Data-driven, Physics informed and Hybrid models on out-of-distribution data

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01 The Bottleneck of Classical CFD

- Traditional Computational Fluid Dynamics (CFD) solvers are computationally **expensive and complex** → Long runtimes
- Surrogate models offer **cheaper approximations** up to **1,000x faster** than traditional solvers
- **Goal:** Analyze and compare generalization behavior of surrogate model classes

02 Three approaches

Classes

Data-driven	Physics-Informed	Hybrid
↓	↓	↓
FNO	PiFNO	PINO

Models

03 Partial Differential Equations

- Darcy flow:

$$-\nabla \cdot (a(x))\nabla u(x)) = f(x)$$
$$x \in (0,1)^2$$

- 1-D viscous Burgers' equation:

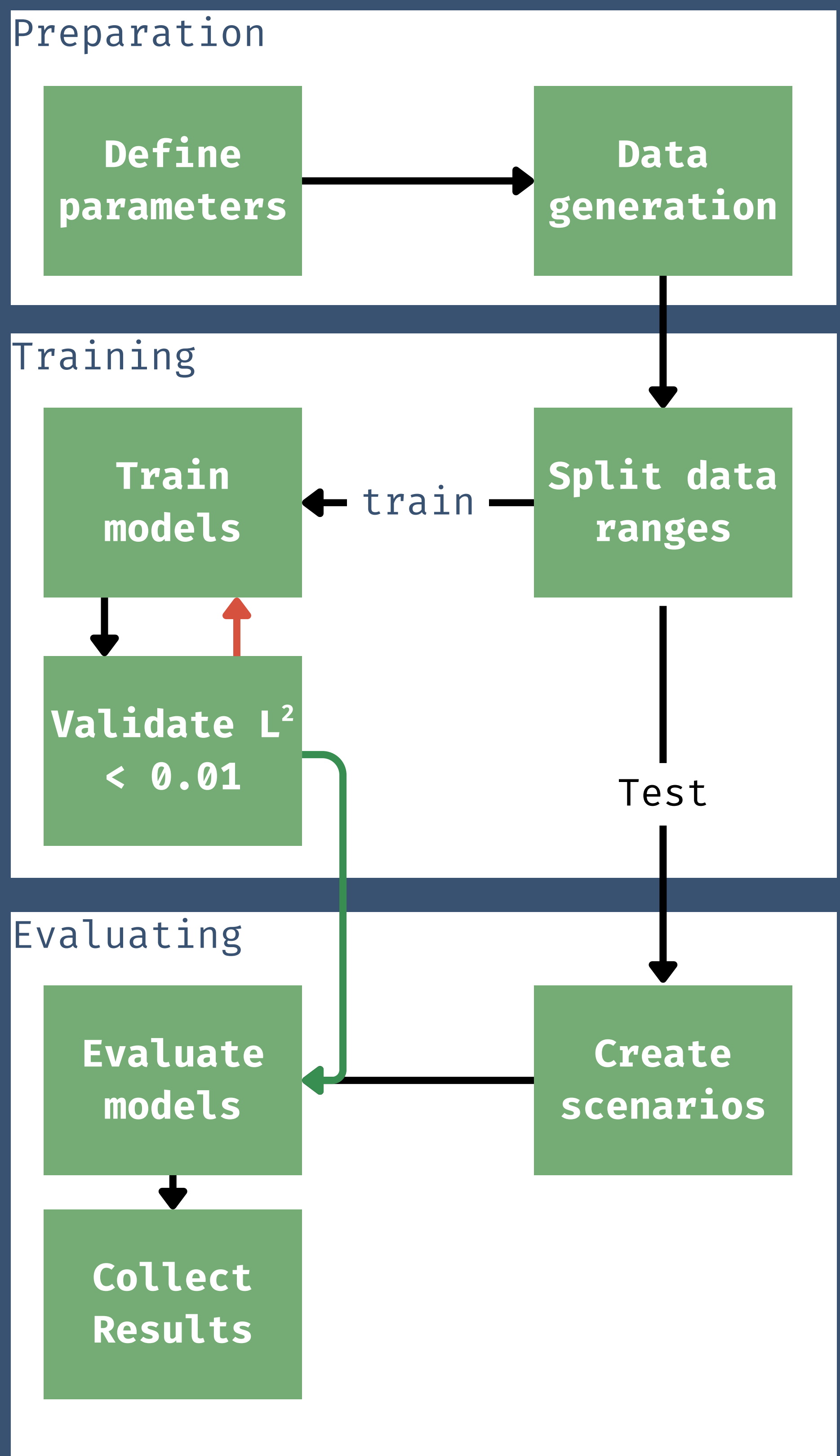
$$\partial_t u(x,t) + \partial_x (u^2(x,t)/2) = \nu \partial_{xx} u(x,t),$$
$$x \in (0,1), t \in (0,1]$$

Research Question:

How does the performance of data-driven, physics informed, and hybrid models change when evaluated outside the training distribution?

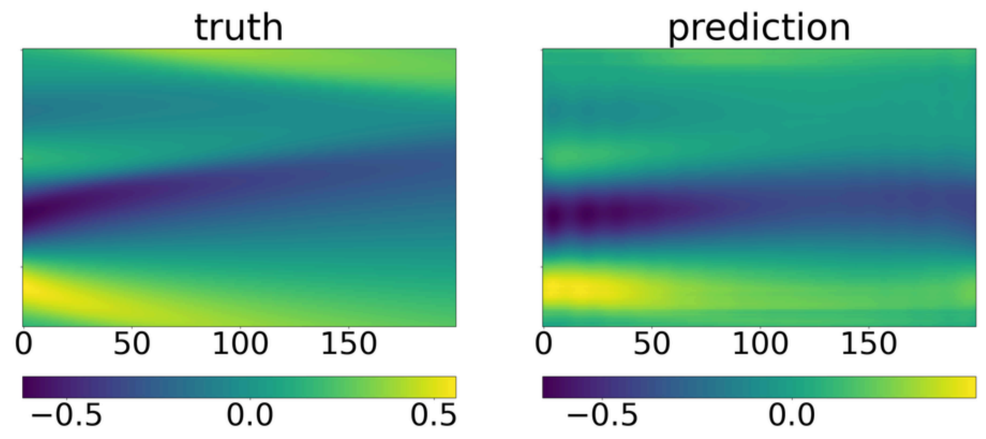
04 Methodology

The evaluation pipeline

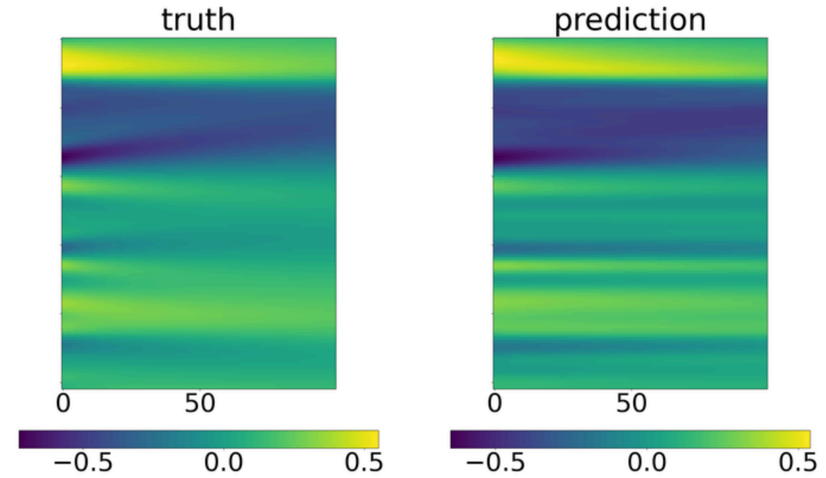


05 Results

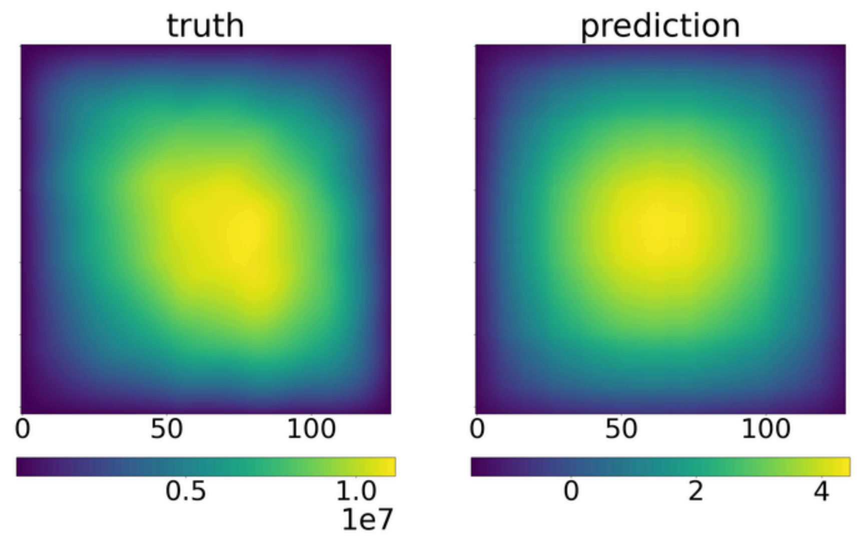
Some noticeable results. All models exhibit struggles to **adjust for scale difference** from training.



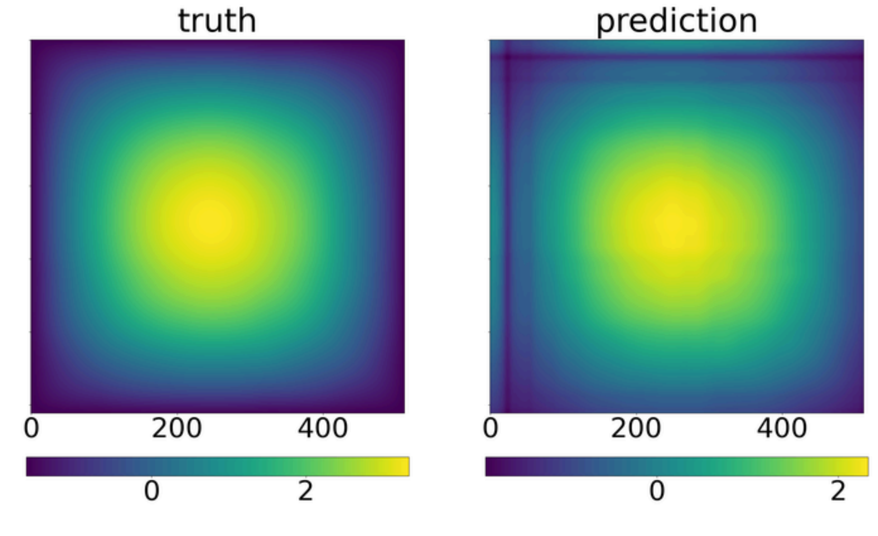
BURGERS' EQUATION: Long extrapolation FNO, Error 0.561



BURGERS' EQUATION: High complexity, PINO Error 0.212



DARCY FLOW: Extreme low permeability FNO Error 1.00



DARCY FLOW: super-resolution 128 → 512, PINO Error: 0.489

PiFNO failed to optimize On Darcy Flow. Converging at "zero-solutions". The residual loss remained to high to train on.

A) Burgers' equation

	FNO	PINO	PiFNO
Standard Train	0.008	0.007	0.006
Low Viscosity	0.023	0.021	0.022
Extreme Low Visc.	0.035	0.032	0.034
High Viscosity	0.074	0.080	0.089
Larger Amp (x1.5)	0.018	0.017	0.017
Smaller Amp (x0.5)	0.010	0.009	0.006
High Complexity IC	0.144	0.212	0.225
Smooth IC	0.007	0.007	0.005
Spatial SuperRes	0.075	0.066	0.064
Temporal SuperRes	0.050	0.043	0.042
Full SuperRes	0.089	0.081	0.079
Temp Extrap (t=2.0)	0.455	0.243	0.304
Long Extrap (t=5.0)	4.195	1.558	2.950

Model Architecture; Mean L2 Error (color scale 0.0–1.0)

B) Darcy Flow

	FNO	PINO
Standard Train	0.014	0.022
Narrower Range	0.241	0.257
Broader Range	0.958	0.958
Light Underflow	0.867	0.860
Light Overflow	0.578	0.394
Light Low Permeability	0.748	0.713
Medium Low Permeability	0.996	0.996
Extreme Low Permeability	1.000	1.000
Medium High Permeability	0.455	0.235
Extreme High Permeability	1.094	0.584
Half Viscosity	0.377	0.247
Double Viscosity	0.396	0.370
High Complexity	0.071	0.078
Super Res (x2)	0.292	0.222
Super Res (x4)	0.556	0.498

Model Architecture; Mean L2 Error (color scale 0.0–1.0)

average L^2 error of three test iterations for different scenarios

06 Conclusion

- **Parameter shifts:** Similar performance for all methods, with small outliers
- **Resolution shifts:** Physics-Informed architectures PINO and PiFNO show a marginally lower error.
- **Comparison of architectures:** There is no absolute superior architecture.
- **Future work:** Investigate **instance wise finetuning**

References: