



Don't trust neural networks? Me neither, but here's how I use them anyway

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21 MAY 2024



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Neural networks and their reliability (or lack thereof)

- Large language models (and their limitations...)

ChatGPT 3.5

F Florent Leclercq
What is 1568 times 9762?

ChatGPT
1568 times 9762 equals 15,316,416.

F Florent Leclercq
Now what is the correct result?

ChatGPT
Apologies for the error. Let me recalculate that for you.

1568 times 9762 equals 15,322,016.

F Florent Leclercq
No, that's still wrong!

ChatGPT
My apologies for the mistake. Let me calculate it again.

1568 times 9762 equals 15,318,816.

ChatGPT 4

F Florent Leclercq
What is 1568 times 9762?

ChatGPT
The result of multiplying 1568 by 9762 is 15,306,816.

Analysis

```
python  Copy code
```

```
# Calculating the product of 1568 and 9762  
1568 * 9762
```

Result
15306816

1568 x 9762 =
15306816



Gentoo Linux tells AI-generated code contributions to fork off

Tue 16 Apr 2024 // 18:30 UTC

AI-generated and assisted code contributions are no longer allowed in the Gentoo Linux distribution.

AI hallucinates software packages and devs download them – even if potentially poisoned with malware

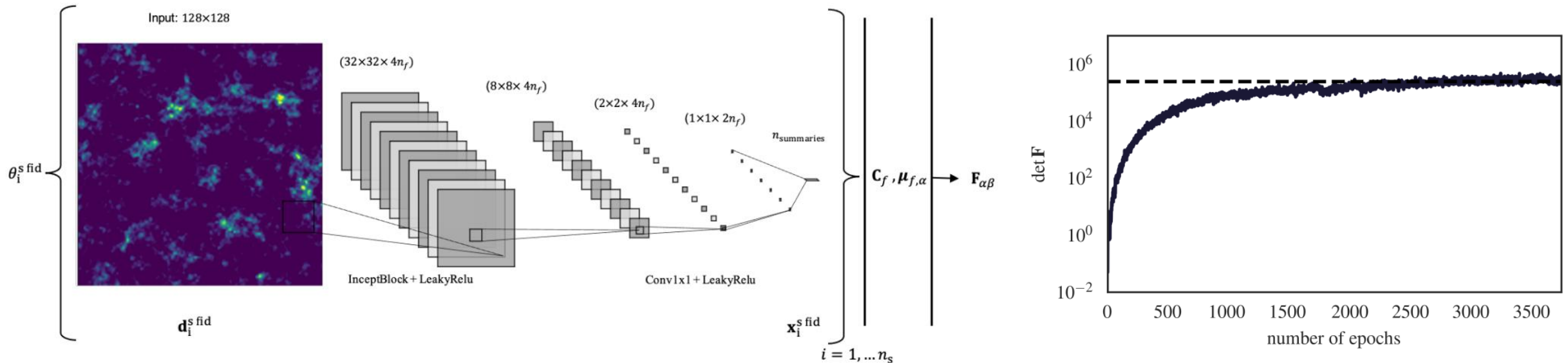
Simply look out for libraries imagined by ML and make them real, with actual malicious code. No wait, don't do that

Thu 28 Mar 2024 // 07:01 UTC



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

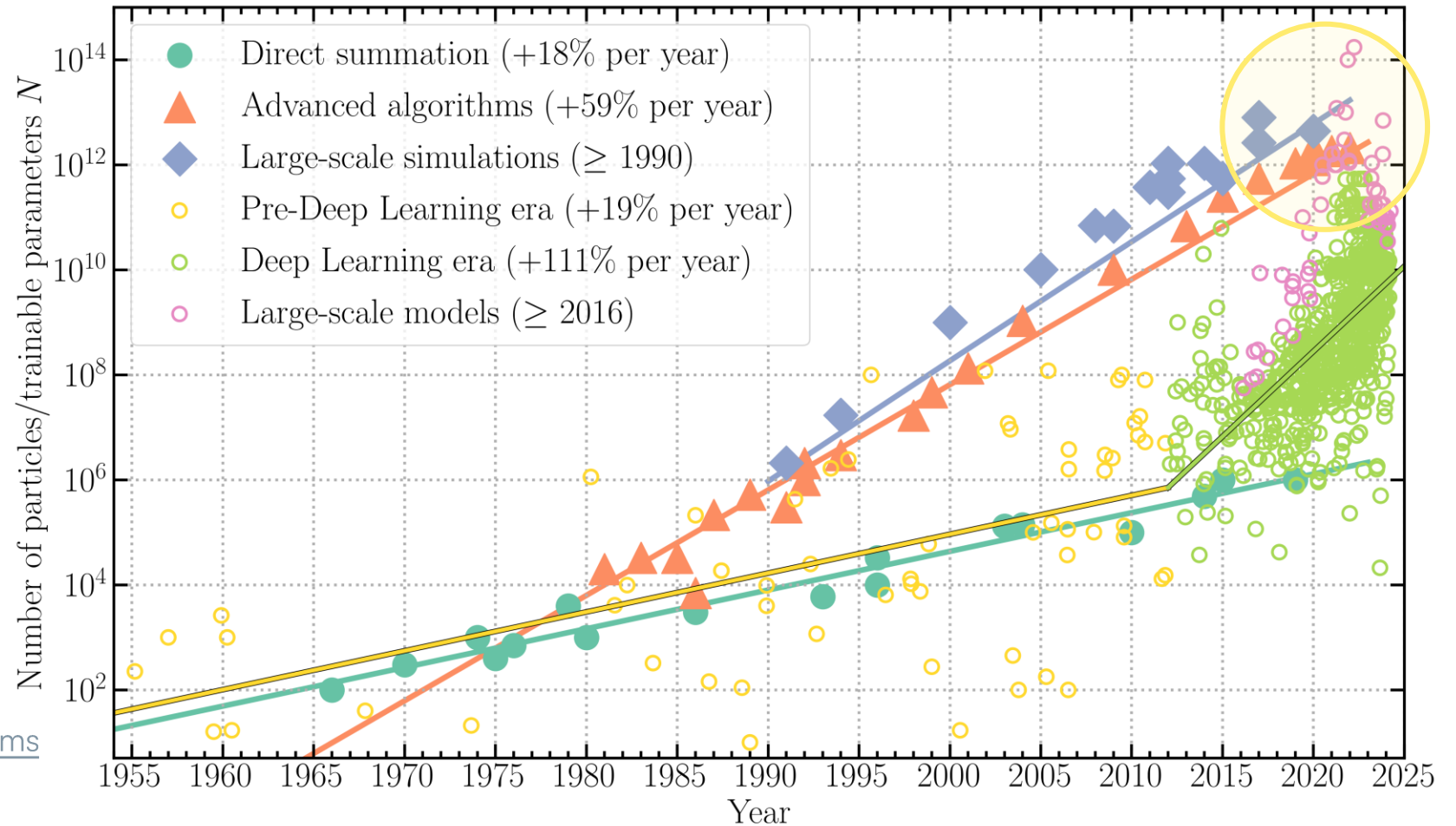


Comparative growth of models and methods

- Amdahl's law: latency kills the gains of parallelisation.

[Amdahl 1967, doi:10.1145/1465482.1465560](https://doi.org/10.1145/1465482.1465560)

- Machine learning (ML) has caught up with the largest cosmological simulations!



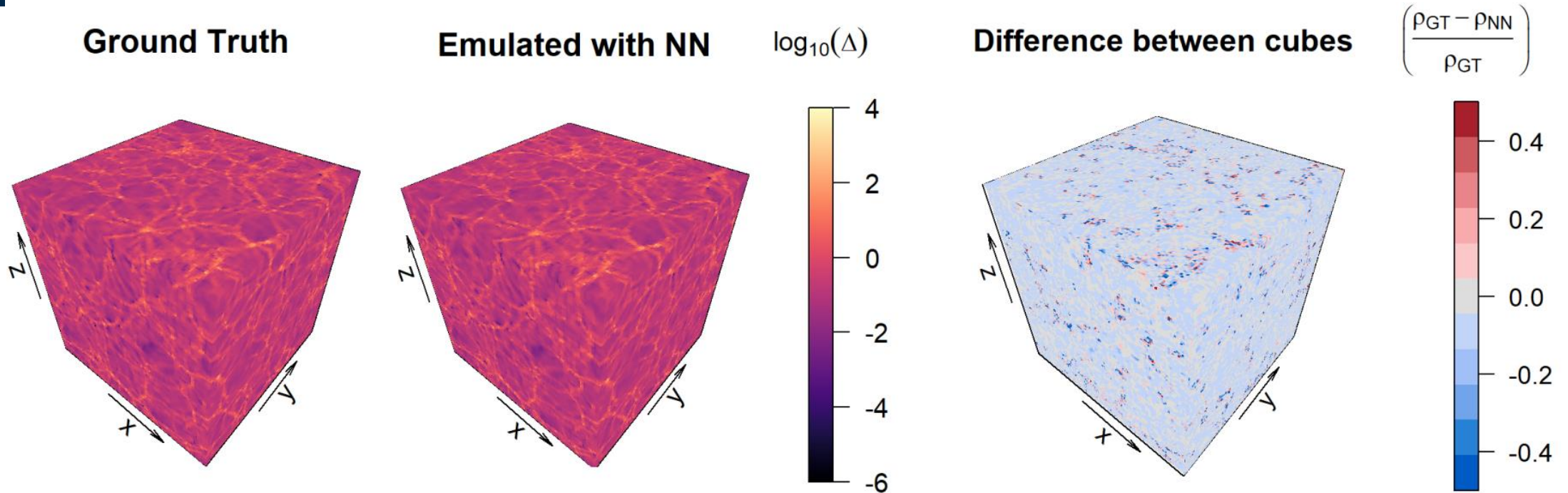
Cosmological simulations:

[Github:florent-leclercq/Moore_low_cosmosims](https://github.com/florent-leclercq/Moore_low_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](#)



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:

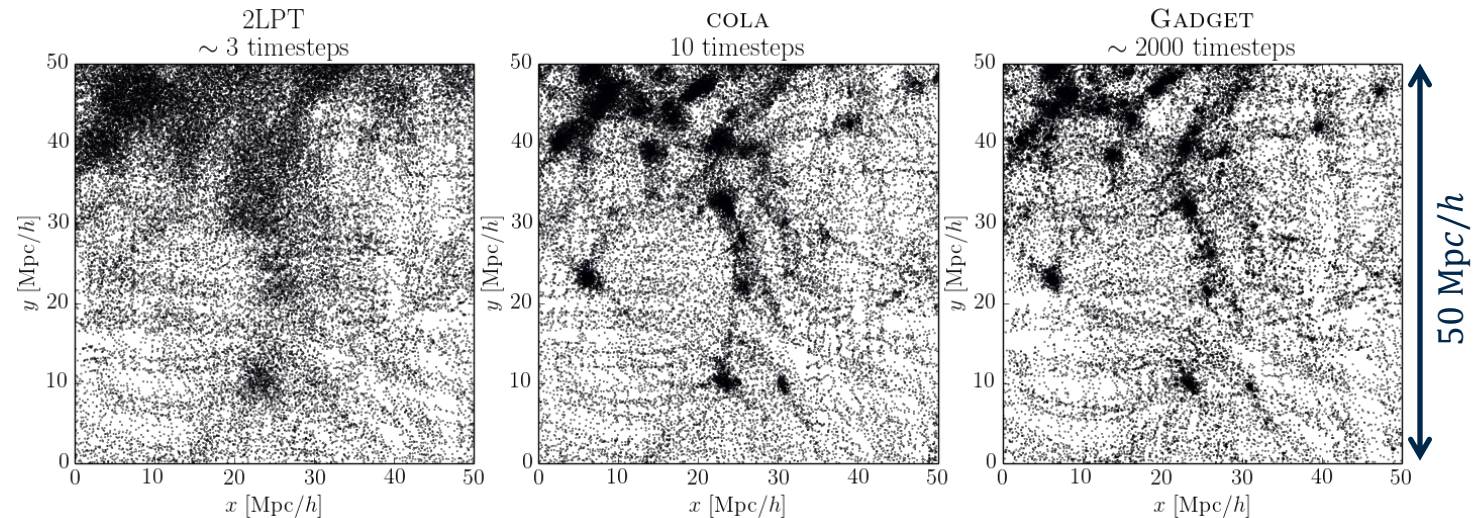
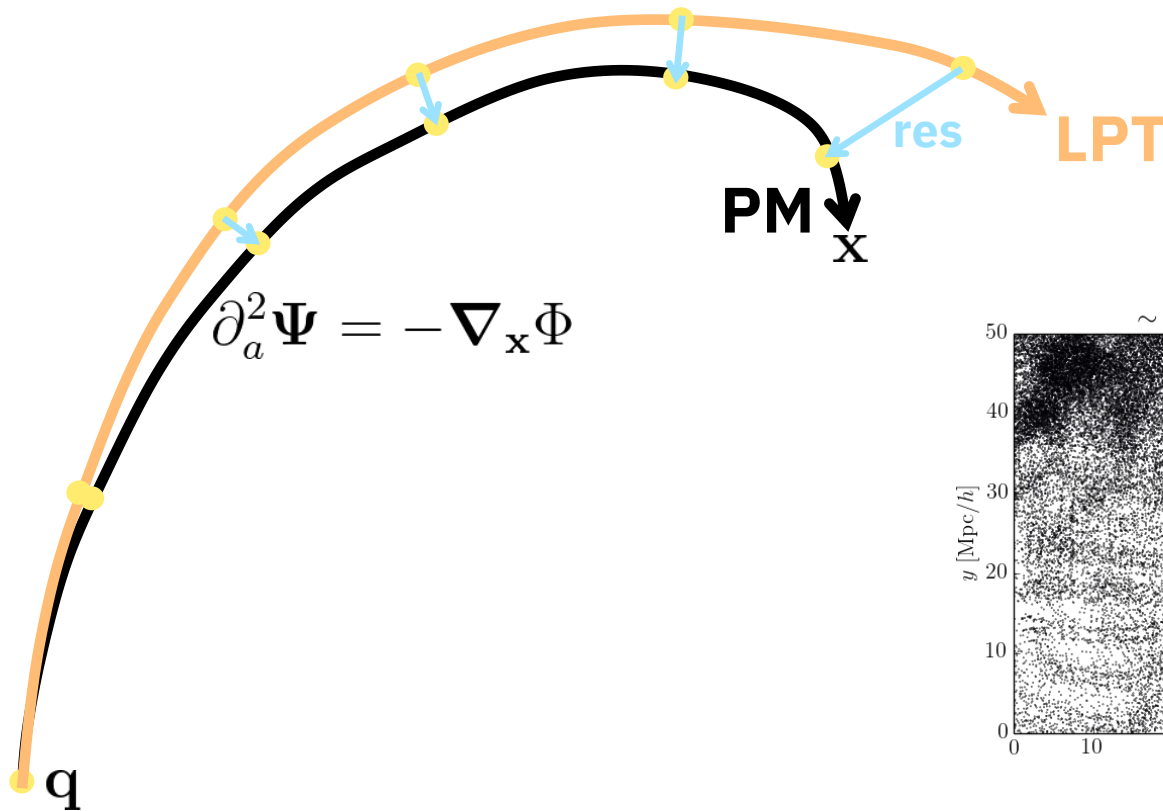
$$\Psi = \Psi_{\text{LPT}} + \Psi_{\text{res}}^{\text{COLA}} \quad (\mathbf{x} = \mathbf{q} + \Psi)$$

Tassev & Zaldarriaga, 1203.5785

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

$$\partial_a^2 \Psi_{\text{res}}^{\text{COLA}} = \partial_a^2 (\Psi - \Psi_{\text{LPT}}) = -\nabla_{\mathbf{x}} \Phi - \partial_a^2 \Psi_{\text{LPT}}$$

Analytical solutions!

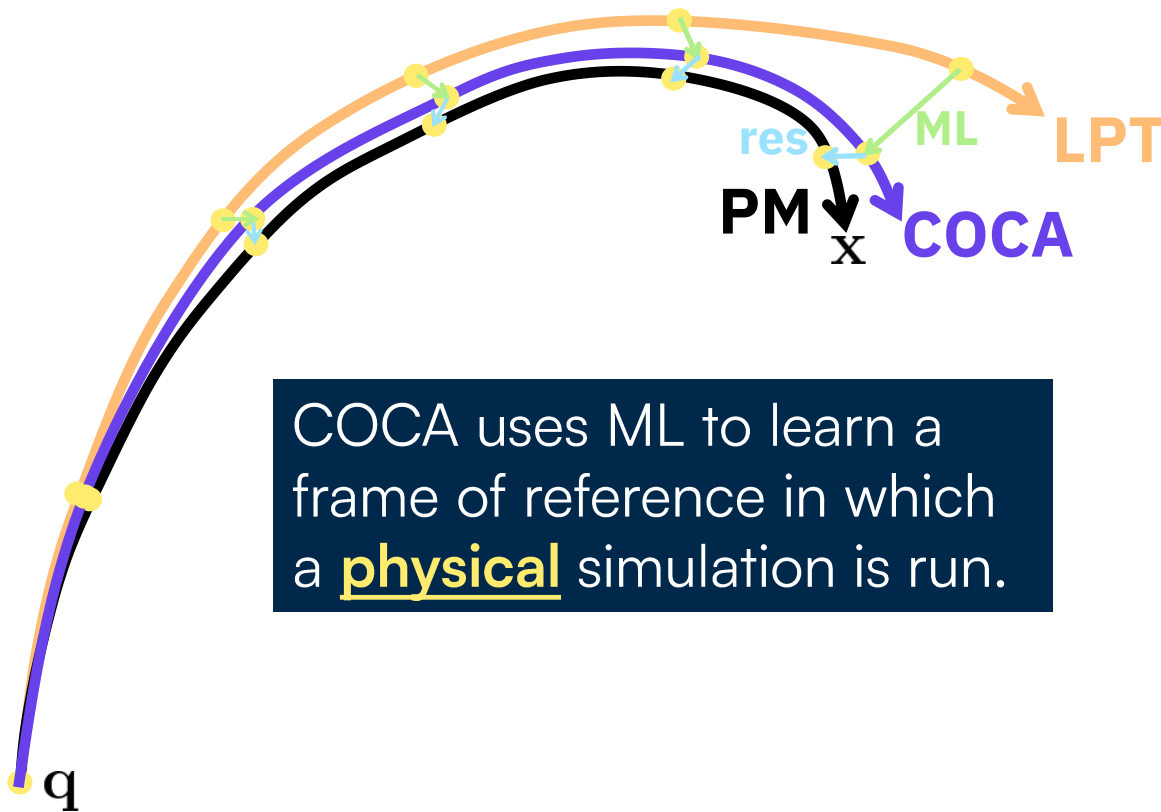


Tassev, Zaldarriaga & Eisenstein, 1301.0322



The tCOCA framework: (temporal) COmoving Computer Acceleration

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



- Write the displacement vector as:

$$\Psi = \Psi_{\text{LPT}} + \Psi_{\text{ML}} + \Psi_{\text{res}}^{\text{COCA}} \quad (\mathbf{x} = \mathbf{q} + \Psi)$$

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

$$\partial_a^2 \Psi_{\text{res}}^{\text{COCA}} = -\nabla_{\mathbf{x}} \Phi - \partial_a^2 \Psi_{\text{LPT}} - \partial_a^2 \Psi_{\text{ML}}$$

$$\Leftrightarrow \partial_a^2 \Psi = -\nabla_{\mathbf{x}} \Phi$$

- 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, in prep.

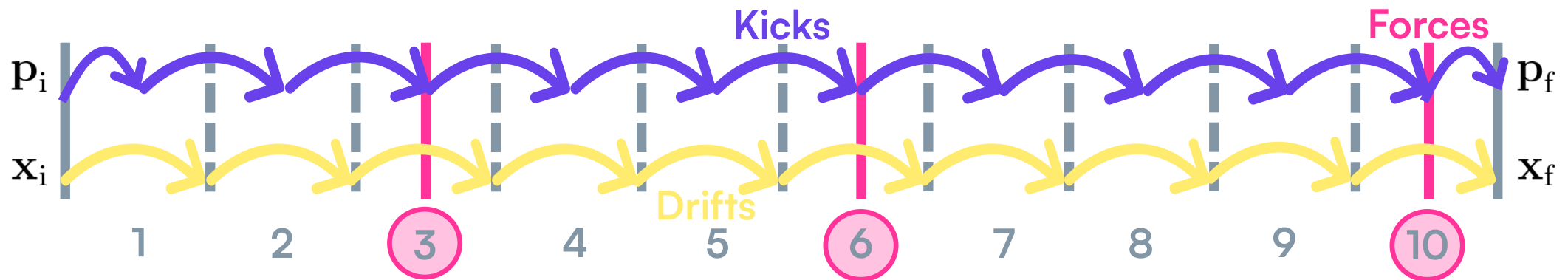


Time stepping and force calculations in COCA

- Our implementation of COCA in the Simbelmyne code uses the standard [Kick-Drift-Kick](#) (leapfrog) discretisation of the equation of motion.

<https://simbelmyne.florent-leclercq.eu> — [Bitbucket:florent-leclercq/simbelmyne](https://bitbucket.org/florent-leclercq/simbelmyne)

- Learning the new frame of reference means emulating the COLA residual momenta at every time step: $\mathbf{p}_{\text{res}}^{\text{COLA}} = \mathbf{p} - \mathbf{p}_{\text{LPT}}$.
- When the emulation error is small ($\mathbf{p}_{\text{ML}} \approx \mathbf{p}_{\text{res}}^{\text{COLA}}$), particles are already at rest in the COCA frame of reference, so it is [unnecessary to compute forces at every step](#).



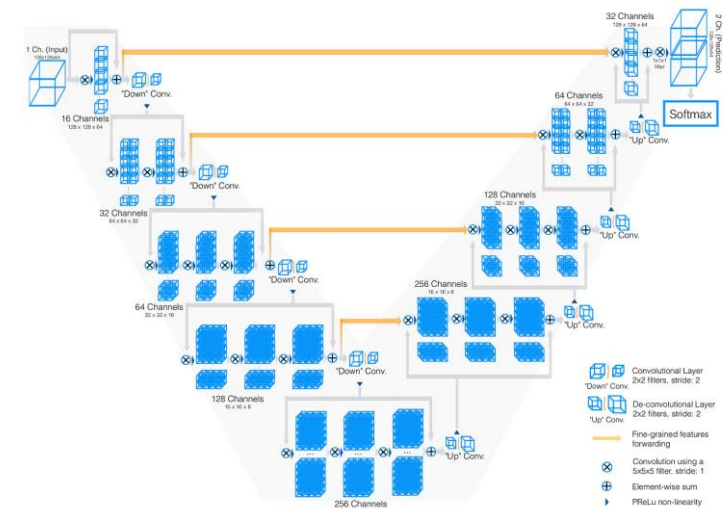
- A good frame-of-reference emulator therefore makes COCA cheaper than COLA.

Bartlett, Chiarenza, Doeser & FL, in prep.

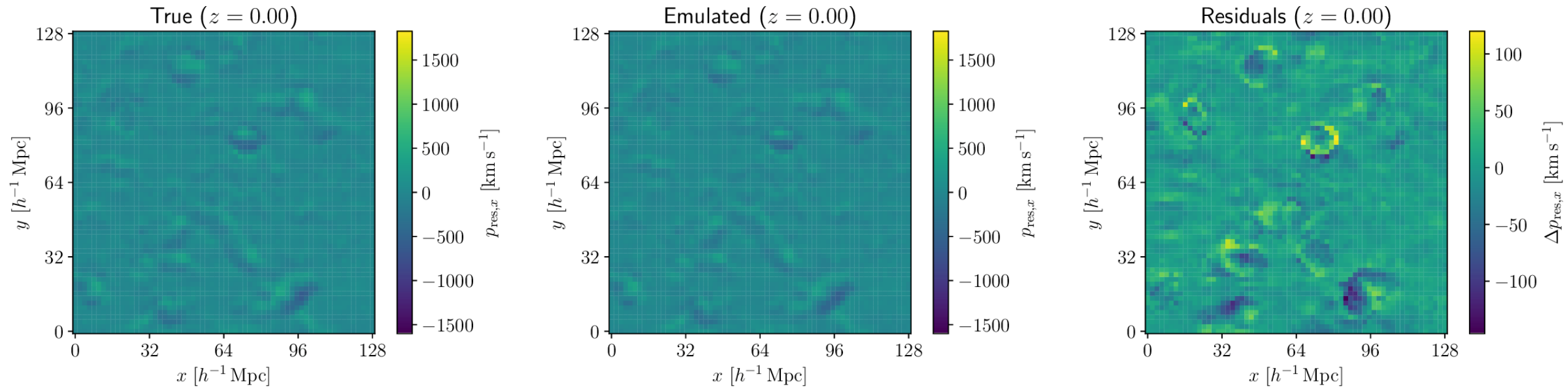


Training a frame-of-reference emulator for COCA

- 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 $L=128 \text{ Mpc}/h$, $N=64^3$ particles, and 200 epochs.
- We can predict the frame of reference to run test COCA simulations:



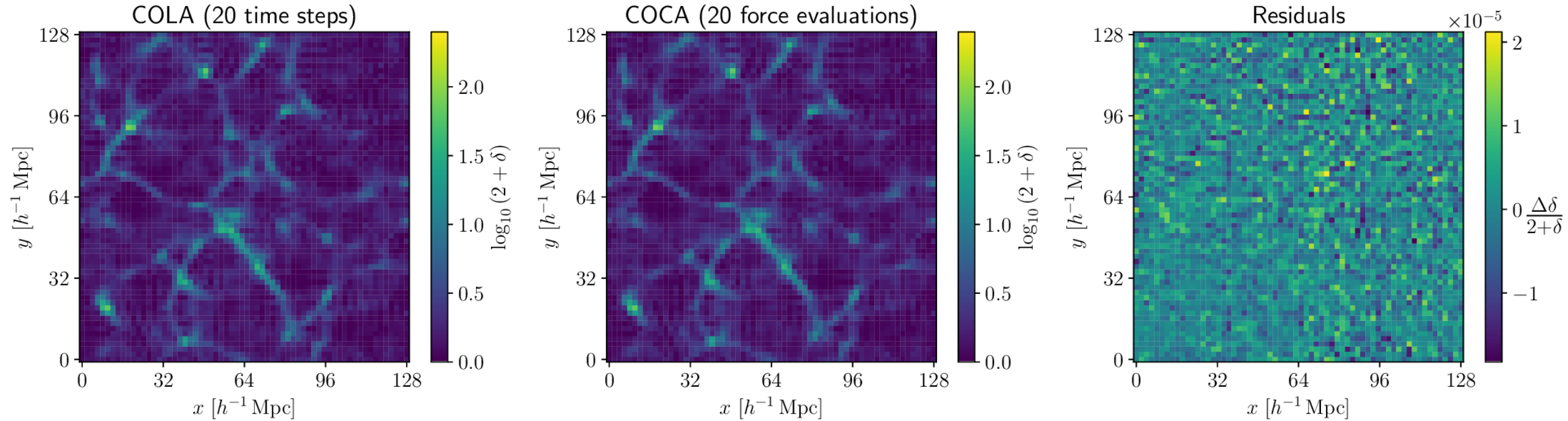
Milletari, Navab & Ahmadi, 1606.04797



Bartlett, Chiarenza, Doeser & FL, in prep.



Results: COCA density field



Bartlett, Chiarenza, Doeser & FL, in prep.



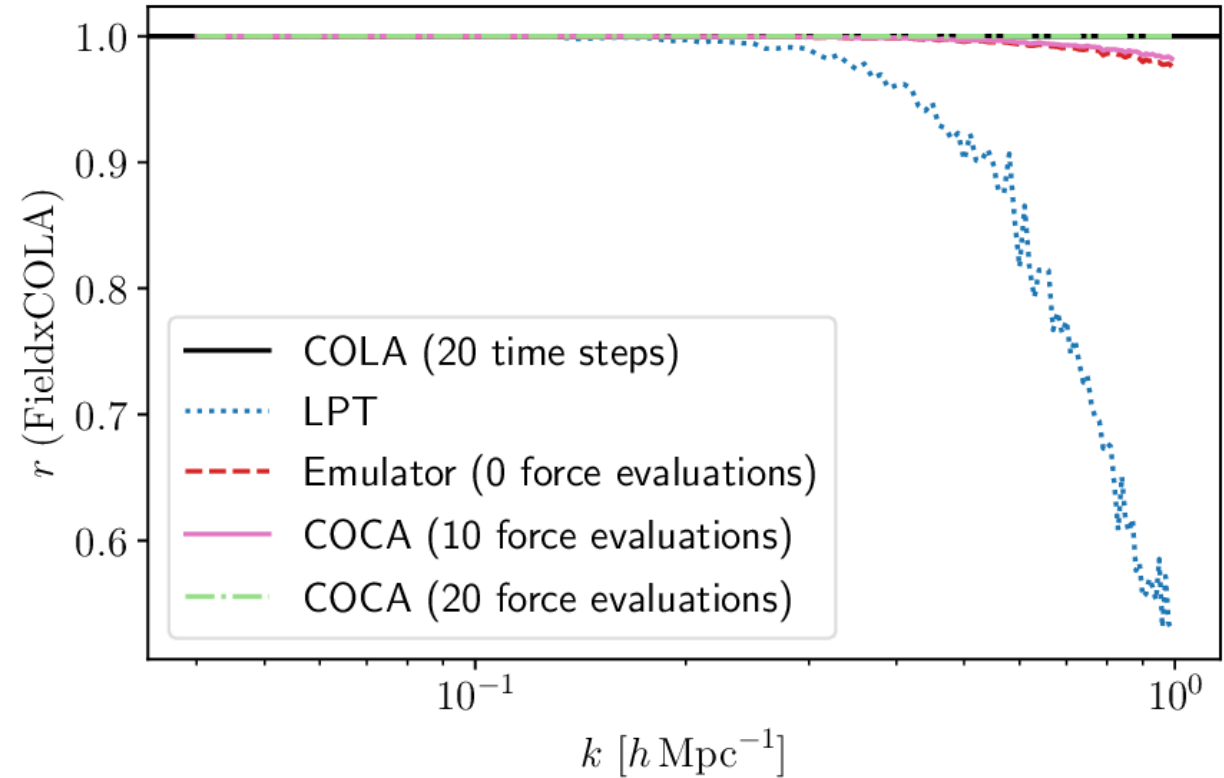
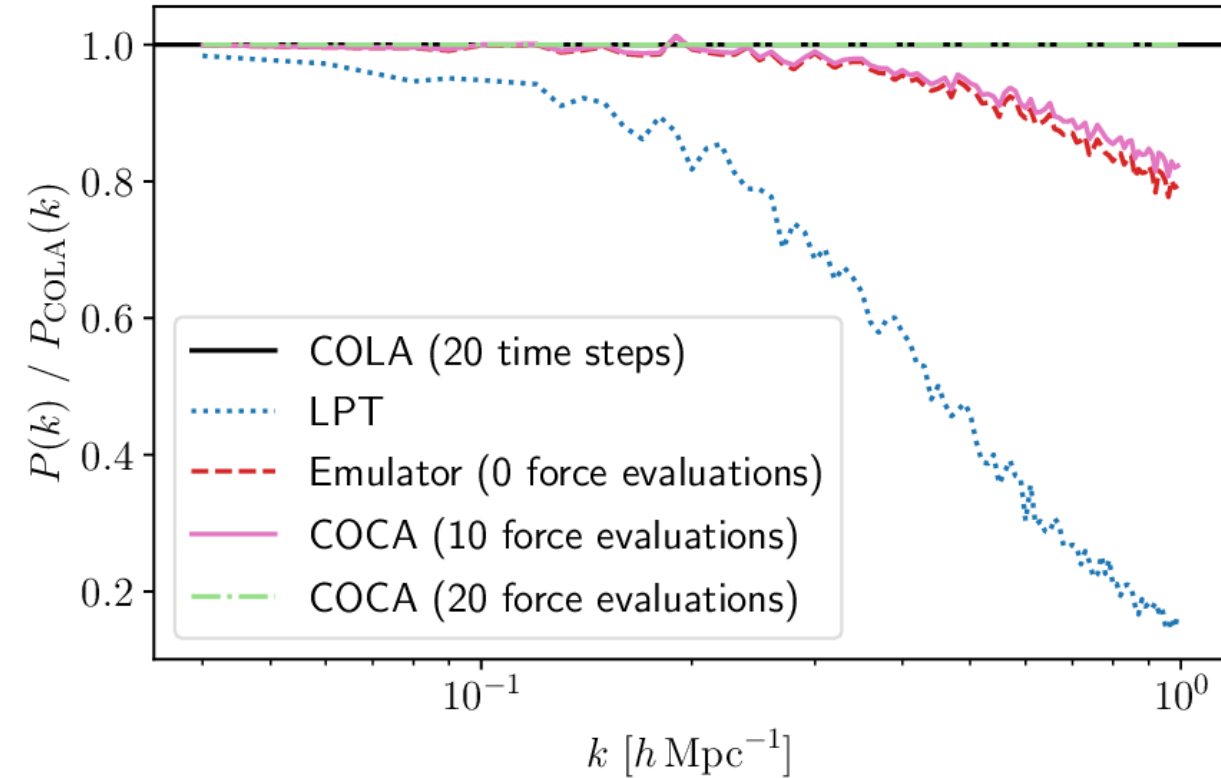
Florent Leclercq

COmoving Computer Acceleration (COCA)

21/05/2024

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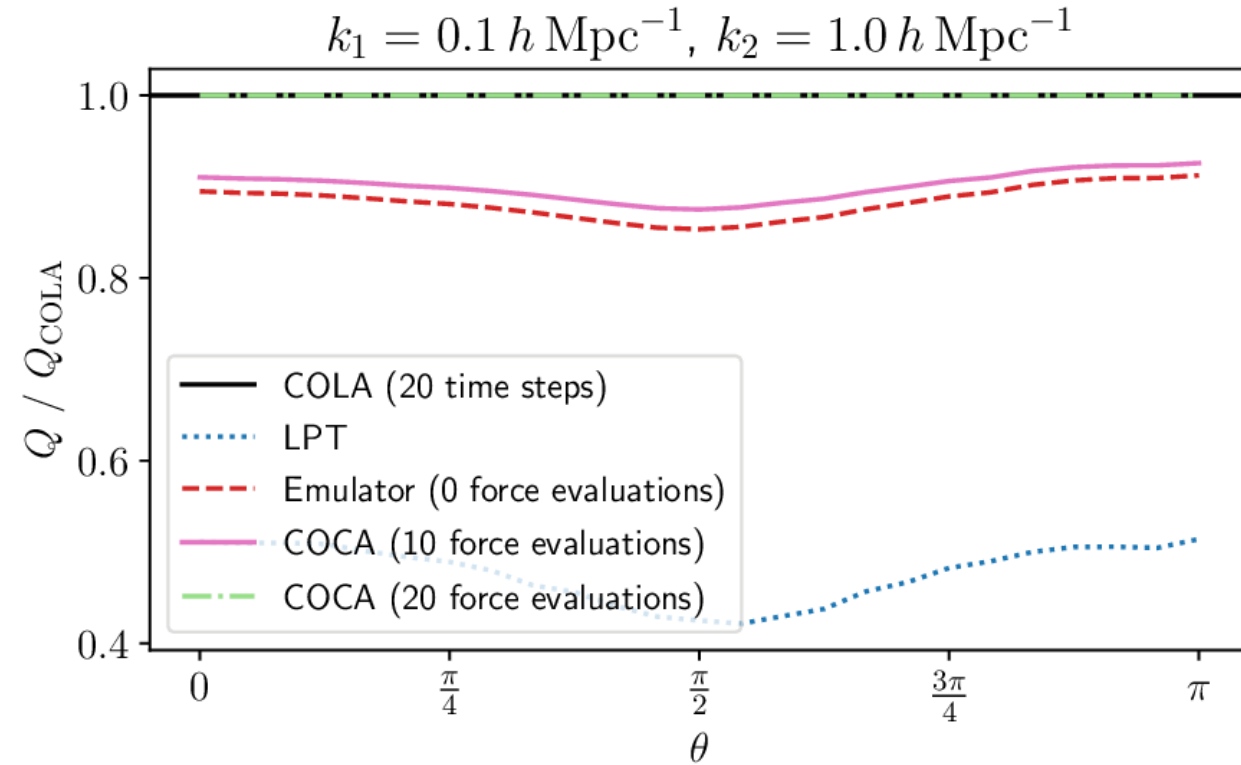
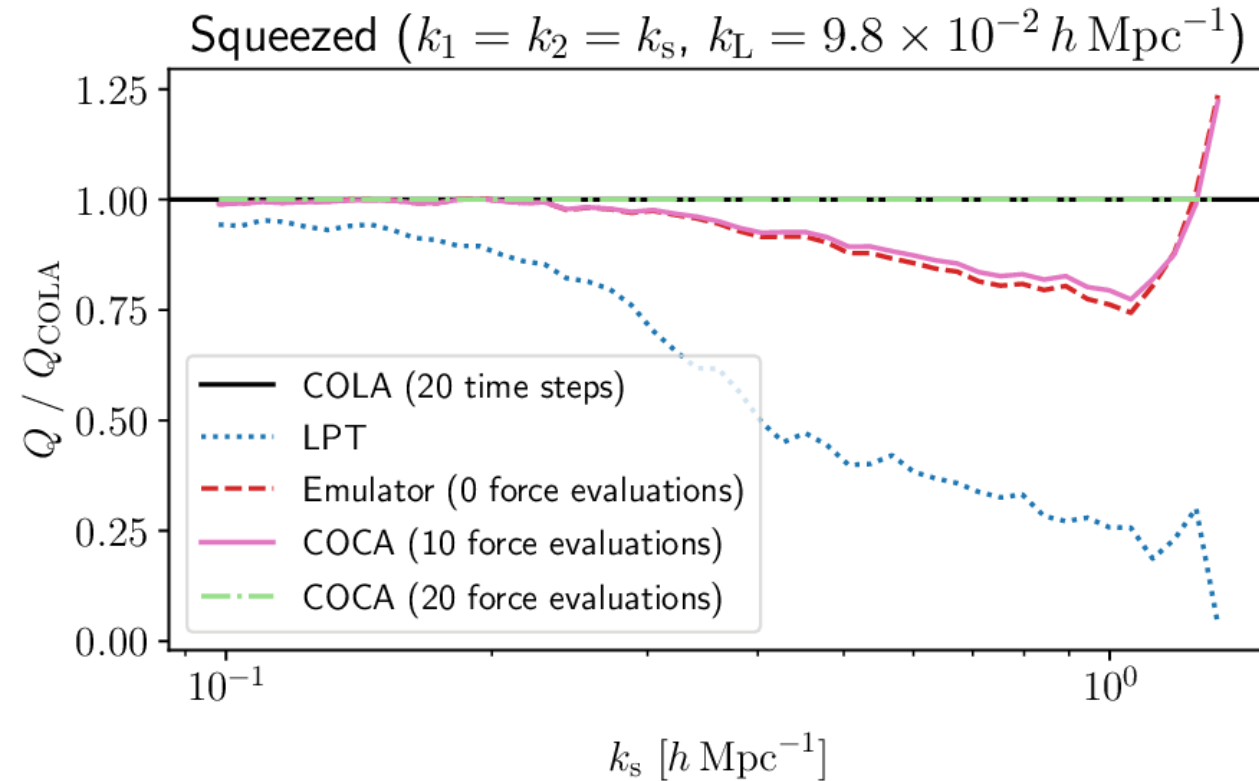
Results: COCA two-point statistics



Bartlett, Chiarenza, Doeser & FL, in prep.



Results: COCA three-point statistics



Bartlett, Chiarenza, Doeser & FL, in prep.

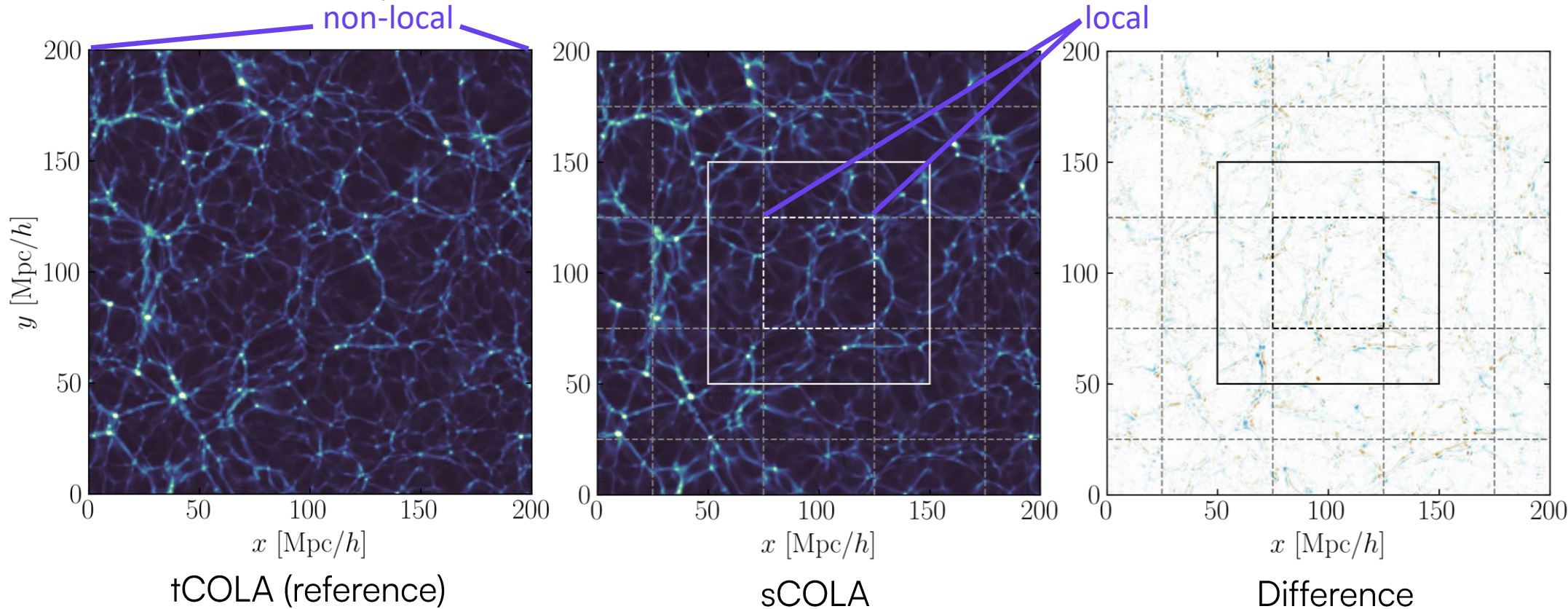


Perfectly parallel cosmological simulations using **spatial** comoving Lagrangian acceleration (sCOLA)

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

$$\partial_a^2 \Psi = -\nabla_x \left[\underbrace{\Delta^{-1} \delta}_{\text{non-local}} \right] \iff \partial_a^2 (\Psi - \underbrace{\Psi_{1.s.}}_{\text{LPT so far}}) = -\nabla_x \left[\underbrace{\Delta^{-1} (\delta - \underbrace{\delta_{1.s.}}_{\text{soon ML solution}})}_{\text{local}} \right]$$

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



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

Publicly available implementation:
[Bitbucket:florent-leclercq/simbelmyne/](https://bitbucket.org/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, Doerer & Leclercq, in prep.

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