Microsoft

PDE-Refiner: Achieving Accurate Long Rollouts with Neural PDE Solvers

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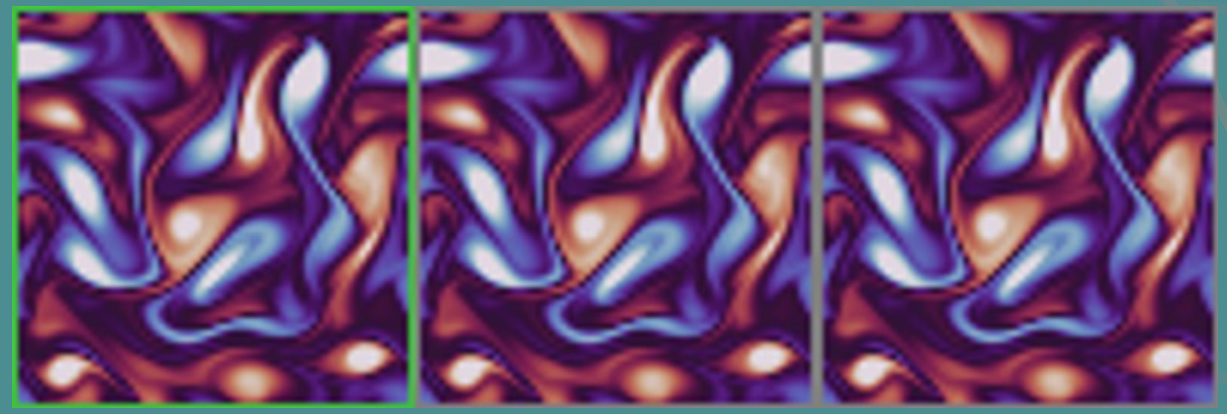
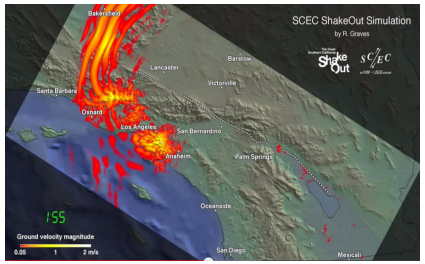
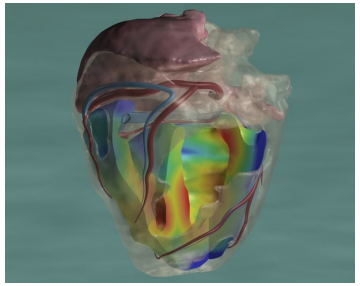


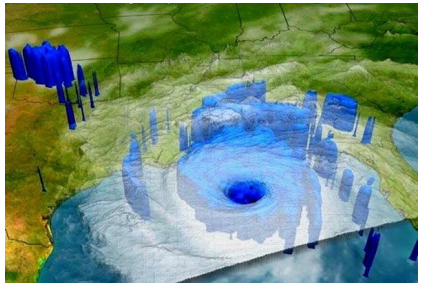
(Large-scale) PDE systems are ubiquitous



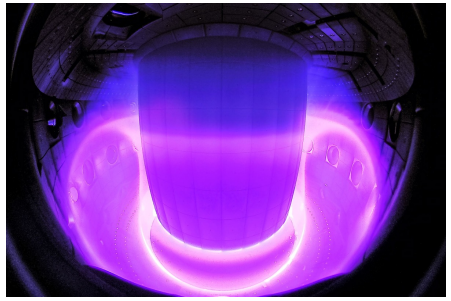
Earthquakes



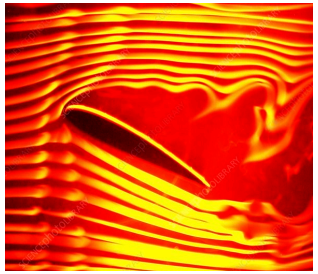
Heart dynamics



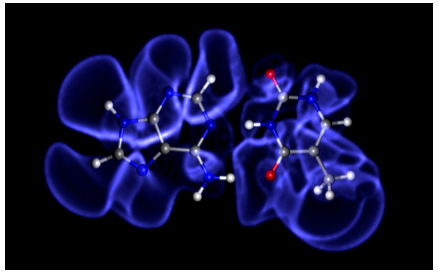
Weather prediction



Plasma physics



Airplane design

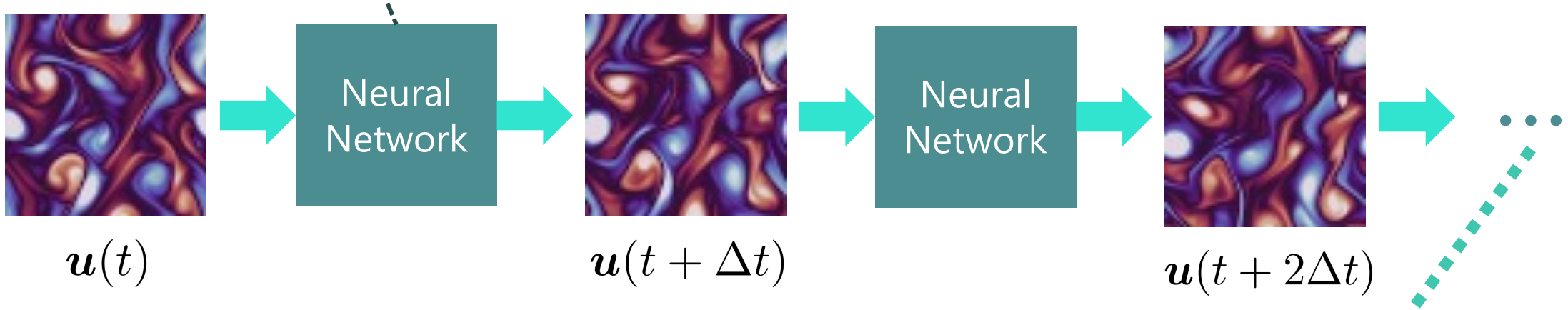


Electronic structure

Neural PDE Solvers

- Neural Operators learn to predict future solutions

$$\boldsymbol{u}(t + \Delta t) = \mathcal{G}_t(\Delta t, \boldsymbol{u}(t))$$



- Trained on one-step predictions
- Long horizon predictions via autoregressive rollout

How can Neural Operators obtain long accurate rollouts?

Case Study: Kuramoto-Sivashinsky

- Example: 1D Kuramoto-Sivashinsky equation (KS)

$$u_t + uu_x + u_{xx} + \nu u_{xxxx} = 0$$

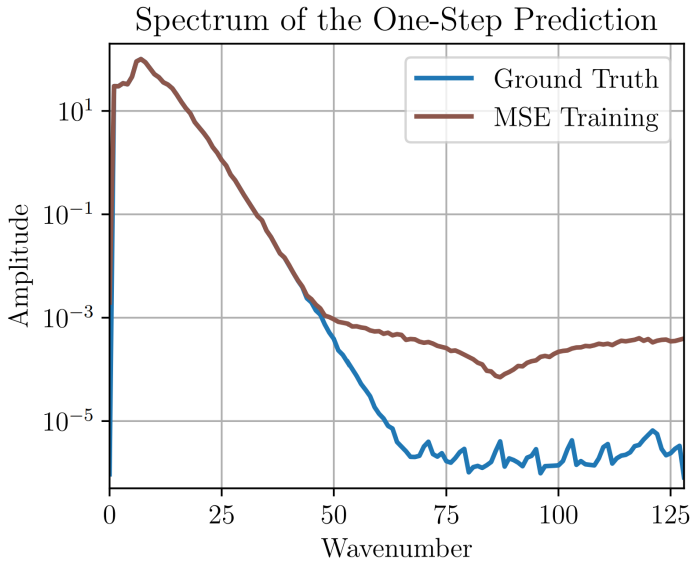
Non-linear term causes all spatial frequencies to interact long-term

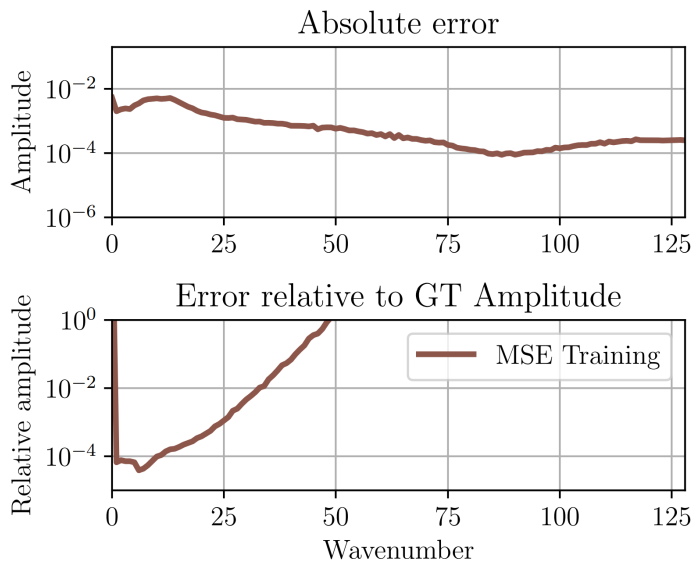
High-order derivatives increase importance of high frequencies in spatial domain

For long accurate rollouts, model **all** spatial frequencies accurately
Errors in higher frequencies have low short-term, but **high long-term impact**

Case Study: Kuramoto-Sivashinsky

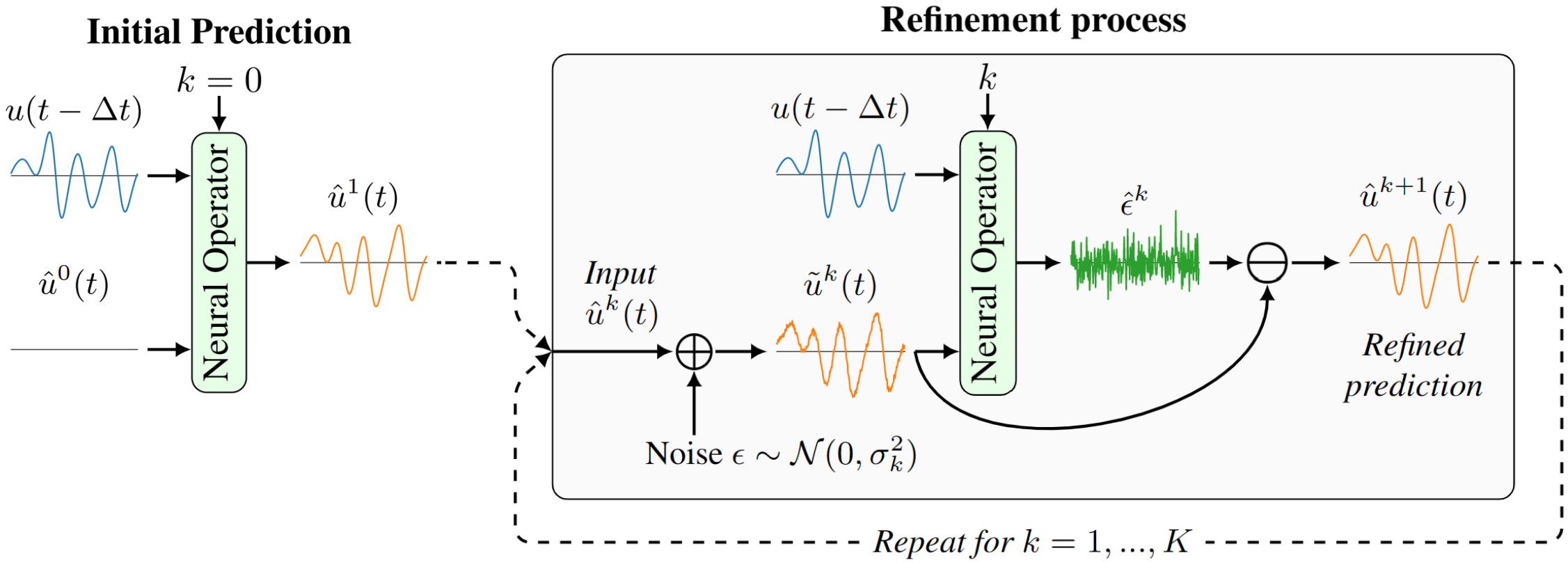
- How well do MSE-trained surrogates cover the frequency spectrum?





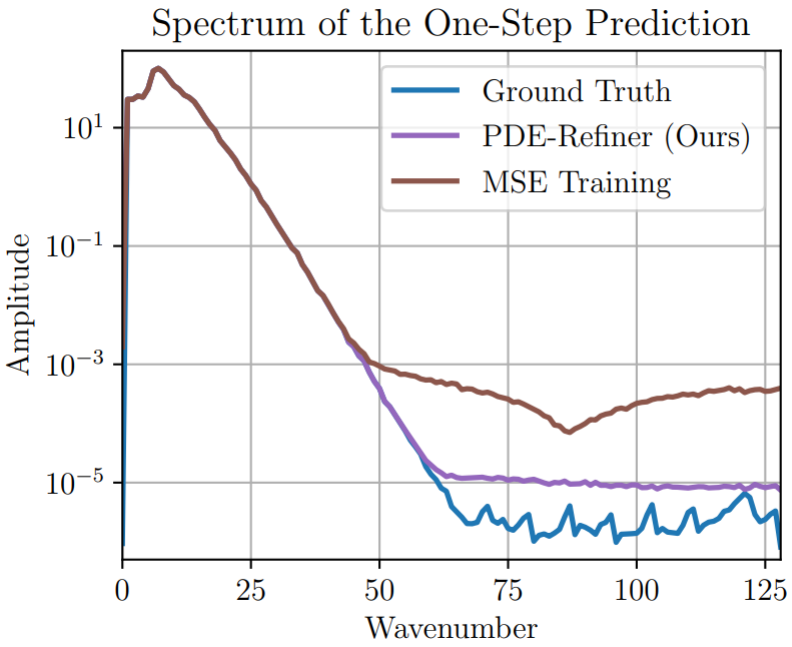
- Neural surrogates focus on **dominating** frequencies, losing high frequencies
- Inherently limits the maximum rollout time

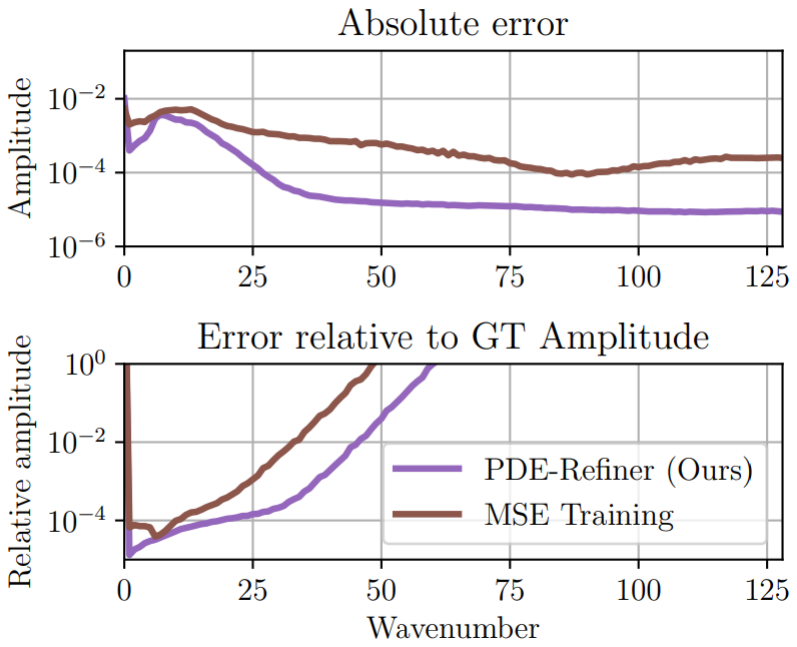
PDE-Refiner


Initial Prediction
Refinement process
$u(t-\Delta t)$
$k=0$
Neural Operator
$\hat{u}^1(t)$
$\hat{u}^0(t)$
$u(t-\Delta t)$
k
Neural Operator
$\hat{\epsilon}^k$
$\hat{u}^{k+1}(t)$
Input
$\hat{u}^k(t)$
$\tilde{u}^k(t)$
Refined prediction
Noise $\epsilon \sim \mathcal{N}(0, \sigma_k^2)$
Repeat for $k = 1, ..., K$

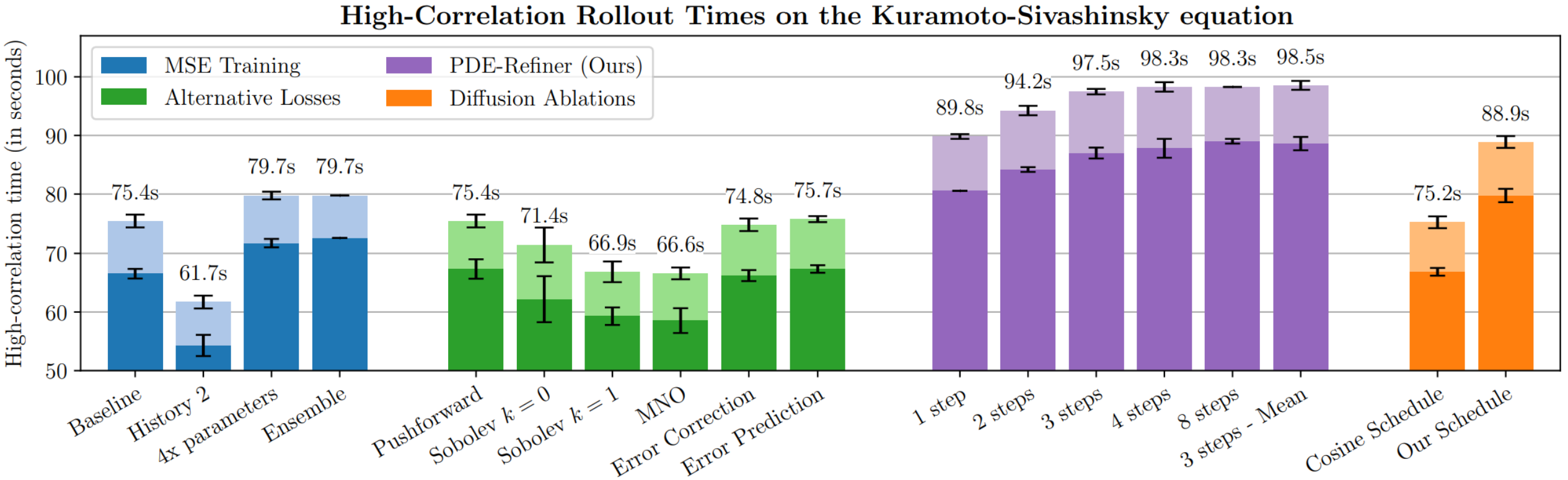
PDE-Refiner – Frequency Spectrum KS equation

- PDE-Refiner models a larger frequency band accurately



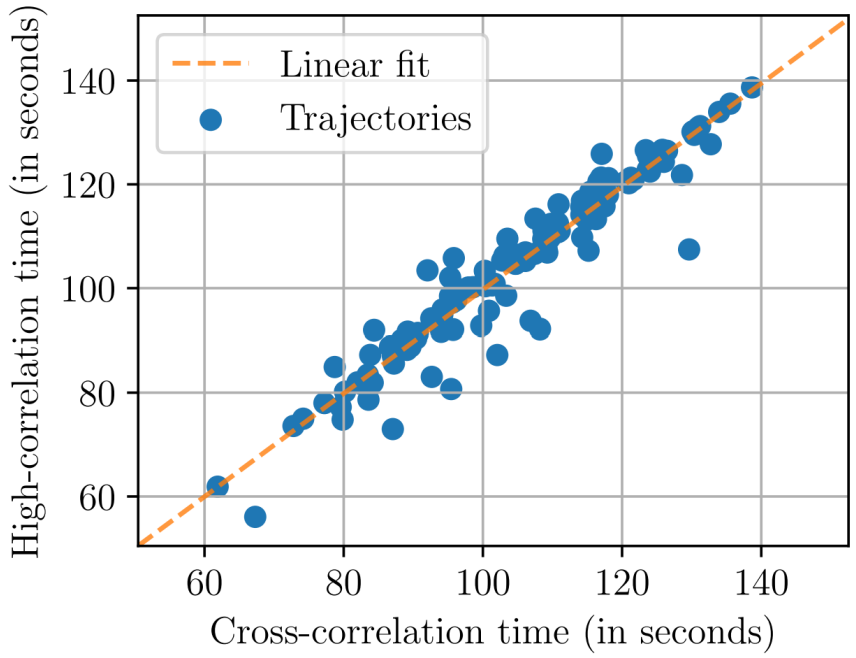


PDE-Refiner – Rollout Performance

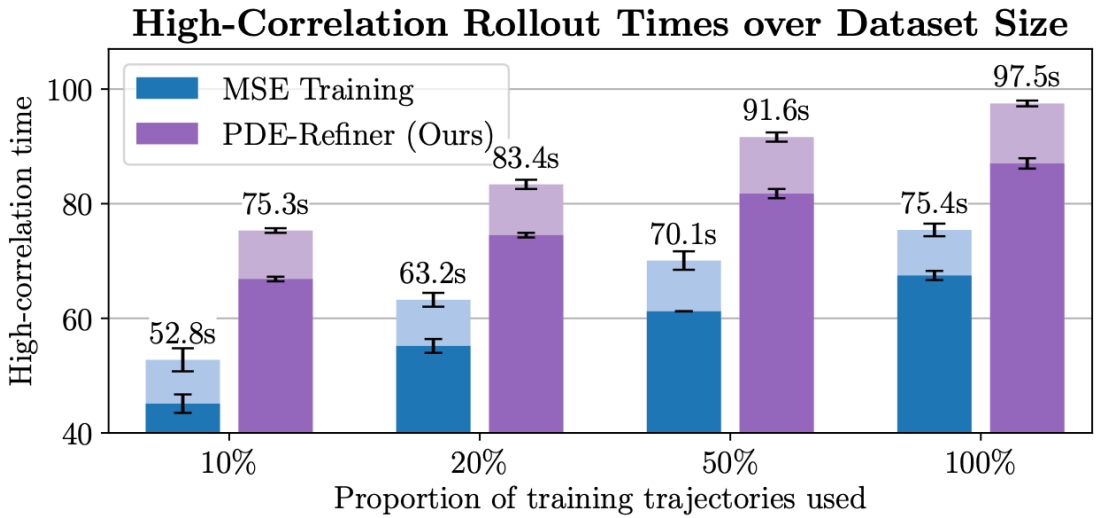


PDE-Refiner – Benefits

Accurate Uncertainty Estimates



Improved Low-Data Regime Performance



Summary

- Modeling a large spatial frequency band is key for long accurate rollouts
- PDE-Refiner achieves this by an iterative refinement process, gaining up to 30% longer rollouts
- Denoising process inherently learns accurate uncertainty estimate
- PDE-Refiner offers flexible tradeoff between accuracy and speed

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Code available

Project Website