LOS}}$$

As propagator:



Upgrade to photon absorption probability using FGPA



redshift-space transmitted flux

-> fast field-level forward model

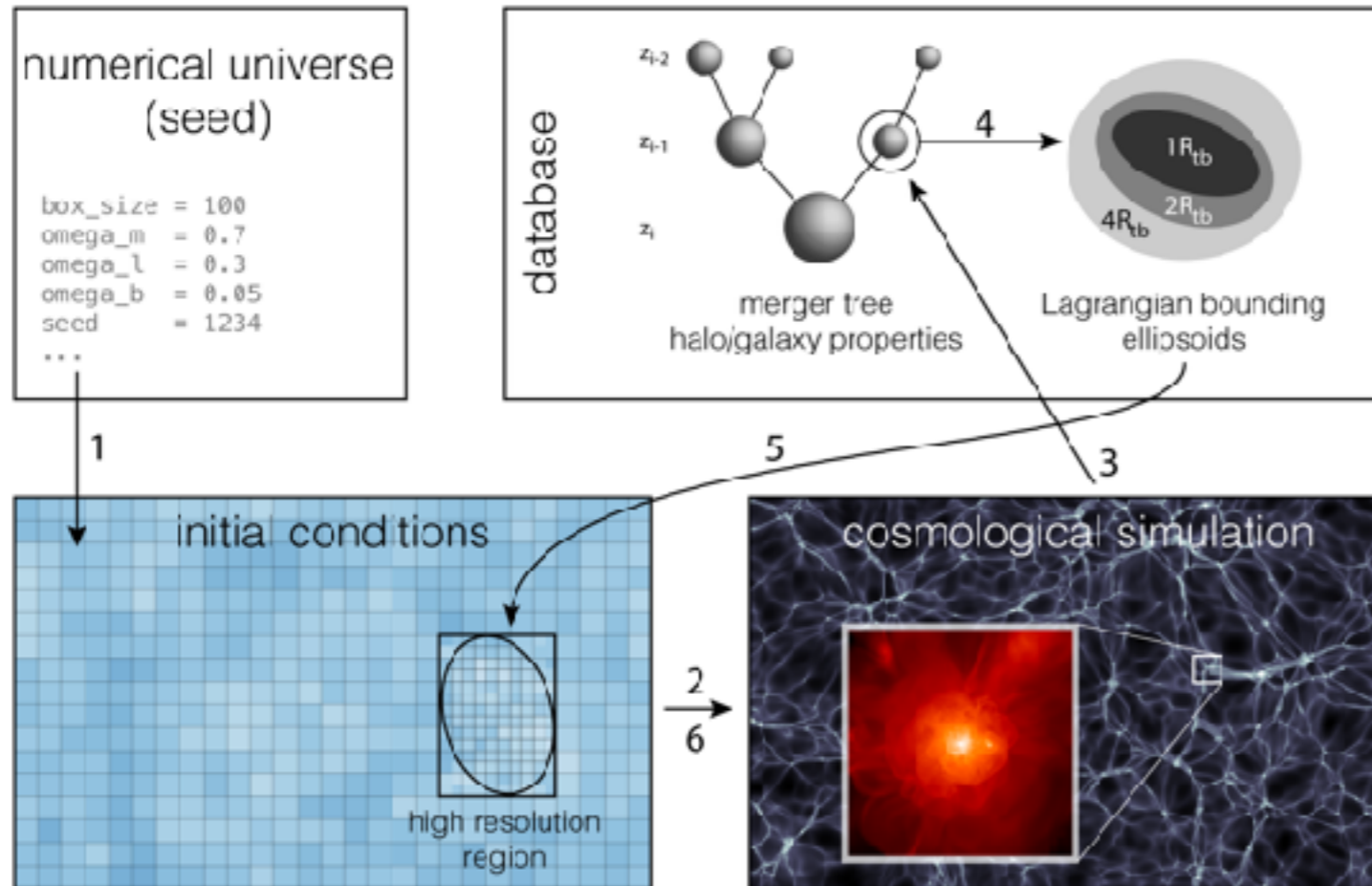
Porqueres+2020

# The cosmlCweb platform - a protohalo database for Zooms

Enhancing the MUSIC1 ecosystem for the next decade

w/ Michael Buehlmann

<http://cosmicweb.astro.univie.ac.at>



1: create ICs from cosmo parameters and random seed

2: running simulation, storing snapshots

3: structure finding and linking across time: merger trees

4: for each halo, find Lagrangian patch (origin)

5: for chosen halo, refine that patch in ICs

6: run zoom simulation with additional physics, etc.

## cosmlCweb:

A database and web interface for

1. **Finding** the right objects to re-simulate

2. **Obtaining** initial conditions for these objects

3. **Referencing** objects in articles / papers

**If interested, do get in touch!**

Buehlmann, OH, et al. 2023, in prep.

slide courtesy M. Buehlmann



# SUMMARY

- LPT has key role in ICs for cosmological simulations
- Demonstrated convergence of LPT beyond shell-crossing
- 3LPT needed for precision era N-body simulations, push to late starts to reduce errors
- new propagator approach for LPT on the grid
  - can be used for Eulerian grid code ICs
  - and for IGM/field-level forward modelling
- new LPT inspired integrators (beyond 'FastPM')

## **MUSIC2 monofonIC** <https://bitbucket.org/ohahn/monofonic>

**single resolution (=only full cosmological volume) version**

- direct integration of CLASS
- up to 3LPT, (nLPT exists already, not public just yet)
- PLT corrections
- more accurate treatment of baryons
- new propagator approach for Eulerian baryons
- modular architecture: multi code, easily extensible
- MPI+threads (no more memory limits)

## **MUSIC2 cosmICweb** <https://cosmicweb.univie.ac.at>

- proto-halo patches for full merger tree (incl. Agora, Eagle, ...)
- numerical observatory (unified framework for zoom resimulations)