Paper:

Physics-Informed Deep B-Spline Networks

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Code:

Motivation

Solving **parametric** partial differential equations (**PDEs**) with **varying** initial and boundary conditions (**ICBCs**) is challenging.

- Classical solvers need to rerun for each parametric configuration.
- Physics-informed learning solvers often struggle with enforcing ICBCs with soft loss penalties.
- Hard ICBC constraint (ansatz) approaches can restrict model flexibility and potentially degrade interior solution accuracy.

Method

Parametric PDE formulation:

- Ground truth PDE solution s with state-time $x \in \mathbb{R}^d$, satisfying the following physics law and ICBC

$$\mathcal{F}(s, x, u) = 0, x \in \Omega(\alpha)$$

$$\mathcal{B}(s, x, u) = 0, x \in \partial\Omega(\alpha)$$

where u is the PDE parameter and α is the ICBC parameter.

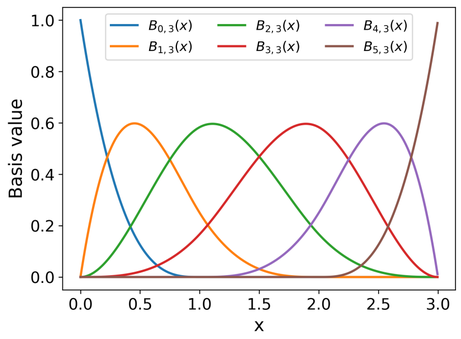
Key insight: leverage **B-spline representation** in **physics-informed learning**

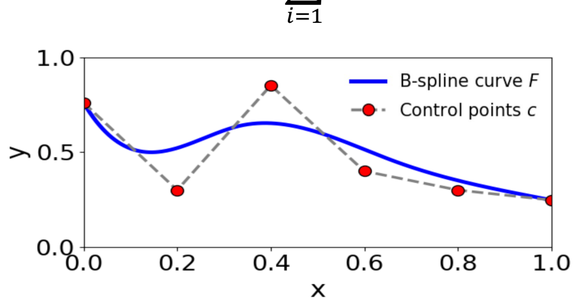
B-spline basis functions
generated through Cox-de Boor formula

$B_{i,d}(x)$: i –th basis with order d
c: weights of the B-spline (control points)

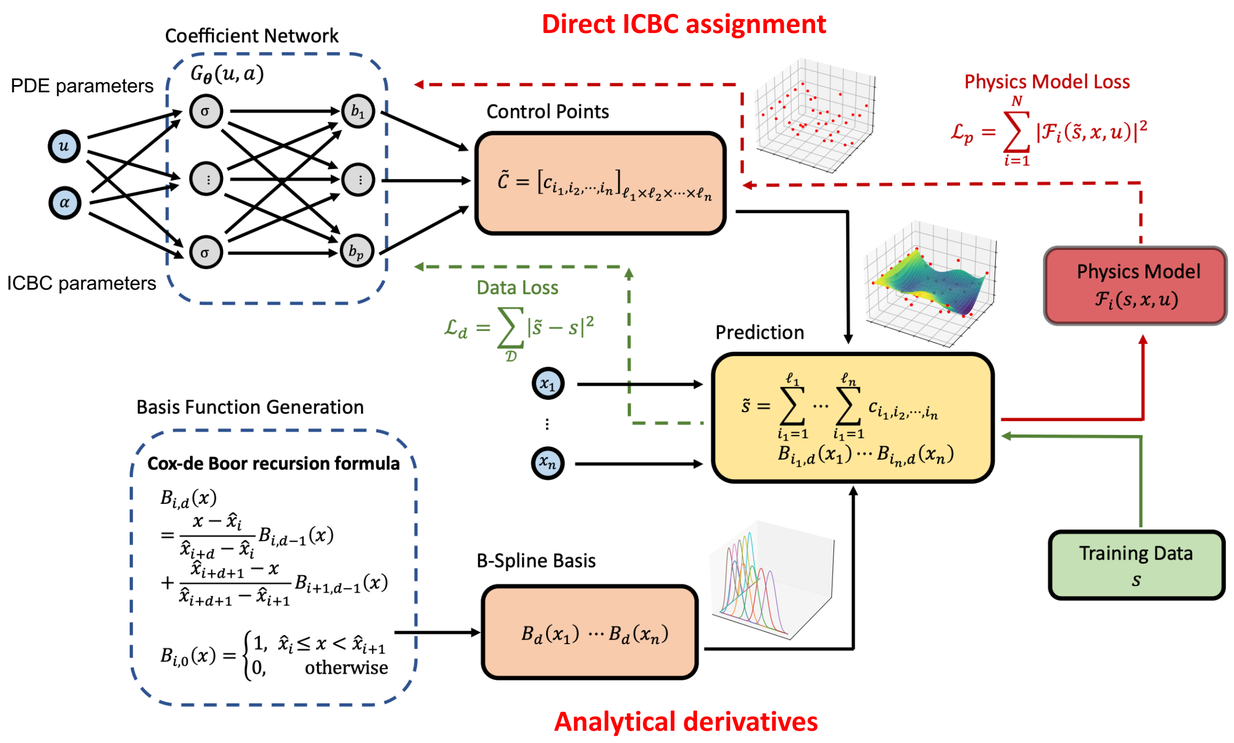
B-spline approximation w/ boundary compliance
with clamped knot points

$$\hat{s}(x) = \sum_{i=1}^{\ell} c_i \, B_{i,d}(x)$$

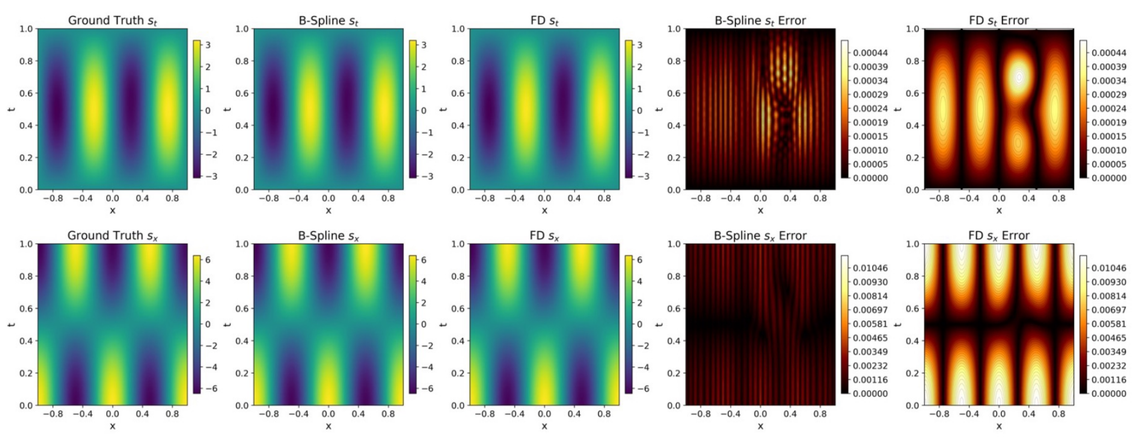




Physics-Informed Deep B-Spline Networks (PI-BSNet):



Analytical B-Spline derivatives for PDE loss with approximated solution:



Theoretical Analysis

Definitions:

- PDE and ICBC parameters u and α in bounded domain $\mathcal{U}$ and $\mathcal{A}$
- Ground truth PDE solution $s_{u,\alpha}(x,t)$, where $(x,t) \in [a_1, b_1] \times \cdots \times [a_n, b_n] \subset \mathbb{R}^n$.
- PI-BSNet prediction $\hat{s}_{u,\alpha}(x,t)$

Theorem (universal approximator):

For any PDE and ICBC parameters $u \in \mathcal{U}$ and $a \in \mathcal{A}$, with corresponding solution $s_{u,\alpha}$, there exists a PI-BSNet configuration such that for any $\epsilon > 0$,

$$\left\| \hat{s}_{u,\alpha} - s_{u,\alpha} \right\|_2 < \epsilon,$$

where $\|\cdot\|_2$ is the L_2 norm.

Theorem (generalization error bound):

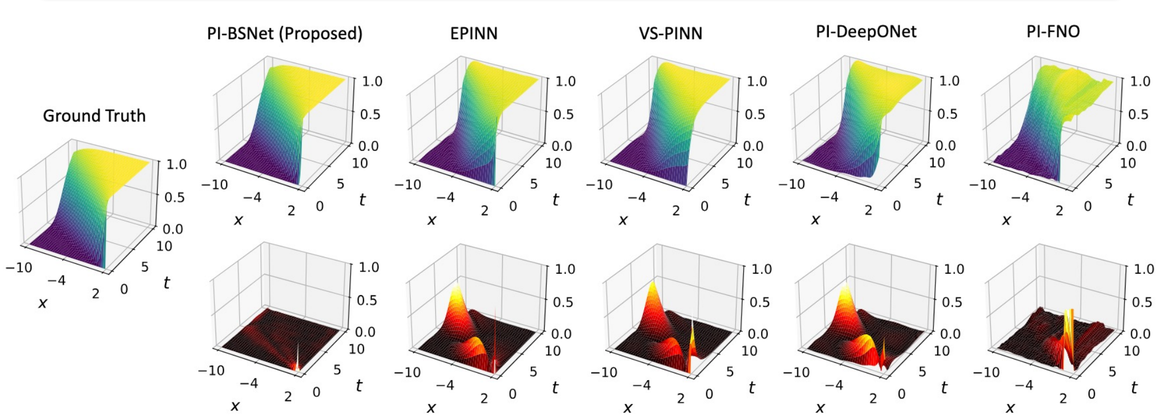
For any elliptic or parabolic PDE, for any $u \in \mathcal{U}$ and $a \in \mathcal{A}$, given the taining loss enforcement density Δu and $\Delta\alpha$ and final training loss δ, the prediction error is bounded by

$$\sup_{(x,t)} \left| \hat{s}_{u,\alpha}(x,t) - s_{u,\alpha}(x,t) \right| < c\delta + L(\Delta u + \Delta\alpha),$$

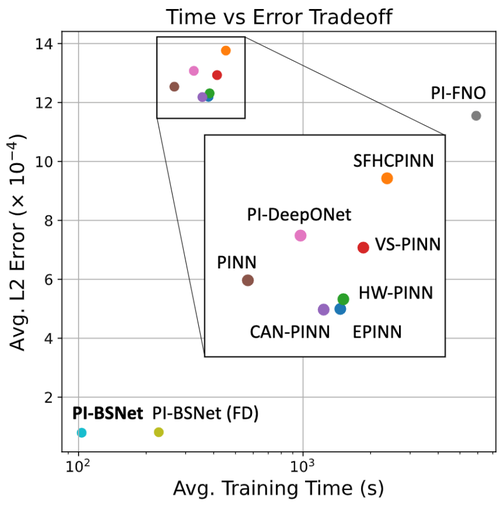
where c, L are constants.

Experiments

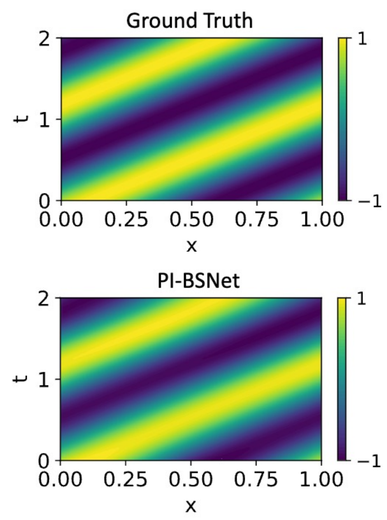
1. Assured boundary compliance



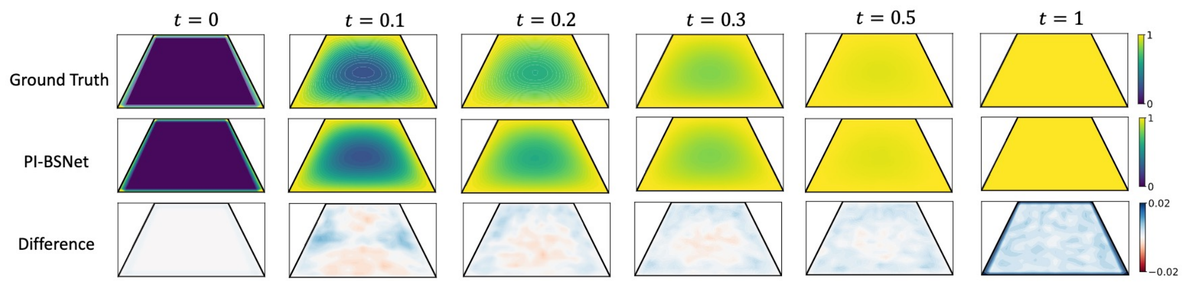
2. Efficient and accurate learning



3. Handles nonhomogeneous ICBC



4. Handles complex domain & long horizon



References

[1] Wang, Zhuoyuan, Raffaele Romagnoli, Saviz Mowlavi, and Yorie Nakahira. "Physics-Informed Deep B-Spline Networks." *Transactions on Machine Learning Research* (2026).

[2] Wang, Zhuoyuan, Raffaele Romagnoli, Kamyar Azizzadenesheli, and Yorie Nakahira. "Neural Spline Operators for Risk Quantification in Stochastic Systems." *In 2025 IEEE 64th Conference on Decision and Control (CDC)*, 2025.

OpInf-LLM: Parametric PDE Solving with LLMs via Operator Inference

Paper:

Code:

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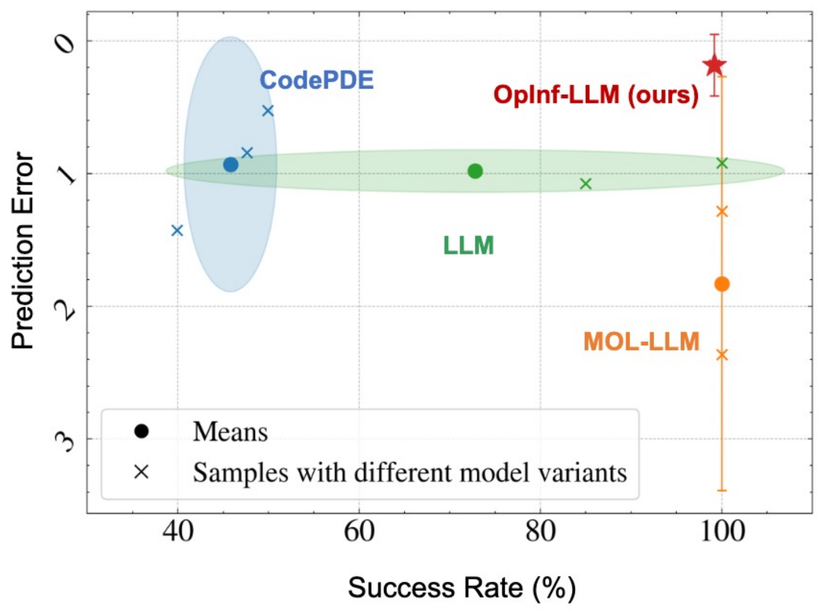
Motivation

LLM-based partial differential equation (PDE) solving is difficult due to the following challenges:

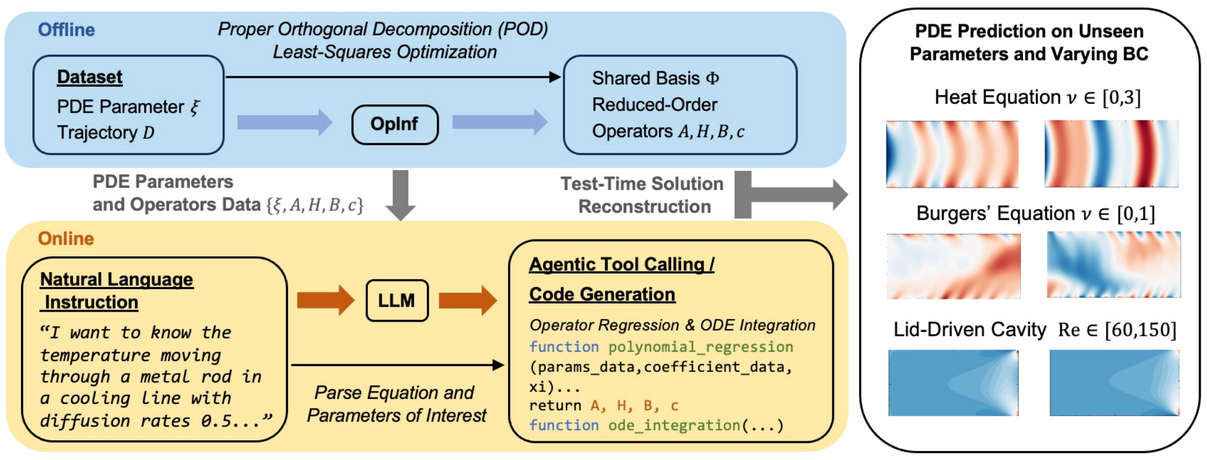
- LLM is not able to predict diverse PDE solutions directly from human instruction.
- LLM-based solver generation suffers from code execution failures and does not incur consistently high accuracy.
- Foundation model (FM) based methods require large dataset and hard to generalize to settings beyond training regime without fine-tuning.



Method

Key insights:

- leverage **operator inference** insight, to enable **LLM** generate reliable parametric **PDE solving** pipeline



Parametric operator inference (OpInf):

- Convert **parametric PDE solving** of diverse boundary conditions to **regression on operator space** and ODE integration

Consider a general class of nonlinear parametric PDEs

$$\frac{\partial y}{\partial t} = \mathcal{F}(\frac{\partial y}{\partial x}, \frac{\partial^2 y}{\partial x^2}, \cdots, s, \xi), \quad x \in \Omega, \quad t \in [0, T],$$

with initial and boundary conditions

$$\mathcal{I}[y](x,0) = g(x), \quad x \in \Omega, \qquad \mathcal{B}[y](x,t) = u(t), \quad x \in \partial\Omega,$$

OpInf approximates the PDE dynamics within a finite subspace spanned by a set of basis functions $\phi_1(x), \ldots, \phi_r(x)$

$$y(x,t,\xi) = \sum_{i=1}^{r} a_i(t,\xi)\phi_i(x),$$

where the modal coefficients $a_i(t,\xi)$ inherit reduced dynamics given ξ

$$\frac{da}{dt} = A(\xi)a + H(\xi)(a \otimes a) + B(\xi)u + c(\xi) \qquad (1)$$

The operators A, H, B, c can be obtained through the following optimization

$$\min_{A,H,B,c} \sum_{k=1}^{K} \left\| \left[Aa + H\,(a \otimes a) + Bu + c - \dot{a} \right](t_k) \right\|_F^2 + \lambda \left(\|A\|_F^2 + \|H\|_F^2 + \|B\|_F^2 + \|c\|_2^2 \right) \qquad (2)$$

where a and $\dot{a}$ can be obtained from the snapshot data at available ξ, and λ is the hyperparameter for regularization intensity

LLM online PDE solving:

- Parse diverse human instruction, including **non-technical** description

I want to study how temperature moves through a metal rod in a cooling line, with diffusion rates 0.1 and 0.5.

Heat equation with $\nu = 0.1, 0.5$

Method	Exact Match	Field Accuracy
Static Parser	52% (26/50)	75.7% (109/144)
OpInf-LLM	**100% (50/50)**	**100% (144/144)**

- **Reason** over correct operator dependence according to **physical law** without explicit prompts
  - ➢ Obtain correct regression parameterization without explicit prompting

Method	Test Re	Distribution	Feature	Error
OpInf	110	In-distribution	Re	3.57e−2
OpInf-LLM	110	In-distribution	1/Re	2.57e−2
OpInf	200	OOD	Re	instability
OpInf-LLM	200	OOD	1/Re	7.47e−2

- **Construct solver** based on OpInf for diverse PDE solving, through either **tool-calling** or **code generation**
  - ➢ Use regression on available A, H, B, c from optimization (2) to obtain operators for PDE parameters ξ of interest
  - ➢ Solve ODE (1) to obtain PDE solution of diverse BC

Metric	Value
Bug-free rate	100%
Success rate	99.2% (1 ROM instability)
Avg. code attempts	1.00 (tool-calling) 1.89 (code generation)

Experiments

- Require only **small amount** of **data**
- **High execution success rate** for both tool-calling and code generation
- Accurately generalize to **unseen parameters** and **BCs**, and to **longer time horizon**

Table 1. Results summary. Average relative L_2 error is reported for each equation. **Bold** denotes the best result, and underline denotes the second best. ↑ higher is better, ↓ lower is better.

Method	Data	Train time (s)	Success rate ↑	Heat ↓	Burgers ↓	Cavity ↓
CodePDE (GPT-4.1)	–	–	49.9%	1.59e−2	**1.50e−1**	1.41e0
CodePDE (GPT-4o)	–	–	39.9%	1.60e−1	1.23e0	2.89e0
CodePDE (Gemini-2.0-flash)	–	–	47.6%	1.74e−2	9.56e−1	1.55e0
MOL-LLM	449	14306	**100.0%**	1.69e0	1.44e0	7.24e−1
MOL-LLM (large dataset)	15000	35915	**100.0%**	4.87e0	1.58e0	6.44e−1
LLM (GPT-4.1)	–	–	**100.0%**	7.79e−1	9.82e−1	1.00e0
LLM (GPT-4o)	–	–	85.0%	9.24e−1	1.30e0	1.00e0
LLM (Gemini-2.0-flash)	–	–	33.3%	9.02e−1	failed	failed
OpInf-LLM (GPT-4.1)	449	30	99.2%	**1.29e−2**	4.91e−1	**4.63e−2**
OpInf-LLM (GPT-4o)	449	30	99.2%	**1.29e−2**	4.91e−1	**4.63e−2**
OpInf-LLM (Gemini-2.0-flash)	449	30	99.2%	**1.29e−2**	4.91e−1	**4.63e−2**

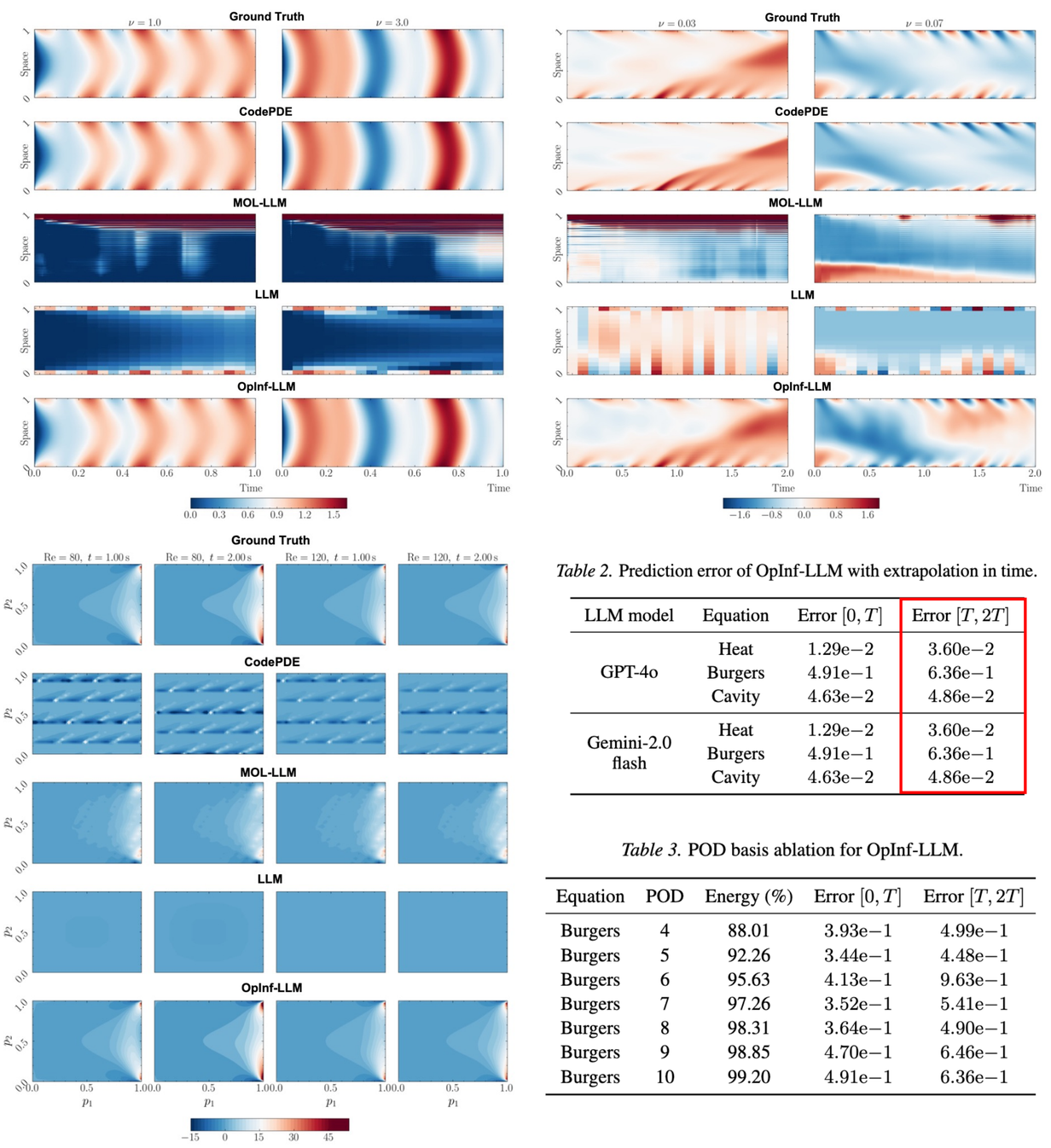


Table 2. Prediction error of OpInf-LLM with extrapolation in time.

LLM model	Equation	Error $[0, T]$	Error $[T, 2T]$
GPT-4o	Heat	1.29e−2	3.60e−2
	Burgers	4.91e−1	6.36e−1
	Cavity	4.63e−2	4.86e−2
Gemini-2.0 flash	Heat	1.29e−2	3.60e−2
	Burgers	4.91e−1	6.36e−1
	Cavity	4.63e−2	4.86e−2

Table 3. POD basis ablation for OpInf-LLM.

Equation	POD	Energy (%)	Error $[0, T]$	Error $[T, 2T]$
Burgers	4	88.01	3.93e−1	4.99e−1
Burgers	5	92.26	3.44e−1	4.48e−1
Burgers	6	95.63	4.13e−1	9.63e−1
Burgers	7	97.26	3.52e−1	5.41e−1
Burgers	8	98.31	3.64e−1	4.90e−1
Burgers	9	98.85	4.70e−1	6.46e−1
Burgers	10	99.20	4.91e−1	6.36e−1