Accurate Small Scale Dynamics in COLA

Les Houches School of Physics — The Dark Universe

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BASTILLE DAY, 2025

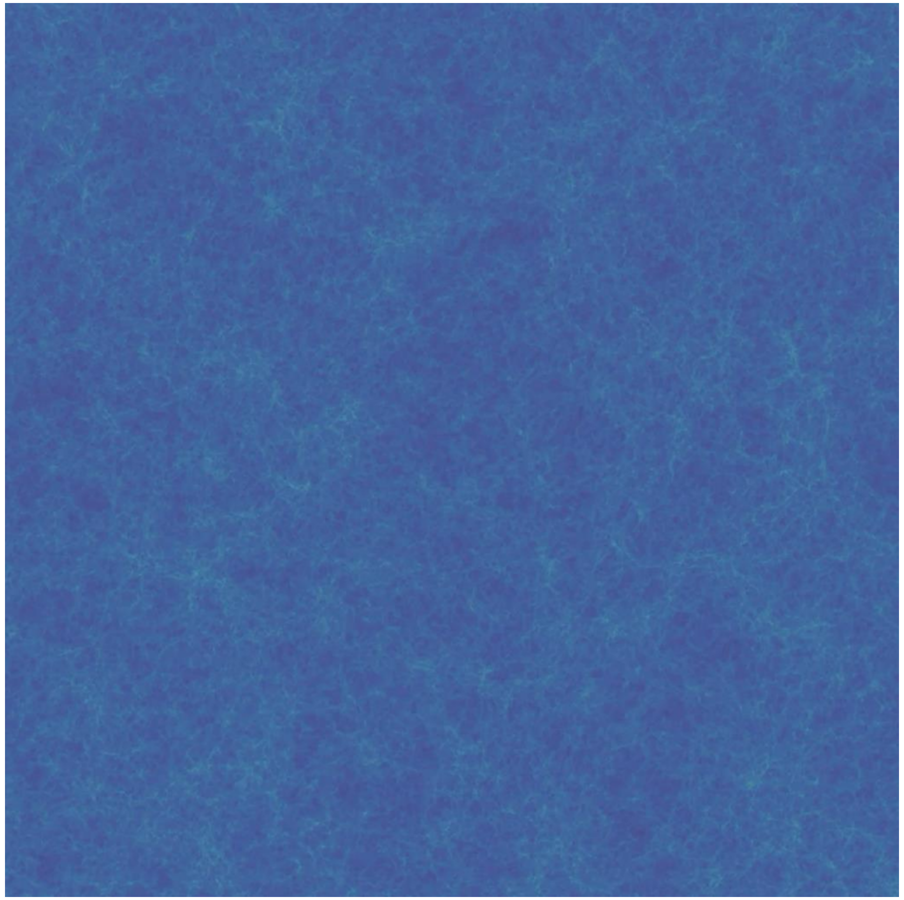
Bastille Day in Les Houches, Midjourney

Outline

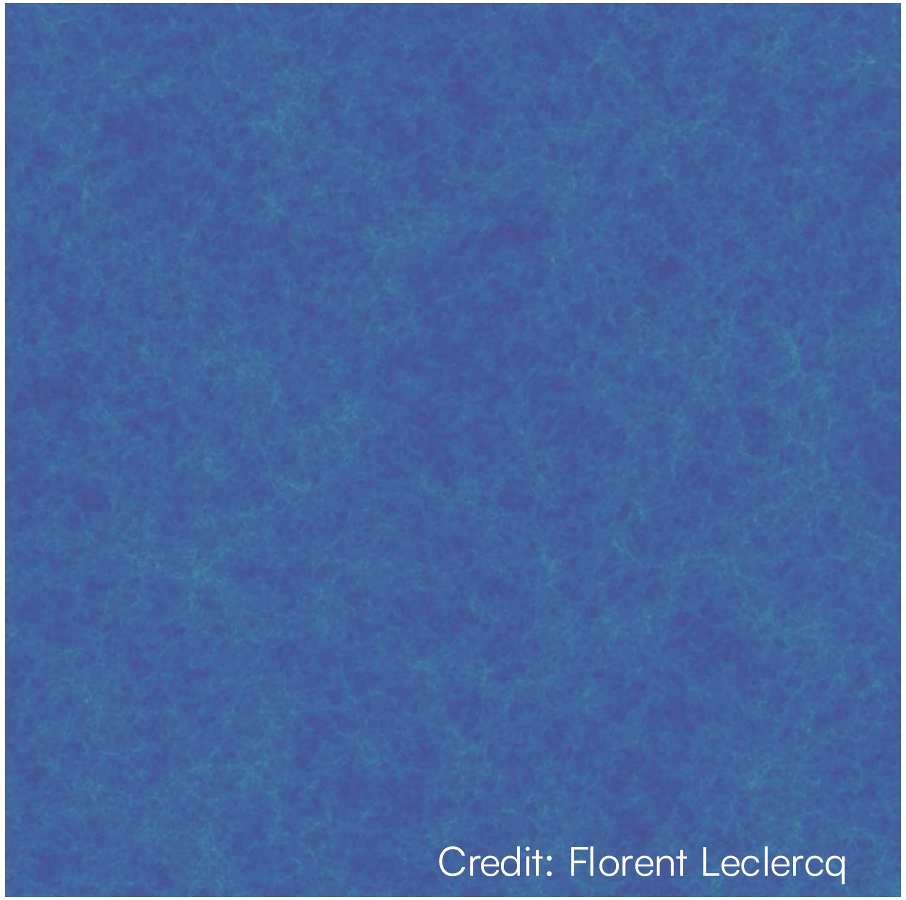
Why small scales matter?

Large Scale Galaxy Surveys: Why small scales matter?

Lagrangian Perturbation Theory



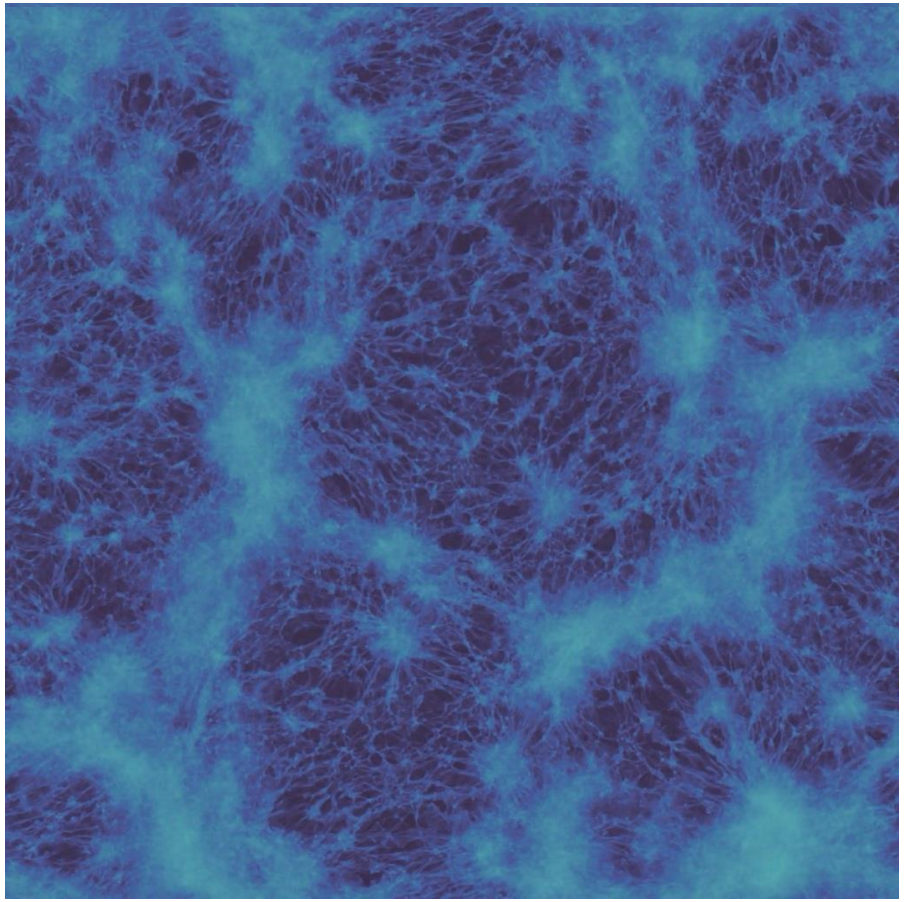
N-body: Particle-Mesh



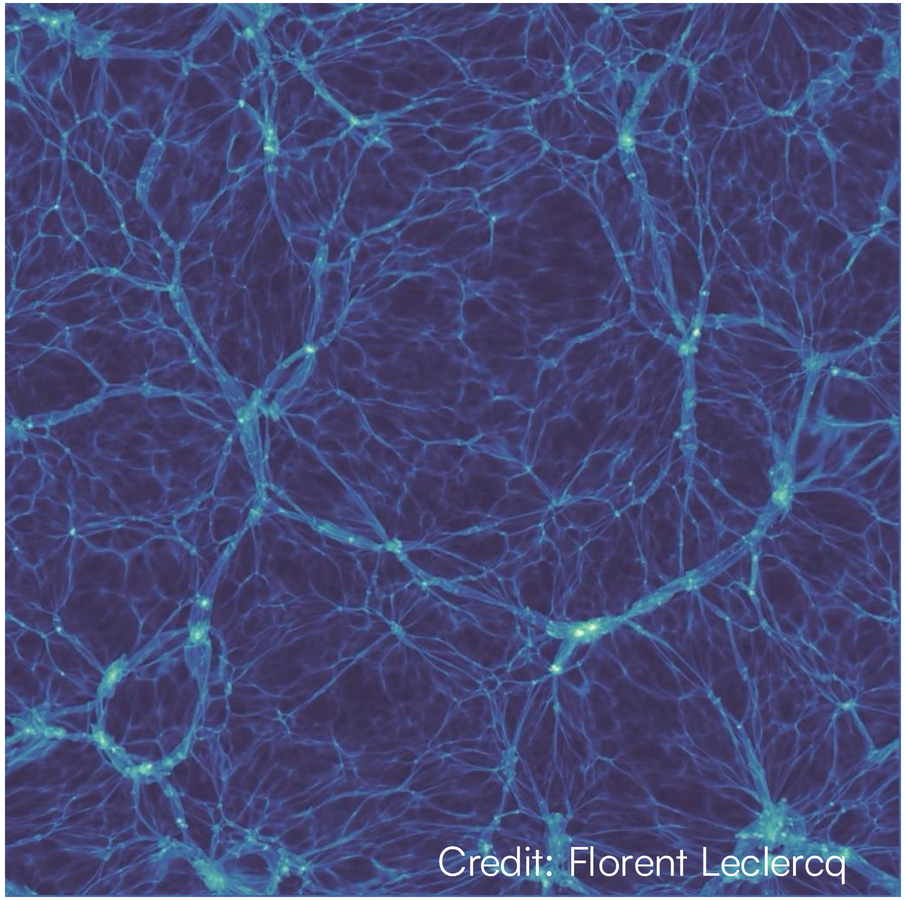
Credit: Florent Leclercq

Large Scale Galaxy Surveys: Why small scales matter?

Lagrangian Perturbation Theory

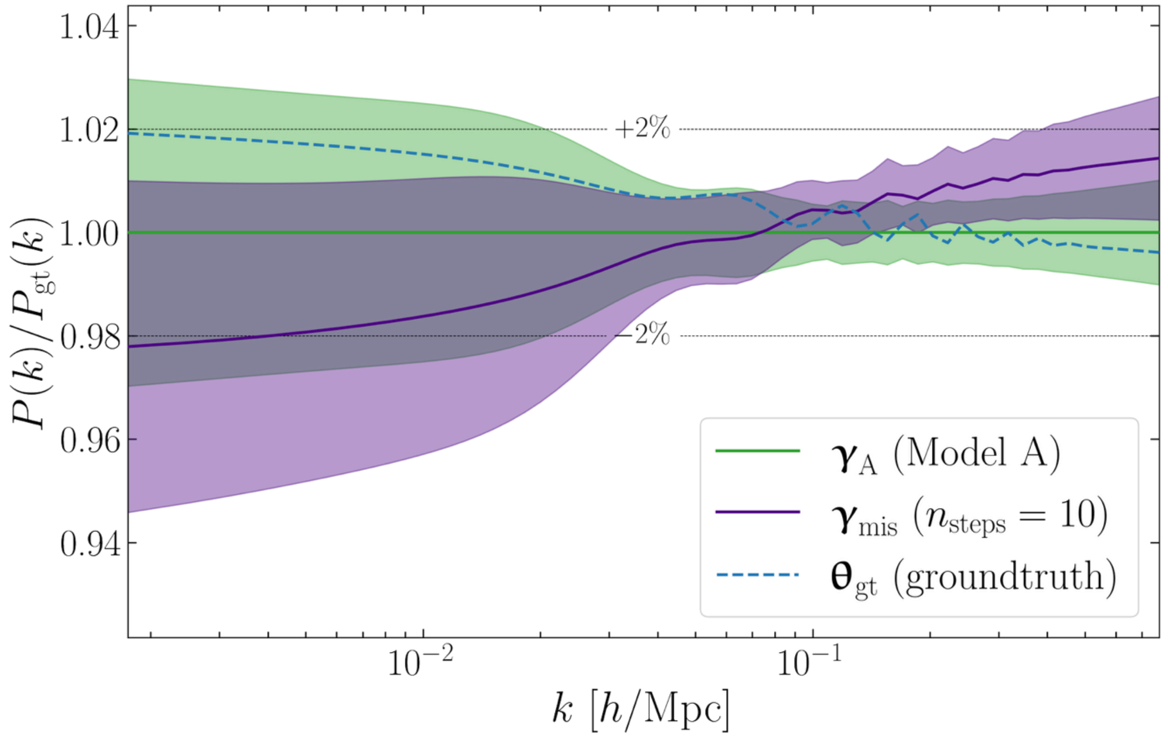


N-body: Particle-Mesh



Large Scale Galaxy Surveys: Why small scales matter?

- Stage-IV surveys: unprecedented volume & precision.
- Small scales contain most of the information: $N_{\text{modes}} \propto k_{\max}^3$.
- Cosmological inferences sensitive to model misspecification, which risks biasing posteriors.

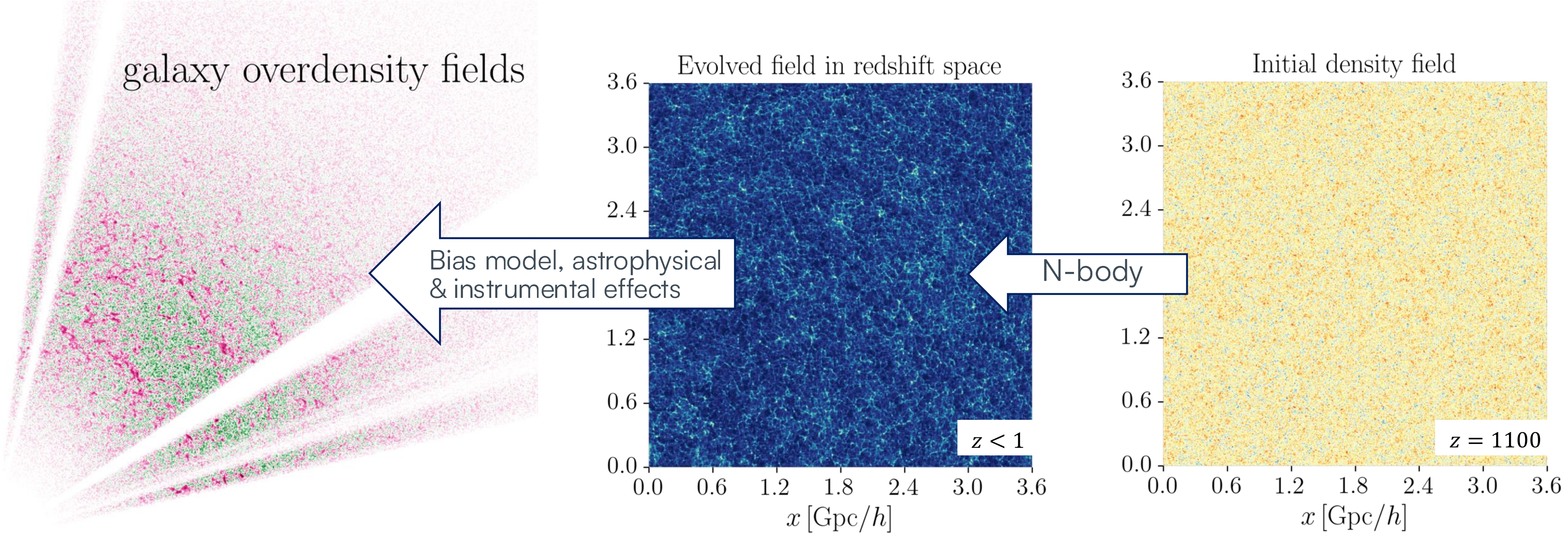


Impact of using 10 versus 20 time steps in the gravity solver, on the initial matter power spectrum inferred with SELFI. We guaranteed 1% precision on simulated galaxy power spectra down to the smallest scales; not enough to avoid biasing the posterior.

TH & Leclercq 2024, 2412.04443

One slide on Implicit Likelihood Inference

The likelihood is implicitly represented by a simulator.



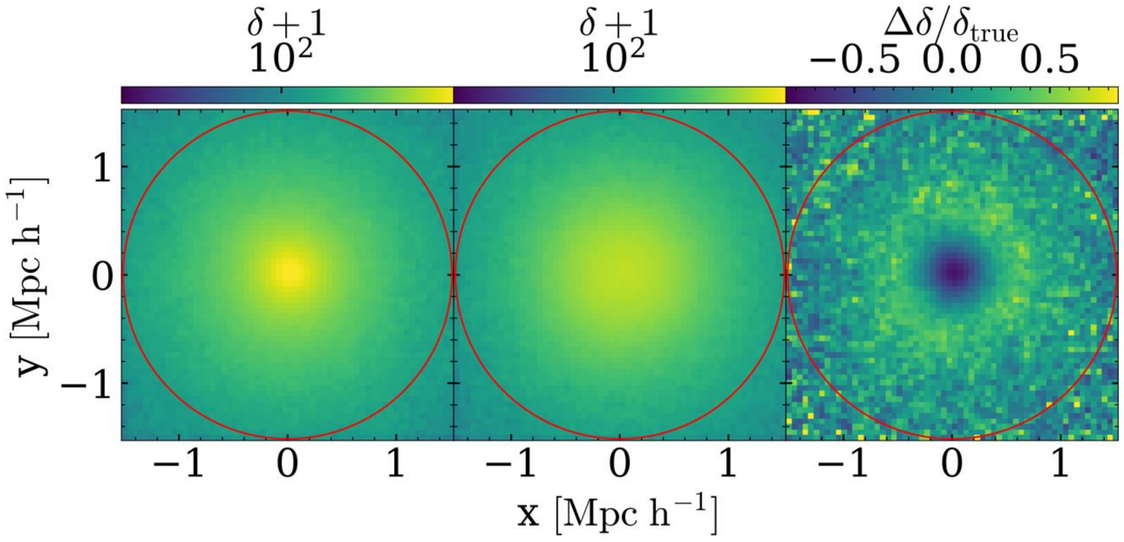
Evolution with *Simbelmynë*, Leclercq, Jasche & Wandelt 2015, 1502.02690

Adapted from TH & Leclercq 2024, 2412.04443

What do we need?

What do we need?

- Cosmological inference demand thousands of N-body simulations.
- Need fast simulations spanning vast cosmological volumes and reaching deep into the non-linear regime.
- ML emulators are useful, but make mistakes: we need to be cautious.



Left panel. Average density for 500 halos in N-body simulations. **Middle panel.** Same for the ML emulator. **Right panel.** Residual.

Scoggins et al. 2025 (2502.13242)

Collisionless dynamics of dark matter in an expanding Universe

Collisionless dynamics of dark matter in an expanding Universe

- Newtonian gravity in an expanding background Universe:

Vlasov equation

coupled to

the Cosmological Poisson equation

$$\Delta\Phi = 4\pi G a^2 \bar{\rho}\delta$$

- **N-body**: Sample phase-space density with N tracer particles, then numerically integrate the equations of motion of these particles.

Collisionless dynamics of dark matter in an expanding Universe

- Newtonian gravity in an expanding background Universe:

Equations of motion

$$\partial_\tau \mathbf{p} = -a\nabla\Phi \quad \text{with} \quad \mathbf{p} = a\partial_\tau \mathbf{x}$$

Cosmological Poisson equation

$$\Delta\Phi = 4\pi G a^2 \bar{\rho}\delta$$

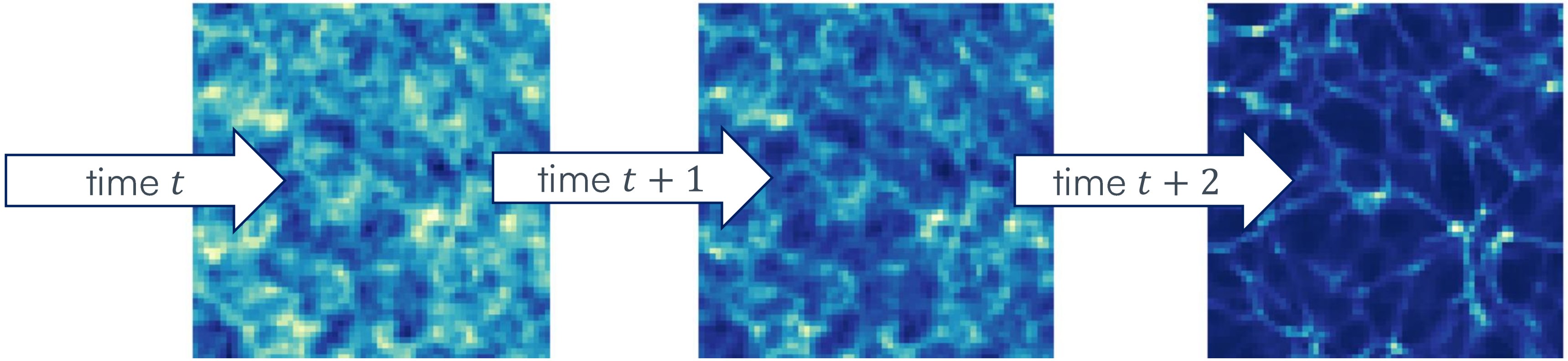
- $\Phi(\mathbf{x}, \tau)$ is the peculiar gravitational potential, τ is the conformal time.

Collisionless dynamics of dark matter in an expanding Universe

- Two ingredients in numerical gravity solvers:
  1. A method for solving the cosmological Poisson equation,
  2. A method for integrating the equations of motion.

$$\partial_\tau \mathbf{p} = -a\nabla\Phi \quad \text{with} \quad \mathbf{p} = a\partial_\tau \mathbf{x}$$

- Say we solved the Poisson equation. How do we evolve particles in time?



Collisionless dynamics of dark matter in an expanding Universe

- Equations of motion:

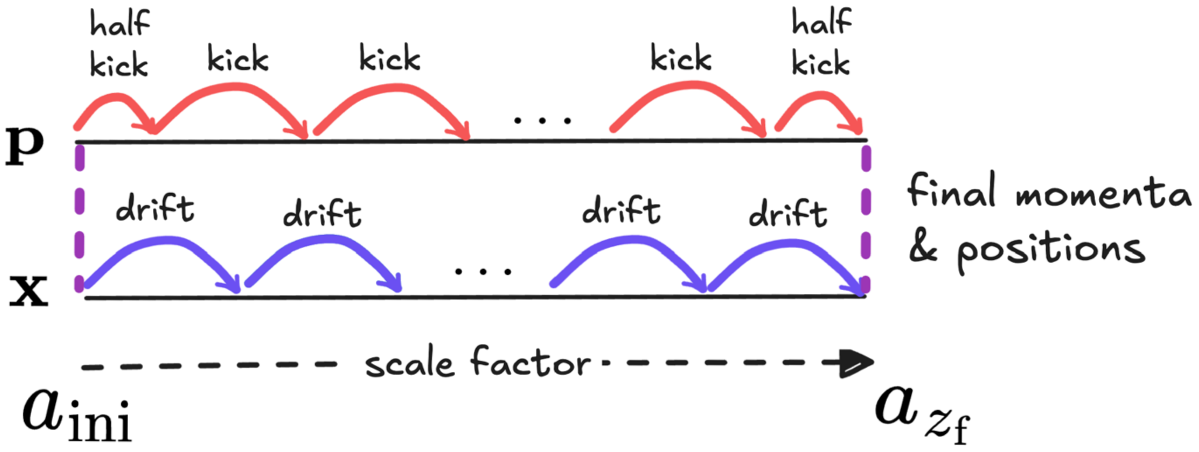
$$\partial_a \mathbf{x} = \mathcal{D}(a)\mathbf{p}$$
$$\partial_a \mathbf{p} = \mathcal{K}(a)\nabla\left(\Delta^{-1}\delta\right)$$

$\Delta^{-1}\delta$ denotes the solution of the Poisson equation $\Delta\Phi = \delta$.

The Drift and Kick pre-factors depend only on background quantities.

Details: Florent Leclercq's thesis, Appendix B

- The EoM are integrated in time typically using a Leapfrog integrator.



$$\mathbf{x}(a_{k+1}) = \mathbf{x}(a_k) + \dots \quad \text{(Drift)}$$
$$\mathbf{p}(a_{k+1}) = \mathbf{p}(a_k) + \dots \quad \text{(Kick)}$$

Collisionless dynamics of dark matter in an expanding Universe

Now, how do we get the potential & the force?

- Take N particles in a toroidal Universe of comoving size L^3

$$\delta(\mathbf{x}) = \sum_{n\in\mathbb{Z}^3}\left[-\frac{N}{L^3} + \sum_{j=1}^{N}\delta_{\mathrm{D}}\left(\mathbf{x}-\mathbf{x}_{j\mathbf{n}}\right)\right],$$

where $\mathbf{x}_{j\mathbf{n}} = \mathbf{x}_j + L\mathbf{n}$ is a commensurable image of the *j*-th particle.

Collisionless dynamics of dark matter in an expanding Universe

Now, how do we get the potential & the force?

- Approximate $\delta(\mathbf{x})$ by replacing δ_{D} with a smooth particle shape S_ϵ

$$\delta(\mathbf{x}) = \sum_{n\in\mathbb{Z}^3}\left[-\frac{N}{L^3} + \sum_{j=1}^{N} S_\epsilon\left(\mathbf{x} - \mathbf{x}_{j\mathbf{n}}\right)\right],$$

S_ϵ smoothens the density field below some characteristic scale ϵ.

Collisionless dynamics of dark matter in an expanding Universe

Now, how do we get the potential & the force?

- The Green function $\mathcal{G} \propto |\mathbf{x}|^{-1}$ of the Laplacian gives the solution of the Poisson equation for Dirac-like particles

$$\Phi(\mathbf{x}) \propto \sum_{j=1}^{N} \sum_{\mathbf{n}\in\mathbb{Z}^3} |\mathbf{x} - \mathbf{x}_{j\mathbf{n}}|^{-1}.$$

- For a particle shape S, the ”dressed Green function” $\mathcal{G}_S \,\tilde{\propto}\, |\mathbf{x}|_S^{-1}$ (notation) gives

$$\Phi(\mathbf{x}) \propto \sum_{j=1}^{N} \sum_{\mathbf{n}\in\mathbb{Z}^3} |\mathbf{x} - \mathbf{x}_{j\mathbf{n}}|_S^{-1}.$$

The Particle-Particle (PP) method.

- The comoving force $\mathbf{f}_i \propto \nabla\Phi(\mathbf{x}_i)$ acting on a particle is

$$\mathbf{f}_i \propto \sum_{\substack{j=1 \\ j\neq i}}^{N} \sum_{\mathbf{n}\in\mathbb{Z}^3} (\mathbf{x}_i - \mathbf{x}_{j\mathbf{n}})\left|\mathbf{x}_i - \mathbf{x}_{j\mathbf{n}}\right|_S^{-3}$$

$\left|\mathbf{x}_i - \mathbf{x}_{j\mathbf{n}}\right|_S^{-3}$ is just a notation—the meaning of which depends on *S*.

More details in Hockney & Eastwood 1988 & Dakin, Hannestad & Tram 2022, 2112.01508

- PP: determine $\mathbf{f}_i$ by computing all interactions.
- Force profile exact down to the smoothing length. Prohibitive $\mathcal{O}\left(N^2\right)$ complexity.

The Particle-Mesh (PM) method.

- The PM method solves the potential in Fourier space over a finite cubic grid. The forces are then obtained numerically.

- Main steps to compute the forces:
  1. Deposit / interpolate the particle masses onto a grid, yielding $\delta\rho(\mathbf{x})$ on a grid,
  2. $\delta\rho(\mathbf{x}) \xrightarrow{\text{FFT}} \delta\rho(\mathbf{k}) \xrightarrow{\times k^2} \Phi(\mathbf{k}) \xrightarrow{\text{iFFT}} \Phi(\mathbf{x})$ on the grid,
  3. Differentiate the potential to obtain the force $\mathbf{f}(\mathbf{x})$on the grid,
  4. Interpolate back to the particles' positions $\mathbf{x}_i$.

The Particle-Mesh (PM) method.

- $\mathcal{O}\left(N \log N\right)$ complexity. Drawback: force resolution limited by grid & large FFT.

- Main steps to compute the forces:
  1. Deposit / interpolate the particle masses onto a grid, yielding $\delta\rho(\mathbf{x})$ on a grid,
  2. $\delta\rho(\mathbf{x}) \xrightarrow{\text{FFT}} \delta\rho(\mathbf{k}) \xrightarrow{\times k^2} \Phi(\mathbf{k}) \xrightarrow{\text{iFFT}} \Phi(\mathbf{x})$ on the grid,
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The Particle-Particle—Particle-Mesh (P3M) method.

Hockney, Goel & Eastwood, 1974

The best of both worlds.

- Use PM for large-scale gravity.
- Supply the missing short-range gravity using direct summation (PP).

- **Ewald summation**

  At the crux of the P3M method is the Ewald summation technique.

  Brush, Sahlin & Teller, 1966 (same Teller as the hydrogen bomb); Hernquist, Bouchet & Suto, 1991.

  Start by writing $|\mathbf{x}|^{-1}$ (~ the Green function of the Laplacian) as a sum of a long-range and a short-range contribution:

$$|\mathbf{x}|^{-1} = \mathcal{G}_{\mathrm{sr}}(\mathbf{x}) + \mathcal{G}_{\mathrm{lr}}(\mathbf{x})$$

The Particle-Particle—Particle-Mesh (P3M) method.

- Now how does P3M work?
- Start with the softened potential seen earlier: $\Phi(\mathbf{x}) \propto \sum_{j=1}^{N} \sum_{\mathbf{n}\in\mathbb{Z}^3} |\mathbf{x} - \mathbf{x}_{j\mathbf{n}}|_S^{-1}.$
- Make the true, unsoftened Green function appear:

$$\phi(\mathbf{x}) \propto \sum_{j=1}^{N} \sum_{\mathbf{n}} \overbrace{|\mathbf{x} - \mathbf{x}_{j\mathbf{n}}|^{-1}}^{\text{unsoftened}} + \overbrace{\left(|\mathbf{x} - \mathbf{x}_{j\mathbf{n}}|_S^{-1} - |\mathbf{x} - \mathbf{x}_{j\mathbf{n}}|^{-1}\right)}^{\text{deviation from the softened potential}}$$

- Then, split the unsoftened potential using the Ewald technique:

$$\phi(\mathbf{x}) \propto \sum_{j=1}^{N} \sum_{\mathbf{n}} \mathcal{G}_{\mathrm{sr}}(\mathbf{x} - \mathbf{x}_{j\mathbf{n}}) + |\mathbf{x} - \mathbf{x}_{j\mathbf{n}}|_S^{-1} - |\mathbf{x} - \mathbf{x}_{j\mathbf{n}}|^{-1} + \underbrace{\mathcal{G}_{\mathrm{lr}}(\mathbf{x} - \mathbf{x}_{j\mathbf{n}})}_{\text{solved with PM}}$$

The Particle-Particle—Particle-Mesh (P3M) method.

- After some tricks and algebra, one obtains a finite expression for the force:

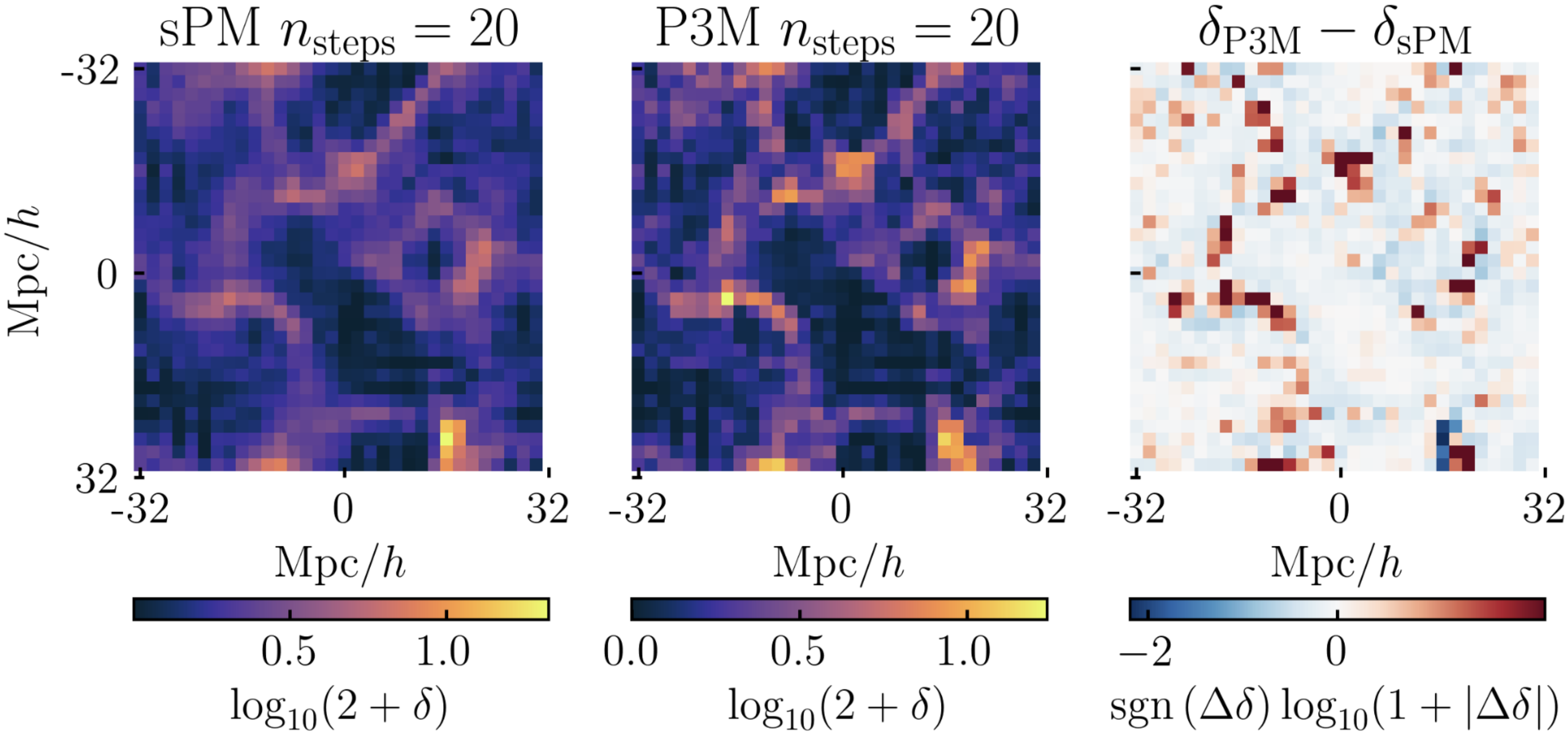
$$\mathbf{f}_i = \underbrace{\text{finite short-range part}}_{\text{solved with direct summation}} + \underbrace{\text{smooth long-range part}}_{\text{solved with standard PM}}$$

More details in Efstathiou & Eastwood 1981, Hockney & Eastwood 1988, Dakin, Hannestad & Tram 2022, 2112.01508

- Since the long-range force is provided with PM, the short-range summation is computed only in a local neighborhood of each particle.

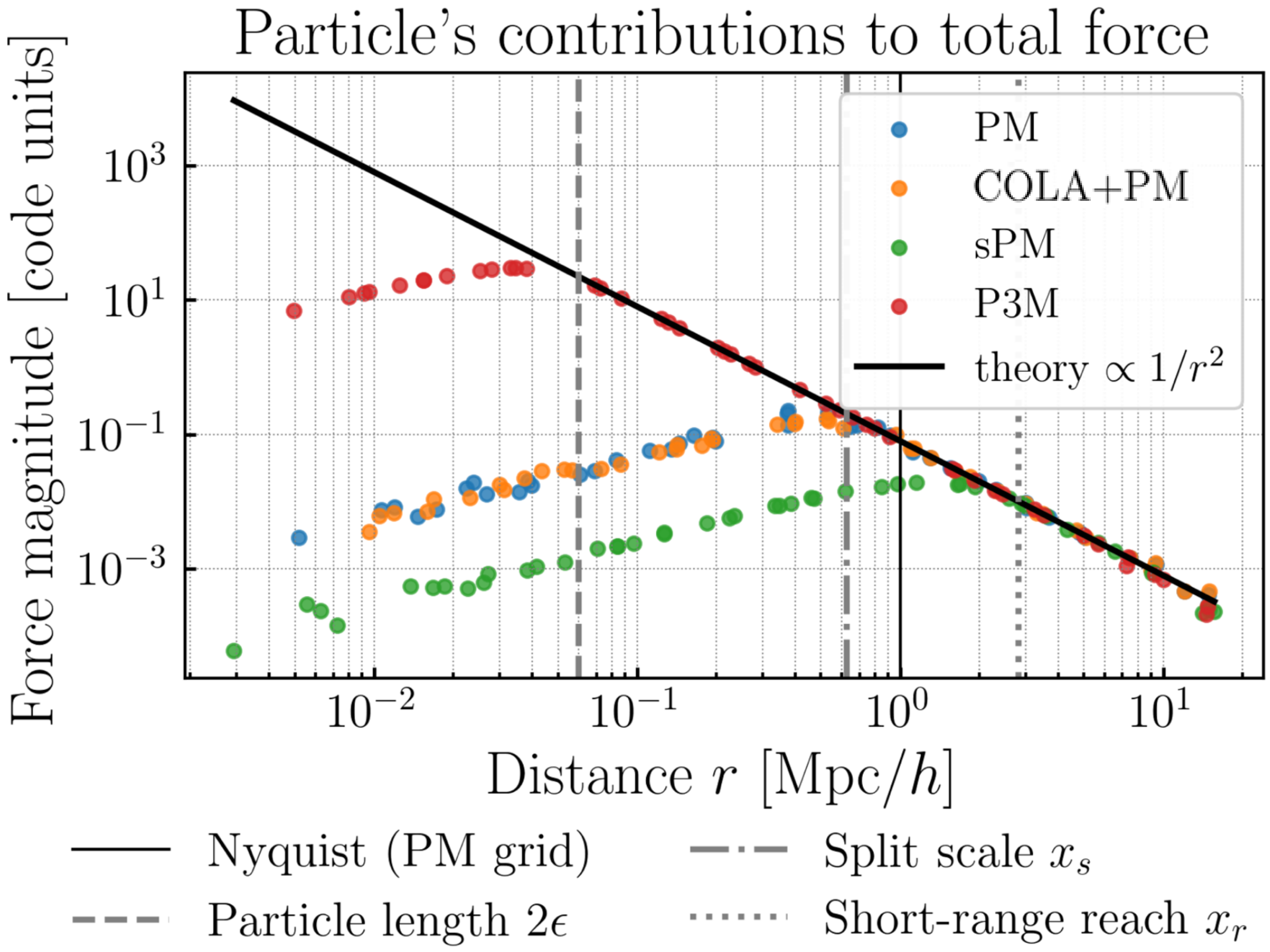
- This allows beating the $\mathcal{O}\left(N^2\right)$ complexity of standard PP summation!

Collisionless dynamics of dark matter in an expanding Universe



Plot computed using a modified version of the Simbelmynë cosmological solver.

Collisionless dynamics of dark matter in an expanding Universe



Plot computed using a modified version of the Simbelmynë cosmological solver.

COmoving Lagrangian Acceleration (COLA) with P3M

COLA: COmoving Lagrangian Acceleration

- Separate the temporal evolution of large and small scales.

$$\mathbf{\Psi}(\mathbf{q}, a) \equiv \mathbf{\Psi}_{\mathrm{LPT}}(\mathbf{q}, a) + \mathbf{\Psi}^{\mathrm{COLA}}_{\mathbf{res}}(\mathbf{q}, a).$$

- $\mathbf{q}$ denotes the Lagrangian position, $\mathbf{x} = \mathbf{q} + \mathbf{\Psi}$.

- $\mathbf{\Psi}_{\mathrm{LPT}}(\mathbf{q}, a)$ is the LPT displacement field, $\mathbf{\Psi}^{\mathrm{COLA}}_{\mathbf{res}}(\mathbf{q}, a)$ denotes the residual displacement of particles seen from a frame comoving with an "LPT observer".

Tassev, Zaldarriaga & Eisenstein, 2013; Tassev & Zaldarriaga, 2012

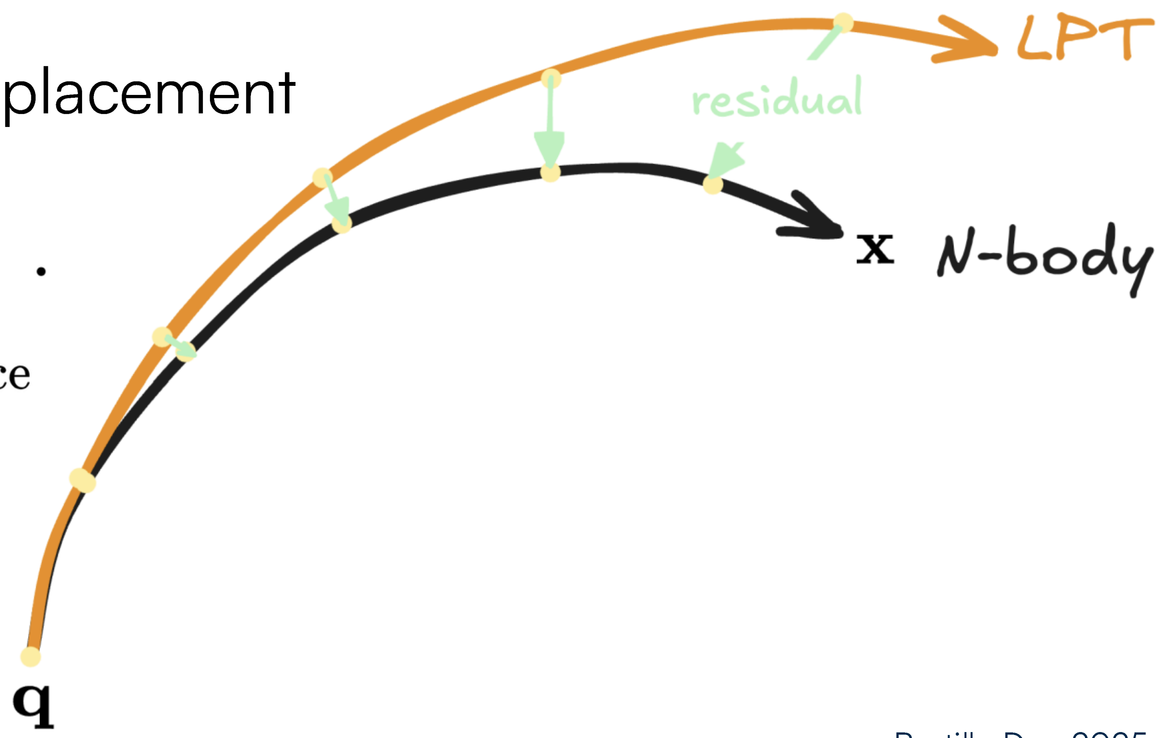
COLA: COmoving Lagrangian Acceleration

- Separate the temporal evolution of large and small scales.

$$\boldsymbol{\Psi}(\mathbf{q}, a) \equiv \boldsymbol{\Psi}_{\mathrm{LPT}}(\mathbf{q}, a) + \boldsymbol{\Psi}_{\mathrm{res}}^{\mathrm{COLA}}(\mathbf{q}, a).$$

- Equations of motion for the residual displacement

$$\partial_a^2 \boldsymbol{\Psi}_{\mathrm{res}}^{\mathrm{COLA}} = -\nabla_{\mathbf{x}}\Phi - \underbrace{\partial_a^2 \boldsymbol{\Psi}_{\mathrm{LPT}}}_{\text{fictitious force}} .$$

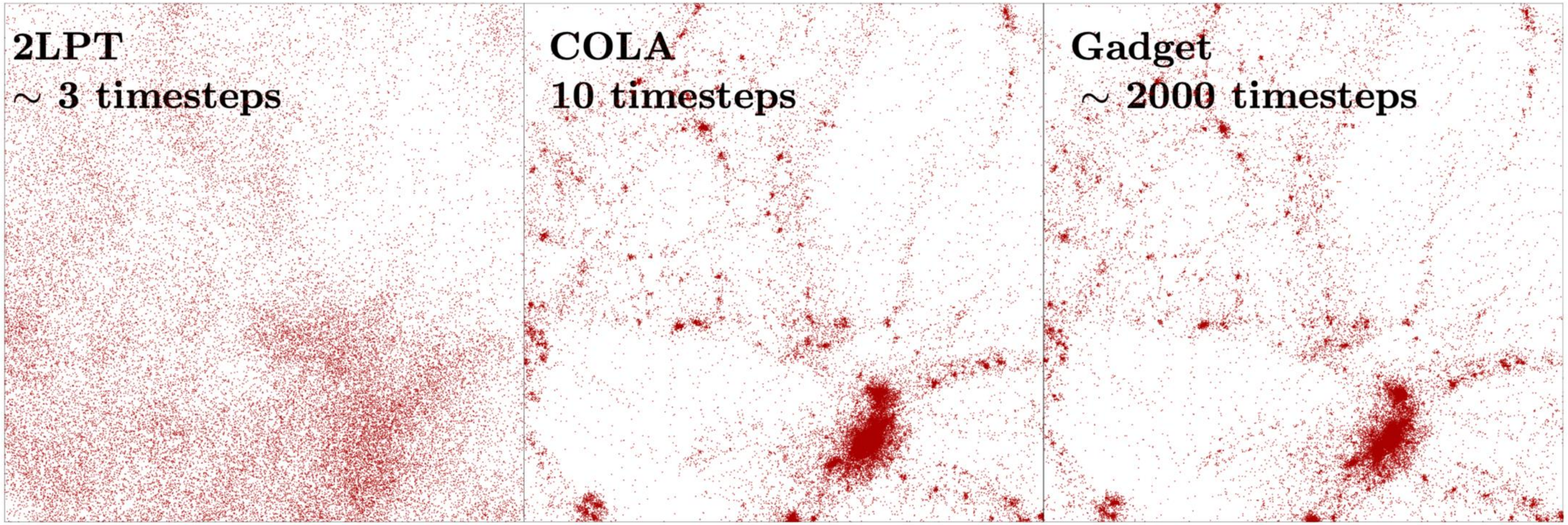


Tassev, Zaldarriaga & Eisenstein, 2013; Tassev & Zaldarriaga, 2012

COLA: COmoving Lagrangian Acceleration

- Introduced by Tassev, Zaldarriaga & Eisenstein 2013, 1301.0322.

Famously applied to a PM code, solving the large-scale structure in 10 time steps.



Tassev, Zaldarriaga & Eisenstein, 2013

COLA with P3M forces

COLA: COmoving Lagrangian Acceleration

- A common missconception is that COLA sacrifices small-scale accuracy for speed! **It does not**.

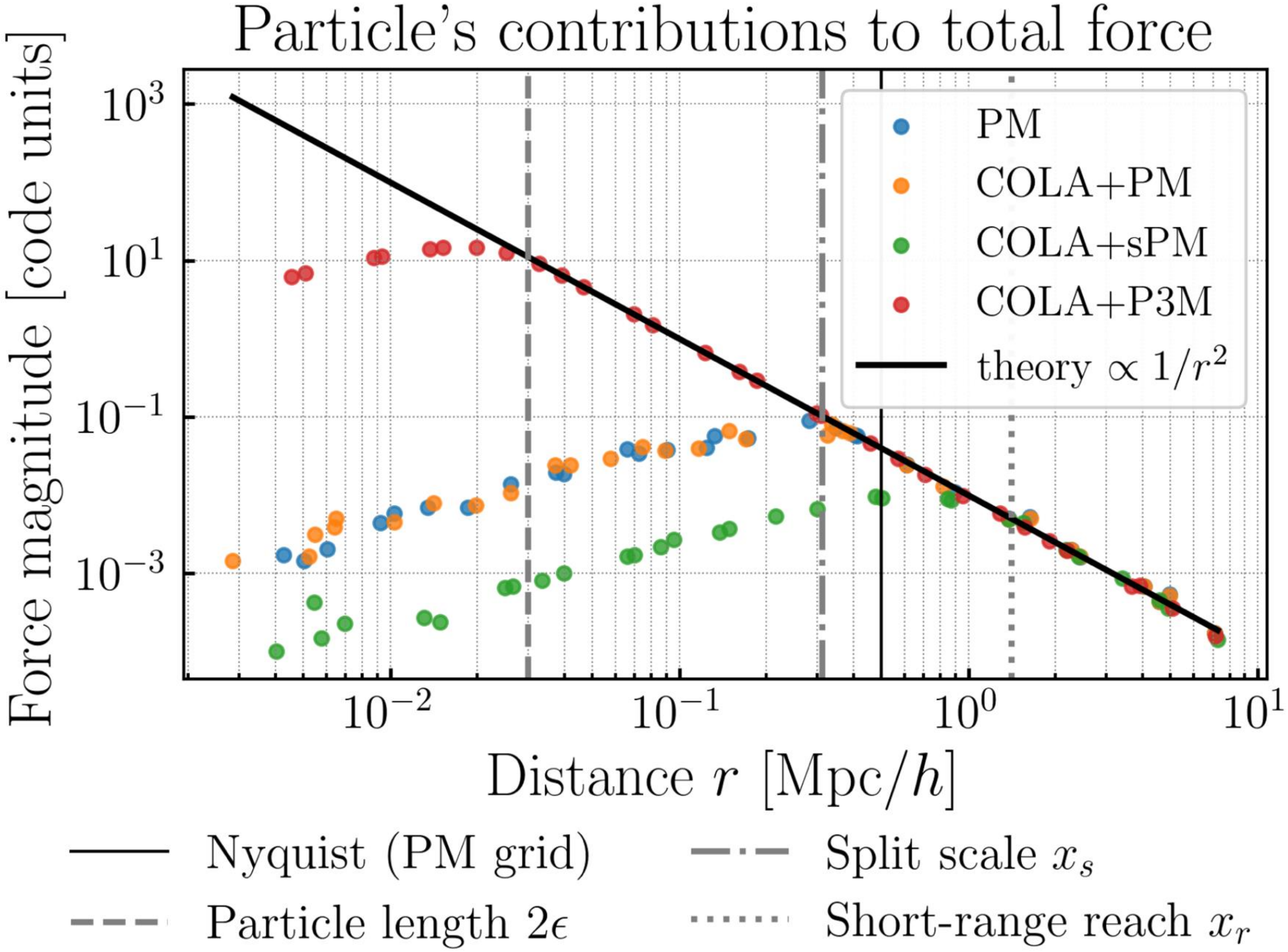
- The LPT change of frame of reference can be done with *any* force calculation.

- Accurate **small-scales in 200 time steps** using **COLA** with **P3M forces**.

COLA with P3M forces

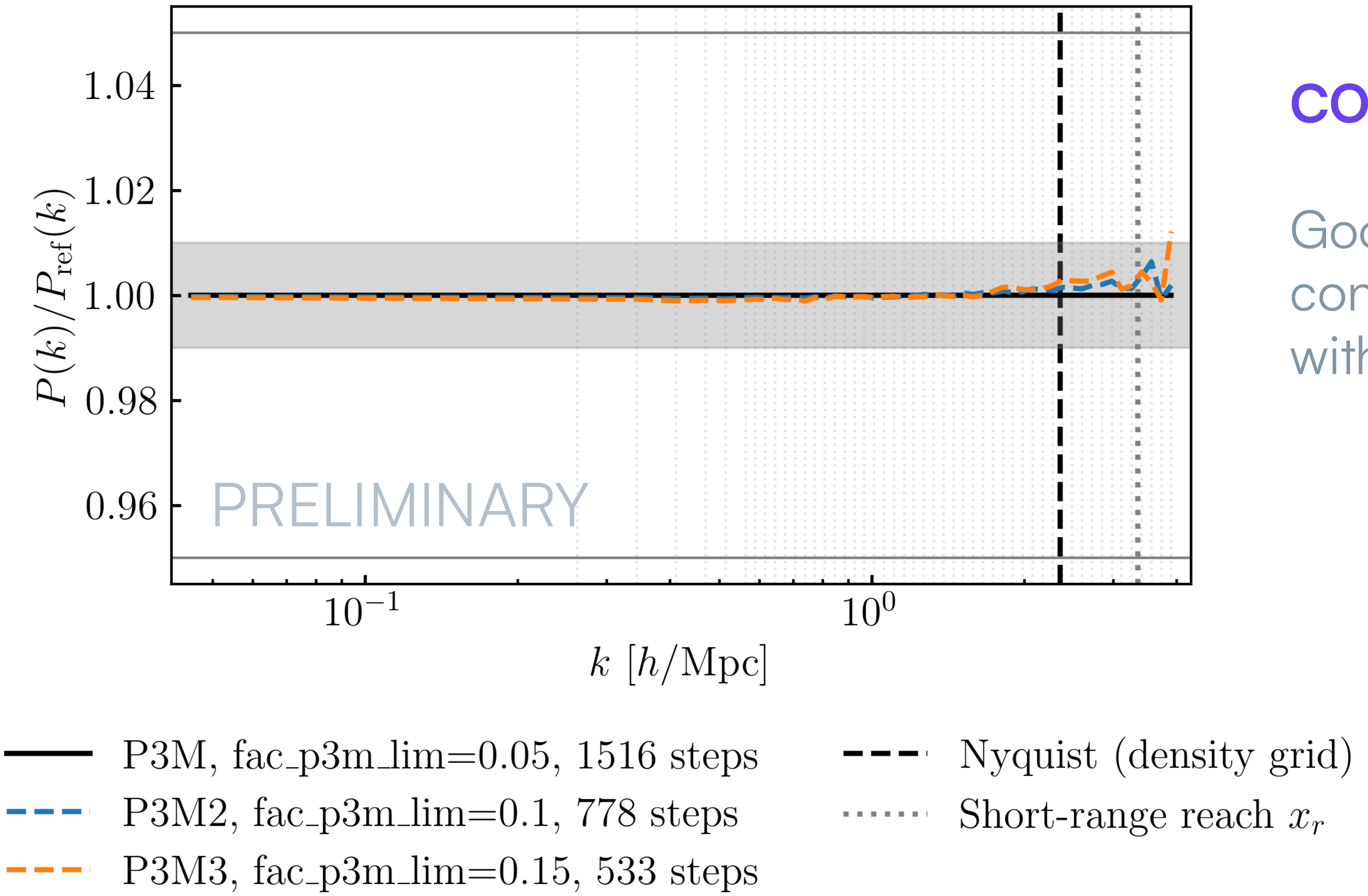
- Objective: Get **accurate gravitational forces** at small scales, at an affordable cost, usable in actual cosmological inferences. *As accurate as Tree-based codes e.g. GADGET4.*
- What for? Exploit small scale information of Stage-IV surveys.
- The COLA change of frame makes it possible to start the simulation later and use fewer time steps. *Preliminary result — to be confirmed.*

COLA with P3M forces



Plot computed using a modified version of the Simbelmynë cosmological solver.

COLA with P3M forces

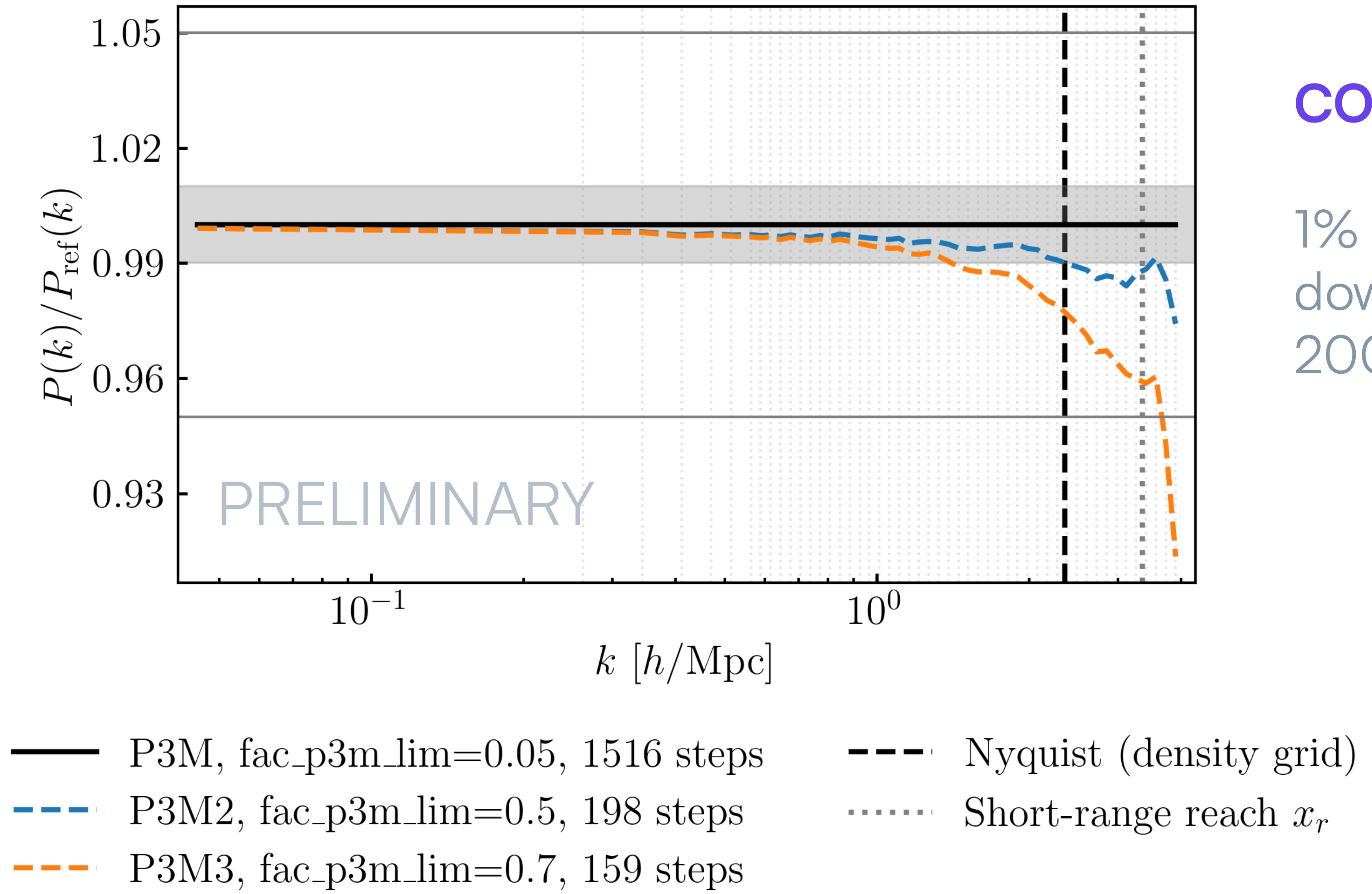


COLA+P3M

Good P(k) convergence with ~500 steps.

Plot computed using a modified version of the Simbelmynë cosmological solver.

COLA with P3M forces



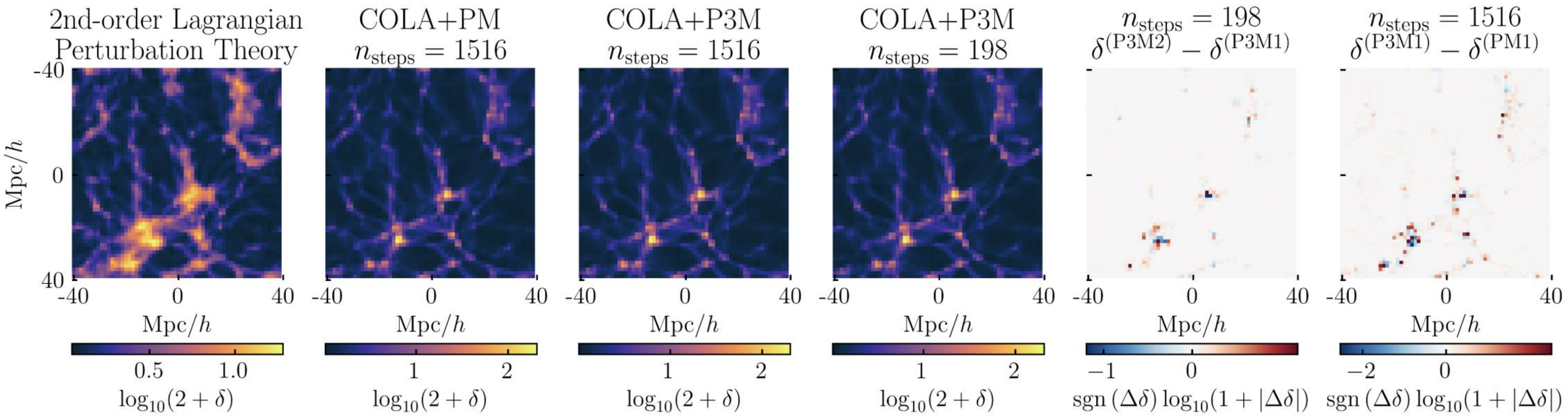
COLA+P3M

1% agreement down to *k*=2 with 200 time steps.

Plot computed using a modified version of the Simbelmynë cosmological solver.

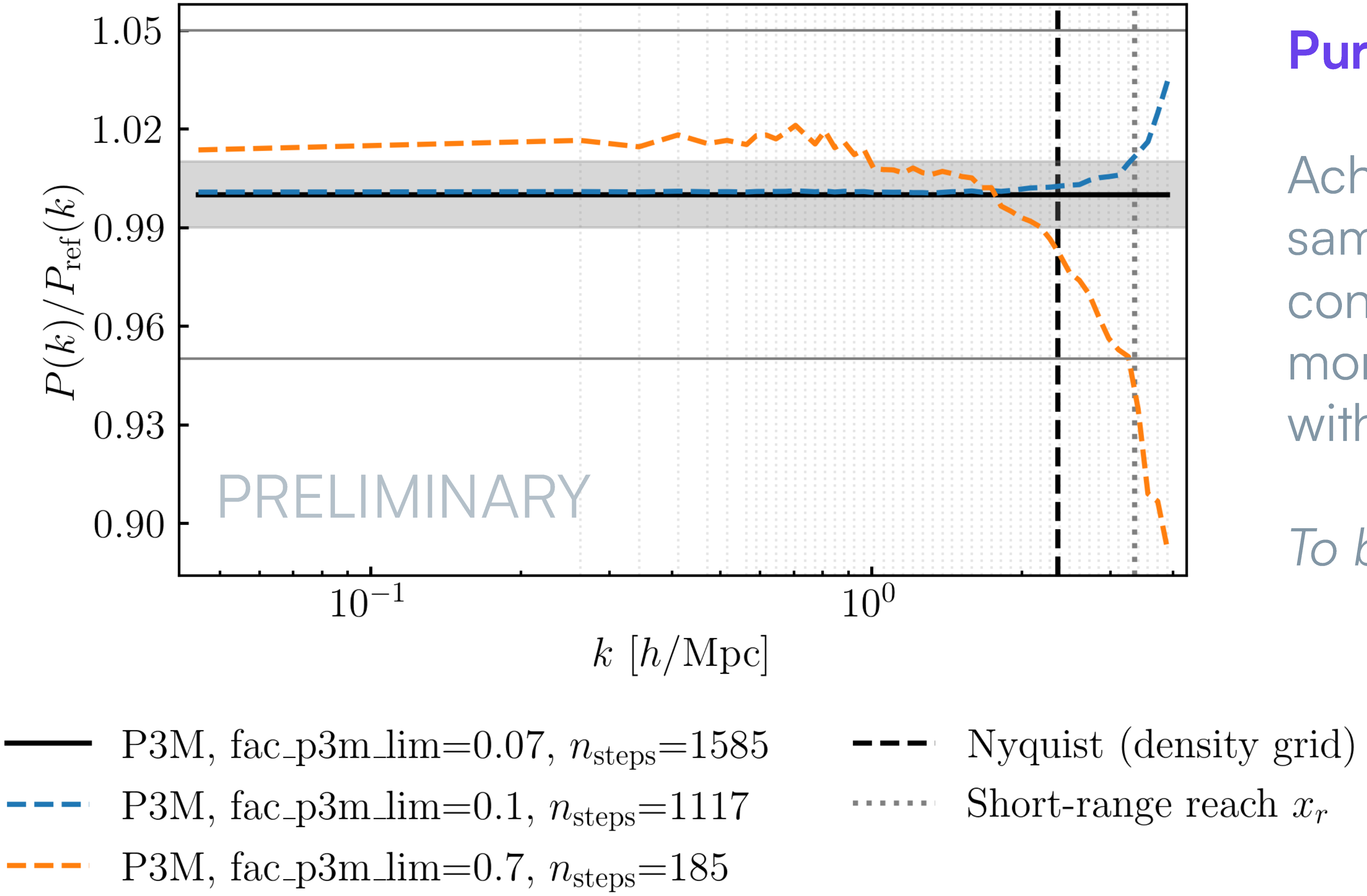
COLA with P3M forces

- Next step: look how residuals with ~200 time steps affects halos and other stats.



Plot computed using a modified version of the Simbelmynë cosmological solver.

COLA with P3M forces



Pure P3M

Achieving the same level of convergence is more expensive without COLA.

To be confirmed!

Plot computed using a modified version of the Simbelmynë cosmological solver.

What next?

What next?

Where we are now.

- COLA+P3M force evaluation: proof-of-concept validated based on *P(k)* for box sizes between 60 and 2048 Mpc/*h*.
- 200 time steps were consistently enough to guarantee <1% precision down to *k*=2 in all setups tested with mass resolutions down to $1 \times 10^{10}\ M_\odot$.
- This seems to be a significant improvement compared to not using COLA.

What next?

What needs to be done / ongoing work

- Check the halo mass function, and other statistics.
- Implement non-periodic boundary conditions.

- Further reduce the number of force evaluations. How?
  Forces need not be evaluated at each time step.
  Use an emulated frame of reference (as in Bartlett et al. 2025, 2409.02154).

$$\Psi = \Psi_{\mathrm{LPT}} + \Psi_{\mathrm{ML}} + \Psi_{\mathrm{res}}^{\mathrm{COCA}}$$

$$\partial_t^2 \Psi_{\mathrm{res}}^{\mathrm{COCA}} = -\nabla\Phi - \partial_t^2 \Psi_{\mathrm{LPT}} - \partial_t^2 \Psi_{\mathrm{ML}}$$

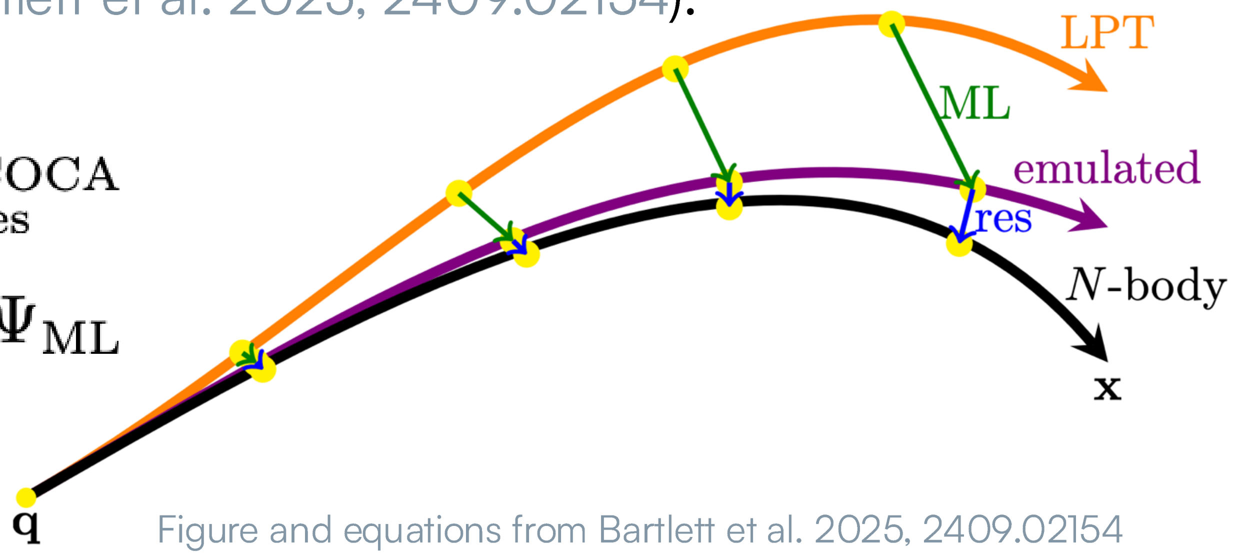


Figure and equations from Bartlett et al. 2025, 2409.02154

Acknowledgements, credits, contacts

Thanks!

Questions? hoelling@iap.fr

References

- **Simbelmynë**: Leclercq, Jasche & Wandelt 2015, 1502.02690
- **GADGET**: Springel 2005, astro-ph/0505010
- **CONCEPT**: Dakin, Hannestad & Tram 2022, 2112.01508
- **COCA**: Bartlett et al. 2025, 2409.02154

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BACKUP SLIDES

The Particle-Particle—Particle-Mesh (P3M) method.

$$\mathcal{G}_{\rm sr}(\mathbf{x}) = \mathrm{erfc}(|\mathbf{x}|/[2x_{\rm s}])|\mathbf{x}|^{-1} \qquad \mathcal{G}_{\rm lr}(\mathbf{x}) = \mathrm{erf}(|\mathbf{x}|/[2x_{\rm s}])|\mathbf{x}|^{-1}$$

This form of long-range potential is essentially the solution of the Poisson equation for a Gaussian distribution of mass—it is therefore the same as the dressed Green function obtained by replacing a point particle by a Gaussian shape.

The Ewald procedure, however, introduces no smoothing in the total potential.

COLA with P3M forces

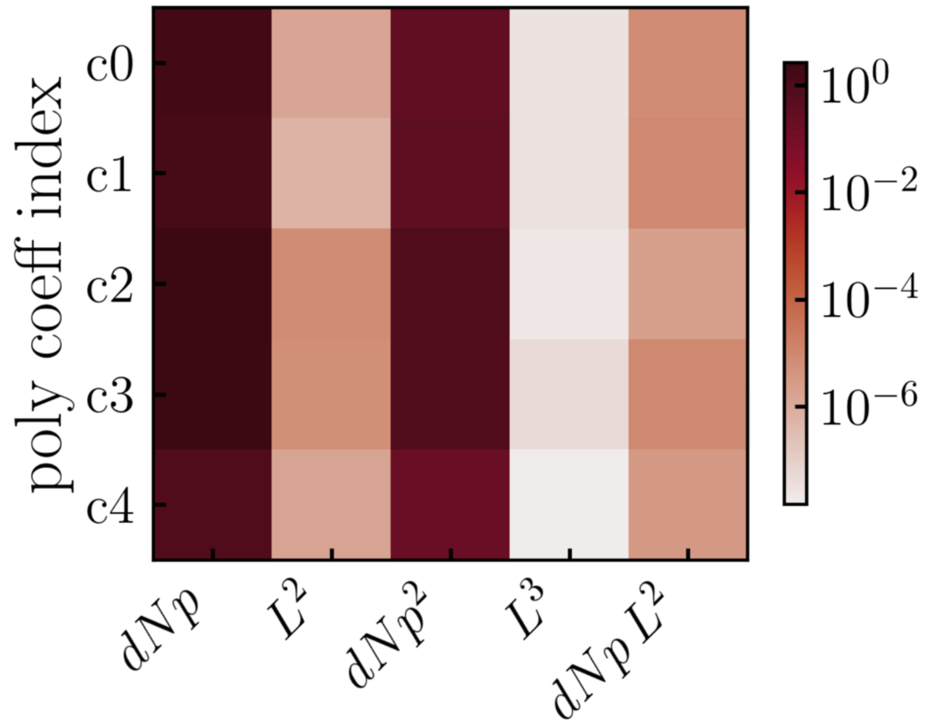
- PP summation requires fine steps at late times.

  Use time step limiters to avoid unnecessary fine steps earlier on.

- Some limiters are “linear”—they do not depend on the particle system,

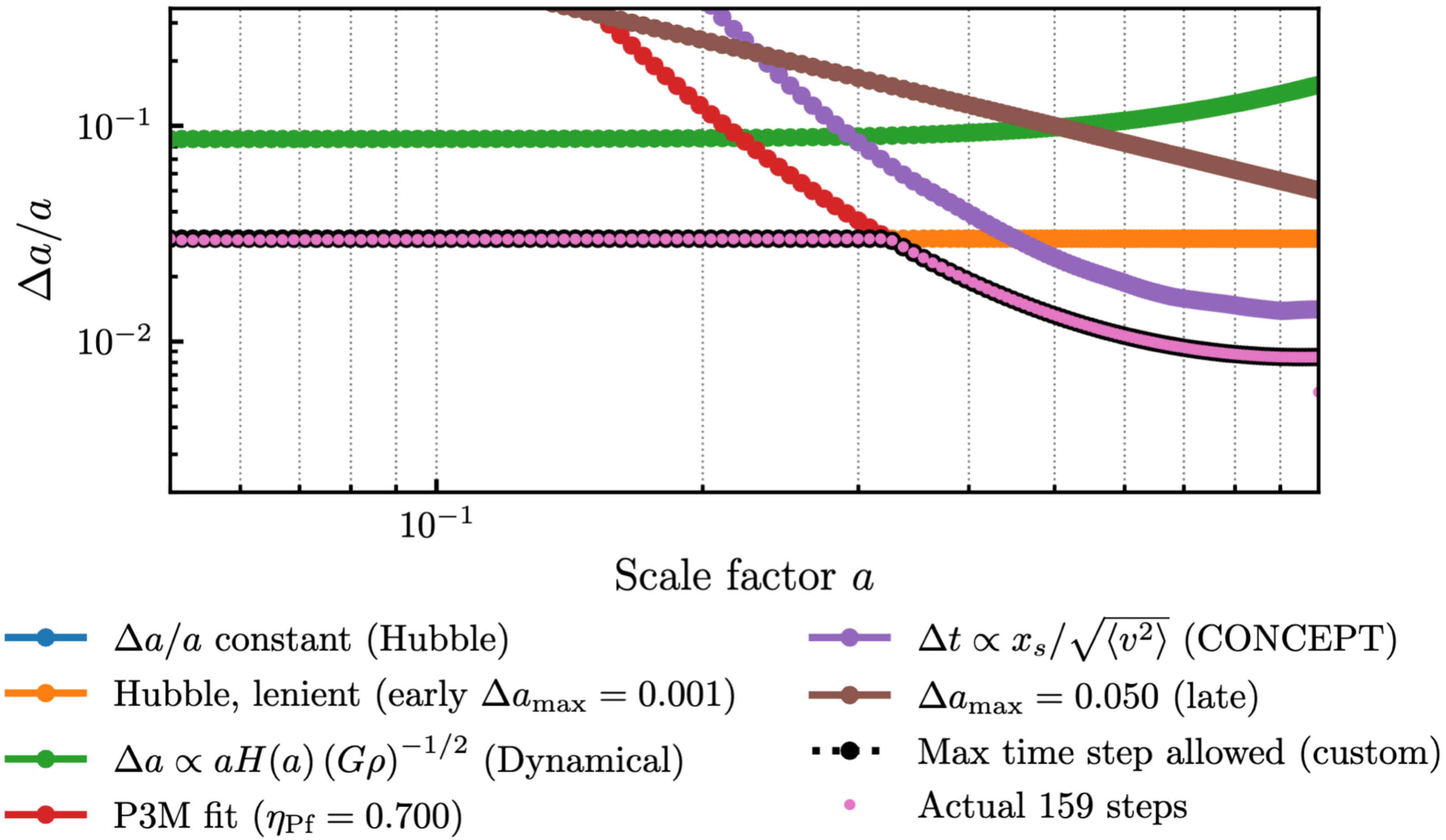
- Some are non-linear.

- Fit the P3M time step limiter with quintic polynomials (coefficients regressed against L and L/N_p).



COLA with P3M forces

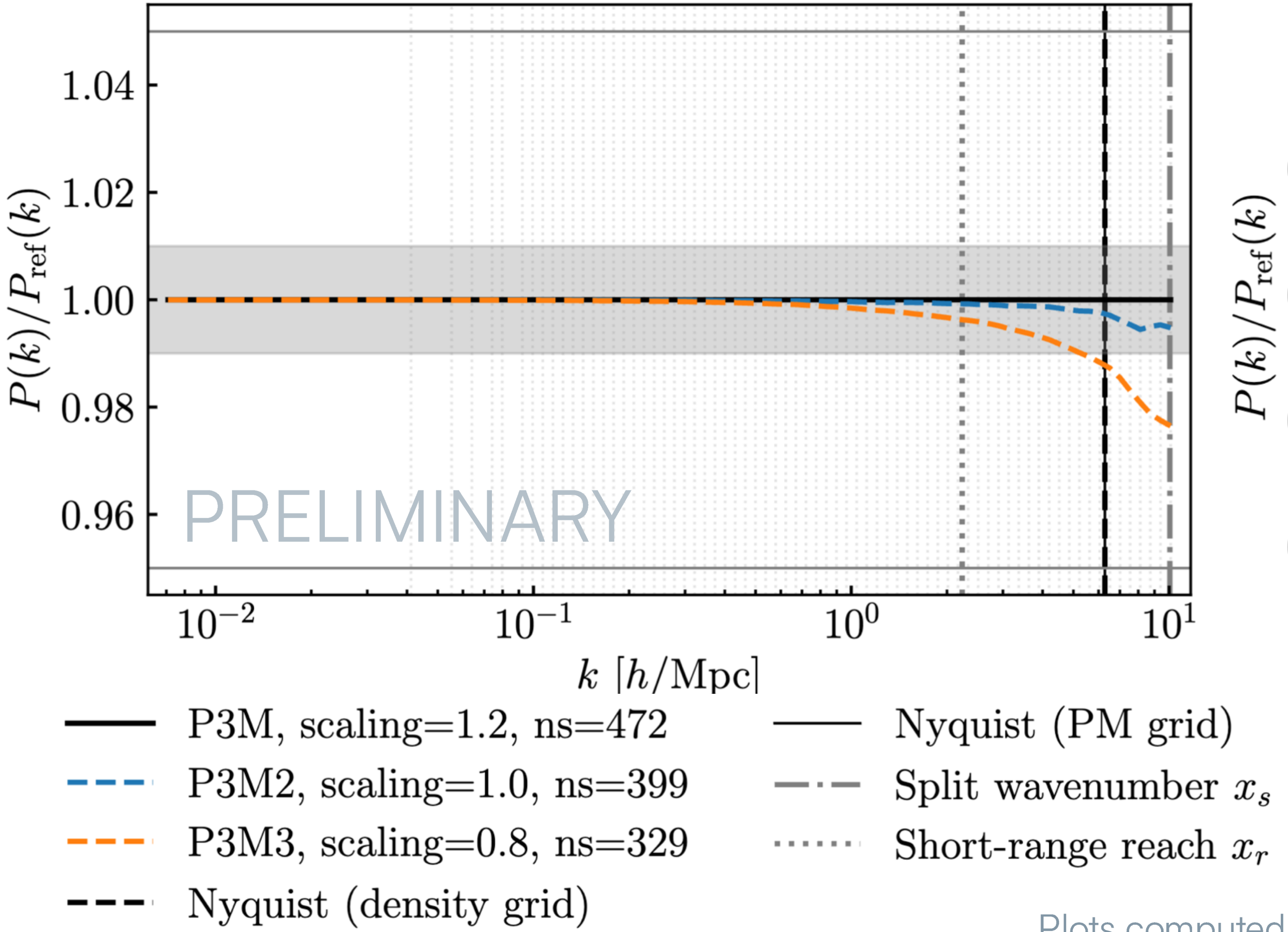
Limiters based on Dakin, Hannestad & Tram 2022, 2112.01508.

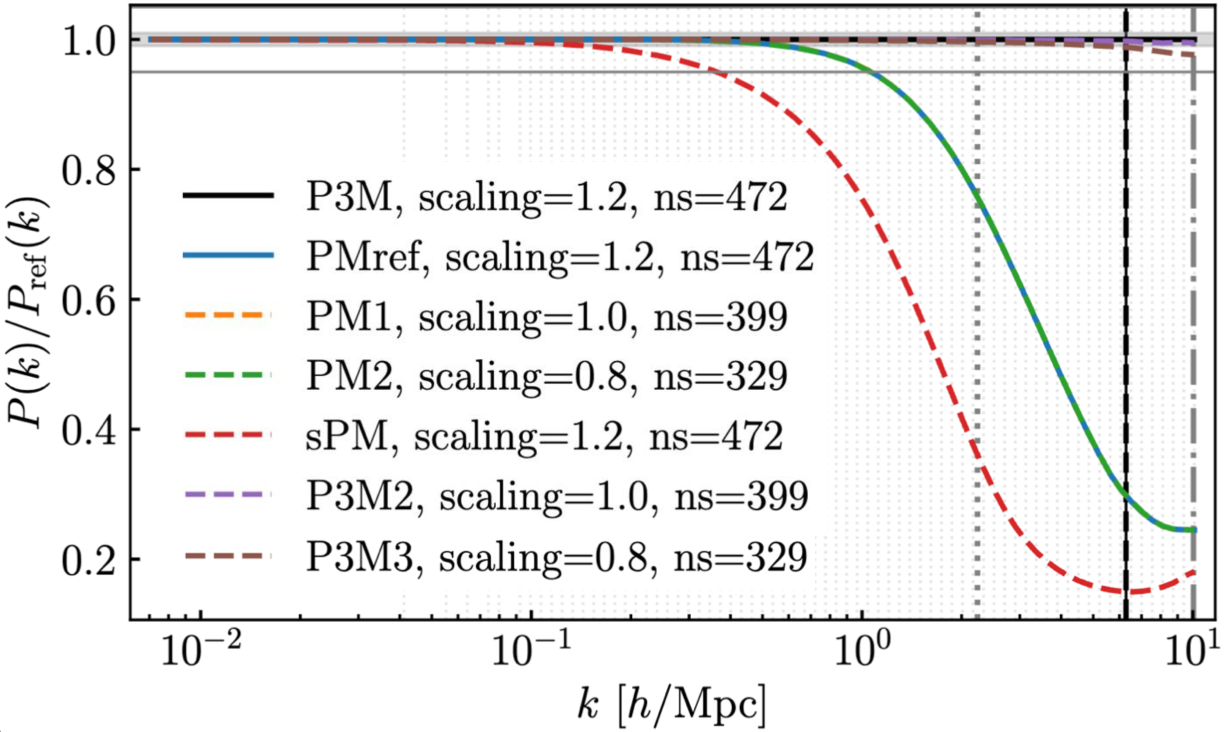


Plot computed using a modified version of the Simbelmynë cosmological solver.

COLA with P3M forces

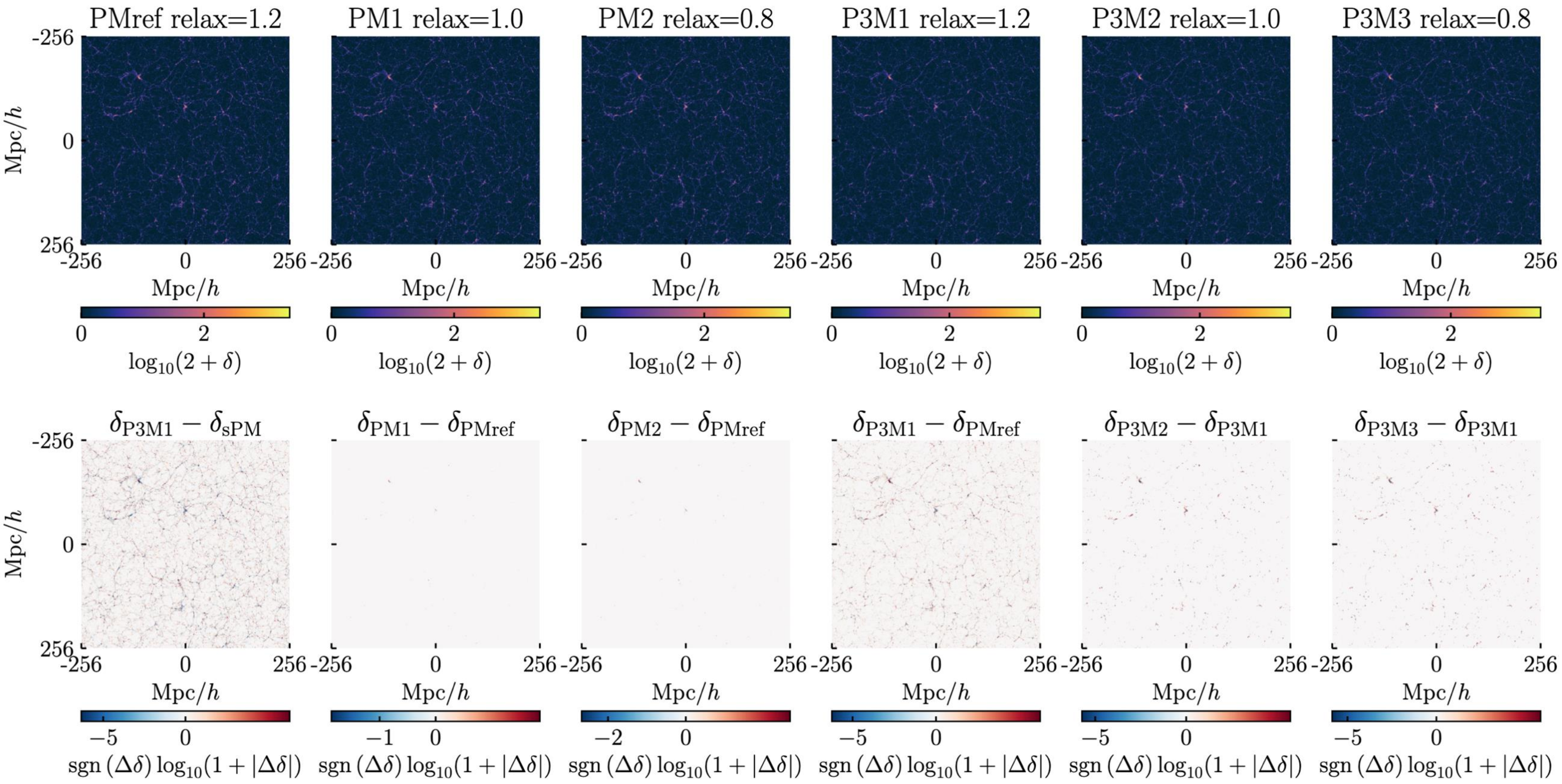
- Much larger box (+ slightly coarser mass resolution).





Plots computed using a modified version of the Simbelmynë cosmological solver.

COLA with P3M forces



Collisionless dynamics of dark matter in an expanding Universe

Deriving the actual expression for the potential with direct summation.

$$\phi(\mathbf{x}) \overset{\Delta}{=} \frac{-Gm}{a} \sum_{j=1}^{N} \sum_{\mathbf{n}\in\mathbb{Z}^3} |\mathbf{x}-\mathbf{x}_{jn}|_{\bullet}^{-1} \quad \text{start with the total softened potential}$$

$$= \frac{-Gm}{a} \sum_{j=1}^{N} \sum_{\mathbf{n}\in\mathbb{Z}^3} \overbrace{|\mathbf{x}-\mathbf{x}_{jn}|^{-1}}^{\text{Newtonian}} + \overbrace{\left(|\mathbf{x}-\mathbf{x}_{jn}|_{\bullet}^{-1} - |\mathbf{x}-\mathbf{x}_{jn}|^{-1}\right)}^{\text{deviation of Newtonian from softened potential}} \quad \text{make the true unsoftened Green function appear}$$

$$= \frac{-Gm}{a} \sum_{j=1}^{N} \sum_{\mathbf{n}\in\mathbb{Z}^3} \mathcal{G}_{\text{sr}}(\mathbf{x}-\mathbf{x}_{jn}) + \mathcal{G}_{\text{lr}}(\mathbf{x}-\mathbf{x}_{jn}) + \left(|\mathbf{x}-\mathbf{x}_{jn}|_{\bullet}^{-1} - |\mathbf{x}-\mathbf{x}_{jn}|^{-1}\right) \quad \text{split the true potential (Ewald)}$$

$$= \frac{-Gm}{a} \sum_{j=1}^{N} \left[\underbrace{\sum_{\mathbf{n}\in\mathbb{Z}^3} \mathcal{G}_{\text{sr}}(\mathbf{x}-\mathbf{x}_{jn}) + \overbrace{\underbrace{\left(|\mathbf{x}-\mathbf{x}_{jn}|_{\bullet}^{-1} - |\mathbf{x}-\mathbf{x}_{jn}|^{-1}\right)}_{\text{is why we write it here}}}^{\text{the deviation of the Newtonian from the softened potential affects only the short range part, which}}}_{\text{short range contribution of all particles images to the potential}} + \underbrace{\sum_{\mathbf{n}\in\mathbb{Z}^3} \mathcal{G}_{\text{lr}}(\mathbf{x}-\mathbf{x}_{jn})}_{\text{long range}} \right]$$

$$\overset{\text{Fourier}}{=} \frac{-Gm}{a} \sum_{j=1}^{N} \left[\underbrace{\sum_{\mathbf{n}\in\mathbb{Z}^3} \overbrace{\underbrace{\mathcal{G}_{\text{sr}}(\mathbf{x}-\mathbf{x}_{jn})}_{\text{vanishingly small at a distance } x_r \text{ a few times greater than } x_s}}^{\equiv \text{ complementary error function, over } r} + \overbrace{\left(|\mathbf{x}-\mathbf{x}_{jn}|_{\bullet}^{-1} - |\mathbf{x}-\mathbf{x}_{jn}|^{-1}\right)}^{\text{cancels out at large distance (above } x_B)}}_{\text{short range}} + \underbrace{L_{\text{box}}^{-3} \sum_{\mathbf{h}\in\mathbb{Z}^3\setminus\{\mathbf{0}\}} \mathcal{G}_{\text{lr}}(k_{\mathbf{h}}) \cos\left[k_{\mathbf{h}} \cdot (\mathbf{x}-\mathbf{x}_j)\right]}_{\text{Fourier decomposition of the long range contribution (details below, Poisson summation formula for Ewald)}} \right]$$

Based on Dakin, Hannestad & Tram 2022, 2112.01508.

Collisionless dynamics of dark matter in an expanding Universe

Deriving the actual expression for the potential with direct summation.

$$\phi(\mathbf{x}) = \frac{-Gm}{a}\sum_{j=1}^{N}\left[\underbrace{\sum_{\mathbf{n}\in\mathbb{Z}^3}\underbrace{\overbrace{\mathcal{G}_{\rm sr}(\mathbf{x}-\mathbf{x}_{jn})}^{\equiv\text{ complementary error function, over } r}}_{\text{vanishingly small at a distance } x_r \text{ a few times greater than } x_s} + \overbrace{\left(|\mathbf{x}-\mathbf{x}_{jn}|_\bullet^{-1} - |\mathbf{x}-\mathbf{x}_{jn}|^{-1}\right)}^{\text{cancels out at large distance (above } x_B)}}_{\text{short range}} + \underbrace{L_{\rm box}^{-3}\sum_{\mathbf{h}\in\mathbb{Z}^3\setminus\{\mathbf{0}\}}\mathcal{G}_{\rm lr}(k_{\mathbf{h}})\cos\left[k_{\mathbf{h}}\cdot(\mathbf{x}-\mathbf{x}_j)\right]}_{\text{Fourier decomposition of the long range contribution (details below, Poisson summation formula for Ewald)}}\right]$$

where $\mathbf{k_h} \overset{\Delta}{=} 2\pi L_{\rm box}^{-1}\mathbf{h}$ and we recall that $\mathbf{x}_{jn} \overset{\Delta}{=} \mathbf{x}_j + L_{\rm box}\mathbf{n}$. Using the Poisson summation formula, one has:

$$\sum_{\mathbf{n}\in\mathbb{Z}^3}\mathcal{G}_{\rm lr}(\mathbf{x}-\mathbf{x}_{jn}) = \sum_{\mathbf{n}\in\mathbb{Z}^3}\mathcal{G}_{\rm lr}(\mathbf{x}-\mathbf{x}_j - L_{\rm box}\mathbf{n}) \overset{\text{Poisson}}{=} L_{\rm box}^{-3}\sum_{\mathbf{h}\in\mathbb{Z}^3}\mathcal{G}_{\rm lr}(k_{\mathbf{h}})\exp\left[ik_{\mathbf{h}}\cdot(\mathbf{x}-\mathbf{x}_j)\right] \overset{\mathcal{G}_{\rm lr}\text{ even}}{=} L_{\rm box}^{-3}\sum_{\mathbf{h}\in\mathbb{Z}^3}\mathcal{G}_{\rm lr}(k_{\mathbf{h}})\cos\left[k_{\mathbf{h}}\cdot(\mathbf{x}-\mathbf{x}_j)\right],$$

which is how the real space sum over all integer triplets $\mathbf{n}$ is replaced by a reciprocal space sum over all integer triplets $\mathbf{k}$. This trick is one of the core principles of the Ewald summation: the sum converges much faster in Fourier space.

Based on Dakin, Hannestad & Tram 2022, 2112.01508.

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Deriving the actual expression for the force with direct summation.

$$\nabla \mathcal{G}_{\rm sr}(\mathbf{x}) = \nabla\left(\frac{\mathrm{erfc}(|\mathbf{x}|/[2x_{\rm s}])}{|\mathbf{x}|}\right) = -\frac{\mathbf{x}}{|\mathbf{x}|^3}\mathrm{erfc}\left(\frac{|\mathbf{x}|}{2x_{\rm s}}\right) - \frac{1}{2x_{\rm s}|\mathbf{x}|}\frac{2}{\sqrt{\pi}}\frac{\mathbf{x}}{|\mathbf{x}|}\exp\left(-\frac{|\mathbf{x}|^2}{4x_{\rm s}^2}\right) = \left[-|\mathbf{x}|^{-3}\mathrm{erfc}\left(\frac{|\mathbf{x}|}{2x_{\rm s}}\right) - \frac{|\mathbf{x}|^{-2}}{\sqrt{\pi}x_s}\exp\left(-\frac{|\mathbf{x}|^2}{4x_{\rm s}^2}\right)\right]\mathbf{x}$$

$$\nabla \mathcal{G}_{\rm lr}(\mathbf{x}) = \nabla\left(\frac{\mathrm{erf}(|\mathbf{x}|/[2x_{\rm s}])}{|\mathbf{x}|}\right) = -\frac{\mathbf{x}}{|\mathbf{x}|^3}\mathrm{erf}\left(\frac{|\mathbf{x}|}{2x_{\rm s}}\right) + \frac{1}{2x_{\rm s}|\mathbf{x}|}\frac{2}{\sqrt{\pi}}\frac{\mathbf{x}}{|\mathbf{x}|}\exp\left(-\frac{|\mathbf{x}|^2}{4x_{\rm s}^2}\right) = \left[-|\mathbf{x}|^{-3}\mathrm{erf}\left(\frac{|\mathbf{x}|}{2x_{\rm s}}\right) + \frac{|\mathbf{x}|^{-2}}{\sqrt{\pi}x_s}\exp\left(-\frac{|\mathbf{x}|^2}{4x_{\rm s}^2}\right)\right]\mathbf{x}.$$

Denoting $\mathbf{x}_{ij\mathbf{n}} \stackrel{\Delta}{=} \mathbf{x}_i - \mathbf{x}_{jn}$ and $\nabla \equiv \nabla_{\mathbf{x}_i}$, it follows that the comoving force acting on particle i is:

$$\begin{aligned}\mathbf{f}_i &\stackrel{\Delta}{=} -am\nabla\phi(\mathbf{x}_i) = Gm^2\nabla\sum_{j=1}^{N}\left(\sum_{\mathbf{n}\in\mathbb{Z}^3}\mathcal{G}_{\rm sr}(\mathbf{x}-\mathbf{x}_{jn}) + \left(|\mathbf{x}-\mathbf{x}_{jn}|_\bullet^{-1} - |\mathbf{x}-\mathbf{x}_{jn}|^{-1}\right) + L_{\rm box}^{-3}\sum_{\mathbf{h}\in\mathbb{Z}^3\setminus\{0\}}\mathcal{G}_{\rm lr}(k_{\mathbf{h}})\cos\left[k_{\mathbf{h}}\cdot(\mathbf{x}-\mathbf{x}_j)\right]\right)\\
&= Gm^2\nabla\sum_{j=1}^{N}\left(\sum_{\mathbf{n}\in\mathbb{Z}^3}\mathcal{G}_{\rm sr}(\mathbf{x}_{ij\mathbf{n}}) + \left(|\mathbf{x}_{ij\mathbf{n}}|_\bullet^{-1} - |\mathbf{x}_{ij\mathbf{n}}|^{-1}\right) + 4\pi L_{\rm box}^{-3}\sum_{\mathbf{h}\in\mathbb{Z}^3\setminus\{0\}}\frac{\exp(-x_{\rm s}^2k_{\mathbf{h}}^2)}{k_{\mathbf{h}}^2}\cos(k_{\mathbf{h}}[\mathbf{x}_i-\mathbf{x}_j])\right)\\
&= -Gm^2\sum_{j=1}^{N}\left[\sum_{\mathbf{n}\in\mathbb{Z}^3}-\nabla\mathcal{G}_{\rm sr}(\mathbf{x}_{ij\mathbf{n}}) - \nabla\left(|\mathbf{x}_{ij\mathbf{n}}|_\bullet^{-1} - |\mathbf{x}_{ij\mathbf{n}}|^{-1}\right) - 4\pi L_{\rm box}^{-3}\sum_{\mathbf{h}\in\mathbb{Z}^3\setminus\{0\}}\mathcal{G}_{\rm lr}(k_{\mathbf{h}})\nabla\left\{\cos(k_{\mathbf{h}}[\mathbf{x}_i-\mathbf{x}_j])\right\}\right],\end{aligned}$$

Based on Dakin, Hannestad & Tram 2022, 2112.01508.

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The PM method: analytical expression.

$$\mathbf{f}_i = \frac{4\pi G m^2}{L_\phi^4} \sum_{\substack{\mathbf{m} \\ \text{such that} \\ |\mathbf{x}_{i\mathbf{m}}|_\infty < \frac{p_i L_\phi}{2}}} W_{p_\mathrm{i}}\left(\frac{\mathbf{x}_i - \mathbf{x}_\mathbf{m}}{L_\phi}\right) \mathbf{D}_{p_\mathrm{d}} \mathcal{F}_\varnothing^{-1}\left[\left(\frac{W_{p_\mathrm{i}}(L_\phi \mathbf{k}_\mathbf{h})}{L_\phi^3}\right)^{-2} \frac{1}{k_\mathbf{h}^2} \mathcal{F}\left[\underbrace{\sum_{j=1}^{N} W_{p_\mathrm{i}}\left(\frac{\mathbf{x}_\mathbf{m} - \mathbf{x}_\mathbf{n}}{L_\phi}\right)}_{\substack{\text{the sum over } \mathbb{Z}^3 \text{ is automatically} \\ \text{accounted for by the} \\ \text{periodicity of the FFT}}}\right](\cdot)\right](\mathbf{m})$$

Based on Dakin, Hannestad & Tram 2022, 2112.01508.

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The P3M method: summarised analytical expression.

$$\mathbf{f}_i = \frac{4\pi G m^2}{L_\phi^4} \sum_{\substack{\mathbf{m}\in\mathbb{Z}^3 \\ |\mathbf{x}_{i\mathbf{m}}|_\infty < \frac{p_\mathrm{i} L_\phi}{2}}} \overbrace{W_{p_\mathrm{i}}\left(\frac{\mathbf{x}_i - \mathbf{x}_\mathbf{m}}{L_\phi}\right) \underbrace{\mathbf{D}_{p_\mathrm{d}}}_{\substack{\text{finite} \\ \text{difference}}} \underbrace{\mathcal{F}_\varnothing^{-1}}_{\text{iFFT}}}^{\text{operations in real space}} \left[\overbrace{\underbrace{\left(\frac{W_{p_\mathrm{i}}(L_\phi \mathbf{k}_{\mathbf{h}'})}{L_\phi^3}\right)^{-2}}_{\text{deconvolve twice}} \overbrace{\frac{\exp\left(-x_s k_{\mathbf{h}'}^2\right)}{k_{\mathbf{h}'}^2}}^{\substack{\text{non-Newtonian} \\ \text{long-range kernel}}}}^{\text{operations in Fourier space}} \underbrace{\mathcal{F}}_{\text{FFT}} \overbrace{\left(\underbrace{\sum_{j=1}^{N} W_{p_\mathrm{i}}\left(\frac{\mathbf{x}_{\mathbf{m}'} - \mathbf{x}_j}{L_\phi}\right)}_{\substack{\text{particles } x_j \text{ with shape } W_{p_\mathrm{i}-1} \\ \text{deposit mass on the real grid} \\ \text{at position } x_{\mathbf{m}'} \text{ through top-hat}}} \right)}^{\text{operations in real space}} (k_{\mathbf{h}'}) \right] (\mathbf{x}_\mathbf{m}) \quad \text{long-range}$$

$$- G m^2 \sum_{\substack{\mathbf{n}\in\mathbb{Z}^3 \\ j\in[\![1,N]\!] \\ j\neq i \\ |\mathbf{x}_{ij\mathbf{n}}|<x_r}} \left[|\mathbf{x}_{ij\mathbf{n}}|^{-3} \operatorname{erfc}\left(\frac{|\mathbf{x}_{ij\mathbf{n}}|}{2x_\mathrm{s}}\right) + \frac{|\mathbf{x}_{ij\mathbf{n}}|^{-2}}{\sqrt{\pi} x_s} \exp\left(-\frac{|\mathbf{x}_{ij\mathbf{n}}|^2}{4x_\mathrm{s}^2}\right) + \overbrace{\underbrace{|\mathbf{x}_{ij\mathbf{n}}|_\bullet^{-3} - |\mathbf{x}_{ij\mathbf{n}}|^{-3}}_{\substack{|\mathbf{x}|_\bullet^{-3} \text{ is just a notation and} \\ \text{differs from } \left(|\mathbf{x}|_\bullet^{-1}\right)^3 \text{ in general}}}}^{\text{softening}} \right] \mathbf{x}_{ij\mathbf{n}} \quad \text{short-range summation.}$$

In the above formula, the primes in the primed variables (within the Fourier transforms) indicate that they are defined all over the grid—they appear in the expression solely to indicate the type of the argument of the corresponding function.

Based on Dakin, Hannestad & Tram 2022, 2112.01508.