COmoving Computer Acceleration: N-body simulations in an emulated frame of reference

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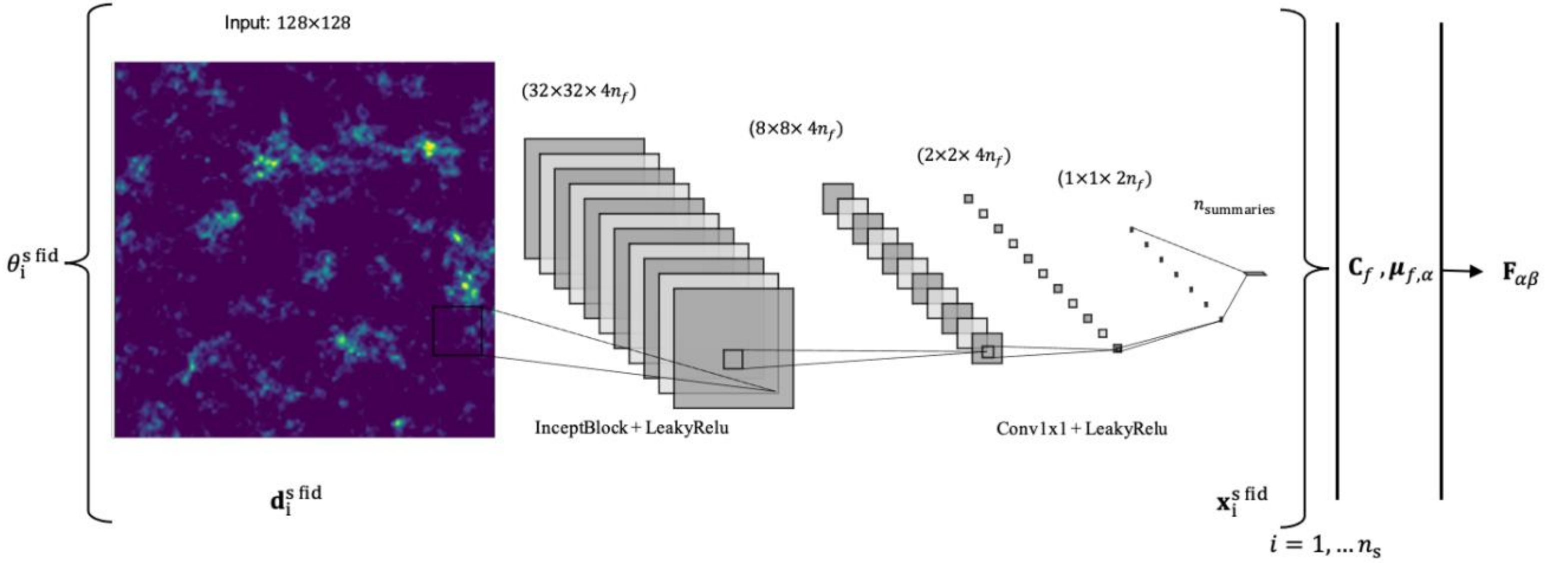
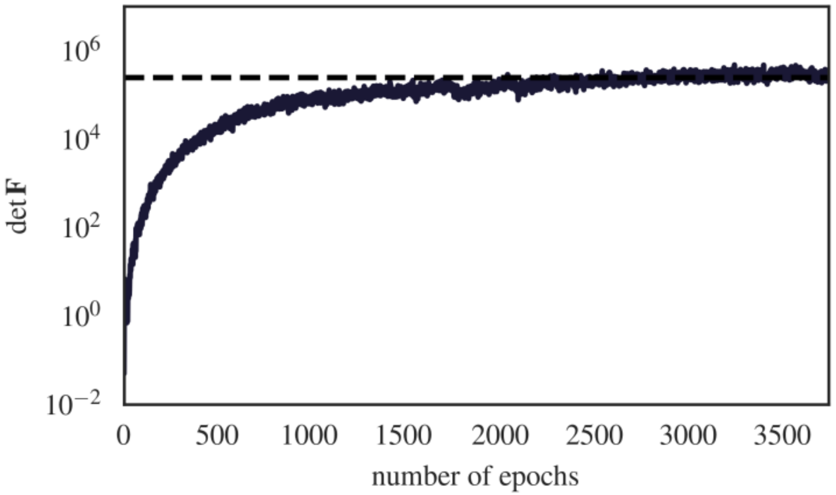
Safe uses of machine learning

- Safe use: applying machine learning (ML) — in particular neural networks (NNs) — in a way that ensures the results are either correct by construction or, at worst, suboptimal.
- Safe uses of ML include:
  - Ensuring certifiability of the model used for parameter inference and model comparison.
  - Eliminating the requirement for explainability.
- Examples: denoising autoencoders (DAE) to build summaries, information-maximising neural networks (IMNN) for simulation-based inference (SBI).

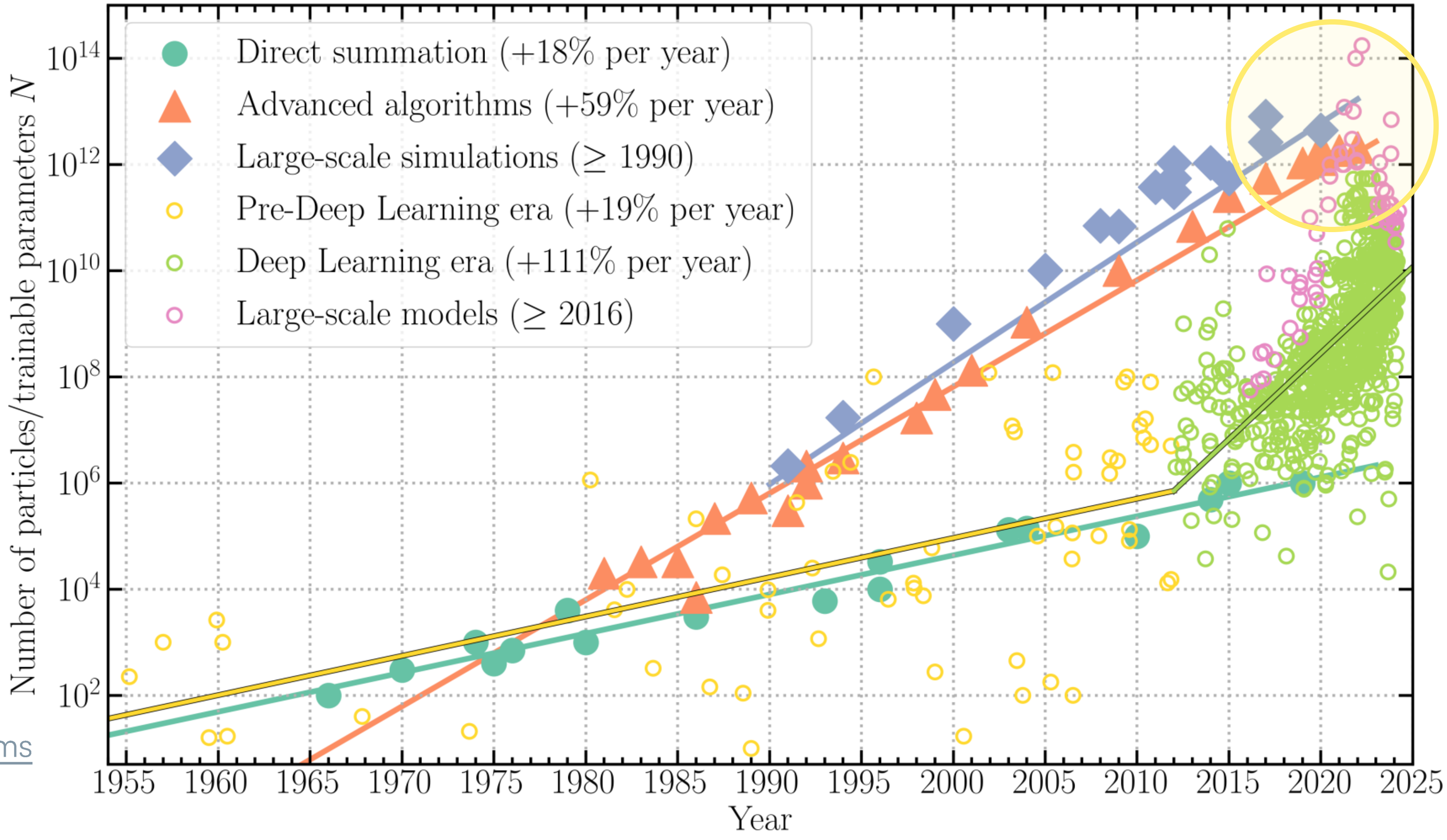




Charnock *et al.*, 1802.03537, Makinen *et al.*, 2107.07405, Makinen *et al.*, 2410.07548

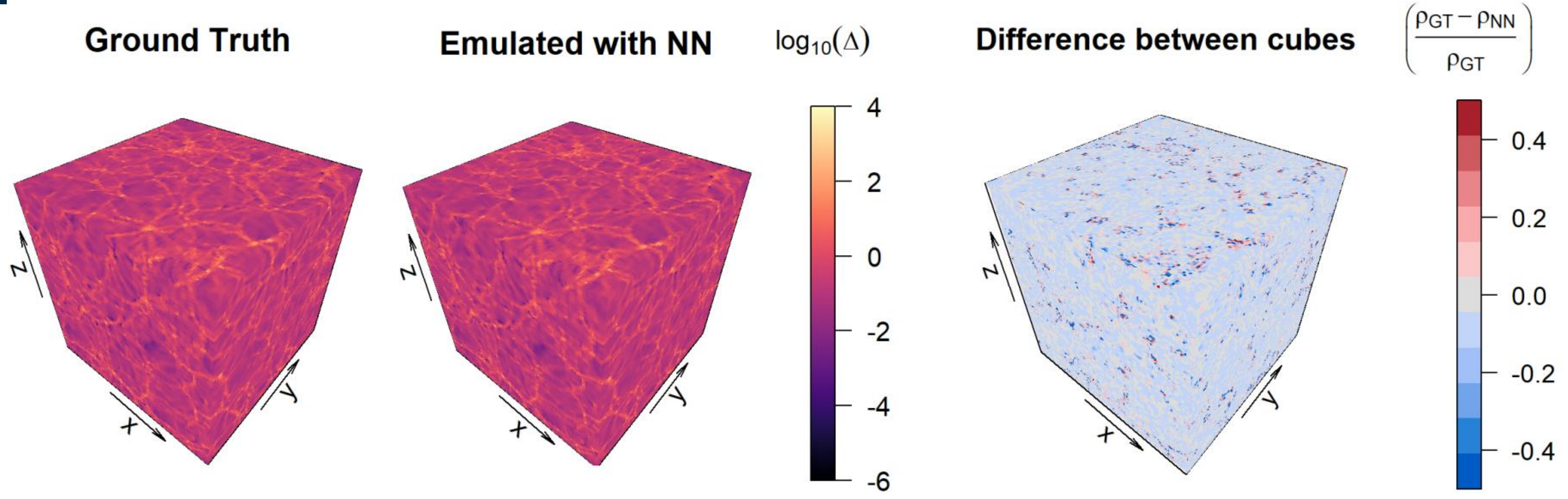
Comparative growth of models and methods

- Amdahl's law: latency kills the gains of parallelisation. Amdahl 1967, doi:10.1145/1465482.1465560
- Machine learning (ML) has caught up with the largest cosmological simulations!



Cosmological simulations: Github:florent-leclercq/Moore_law_cosmosims
IA models: data from epochai.org

Emulation of N-body simulations

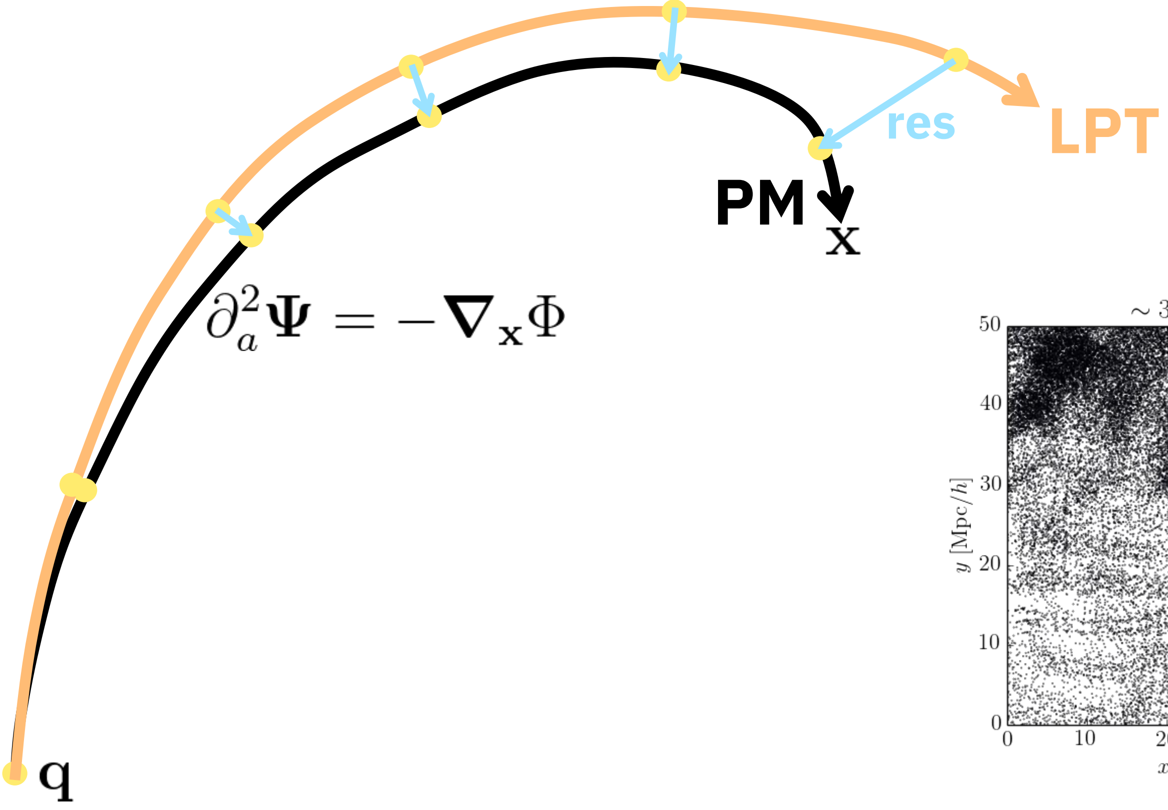


- Pleasantly fast, but what about the accuracy?
- There remains an emulation error [up to $\mathcal{O}(10\%)$] that we cannot ever correct for.
- Using these emulators as forward models does not qualify as a safe use of NNs.

He *et al.*, 1811.06533, Lucie-Smith *et al.*, 1802.04271, Jamieson *et al.*, 2206.04594, Conceição *et al.*, 2304.06099, Doeser *et al.*, 2312.09271, Jamieson *et al.*, 2408.07699

The tCOLA framework: (temporal) COmoving Lagrangian Acceleration

- Idea behind tCOLA: we can make use of the analytical solution at large scales and early times: Lagrangian perturbation theory (LPT).



- Write the displacement vector as:

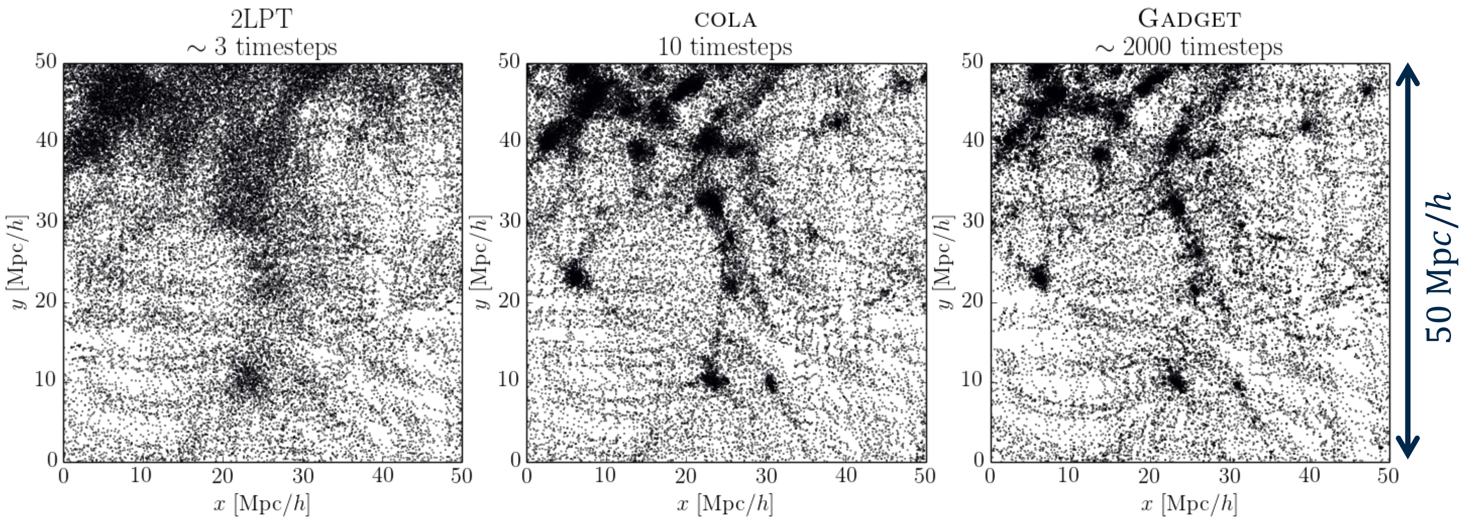
$$\boldsymbol{\Psi} = \boldsymbol{\Psi}_\mathrm{LPT} + \boldsymbol{\Psi}^\mathrm{COLA}_\mathrm{res} \qquad (\mathbf{x} = \mathbf{q} + \boldsymbol{\Psi})$$

Tassev & Zaldarriaga, 1203.5785

- Equation of motion (omitted constants and Hubble expansion):

Analytical solutions!

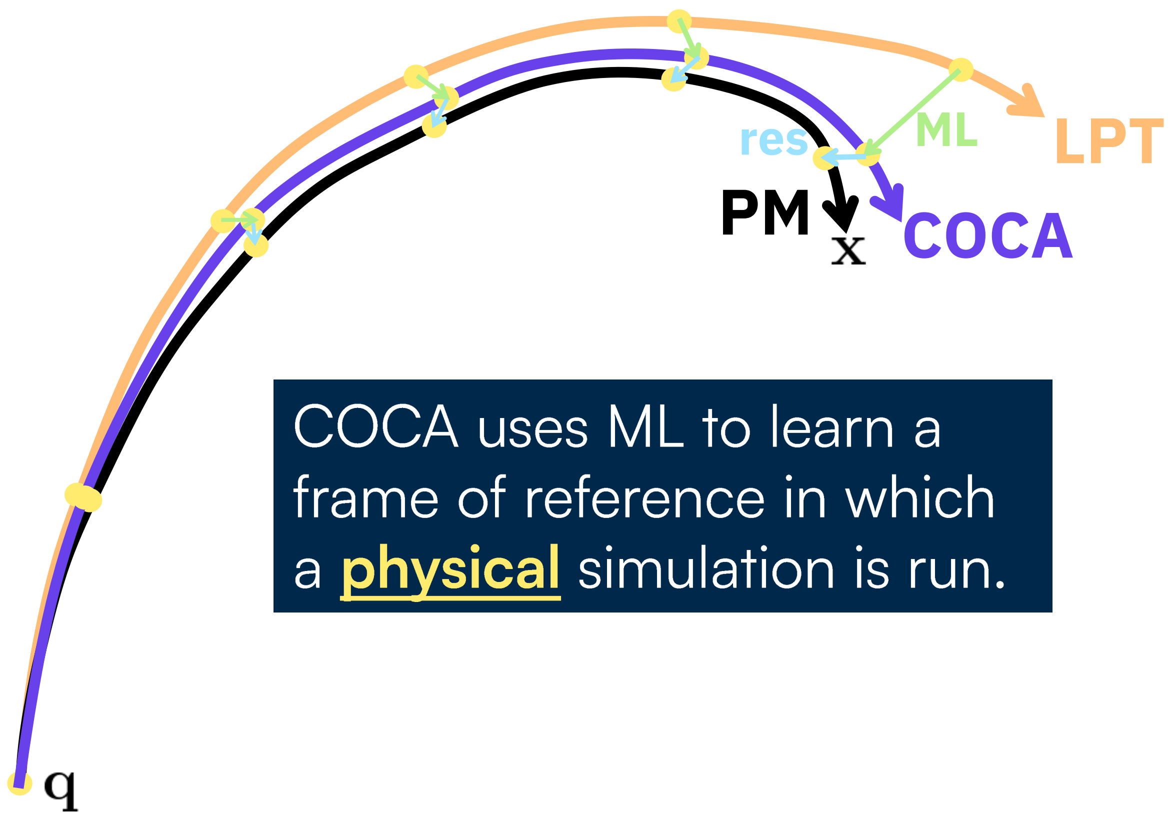
$$\partial_a^2 \boldsymbol{\Psi}^\mathrm{COLA}_\mathrm{res} = \partial_a^2 (\boldsymbol{\Psi} - \boldsymbol{\Psi}_\mathrm{LPT}) = -\boldsymbol{\nabla}_\mathbf{x}\Phi - \partial_a^2 \boldsymbol{\Psi}_\mathrm{LPT}$$



Tassev, Zaldarriaga & Einsenstein, 1301.0322

The tCOCA framework: (temporal) COmoving Computer Acceleration

- The idea behind tCOCA: the easiest simulation to run is the one where nothing moves!



COCA uses ML to learn a frame of reference in which a **physical** simulation is run.

- Write the displacement vector as:

$$\boldsymbol{\Psi} = \boldsymbol{\Psi}_{\mathrm{LPT}} + \boldsymbol{\Psi}_{\mathrm{ML}} + \boldsymbol{\Psi}_{\mathrm{res}}^{\mathrm{COCA}} \qquad (\mathbf{x} = \mathbf{q} + \boldsymbol{\Psi})$$

- Equation of motion (omitted constants and Hubble expansion):

$$\partial_a^2 \boldsymbol{\Psi}_{\mathrm{res}}^{\mathrm{COCA}} = -\boldsymbol{\nabla}_{\mathbf{x}}\Phi - \partial_a^2 \boldsymbol{\Psi}_{\mathrm{LPT}} - \partial_a^2 \boldsymbol{\Psi}_{\mathrm{ML}}$$

$$\Leftrightarrow \partial_a^2 \boldsymbol{\Psi} = -\boldsymbol{\nabla}_{\mathbf{x}}\Phi$$

- With COCA:
  - Any emulation error will be corrected by solving the *correct* physical equation of motion.
  - Any ML algorithm can do the job!
  - Building a data model is a safe use of ML.

Bartlett, Chiarenza, Doeser & FL, 2409.02154

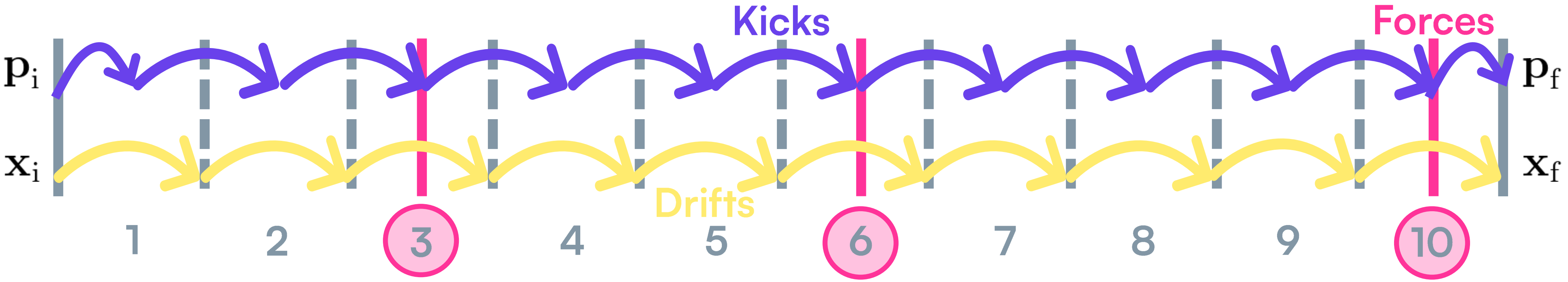
Time stepping and force calculations in COCA

- Our implementation of COCA in the Simbelmynë code uses the standard Kick-Drift-Kick (leapfrog) discretisation of the equation of motion.

  https://simbelmyne.florent-leclercq.eu — Bitbucket:florent-leclercq/simbelmyne

- Learning the new frame of reference means emulating the COLA residual momenta at every time step: $\mathbf{p}_{\mathrm{res}}^{\mathrm{COLA}} = \mathbf{p} - \mathbf{p}_{\mathrm{LPT}}$.

- When the emulation error is small $\left(\mathbf{p}_{\mathrm{ML}} \approx \mathbf{p}_{\mathrm{res}}^{\mathrm{COLA}}\right)$, particles are already at rest in the COCA frame of reference, so it is unnecessary to compute forces at every step.

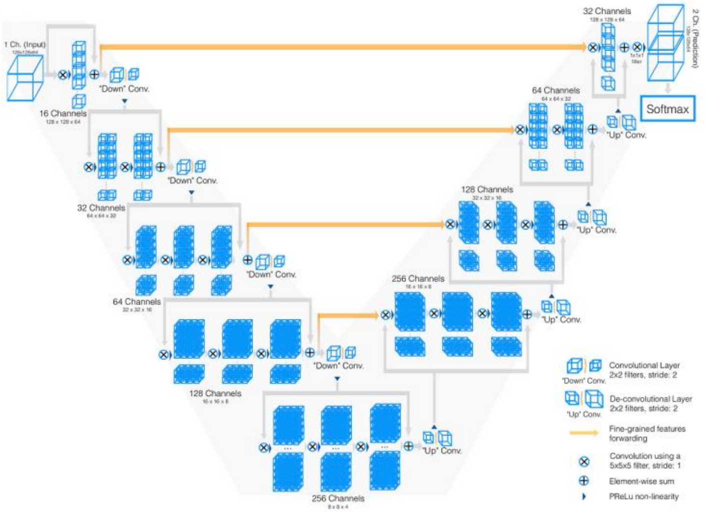


- A good frame-of-reference emulator therefore makes COCA cheaper than COLA.

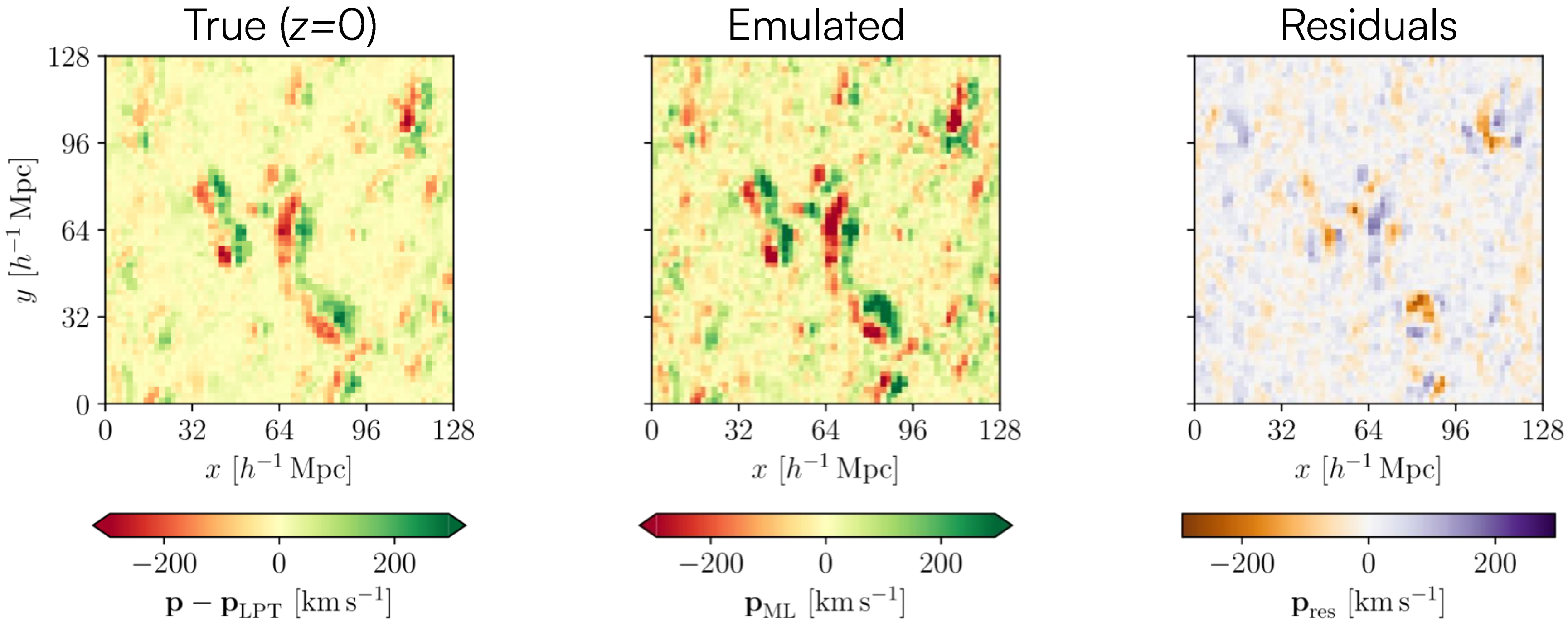
Bartlett, Chiarenza, Doeser & FL, 2409.02154

Training a frame-of-reference emulator for COCA

- We trained a styled V-net with initial density field and scale factor as inputs; frame of reference (particles' residual momenta) as output.
- We used 100 training COLA simulations with L=128 Mpc/h, N=64^3 particles, and 277 epochs.
- We can predict the frame of reference to run test COCA simulations:

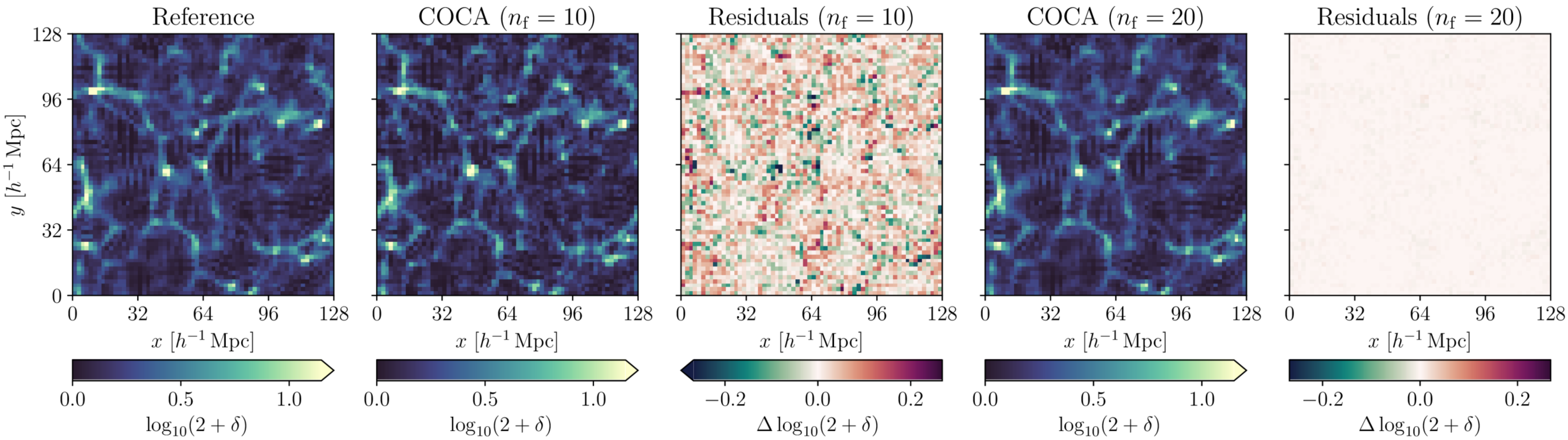


Milletari, Navab & Ahmadi, 1606.04797



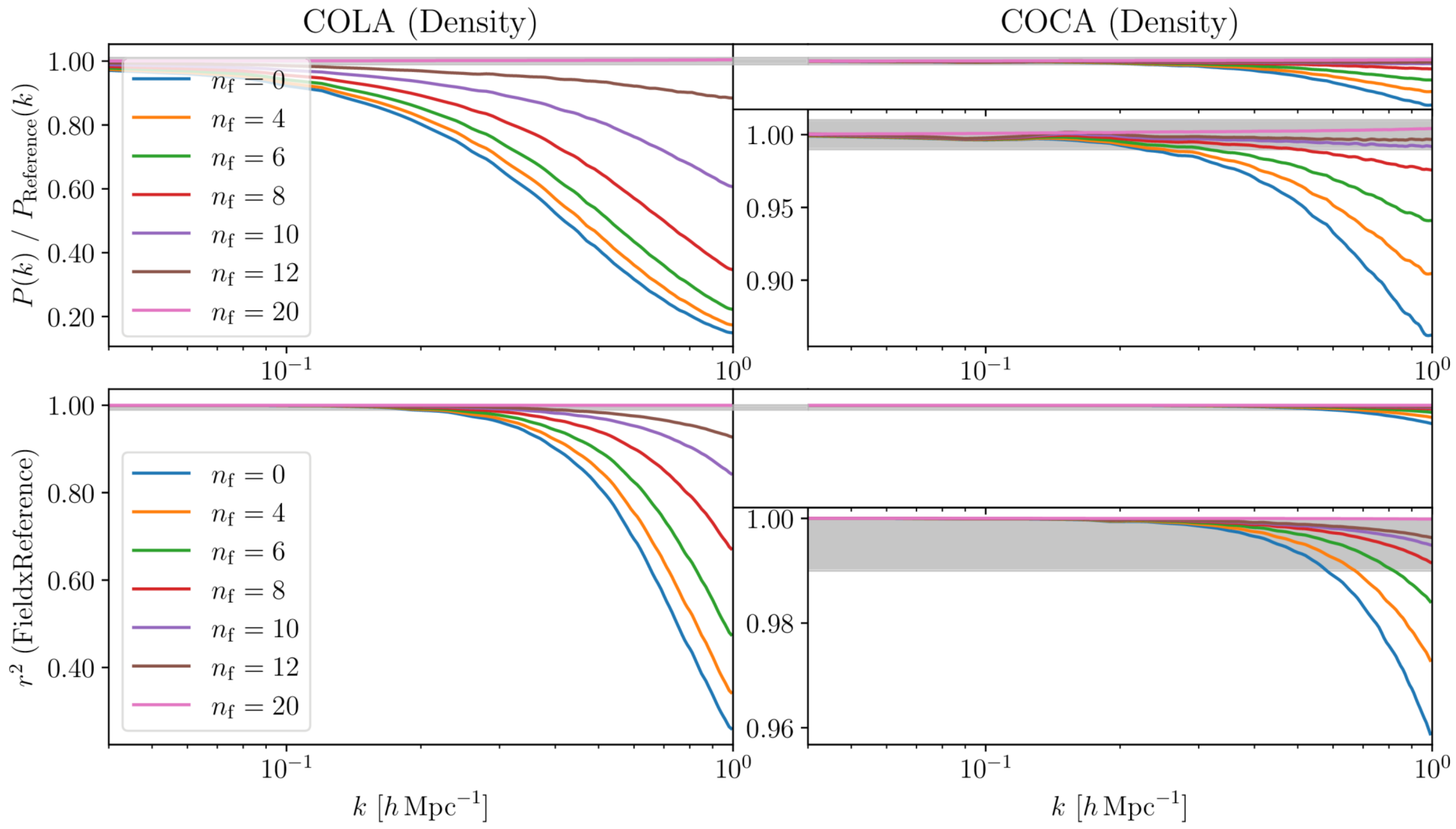
Bartlett, Chiarenza, Doeser & FL, 2409.02154

Results: COCA density field



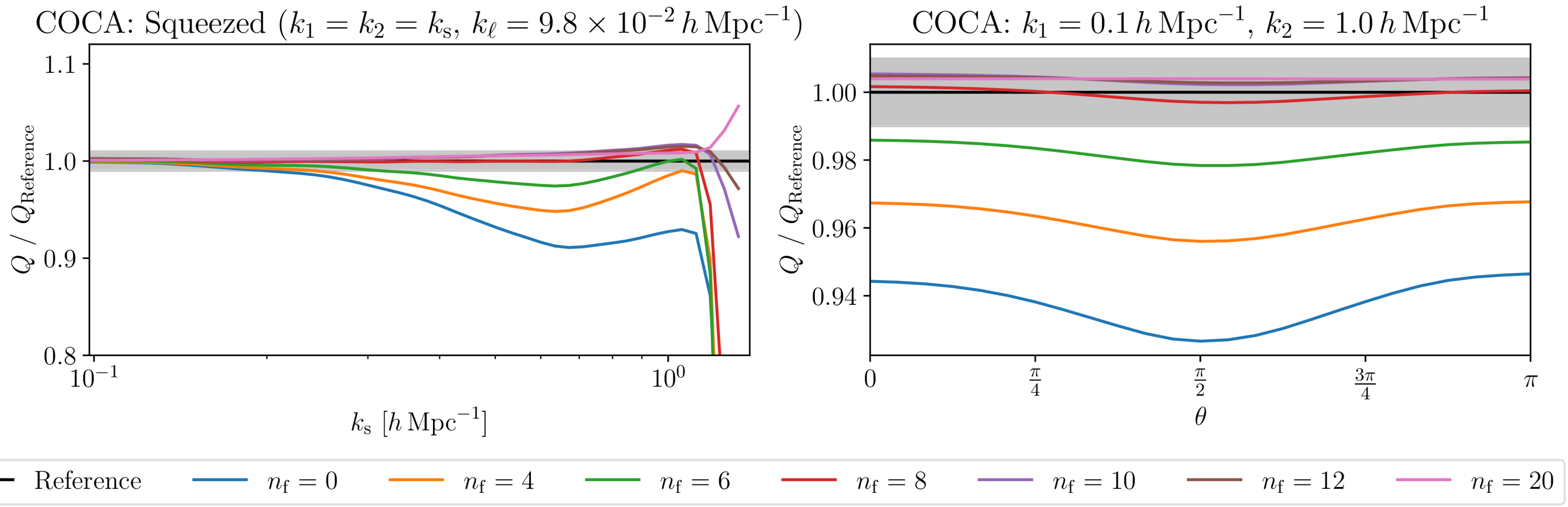
Bartlett, Chiarenza, Doeser & FL, 2409.02154

Results: COCA two-point statistics



Bartlett, Chiarenza, Doeser & FL, 2409.02154

Results: COCA three-point statistics



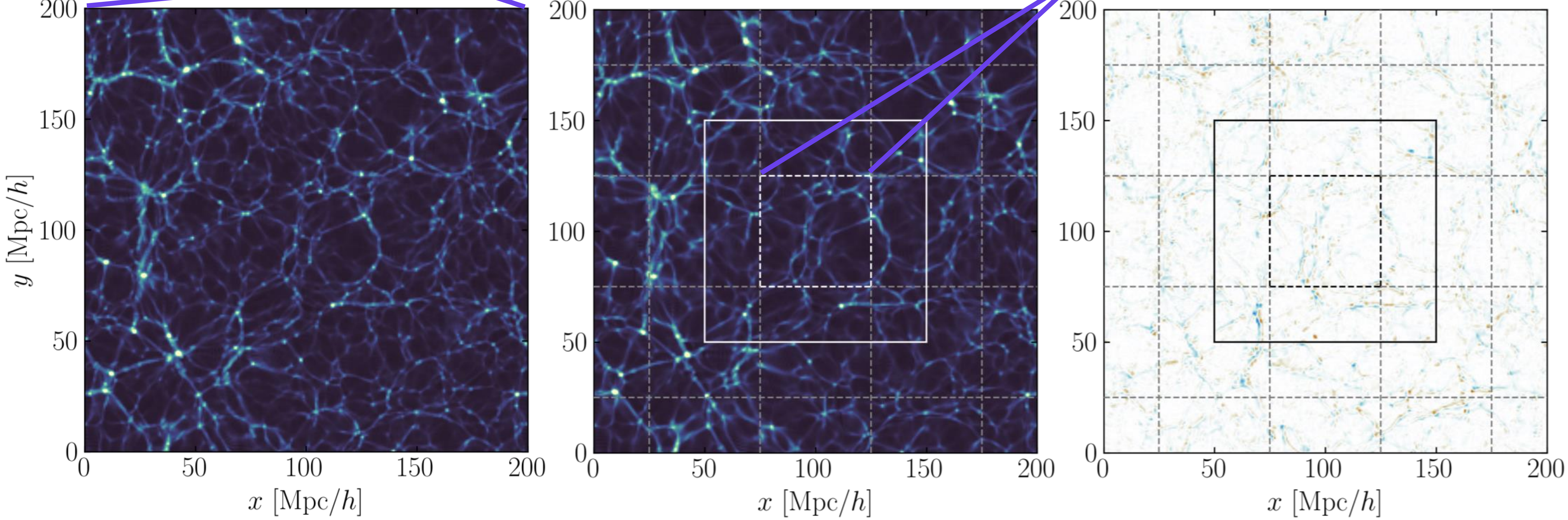
Bartlett, Chiarenza, Doeser & FL, 2409.02154

Perfectly parallel cosmological simulations using spatial comoving Lagrangian acceleration (sCOLA)

- Can we decouple sub-volumes by using the large-scale solution?

LPT so far (analytical solution) → sCOLA; soon ML solution → sCOCA

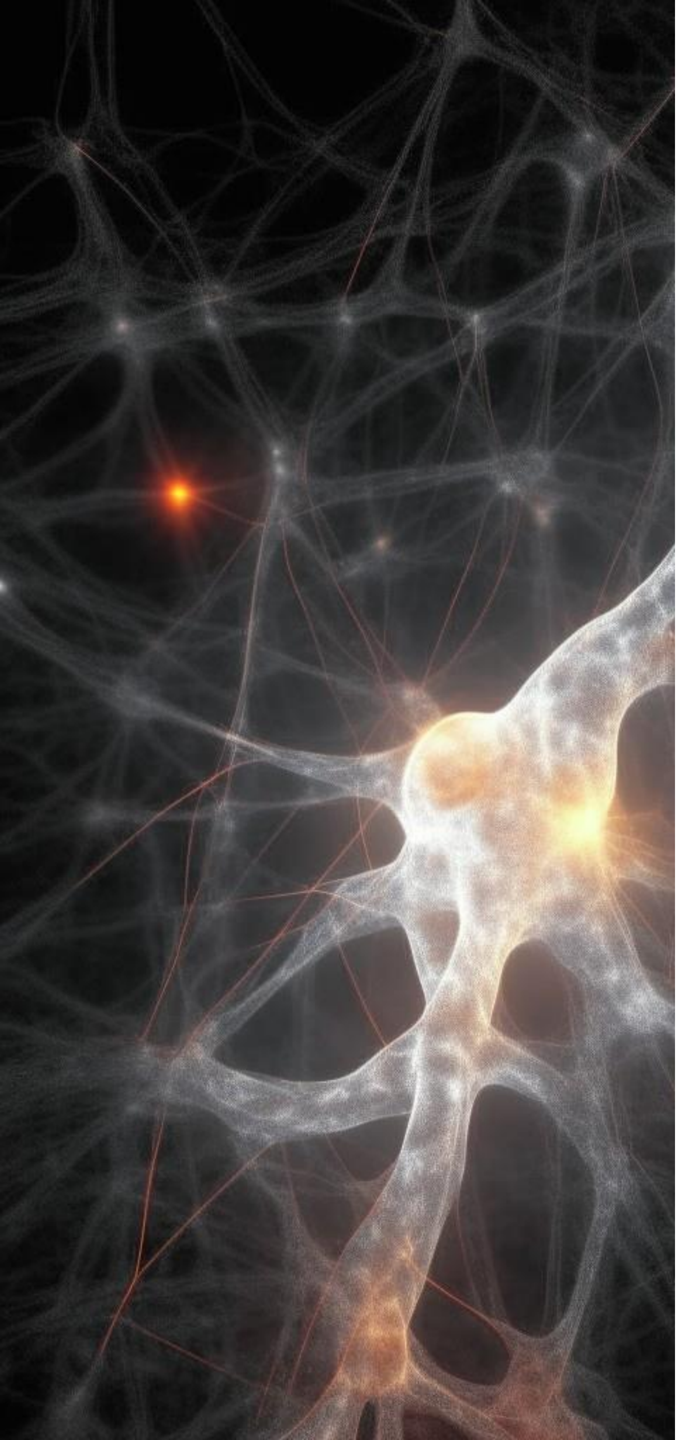
$$\partial_a^2 \boldsymbol{\Psi} = -\boldsymbol{\nabla}_{\mathbf{x}} \left[\underbrace{\Delta^{-1}\delta}_{\text{non-local}} \right] \Leftrightarrow \partial_a^2 (\boldsymbol{\Psi} - \boldsymbol{\Psi}_{\mathrm{l.s.}}) = -\boldsymbol{\nabla}_{\mathbf{x}} \left[\underbrace{\Delta^{-1}(\delta - \delta_{\mathrm{l.s.}})}_{\text{local}} \right]$$



tCOLA (reference) sCOLA Difference

FL, Faure, Lavaux, Wandelt, Jaffe, Heavens, Percival & Noûs, 2003.04925

Publicly available implementation: Bitbucket:florent-leclercq/simbelmyne/



Conclusions

- Safe uses of neural networks exist, where:
  - The answer is correct by construction or suboptimal,
  - Use for physics (parameter inference, model comparison) is certifiably robust,
  - Explainability is not needed.

- tCOCA reimagines the use of neural networks for emulating *N*-body simulations:
  - It generalises the idea of tCOLA: running simulations in a new frame of reference,
  - It solves the correct equations of motion, so it is a safe use of neural networks,
  - It makes simulations cheaper by skipping unnecessary force evaluations.

- The large-scale ML solution can also be used to decouple sub-volumes, in the same spirit as sCOLA: the sCOCA framework!

Acknowledgements, credits, contacts

References:
- **Simbelmynë**: Leclercq, Jasche & Wandelt 2014, 1403.1260, *Bayesian analysis of the dynamic cosmic web in the SDSS galaxy survey* — https://simbelmyne.florent-leclercq.eu
- **sCOLA**: Leclercq *et al.* 2020, 2003.04925, *Perfectly parallel cosmological simulations using spatial comoving Lagrangian acceleration*
- **COCA**: Bartlett, Chiarenza, Doeser & Leclercq 2024, 2409.02154, *COmoving Computer Acceleration (COCA): N-body simulations in an emulated frame of reference*

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