Multi-Fidelity Emulation for matter power spectrum and Ly*α* flux power spectrum

Cosmology from Home 2022

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Multi-fidelity emulation for matter power spectrum using Gaussian processes
Ming-Feng Ho[1,3], Simeon Bird[1], Christian R. Shelton[2] (2022 MNRAS)
arXiv:2105.01081

A multi-fidelity emulator for Lyα forest
Martin Fernandez[1,4], Ming-Feng Ho[1,3], Simeon Bird[1] (in prep)

Multi-fidelity emulation using simulation from different boxsizes
Ming-Feng Ho[1,3], Simeon Bird[1], Christian R. Shelton[2] (in prep)

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PHYSICS & ASTRONOMY

July 2022 Virtual

Outline

- What's the problem? Why multi-fidelity
- What's emulation?
- What's multi-fidelity?
- Example 1: matter power spectrum
- Example 2: emulation for different simulation box sizes
- Example 3: Lyα 1-D flux power

Why multi-fidelity emulation?
Problem of current emulation

- **Problem:** As the simulations become increasingly more realistic & expensive, the simulation data needed to train an accurate emulator can be difficult to generate.
  - EuclidEmulator2 (2020): **needs 200+ simulations (3000^3)** in 8D even though using Latin hypercube
  - And we need to emulate beyond ΛCDM in the future … (more dimensions!)

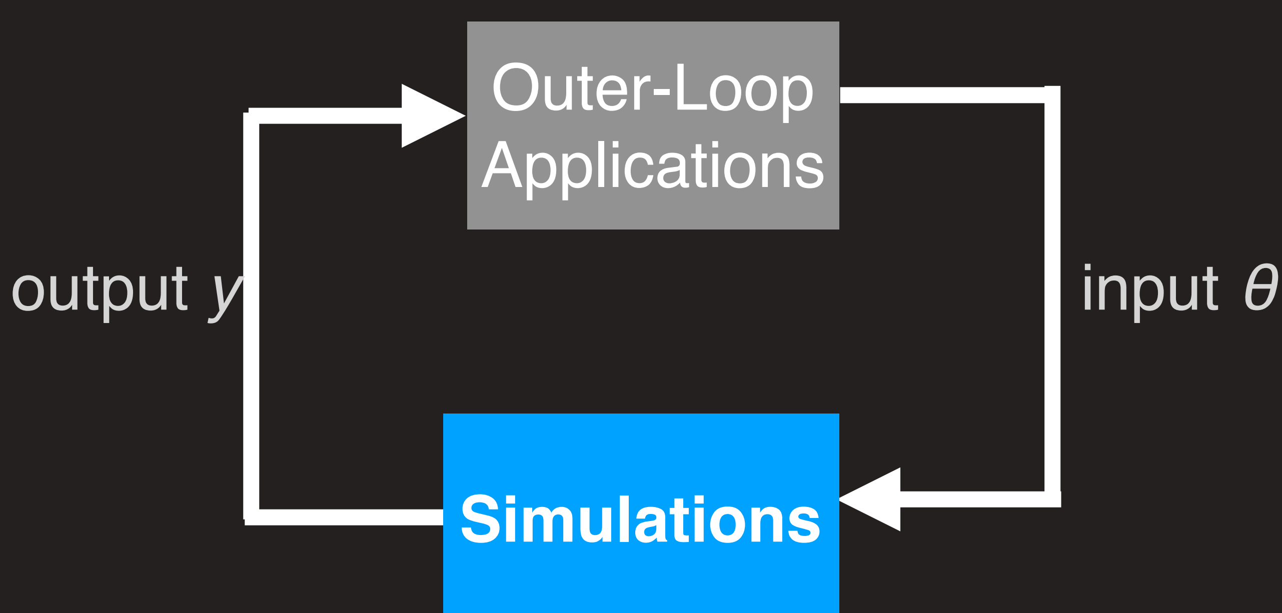
*Emulator: A model learns the mapping relationship from cosmological parameters θ to summary statistics (e.g., matter power spectrum) through a statistical learning process

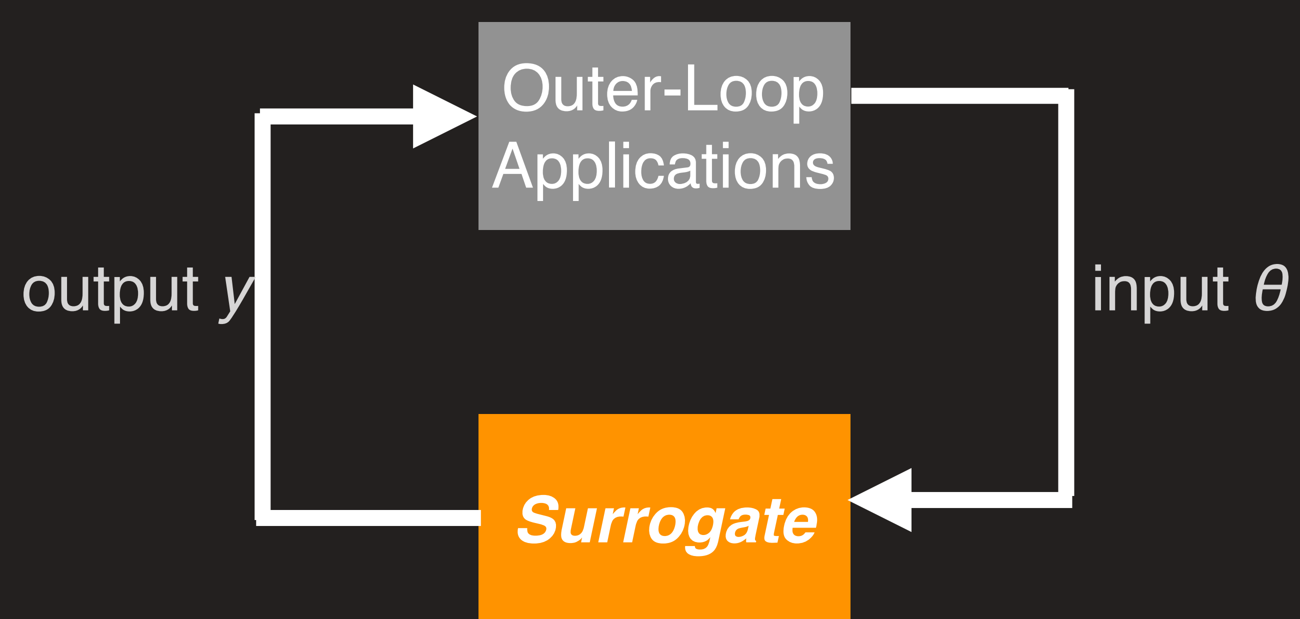
What’s emulation?
Cosmic calibration

- History: analytical calculation is not enough anymore for future surveys, we have to rely on numerical simulations to give accurate theoretical predictions …

- Key ingredients for emulation:
  - Experimental design: space filling
  - Surrogate modelling: interpolation

- Outer-loop applications:
  - Uncertainty quantification
  - Inference
  - Optimization





Perherstorfer et al (2018)
Survey of Multifidelity Methods in Uncertainty Propagation, Inference, and Optimization

What's emulation? ~~Cosmic calibration~~

Bayesian calibration for computer experiments

- History: analytical calculation is not enough anymore for future surveys, we have to rely on numerical simulations to give accurate theoretical predictions …

- Key ingredients for ~~emulation~~ *Bayesian* modelling:
  - Experimental design: ~~space filling~~ ***Data***
  - Surrogate modelling: ~~interpolation~~ ***Prior***

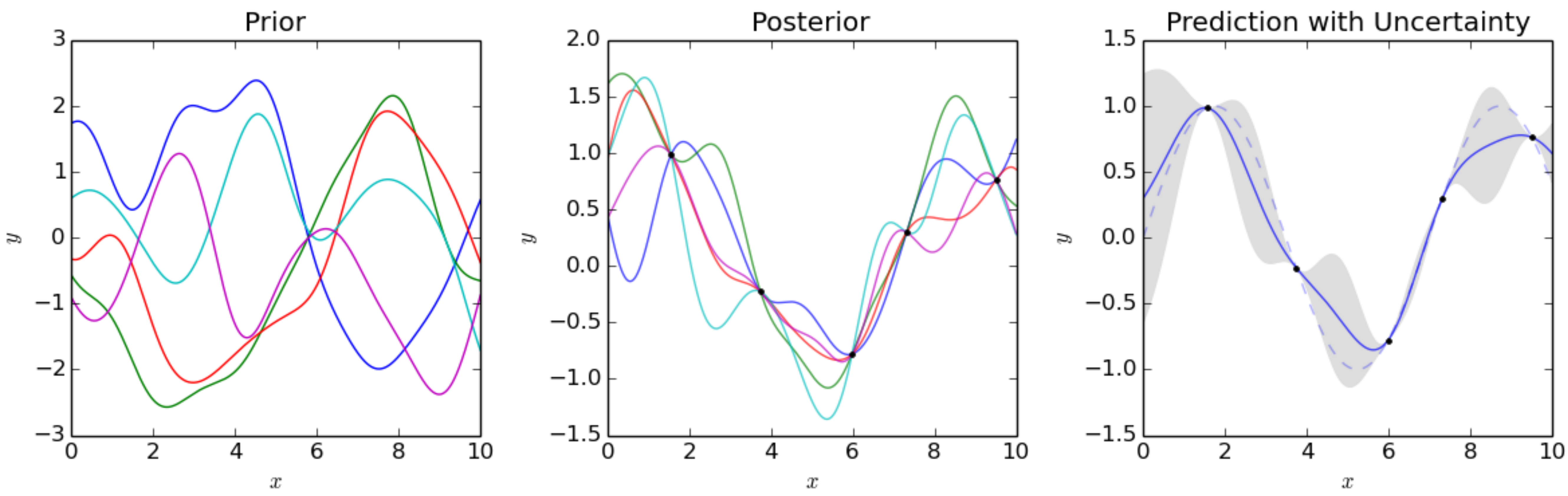
Simulations ↑

Emulation = *Posterior* predictions given *Prior* and *Data*

↓ Simulations you haven't run

↓ A distribution over smooth functions

Gaussian process: Bayesian function prediction



- Gaussian process prior: Smoothness and monotonicity features of y(x) before data are collected.
- Bayesian approach: Choose a flexible prior allowing many shapes of y(x), and let the Bayesian machinery to direct the details of the predictions.*

image credit: wikipedia

* This Bayesian attitude is mentioned in Santner (2003), The Design and Analysis of Computer Experiments

What's emulation?
Roadmap of building an emulator

Bayesian calibration of computer experiments

Simulations

- **N-body simulations** — Most of current applications are N-Body
- **Baryonification** — BACCO: Arico (2020), Giri (2021)
- **Hydro simulations** — CAMELS: F Villaescusa-Navarro et al, Lyman-α: Bird (2019), Rogers (2019)

… *More*!

Surrogates

- **Gaussian process**
- **Neural Network**

… *More*!

Applications

- **Matter power** — Heitmann (2006), Habib (2007), etc. Coyote Universe: 37 highRes; Mira-Titan: 36 highRes; EuclidEmulator: 250 highRes
- **Halo mass functions** — Aemulus: T McClintock (2018); Mira-Titan: Bocquent (2020)
- **Cosmic shear** — Harnois-De´raps (2019), Giblin (2019)
- **Field level** — KiDs: Yiu (2021); Neerav (2021), CAMELS papers
- **Lyα flux power** — Bird (2019), Rogers (2019), Rogers (2021), Pedersen (2021)
- **21cm power** — Sudipta (2022)
- **Gravitational wave** — Damon H. T. (2022)
- **Exoplanet** — Rogers (2021), they use Random Forest

… *More*!

What's emulation?
Roadmap of building an emulator

Simulations

First cosmic emulator- Heitmann (2006)

Bayesian calibration of computer experiments

N-body simulations
Most of current applications are N-Body

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… *More*!

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Neural Network

… *More*!

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CAMELS

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… *More*!

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… *More*!

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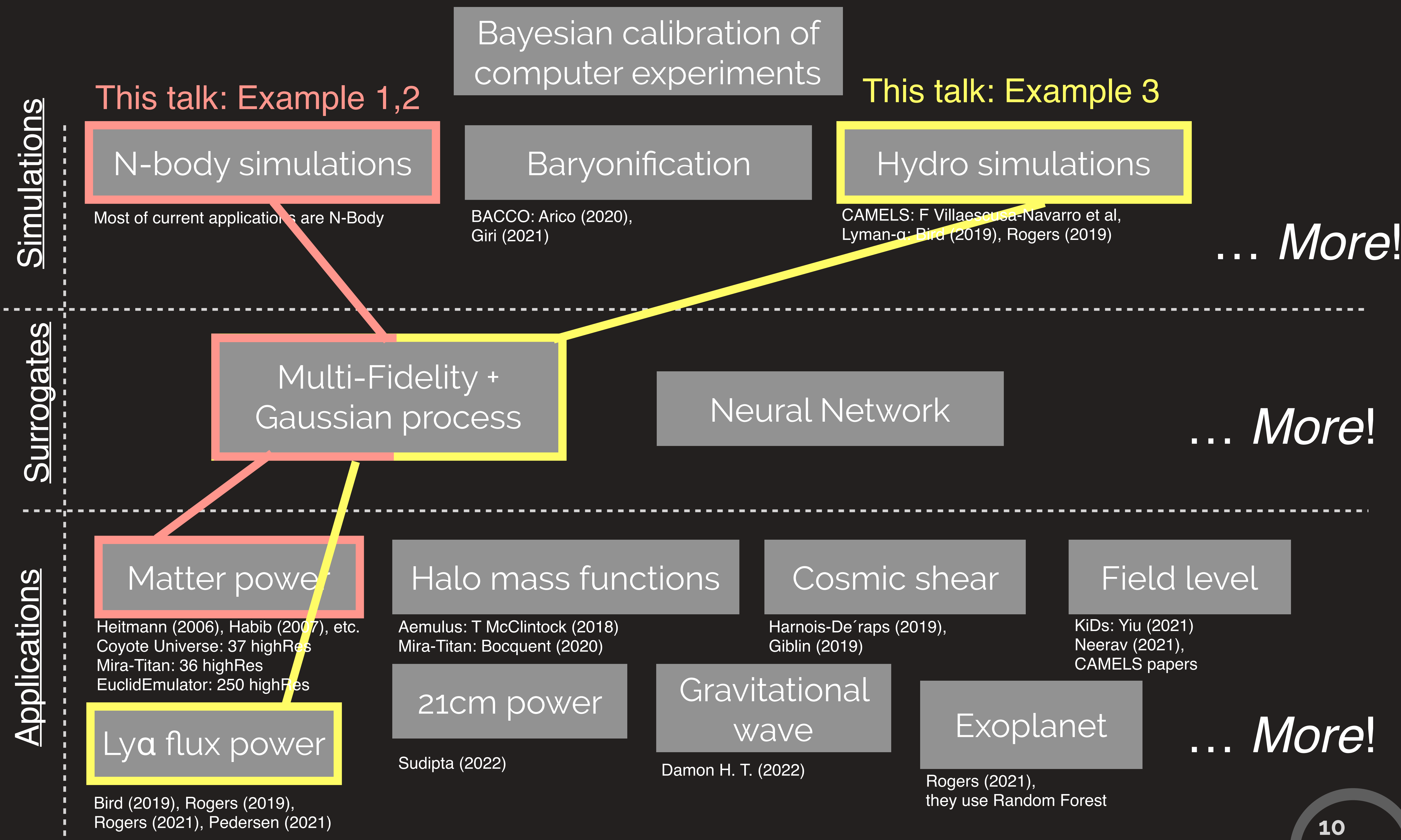
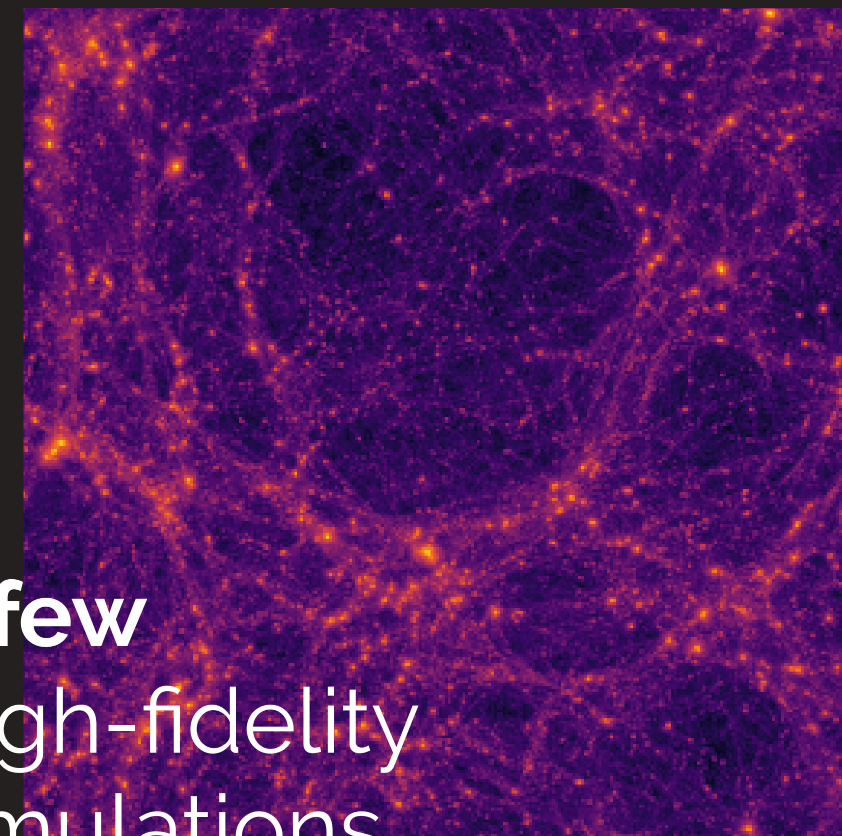


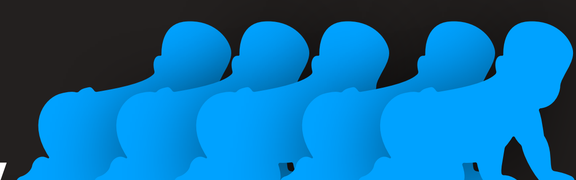
What’s multi-fidelity?
An analogy

Many
Low-fidelity
simulations

+



A few
High-fidelity
simulations



Many
Grad Student Researchers

+

A few
Professors

= efficiency + accuracy

What's multi-fidelity?
Statistical modelling - regression view

- KO method (AR1): linear autoregressive GP

$$f_{\mathrm{HF}}(x) = \rho f_{\mathrm{LF}}(x) + \delta(x).$$

Bias function, a GP

Low-fidelity output, a GP

Scale, a value

- Nonlinear Autoregressive Gaussian Process (NARGP): An improved KO method using a deep GP

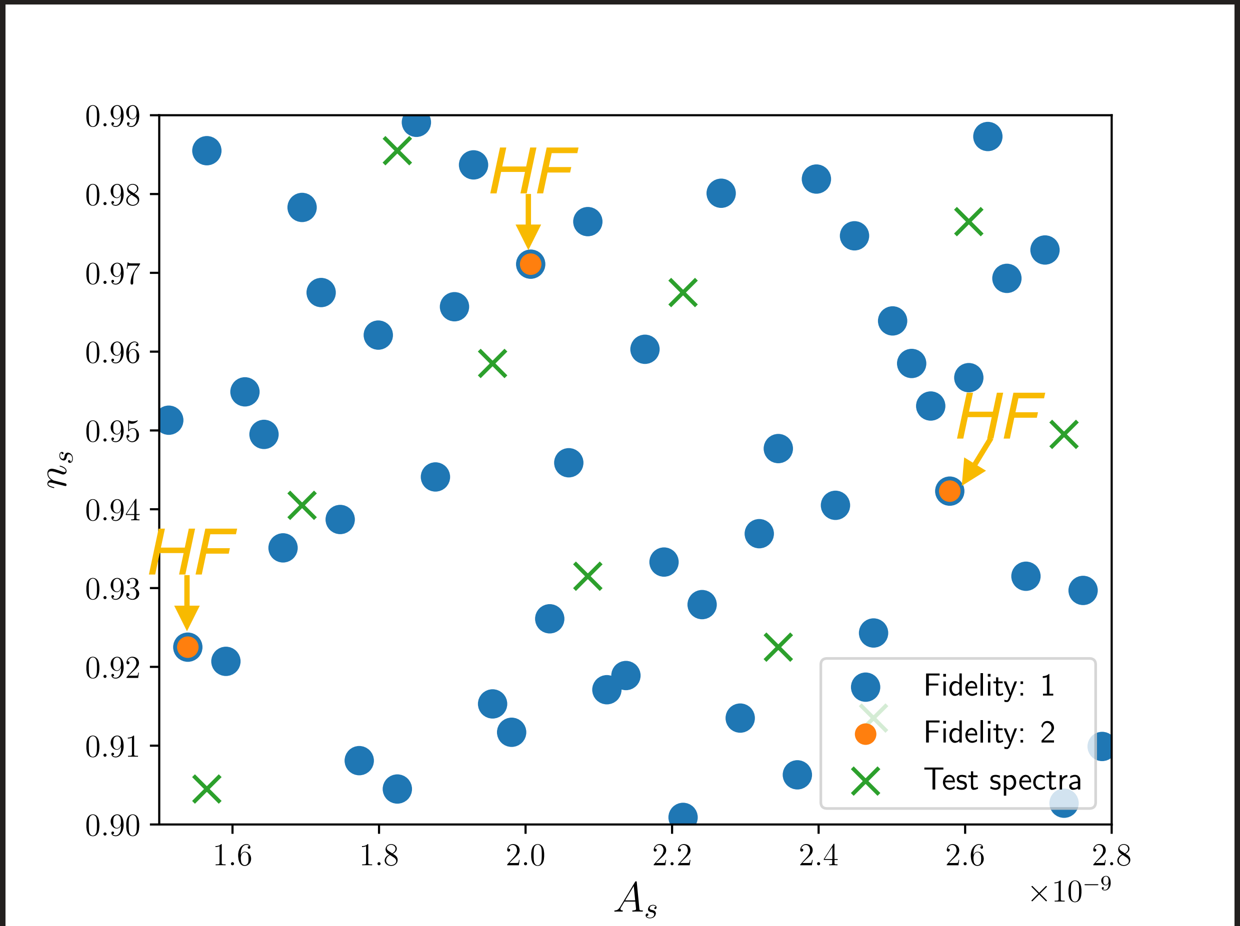
$$f_{\mathrm{HF}}(x) = \rho(x, f_{\mathrm{LF}}(x)) + \delta(x).$$

Scale function, a GP

KO: Kennedy & O'Hagan (2000)
NARGP: Perdikaris et al. (2017)

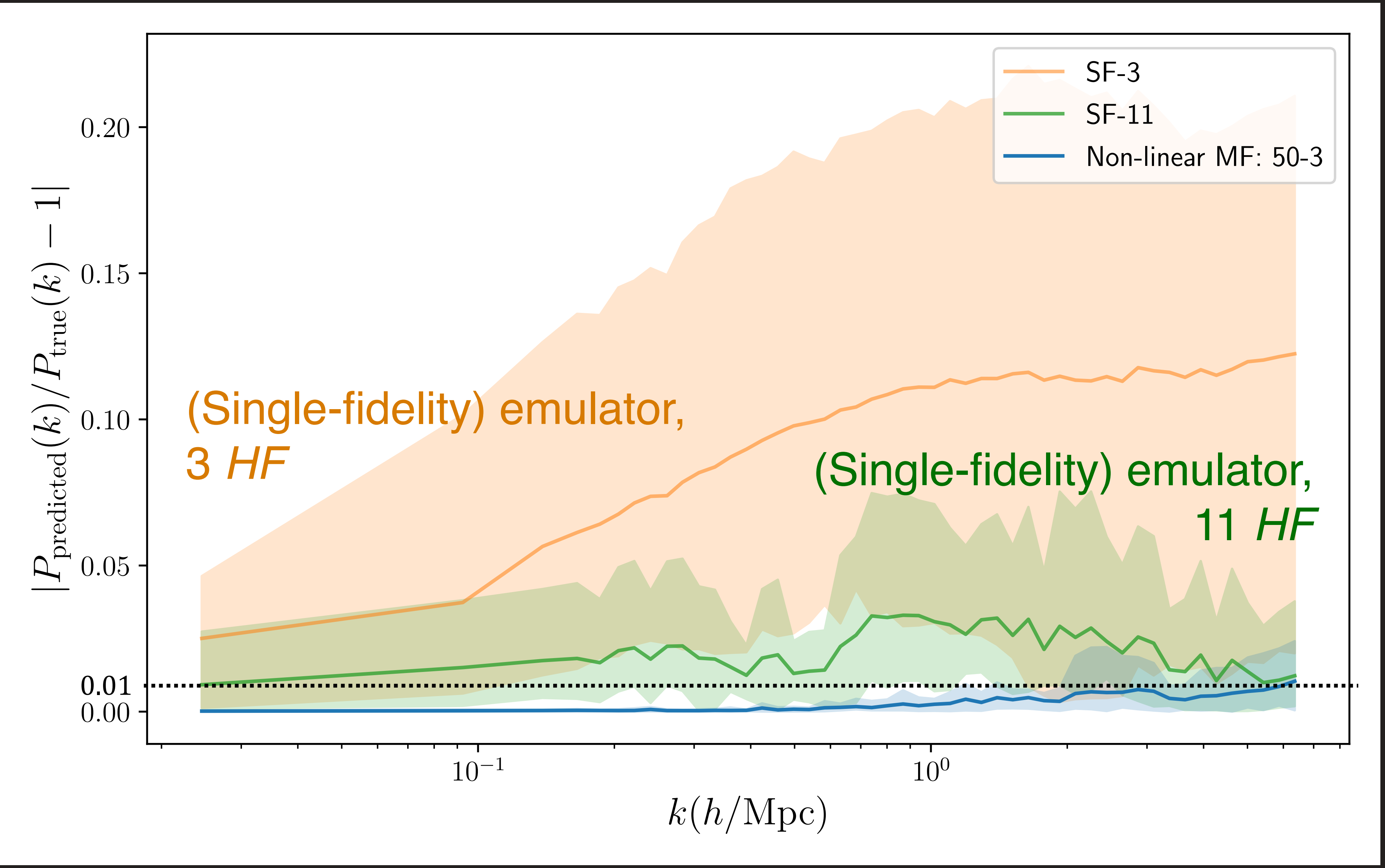
Example 1: matter power spectrum
Experimental design

- Parameters: $(h, \Omega_0, \Omega_b, A_s, n_s)$
- *Low-fidelity*: space-filling strategy (Latin hypercube)
  - $128^3, 256\,\mathrm{Mpc\,h^{-1}}$
- *High-fidelity*: a subset of low-fidelity runs
  - $512^3, 256\,\mathrm{Mpc\,h^{-1}}$
- *HF* choices were optimized using *LF* simulations



Ho, Bird, Shelton (2022)

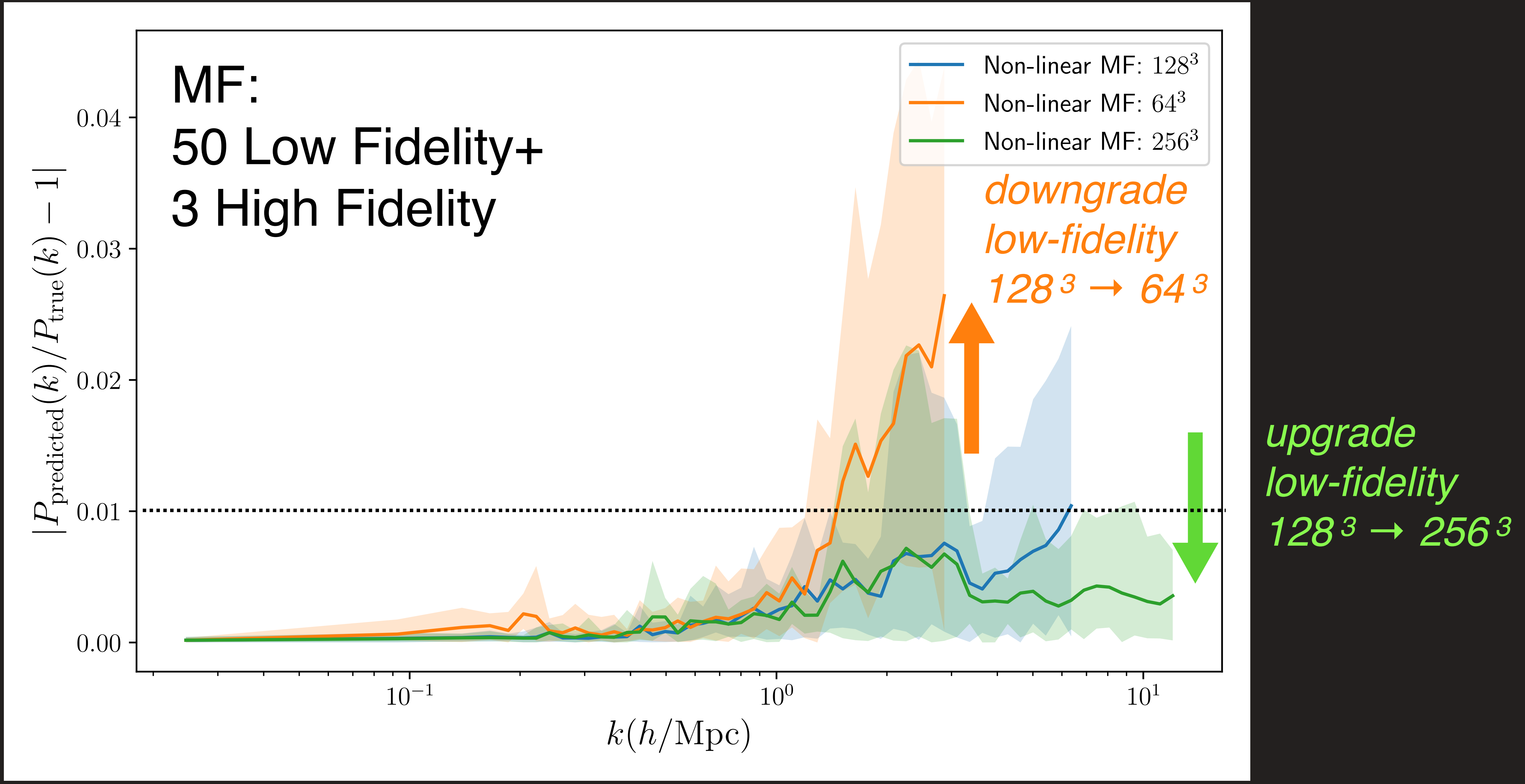
Example 1: matter power spectrum
Emulation error (z = 0)



Multi-fidelity, 50 *LF* + 3 *HF*

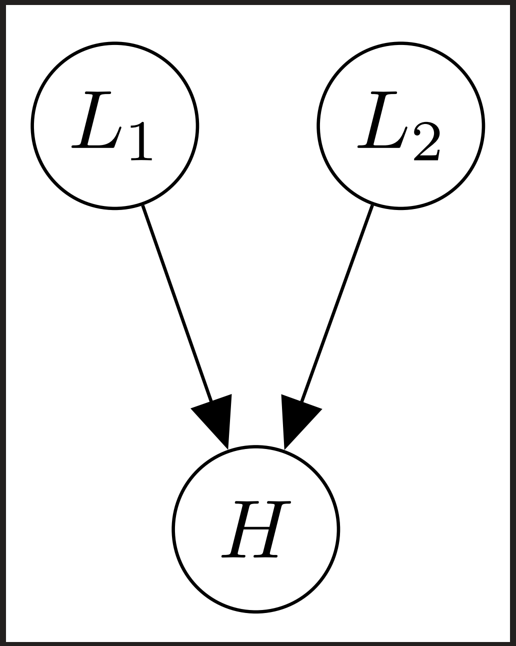
- The cost of 50 LF + 3 HF simulations is ~ 4 HF simulations.
- Still, the accuracy of MFEmulator is even better than using 11 HF.

Example 1: matter power spectrum
Accuracy increases with a better LF training set



- The quality of LF simulations affects the accuracy of MF emulation
- Small scales emulation can be improved with a better quality of LF simulation suite. → *Question: Can we use small box LF to improve emulation?*

Example 2: matter power spectrum
Extending to using **boxsize** as a fidelity



- L_1: 128^3, 256 Mpc/h
- L_2: 128^3, 100 Mpc/h
- H: 512^3, 256 Mpc/h

- Number of particles is not the only fidelity variable, ***boxsize*** is also a fidelity variable
- A smaller boxsize, ***better*** resolution at ***small scales***
- We can combine both ***large box (L1)*** and ***small box (L2)*** information through a graphical model construction.
- A graphical GP (Ji et al., 2021) allows us to do so.

Deep Graphical Multi-fidelity GP (dGMGP)

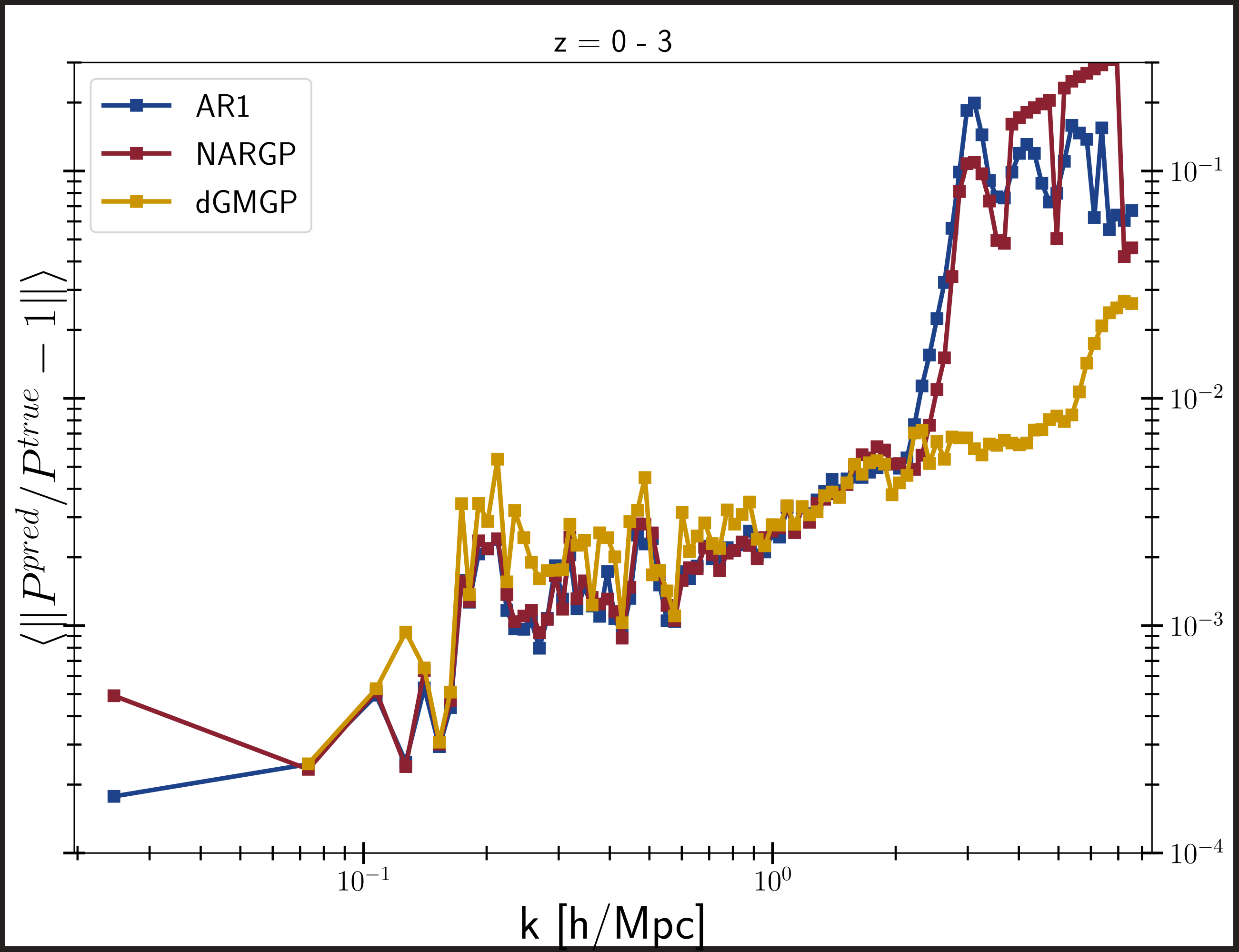
$$f_{\mathrm{HF}}(x) = \rho(\{f_{\mathrm{LF},1}, f_{\mathrm{LF},2}\} \cup x) + \delta(x)$$

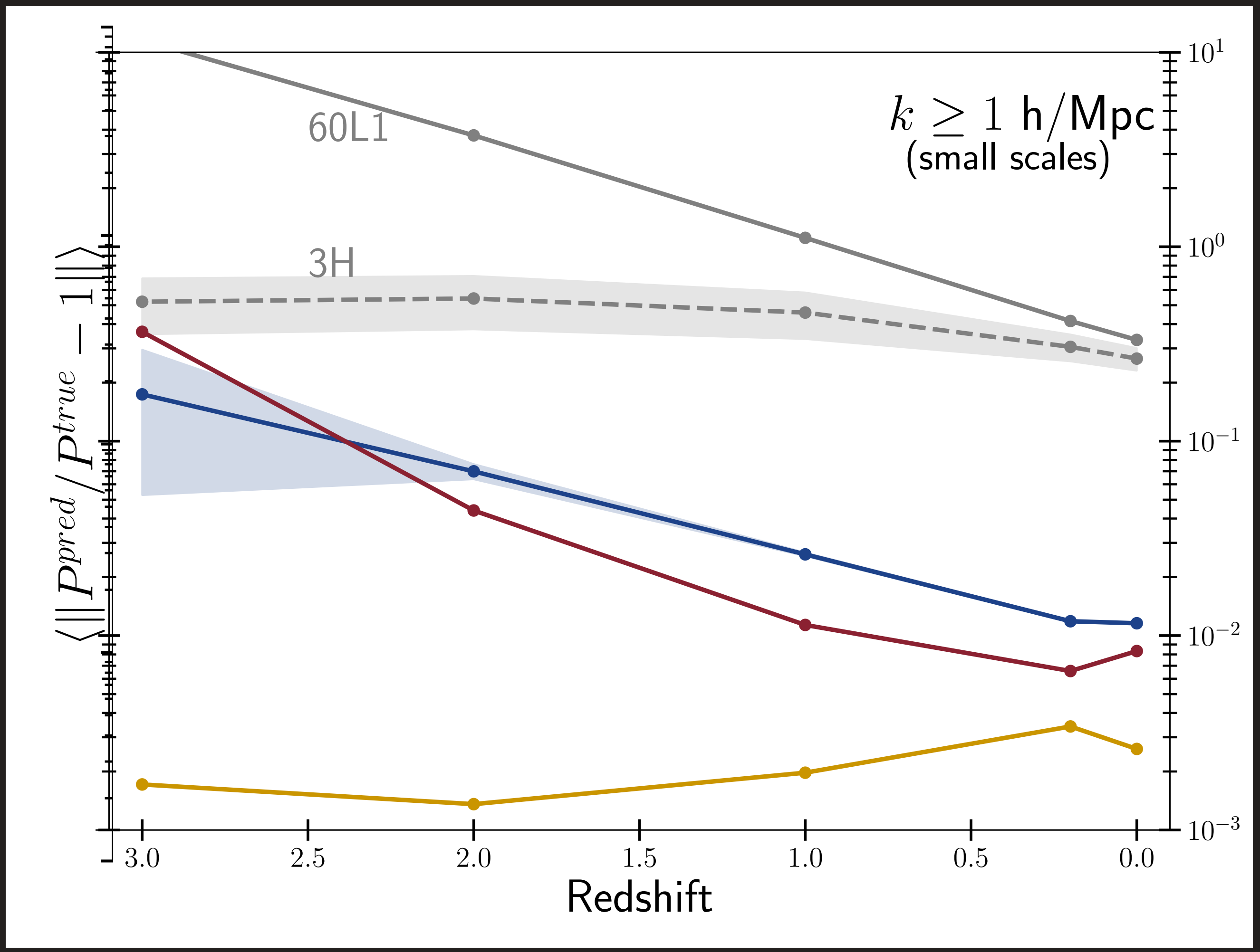
$$K([x, f_{\mathrm{LF}}], [x', f'_{\mathrm{LF}}]) = K_{\mathrm{SE}}(x, x')[K_{\mathrm{LIN}}(f_{\mathrm{LF}}, f'_{\mathrm{LF}}) + K_{\mathrm{SE}}(f_{\mathrm{LF}}, f'_{\mathrm{LF}})] + K_{\mathrm{SE}}(x, x')$$

K_{SE} : Squared-exponential kernel, guarantees smooth functions
K_{LIN} : Linear kernel, doing Bayesian linear regression

GMGP: Ji (2021)
A graphical multi-fidelity Gaussian process model, with application to emulation of expensive computer simulations

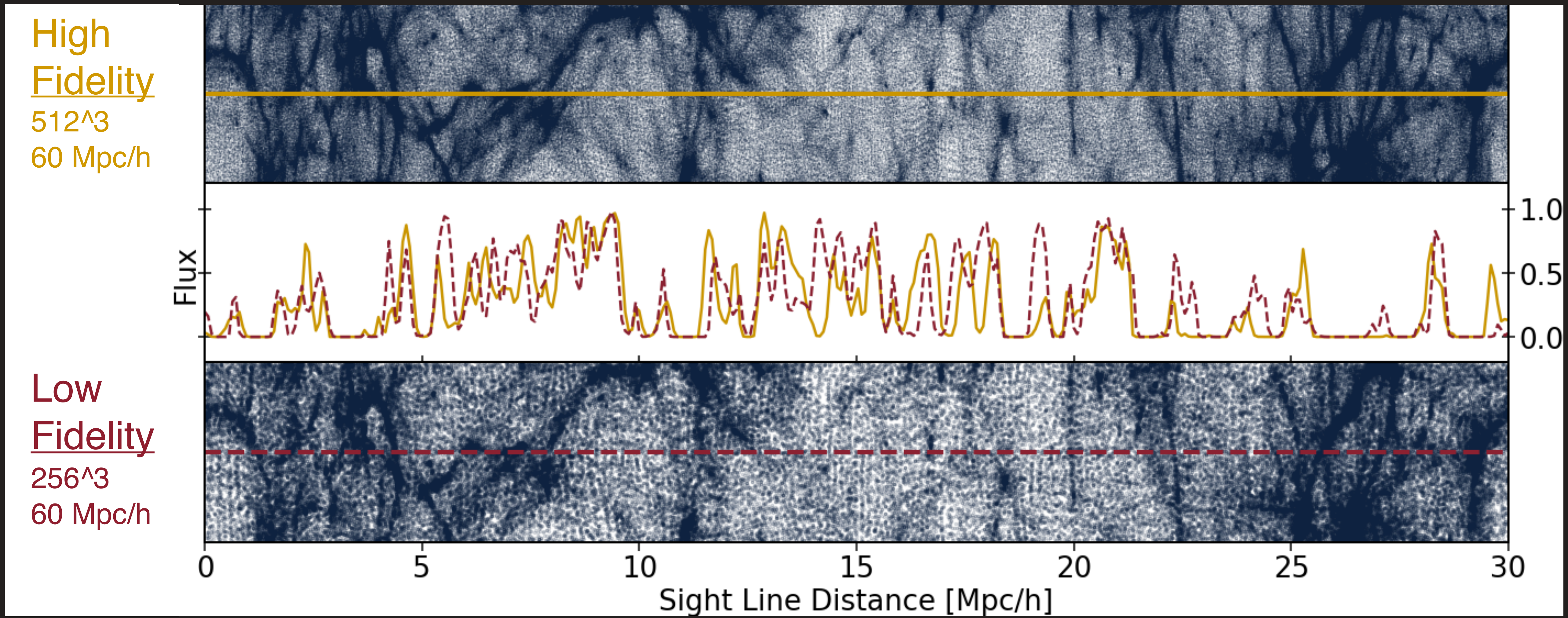
Example 2: matter power spectrum
Extending to using **boxsize** as a fidelity





- GMGP uses smaller boxsize simulations to enhance the emulation accuracy at small scales.
- GMGP outperforms AR1 and NARGP at z ≧ 1.
- It is possible to emulate HF using LF from various box sizes.

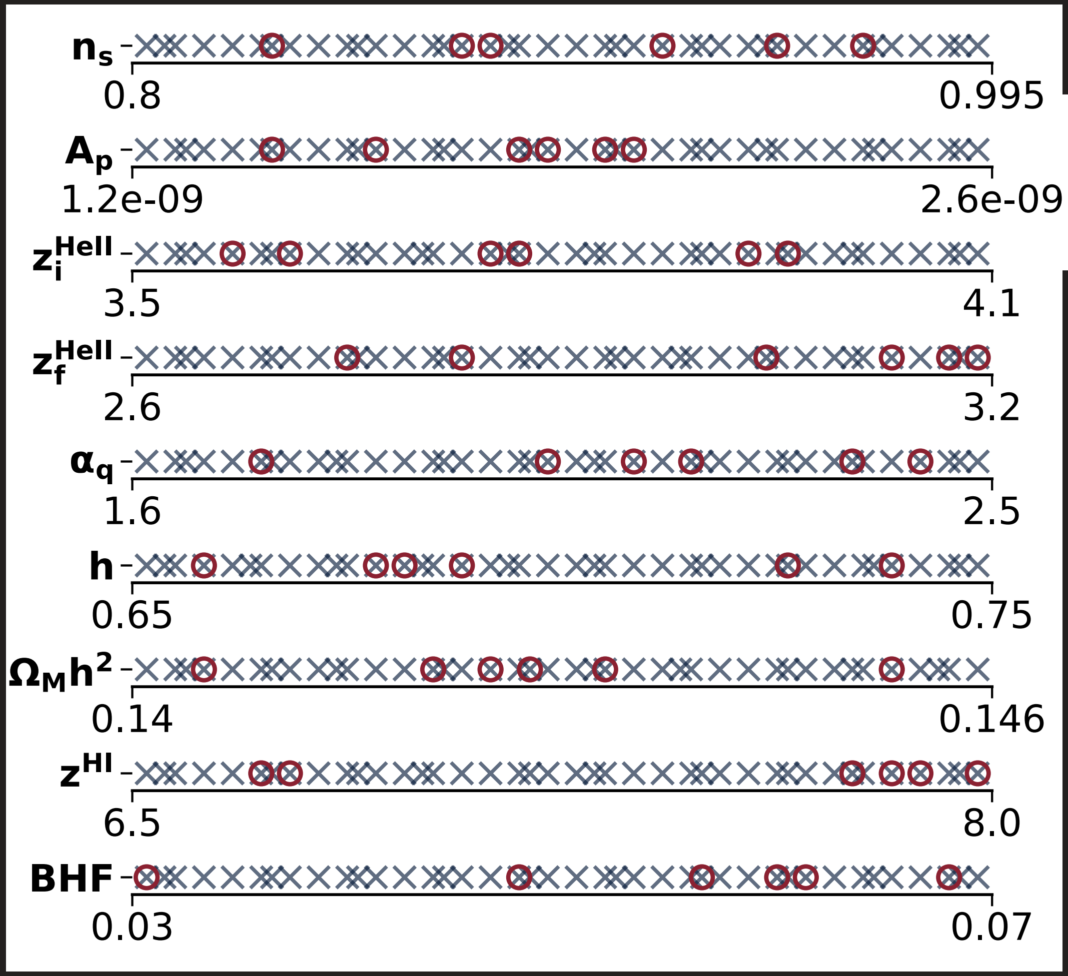
Example 3: Lya flux power spectrum
Simulated spectra generation



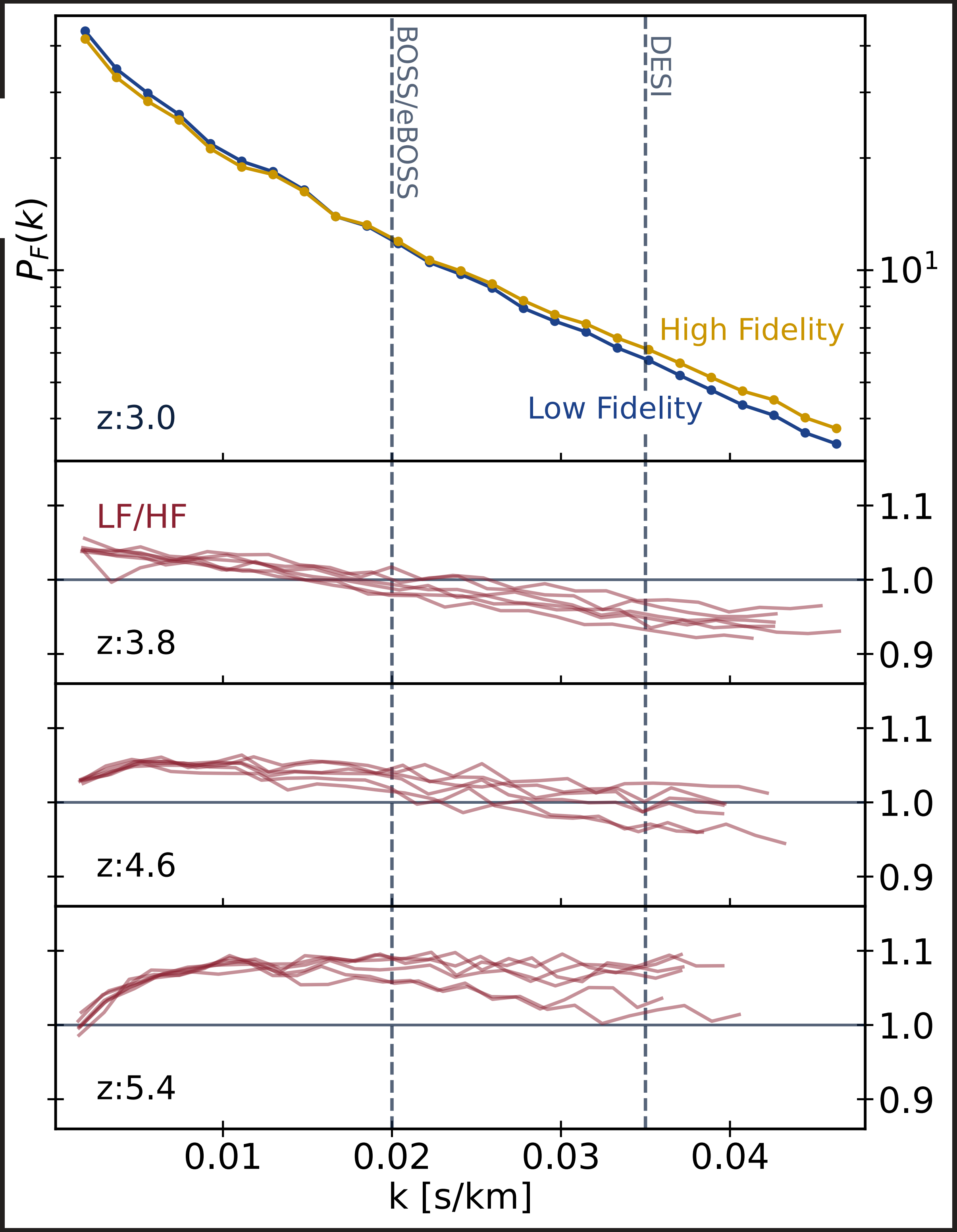
- Fake spectra: 32,000 (seeded) random skewers per snapshot using Bird (2017).
- Lya flux power spectrum: Measure correlation between neutral hydrogen within a slightline

figure credit: Martin Fernandez

Example 3: Lya flux power spectrum
Experimental design in 9 dimensions



x: LF
o: HF

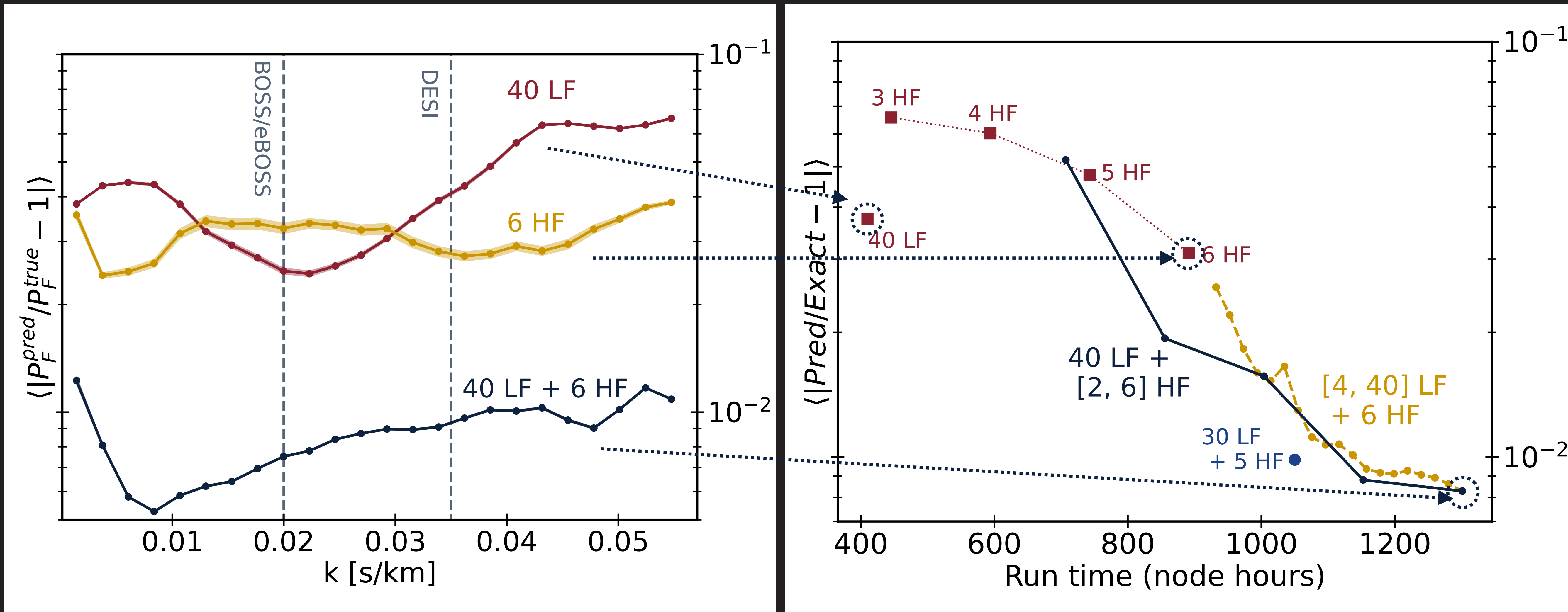


- 9 parameters (z = 2 - 5.4), including reionization parameters and black hole feedback
- The discrepancy between LF/HF appears across scales (k), varies with redshifts

figure credit: Martin Fernandez

Fernandez, Ho, Bird (2022 in prep)

Example 3: Lya flux power spectrum
Emulation errors and computational cost



- MFEmulator with 40 LF + 6 HF has ≈ 1% accuracy across all scales.
- Effectively increase the emulation accuracy by combining existing low and high-fidelity simulations.

figure credit: Martin Fernandez

Conclusion

- Save computation budget with multi-fidelity experimental designs.
- Multi-fidelity emulation can be directly applied to existing simulation suite.
- Cheaply increasing dynamic range of simulations.
- Example 1: matter power spectrum
- Example 2: matter power spectrum, emulating with different box sizes
- Example 3: Lya flux power spectrum
- Future applications: Halo mass function, cosmic shear power spectrum

arXiv:2105.01081
github.com/jibanCat/matter_multi_fidelity_emu
Papers for example 2 and 3 are expected to be submitted later this year.

We thanks Yi Ji (Duke, Stat) and Simon Mak (Duke, Stat) for kindly providing the GMGP code in Python.