COmoving Computer Acceleration (COCA)

Correcting Emulation Errors for Trustworthy N-Body Simulations

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Key idea

- Neural networks can emulate expensive N-body simulations.
- These have (until now) **un-correctable emulation errors**.
- By learning a frame of reference rather than the output, we can **correct for emulation errors** by adding a few force evaluations.

Solve in an emulated reference frame

Split the Lagrangian displacement field into three contributions:

$$\boldsymbol{\Psi}(\boldsymbol{q}, a) \equiv \boldsymbol{\Psi}_{\rm LPT}(\boldsymbol{q}, a) + \boldsymbol{\Psi}_{\rm ML}(\boldsymbol{q}, a) + \boldsymbol{\Psi}_{\rm res}(\boldsymbol{q}, a).$$

These are:

- $\boldsymbol{\Psi}_{\rm LPT}$ - Lagrangian Perturbation Theory (LPT) prediction. Matches truth on large scales and at early times.
- $\boldsymbol{\Psi}_{\rm ML}$ - Machine-Learning correction. Improves prediction on small scales.
- $\boldsymbol{\Psi}_{\rm res}$ - Residual (emulation error). We cannot remove this if our emulator directly predicts $\boldsymbol{\Psi}$.

By **solving equation of motion in emulated frame**, we can correct for emulation errors:

$$\partial_a^2 \boldsymbol{\Psi}_{\rm res}(\boldsymbol{q}, a) = \underbrace{-\boldsymbol{\nabla}\Phi(\boldsymbol{x}, a)}_{\text{Gravity}} \underbrace{-\partial_a^2 \boldsymbol{\Psi}_{\rm LPT}(\boldsymbol{q}, a) - \partial_a^2 \boldsymbol{\Psi}_{\rm ML}(\boldsymbol{q}, a)}_{\text{Fictitious Forces}}.$$

Similar to COmoving Lagrangian Acceleration (COLA) scheme [1], where one solves in LPT frame. Using the more accurate ML frame means we need **fewer force evaluations than COLA**.

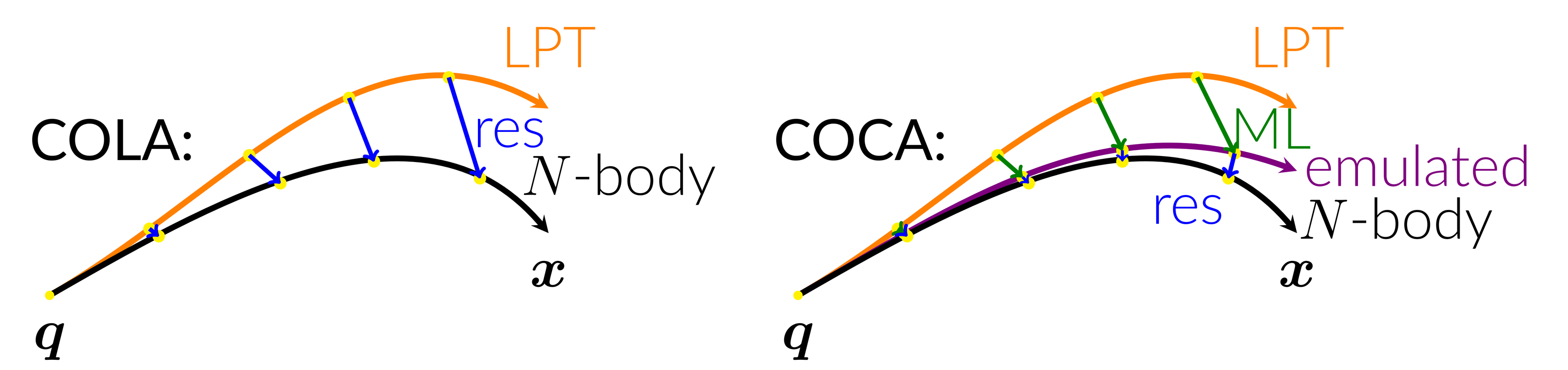

Figure 1. COLA (left) and COCA (right) formalisms for cosmological simulations.

Styled V-net to predict frame from initial conditions

We use a "V-net" architecture [2, 3], with initial conditions as input (1 channel) and the momentum of the frame of reference as output (3 channels). A "style" parameter specifies the time dependence.

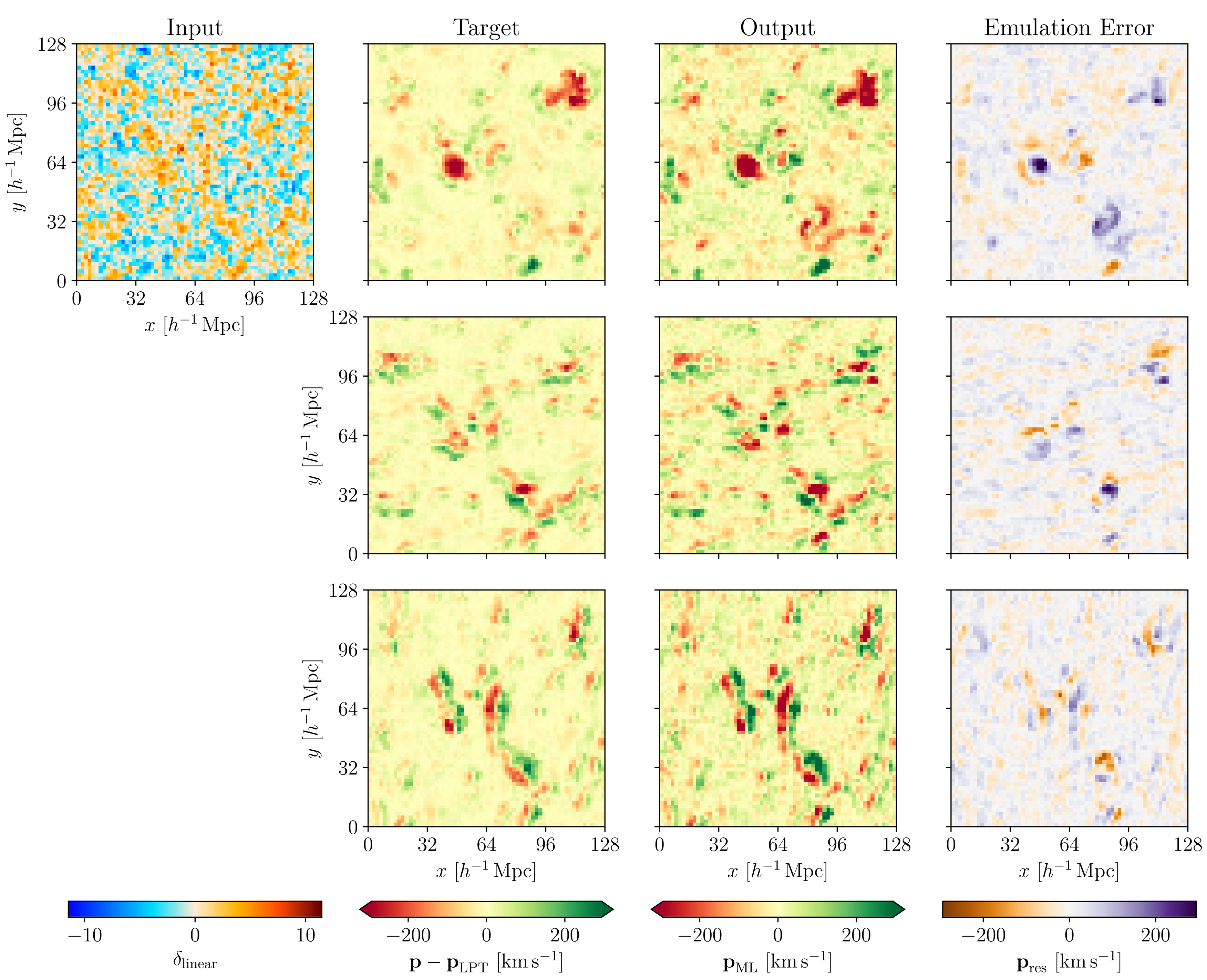

Figure 2. Slices of the input, target, output, and error of the frame of reference emulator at the final time step.

Force evaluations correct emulation errors

- Only need $n_{\rm f} = 8$ force evaluations to practically **eliminate emulation errors**.
- **4 to 5 times more accurate** than a Lagrangian displacement emulator when the frame of reference emulator is trained with the **same resources** as the Lagrangian displacement emulator.
- Can correct for **extrapolation** errors.

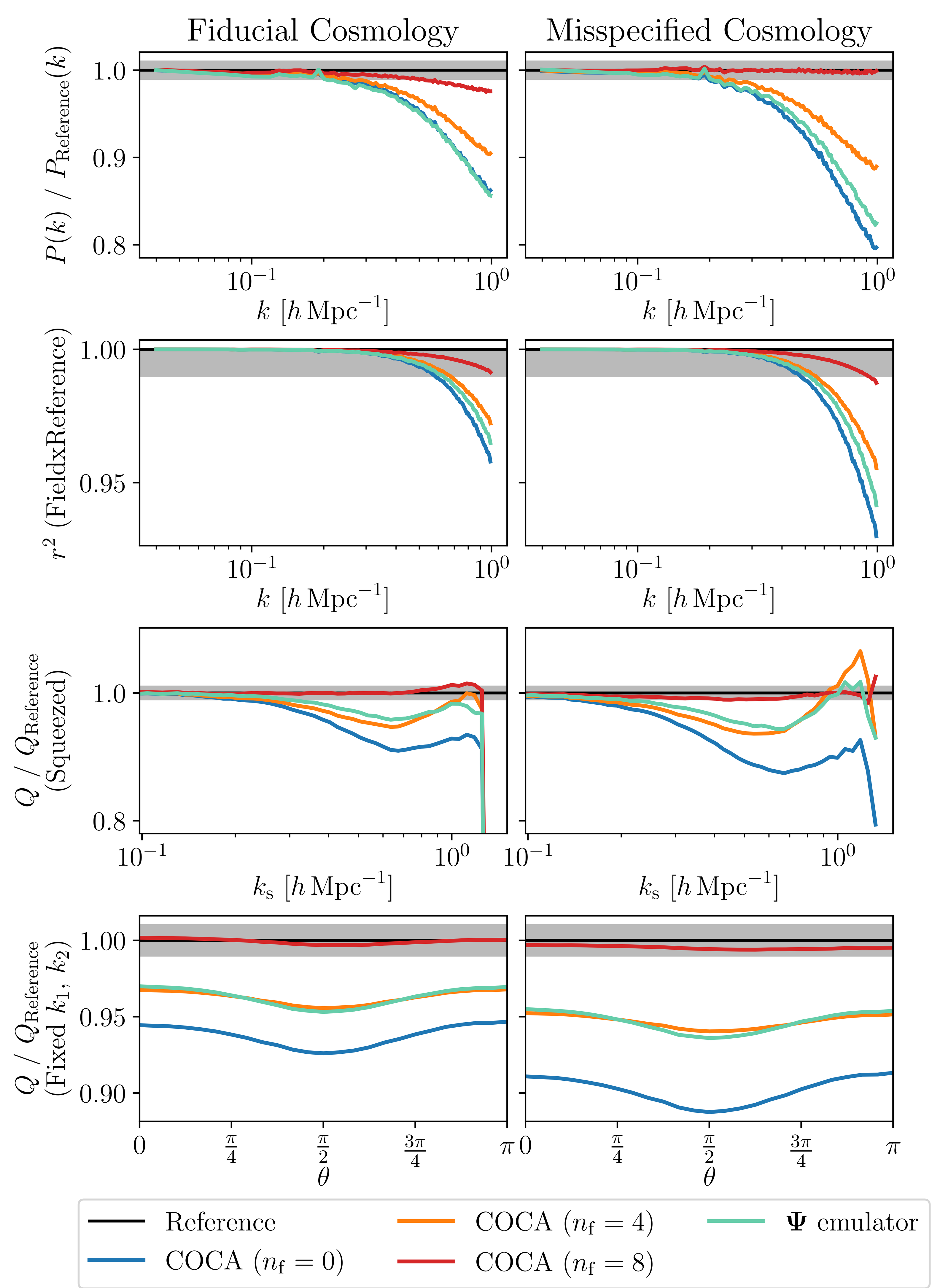

Figure 3. COCA gives **percent-level correct** power spectra (top row), cross-correlation (second row), and bispectra (third and fourth rows) for the density field when used within (left) and outside (right) the range of the training data.

Summary

COCA makes N-body simulations **cheaper** by skipping unnecessary force evaluations, while still solving the correct equations of motion and **correcting for emulation errors** made by machine learning.

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