Physics-informed Temporal Alignment for Auto-regressive PDE Foundation Models

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Background & Motivation

- Auto-regressive foundation models for partial differential equations (PDEs) have shown promise over traditional methods:
  Higher Generalization Capacity
  Lower Computational Costs
  Towards General Scientific Intelligence
- It takes T_{in} frames as input and predict the next frames based on previous ones
$$\hat{\boldsymbol{u}}_{t+1} = G_{\boldsymbol{\theta}}(\{\boldsymbol{u}_i\}_{i=t-T_{in}+1}^{t})$$
- But it suffers from error accumulation over long rollout horizons due to shortcut learning phenomena.

Illustration of Error Accumulation

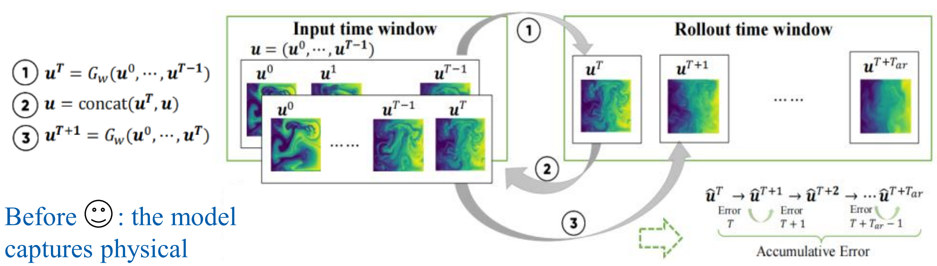
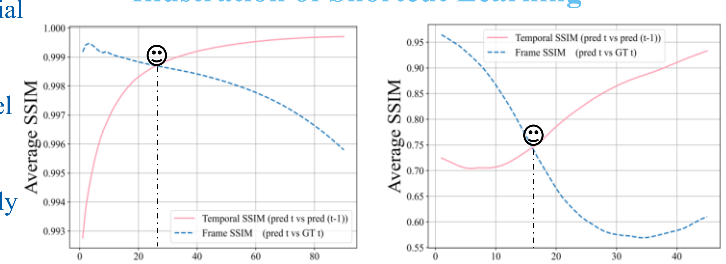


Illustration of Shortcut Learning

Before ☺: the model captures physical dynamics encoded in the PDEs rather than relying on superficial shortcut features.

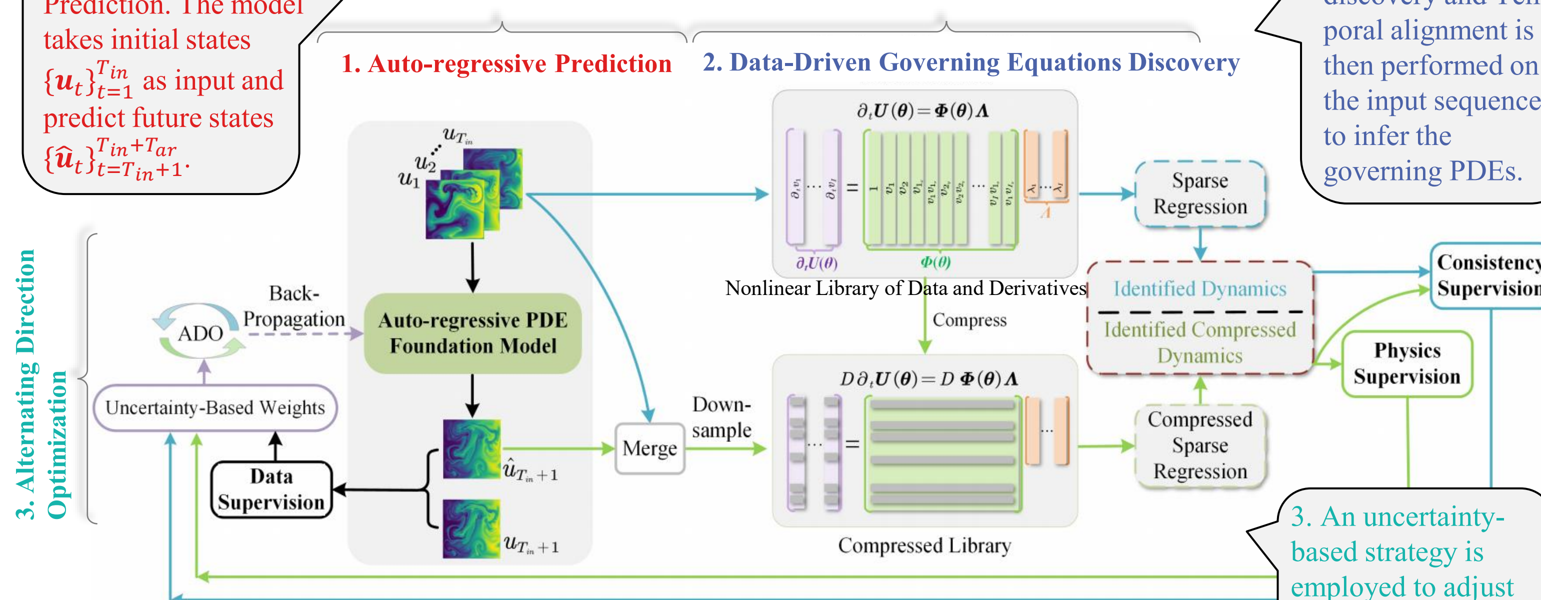
After ☺: the model fail to learn true physical features instead it recursively replicates prior predictions.



Methodology

1. Auto-regressive Prediction. The model takes initial states $\{\boldsymbol{u}_t\}_{t=1}^{T_{in}}$ as input and predict future states $\{\hat{\boldsymbol{u}}_t\}_{t=T_{in}+1}^{T_{in}+T_{ar}}$.

2. Data-driven PDE discovery and Temporal alignment is then performed on the input sequence to infer the governing PDEs.



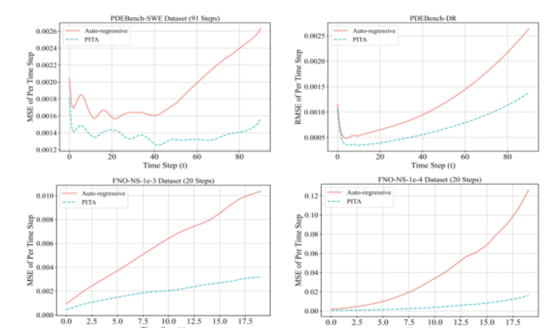
3. An uncertainty-based strategy is employed to adjust the weights between L_{Data}, L_{Phy} and L_{Con}

Experiments

- **In Distribution Test**

Model	Finetune Strategy	FNO-NS-ν 1e-5	1e-4	1e-3	PDEBench DR	SWE	PDEBench-CNS-(M,η) 1,0.1	1,0.01	M1	0.1,0.1	0.1,0.01	M0.1	PDEArena NS-Force	NS	CFDBench -
							Predict short trajectory								
DPOT-Ti	Auto-regress	0.05200	0.00385	0.00380	0.01326	0.00208	0.01120	0.01950	0.01535	0.01740	0.01380	0.01560	0.10269	0.09100	0.00391
7M	PITA	0.05629	0.00499	0.00218	0.02119	0.00202	0.01793	0.01565	0.01679	0.01080	0.01250	0.01165	0.11988	0.06465	0.00360
DPOT-S	Auto-regress	0.03220	0.00641	0.00301	0.01239	0.00210	0.01290	0.01670	0.01480	0.0152	0.01260	0.01390	0.07598	0.08670	0.00382
30M	PITA	0.02240	0.00232	0.00157	0.01346	0.00150	0.01057	0.01217	0.01137	0.01750	0.01140	0.01445	0.06769	0.04190	0.00335
MPP-Ti	Auto-regress	-	-	-	0.03510	0.00645	-	-	0.05841	-	-	0.04611	-	-	-
7M	PITA	-	-	-	0.03384	0.00605	-	-	0.04370	-	-	0.04025	-	-	-
MPP-S	Auto-regress	-	-	-	0.02974	0.00281	-	-	0.04287	-	-	0.02012	-	-	-
30M	PITA	-	-	-	0.03024	0.00274	-	-	0.04051	-	-	0.01906	-	-	-
DPOT-M	Auto-regress	0.02290	0.00385	0.00297	0.01209	0.00219	0.00998	0.01460	0.01230	0.01610	0.00947	0.01280	0.05571	0.02940	0.00373
122M	PITA	0.03199	0.00185	0.00193	0.00957	0.00154	0.01101	0.01032	0.01067	0.00945	0.01010	0.00958	0.05829	0.02191	0.00289
FNO-M	Auto-regress	0.08036	0.00577	0.00302	0.08608	0.00501	0.27849	0.03345	0.15597	0.13200	0.04449	0.08825	0.15190	0.15590	0.01382
170M	PITA	0.07668	0.00552	0.00152	0.07014	0.00423	0.10947	0.03483	0.07215	0.10224	0.05686	0.07955	0.15594	0.14066	0.00756
DPOT-L	Auto-regress	0.02130	0.00400	0.00298	0.00801	0.00184	0.01080	0.01310	0.01195	0.01600	0.00905	0.01253	0.05493	0.02780	0.00322
500M	PITA	0.01059	0.00198	0.00139	0.01084	0.00172	0.01001	0.00995	0.00998	0.02004	0.01871	0.01938	0.04965	0.02048	0.00302
							Predict long trajectory								
DPOT-Ti	Auto-regress	-	0.03670	0.00580	0.01480	0.00241	-	-	-	-	-	-	0.30034	-	-
7M	PITA	-	0.01718	0.00327	0.01090	0.00199	-	-	-	-	-	-	0.31012	-	-
DPOT-S	Auto-regress	-	0.02370	0.00437	0.01350	0.00235	-	-	-	-	-	-	0.26800	-	-
30M	PITA	-	0.00854	0.00223	0.00994	0.00137	-	-	-	-	-	-	0.22620	-	-
MPP-Ti	Auto-regress	-	-	-	0.05212	0.03291	-	-	-	-	-	-	-	-	-
7M	PITA	-	-	-	0.03844	0.02174	-	-	-	-	-	-	-	-	-
MPP-S	Auto-regress	-	-	-	0.04258	0.01631	-	-	-	-	-	-	-	-	-
30M	PITA	-	-	-	0.03704	0.00950	-	-	-	-	-	-	-	-	-
DPOT-M	Auto-regress	-	0.0126	0.00335	0.01030	0.00227	-	-	-	-	-	-	0.17200	-	-
122M	PITA	-	0.00694	0.00139	0.00904	0.00135	-	-	-	-	-	-	0.16390	-	-
FNO-M	Auto-regress	-	0.01761	0.00425	0.04101	0.00924	-	-	-	-	-	-	0.43136	-	-
170M	PITA	-	0.01710	0.00227	0.02884	0.00614	-	-	-	-	-	-	0.38731	-	-
DPOT-L	Auto-regress	-	0.0104	0.00323	0.00739	0.00170	-	-	-	-	-	-	0.17000	-	-
500M	PITA	-	0.00708	0.00199	0.00670	0.00121	-	-	-	-	-	-	0.16488	-	-

- **Performance on Shortcut Issue Resolution**



- **Out of Distribution Test**

Model	Strategy \ Epoch	PDEArena-SWE 500	1000	1500	Burgers 500	1000	1500
DPOT-Ti	Finetune (Auto-regress)	18.46497	5.24994	1.01142	0.03712	0.02543	0.00455
	Train from Scratch (Auto-regress)	5.98731	**3.20792**	0.99990	**0.06691**	0.01526	0.00419
	Train from Scratch (PITA)	**2.07097**	3.89625	**0.99710**	0.06945	**0.01318**	**0.00374**
DPOT-S	Finetune (Auto-regress)	44.70683	2.69744	0.99152	0.04679	0.01627	0.00304
	Train from Scratch (Auto-regress)	**8.00870**	2.66849	0.99414	0.06251	0.02703	0.00383
	Train from Scratch (PITA)	16.16088	**1.87741**	**0.99051**	**0.04121**	**0.01943**	**0.00307**