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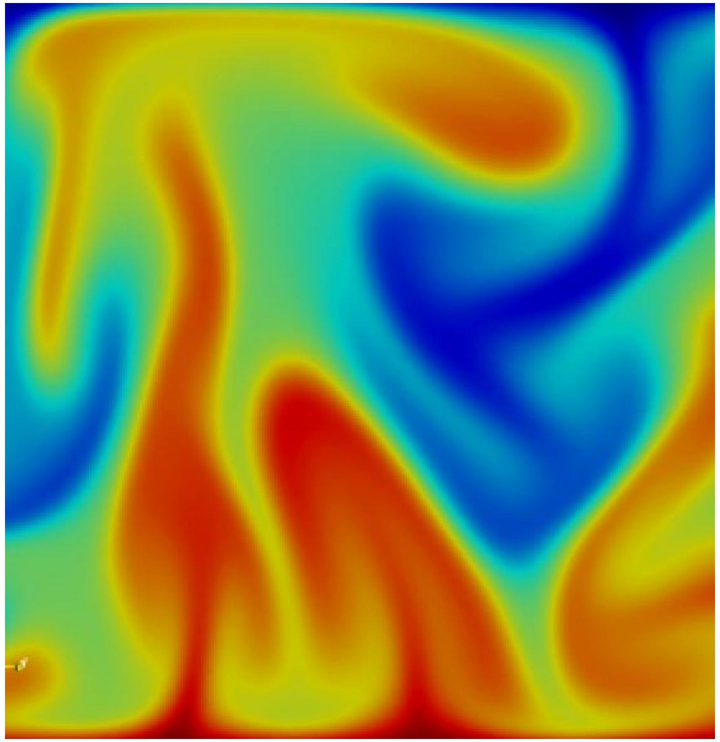
Surrogate modeling: Accelerating Scientific Discovery with Machine Learning



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Lamarr Lab Visits 2025

18.02.2025

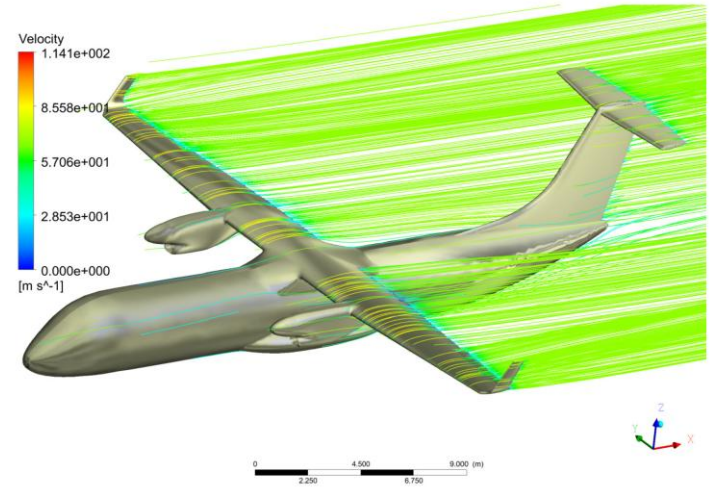
Outline of the session

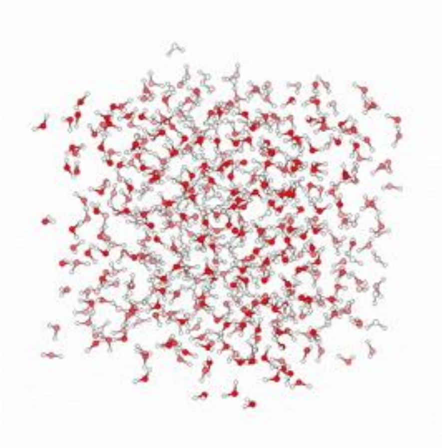
Discussing Machine Learning in physics applications and using physics to improve Machine Learning

- **Talks (14:30-15:30)**
  - Surrogate modeling using Machine Learning (Michiel Straat)
  - Physics-informed machine learning (Thorben Markmann)
  - Application of physics-informed ML in Water Distribution Networks (André Artelt)
  - Symmetry-Informed Reinforcement Learning (Sebastian Peitz)
- **Time for discussion (15:30-)**

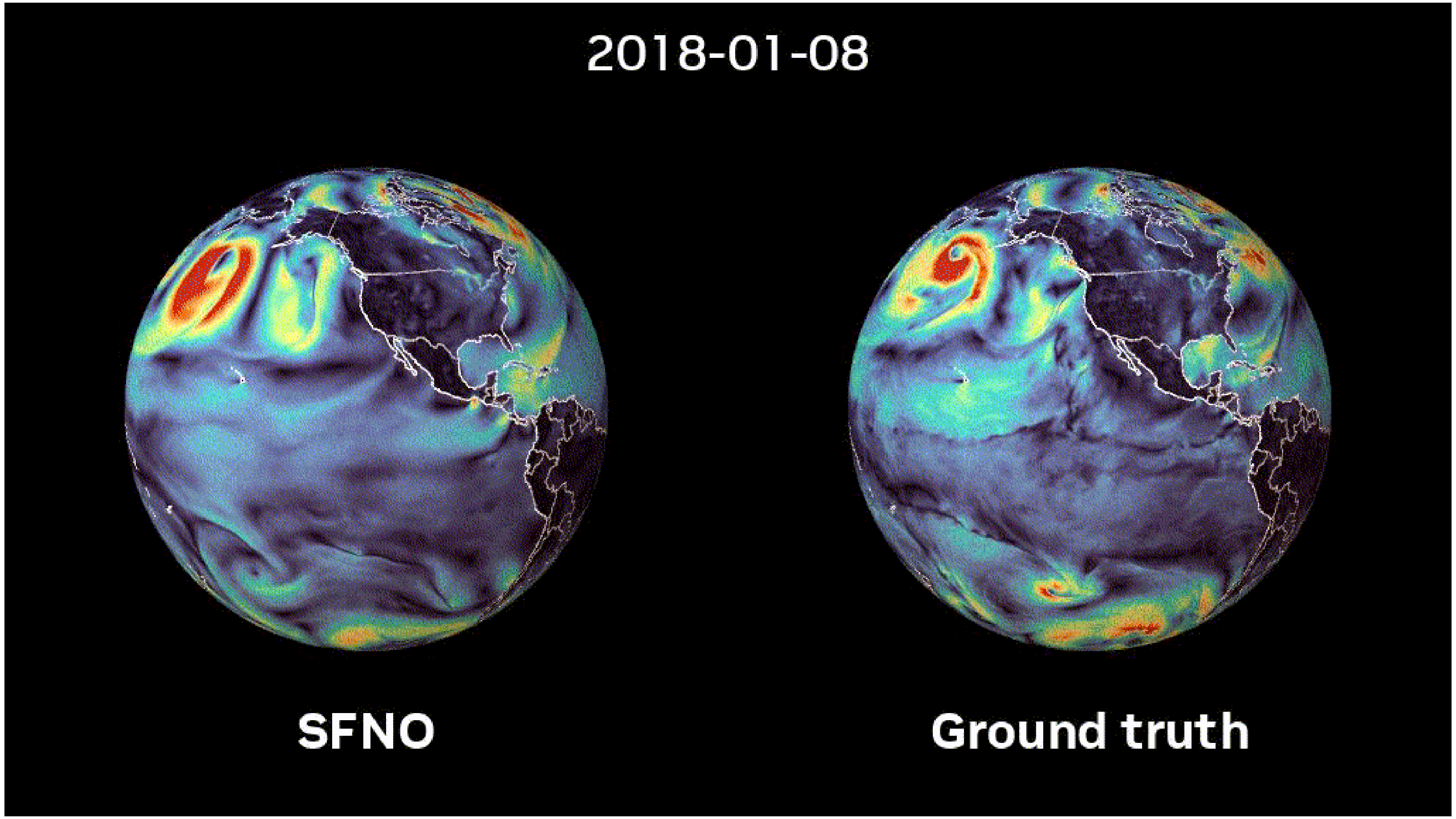
Introduction to Surrogate Modeling

- A surrogate model approximates a more complex or expensive model, and it is used to accelerate simulations, optimization, and decision-making.
- Often used when direct simulations or experiments are too costly
  - Reinforcement learning environments
  - Parameter studies and inverse problems.
- Examples and application areas:
  - Climate science: Estimating climate patterns based on computationally intensive weather simulations.
  - Engineering: Predicting the behavior of an aircraft wing under different conditions without running full CFD simulations.
  - Material science: Predicting material properties without running full molecular dynamics simulations.





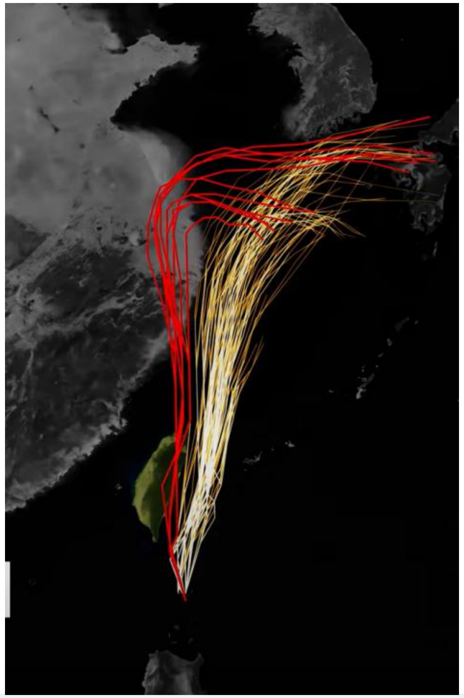
Weather prediction

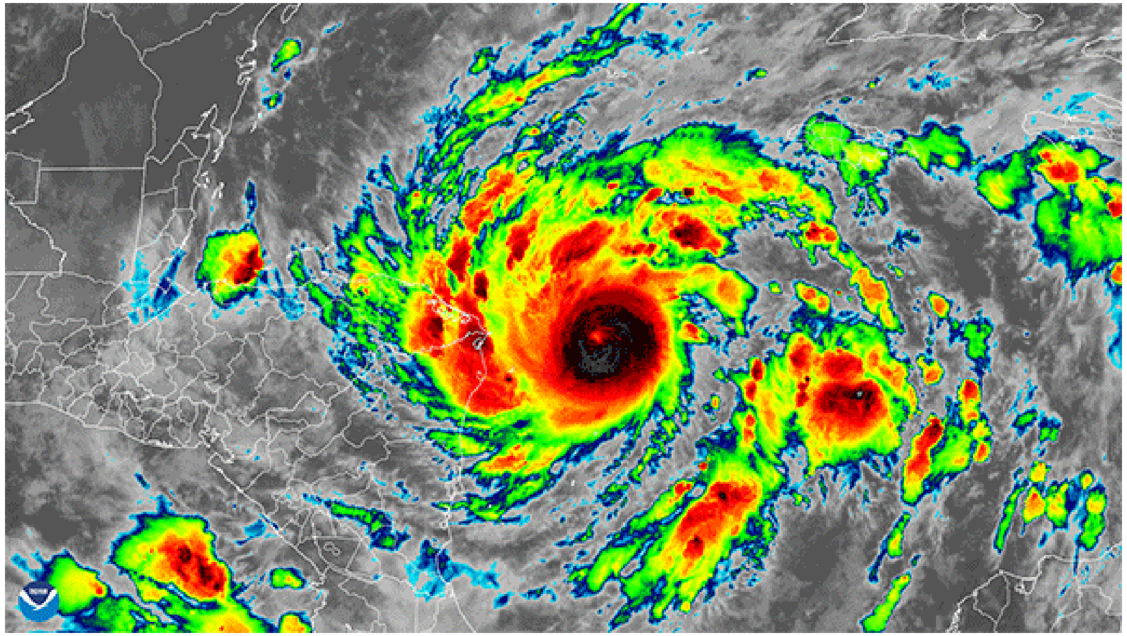


1-month-long rollout of SFNO. Surface windspeed predictions with SFNO and ground truth data are compared to each other, trained on the ERA5 dataset.
1 year rollout (1460 steps), takes about 13 minutes

Ensemble Weather Forecast

- simulations with many slightly different initial conditions and model details (*parameter studies*)
  - Gives possible developments (e.g. different tracks of a storm) and uncertainty quantification.





https://developer.nvidia.com/blog/ai-accurately-forecasts-extreme-weather-up-to-23-days-ahead/

Application area: Inverse problems

- Determine unknown inputs from observed outputs.
- Examples are in engineering: airfoil optimization, ocean current prediction from sparse temperature measurements.
- Surrogates help in solving the problem by:
  - Rapid forward evaluations: $y = f(\theta) \approx s(\theta)$
  - Approximating the inverse mapping directly: $\theta = f^{-1}(y) \approx s(\theta)$
  - (Combine both approaches).

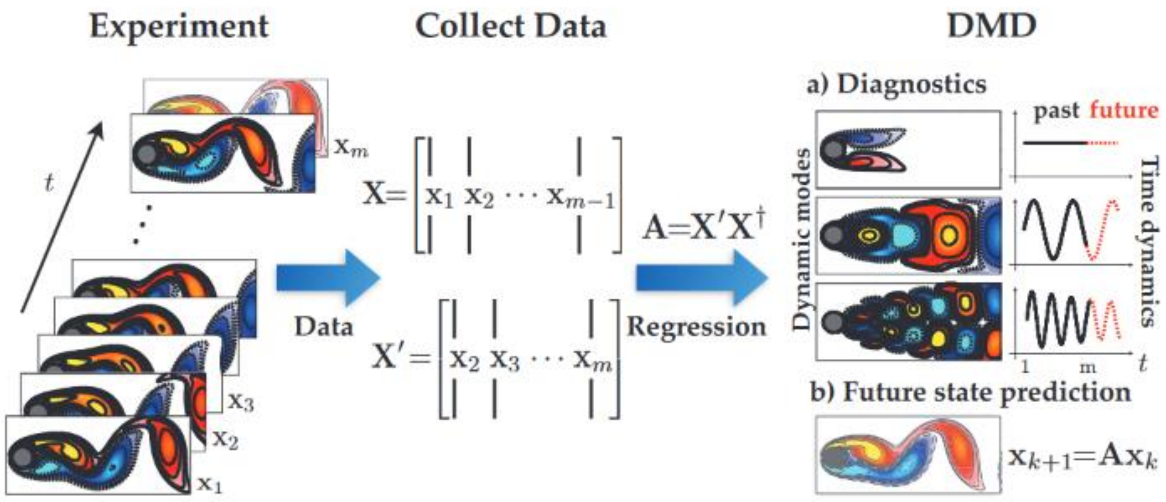
Machine Learning and Surrogate Modeling

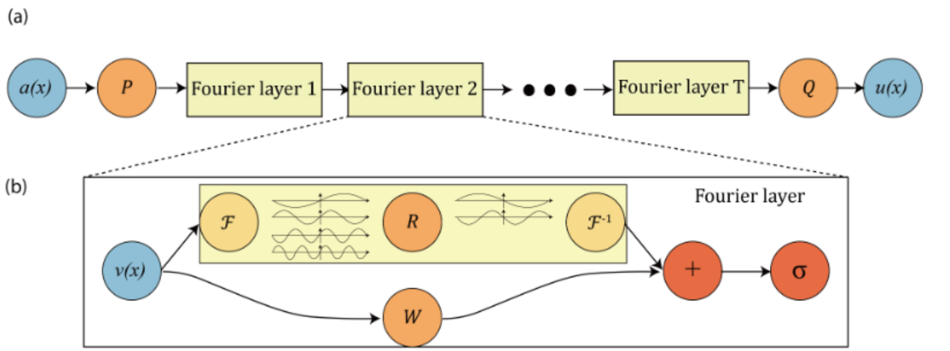
- Traditional models: polynomial approximations, kriging, Reduced Order Models (ROMs).
- Big-data and compute era: ML-based models, such as (Convolutional) Neural Networks, Gaussian Processes, Neural Operators.
- ML techniques can capture complex, high-dimensional dependencies that traditional methods struggle with.
- After the computational effort of training, the models provide very fast predictions.
- Surrogate models can be fully data-driven or include physics to accelerate training, improve generalization and alleviate data requirements.

Surrogate modeling in Reinforcement Learning

- Many RL environments rely on expensive simulations (e.g. robotics, autonomous systems, finance).
- Model-Based Reinforcement Learning
  - Surrogate models (a.k.a. World Models) make training more efficient by approximating system dynamics.

Case study: ML surrogate modeling in fluid dynamics

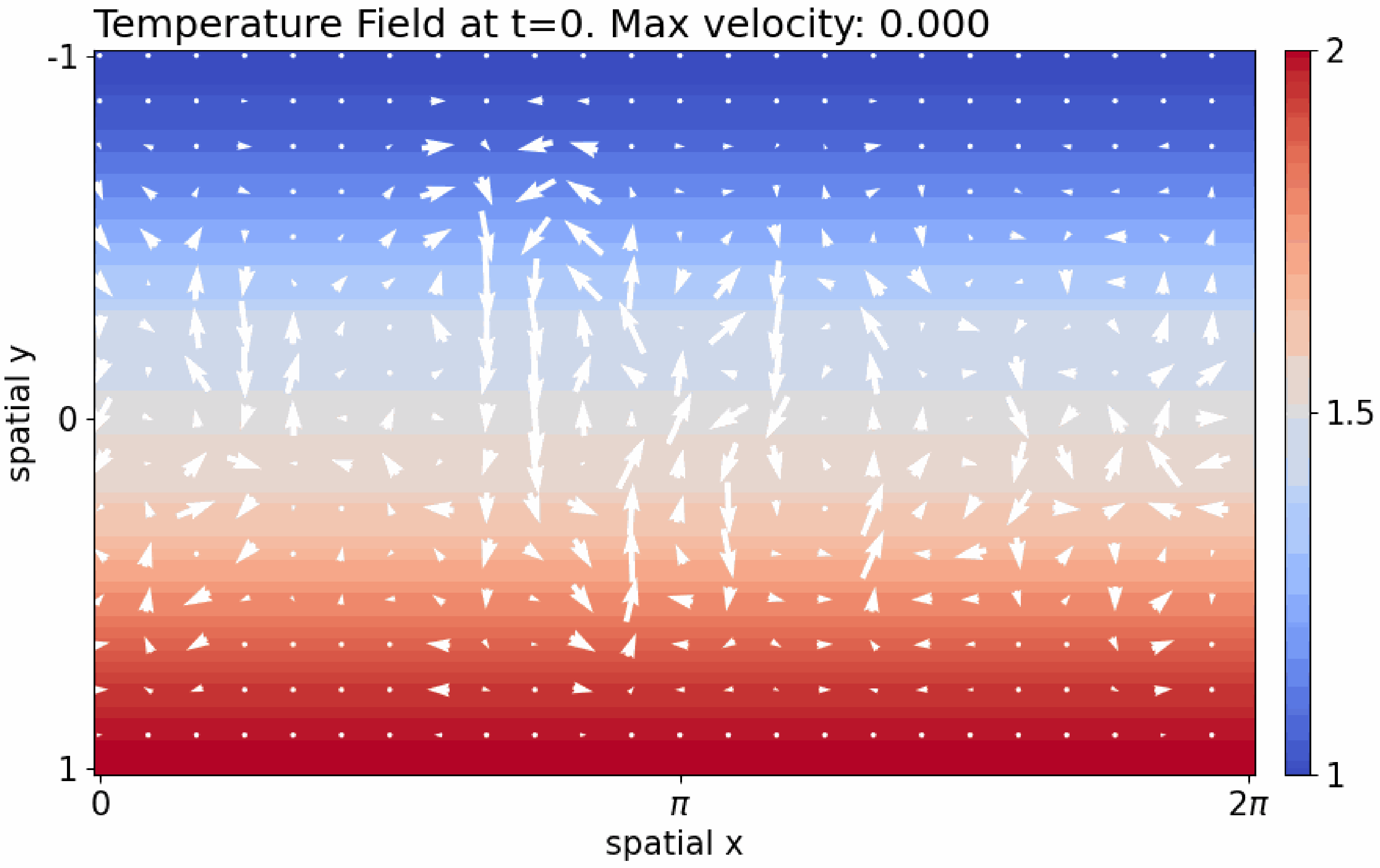




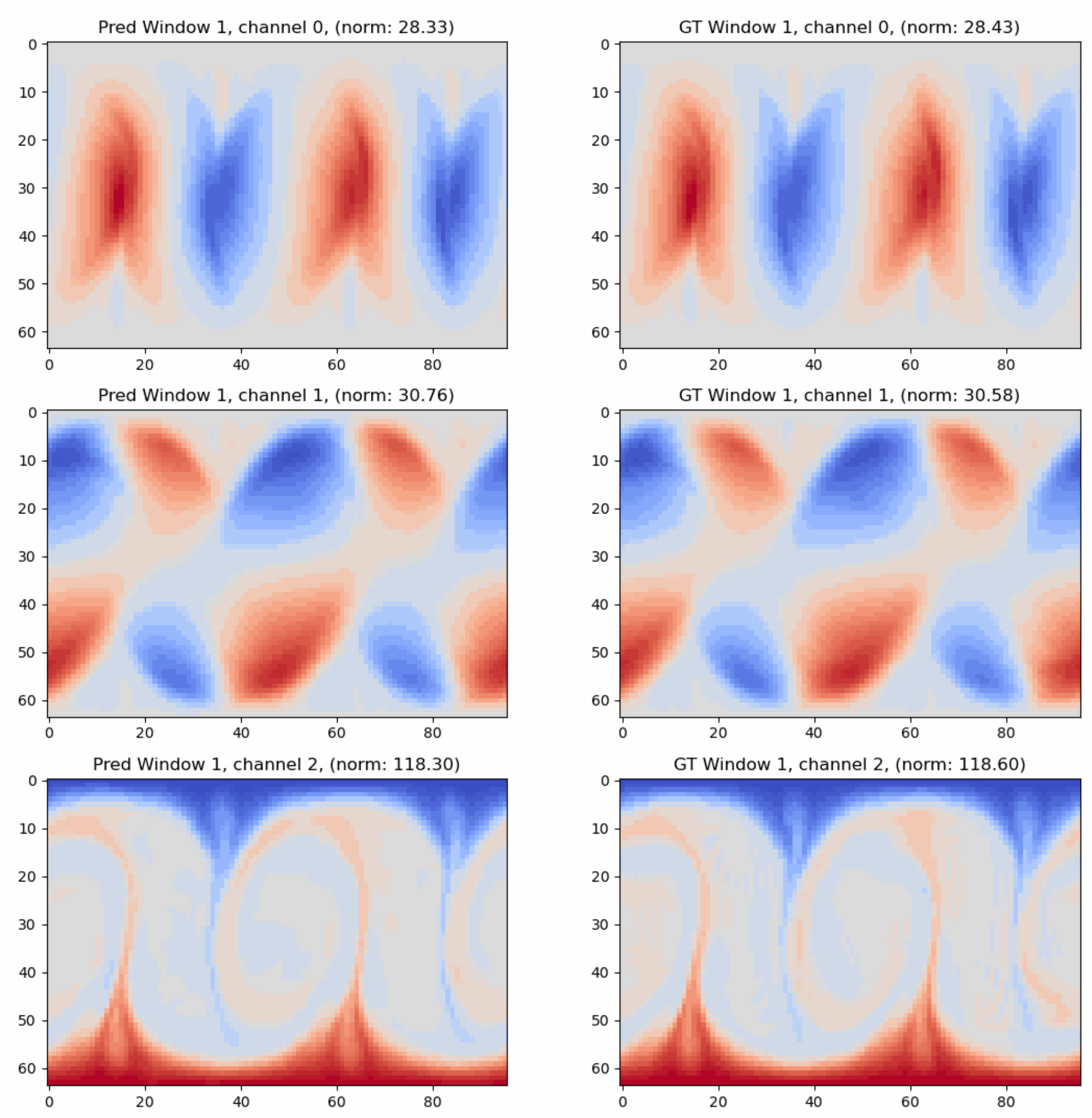
(a) The full architecture of neural operator: start from input a. 1. Lift to a higher dimension channel space by a neural network P. 2. Apply four layers of integral operators and activation functions. 3. Project back to the target dimension by a neural network Q. Output u. **(b) Fourier layers**: Start from input v. On top: apply the Fourier transform $\mathcal{F}$; a linear transform R on the lower Fourier modes and filters out the higher modes; then apply the inverse Fourier transform $\mathcal{F}^{-1}$. On the bottom: apply a local linear transform W.

Figure 2: **top:** The architecture of the neural operators; **bottom:** Fourier layer.

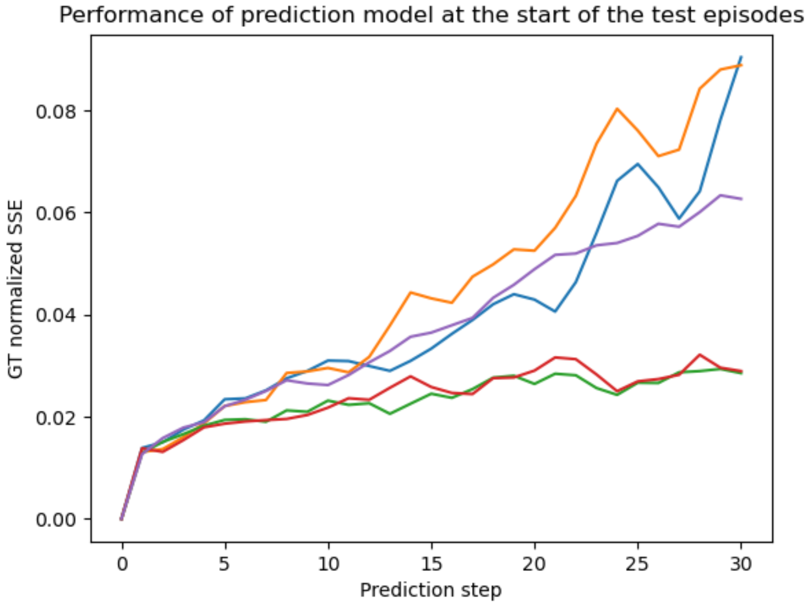
Predicting convection patterns



Results FNO $Ra = 2 * 10^6$



Parameter	Value	Parameter	Value
Hidden channels	32	Nr Episodes	20
Lifting channels	64	Projection Channels	64
Nr Layers	6	Seq. Delay	0.7
Nr Modes x	16	Seq. Length	2
Nr Modes y	16		



Challenges in Surrogate Modeling

- Generalization beyond the training data.
- Integrate physical constraints and domain knowledge into ML models (increase generalization and data efficiency)
  - Physics Informed Neural Networks
  - Hybrid AI-Simulation: e.g. in computation fluid dynamics, AI-based surrogate model predicts turbulence behavior while the rest of the simulation is handled by classical numerical solvers.
- Transfer learning: Encourage re-use of surrogate models for slight changes in tasks or domains, fine-tune to problem specifics using small datasets. Sim-to-Real Transfer.

Summary

- Surrogate models enable faster and more efficient simulations.
- Machine learning-based surrogates have shown impressive results for high-dimensional problems.
- Open question: How to best combine physics, machine learning and domain expertise?

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Thank you for your attention!

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