Accelerated forward modelling of dark matter dynamics: ML-safety and perfect parallelism

MIAPbP workshop “Big Data, Big Questions: The Future of Cosmological Surveys”

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and the Aquila Consortium

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Let's define some concepts

- Machine-Learning safety: 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 eliminates the requirement for explainability.
  - Example: data compression, e.g. denoising autoencoders (DAE) to build summaries, information-maximising neural networks (IMNN) for implicit likelihood inference.

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

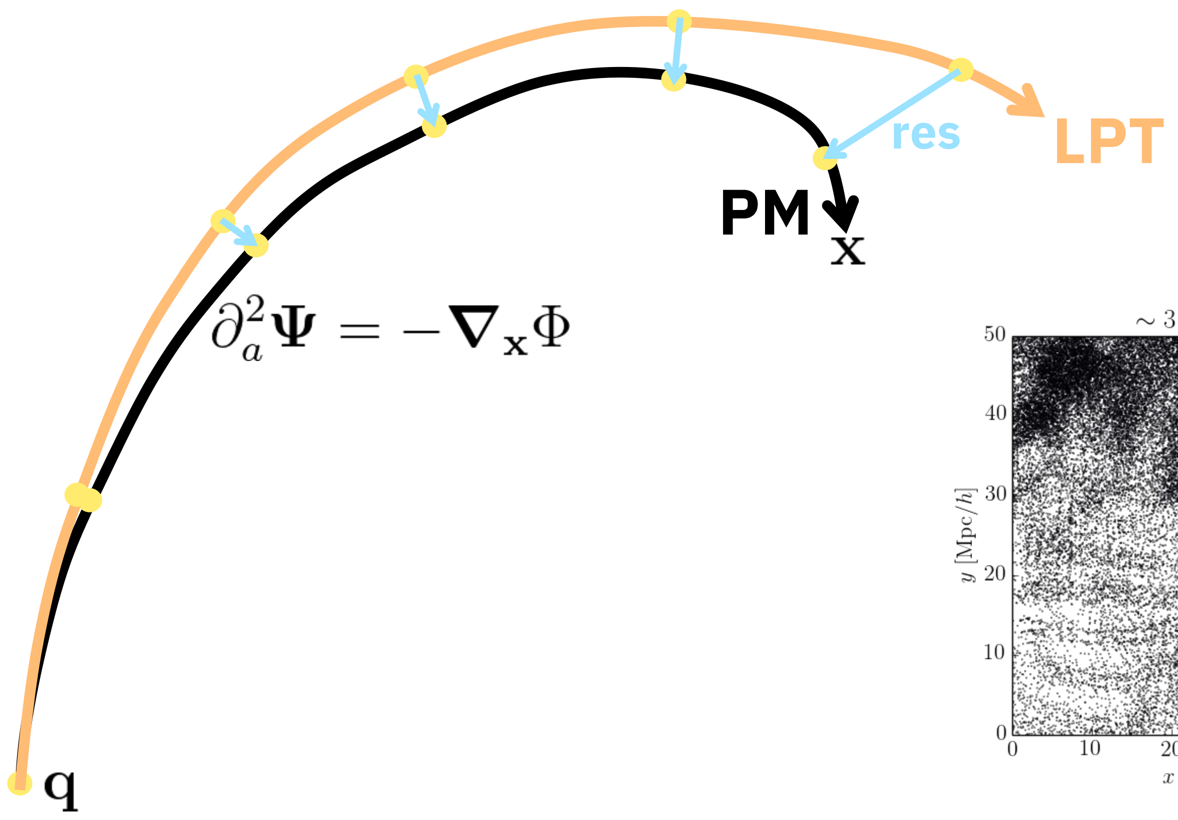
  - Counter-example: emulation of *N*-body simulations. There remains an emulation error [up to $\mathcal{O}(10\%)$] that we cannot ever correct for.

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

- Perfect parallelism: dividing a computational task into independent sub-tasks with no communication between them, allowing for highly efficient parallel processing.
  - It is a.k.a. an "embarrassingly parallel workload" — but there's nothing to be embarrassed about, really.
  - Examples: computer simulations comparing many independent scenarios, ensemble calculation of i.i.d. numerical model predictions (e.g. for covariance matrix estimation).
  - Counter-examples: usual *N*-body simulation codes, recursive algorithms, Markov Chain Monte Carlo.

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:

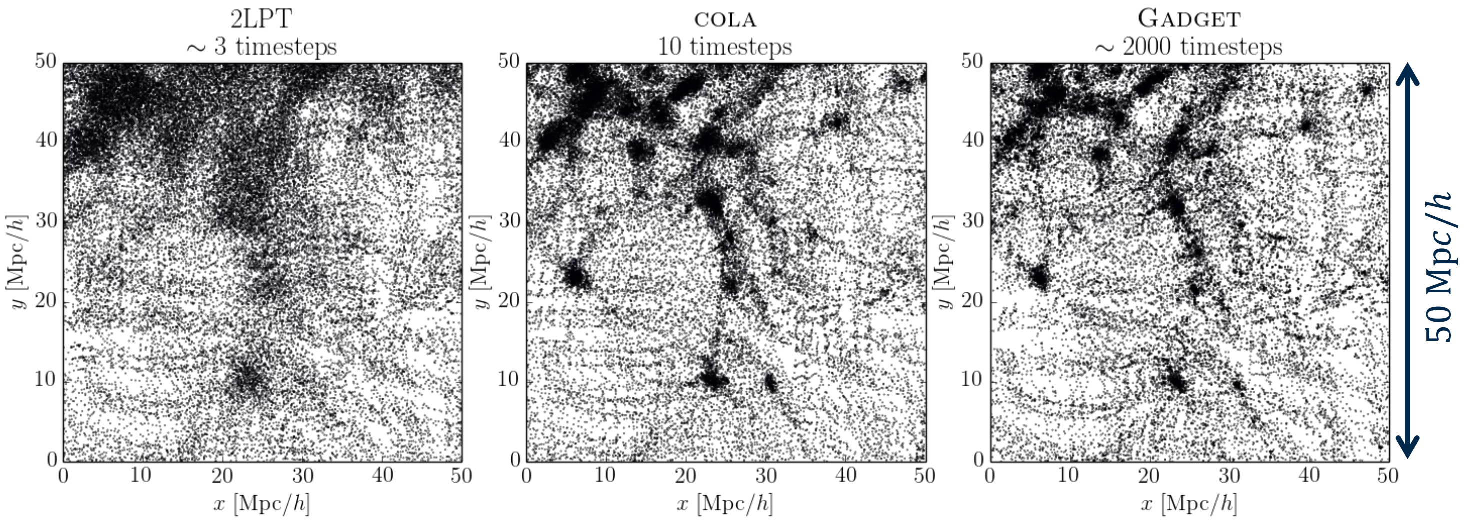
$$\boldsymbol{\Psi} = \boldsymbol{\Psi}_{\mathrm{LPT}} + \boldsymbol{\Psi}_{\mathrm{res}}^{\mathrm{COLA}} \qquad (\mathbf{x} = \mathbf{q} + \boldsymbol{\Psi})$$

Tassev & Zaldarriaga, 1203.5785

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

Analytical solutions!

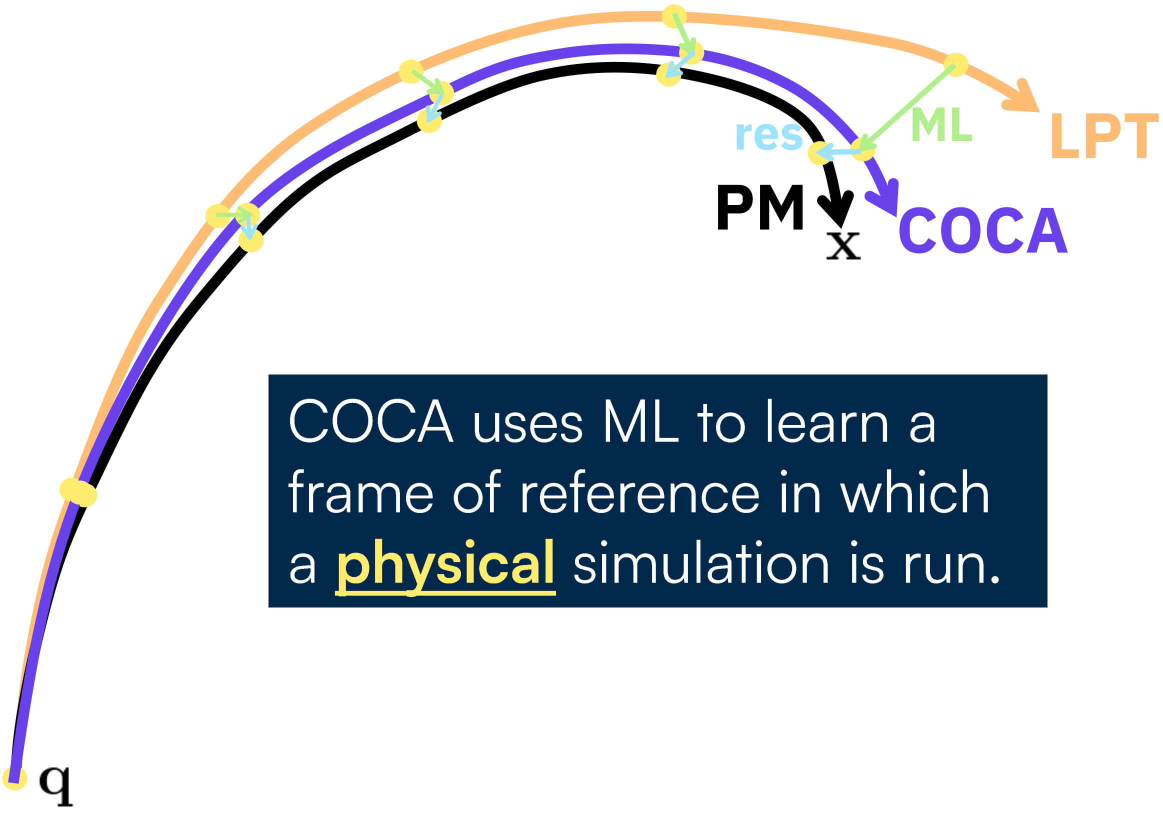
$$\partial_a^2 \boldsymbol{\Psi}_{\mathrm{res}}^{\mathrm{COLA}} = \partial_a^2 (\boldsymbol{\Psi} - \boldsymbol{\Psi}_{\mathrm{LPT}}) = -\boldsymbol{\nabla}_{\mathbf{x}} \Phi - \partial_a^2 \boldsymbol{\Psi}_{\mathrm{LPT}}$$



Tassev, Zaldarriaga & Einsenstein, 1301.0322

The tCOCA framework: (temporal) COmoving Computer Acceleration

- 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):

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

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

- 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

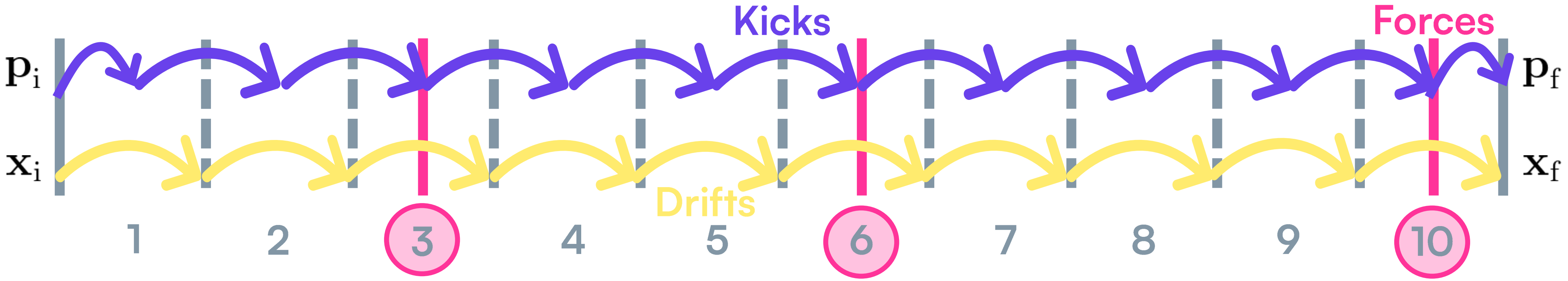
Time stepping and force calculations in COCA

- 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.

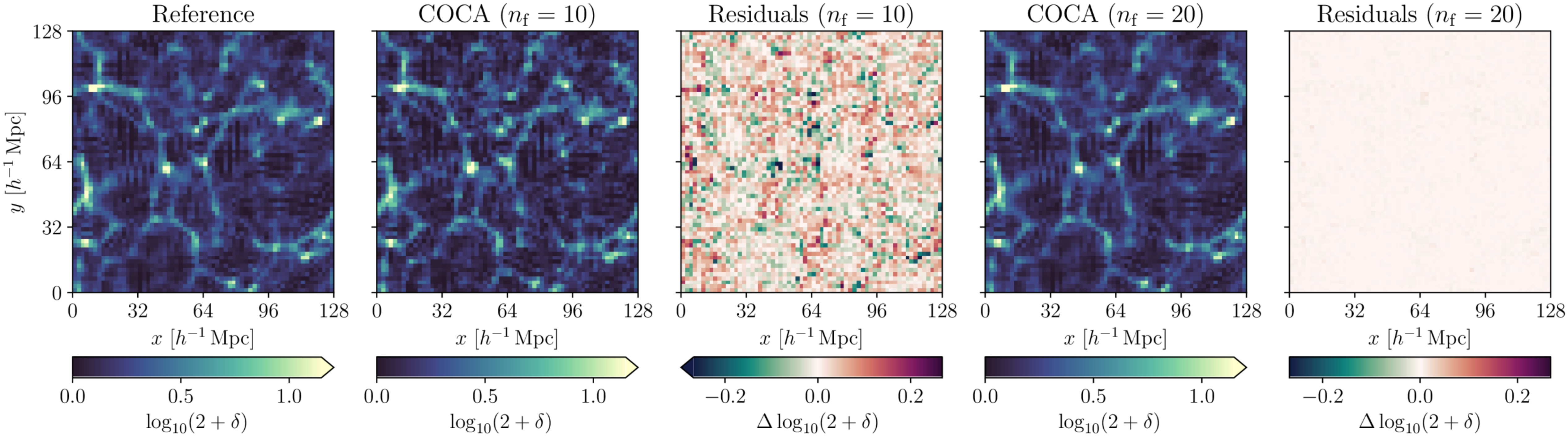


- A good frame-of-reference emulator therefore makes COCA cheaper than COLA.

Bartlett, Chiarenza, Doeser & FL, 2409.02154

Results: COCA density field

Deaglan Bartlett
(PDRA at IAP → Oxford)



We reach percent-level accuracy up to $k = 1\ h/\mathrm{Mpc}$ on standard correlations functions, using only 8 to 10 particle-mesh (PM) force evaluations (see the paper).

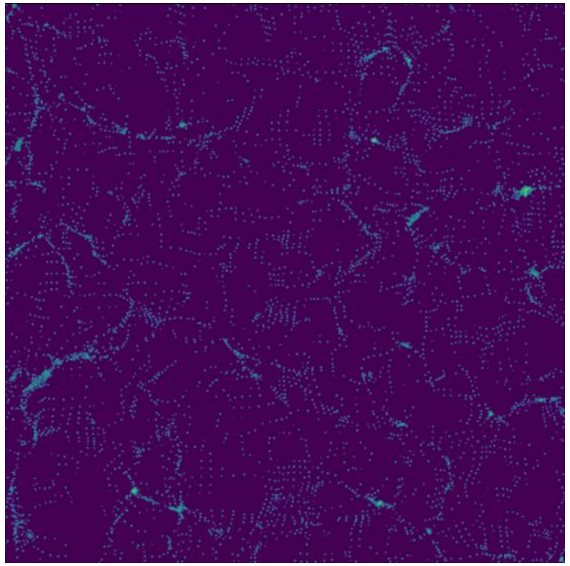
Bartlett, Chiarenza, Doeser & FL, 2409.02154

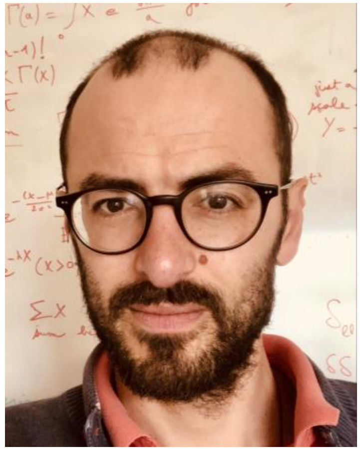
Force calculation and the small-scale accuracy of COLA/COCA

- A common misconception: COLA (or COCA) does not necessarily sacrifice small-scale accuracy for speed! (only implementations with PM forces usually do).
- Changing the frame of reference (to LPT or LPT+ML) can be done with *any* force calculation technique. Therefore, trajectories can be integrated to arbitrary accuracy.

Spectral sheet interpolation

(PRELIMINARY)





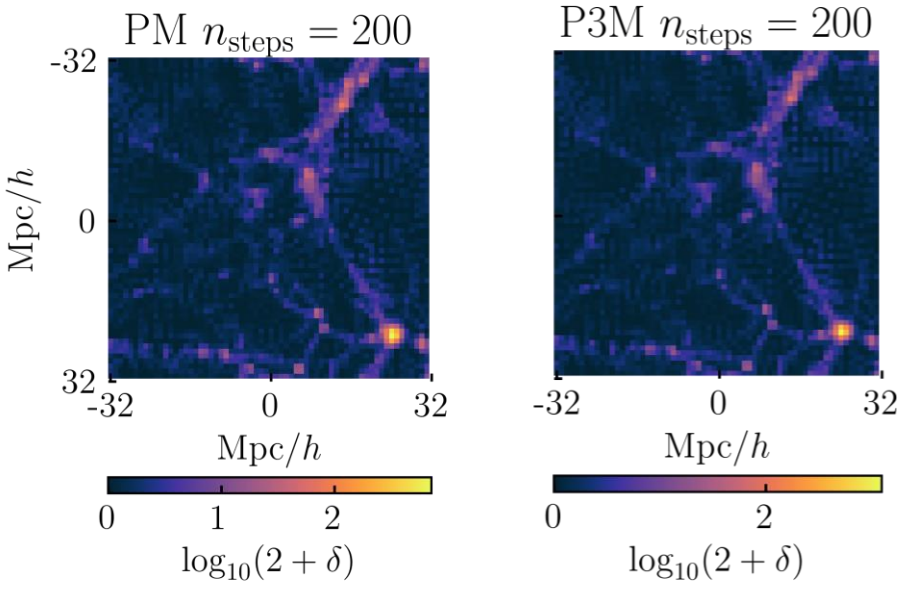
Rémi Fahed
(Research engineer at IAP)

Implemented as in List *et al.*, 2309.10865

Particle-particle particle-mesh (P3M) dynamics

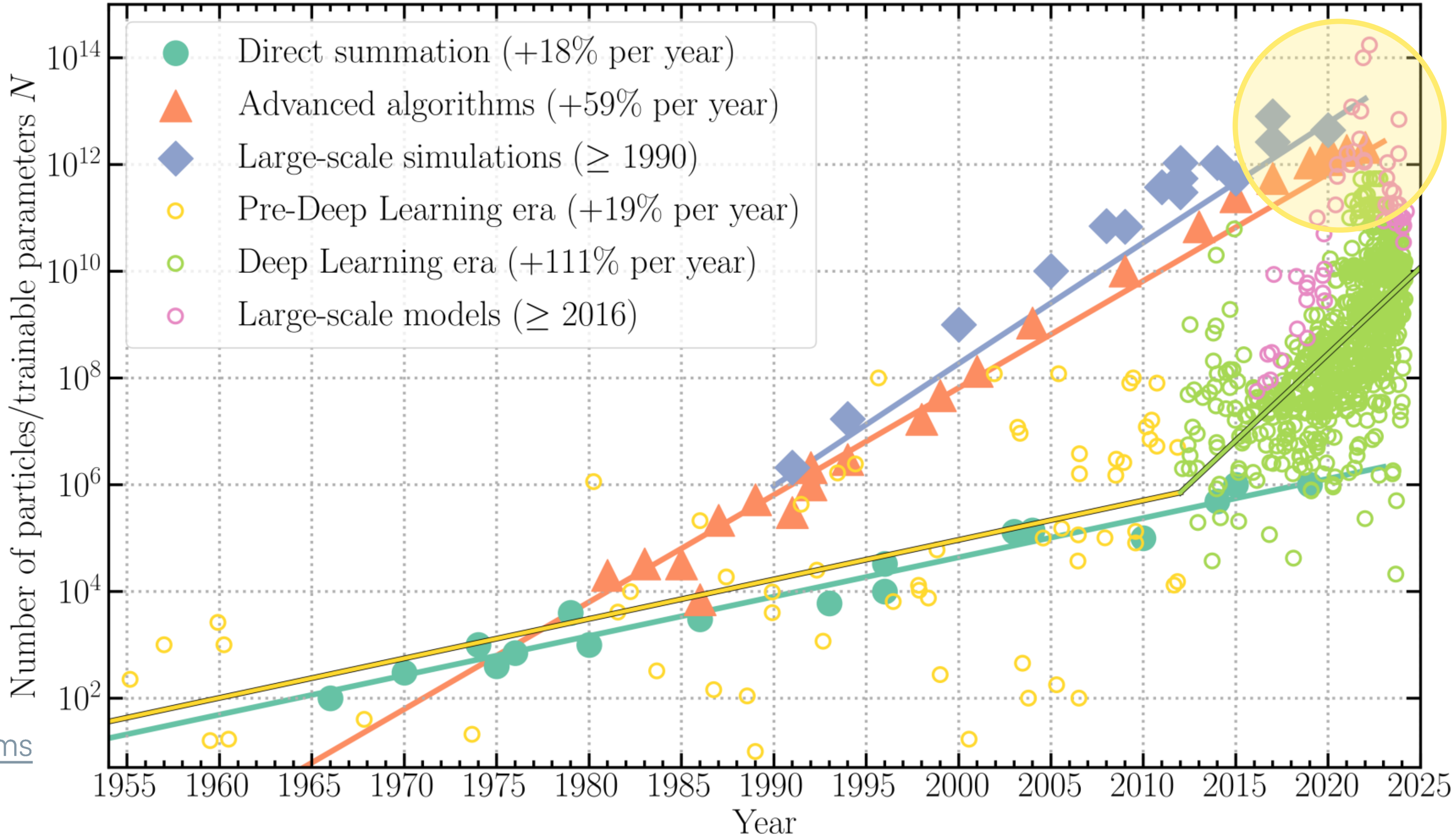
(PRELIMINARY)

Tristan Hoellinger
(doctoral researcher at IAP)



Implemented as in Dakin *et al.*, 2112.01508

Comparative growth of methods and models



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

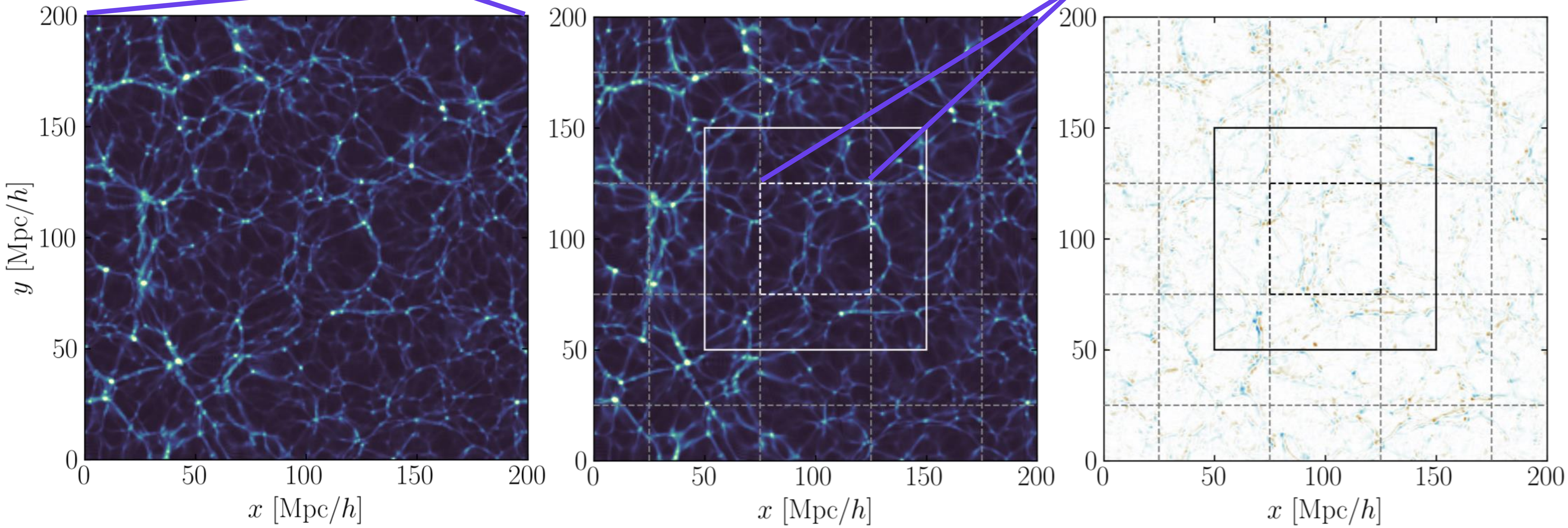
- Machine learning (ML) has caught up with the largest cosmological simulations!
- The real challenge for N-body simulations is Amdahl's law: latency kills the gains of parallelisation. Amdahl 1967, doi:10.1145/1465482.1465560

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

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

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

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



tCOLA (reference) sCOLA Difference

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

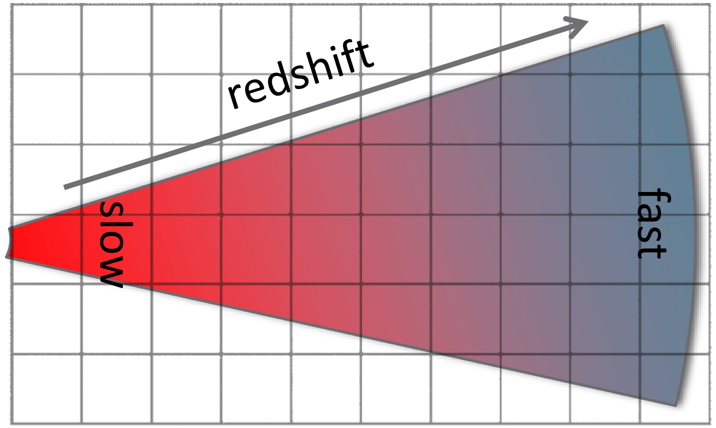
Publicly available implementation: Bitbucket:florent-leclercq/simbelmyne/

Lightcones and mock catalogues with sCOLA

- The workload in sCOLA is perfectly parallel, with a parallelisation potential factor:

$$p = s\left(\frac{L}{L_{\mathrm{sCOLA}}}\right)^3$$

hardware "boost" factor due to small memory requirements

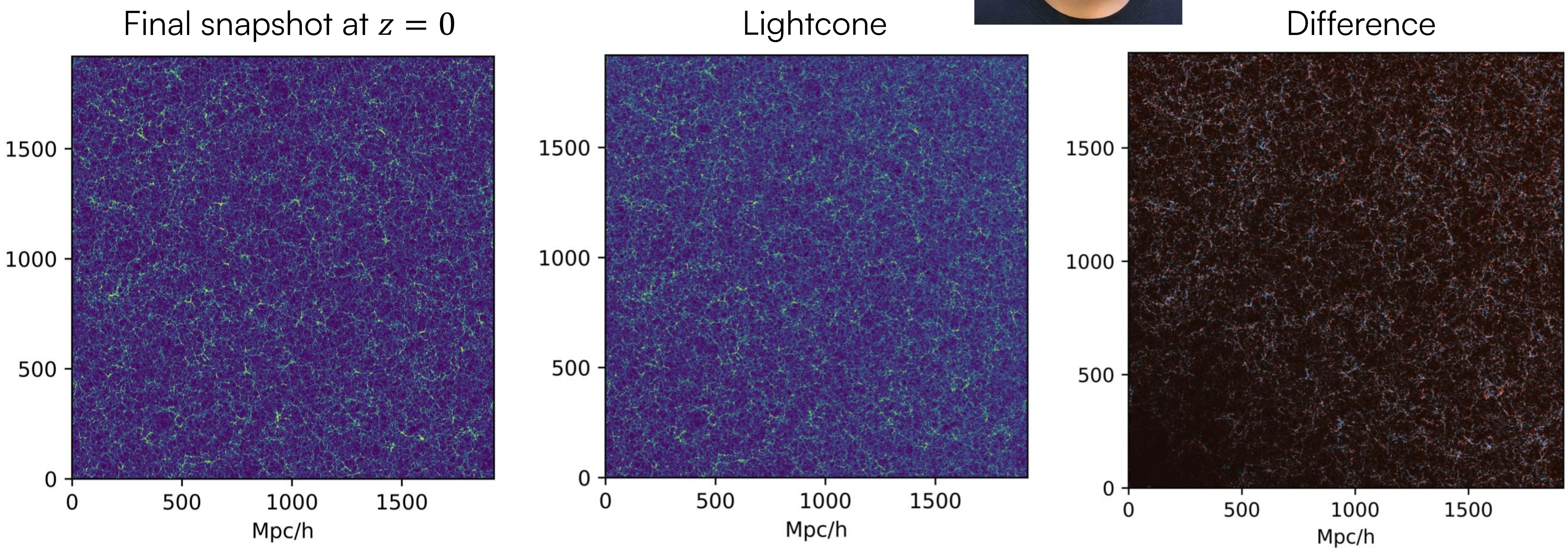


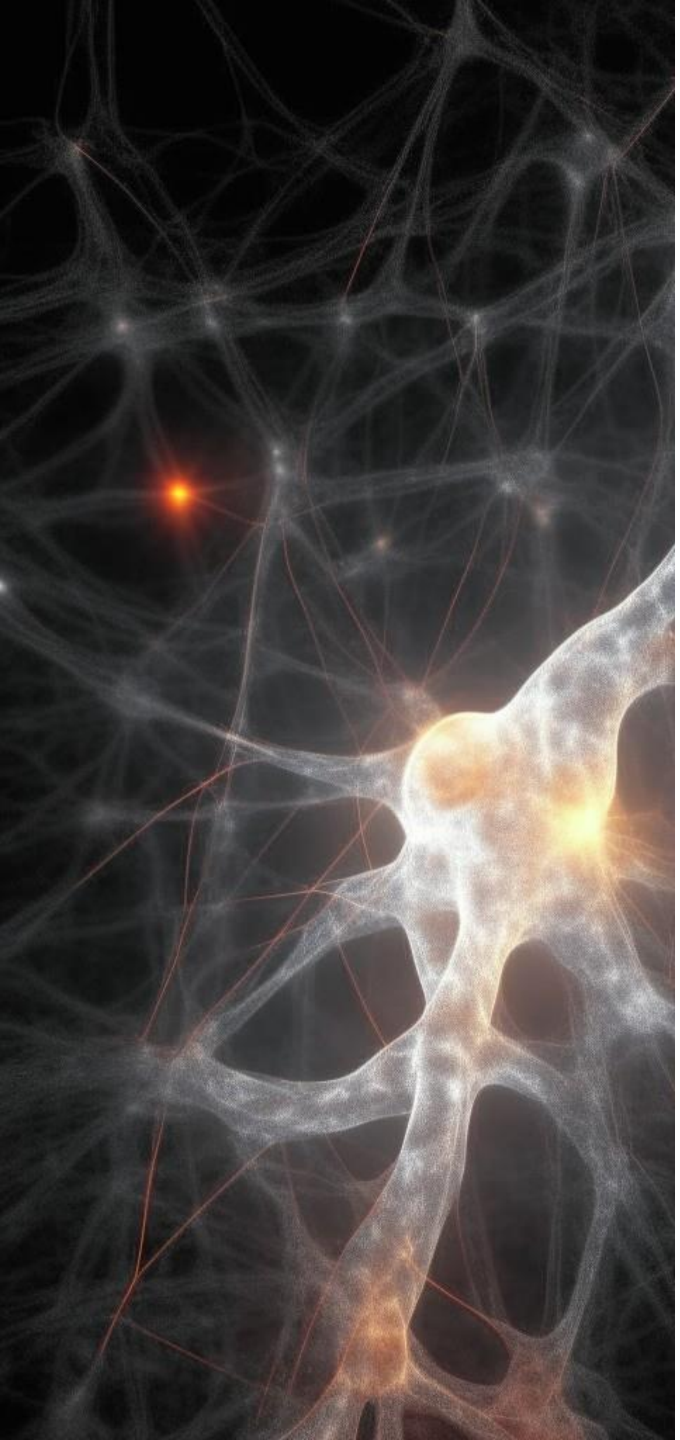
- Generation of lightcones and mock catalogues:
  - sCOLA boxes only need to run until they intersect the observer's past lightcone.
  - Most of the high-z volume will run faster than $z = 0$.
  - Many unobserved sCOLA boxes do not even have to run!
  - The wall-clock time limit is the time for running a single sCOLA box to $z = 0$ at the observer's position.

- Additional benefits:
  - Grid computing: the algorithm is suitable for inexpensive, strongly asynchronous networks
  - Robustness to node failure

One sCOLA lightcone simulation
(PRELIMINARY)

Mayeul Aubin
(doctoral researcher at IAP)





Conclusions – ML-safety and perfect parallelism

- 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. But it is not an emulator!
  - It solves the correct equations of motion, so it is a ML-safe use of neural networks. Explainability is not needed!
  - It makes simulations cheaper by skipping unnecessary force evaluations. But any force calculation technique (e.g. P3M) can be used.
- sCOLA uses the large-scale approximate solution to spatially split simulations in independent tiles:
  - It achieves perfect parallelism by fully removing the need for communications across the full computational volume.
  - It allows for fast lightcone and mock catalogue generation.
- Outlook: 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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