AI for PDEs

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*work performed at the University of Pennsylvania

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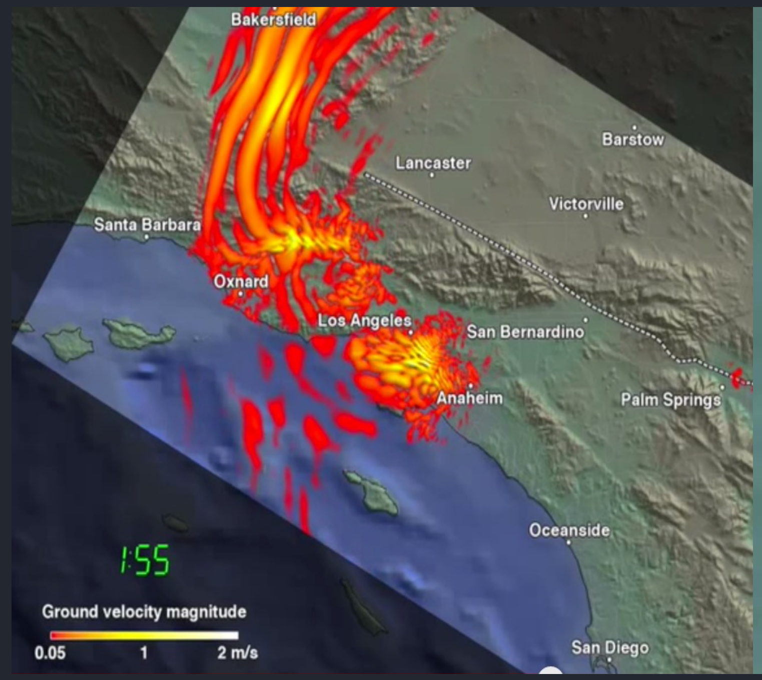
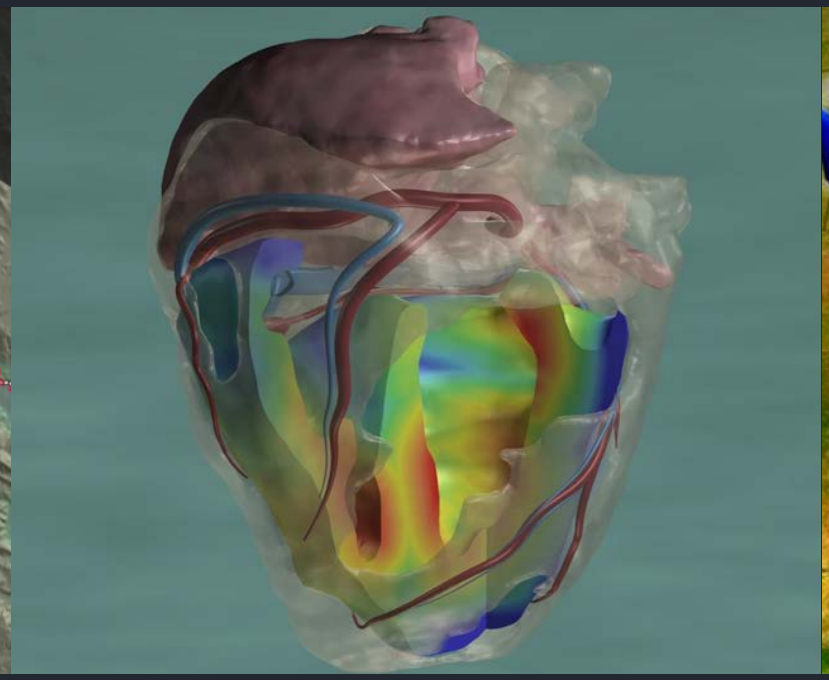
Partial Differential Equations (PDEs)

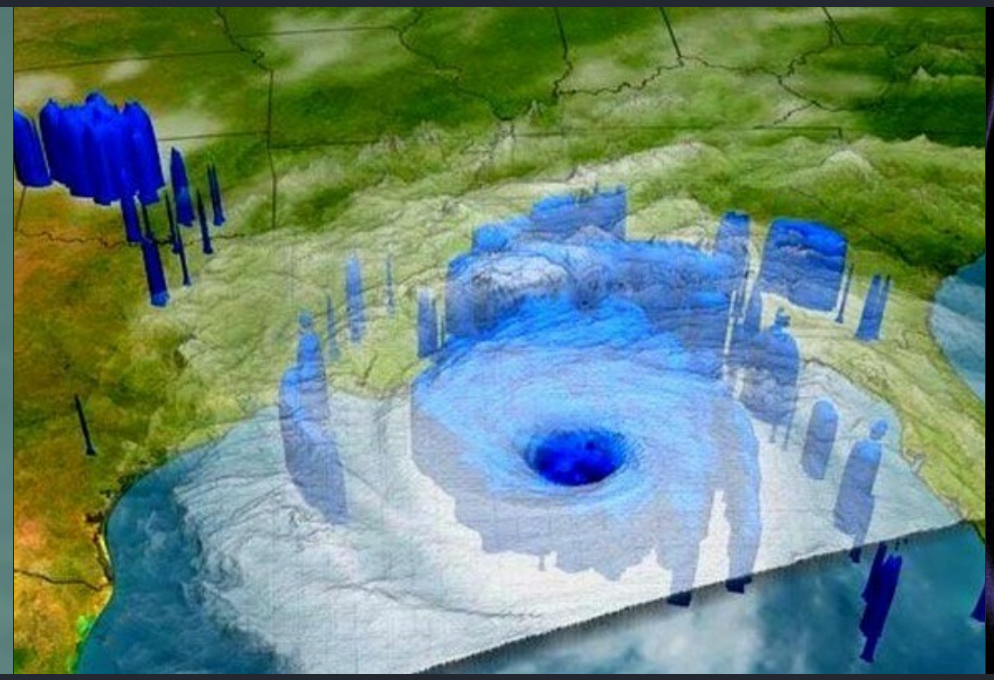
- PDEs describe the evolution of continuous fields (e.g. velocity, temperature)
- They model local, causal and continuous relationships in spatio-temporal fields



Earthquake prediction

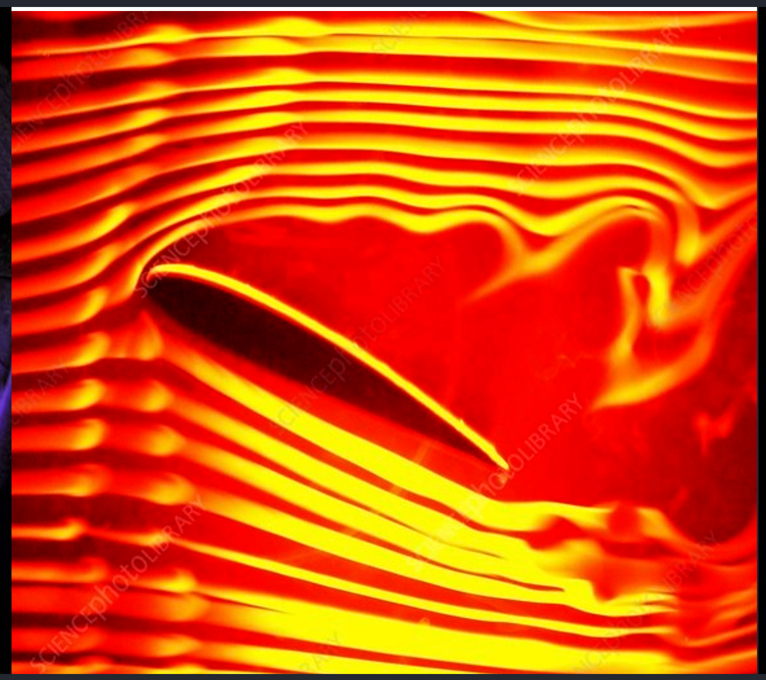


Heart modeling

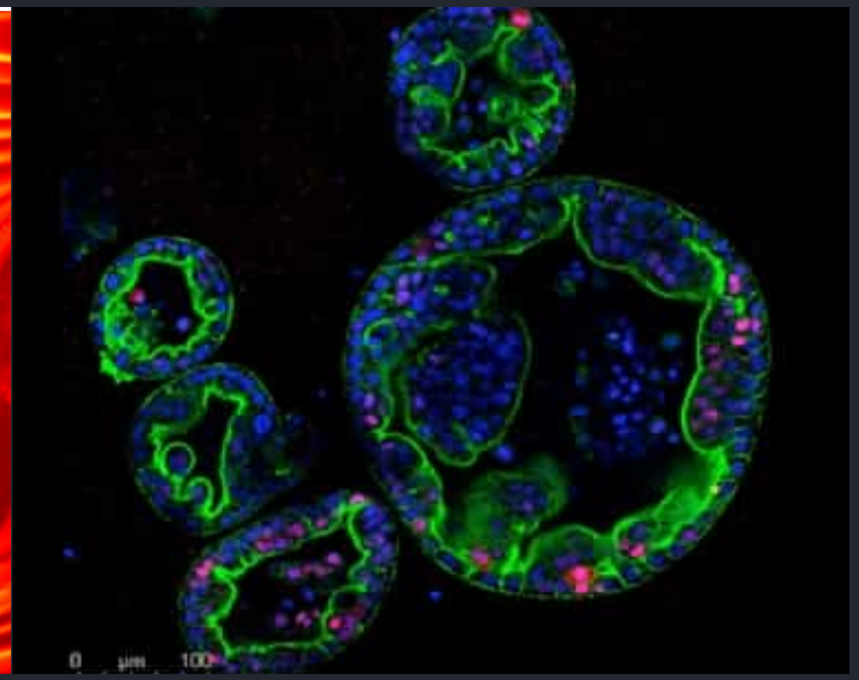


Weather prediction

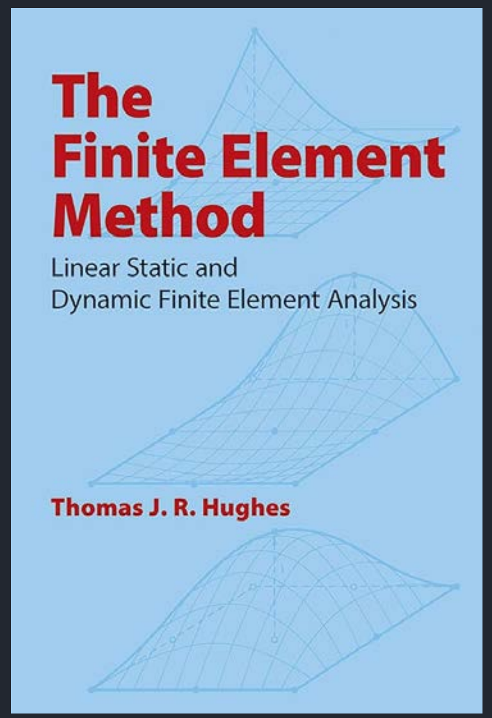
Plasma physics



Hydro/ Aerodynamic design



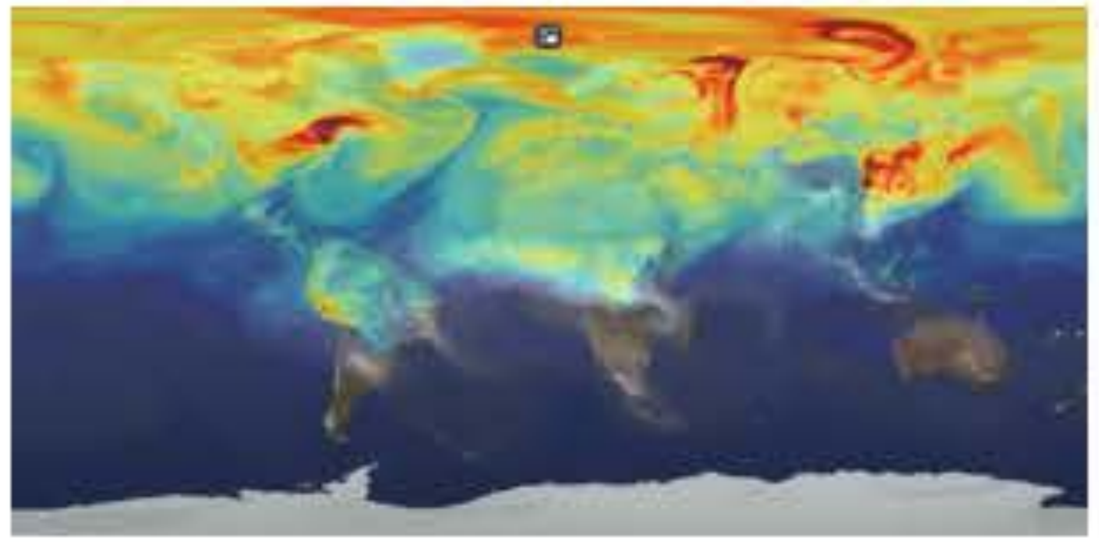
Tumor growth prediction



- Decades of software development
- Specialized solvers (~10^6 lines of C++ code)
- High simulation cost (~days on 10^4 cores)
- Solving parametrized problems is prohibitive

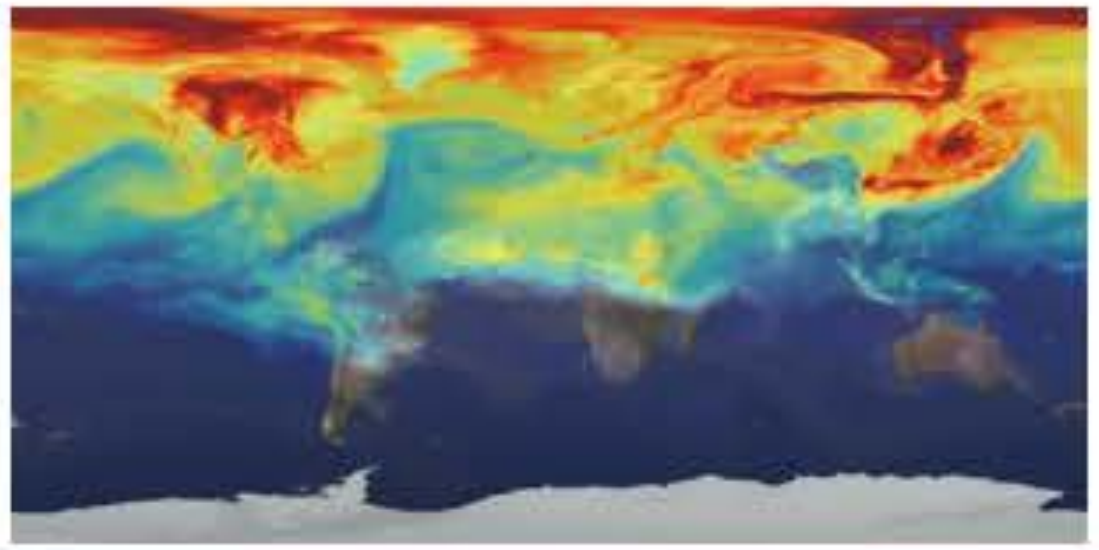
Highlights: Weather Forecasting

NWP

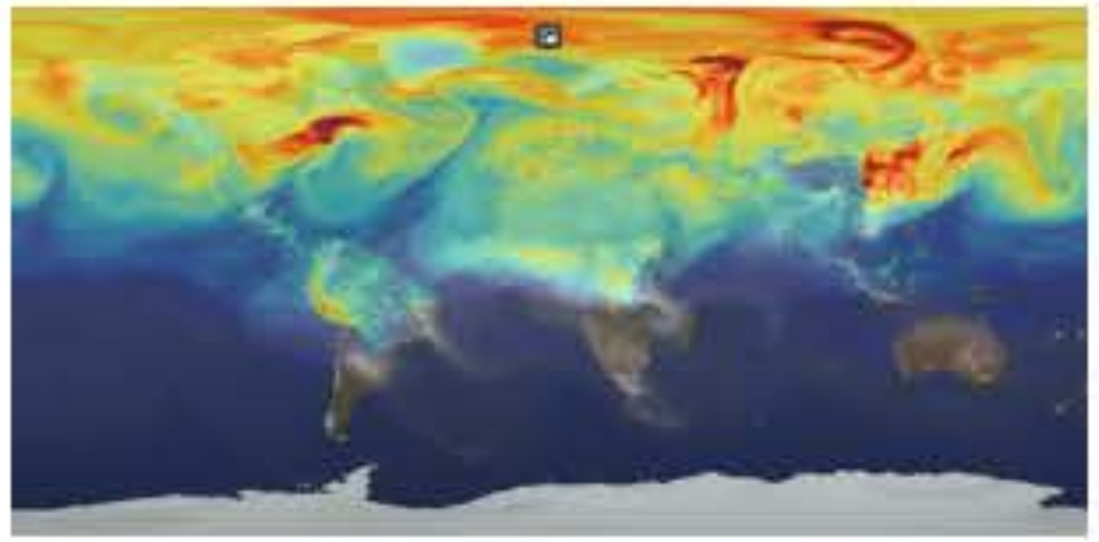


$$\overbrace{\underbrace{\frac{\partial \mathbf{u}}{\partial t}}_{\text{Variation}} + \underbrace{(\mathbf{u}\cdot\nabla)\mathbf{u}}_{\text{Divergence}}}^{\text{Inertia (per volume)}} = \overbrace{\underbrace{-\nabla w}_{\text{Internal source}} + \underbrace{\nu\nabla^2\mathbf{u}}_{\text{Diffusion}}}^{\text{Divergence of stress}} + \underbrace{\mathbf{g}}_{\text{External source}} .$$

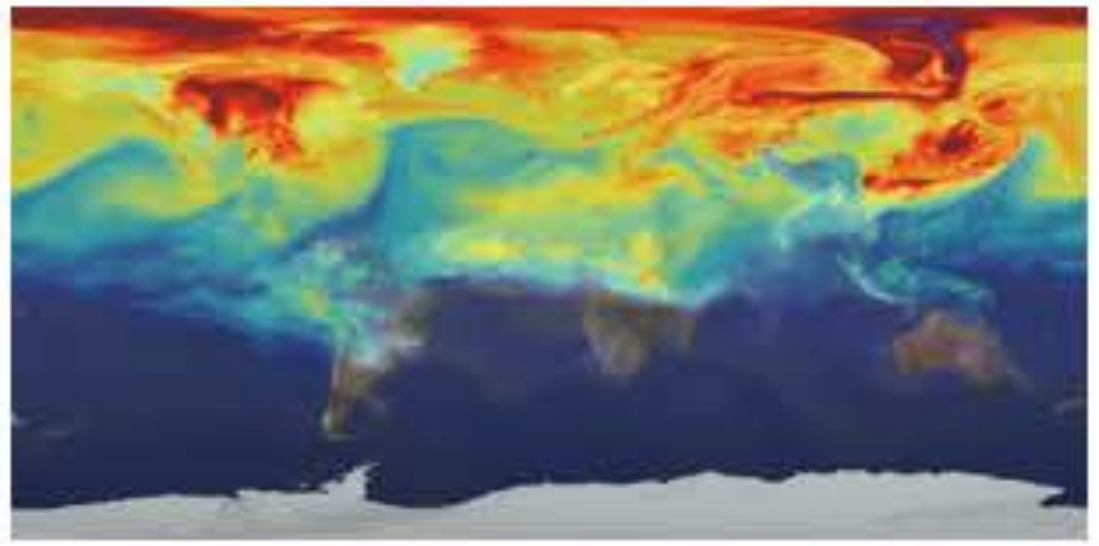
t $\longrightarrow$ t+Δt



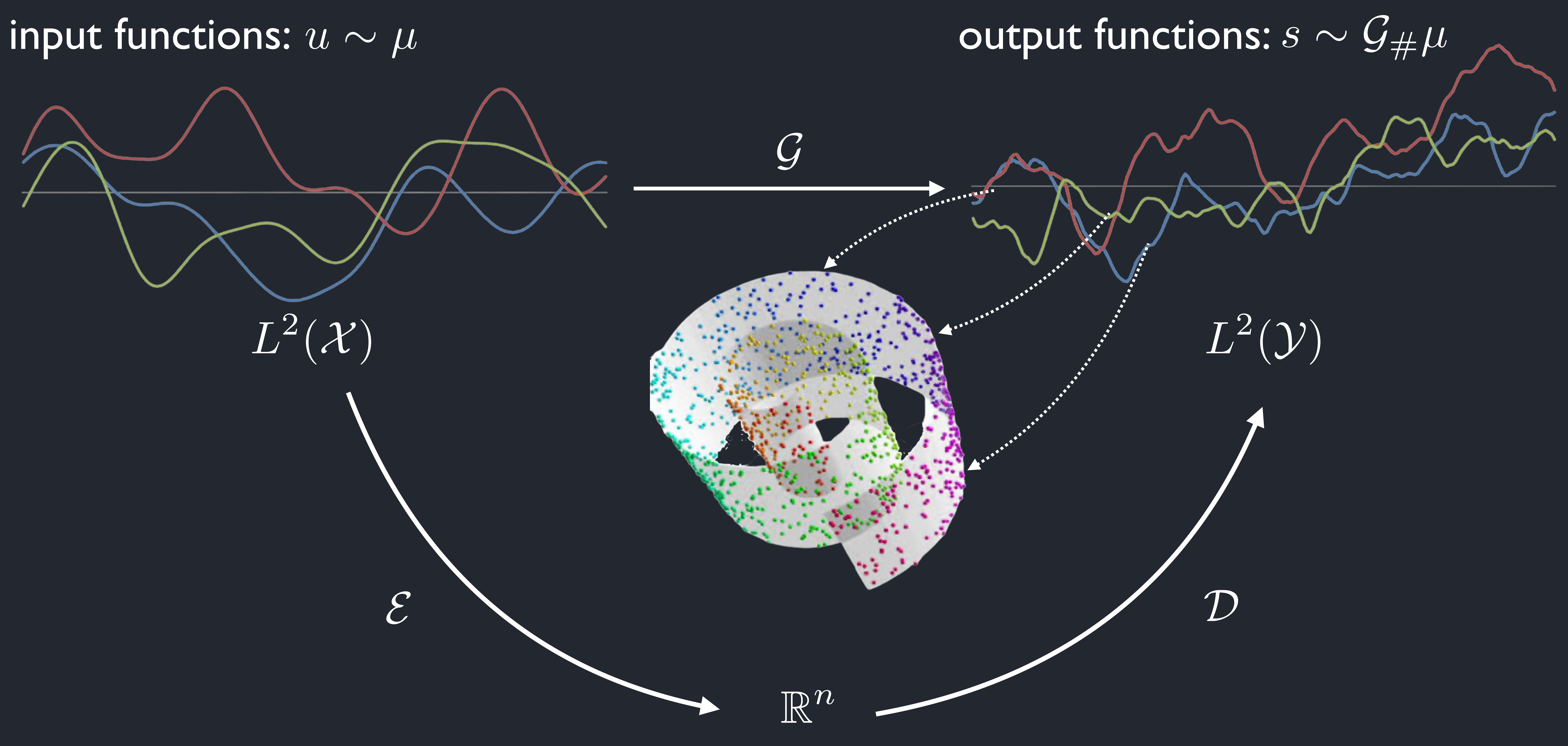
AI



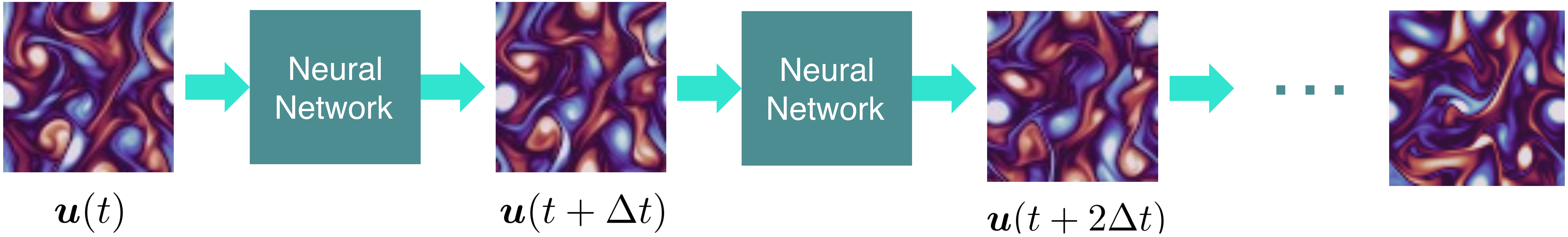
t $\longrightarrow$ t+Δt

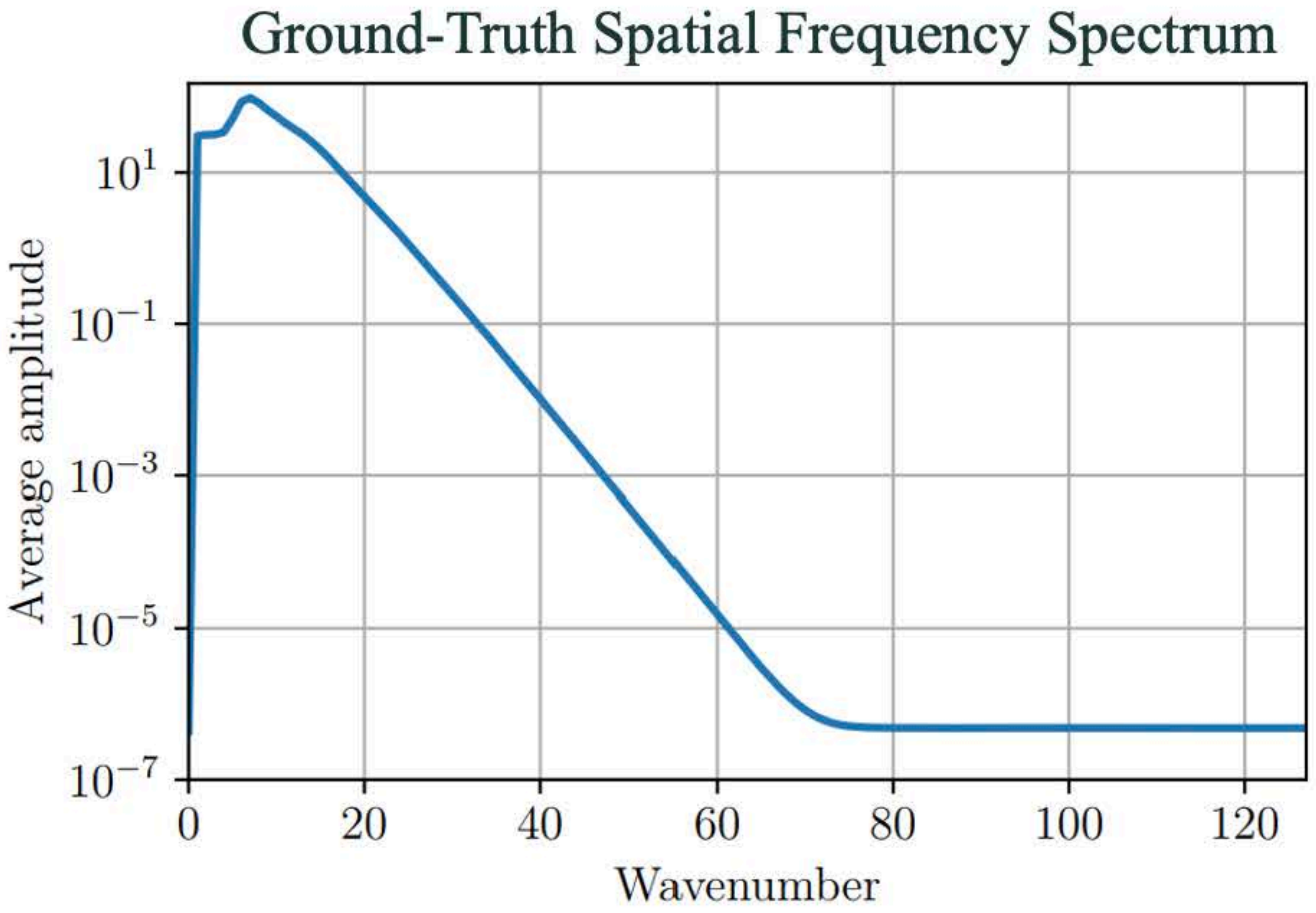


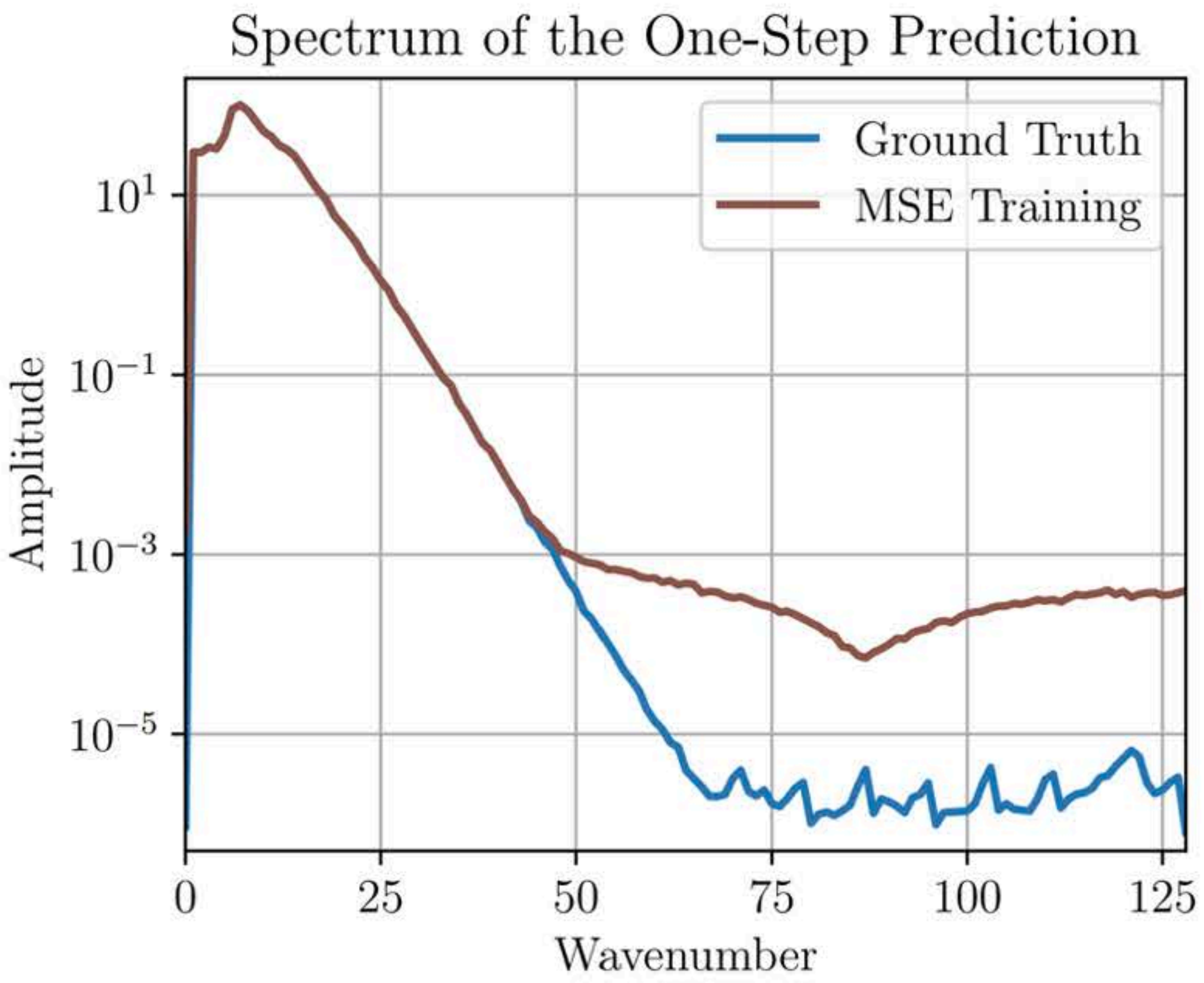
Neural Operators

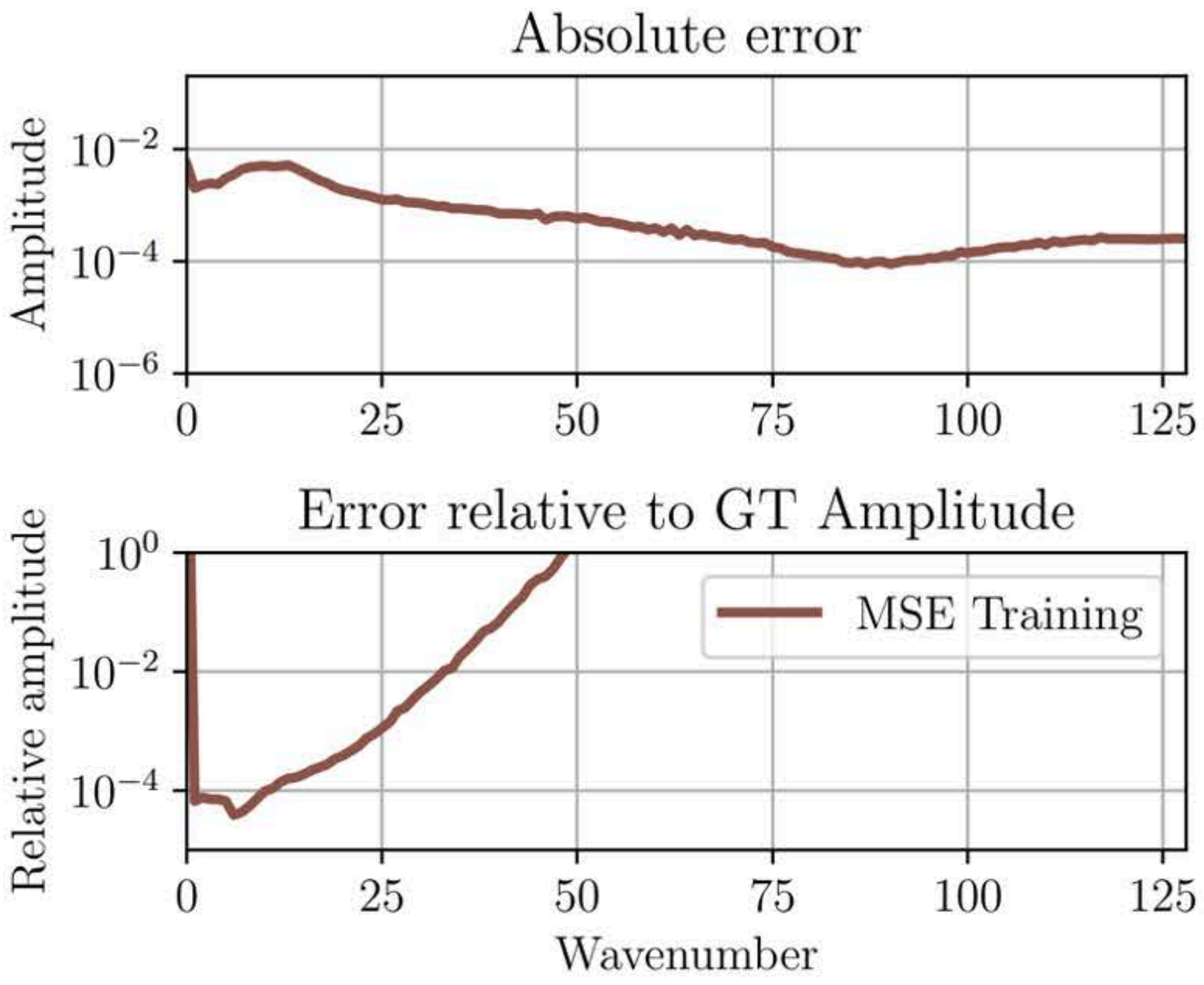


Challenges: Autoregressive Rollouts





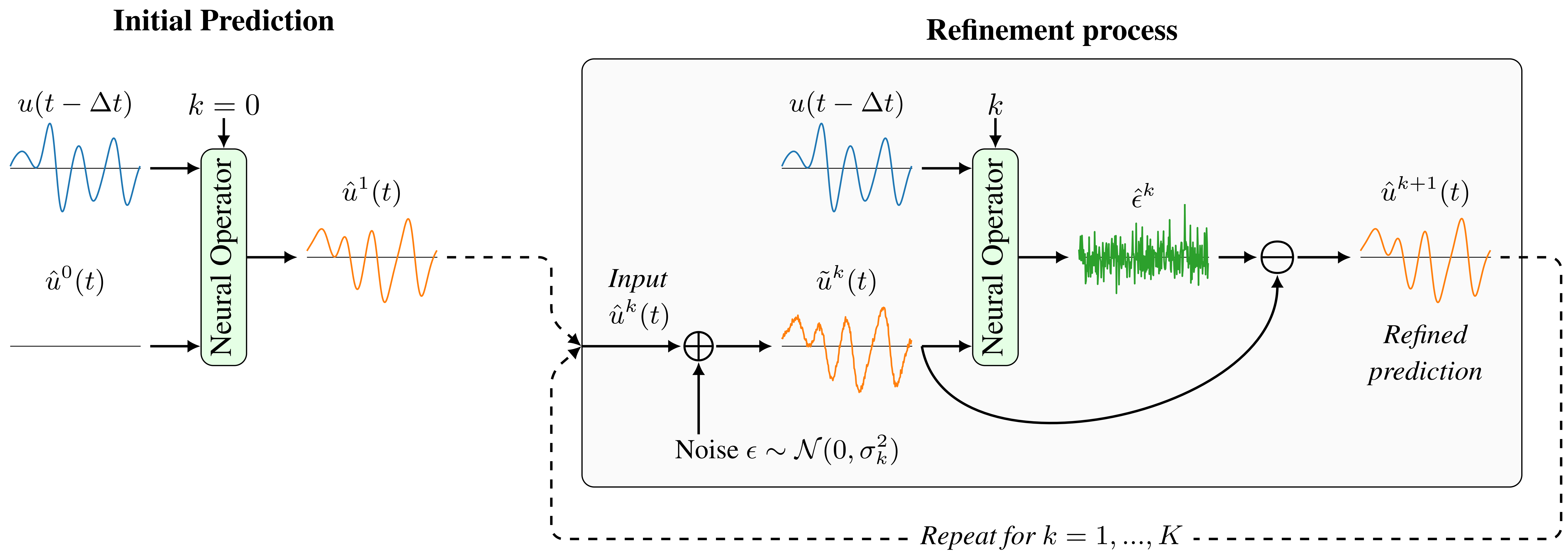


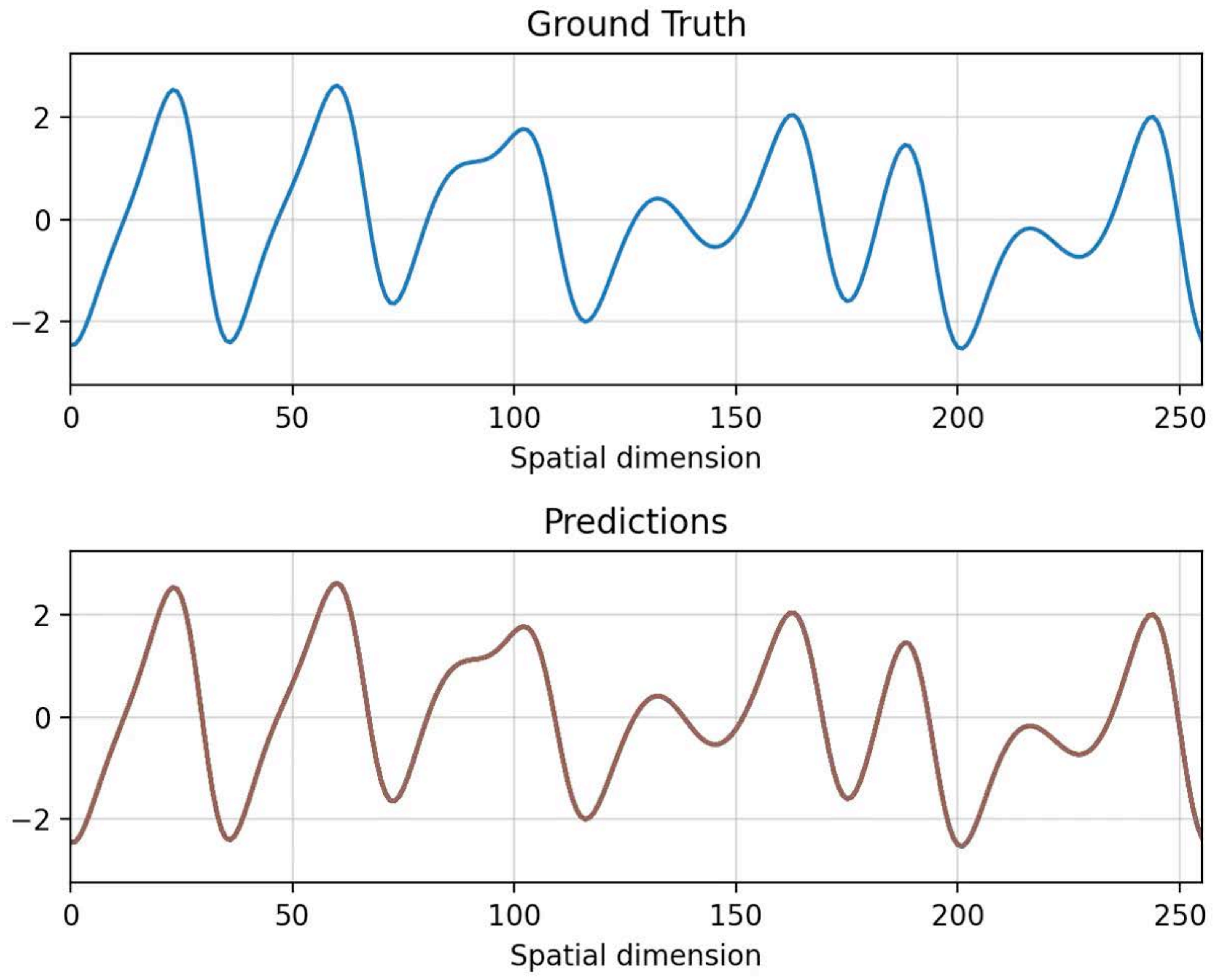


- Training on MSE fails to accurately capture low-amplitude/high-frequency modes.

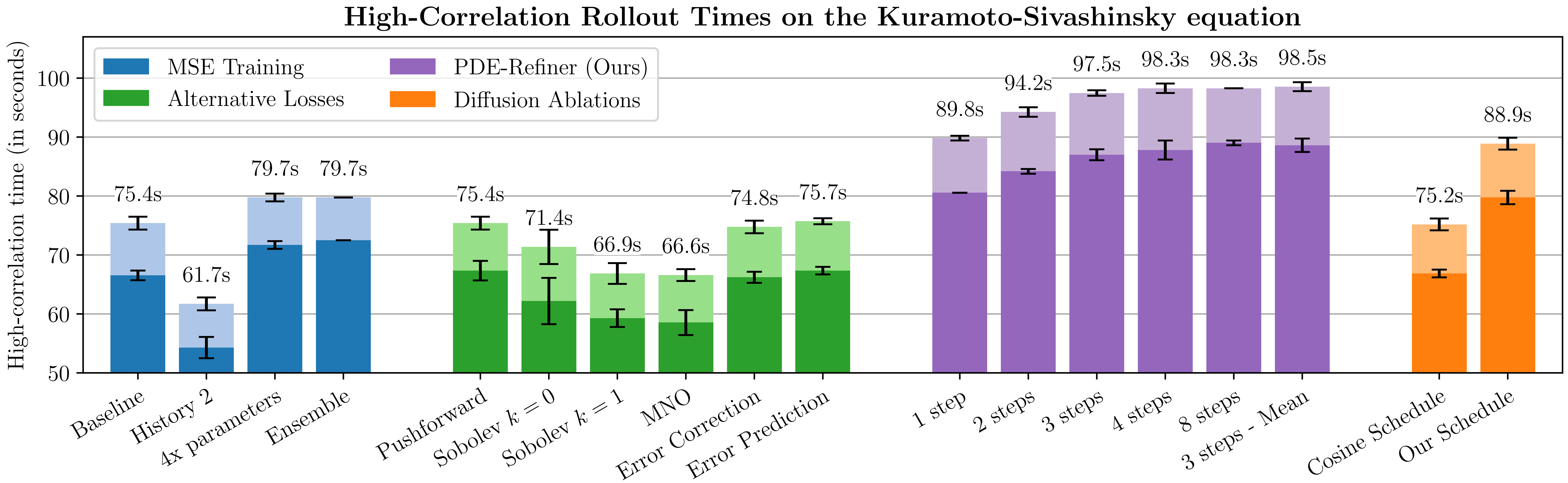
Lippe, P., Veeling, B. S., Perdikaris, P., Turner, R. E., & Brandstetter, J. (2023). Pde-refiner: Achieving accurate long rollouts with neural pde solvers.

Challenges: Autoregressive Rollouts





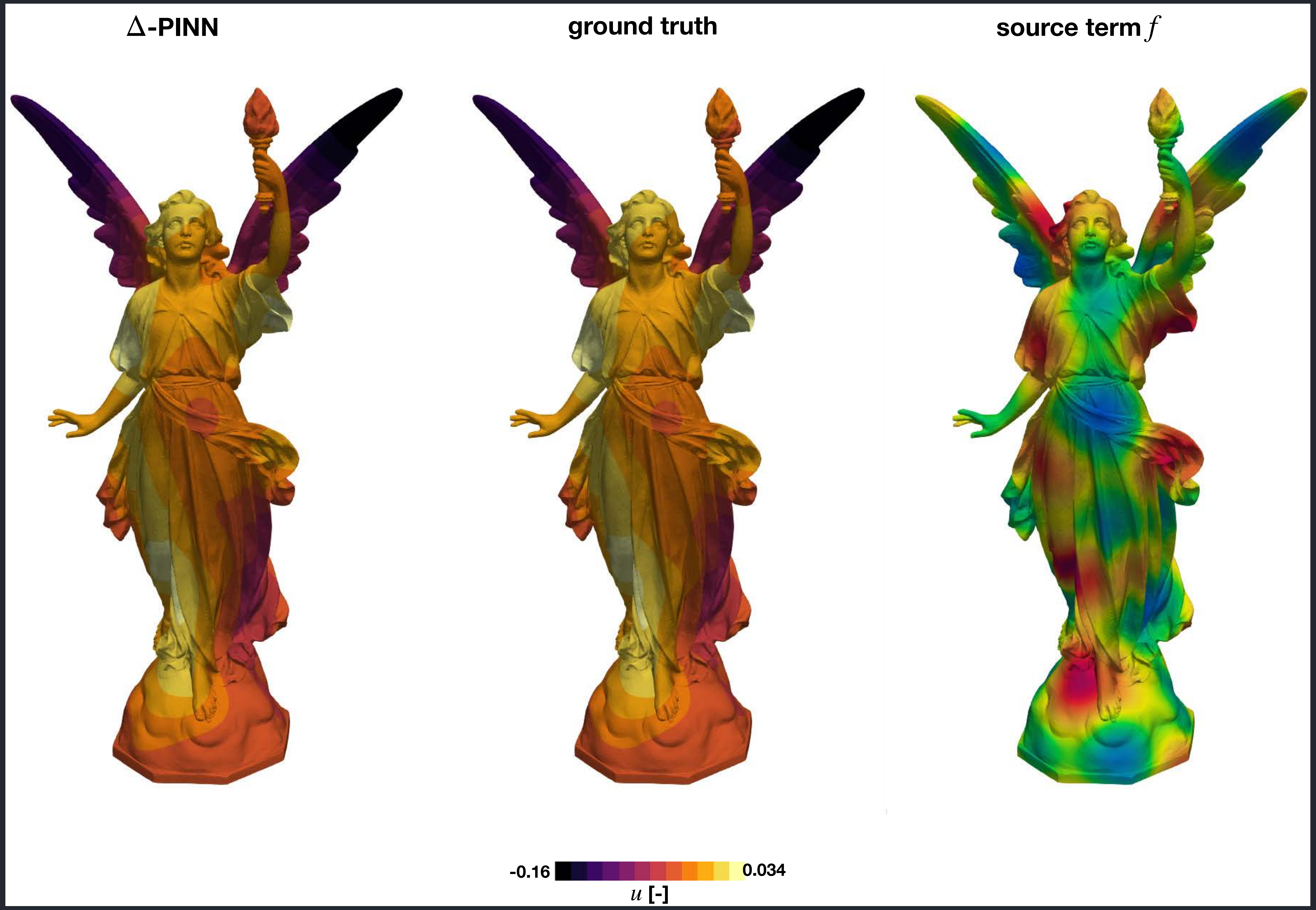
$$\mathcal{L}^k(u,t) = \mathbb{E}_{\epsilon^k \sim \mathcal{N}(0,1)} \left[\| \epsilon_k - \texttt{NO}\left(u(t) + \sigma_k \epsilon_k, u(t-\Delta t), k\right) \|_2^2 \right]$$



Challenges: PDEs on Complex Geometries

- Encode geometry via appropriate coordinate embeddings (=Laplace-Beltrami eigenfunctions)

Challenges: PDEs on Complex Geometries



Costabal, F. S., Pezzuto, S., & Perdikaris, P. (2024). Δ-PINNs: Physics-informed neural networks on complex geometries.

Challenges: Data Efficiency

- Current data-driven frameworks require $\mathcal{O}(10^3)$ labelled examples.
- This can be prohibitive for applications where the cost of data acquisition is high.

Data augmentation

- Multi-fidelity data-sets
- Lie groups & symmetry transformations

Inductive bias

- Equivariant layers
- Clifford layers
- Differentiable PDE solver layers

Soft constraints

- PDE residual penalties

Transfer learning

- Unsupervised pretraining
- Supervised fine-tuning

Thank you for your attention! Questions?