How to obtain Accurate Long Rollouts for Neural PDE Modeling

Modeling Accurate Long Rollouts with Temporal Neural PDE Solvers

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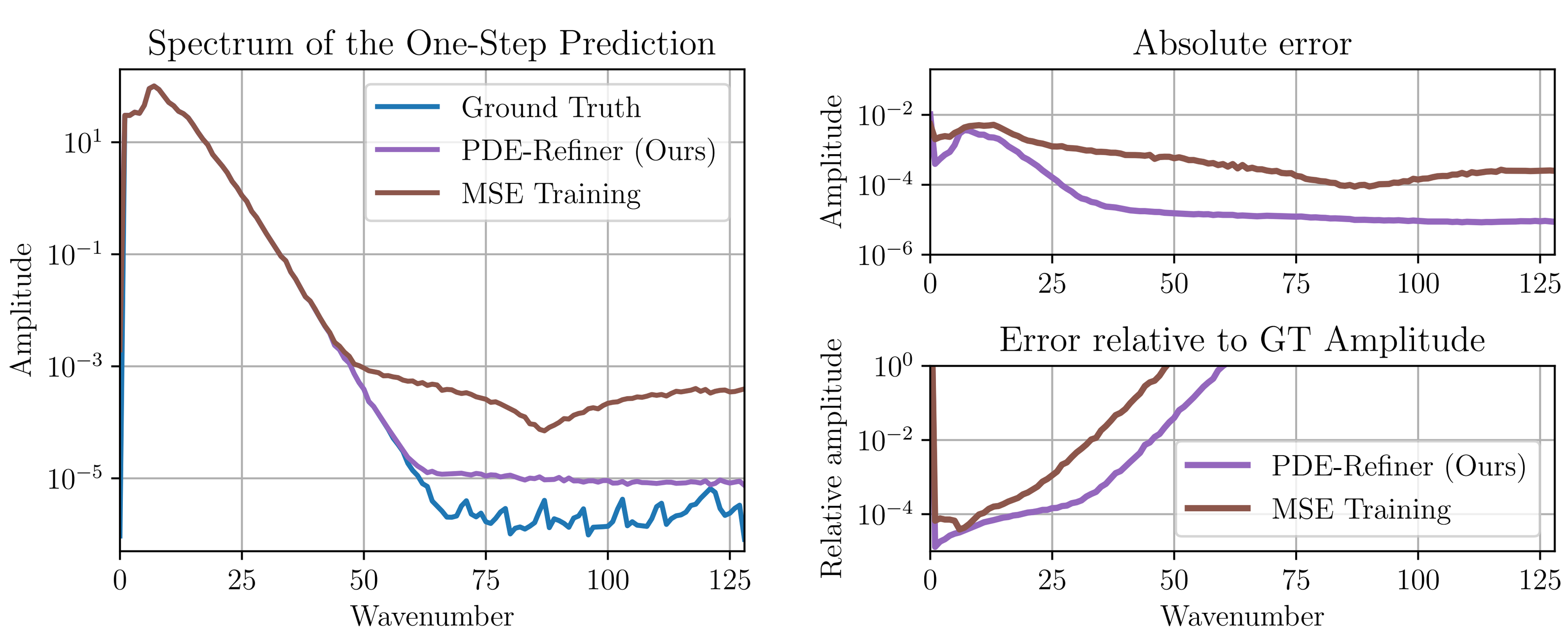
PROBLEM SETTING

- Task: use NNs to predict next time step of a PDE
- Insights on long-horizon autoregressive predictions:
  - **MSE models neglect low-amplitude spatial frequencies**
  - **Low short-term impact, but high long-term impact**

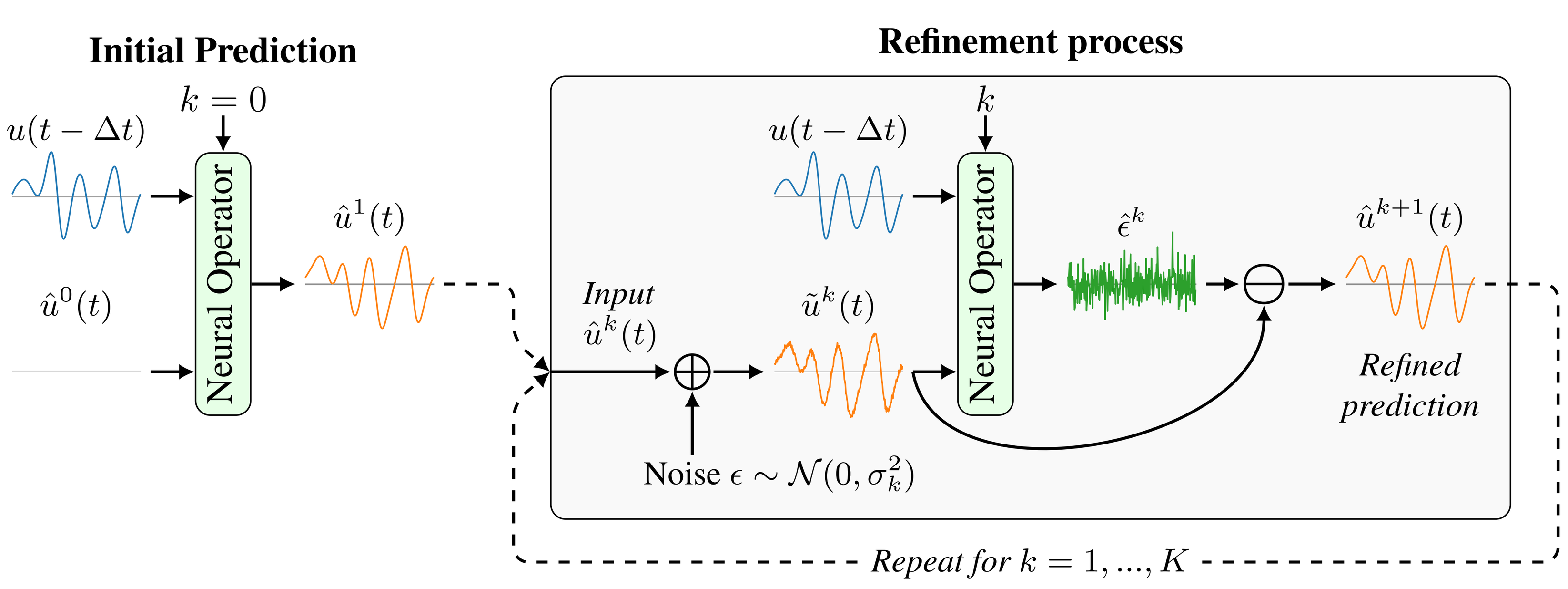
Example: Kuramoto-Sivashinsky 1D equation

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



PDE-REFINER

- Iterative refinement process to improve low amplitudes
- Denoising process with initial prediction of common MSE
- Noise removes low-amplitude info, reconstruct to refine
- Decreasing noise variance to focus on all amplitude levels

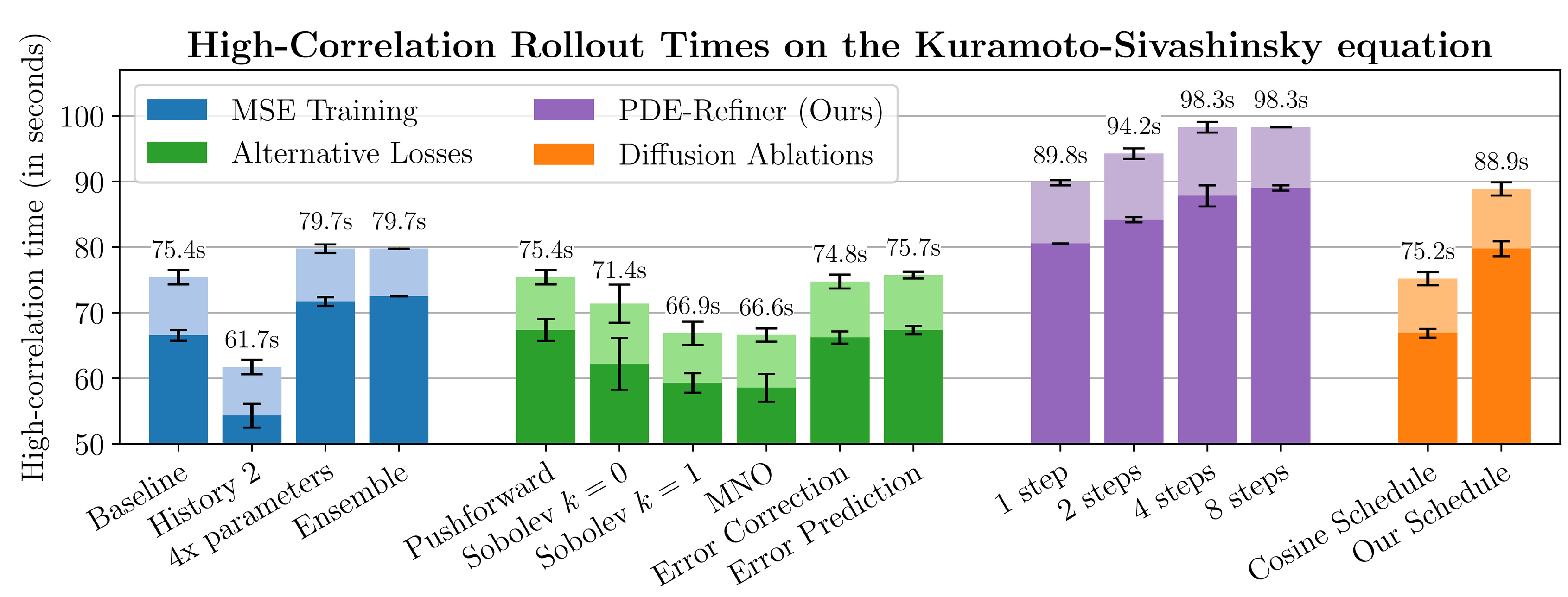


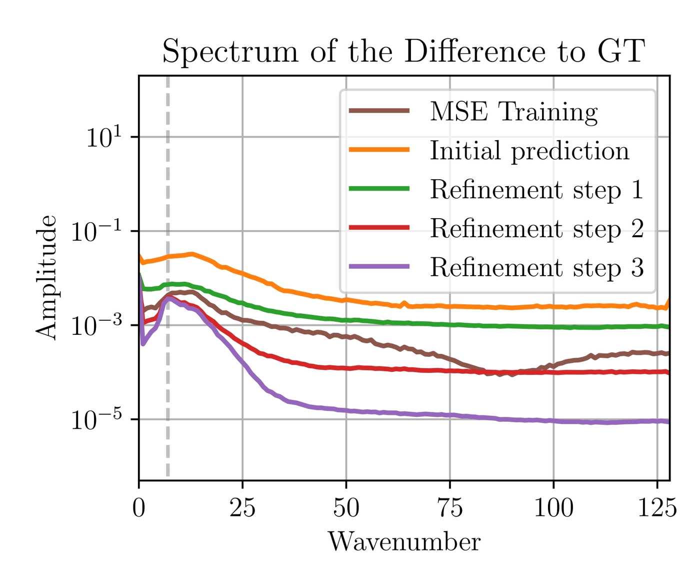
Key differences to common Diffusion models:

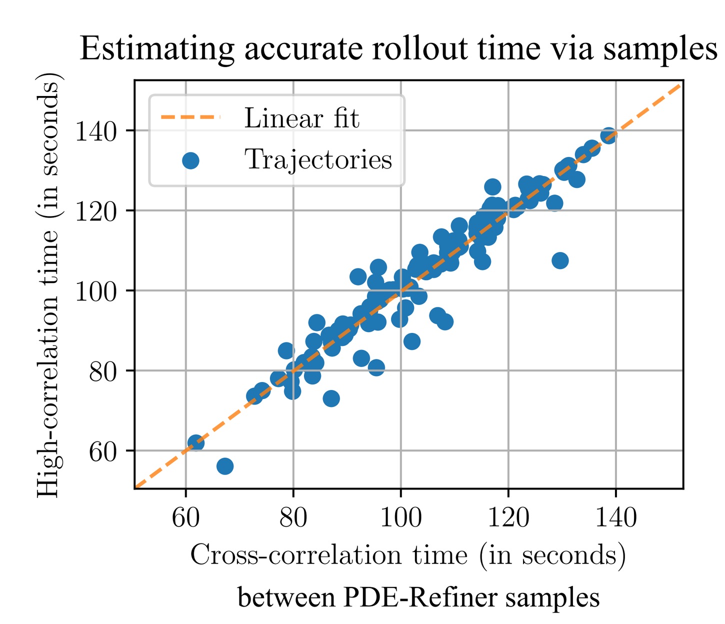
- Target is deterministic and initial prediction is the signal
- Exponential noise schedule with very few steps (1-4)

EXPERIMENTS – 1D Kuramoto-Sivashinsky Equation

- Trained on 1D KS with res 256, Δt=0.8s, U-Net operators
- PDE-Refiner significantly improves long-horizon preds
- Denoising gives accurate long-horizon uncertainty estim.

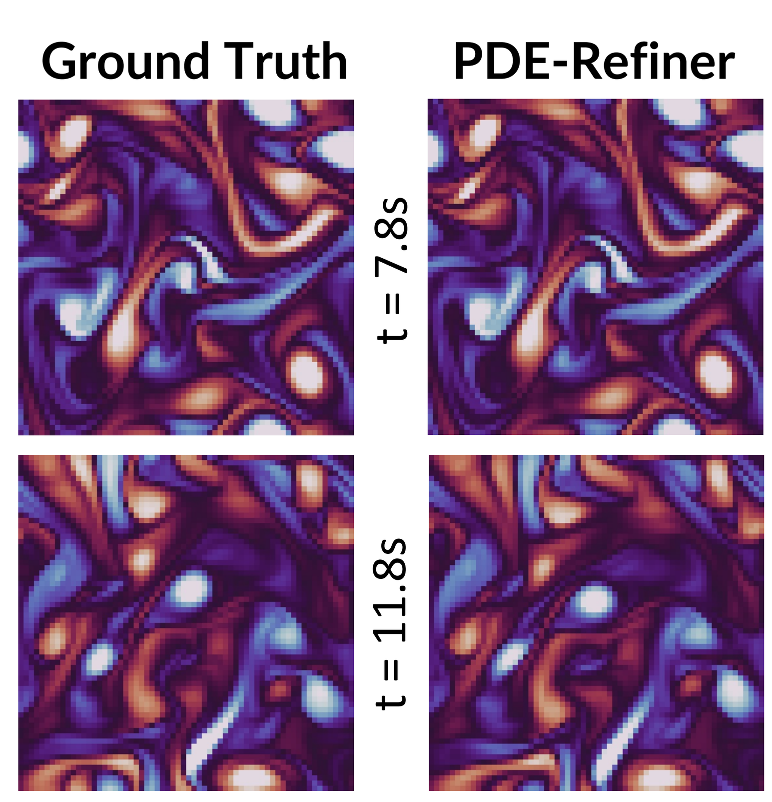






EXPERIMENTS – 2D Kolmogorov Flow

- Variant of incompressible Navier-Stokes
- GT is classical solver on 2048x2048, trained on 64x64
- PDE-Refiner outperforms neural and hybrid solvers



Method	Corr. > 0.8 time
Classical PDE Solvers	
DNS - 64 × 64	2.805
DNS - 1024 × 1024	8.752
Hybrid Methods	
LC (Kochkov et al., 2021)	7.630
LI (Kochkov et al., 2021)	7.910
TSM (Sun et al., 2023)	9.481
ML Surrogates	
MSE training - FNO	6.451 ± 0.105
MSE training - U-Net	9.663 ± 0.117
PDE-Refiner - U-Net	**10.659** ± 0.092

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Check out the full paper!