

OPINF-LLM: PARAMETRIC PDE SOLVING WITH LLMS VIA OPERATOR INFERENCE

Wang, Zhuoyuan; Hu, Hanjiang; Deng, Xiyu; Mowlavi, Saviz; Nakahira, Yorie

TR2026-043 April 24, 2026

Abstract

Solving diverse partial differential equations (PDEs) is fundamental in science and engineering. Large language models (LLMs) have demonstrated strong capabilities in code generation, symbolic reasoning, and tool use, but reliably solving PDEs across heterogeneous settings remains challenging. Prior work on LLM-based code generation and transformer-based foundation models for PDE learning has shown promising advances. However, a persistent trade-off between execution success rate and numerical accuracy arises, particularly when generalization to unseen parameters and boundary conditions is required. In this work, we propose OpInf-LLM, an LLM parametric PDE solving framework based on operator inference. The proposed framework leverages a small amount of solution data to enable accurate prediction of diverse PDE instances, including unseen parameters and configurations, and provides seamless integration with LLMs for natural language specification of PDE solving tasks. Its low computational demands and unified tool interface further enable a high execution success rate across heterogeneous settings. By combining operator inference with LLM capabilities, OpInf-LLM opens new possibilities for generalizable reduced-order modeling in LLM-based PDE solving.

International Conference on Learning Representations (ICLR) Workshop on AI and Partial Differential Equations (AI&PDE) 2026

© 2026 MERL. This work may not be copied or reproduced in whole or in part for any commercial purpose. Permission to copy in whole or in part without payment of fee is granted for nonprofit educational and research purposes provided that all such whole or partial copies include the following: a notice that such copying is by permission of Mitsubishi Electric Research Laboratories, Inc.; an acknowledgment of the authors and individual contributions to the work; and all applicable portions of the copyright notice. Copying, reproduction, or republishing for any other purpose shall require a license with payment of fee to Mitsubishi Electric Research Laboratories, Inc. All rights reserved.

OPINF-LLM: PARAMETRIC PDE SOLVING WITH LLMs VIA OPERATOR INFERENCE

Zhuoyuan Wang¹ Hanjiang Hu¹ Xiyu Deng¹ Saviz Mowlavi² Yorie Nakahira¹

¹Carnegie Mellon University ²MERL Correspondence: zhuoyuaw@andrew.cmu.edu

ABSTRACT

Solving diverse partial differential equations (PDEs) is fundamental in science and engineering. Large language models (LLMs) have demonstrated strong capabilities in code generation, symbolic reasoning, and tool use, but reliably solving PDEs across heterogeneous settings remains challenging. Prior work on LLM-based code generation and transformer-based foundation models for PDE learning has shown promising advances. However, a persistent trade-off between execution success rate and numerical accuracy arises, particularly when generalization to unseen parameters and boundary conditions is required. In this work, we propose OpInf-LLM, an LLM parametric PDE solving framework based on operator inference. The proposed framework leverages a small amount of solution data to enable accurate prediction of diverse PDE instances, including unseen parameters and configurations, and provides seamless integration with LLMs for natural language specification of PDE solving tasks. Its low computational demands and unified tool interface further enable a high execution success rate across heterogeneous settings. By combining operator inference with LLM capabilities, OpInf-LLM opens new possibilities for generalizable reduced-order modeling in LLM-based PDE solving.

1 INTRODUCTION

Solving diverse partial differential equations (PDEs) is fundamental in science and engineering, underpinning applications ranging from fluid dynamics and heat transfer to electromagnetics, materials science, and climate modeling (Cai et al., 2021; Oommen et al., 2024; Nohra & Dufour, 2024; Pathak et al., 2022). In practice, modern PDE workflows must accommodate heterogeneous governing equations, parameter regimes, and boundary and initial conditions, often under strict accuracy and robustness requirements. As a result, there is growing interest in automated and generalizable PDE solvers that can flexibly adapt to new problem instances without extensive manual intervention or retraining (Karniadakis et al., 2021; Li et al., 2020; Lu et al., 2019; Sun et al., 2025; Ye et al., 2024; Liu et al., 2024a).

Large language models (LLMs) have recently demonstrated strong capabilities in code generation (Jiang et al., 2024; Huynh & Lin, 2025), symbolic reasoning (Xu et al., 2024; Shojaee et al., 2024), and tool use (Xu et al., 2025b), motivating a new line of work on language-driven scientific computing (Nejjar et al., 2025). In the context of PDEs, prior work on LLM-based code generation and transformer-based foundation models for PDE learning has shown promising advances, including automatic solver synthesis and data-driven surrogate modeling (Li et al., 2025; Gaonkar et al., 2025; Wu et al., 2025; Negrini et al., 2025). However, reliably solving PDEs across heterogeneous settings remains challenging for LLM-based approaches. In particular, a persistent trade-off between execution success rate and numerical accuracy arises, especially when generalization to unseen parameters, boundary conditions, and domain configurations is required (Fig. 1). Code-generation-based methods often suffer from brittle execution and

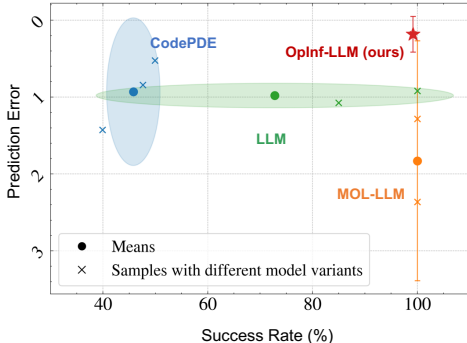


Figure 1: Trade-offs in prediction error and success rate.

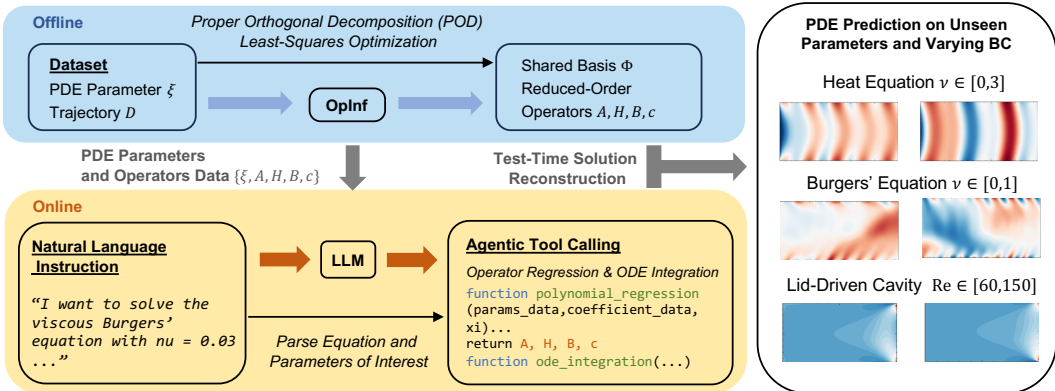


Figure 2: Overall diagram of the OpInf-LLM framework.

solver instability, while purely data-driven neural surrogates can exhibit poor extrapolation and high training costs.

These limitations highlight a fundamental gap between expressive, flexible language-driven interfaces and robust, generalizable numerical solvers. On the one hand, LLMs provide a powerful abstraction layer for specifying PDEs and solver configurations via natural language (Li et al., 2024a). On the other hand, classical reduced-order modeling techniques, such as operator inference, offer principled mechanisms for constructing compact, interpretable, and generalizable dynamical system representations from limited data, but cannot handle diverse PDEs at once with language specifications (Peherstorfer & Willcox, 2016; Kramer et al., 2024). Bridging these two paradigms offers a promising pathway toward reliable, language-driven PDE solving.

In this work, we propose OpInf-LLM, an LLM parametric PDE solving framework via operator inference (Fig. 2). We first leverage operator inference to learn reduced-order models for diverse parametric PDE instances from a small amount of solution data over a finite set of parameter values and configuration settings, yielding a shared reduced basis and parameter-dependent reduced operators. We then integrate large language models to infer and solve new reduced-order models via agentic tool calling, enabling the prediction of PDE solutions for diverse instances, including previously unseen parameters and varying boundary conditions. By construction, the reduced-order model effectively reduces the complexity of PDE generalization to polynomial fitting over learned operators and time integration of a low-dimensional ODE system, resulting in low computational demands at test time and a high execution success rate across heterogeneous PDE settings. Moreover, the use of LLMs naturally admits natural language instructions for specifying PDEs parameters and configurations, providing a flexible and unified interface for diverse PDE-solving tasks. The key advantages of OpInf-LLM are:

- Accurate zero-shot prediction of PDE solutions under unseen parameters and configuration settings.
- Lightweight training with high execution success rates across heterogeneous PDEs and settings.
- Seamless natural language specification and solution of diverse PDEs within a single unified framework.

2 RELATED WORK

Operator Inference. Reduced-order modeling (ROM) (Benner et al., 2015; Brunton & Kutz, 2022) is a class of model reduction techniques that aims to reduce the computational cost of simulating large-scale dynamical systems governed by PDEs by leveraging a low-dimensional latent space. Among model reduction techniques, operator inference (OpInf) (Kramer et al., 2024; Peherstorfer & Willcox, 2016) is a data-driven ROM method that learns structured reduced dynamics consistent with PDE nonlinearities, allowing accurate prediction with improved generalization and lower data requirements compared to black-box approaches. OpInf has been applied to parametric settings (McQuarrie et al., 2023), used to simulate complex physics such as combustion chamber dynamics (McQuarrie et al., 2021; Swischuk et al., 2020), and enhancements have been proposed to account for a wider class of PDE nonlinearities (Qian et al., 2020; 2022) or enhance robustness of the predictions (Sawant et al.,

2023). To the best of our knowledge, ROMs have not been explored for language-model-driven PDE solving or for extending beyond single parametric PDE families. We address this gap by bridging OpInf with expressive LLM interfaces and tool-use capabilities to enable reliable multi-PDE-family solving across diverse instances.

PDE Foundation Models. Recent advances in AI/ML have led to the development of a broad class of data-driven PDE solvers, including physics-informed neural networks (PINNs) (Raissi et al., 2019; Han et al., 2018; Cuomo et al., 2022; Cho et al., 2024; Huang et al., 2022), neural operators (Kovachki et al., 2023; Li et al., 2020; Lu et al., 2019; 2021; 2022; Li et al., 2024b; Goswami et al., 2023), and neural PDE solvers (Brandstetter et al., 2022; Takamoto et al., 2023; Hsieh et al., 2019). More recently, PDE foundation models that learn generalizable representations across diverse equation families have been proposed (Herde et al., 2024; Liu et al., 2024b; Ye et al., 2024; Sun et al., 2025; Shen et al., 2024; Rautela et al., 2025; Zhu et al., 2025; Zhou et al., 2025; Hao et al., 2024; Wiesner et al., 2025). These models aim to solve multiple PDEs with a single pre-trained architecture, reducing the need for equation-specific training. Building on this direction, multimodal approaches have emerged that incorporate language inputs to enhance flexibility and interpretability (Negrini et al., 2025; Bao et al., 2025). In parallel, diffusion-based neural PDE solvers have been developed to support text-conditioned simulation using captions generated by multimodal LLMs (Zhou et al., 2024). Additionally, LLMs have been explored as auxiliary modalities to improve surrogate model performance (Lorsung & Farimani, 2024). Despite this progress, robust generalization to unseen parameters and initial and boundary condition settings remains a significant challenge.

LLMs for Scientific Machine Learning. Large language models have shown promising capabilities in scientific machine learning. Prior works focus on using LLMs to directly generate executable PDE solvers from natural language descriptions (Li et al., 2025; Wu et al., 2025), as well as leveraging LLMs to write code for broader scientific machine learning problems (Gaonkar et al., 2025; Jiang et al., 2025; He et al., 2025). Beyond code generation, Yang et al. (2025) fine-tunes LLMs for in-context operator learning, while Xu et al. (2025a) explores PDE discovery by training generative models with textbook information. LLM-based agents have also adopted agentic workflows for PDE solving (Jiang & Karniadakis, 2025; Liu et al., 2025). In parallel, many efforts have explored LLM-driven autoformalization of PDEs, translating language descriptions into formal mathematical representations (Soroco et al., 2025; Mensfelt et al., 2025), building on broader autoformalization research that maps informal mathematical content into formal, machine-verifiable languages (Wu et al., 2022; Weng et al., 2025). Equation discovery from data has also been explored in Du et al. (2024); Grayeli et al. (2024). Despite these advances, solver reliability and execution robustness remain key challenges.

3 PROPOSED METHOD

In this section, we present the proposed OpInf-LLM method. The overall diagram is shown in Fig. 2. The method consists of two stages. In the offline stage, operator inference (OpInf) is used to construct a parametric reduced-order model (ROM) by learning a projection basis and reduced modal dynamics from PDE data with finite parameter coverage. In the online stage, a large language model (LLM) is integrated at test time to enable the prediction of solutions for diverse PDE instances based on natural-language instructions, while generalizing to previously unseen parameters and configurations.

3.1 OPERATOR INFERENCE

We start by introducing OpInf, which is a data-driven model reduction method for PDEs (Kramer et al., 2024; Peherstorfer & Willcox, 2016) and is the key component in the offline stage of the proposed method. Consider a general class of nonlinear parametric PDEs:

$$\frac{\partial y}{\partial t} = \mathcal{F}\left(\frac{\partial y}{\partial x}, \frac{\partial^2 y}{\partial x^2}, \dots, s, \xi\right), \quad x \in \Omega, \quad t \in [0, T], \quad (1)$$

with initial and boundary conditions

$$\mathcal{I}[y](x, 0) = g(x), \quad x \in \Omega, \quad \mathcal{B}[y](x, t) = u(t), \quad x \in \partial\Omega, \quad (2)$$

where $\Omega \subset \mathbb{R}^d$ is the spatial domain, s is a known source term, $\xi \in \mathbb{R}$ is the PDE parameter, and \mathcal{F} is the generic nonlinear PDE operator.

OpInf learns a ROM approximating the PDE dynamics within a finite r -dimensional subspace spanned by a set of basis functions $\phi_1(x), \dots, \phi_r(x)$. Specifically, the PDE state is decomposed as

$$y(x, t, \xi) = \sum_{i=1}^r a_i(t, \xi) \phi_i(x), \quad (3)$$

where $a_i(t, \xi)$ are time-dependent modal coefficients. In classical model reduction, the dynamics for these modal coefficients can be derived from the PDE itself using Galerkin projection (Holmes et al., 2012). For PDE operators \mathcal{F} with at most quadratic nonlinearities, which encompass a broad class of PDEs commonly arising in physics (e.g., the diffusion equation modeling heat transfer or the Navier-Stokes equations modeling fluid dynamics), the modal coefficients inherit reduced dynamics of the following form given ξ :

$$\frac{da}{dt} = A(\xi)a + H(\xi)(a \otimes a) + B(\xi)u + c(\xi), \quad (4)$$

where $A \in \mathbb{R}^{r \times r}$ is a linear operator, $H \in \mathbb{R}^{r \times r^2}$ is a quadratic operator, $B \in \mathbb{R}^{r \times d}$ is a control input matrix, and $c \in \mathbb{R}^r$ is an offset vector, with \otimes denoting the Kronecker product. This procedure naturally applies to PDE operators \mathcal{F} with higher-order or non-polynomial nonlinearities, leading to modal dynamics with structures that differ from equation 4, for example through the inclusion of cubic terms (Qian et al., 2022). In this paper, we stick to quadratically nonlinear PDEs with the formulation in equation 4 for clarity.

For a fixed ξ , OpInf composes the following two steps: 1) identify an appropriate basis $\phi_1(x), \dots, \phi_r(x)$; 2) identify the corresponding reduced-order operators A, H, B, c . These procedures yield a reduced order model defined by equation 3 and equation 4 for solving PDEs with varying boundary conditions. For the rest of this subsection, we consider a single fixed ξ and we omit ξ dependency in the notation for conciseness.

Basis identification. We collect a dataset \mathcal{D} , obtained either from physical experiments or numerical simulations of the PDE in equation 1. The dataset consists of time series of the solution and its temporal derivatives over a discretization \mathbf{x} of the full spatial domain

$$\mathcal{D} = \{y(\mathbf{x}, t_1), \dots, y(\mathbf{x}, t_K)\} \cup \left\{ \frac{\partial y}{\partial t}(\mathbf{x}, t_1), \dots, \frac{\partial y}{\partial t}(\mathbf{x}, t_K) \right\}. \quad (5)$$

For notational simplicity, equation 5 is written for a single trajectory. In practice, the dataset may include multiple trajectories corresponding to different initial conditions and boundary conditions. Then, for a given reduced-order basis dimension r , OpInf computes the basis functions by conducting a proper orthogonal decomposition (POD) (Chatterjee, 2000) of the concatenated solution values y contained in the dataset \mathcal{D} , which yields an optimal basis that maximizes the captured energy. Specifically, $\Phi := [\phi_1(\mathbf{x}), \dots, \phi_r(\mathbf{x})]$ are the first r left-singular vectors of the trajectory data matrix $\{y(\mathbf{x}, t_1), \dots, y(\mathbf{x}, t_K)\}$, corresponding to the r largest singular values.¹ The number of basis functions r can be tuned based on the desired level of captured energy (Peherstorfer & Willcox, 2016). Ablations on the effects of the basis function number r can be found in Section 4.4.

Operator identification. Once the POD basis has been obtained, we project the dataset \mathcal{D} onto the basis functions to form a reduced-order dataset \mathcal{A} of modal coefficients and their time derivatives. Specifically,

$$\mathcal{A} = \{a(t_1), \dots, a(t_K)\} \cup \{\dot{a}(t_1), \dots, \dot{a}(t_K)\}, \quad (6)$$

where

$$a_i(t_j) = \langle y(\mathbf{x}, t_j), \phi_i(\mathbf{x}) \rangle, \quad \dot{a}_i(t_j) = \left\langle \frac{\partial y}{\partial t}(\mathbf{x}, t_j), \phi_i(\mathbf{x}) \right\rangle, \quad (7)$$

for $i = 1, \dots, r$ and $j = 1, \dots, K$. Here $\langle \cdot, \cdot \rangle$ denotes the L_2 inner product. Then, OpInf calculates the operators A, H, B and c such that the reduced dynamics in equation 4 best fits the data in the least-squares sense, which can be formulated as the least-squares problem

$$\min_{A, H, B, c} \sum_{k=1}^K \|[Aa + H(a \otimes a) + Bu + c - \dot{a}](t_k)\|_F^2 + \lambda (\|A\|_F^2 + \|H\|_F^2 + \|B\|_F^2 + \|c\|_2^2), \quad (8)$$

¹For PDEs with $d > 1$ spatial dimensions, solution snapshots $y(x, t)$ in the trajectory data matrix are vectorized (flattened) before performing the POD.

where $\|\cdot\|_F$ denotes the Frobenius norm, and λ is a Tikhonov regularization coefficient that prevents model overfitting and is often selected through a line search (Swischuk et al., 2020). Ablations on the effects of the regularization intensity λ can be found in Section 4.4.

During online inference, given any initial condition and boundary conditions of interest, the ROM approximates the PDE solution by first calculating the initial modal coefficients corresponding to the initial condition, then propagating the modal coefficients over time according to the reduced dynamics in equation 4, and reconstructing the full-order solution via equation 3.

3.2 PARAMETRIC OPINF AND LLM INTEGRATION

In the previous section, we discussed how OpInf can learn ROMs for PDEs with a single fixed parameter ξ . In this section, we will discuss how OpInf can be extended to parametric PDEs, and how we integrate it with LLMs to solve diverse equations with natural language instructions.

The key insight behind parametric OpInf is as follows (McQuarrie et al., 2023). First, the ROM can share a common basis Φ within a parametric PDE family. Second, once reduced dynamics operators A , H , B , c have been separately obtained for a set of training parameters ξ_1, ξ_2, \dots , reduced dynamics operators for any unseen ξ can be obtained via polynomial regression among the existing operators. Based on those insights, the proposed OpInf-LLM performs the following procedures to solve diverse parametric PDEs.

Basis identification. We collect a trajectory dataset \mathcal{D} in the form of time series of solutions and time derivatives similar to equation 5, but for multiple parameters ξ

$$\begin{aligned} \mathcal{D} = & \{y(\mathbf{x}, t_1, \xi_1), \dots, y(\mathbf{x}, t_K, \xi_1)\} \cup \{y(\mathbf{x}, t_1, \xi_2), \dots\} \\ & \dots \cup \left\{ \frac{\partial y}{\partial t}(\mathbf{x}, t_1, \xi_1), \dots \right\} \cup \left\{ \frac{\partial y}{\partial t}(\mathbf{x}, t_1, \xi_2), \dots \right\} \dots \end{aligned} \quad (9)$$

Here equation 9 shows a single trajectory for each ξ_i for notation conciseness, but multiple trajectories can be used. Then, for a given number of basis functions r , the shared basis $\Phi := [\phi_1(\mathbf{x}), \dots, \phi_r(\mathbf{x})]$ can be obtained via proper orthogonal decomposition (POD) of all solution data y in equation 9.

Operator identification. Once the POD basis is determined, the reduced-order dataset \mathcal{A} of modal coefficients and their time derivatives can be obtained by projecting equation 7 on equation 9

$$\begin{aligned} \mathcal{A} = & \{a(t_1, \xi_1), \dots, a(t_K, \xi_1)\} \cup \{a(t_1, \xi_2), \dots\} \dots \\ & \cup \{\dot{a}(t_1, \xi_1), \dots, \dot{a}(t_K, \xi_1)\} \cup \{\dot{a}(t_1, \xi_2), \dots\} \dots \end{aligned} \quad (10)$$

Then for each ξ_i in the dataset \mathcal{A} , we solve the least-squares problem in equation 8 to obtain the reduced operators $A(\xi_i)$, $H(\xi_i)$, $B(\xi_i)$, $c(\xi_i)$.

OpInf-LLM. Once the above procedures are executed, we integrate large language models (LLMs) to admit natural language instructions specifying the target PDE and its configurations, and leverage LLM tool-calling capabilities to infer the reduced operators and perform time integration, enabling parametric PDE solving across diverse settings. Specifically, given a natural language description of a PDE-solving task (e.g., “solve the viscous Burgers’ equation with viscosity $\nu = 0.03\dots$ ”), the LLM first parses the governing equation and the specified parameters. Based on this information, the LLM calls existing tools to perform polynomial regression to infer the parameter-dependent reduced operators $A(\xi)$, $H(\xi)$, $B(\xi)$, and $c(\xi)$, and then integrates the reduced-order ODE system in equation 4 using the parsed initial and boundary condition specifications. The key features of this integration include: **(i)**. Natural language descriptions of diverse PDEs as instructions; **(ii)**. Low execution failure rate enabled by moderate polynomial fitting and reduced-order ODE integration demands; **(iii)**. Zero-shot generalization to unseen PDE parameters and ICBC configurations from unified ROM structure.

4 EXPERIMENTS

In this section, we evaluate the performance of the proposed OpInf-LLM framework and compare it against representative baseline methods. While many widely used PDE benchmarks focus on fixed or periodic boundary conditions (Li et al., 2020; Raissi et al., 2019; Takamoto et al., 2022;

Gupta & Brandstetter, 2022), we consider parametric PDEs with varying non-homogeneous boundary conditions to highlight the generalization capabilities of the proposed approach. Full experimental details are provided in Appendix A.

4.1 PDES OF INTEREST

Heat Equation. We consider the one-dimensional heat equation

$$y_t(x, t) = \nu y_{xx}(x, t), \quad x \in [0, 1], \quad (11)$$

subject to Dirichlet boundary conditions $y(0, t) = y(1, t) = u(t)$ and a fixed smooth initial condition $y(x, 0) = g(x)$. The boundary input $u(t)$ is a multi-sine signal

$$u(t) = b + \sum_{k=1}^3 A_k \sin(2\pi f_k t + \phi_k), \quad (12)$$

where the amplitudes A_k , frequencies f_k , phases ϕ_k , and bias b are independently randomized for each trajectory. This construction provides persistent excitation across a range of temporal modes.

Training data are generated over a time horizon $T = 1.0$ using diffusivity values $\nu \in \{0.1, 0.5, 2.0\}$ with 3 trajectories per parameter. Number of POD modes is set to $r = 6$ for OpInf and regularization $\lambda = 10^{-6}$. Evaluation is performed on 20 trajectories each corresponding to diffusivity values $\nu \in \{0.5, 1.0, 3.0\}$.

Burgers' Equation. We consider the forced viscous Burgers' equation

$$y_t(x, t) + y y_x(x, t) = \nu y_{xx}(x, t) + s(x, t), \quad x \in [0, 1], \quad (13)$$

with Dirichlet boundary conditions

$$y(0, t) = u_1(t), \quad y(1, t) = u_2(t). \quad (14)$$

The boundary inputs $u_1(t)$ and $u_2(t)$ represent time-dependent boundary conditions, while $s(x, t)$ denotes an internal source term. Both the boundary inputs and the source term are constructed using multi-sine signals, with a fixed spatial profile used to localize the source term. The initial condition is chosen to be smooth and consistent with the boundary values at $t = 0$.

Training data are generated over a time horizon $T = 2.0$ using viscosity parameters $\nu \in \{0.01, 0.02, 0.05, 0.1\}$ with 100 trajectories per parameter. Number of POD modes is set to $r = 10$ for OpInf and regularization $\lambda = 0.5$. Evaluation is performed on 20 trajectories each corresponding to previously unseen viscosity values $\nu \in \{0.03, 0.07\}$, while maintaining the same boundary and forcing input structure.

2D Lid-Driven Cavity Flow. We consider two-dimensional incompressible flow in a square cavity using the vorticity-stream function formulation

$$\omega_t + v_1 \omega_{p_1} + v_2 \omega_{p_2} = \frac{1}{\text{Re}} (\omega_{p_1 p_1} + \omega_{p_2 p_2}), \quad \Delta \psi = -\omega, \quad (15)$$

where ω is the vorticity, $x = (p_1, p_2) \in [0, 1]^2$ denotes the two-dimensional spatial coordinate, subscripts p_1 and p_2 indicate corresponding partial derivatives, and the velocity $v = (v_1, v_2)$ is related to the stream function ψ as

$$v_1 = \psi_{p_2}, \quad v_2 = -\psi_{p_1}. \quad (16)$$

No-slip boundary conditions are enforced on all cavity walls. The top lid is driven by a spatially varying and time-dependent horizontal velocity

$$v_1(x, t) = h(p_1) u(t), \quad v_2 = 0, \quad (17)$$

where $h(p_1)$ is a fixed, non-symmetric spatial profile, and $u(t)$ is a randomized sinusoidal input.

Training data are generated over a time horizon $T = 2.0$ using Reynolds numbers $\text{Re} \in \{50, 75, 100, 125, 150\}$ with 8 trajectories per parameter. The number of POD modes is set to $r = 20$ for OpInf and the regularization strength is fixed to $\lambda = 3$. Model evaluation is carried out on 2 trajectories for each unseen Reynolds numbers $\text{Re} \in \{60, 80, 90, 110, 120, 140\}$.

4.2 BASELINES

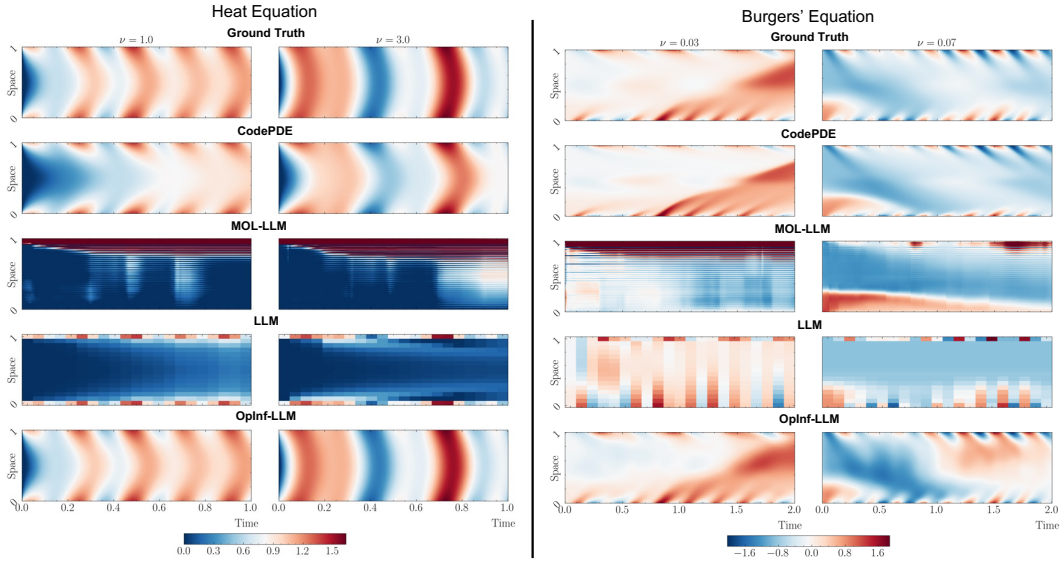


Figure 3: Predictions on Heat and Burgers’ equations with varying parameters. Results are shown for CodePDE, LLM and OpInf-LLM with GPT-4.1.

CodePDE (Li et al., 2025). CodePDE represents a class of LLM-based approaches that directly generate executable PDE solvers in a programming language from a textual description of the governing equations, initial conditions, and boundary conditions. It employs a self-debugging mechanism that iteratively refines generated code using execution feedback. We apply test-time scaling with 5 independent solver generation rounds, each allowing 5 debugging trials, and report the best-performing solver.

MOL-LLM (Negrini et al., 2025). MOL-LLM represents multimodal PDE foundation models with language integration, combining a transformer-based PDE foundation model with language inputs. The model takes as input the initial state of the discretized solution, the PDE parameter vector, and boundary condition parameters, together with textual tokens describing the governing equation. Given these inputs, MOL-LLM outputs the full solution trajectory over a fixed time grid.

MOL-LLM (large dataset). Following the original MOL-LLM work, which is trained on large-scale datasets, we also evaluate a large-data variant of this baseline. In this setting, the same MOL-LLM model and training procedure are used, but the training set is expanded to 5000 trajectories per equation sampled from the same underlying distribution.

LLMs. We directly prompt large language models with the governing PDE, full initial and boundary conditions, external inputs, and a coarse output grid for tractability (heat/Burgers: 16 spatial points \times 41 time steps; cavity: 6 \times 6 spatial points \times 21 time steps), and ask it to return the full spatiotemporal state array in JSON format (3-decimal precision) for a single parameter setting and trajectory. The LLM is treated as a black-box simulator, and its predicted field is compared against downsampled ground truth data using the relative L_2 error. For each parameter instance and equation, the LLM is queried 10 times, and the averaged error over all successful cases is reported. Example prompts are provided in Appendix B.3.

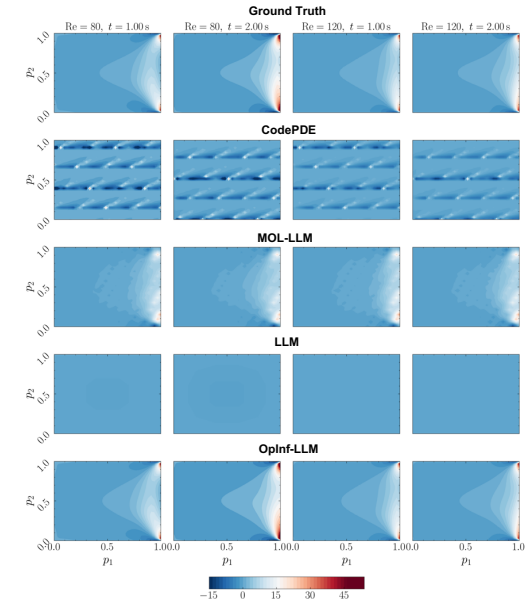


Figure 4: Lid-driven cavity predictions.

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. \uparrow higher is better, \downarrow lower is better.

Method	Data	Train time (s)	Success rate \uparrow	Heat \downarrow	Burgers \downarrow	Cavity \downarrow
CodePDE (GPT-4.1)	–	–	49.9%	<u>1.59e-2</u>	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	<u>6.44e-1</u>
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	<u>99.2%</u>	1.29e-2	<u>4.91e-1</u>	4.63e-2
OpInf-LLM (GPT-4o)	449	30	<u>99.2%</u>	1.29e-2	<u>4.91e-1</u>	4.63e-2
OpInf-LLM (Gemini-2.0-flash)	449	30	<u>99.2%</u>	1.29e-2	<u>4.91e-1</u>	4.63e-2

4.3 RESULTS

We report the results of the proposed OpInf-LLM framework and compare them with baseline methods. Table 1 summarizes the number of training samples, training time, code success rate, and the average relative L_2 error over $[0, T]$ for the heat, Burgers’, and lid-driven cavity flow equations. Visualizations of prediction results across equation parameters and methods are shown in Fig. 3–4.

It can be seen that CodePDE does not consistently produce high-quality solvers, often resulting in either code failures or inaccurate numerical solutions. MOL-LLM achieves a high execution success rate since it is primarily a transformer-based method, but its prediction error becomes large when generalizing to different parameters and boundary conditions is required, and its training cost is substantially higher than that of the other methods. Direct LLM prediction of PDE solutions remains challenging, as existing LLMs tend to infer boundary conditions correctly but zero out or purely interpolate the interior values, and their success rate is further reduced by shape or format mismatches. In contrast, OpInf-LLM yields accurate predictions across all equations while maintaining a high code execution success rate. It requires only a small amount of training data, accepts natural language instructions, and accurately predicts diverse PDE solutions with varying boundary conditions across different instances and previously unseen parameters and configurations.

4.4 ABLATIONS

Extrapolation in time. We examine the capability of OpInf-LLM to extrapolatively predict solutions beyond the time horizons observed during training. Specifically, we evaluate its performance on the interval $[T, 2T]$ for the three equations considered, following the settings in Section 4.1, and report the relative L_2 error in Table 2. Although the framework has never seen any data on $[T, 2T]$, the prediction error remains consistently low and comparable to that on $[0, T]$, demonstrating strong temporal generalization of the proposed method. Additional visualizations on extended horizons are provided in Fig. 5-8 in the Appendix.

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

Number of POD modes. We further examine the effect of the number of POD basis modes in the proposed OpInf-LLM method. Specifically, we follow the settings in Section 4.1 and vary the number of POD modes r from 4 to 10 for each equation instance. We report the total energy captured by the POD basis on the training data, along with the prediction errors on test parameters and configurations for both the original and extended time horizons. Table 3 summarizes the results for Burgers’ equation with full results available in Table 7 in the Appendix. As expected, increasing the number of POD modes captures more energy in the training data and generally improves prediction accuracy, provided

Table 3: POD basis number (r) ablation.

Equation	r	Energy (%)	Error $[0, T]$
Burgers	4	88.01	3.93e-1
Burgers	5	92.26	3.44e-1
Burgers	6	95.63	4.13e-1
Burgers	7	97.26	3.52e-1
Burgers	8	98.31	3.64e-1
Burgers	9	98.85	4.70e-1
Burgers	10	99.20	4.91e-1

Table 4: Regularization intensity (λ) ablation.

Equation	λ	Norm	Error $[0, T]$
Burgers	0	1730.53	2.25e1
Burgers	10^{-6}	1730.53	2.25e1
Burgers	10^{-4}	1645.28	2.25e1
Burgers	10^{-2}	1377.88	2.96e1
Burgers	10^{-1}	346.36	1.81e1
Burgers	1	76.14	3.31e-1
Burgers	10	33.22	3.34e-1

that the additional modes are not overfitting. In practice, capturing around 99% of the energy serves as a useful guideline for selecting the number of POD modes (Kramer et al., 2024). Overly large POD bases can lead to solver instability, as observed for the heat equation with a large number of modes. Nevertheless, the OpInf-LLM framework remains executable across these settings with 100% code success rate, indicating robustness with respect to the choice of POD dimension.

Regularization intensity. We next examine the effect of the regularization strength λ in equation 8 on the proposed OpInf-LLM scheme. Following the settings in Section 4.1, we vary λ logarithmically from 0 to 10 for each equation instance, and report the averaged operator norm $\sqrt{\|A\|_F^2 + \|H\|_F^2 + \|B\|_F^2 + \|c\|_F^2}$ on the training set, together with the prediction errors on test configurations for both the original and extended time horizons. Table 4 shows the results for Burgers’ equation and full results are available in Table 8 in the Appendix. The averaged operator norms decrease as the regularization strength increases, and the best λ for test performance can be identified, which is typically within a range spanning one order of magnitude or more. However, certain regularization values (e.g., $\lambda = 0$ and 10^{-6} for the cavity flow) can lead to failed least-squares optimization due to numerical singularity. In practice, ablations over a range of regularization values are typically performed on a validation set, and the operator norm is jointly considered to determine an appropriate λ , with low validation error and a moderate operator norm being desired (Golub et al., 1979; McQuarrie et al., 2021).

5 DISCUSSION

In this section, we discuss limitations and potential extensions of the proposed OpInf-LLM method. For a given PDE family, the same reduced basis can be reused across different parameter values and configurations, but new bases are usually constructed when introducing new governing equations, although such cost is incurred upfront offline rather than introducing additional computation at inference time. Notably, the OpInf framework does not require explicit knowledge of the full PDE form and only assumes the type of nonlinearity in the reduced dynamics, such as linear or quadratic structure, without needing the specific PDE instance or parameter values, which makes it well suited for settings in which the governing equations are partially unknown or difficult to identify. In addition, although we employ the standard OpInf in our framework (Peherstorfer & Willcox, 2016), extensions of the OpInf framework that improve its robustness and accuracy (Sawant et al., 2023; Geng et al., 2024) can be potentially used to further enhance the performance of OpInf-LLM.

6 CONCLUSIONS

In this work, we provide a new perspective on reduced order modeling for LLM-based PDE solving, and propose OpInf-LLM, an LLM parametric PDE solving framework via operator inference. The proposed framework leverages shared reduced-order bases across each PDE family to support accurate, generalizable solutions under varying boundary conditions from limited data. By reformulating parametric PDE solving as polynomial regression in a reduced-order operator space followed by ODE integration, OpInf-LLM is able to solve unseen PDE instances from natural language instructions while achieving improved trade-offs between accuracy and execution success rate. Ablations further show robustness over extended test horizons and different OpInf configurations. Future directions include integrating more advanced operator inference techniques and developing richer language–solver interfaces for scalable scientific computing.

ACKNOWLEDGMENTS

This material is based upon work supported in part by the National Science Foundation under Grant number 2442948, and in part by a grant from the Commonwealth of Pennsylvania, Department of Community and Economic Development. Saviz Mowlavi is supported solely by Mitsubishi Electric Research Laboratories.

REFERENCES

- Jiajun Bao, Nicolas Boullé, Toni JB Liu, Raphaël Sarfati, and Christopher J Earls. Text-trained llms can zero-shot extrapolate pde dynamics. *arXiv preprint arXiv:2509.06322*, 2025.
- Peter Benner, Serkan Gugercin, and Karen Willcox. A survey of projection-based model reduction methods for parametric dynamical systems. *SIAM review*, 57(4):483–531, 2015.
- Johannes Brandstetter, Daniel Worrall, and Max Welling. Message passing neural pde solvers. *arXiv preprint arXiv:2202.03376*, 2022.
- Steven L Brunton and J Nathan Kutz. *Data-driven science and engineering: Machine learning, dynamical systems, and control*. Cambridge University Press, 2022.
- Shengze Cai, Zhicheng Wang, Sifan Wang, Paris Perdikaris, and George Em Karniadakis. Physics-informed neural networks for heat transfer problems. *Journal of Heat Transfer*, 143(6), 2021.
- Anindya Chatterjee. An introduction to the proper orthogonal decomposition. *Current science*, pp. 808–817, 2000.
- Woojin Cho, Minju Jo, Haksoo Lim, Kookjin Lee, Dongeun Lee, Sanghyun Hong, and Noseong Park. Parameterized physics-informed neural networks for parameterized pdes. *arXiv preprint arXiv:2408.09446*, 2024.
- Salvatore Cuomo, Vincenzo Schiano Di Cola, Fabio Giampaolo, Gianluigi Rozza, Maziar Raissi, and Francesco Piccialli. Scientific machine learning through physics-informed neural networks: Where we are and what’s next. *Journal of Scientific Computing*, 92(3):88, 2022.
- Mengge Du, Yuntian Chen, Zhongzheng Wang, Longfeng Nie, and Dongxiao Zhang. Llm4ed: Large language models for automatic equation discovery. *arXiv preprint arXiv:2405.07761*, 2024.
- Saarth Gaonkar, Xiang Zheng, Haocheng Xi, Rishabh Tiwari, Kurt Keutzer, Dmitriy Morozov, Michael W Mahoney, and Amir Gholami. Sciml agents: Write the solver, not the solution. *arXiv preprint arXiv:2509.09936*, 2025.
- Yuwei Geng, Jasdeep Singh, Lili Ju, Boris Kramer, and Zhu Wang. Gradient preserving operator inference: Data-driven reduced-order models for equations with gradient structure. *Computer Methods in Applied Mechanics and Engineering*, 427:117033, 2024.
- Gene H Golub, Michael Heath, and Grace Wahba. Generalized cross-validation as a method for choosing a good ridge parameter. *Technometrics*, 21(2):215–223, 1979.
- Somdatta Goswami, Aniruddha Bora, Yue Yu, and George Em Karniadakis. Physics-informed deep neural operator networks. In *Machine learning in modeling and simulation: methods and applications*, pp. 219–254. Springer, 2023.
- Arya Grayeli, Atharva Sehgal, Omar Costilla Reyes, Miles Cranmer, and Swarat Chaudhuri. Symbolic regression with a learned concept library. *Advances in Neural Information Processing Systems*, 37: 44678–44709, 2024.
- Jayesh K Gupta and Johannes Brandstetter. Towards multi-spatiotemporal-scale generalized pde modeling. *arXiv preprint arXiv:2209.15616*, 2022.
- Jiequn Han, Arnulf Jentzen, and Weinan E. Solving high-dimensional partial differential equations using deep learning. *Proceedings of the National Academy of Sciences*, 115(34):8505–8510, 2018.

- Zhongkai Hao, Chang Su, Songming Liu, Julius Berner, Chengyang Ying, Hang Su, Anima Anandkumar, Jian Song, and Jun Zhu. Dpot: Auto-regressive denoising operator transformer for large-scale pde pre-training. *arXiv preprint arXiv:2403.03542*, 2024.
- Xin He, Liangliang You, Hongduan Tian, Bo Han, Ivor Tsang, and Yew-Soon Ong. Lang-pinn: From language to physics-informed neural networks via a multi-agent framework. *arXiv preprint arXiv:2510.05158*, 2025.
- Maximilian Herde, Bogdan Raonic, Tobias Rohner, Roger Käppeli, Roberto Molinaro, Emmanuel de Bézenac, and Siddhartha Mishra. Poseidon: Efficient foundation models for pdes. *Advances in Neural Information Processing Systems*, 37:72525–72624, 2024.
- Philip Holmes, John L. Lumley, Gahl Berkooz, and Clarence W. Rowley. *Turbulence, Coherent Structures, Dynamical Systems and Symmetry*. Cambridge University Press, 2 edition, 2012. ISBN 9781107008250. doi: 10.1017/CBO9780511919701.
- Jun-Ting Hsieh, Shengjia Zhao, Stephan Eismann, Lucia Mirabella, and Stefano Ermon. Learning neural pde solvers with convergence guarantees. *arXiv preprint arXiv:1906.01200*, 2019.
- Xiang Huang, Zhanhong Ye, Hongsheng Liu, Shi Ji, Zidong Wang, Kang Yang, Yang Li, Min Wang, Haotian Chu, Fan Yu, et al. Meta-auto-decoder for solving parametric partial differential equations. *Advances in Neural Information Processing Systems*, 35:23426–23438, 2022.
- Nam Huynh and Beiyu Lin. Large language models for code generation: A comprehensive survey of challenges, techniques, evaluation, and applications. *arXiv preprint arXiv:2503.01245*, 2025.
- Juyong Jiang, Fan Wang, Jiasi Shen, Sungju Kim, and Sunghun Kim. A survey on large language models for code generation. *arXiv preprint arXiv:2406.00515*, 2024.
- Qile Jiang and George Karniadakis. Agenticsciml: Collaborative multi-agent systems for emergent discovery in scientific machine learning. *arXiv preprint arXiv:2511.07262*, 2025.
- Qile Jiang, Zhiwei Gao, and George Em Karniadakis. Deepseek vs. chatgpt vs. claude: A comparative study for scientific computing and scientific machine learning tasks. *Theoretical and Applied Mechanics Letters*, 15(3):100583, 2025.
- George Em Karniadakis, Ioannis G Kevrekidis, Lu Lu, Paris Perdikaris, Sifan Wang, and Liu Yang. Physics-informed machine learning. *Nature Reviews Physics*, 3(6):422–440, 2021.
- Nikola Kovachki, Zongyi Li, Burigede Liu, Kamyar Azizzadenesheli, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. Neural operator: Learning maps between function spaces with applications to pdes. *Journal of Machine Learning Research*, 24(89):1–97, 2023.
- Boris Kramer, Benjamin Peherstorfer, and Karen E Willcox. Learning nonlinear reduced models from data with operator inference. *Annual Review of Fluid Mechanics*, 56(1):521–548, 2024.
- Shanda Li, Tanya Marwah, Junhong Shen, Weiwei Sun, Andrej Risteski, Yiming Yang, and Ameet Talwalkar. Codepde: An inference framework for llm-driven pde solver generation. *arXiv preprint arXiv:2505.08783*, 2025.
- Zenan Li, Yifan Wu, Zhaoyu Li, Xinming Wei, Xian Zhang, Fan Yang, and Xiaoxing Ma. Autoformalize mathematical statements by symbolic equivalence and semantic consistency. *Advances in Neural Information Processing Systems*, 37:53598–53625, 2024a.
- Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. Fourier neural operator for parametric partial differential equations. *arXiv preprint arXiv:2010.08895*, 2020.
- Zongyi Li, Hongkai Zheng, Nikola Kovachki, David Jin, Haoxuan Chen, Burigede Liu, Kamyar Azizzadenesheli, and Anima Anandkumar. Physics-informed neural operator for learning partial differential equations. *ACM/JMS Journal of Data Science*, 1(3):1–27, 2024b.
- Jianming Liu, Ren Zhu, Jian Xu, Kun Ding, Xu-Yao Zhang, Gaofeng Meng, and Cheng-Lin Liu. Pde-agent: A toolchain-augmented multi-agent framework for pde solving. *arXiv preprint arXiv:2512.16214*, 2025.

- Xin-Yang Liu, Min Zhu, Lu Lu, Hao Sun, and Jian-Xun Wang. Multi-resolution partial differential equations preserved learning framework for spatiotemporal dynamics. *Communications Physics*, 7(1):31, 2024a.
- Yuxuan Liu, Jingmin Sun, Xinjie He, Griffin Pinney, Zecheng Zhang, and Hayden Schaeffer. Prose-fd: A multimodal pde foundation model for learning multiple operators for forecasting fluid dynamics. *arXiv preprint arXiv:2409.09811*, 2024b.
- Cooper Lorsung and Amir Barati Farimani. Explain like i'm five: Using llms to improve pde surrogate models with text. *arXiv preprint arXiv:2410.01137*, 2024.
- Lu Lu, Pengzhan Jin, and George Em Karniadakis. Deeponet: Learning nonlinear operators for identifying differential equations based on the universal approximation theorem of operators. *arXiv preprint arXiv:1910.03193*, 2019.
- Lu Lu, Pengzhan Jin, Guofei Pang, Zhongqiang Zhang, and George Em Karniadakis. Learning nonlinear operators via deeponet based on the universal approximation theorem of operators. *Nature machine intelligence*, 3(3):218–229, 2021.
- Lu Lu, Xuhui Meng, Shengze Cai, Zhiping Mao, Somdatta Goswami, Zhongqiang Zhang, and George Em Karniadakis. A comprehensive and fair comparison of two neural operators (with practical extensions) based on fair data. *Computer Methods in Applied Mechanics and Engineering*, 393:114778, 2022.
- Shane A McQuarrie, Cheng Huang, and Karen E Willcox. Data-driven reduced-order models via regularised operator inference for a single-injector combustion process. *Journal of the Royal Society of New Zealand*, 51(2):194–211, 2021.
- Shane A McQuarrie, Parisa Khodabakhshi, and Karen E Willcox. Nonintrusive reduced-order models for parametric partial differential equations via data-driven operator inference. *SIAM Journal on Scientific Computing*, 45(4):A1917–A1946, 2023.
- Agnieszka Mensfelt, David Tena Cucala, Santiago Franco, Angeliki Koutsoukou-Argraki, Vince Trencsenyi, and Kostas Stathis. Towards a common framework for autoformalization. *arXiv preprint arXiv:2509.09810*, 2025.
- Elisa Negrini, Yuxuan Liu, Liu Yang, Stanley J Osher, and Hayden Schaeffer. A multimodal pde foundation model for prediction and scientific text descriptions. *arXiv preprint arXiv:2502.06026*, 2025.
- Mohamed Nejjar, Luca Zacharias, Fabian Stiehle, and Ingo Weber. Llms for science: Usage for code generation and data analysis. *Journal of Software: Evolution and Process*, 37(1):e2723, 2025.
- Michel Nohra and Steven Dufour. Physics-informed neural networks for the numerical modeling of steady-state and transient electromagnetic problems with discontinuous media. *arXiv preprint arXiv:2406.04380*, 2024.
- Vivek Oommen, Khemraj Shukla, Saaketh Desai, Rémi Dingreville, and George Em Karniadakis. Rethinking materials simulations: Blending direct numerical simulations with neural operators. *npj Computational Materials*, 10(1):145, 2024.
- Jaideep Pathak, Shashank Subramanian, Peter Harrington, Sanjeev Raja, Ashesh Chattopadhyay, Morteza Mardani, Thorsten Kurth, David Hall, Zongyi Li, Kamyar Azizzadenesheli, et al. Fourcast-net: A global data-driven high-resolution weather model using adaptive fourier neural operators. *arXiv preprint arXiv:2202.11214*, 2022.
- Benjamin Peherstorfer and Karen Willcox. Data-driven operator inference for nonintrusive projection-based model reduction. *Computer Methods in Applied Mechanics and Engineering*, 306:196–215, 2016.
- Elizabeth Qian, Boris Kramer, Benjamin Peherstorfer, and Karen Willcox. Lift & learn: Physics-informed machine learning for large-scale nonlinear dynamical systems. *Physica D: Nonlinear Phenomena*, 406:132401, 2020.

- Elizabeth Qian, Ionut-Gabriel Farcas, and Karen Willcox. Reduced operator inference for nonlinear partial differential equations. *SIAM Journal on Scientific Computing*, 44(4):A1934–A1959, 2022.
- Maziar Raissi, Paris Perdikaris, and George E Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational physics*, 378:686–707, 2019.
- Mahindra Singh Rautela, Alexander Most, Siddharth Mansingh, Bradley C Love, Ayan Biswas, Diane Oyen, and Earl Lawrence. Morph: Pde foundation models with arbitrary data modality. *arXiv preprint arXiv:2509.21670*, 2025.
- Nihar Sawant, Boris Kramer, and Benjamin Peherstorfer. Physics-informed regularization and structure preservation for learning stable reduced models from data with operator inference. *Computer Methods in Applied Mechanics and Engineering*, 404:115836, 2023.
- Junhong Shen, Tanya Marwah, and Ameet Talwalkar. Ups: Efficiently building foundation models for pde solving via cross-modal adaptation. *arXiv preprint arXiv:2403.07187*, 2024.
- Parshin Shojaee, Kazem Meidani, Shashank Gupta, Amir Barati Farimani, and Chandan K Reddy. Llm-sr: Scientific equation discovery via programming with large language models. *arXiv preprint arXiv:2404.18400*, 2024.
- Mauricio Soroco, Jialin Song, Mengzhou Xia, Kye Emond, Weiran Sun, and Wuyang Chen. Pde-controller: Llms for autoformalization and reasoning of pdes. *arXiv preprint arXiv:2502.00963*, 2025.
- Jingmin Sun, Yuxuan Liu, Zecheng Zhang, and Hayden Schaeffer. Towards a foundation model for partial differential equations: Multioperator learning and extrapolation. *Physical Review E*, 111(3):035304, 2025.
- Renee Swischuk, Boris Kramer, Cheng Huang, and Karen Willcox. Learning physics-based reduced-order models for a single-injector combustion process. *AIAA Journal*, 58(6):2658–2672, 2020.
- Makoto Takamoto, Timothy Praditia, Raphael Leiteritz, Daniel MacKinlay, Francesco Alesiani, Dirk Pflüger, and Mathias Niepert. Pdebench: An extensive benchmark for scientific machine learning. *Advances in Neural Information Processing Systems*, 35:1596–1611, 2022.
- Makoto Takamoto, Francesco Alesiani, and Mathias Niepert. Learning neural pde solvers with parameter-guided channel attention. In *International Conference on Machine Learning*, pp. 33448–33467. PMLR, 2023.
- Ke Weng, Lun Du, Sirui Li, Wangyue Lu, Haozhe Sun, Hengyu Liu, and Tiancheng Zhang. Autoformalization in the era of large language models: A survey. *arXiv preprint arXiv:2505.23486*, 2025.
- Florian Wiesner, Matthias Wessling, and Stephen Baek. Towards a physics foundation model. *arXiv preprint arXiv:2509.13805*, 2025.
- Haoyang Wu, Xinxin Zhang, and Lailai Zhu. Automated code development for pde solvers using large language models. *arXiv preprint arXiv:2509.25194*, 2025.
- Yuhuai Wu, Albert Qiaochu Jiang, Wenda Li, Markus Rabe, Charles Staats, Mateja Jamnik, and Christian Szegedy. Autoformalization with large language models. *Advances in neural information processing systems*, 35:32353–32368, 2022.
- Hao Xu, Yuntian Chen, Rui Cao, Tianning Tang, Mengge Du, Jian Li, Adrian H Callaghan, and Dongxiao Zhang. Generative discovery of partial differential equations by learning from math handbooks. *Nature Communications*, 16(1):10255, 2025a.
- Jundong Xu, Hao Fei, Liangming Pan, Qian Liu, Mong-Li Lee, and Wynne Hsu. Faithful logical reasoning via symbolic chain-of-thought. *arXiv preprint arXiv:2405.18357*, 2024.
- Weikai Xu, Chengrui Huang, Shen Gao, and Shuo Shang. Llm-based agents for tool learning: A survey: W. xu et al. *Data Science and Engineering*, pp. 1–31, 2025b.

Liu Yang, Siting Liu, and Stanley J Osher. Fine-tune language models as multi-modal differential equation solvers. *Neural Networks*, pp. 107455, 2025.

Zhanhong Ye, Xiang Huang, Leheng Chen, Hongsheng Liu, Zidong Wang, and Bin Dong. Pdeformer: Towards a foundation model for one-dimensional partial differential equations. *arXiv preprint arXiv:2402.12652*, 2024.

Anthony Zhou, Zijie Li, Michael Schneier, John R Buchanan Jr, and Amir Barati Farimani. Text2pde: Latent diffusion models for accessible physics simulation. *arXiv preprint arXiv:2410.01153*, 2024.

Hang Zhou, Yuezhou Ma, Haixu Wu, Haowen Wang, and Mingsheng Long. Unisolver: Pde-conditional transformers are universal neural pde solvers. In *ICLR 2025 Workshop on Foundation Models in the Wild*, 2025.

Min Zhu, Jingmin Sun, Zecheng Zhang, Hayden Schaeffer, and Lu Lu. Pi-mfm: Physics-informed multimodal foundation model for solving partial differential equations. *arXiv preprint arXiv:2512.23056*, 2025.

A EXPERIMENT DETAILS

Below we provide additional details on input signal generation, numerical discretization, dataset construction, and simulation settings for the PDE systems described in Section 4.1.

A.1 HEAT EQUATION

The initial condition for the heat equation is fixed across all trajectories and given by

$$g(x) = \exp(\alpha(x - 1)) + \exp(-\alpha x) - \exp(-\alpha), \quad \alpha = 100. \quad (18)$$

The Dirichlet boundary input $u(t)$ applied at both ends of the domain is constructed as a three-component multi-sine signal

$$u(t) = b + \sum_{k=1}^3 A_k \sin(2\pi f_k t + \phi_k), \quad (19)$$

where, for each trajectory, the amplitudes $A_k \sim \mathcal{U}(0.1, 0.5)$, frequencies $f_k \sim \mathcal{U}(0.2, 5.0)$, phases $\phi_k \sim \mathcal{U}(0, 2\pi)$, and bias $b \sim \mathcal{U}(0.8, 1.2)$ are sampled independently. Independent realizations of the boundary input are used for training and test datasets.

The spatial domain $x \in [0, 1]$ is discretized using 1023 uniformly spaced interior points, and the second-order central finite difference scheme is used to generate full-order PDE solution. Training trajectories are sampled at 1001 uniformly spaced time instances over the horizon $T = 1.0$, with BDF integrator. For evaluation, trajectories are generated over the extended horizon $T_{\text{test}} = 2.0$ using 2001 time steps.

A.2 BURGERS' EQUATION

The Burgers' equation includes an internal source term $s(x, t)$ with a fixed spatial profile and a time-dependent amplitude. The spatial component of the source is defined as

$$s_0(x) = \cosh\left(\frac{x - 0.5}{0.05}\right)^{-1}, \quad (20)$$

and the full source term is given by

$$s(x, t) = s_0(x) \sigma(t), \quad (21)$$

where the temporal modulation $\sigma(t)$ is generated as a single-component sinusoidal signal

$$\sigma(t) = b_s + A_s \sin(2\pi f_s t + \phi_s). \quad (22)$$

The parameters are sampled independently for each trajectory according to $A_s \sim \mathcal{U}(0.1, 3.0)$, $f_s \sim \mathcal{U}(0.2, 1.0)$, $\phi_s \sim \mathcal{U}(0, 2\pi)$, and $b_s \sim \mathcal{U}(-1.0, 1.0)$.

The system is subject to time-dependent Dirichlet boundary conditions

$$y(0, t) = u_1(t), \quad y(1, t) = u_2(t), \quad (23)$$

where the boundary inputs $u_1(t)$ and $u_2(t)$ are generated independently as three-component multi-sine signals of the form

$$u_i(t) = b_i + \sum_{k=1}^3 A_{i,k} \sin(2\pi f_{i,k} t + \phi_{i,k}), \quad i \in \{1, 2\}. \quad (24)$$

For each trajectory, the amplitudes $A_{i,k} \sim \mathcal{U}(0.1, 1.0)$, frequencies $f_{i,k} \sim \mathcal{U}(0.2, 5.0)$, phases $\phi_{i,k} \sim \mathcal{U}(0, 2\pi)$, and biases $b_i \sim \mathcal{U}(-0.5, 0.5)$ are sampled independently.

The initial condition is constructed to be smooth and consistent with the boundary values at $t = 0$:

$$y(x, 0) = u_2(0) + \frac{1}{2}(u_1(0) - u_2(0)) \left[1 - \tanh\left(\frac{x - 0.3}{0.1}\right) \right]. \quad (25)$$

The spatial discretization uses Chebyshev collocation with $N = 64$ interior points. For evaluation and visualization, the solution is interpolated onto a uniform grid with 1001 points. Training trajectories span the time horizon $T = 2.0$ with 1001 time steps, while test trajectories span $T_{\text{test}} = 4.0$ with 2001 time steps. All source and boundary signals are sampled independently across trajectories. RK45 integrator is used for full-order solution generation.

A.3 2D LID-DRIVEN CAVITY FLOW

The no-slip boundary conditions enforce zero velocity on all walls except the top lid. The horizontal velocity on the top boundary is prescribed as

$$v_1(x, t) = h(p_1) u(t), \quad v_2(x, t) = 0, \quad (26)$$

where the fixed spatial profile is

$$h(p_1) = 1 + 0.3 \sin(2\pi p_1) + 0.2 p_1. \quad (27)$$

The temporal modulation $u(t)$ is generated as a single-sine signal

$$u(t) = b + A \sin(2\pi f t + \phi), \quad (28)$$

where $b \sim \mathcal{U}(0.7, 1.3)$, $A \sim \mathcal{U}(0.1, 0.4)$, $f \sim \mathcal{U}(0.5, 2.0)$, and $\phi \sim \mathcal{U}(0, 2\pi)$ are sampled independently for each trajectory.

The cavity domain is defined on $x = (p_1, p_2) \in [0, 1]^2$ and discretized using a uniform grid with 32 interior points in each spatial direction, resulting in a (34×34) grid including boundary points. The full-order solver uses a fixed time step $\Delta t = 10^{-3}$, with second-order finite difference scheme in space and forward Euler temporal integration. Training data are collected over the horizon $T = 2.0$, with solution snapshots recorded every 0.02 time units, yielding 101 snapshots per trajectory. For evaluation, trajectories are simulated over $T_{\text{test}} = 4.0$ using the same solver and snapshot spacing.

A.4 DATASET CONSTRUCTION

For all PDE systems, training and test datasets are generated using independent random seeds for boundary and forcing inputs. Each dataset consists of multiple trajectories corresponding to different realizations of input signals and, where applicable, different physical parameter values.

All reported results are obtained using identical datasets across methods to ensure fair comparison. Numerical solvers, discretization schemes, and time-stepping parameters are fixed across training and testing, and no test-time information is used during model training.

B IMPLEMENTATION DETAILS

B.1 CODEPDE

We evaluate CodePDE (Li et al., 2025) using 5 rounds of solver generation for each PDE, with 5 debug trials for each round. The test performance is measured using the relative L_2 error over the full time horizon. The best solver for each equation is reported for prediction errors. Success rate is calculated based on trial-level failures. The prompts and solver templates for all equations are shown below.

Prompts:

```
heat_description = '''
The PDE is the 1D heat equation with time-varying Dirichlet boundary
conditions, given by

\\[
\\begin{{cases}}
\\partial_t u(t, x) = \\nu \\partial_{{xx}} u(t, x), & x \\in (0,1), \\;
t \\in (0,T) \\\\
u(0, x) = u_0(x), & x \\in (0,1) \\\\
u(t, 0) = u_{{bc}}(t), & t \\in (0,T) \\\\
u(t, 1) = u_{{bc}}(t), & t \\in (0,T)
\\end{{cases}}
\\]

where $\\nu$ is the thermal diffusivity coefficient. **Note that the
boundary conditions are symmetric** (same function at both
boundaries) and time-varying.
```

```

**Initial Condition (Fixed)**: The initial condition is a fixed
    exponential profile given by
    \[
    u_0(x) = e^{\{100(x-1)\}} + e^{\{-100x\}} - e^{\{-100\}}
    \]
    This creates steep gradients near the boundaries with approximate zero
    values at both ends.

**Boundary Conditions (Time-varying)**: The boundary value  $u_{\{bc\}}(t)$ 
    is provided as an input array of shape [batch_size, T+1] containing
    the boundary values at each time step. The same values apply to both
     $x=0$  and  $x=1$  (symmetric boundaries).

    Given the discretization of the boundary condition values  $u_{\{bc\}}(t)$ 
    of shape [batch_size, T+1], you need to implement a solver that:
    1. Computes the fixed initial condition for the given spatial grid
    2. Solves the heat equation forward in time while enforcing the
       time-varying boundary conditions
    3. Returns the solution of shape [batch_size, T+1, N] where N=1023
       (interior spatial points)

    In particular, your code should be tailored to the case where
     $\nu = \text{opinf\_heat\_nu}$ , i.e., optimizing it particularly for this
    use case.

**Important implementation notes**:
    - Use 1023 interior spatial points (not including boundaries at  $x=0$ 
      and  $x=1$ )
    - The domain is  $x \in [0,1]$  with  $dx \approx 9.766 \times 10^{\{-4\}}$ 
    - Time horizon is  $T=1.0$  with 1001 time points ( $dt = 10^{\{-3\}}$ )
    - The boundary conditions must be enforced at every time step
    - Consider using implicit methods (e.g., BDF, Crank-Nicolson) for
      stability
    - Use finite difference for spatial discretization (2nd order central
      differences recommended)
    '''

    burgers_description = '''
    The PDE is the 1D Burgers equation with asymmetric time-varying
    Dirichlet boundary conditions and a localized source term, given by

    \[
    \begin{cases}
    \partial_t u(t, x) + u(t, x) \partial_x u(t, x) = \nu
      \partial_{xx} u(t, x) + s(x) \cdot w_3(t), & x \in (0,1), \quad t \\
      \in (0,T) \\
    u(0, x) = u_0(x), & x \in (0,1) \\
    u(t, 0) = w_1(t), & t \in (0,T) \\
    u(t, 1) = w_2(t), & t \in (0,T)
    \end{cases}
    \]

    where  $\nu$  is the viscosity coefficient, and we have three
    time-varying input functions provided as arrays:
    -  $w_1(t)$ : Left boundary condition (shape [batch_size, T+1])
    -  $w_2(t)$ : Right boundary condition (shape [batch_size, T+1])
    -  $w_3(t)$ : Source term temporal modulation (shape [batch_size, T+1])

**Initial Condition (Variable)**: The initial condition depends on the
    boundary values at  $t=0$  and must be computed:
    \[
    u_0(x) = w_2(0) + 0.5(w_1(0) - w_2(0))(1 - \tanh((x - 0.3)/0.1))
    \]
  
```

This creates a smooth transition from the left BC to the right BC, centered at $x=0.3$ with transition width 0.1 .

Source Term (Localized): The spatial source profile is a narrow bell-shaped function centered at $x=0.5$:

$$s(x) = \frac{1}{\cosh^2\left(\frac{x - 0.5}{0.05}\right)} = \frac{1}{\cosh^2\left(\frac{x - 0.5}{0.05}\right)}$$

The full source term is $s(x) \cdot w_3(t)$, where $w_3(t)$ modulates the source strength in time (element-wise multiplication for each spatial point).

Boundary Conditions (Asymmetric, Time-varying): The left and right boundaries have **independent** time-varying values $w_1(t) \neq w_2(t)$.

Given the discretization of the boundary functions $w_1(t)$, $w_2(t)$, and source modulation $w_3(t)$ (each of shape $[batch_size, T+1]$), you need to implement a solver that:

1. Computes the initial condition from $w_1(0)$ and $w_2(0)$
2. Evaluates the spatial source profile $s(x)$ on the grid
3. Solves the Burgers equation forward in time with boundary conditions and source term
4. Returns the solution of shape $[batch_size, T+1, N]$ where N is the number of spatial grid points

In particular, your code should be tailored to the case where $\nu = \text{opinf_burgers_nu}$, i.e., optimizing it particularly for this use case.

Important implementation notes:

- Spatial discretization: 1001 points uniformly spaced in $[0,1]$ (including boundaries) or use spectral methods
- Time horizon is $T=2.0$ with 1001 time points ($dt = 2 \times 10^{-3}$)
- The source term is localized at the center ($x=0.5$) with very narrow width (0.05)
- Boundary conditions are **asymmetric**: $w_1(t) \neq w_2(t)$
- The nonlinear convection term $u \frac{\partial u}{\partial x}$ can cause shocks/steep gradients at low viscosity
- Consider using explicit methods (e.g., RK45) or spectral methods for accuracy
- Pay special attention to handling the localized source term accurately

```
'''
cavity_description = '''
The PDE is the 2D lid-driven cavity flow in vorticity-streamfunction
form:

[[
\omega_t + u \omega_x + v \omega_y = \frac{1}{Re}(\omega_{xx}
+ \omega_{yy}), \quad (x, y) \in (0,1)^2
]]
[[
\Delta \psi = -\omega, \quad u = \psi_y, \quad v = -\psi_x
]]

Boundary conditions are no-slip on all walls. The top lid has a
time-varying velocity:

[[
u_{lid}(x, t) = a(x) f(t), \quad v=0
]]
where the fixed spatial profile is:
[[
```

```

a(x) = 1 + 0.3\\sin(2\\pi x) + 0.2x
\\]
and the input is a scalar function f(t).

Given the discretization of f(t) as an input array of shape [batch_size,
T+1], you need to implement
a solver that returns the vorticity field \\omega(t, x, y) for all
times. The solution should be of shape
[batch_size, T+1, N, N] where N=34 (32 interior points plus boundaries).

In particular, your code should be tailored to the case where
Re={opinf_cavity_re}.

Important implementation notes:
- Initial condition: \\omega(x, y, 0) = 0 and \\psi(x, y, 0) = 0
- Spatial grid: 34x34 uniform grid on [0, 1]^2
- Time step in the full-order model is dt = 0.001 with snapshots every
0.02
- Use finite differences for spatial derivatives and a Poisson solver
for \\psi
- Consider small internal time steps for stability
'''

```

Solver templates:

```

1
2 import numpy as np
3
4 def solver(u_bc, t_coordinate, nu):
5     """Solves the 1D heat equation with time-varying Dirichlet boundary
6     conditions.
7
8     Args:
9         u_bc (np.ndarray): Boundary condition values at both x=0 and x=1
10        Shape: [batch_size, T+1] where T+1 is the number of time
11        points.
12        The same boundary value applies to both boundaries (symmetric
13        ).
14        t_coordinate (np.ndarray): Time coordinates of shape [T+1].
15        It begins with t_0=0 and follows the time steps t_1, ..., t_T
16        .
17        nu (float): Thermal diffusivity coefficient.
18
19    Returns:
20        solutions (np.ndarray): Shape [batch_size, T+1, N] where N=1023 (
21        interior points).
22        solutions[:, 0, :] contains the initial conditions (fixed
23        exponential profile),
24        solutions[:, i, :] contains the solutions at time
25        t_coordinate[i].
26    """
27    # TODO: Implement the solver for the heat equation with time-varying
28    # BCs
29    #
30    # Key implementation steps:
31    # 1. Create spatial grid: N=1023 interior points in [0, 1]
32    #    x = linspace(0, 1, 1025)[1:-1] # Interior points only
33    #    dx = 1/1024
34    #
35    # 2. Compute fixed initial condition:
36    #    u0 = exp(100*(x-1)) + exp(-100*x) - exp(-100)
37    #
38    # 3. Set up finite difference matrix for d^2/dx^2 (2nd order central)
39    #
40    # 4. Time integration loop:

```

```

33 # - Enforce boundary conditions at each time step
34 # - Solve:  $du/dt = \nu * d^2 u/dx^2$ 
35 # - Consider using implicit methods (BDF, Crank-Nicolson) for
stability
36 #
37 # Hints:
38 # - Use scipy.integrate.solve_ivp with method='BDF' or implement
implicit scheme
39 # - Consider using PyTorch or JAX for GPU acceleration
40 # - Remember that u_bc has shape [batch_size, T+1] with same values
for both boundaries
41
42 return solutions
43
44
45
46 def solver(w1_bc, w2_bc, source, t_coordinate, nu):
47     """Solves the 1D Burgers equation with asymmetric time-varying
Dirichlet BCs and source term.
48
49     Args:
50         w1_bc (np.ndarray): Left boundary condition values at x=0
51             Shape: [batch_size, T+1] where T+1 is the number of time
points.
52         w2_bc (np.ndarray): Right boundary condition values at x=1
53             Shape: [batch_size, T+1]. Note: w1 != w2 (asymmetric
boundaries).
54         source (np.ndarray): Source term temporal modulation w3(t)
55             Shape: [batch_size, T+1]. This modulates the spatial source
profile s(x).
56         t_coordinate (np.ndarray): Time coordinates of shape [T+1].
57             It begins with t_0=0 and follows the time steps t_1, ..., t_T.
58
59         nu (float): Viscosity coefficient.
60
61     Returns:
62         solutions (np.ndarray): Shape [batch_size, T+1, N] where N is
spatial grid points.
63         solutions[:, 0, :] contains the initial conditions (computed
from w1(0), w2(0)),
64         solutions[:, i, :] contains the solutions at time
t_coordinate[i].
65     """
66     # TODO: Implement the solver for Burgers equation with BCs and source
term
67     #
68     # Key implementation steps:
69     # 1. Create spatial grid: N=1001 points (including boundaries) or use
spectral
70     #     x = linspace(0, 1, 1001) for uniform grid
71     #     dx = 1/1000
72     #
73     # 2. Compute spatial source profile s(x):
74     #     s_x = 1 / cosh^2((x - 0.5) / 0.05)
75     #     This is a narrow bell-shaped function centered at x=0.5
76     #
77     # 3. Compute initial condition for each batch item:
78     #     u0 = w2_bc[:, 0] + 0.5 * (w1_bc[:, 0] - w2_bc[:, 0]) * (1 - tanh
((x - 0.3) / 0.1))
79     #     Note: u0 depends on boundary values at t=0
80     #
81     # 4. Time integration loop:
82     #     - Enforce boundary conditions at each time step:
83     #         u[:, 0] = w1_bc[:, t_idx] (left)
84     #         u[:, -1] = w2_bc[:, t_idx] (right)

```

```

84 # - Solve:  $du/dt + u*du/dx = \nu*d^2 u/dx^2 + s(x)*source[:, t\_idx]$ 
85 # - Consider using RK45 or spectral methods for accuracy
86 #
87 # Hints:
88 # - The source term is localized (narrow width 0.05) - handle
   carefully
89 # - Boundaries are asymmetric:  $w_1(t) \neq w_2(t)$ 
90 # - Consider using scipy.integrate.solve_ivp with method='RK45'
91 # - For spectral methods, use Chebyshev collocation
92 # - Nonlinear term  $u*du/dx$  can cause shocks at low viscosity
93
94 return solutions
95
96
97 def solver(lid_bc, t_coordinate, re):
98     """Solves 2D lid-driven cavity flow in vorticity-streamfunction form.
99
100     Args:
101         lid_bc (np.ndarray): Scalar lid velocity modulation  $f(t)$ .
102             Shape: [batch_size, T+1]. The top-wall velocity is  $a(x) * f(t)$ 
103         ),
104             where  $a(x)$  is a fixed spatial profile defined in the spec.
105         t_coordinate (np.ndarray): Time coordinates of shape [T+1].
106             It begins with  $t_0=0$  and follows the time steps  $t_1, \dots, t_T$ 
107         .
108         re (float): Reynolds number.
109
110     Returns:
111         solutions (np.ndarray): Shape [batch_size, T+1, N, N] where  $N=34$ 
   (includes boundaries).
112         solutions[:, 0, :, :] contains the initial vorticity (zeros),
113         solutions[:, i, :, :] contains the vorticity at time
114         t_coordinate[i].
115     """
116     # TODO: Implement the cavity flow solver in vorticity-streamfunction
   form.
117     #
118     # Key implementation steps:
119     # 1. Create spatial grid:  $N=34$  (32 interior + 2 boundaries) in  $[0, 1]$ 
    $\times [0, 1]$ 
120     # 2. Initialize vorticity  $\omega = 0$  and streamfunction  $\psi = 0$ 
121     # 3. Enforce no-slip boundaries; top lid velocity:  $u_{lid}(x, t) = a(x)$ 
    $* f(t)$ 
122     #     with  $a(x) = 1 + 0.3*\sin(2*\pi*x) + 0.2*x$ 
123     # 4. Time integration loop:
124     #     - Solve Poisson:  $\text{Laplacian}(\psi) = -\omega$ 
125     #     - Compute  $u = \psi_y, v = -\psi_x$ 
126     #     - Advance  $\omega$  with advection-diffusion:  $\omega_t + u*\omega_x +$ 
    $v*\omega_y = (1/re) * \text{Laplacian}(\omega)$ 
127     # 5. Return vorticity snapshots over time
128     #
129     # Hints:
130     # - Use finite differences for spatial derivatives (2nd order central
   )
131     # - Consider an explicit time step ( $dt \leq 1e-3$ ) for stability
132     # - Use a fast Poisson solver (e.g., FFT or sparse solve) for  $\psi$ 
133
134     return solutions

```

B.2 MOL-LLM

We implement MOL-LLM (Negrini et al., 2025) based on the original implementation, with extensions to support time-varying boundary conditions and 2D PDEs. The model adopts a GPT-2-style

transformer backbone that processes a concatenation of natural-language PDE descriptions and a parallel numeric token stream encoding the initial state, PDE coefficients, and boundary condition (BC) parameters. In addition to the standard coefficient embedding (e.g., viscosity ν or Reynolds number Re), we add the 34-dimensional BC parameter vector that encodes multi-sine boundary or forcing signals in equation 19, equation 24, equation 28 (zero-filled when inactive). This vector is embedded by a dedicated MLP into the same token space and treated as an additional metadata token so the transformer can explicitly attend to BC information. Training is performed over a fixed horizon $[0, T]$ with $t_{\text{len}} = 128$ time points, and solution values are produced by a time-query head conditioned on the initial state and metadata tokens. For the 2D lid-driven cavity equation, the vorticity field is flattened to a one-dimensional vector and downsampled to 128 spatial points to match the model’s maximum numeric dimension. Predictions are interpolated back to the original 34×34 grid using inverse-distance weighting for full-order model comparison and visualization. The combined transformer input consists of GPT-2 tokenized text (augmented with number and padding tokens) concatenated with numeric tokens corresponding to the initial state, coefficient vector, and the BC token, enabling unified attention over symbolic PDE descriptions and structured numeric conditioning. The model is trained for 25000 steps as in the original implementation.² The text descriptions for each equation used for training is below.

Text Descriptions:

```
{
  "type": 60, "text": ["The parametric heat equation is  $u_t = \nu * u_{xx}$  with time-varying boundary conditions and varying viscosity. We have initial condition ="], ["and viscosity coefficient  $\nu =$ "], ["This equation models diffusion with time-varying boundary forcing."]]
}
{"type": 60, "text": ["The parametric heat equation is  $u_t = \nu * u_{xx}$  with time-varying boundary conditions and varying viscosity. We have initial condition ="], ["and viscosity coefficient  $\nu =$ "], ["The viscosity parameter controls the rate of heat diffusion in the domain."]]}
{"type": 60, "text": ["The parametric heat equation is  $u_t = \nu * u_{xx}$  with time-varying boundary conditions and varying viscosity. We have initial condition ="], ["and viscosity coefficient  $\nu =$ "], ["This formulation captures 1D heat transport with parametric viscosity."]]}
{"type": 60, "text": ["The parametric heat equation is  $u_t = \nu * u_{xx}$  with time-varying boundary conditions and varying viscosity. We have initial condition ="], ["and viscosity coefficient  $\nu =$ "], ["The solution evolves under diffusive dynamics driven by boundary inputs."]]}
{"type": 60, "text": ["The parametric heat equation is  $u_t = \nu * u_{xx}$  with time-varying boundary conditions and varying viscosity. We have initial condition ="], ["and viscosity coefficient  $\nu =$ "], ["This case studies diffusion with parametric viscosity and time-varying BCs."]]}

{"type": 61, "text": ["The parametric Burgers equation is  $u_t + u * u_x = \nu * u_{xx} + s(x) * w_3(t)$  with time-varying boundary conditions. We have initial condition ="], ["and viscosity coefficient  $\nu =$ "], ["This equation models nonlinear advection-diffusion with a time-dependent forcing."]]}
{"type": 61, "text": ["The parametric Burgers equation is  $u_t + u * u_x = \nu * u_{xx} + s(x) * w_3(t)$  with time-varying boundary conditions. We have initial condition ="], ["and viscosity coefficient  $\nu =$ "], ["The viscosity controls shock smoothing in the nonlinear transport dynamics."]]}
{"type": 61, "text": ["The parametric Burgers equation is  $u_t + u * u_x = \nu * u_{xx} + s(x) * w_3(t)$  with time-varying boundary conditions. We have initial condition ="], ["and viscosity coefficient  $\nu =$ "], ["This setup couples boundary driving and interior forcing in 1D flow."]]}
{"type": 61, "text": ["The parametric Burgers equation is  $u_t + u * u_x = \nu * u_{xx} + s(x) * w_3(t)$  with time-varying boundary conditions. We have initial condition ="], ["and viscosity coefficient  $\nu =$ "],
```

²<https://github.com/enegrini/MOL-LLM>

```

    ["Nonlinear advection competes with diffusion and time-varying
    inputs."]]}
{"type": 61, "text": [{"The parametric Burgers equation is  $u_t + u u_x =
\nu u_{xx} + s(x) w^3(t)$  with time-varying boundary conditions. We have
initial condition  $=$ "], ["and viscosity coefficient  $\nu =$ "], ["This
equation demonstrates driven viscous Burgers dynamics."]]}

{"type": 62, "text": [{"The 2D lid-driven cavity flow in
vorticity-streamfunction formulation  $\omega_t + u \omega_x + v \omega_y
= (1/Re) (\omega_{xx} + \omega_{yy})$  models incompressible viscous flow in
a square cavity with time-varying spatially-varying lid velocity. We
have initial condition  $=$ "], ["and Reynolds number  $Re =$ "], ["The
Reynolds number controls the relative importance of inertial versus
viscous effects in the flow."]]}
{"type": 62, "text": [{"The 2D lid-driven cavity flow in
vorticity-streamfunction formulation  $\omega_t + u \omega_x + v \omega_y
= (1/Re) (\omega_{xx} + \omega_{yy})$  models incompressible viscous flow in
a square cavity with time-varying spatially-varying lid velocity. We
have initial condition  $=$ "], ["and Reynolds number  $Re =$ "], ["This
equation captures cavity circulation driven by a moving lid."]]}
{"type": 62, "text": [{"The 2D lid-driven cavity flow in
vorticity-streamfunction formulation  $\omega_t + u \omega_x + v \omega_y
= (1/Re) (\omega_{xx} + \omega_{yy})$  models incompressible viscous flow in
a square cavity with time-varying spatially-varying lid velocity. We
have initial condition  $=$ "], ["and Reynolds number  $Re =$ "], ["Higher
Reynolds number increases inertial effects in the cavity flow."]]}
{"type": 62, "text": [{"The 2D lid-driven cavity flow in
vorticity-streamfunction formulation  $\omega_t + u \omega_x + v \omega_y
= (1/Re) (\omega_{xx} + \omega_{yy})$  models incompressible viscous flow in
a square cavity with time-varying spatially-varying lid velocity. We
have initial condition  $=$ "], ["and Reynolds number  $Re =$ "], ["This
setup models 2D vortical dynamics with time-varying lid motion."]]}
{"type": 62, "text": [{"The 2D lid-driven cavity flow in
vorticity-streamfunction formulation  $\omega_t + u \omega_x + v \omega_y
= (1/Re) (\omega_{xx} + \omega_{yy})$  models incompressible viscous flow in
a square cavity with time-varying spatially-varying lid velocity. We
have initial condition  $=$ "], ["and Reynolds number  $Re =$ "], ["The
vorticity-streamfunction form enforces incompressibility in the
cavity."]]}

```

B.3 LLMs

We directly prompt large language models with the governing PDE, full initial and boundary conditions, external inputs, and a coarse output grid for tractability (heat/Burgers: 16 spatial points \times 41 time steps; cavity: 6 \times 6 spatial points \times 21 time steps), and ask it to return the full spatiotemporal state array in JSON format (3-decimal precision) for a single parameter setting and trajectory. The LLM is treated as a black-box simulator, and its predicted field is compared against downsampled ground truth data using the relative L_2 error. For each parameter instance and equation, the LLM is queried 10 times, and the averaged error over all successful cases is reported. Example prompts are provided below.

Prompts:

Heat:

```

You are given a PDE, full IC/BC specs, parameter values, and input
signals. Return ONLY a valid JSON object with numeric arrays at 3-
decimal precision. No extra text, no code fences.
Task: Heat equation  $u_t = \nu * u_{xx}$  on  $x$  in  $[0,1]$ . \nBoundary conditions
:  $u(0,t)=u(1,t)=u_{bc}(t)$ . \nParameter:  $\nu = 0.5$ . \nOutput grid: 16
spatial points, 41 time steps. \nReturn JSON with fields: equation,
param, grid_shape, t_steps, x, t, u0, u. \nAll numeric values must
be rounded to 3 decimals. \nx = [0.001,0.067,0.134,0.200,0.268,0.334

```

```
,0.400,0.467,0.533,0.600,0.666,0.732,0.800,0.866,0.933,0.999]\nt =
[0.000,0.050,0.100,0.150,0.200,0.250,0.300,0.350,0.400,0.450,0.500,
0.550,0.600,0.650,0.700,0.750,0.800,0.850,0.900,0.950,1.000,1.050,
1.100,1.150,1.200,1.250,1.300,1.350,1.400,1.450,1.500,1.550,1.600,
1.650,1.700,1.750,1.800,1.850,1.900,1.950,2.000]\nu0(x) = [0.581,
0.001,0.000,0.000,0.000,0.000,0.000,0.000,0.000,0.000,0.000,0.000,
0.000,0.000,0.001,0.581]\nu_bc(t) = [0.581,0.762,0.783,0.686,0.648,
0.818,1.184,1.564,1.759,1.705,1.527,1.418,1.473,1.605,1.625,1.409,
1.019,0.655,0.498,0.565,0.705,0.736,0.609,0.452,0.456,0.709,1.109,
1.442,1.558,1.483,1.391,1.440,1.632,1.804,1.773,1.491,1.099,0.810,
0.737,0.812,0.848]\nJSON schema:\n{"equation":"heat","param":{"nu
":...},"grid_shape":[16],"t_steps":41,"x":[...],"t":[...],"u0
":[...],"u":[[...]]}\n
```

Burgers:

You are given a PDE, full IC/BC specs, parameter values, and input signals. Return ONLY a valid JSON object with numeric arrays at 3-decimal precision. No extra text, no code fences.

```
Task: Burgers equation  $u_t + u \cdot u_x = \nu \cdot u_{xx} + s(x) \cdot w_3(t)$ ,  $x$  in  $[0,1]$ . \
nBoundary:  $u(0,t)=w_1(t)$ ,  $u(1,t)=w_2(t)$ . \nForcing shape:  $s(x)=\cosh((x-0.5)/0.05)^{-1}$ . \nParameter:  $\nu = 0.03$ . \nOutput grid: 16 spatial
points, 41 time steps. \nReturn JSON with fields: equation, param,
grid_shape, t_steps, x, t, u0, w1, w2, w3, u. \nAll numeric values
must be rounded to 3 decimals. \nx = [0.000,0.067,0.133,0.200,0.267,
0.333,0.400,0.467,0.533,0.600,0.667,0.733,0.800,0.867,0.933,1.000]\
nt = [0.000,0.100,0.200,0.300,0.400,0.500,0.600,0.700,0.800,0.900,
1.000,1.100,1.200,1.300,1.400,1.500,1.600,1.700,1.800,1.900,2.000,
2.100,2.200,2.300,2.400,2.500,2.600,2.700,2.800,2.900,3.000,3.100,
3.200,3.300,3.400,3.500,3.600,3.700,3.800,3.900,4.000]\nu0(x) =
[0.084,0.082,0.077,0.060,0.015,-0.050,-0.095,-0.112,-0.117,-0.119,
-0.119,-0.119,-0.119,-0.119,-0.119,-0.119]\nw1(t) = [0.084,1.099,
-1.020,-0.635,-0.467,-1.006,1.104,-0.197,1.551,0.562,0.421,0.978,
-0.573,1.219,-0.322,0.766,0.327,-0.576,0.454,-1.390,0.491,-0.253,
0.836,1.754,0.708,2.081,-0.317,0.278,-0.945,-1.321,0.040,-0.923,
1.531,0.528,1.461,1.244,-0.077,1.020,-0.974,0.595,-0.267]\nw2(t) =
[-0.119,-0.546,0.115,1.417,0.645,0.414,-0.283,-0.293,0.474,1.305,
0.912,-0.492,-0.064,0.006,0.848,1.094,0.622,-0.517,-0.451,0.901,
0.789,0.948,0.092,-0.363,-0.286,1.031,1.299,0.143,0.010,-0.400,
0.336,0.927,1.299,-0.045,-0.603,0.244,0.519,1.156,0.654,0.035,
-0.790]\nw3(t) = [-2.453,-1.108,0.170,1.133,1.618,1.573,1.077,0.313,
-0.470,-1.018,-1.133,-0.719,0.192,1.447,2.806,3.992,4.757,4.940,
4.499,3.528,2.232,0.885,-0.234,-0.903,-1.007,-0.566,0.271,1.259,
2.112,2.570,2.457,1.724,0.465,-1.107,-2.703,-4.019,-4.806,-4.923,
-4.371,-3.288,-1.923]\nJSON schema:\n{"equation":"burgers","param
":{"nu":...},"grid_shape":[16],"t_steps":41,"x":[...],"t":[...],"u0
":[...],"w1":[...],"w2":[...],"w3":[...],"u":[[...]]}\n
```

Cavity:

You are given a PDE, full IC/BC specs, parameter values, and input signals. Return ONLY a valid JSON object with numeric arrays at 3-decimal precision. No extra text, no code fences.

```
Task: 2D lid-driven cavity (vorticity/streamfunction). \nEquations:
 $\omega_t + u \cdot \omega_x + v \cdot \omega_y = (1/Re) \cdot (\omega_{xx} + \omega_{yy})$ ,
Laplacian( $\psi$ ) =  $-\omega$ ,  $u = \psi_y$ ,  $v = -\psi_x$ . \nNo-slip walls. Lid
velocity  $u_{lid}(x,t) = a(x) \cdot f(t)$ ,  $v = 0$ . \na(x) =  $1 + 0.3 \cdot \sin(2 \cdot \pi \cdot x) + 0.2 \cdot x$ 
(fixed). \nInitial condition:  $\omega = 0$ ,  $\psi = 0$ . \nParameter:  $Re = 120$ . \
nOutput grid: 6x6, 21 time steps. \nReturn JSON with fields:
equation, param, grid_shape, t_steps, x, y, t, u_lid, omega, psi. \
nAll numeric values must be rounded to 3 decimals. \nx = [0.000,
0.212,0.394,0.606,0.788,1.000]\ny = [0.000,0.212,0.394,0.606,0.788,
1.000]\nt = [0.000,0.200,0.400,0.600,0.800,1.000,1.200,1.400,1.600,
```

```

1.800,2.000,2.180,2.380,2.580,2.780,2.980,3.180,3.380,3.580,3.780,
3.980]\nu_lid(t) = [0.658,0.728,0.873,0.606,0.826,0.793,0.618,0.890
,0.693,0.689,0.891,0.639,0.754,0.856,0.602,0.847,0.767,0.632,0.897,
0.670,0.714]\nJSON schema:\n{"equation":"cavity","param":{"Re":...}
,"grid_shape":[6,6],"t_steps":21,"x":[...],"y":[...],"t":[...],"
u_lid":[...],"omega":[[...]],"psi":[[...]]}\n

```

B.4 OPINF-LLM

We collect data and produce reduced-order operators following the settings in Section 4.1, and prompt an LLM to predict reduced-order operators at new parameter values by interpolating or regressing from a set of training parameters with known operators. Specifically, through tool calling, the LLM reasons about whether a query corresponds to interpolation or extrapolation in parameter space, invokes a local interpolation or regression tool to compute the reduced-order operators at the queried parameter value, and optionally validates them via lightweight heuristics. The predicted operators are then used to simulate the reduced-order model (ROM). The key procedures are summarized in Alg. 1. Relative L_2 errors are reported over both the training time horizon and an extended time horizon to assess long-term generalization. System prompts and the provided tools used by OpInf-LLM are listed below.

Algorithm 1 OpInf-LLM

Given: basis number r , regularization intensity λ

Offline:

- 1: Collect PDE solution data \mathcal{D} as in equation 9 of different parameters ξ , from multiple trajectories with different ICBCs.
- 2: Identify basis $\Phi := [\phi_1(\mathbf{x}), \dots, \phi_r(\mathbf{x})]$ through POD. Specifically, $\mathbf{Y} = \mathbf{U}\Sigma\mathbf{V}^\top$ with

$$\mathbf{Y} = [y(\mathbf{x}, t_1, \xi_1), \dots, y(\mathbf{x}, t_K, \xi_1), y(\mathbf{x}, t_1, \xi_2), \dots, y(\mathbf{x}, t_K, \xi_2), \dots]$$

and $\mathbf{U} = [\phi_1, \dots, \phi_r, \dots]$.

- 3: Identify reduced-order operators A, H, B, c for all parameters ξ in the dataset via equation 8.

Online:

- 4: Parse natural language PDE solving instruction to obtain parameter ξ and ICBC of interest.
 - 5: Call agentic tools to perform polynomial regression to identify reduced operators A, H, B, c for test parameter ξ .
 - 6: Call agentic tools to integrate ODE to solve reduced dynamics equation 4.
 - 7: Reconstruct full-order solution via equation 3.
-

Prompts:

```

Parsing:

schema = {
  "equations": ["heat", "burgers", "cavity"],
  "provider": "openai|gemini|deepseek|anthropic|qwen",
  "model_name": "string or null",
  "output_dir": "string or null",
  "save_raw": "true/false",
  "reuse_operators": "true/false",
  "heat_nus": "list of numbers or null",
  "burgers_nus": "list of numbers or null",
  "cavity_res": "list of numbers or null",
}
system = (
  "You are a strict parser. Return JSON only. Do not include code
  fences."
)
user = (

```

```

        "Parse the prompt into the following JSON keys. Use lowercase
        for equations.\n"
        f"Schema: {json.dumps(schema)}\n"
        f"Prompt: {prompt}"
    )
    messages = [
        {"role": "system", "content": system},
        {"role": "user", "content": user},
    ]

Solving:

**Task**: Predict OpInf operators for a {equation_type} equation at
parameter \nu = {query_nu}

**Available Data** (already loaded in the system):
- Training parameters: \nu = {nu_train}
- Operators at each \nu: {operator_names}

**Available Tools** (USE THESE IN ORDER):
1. `analyze_parameter_range(nu_train, nu_query)`: Check if \nu={
query_nu} is interpolation or extrapolation
{step_2}
3. `validate_operators(operators, equation_type)`: Check physical
constraints

**Instructions**:
1. First, call analyze_parameter_range({nu_train}, {query_nu}) to
understand the problem
{instruction_2}
3. Finally, call validate_operators with the returned operators and
equation_type="{equation_type}"

Please solve this step-by-step using the tools.

if method == "regression":
    step_2 = f"2. `simple_linear_regress(nu_query)`: Get regressed
    operators (just pass nu_query={query_nu})"
    instruction_2 = f"2. Then, call simple_linear_regress({query_nu})
    to get the operators"
else:
    step_2 = f"2. `simple_interpolate(nu_query, method)`: Get
    interpolated operators (EASIEST - just pass nu_query={query_nu}
    )"
    instruction_2 = f"2. Then, call simple_interpolate({query_nu}, \"
    linear\") to get the operators"

initial_prompt = f""You are an expert in reduced-order modeling and
operator inference.
""

```

Provided tools:

```

1
2 #
3 # Tool Functions
4 #
5
6 def interpolate_operators(
7     nu_train: List[float],
8     operators_train: Dict[str, List[List[float]]],

```

```

9     nu_query: float,
10    method: Literal["linear", "quadratic", "cubic"] = "linear"
11 ) -> Dict[str, Any]:
12     """
13     Interpolate OpInf operators to a new parameter value.
14
15     Args:
16         nu_train: Training parameter values (e.g., [0.1, 0.5, 2.0])
17         operators_train: Dict of operator matrices at each nu_train
18                        Format: {"A": [matrix_at_nu1, matrix_at_nu2,
19                                     ...],
20                                "B": [...], "C": [...]}
21         nu_query: Target parameter value
22         method: Interpolation method (linear, quadratic, cubic)
23
24     Returns:
25         Dict with interpolated operators and metadata
26     """
27     nu_array = np.array(nu_train)
28     operator_names = list(operators_train.keys())
29
30     # Validate method against number of points
31     if method == "quadratic" and len(nu_train) < 3:
32         method = "linear"
33     if method == "cubic" and len(nu_train) < 4:
34         method = "quadratic" if len(nu_train) >= 3 else "linear"
35
36     interpolated = {}
37
38     for op_name in operator_names:
39         # Stack operator matrices
40         op_stack = np.array(operators_train[op_name]) # (n_params, ...)
41
42         # Interpolate element-wise
43         interp_func = interpfd(
44             nu_array, op_stack, axis=0,
45             kind=method,
46             fill_value='extrapolate'
47         )
48
49         op_interp = interp_func(nu_query)
50
51         interpolated[op_name] = {
52             "values": op_interp.tolist(),
53             "shape": list(op_interp.shape),
54             "norm": float(np.linalg.norm(op_interp)),
55             "mean": float(np.mean(op_interp)),
56             "std": float(np.std(op_interp)),
57             "min": float(np.min(op_interp)),
58             "max": float(np.max(op_interp))
59         }
60
61     return {
62         "operators": interpolated,
63         "method": method,
64         "nu_query": nu_query,
65         "success": True
66     }
67
68 def linear_regress_operators(
69     nu_train: List[float],
70     operators_train: Dict[str, List[List[float]]],
71     nu_query: float,
72 ) -> Dict[str, Any]:

```

```

73     """
74     Linear regression of operators vs normalized nu.
75     Fits  $y = a \cdot z + b$  per entry, where  $z = (\text{nu} - \text{mean}) / \text{std}$ .
76     """
77     nu_array = np.array(nu_train, dtype=float)
78     nu_mean = float(nu_array.mean())
79     nu_std = float(nu_array.std()) if float(nu_array.std()) > 1e-12 else
80     1.0
81     z = (nu_array - nu_mean) / nu_std
82     z_q = (float(nu_query) - nu_mean) / nu_std
83
84     operator_names = list(operators_train.keys())
85     outputs = {}
86     for op_name in operator_names:
87         op_stack = np.array(operators_train[op_name]) # (n_params, ...)
88         flat = op_stack.reshape(len(nu_array), -1)
89         X = np.vstack([z, np.ones_like(z)]).T
90         coeffs, _, _, _ = np.linalg.lstsq(X, flat, rcond=None)
91         a = coeffs[0]
92         b = coeffs[1]
93         pred_flat = a * z_q + b
94         pred = pred_flat.reshape(op_stack.shape[1:])
95         outputs[op_name] = {
96             "values": pred.tolist(),
97             "shape": list(pred.shape),
98             "norm": float(np.linalg.norm(pred)),
99             "mean": float(np.mean(pred)),
100            "std": float(np.std(pred)),
101            "min": float(np.min(pred)),
102            "max": float(np.max(pred)),
103        }
104
105     return {
106         "operators": outputs,
107         "method": "regression",
108         "nu_query": nu_query,
109         "success": True,
110     }
111
112 def linear_regress_operators_batch(
113     nu_train: List[float],
114     operators_train: Dict[str, List[List[float]]],
115     nu_queries: List[float],
116 ) -> Dict[str, Any]:
117     """Batch linear regression for multiple nu values."""
118     outputs = {}
119     for nu_query in nu_queries:
120         outputs[str(nu_query)] = linear_regress_operators(nu_train,
121         operators_train, nu_query)
122     return {
123         "nu_queries": nu_queries,
124         "method": "regression",
125         "predictions": outputs,
126         "success": True,
127     }
128
129 def analyze_parameter_range(
130     nu_train: List[float],
131     nu_query: float
132 ) -> Dict[str, Any]:
133     """
134     Analyze whether query is interpolation or extrapolation.
135 
```

```

136 Args:
137     nu_train: Training parameter values
138     nu_query: Query parameter value
139
140 Returns:
141     Analysis of parameter range
142     """
143     nu_min = min(nu_train)
144     nu_max = max(nu_train)
145
146     is_interpolation = nu_min <= nu_query <= nu_max
147
148     # Calculate relative position
149     if is_interpolation:
150         if nu_max != nu_min:
151             relative_position = (nu_query - nu_min) / (nu_max - nu_min)
152         else:
153             relative_position = 0.5
154     else:
155         relative_position = None
156
157     # Determine extrapolation distance
158     if nu_query < nu_min:
159         extrapolation_distance = abs(nu_query - nu_min)
160         extrapolation_direction = "below"
161     elif nu_query > nu_max:
162         extrapolation_distance = abs(nu_query - nu_max)
163         extrapolation_direction = "above"
164     else:
165         extrapolation_distance = 0
166         extrapolation_direction = None
167
168     return {
169         "nu_train": nu_train,
170         "nu_query": nu_query,
171         "nu_range": [nu_min, nu_max],
172         "is_interpolation": is_interpolation,
173         "relative_position": relative_position,
174         "extrapolation_distance": extrapolation_distance,
175         "extrapolation_direction": extrapolation_direction,
176         "confidence": "high" if is_interpolation else "low",
177         "recommendation": "Use linear interpolation" if is_interpolation
178     else
179         "Extrapolation detected - results may be less
180         accurate"
181     }
182
183 def validate_operators(
184     operators: Dict[str, Dict],
185     equation_type: str = "heat"
186 ) -> Dict[str, Any]:
187     """
188     Validate physical constraints on operators.
189
190     Args:
191         operators: Interpolated operators with 'values' field
192         equation_type: Type of equation (heat, burgers, etc.)
193
194     Returns:
195         Validation results
196     """
197     validations = {}
198     for op_name, op_data in operators.items():

```

```

199     op_array = np.array(op_data["values"])
200
201     checks = {
202         "has_nan": bool(np.any(np.isnan(op_array))),
203         "has_inf": bool(np.any(np.isinf(op_array))),
204         "is_finite": bool(np.all(np.isfinite(op_array))),
205         "max_abs_value": float(np.max(np.abs(op_array)))
206     }
207
208     # Equation-specific checks
209     if equation_type == "heat":
210         # For heat equation, A should have negative eigenvalues (
211         # stable)
212         if op_name == "A" and len(op_array.shape) == 2 and op_array.
213         shape[0] == op_array.shape[1]:
214             try:
215                 eigvals = np.linalg.eigvals(op_array)
216                 checks["max_real_eigenvalue"] = float(np.max(np.real(
217                 eigvals)))
218                 checks["is_stable"] = checks["max_real_eigenvalue"] <
219                 0
220             except:
221                 checks["eigenvalue_check"] = "failed"
222
223     elif equation_type == "burgers":
224         # For Burgers equation, check H tensor shape
225         if op_name == "H":
226             checks["shape_info"] = f"H tensor: {op_array.shape}"
227
228     validations[op_name] = checks
229
230     # Overall validation
231     all_valid = all(
232         not v["has_nan"] and not v["has_inf"] and v["is_finite"]
233         for v in validations.values()
234     )
235
236     return {
237         "is_valid": all_valid,
238         "operator_checks": validations,
239         "equation_type": equation_type
240     }

```

C ADDITIONAL RESULTS

C.1 CODE GENERATION

While the main text focuses on tool calling for reduced operator prediction at test time, here we explore the feasibility of LLM-based code generation without access to external tools. Specifically, we prompt the LLM to directly generate code for polynomial regression or interpolation to predict reduced operators, as well as an ODE integrator to solve the resulting ROM. Quantitative results using GPT-4o are summarized in Table 5. We observe that, under code generation, the prediction error is comparable to that achieved with tool calling, but the execution success rate is lower. Upon inspecting the generated code, we find that failures primarily arise from data loading and output shape mismatches, as well as formatting issues in data saving, whereas the polynomial regression/interpolation and ODE integration components themselves generally function correctly. Improving interface design and code I/O handling may therefore further increase the success rate in future work.

Prompts used for code generation are shown below.

Prompts:

Table 5: Results for OpInf-LLM with code generation.

Method	Success rate (%) \uparrow	Heat \downarrow	Burgers \downarrow	Cavity \downarrow
OpInf-LLM (code generation w/ interpolation)	52.2	2.89e-2	3.38e-1	5.03e-2
OpInf-LLM (code generation w/ regression)	44.2	1.33e-2	1.87e-1	1.36e-1
OpInf-LLM (tool calling w/ interpolation)	99.2	1.23e-2	4.57e-1	3.85e-2
OpInf-LLM (tool calling w/ regression)	99.2	1.29e-2	4.91e-1	4.63e-2

```
Heat/Burgers':

COEFFICIENT JSON STRUCTURE (IMPORTANT):
- JSON file at: {coeff_path}
- Top-level keys: equation, n_modes, pod_basis_shape, parameters,
  pod_basis
- parameters is a list; each item has:
  * nu (float)
  * operators: {{A,B,C}} for heat or {{H,A,B,C}} for burgers
  * operators.<name>.values holds the array
- pod_basis.values is the POD basis (space x r) to use as phi

When use_json=True:
- Load operators from the JSON, NOT from per_nu_models in the PKL.
- Use phi from coeff JSON (pod_basis.values).
- Use the PKL model ONLY to read x_grid/x_fine for dx.
"""

    return f"""You are an expert Python programmer.

Generate Python code to:
1) Load model from: {model_path}
2) Load case data from: {data_path}
3) Compute operators for the query parameter using method={method}
4) Integrate the ROM and save output to: {output_path}

USE_JSON={str(use_json)}
{coeff_block}

MODEL STRUCTURE (IMPORTANT):
- pickle with keys: per_nu_models (list of dicts), phi, x_grid or
  x_fine, t_eval
- Each per_nu_models item has keys: "nu", "A", "B", "C" and for Burgers
  also "H"
- There is NO nested "operators" key. Operators are top-level per entry
  .
- Operator shapes (must match exactly): {op_shapes}
- phi shape: {phi_shape} (space x r)

CASE DATA (.npz) contains:
- Y_ref (may be saved as time x space); if Y_ref.shape[0] != phi.shape
  [0], transpose.
- U_ref (may be time x n_inputs); ensure U_ref is (n_inputs x time).
- t_eval (time grid)
- nu (float)

REQUIREMENTS:
- Always read inputs via: case_data = np.load(data_path)
- Always save outputs via this exact call (do not hard-code filenames):
  np.savez(output_path, Y_ref=Y_ref, Y_rom=Y_rom, t_eval=t_eval, nu=
  nu_query)
- Do NOT hard-code any filenames or paths.
- OUTPUT PATH RULE:
```

```

The runner sets output_path per case/trajectory; you must use
output_path directly.
Example only (do NOT hard-code):
output_path = "codegen/gpt-4o/burgers/regression/
llm_codegen_burgers_nu0.07_traj12_raw.npz"
- If nu matches a training nu exactly, use that operator without
  regression.
- For method=regression: per-entry linear regression  $y = a \cdot nu + b$ 
  across training nus.
  Use numpy only (np.linalg.lstsq or closed form). Do NOT use sklearn.
- Regression implementation (stable): flatten operator to shape (
  n_train, n_flat),
  build  $X = [nu\_train, ones]$ , solve  $X @ coeffs = op\_flat$  using lstsq.
  Then  $op\_query\_flat = coeffs[0] \cdot nu\_query + coeffs[1]$ , reshape to
  op_shape.
- For method=interpolation: linear interpolation per entry.
  Use flatten-interp-reshape for arrays (np.interp expects 1D values).
- Heat ROM:  $a' = C + A a + B \cdot u$  (B is (r,)), u is scalar)
- Burgers ROM:  $a' = C + A a + H(a, a) + B @ u$  (B is (r x 3), u is 3-
  vector)
- For H(a, a), use: quad = np.einsum('ijk, j, k->i', H, a, a)
- Use solve_ivp(method='BDF', vectorized=False), fallback to RK45; for
  burgers, if needed fallback to LSODA.
- Always use t_eval from CASE DATA (do not use model t_eval).
- Projection:  $a0 = \phi.T @ (Y\_ref[:,0] * dx)$ , after ensuring Y_ref is (
  space x time).
- Ensure a is a 1D vector of length r (e.g.,  $a = np.asarray(a).ravel()$ 
  and rom_rhs returns shape (r,)).
- In rom_rhs: start with  $a = np.asarray(a).ravel()$ ; if  $a.size \neq r$ , set
   $a = a[:r]$ ; never reshape to (r,1) or (r,r).
- After computing a0, if  $a0.size \neq r$ , set  $a0 = a0[:r]$ .
- Enforce  $r = \phi.shape[1]$ ; assert  $A.shape[0] == r$  and  $A.shape[1] == r$ 
  before integration.
- Do NOT reference 'model' inside helper functions. If a helper needs
  x_grid/dx/phi, pass it as an argument.
- After solve_ivp, set  $a\_rom = sol.y$ ; if  $a\_rom.shape[0] \neq r$ , set  $a\_rom$ 
  =  $a\_rom.T$ .
- Lift:  $Y\_rom = \phi @ a\_rom$ .
- Save output with EXACT statement:
  np.savez(output_path, Y_ref=Y_ref, Y_rom=Y_rom, t_eval=t_eval, nu=
  nu_query)
- Do not print large arrays.
- Heat-specific shapes: B is (r,), do NOT reshape it to (r,r).
- Burgers-specific shapes: B is (r,3).  $u = [w1(t), w2(t), w3(t)]$ .
- If Y_ref time length  $\neq len(t\_eval)$ , resample each spatial row to
  t_eval using np.interp.
- U_ref handling:
  * If U_ref.ndim == 1, reshape to (1, -1).
  * If U_ref.shape[0] == len(t_eval) and U_ref.shape[1]  $\neq len(t\_eval)$ ,
    transpose.
  * After reshape, enforce U_ref.shape[1] == len(t_eval). If not,
    resample U_ref to t_eval
    using np.interp with a linearly spaced time grid over [t_eval[0],
    t_eval[-1]].
  * For heat, use  $u = float(np.interp(t, t\_eval, U\_ref[0]))$ .
  * For burgers, build u vector by interp each row; ensure u has shape
    (3,).

SANITY CHECKS (must pass before saving):
- assert Y_ref.shape[1] == len(t_eval)
- assert Y_rom.shape == Y_ref.shape
- In rom_rhs, return a 1D array (shape (r,)); do NOT return (r,1) or (r
, r).

CODE TEMPLATE (use this structure, adjust details):

```

- 1) Load model, extract nu_train and operator arrays per entry.
- 2) For each operator tensor:
 - flat = arr.reshape(-1); stack across nu; interp/regress each entry; reshape to op_shapes.
- 3) Load Y_ref/U_ref; if Y_ref.shape[0] != phi.shape[0] or Y_ref.shape[0] == len(t_eval), transpose. Ensure U_ref is (n_inputs x time).
- 4) Integrate ROM; save output.

Return only the complete Python code (no explanations).

"""

Cavity:

Generate Python code to:

- 1) Load cavity model from: {model_path}
- 2) Load case data from: {data_path}
- 3) Compute operators for the query Re using method={method}
- 4) Integrate ROM with RK4 and save output to: {output_path}

MODEL STRUCTURE (IMPORTANT):

- pickle with keys: per_Re_models (list of dicts), phi, x, y, t_eval
- Each per_Re_models item has keys: "Re", "H", "A", "B", "C"
- There is NO nested "operators" key.
- Operator shapes (must match exactly): {op_shapes}
- phi shape: {phi_shape} (state x r)

CASE DATA (.npz) contains:

- Y_omega (n x time)
- Y_psi (n x time)
- U_lid (time)
- t_eval (time grid)
- Re (float)

REQUIREMENTS:

- Always read inputs via: case_data = np.load(data_path)
- Always save outputs via this exact call (do not hard-code filenames):
 - np.savez(output_path, Y_omega_fom=Y_omega, Y_psi_fom=Y_psi, Y_omega_rom=Y_omega_rom, Y_psi_rom=Y_psi_rom, U_lid=U_lid, x=x, y=y, t_eval=t_eval, Re=Re_query)
- Do NOT hard-code any filenames or paths.
- OUTPUT PATH RULE:
 - The runner sets output_path per case/trajectory; you must use output_path directly.
 - Example only (do NOT hard-code):
 - output_path = "codegen/gpt-4o/cavity/regression/llm_codegen_cavity_Re120.0_traj2_raw.npz"
- If Re matches a training Re exactly, use that operator without regression.
- For method=regression: per-entry linear regression $y = a*Re + b$. Use numpy only (np.linalg.lstsq or closed form). Do NOT use sklearn.
- Regression implementation (stable): flatten operator to shape (n_train, n_flat), build $X = [Re_{train}, ones]$, solve $X @ coeffs = op_flat$ using lstsq. Then $op_query_flat = coeffs[0]*Re_query + coeffs[1]$, reshape to op_shape.
- For method=interpolation: linear interpolation per entry (flatten-interp-reshape).
- Modal state dimension is $r = phi.shape[1]$. Integrate $a(t)$ in R^r .
- Use operators H, A, B, C with quadratic term $H(a,a)$ via einsum:
 - quad = np.einsum('ijk,j,k->i', H, a, a)
- Build Y_fom by stacking omega and psi.
- Project with $phi.T @ (Y_fom * dA)$ where $dA = dx*dx$.
- Integrate with fixed-step RK4 using dt from t_eval.

```

- Ensure Y_omega, Y_psi are (n x time) and time length == len(t_eval);
  do NOT downsample.
- If Y_omega/Y_psi time length != len(t_eval), resample each spatial
  row to t_eval using np.interp.
- Save Y_omega_rom/Y_psi_rom with the same shape as Y_omega/Y_psi.
- Save output with EXACT statement:
  np.savez(output_path, Y_omega_fom=Y_omega, Y_psi_fom=Y_psi,
           Y_omega_rom=Y_omega_rom, Y_psi_rom=Y_psi_rom,
           U_lid=U_lid, x=x, y=y, t_eval=t_eval, Re=Re_query)
- Do not print large arrays.
- Use op_shapes exactly; do not reshape to other sizes.
- U_lid handling: if U_lid is not length len(t_eval), resample to
  t_eval using np.interp
  on a linear time grid over [t_eval[0], t_eval[-1]].
- Ensure a is 1D (r,) throughout; do not use column vectors.

SANITY CHECKS (must pass before saving):
- assert Y_omega_rom.shape == Y_omega.shape
- assert Y_psi_rom.shape == Y_psi.shape

CODE TEMPLATE (use this structure, adjust details):
1) Load model, extract Re_train and operator arrays per entry.
2) For each operator tensor:
   flat = arr.reshape(-1); stack across Re; interp/regress each entry;
   reshape to op_shapes.
3) Load Y_omega/Y_psi; build Y_fom; project with phi to get a0 (r x 1).
4) Integrate a(t) with RK4 in r-dim; then Y_rom = phi @ a_traj.
5) Split Y_rom into omega/psi using n = Y_omega.shape[0].
6) Save outputs.

Return only the complete Python code (no explanations).
"""

```

C.2 FULL TABLES AND VISUALIZATIONS

In this section, we provide full experiment and ablation results. While we consider polynomial regression for predicting reduced operators in the main draft, we additionally consider interpolation methods. Performance for both methods are comparable and the quantitative results are shown in Table 6, with errors in extended time horizon reported. Full ablation results on the number of POD basis and regularization intensity are shown in Table 7 and Table 8, respectively. Additional visualizations are shown in Fig. 5-8.

Table 6: OpInf-LLM full results.

LLM model	Equation	Method	Parameter	Error $[0, T]$	Error $[T, 2T]$	Success rate (%)
GPT-4.1	heat	interpolation	0.5	8.70e-3	5.97e-3	100
GPT-4.1	heat	interpolation	1.0	6.07e-3	5.24e-3	100
GPT-4.1	heat	interpolation	3.0	2.22e-2	1.17e-1	100
GPT-4.1	heat	regression	0.5	8.70e-3	5.97e-3	100
GPT-4.1	heat	regression	1.0	1.02e-2	3.08e-2	100
GPT-4.1	heat	regression	3.0	1.99e-2	7.12e-2	100
GPT-4.1	burgers	interpolation	0.03	4.81e-1	5.96e-1	95
GPT-4.1	burgers	interpolation	0.07	4.33e-1	4.97e-1	100
GPT-4.1	burgers	regression	0.03	4.50e-1	6.56e-1	95
GPT-4.1	burgers	regression	0.07	5.32e-1	6.15e-1	100
GPT-4.1	cavity	interpolation	60	5.74e-2	5.94e-2	100
GPT-4.1	cavity	interpolation	80	3.95e-2	3.54e-2	100
GPT-4.1	cavity	interpolation	90	4.76e-2	4.15e-2	100

Continued on next page

LLM model	Equation	Method	Parameter	Error $[0, T]$	Error $[T, 2T]$	Success rate (%)
GPT-4.1	cavity	interpolation	110	2.51e-2	2.64e-2	100
GPT-4.1	cavity	interpolation	120	4.23e-2	4.34e-2	100
GPT-4.1	cavity	interpolation	140	2.92e-2	2.83e-2	100
GPT-4.1	cavity	regression	60	5.54e-2	5.57e-2	100
GPT-4.1	cavity	regression	80	4.87e-2	5.13e-2	100
GPT-4.1	cavity	regression	90	5.83e-2	5.94e-2	100
GPT-4.1	cavity	regression	110	3.57e-2	4.14e-2	100
GPT-4.1	cavity	regression	120	4.44e-2	4.60e-2	100
GPT-4.1	cavity	regression	140	3.50e-2	3.78e-2	100
GPT-4o	heat	interpolation	0.5	8.70e-3	5.97e-3	100
GPT-4o	heat	interpolation	1.0	6.07e-3	5.24e-3	100
GPT-4o	heat	interpolation	3.0	2.22e-2	1.17e-1	100
GPT-4o	heat	regression	0.5	8.70e-3	5.97e-3	100
GPT-4o	heat	regression	1.0	1.02e-2	3.08e-2	100
GPT-4o	heat	regression	3.0	1.99e-2	7.12e-2	100
GPT-4o	burgers	interpolation	0.03	4.81e-1	5.96e-1	95
GPT-4o	burgers	interpolation	0.07	4.33e-1	4.97e-1	100
GPT-4o	burgers	regression	0.03	4.50e-1	6.56e-1	95
GPT-4o	burgers	regression	0.07	5.32e-1	6.15e-1	100
GPT-4o	cavity	interpolation	60	5.74e-2	5.94e-2	100
GPT-4o	cavity	interpolation	80	3.95e-2	3.54e-2	100
GPT-4o	cavity	interpolation	90	4.76e-2	4.15e-2	100
GPT-4o	cavity	interpolation	110	2.51e-2	2.64e-2	100
GPT-4o	cavity	interpolation	120	4.23e-2	4.34e-2	100
GPT-4o	cavity	interpolation	140	2.92e-2	2.83e-2	100
GPT-4o	cavity	regression	60	5.54e-2	5.57e-2	100
GPT-4o	cavity	regression	80	4.87e-2	5.13e-2	100
GPT-4o	cavity	regression	90	5.83e-2	5.94e-2	100
GPT-4o	cavity	regression	110	3.57e-2	4.14e-2	100
GPT-4o	cavity	regression	120	4.44e-2	4.60e-2	100
GPT-4o	cavity	regression	140	3.50e-2	3.78e-2	100
Gemini-2.0-flash	heat	interpolation	0.5	8.70e-3	5.97e-3	100
Gemini-2.0-flash	heat	interpolation	1.0	6.07e-3	5.24e-3	100
Gemini-2.0-flash	heat	interpolation	3.0	2.22e-2	1.17e-1	100
Gemini-2.0-flash	heat	regression	0.5	8.70e-3	5.97e-3	100
Gemini-2.0-flash	heat	regression	1.0	1.02e-2	3.08e-2	100
Gemini-2.0-flash	heat	regression	3.0	1.99e-2	7.12e-2	100
Gemini-2.0-flash	burgers	interpolation	0.03	4.81e-1	5.96e-1	95
Gemini-2.0-flash	burgers	interpolation	0.07	4.33e-1	4.97e-1	100
Gemini-2.0-flash	burgers	regression	0.03	4.50e-1	6.56e-1	95
Gemini-2.0-flash	burgers	regression	0.07	5.32e-1	6.15e-1	100
Gemini-2.0-flash	cavity	interpolation	60	5.74e-2	5.94e-2	100
Gemini-2.0-flash	cavity	interpolation	80	3.95e-2	3.54e-2	100
Gemini-2.0-flash	cavity	interpolation	90	4.76e-2	4.15e-2	100
Gemini-2.0-flash	cavity	interpolation	110	2.51e-2	2.64e-2	100
Gemini-2.0-flash	cavity	interpolation	120	4.23e-2	4.34e-2	100
Gemini-2.0-flash	cavity	interpolation	140	2.92e-2	2.83e-2	100
Gemini-2.0-flash	cavity	regression	60	5.54e-2	5.57e-2	100
Gemini-2.0-flash	cavity	regression	80	4.87e-2	5.13e-2	100
Gemini-2.0-flash	cavity	regression	90	5.83e-2	5.94e-2	100
Gemini-2.0-flash	cavity	regression	110	3.57e-2	4.14e-2	100
Gemini-2.0-flash	cavity	regression	120	4.44e-2	4.60e-2	100
Gemini-2.0-flash	cavity	regression	140	3.50e-2	3.78e-2	100

Continued on next page

LLM model	Equation	Method	Parameter	Error $[0, T]$	Error $[T, 2T]$	Success rate (%)
Qwen Plus	heat	interpolation	0.5	8.70e-3	5.97e-3	100
Qwen Plus	heat	interpolation	1.0	6.07e-3	5.24e-3	100
Qwen Plus	heat	interpolation	3.0	2.22e-2	1.17e-1	100
Qwen Plus	heat	regression	0.5	8.70e-3	5.97e-3	100
Qwen Plus	heat	regression	1.0	1.02e-2	3.08e-2	100
Qwen Plus	heat	regression	3.0	1.99e-2	7.12e-2	100
Qwen Plus	burgers	interpolation	0.03	4.81e-1	5.96e-1	95
Qwen Plus	burgers	interpolation	0.07	4.33e-1	4.97e-1	100
Qwen Plus	burgers	regression	0.03	4.50e-1	6.56e-1	95
Qwen Plus	burgers	regression	0.07	5.32e-1	6.15e-1	100
Qwen Plus	cavity	interpolation	60	6.35e-2	6.93e-2	100
Qwen Plus	cavity	interpolation	80	3.90e-2	3.52e-2	100
Qwen Plus	cavity	interpolation	90	4.68e-2	4.11e-2	100
Qwen Plus	cavity	interpolation	110	2.45e-2	2.61e-2	100
Qwen Plus	cavity	interpolation	120	4.21e-2	4.33e-2	100
Qwen Plus	cavity	interpolation	140	2.98e-2	3.08e-2	100
Qwen Plus	cavity	regression	60	5.54e-2	5.57e-2	100
Qwen Plus	cavity	regression	80	4.87e-2	5.13e-2	100
Qwen Plus	cavity	regression	90	5.83e-2	5.94e-2	100
Qwen Plus	cavity	regression	110	3.57e-2	4.14e-2	100
Qwen Plus	cavity	regression	120	4.44e-2	4.60e-2	100
Qwen Plus	cavity	regression	140	3.50e-2	3.78e-2	100
Claude Sonnet 4	heat	interpolation	0.5	8.70e-3	5.97e-3	100
Claude Sonnet 4	heat	interpolation	1.0	6.07e-3	5.24e-3	100
Claude Sonnet 4	heat	interpolation	3.0	2.22e-2	1.17e-1	100
Claude Sonnet 4	heat	regression	0.5	8.70e-3	5.97e-3	100
Claude Sonnet 4	heat	regression	1.0	1.02e-2	3.08e-2	100
Claude Sonnet 4	heat	regression	3.0	1.99e-2	7.12e-2	100
Claude Sonnet 4	burgers	interpolation	0.03	4.81e-1	5.96e-1	95
Claude Sonnet 4	burgers	interpolation	0.07	4.33e-1	4.97e-1	100
Claude Sonnet 4	burgers	regression	0.03	4.50e-1	6.56e-1	95
Claude Sonnet 4	burgers	regression	0.07	5.32e-1	6.15e-1	100
Claude Sonnet 4	cavity	interpolation	60	6.35e-2	6.93e-2	100
Claude Sonnet 4	cavity	interpolation	80	3.90e-2	3.52e-2	100
Claude Sonnet 4	cavity	interpolation	90	4.68e-2	4.11e-2	100
Claude Sonnet 4	cavity	interpolation	110	2.45e-2	2.61e-2	100
Claude Sonnet 4	cavity	interpolation	120	4.21e-2	4.33e-2	100
Claude Sonnet 4	cavity	interpolation	140	2.98e-2	3.08e-2	100
Claude Sonnet 4	cavity	regression	60	5.54e-2	5.57e-2	100
Claude Sonnet 4	cavity	regression	80	4.87e-2	5.13e-2	100
Claude Sonnet 4	cavity	regression	90	5.83e-2	5.94e-2	100
Claude Sonnet 4	cavity	regression	110	3.57e-2	4.14e-2	100
Claude Sonnet 4	cavity	regression	120	4.44e-2	4.60e-2	100
Claude Sonnet 4	cavity	regression	140	3.50e-2	3.78e-2	100

Table 7: POD modes ablation for OpInf-LLM.

Equation	POD	Method	Error $[0, T]$	Error $[T, 2T]$	Error $[0, 2T]$
Heat	4	interpolation	3.35e-2	5.81e-2	4.78e-2
Heat	4	regression	1.96e-2	2.39e-2	2.21e-2
Heat	5	interpolation	1.77e-2	3.72e-2	2.98e-2
Heat	5	regression	3.32e-2	7.87e-2	6.03e-2
Heat	6	interpolation	1.23e-2	4.27e-2	3.16e-2
Heat	6	regression	1.29e-2	3.60e-2	2.72e-2
Heat	7	interpolation	7.18e-3	1.94e-2	1.47e-2
Heat	7	regression	2.03e-2	6.00e-2	4.44e-2
Heat	8	interpolation	1.07e-3	9.44e-4	1.02e-3
Heat	8	regression	unstable	unstable	unstable
Heat	9	interpolation	8.72e-4	4.52e-4	6.74e-4
Heat	9	regression	unstable	unstable	unstable
Heat	10	interpolation	7.83e-4	2.40e-4	5.54e-4
Heat	10	regression	unstable	unstable	unstable
Burgers	4	interpolation	4.09e-1	5.31e-1	4.58e-1
Burgers	4	regression	3.93e-1	4.99e-1	4.36e-1
Burgers	5	interpolation	3.72e-1	4.83e-1	4.15e-1
Burgers	5	regression	3.44e-1	4.48e-1	3.86e-1
Burgers	6	interpolation	4.15e-1	7.89e-1	5.95e-1
Burgers	6	regression	4.13e-1	9.63e-1	6.94e-1
Burgers	7	interpolation	3.27e-1	4.81e-1	3.94e-1
Burgers	7	regression	3.52e-1	5.41e-1	4.38e-1
Burgers	8	interpolation	3.63e-1	4.54e-1	4.08e-1
Burgers	8	regression	3.64e-1	4.90e-1	4.24e-1
Burgers	9	interpolation	3.95e-1	5.02e-1	4.44e-1
Burgers	9	regression	4.70e-1	6.46e-1	5.50e-1
Burgers	10	interpolation	4.57e-1	5.47e-1	5.04e-1
Burgers	10	regression	4.91e-1	6.36e-1	5.67e-1
Cavity	4	interpolation	8.24e-2	5.73e-2	7.16e-2
Cavity	4	regression	8.64e-2	6.39e-2	7.66e-2
Cavity	5	interpolation	7.40e-2	5.29e-2	6.49e-2
Cavity	5	regression	8.00e-2	6.22e-2	7.21e-2
Cavity	6	interpolation	7.27e-2	5.29e-2	6.40e-2
Cavity	6	regression	7.79e-2	6.17e-2	7.07e-2
Cavity	7	interpolation	7.12e-2	4.92e-2	6.18e-2
Cavity	7	regression	7.58e-2	5.66e-2	6.73e-2
Cavity	8	interpolation	7.08e-2	4.83e-2	6.12e-2
Cavity	8	regression	7.62e-2	5.53e-2	6.72e-2
Cavity	9	interpolation	7.08e-2	4.61e-2	6.05e-2
Cavity	9	regression	7.68e-2	5.53e-2	6.77e-2
Cavity	10	interpolation	7.35e-2	4.93e-2	6.34e-2
Cavity	10	regression	7.74e-2	5.77e-2	6.89e-2

Table 8: Regularization intensity (λ) ablation for OpInf-LLM.

Equation	λ	Method	Error $[0, T]$	Error $[T, 2T]$	Error $[0, 2T]$
Heat	0	interpolation	1.23e-2	4.27e-2	3.16e-2
Heat	0	regression	1.29e-2	3.60e-2	2.72e-2
Heat	10^{-6}	interpolation	1.23e-2	4.27e-2	3.16e-2
Heat	10^{-6}	regression	1.29e-2	3.60e-2	2.72e-2
Heat	10^{-5}	interpolation	1.23e-2	4.27e-2	3.16e-2
Heat	10^{-5}	regression	1.29e-2	3.60e-2	2.72e-2
Heat	10^{-4}	interpolation	1.23e-2	4.27e-2	3.16e-2
Heat	10^{-4}	regression	1.29e-2	3.60e-2	2.72e-2
Heat	10^{-3}	interpolation	1.23e-2	4.27e-2	3.16e-2
Heat	10^{-3}	regression	1.29e-2	3.60e-2	2.72e-2
Heat	10^{-2}	interpolation	1.25e-2	4.4e-2	3.25e-2
Heat	10^{-2}	regression	1.22e-2	3.33e-2	2.54e-2
Heat	10^{-1}	interpolation	4.00e-2	4.43e-1	3.07e-1
Heat	10^{-1}	regression	3.44e-2	1.09e-1	7.97e-2
Heat	1	interpolation	4.37e3	4.43e9	3.01e9
Heat	1	regression	5.67e-2	8.61e-2	7.3e-2
Heat	10	interpolation	3.73e-1	1.52e0	1.12e0
Heat	10	regression	2.71e-1	3.16e-1	2.96e-1
Burgers	0	interpolation	1.34e0	9.17e-1	1.14e0
Burgers	0	regression	2.25e1	2.92e1	2.5e1
Burgers	10^{-6}	interpolation	1.34e0	9.17e-1	1.14e0
Burgers	10^{-6}	regression	2.25e1	2.92e1	2.5e1
Burgers	10^{-5}	interpolation	1.34e0	9.17e-1	1.14e0
Burgers	10^{-5}	regression	2.25e1	2.92e1	2.5e1
Burgers	10^{-4}	interpolation	1.34e0	9.17e-1	1.14e0
Burgers	10^{-4}	regression	2.25e1	2.92e1	2.5e1
Burgers	10^{-3}	interpolation	1.34e0	9.17e-1	1.14e0
Burgers	10^{-3}	regression	2.26e1	2.94e1	2.51e1
Burgers	10^{-2}	interpolation	1.31e0	8.91e-1	1.12e0
Burgers	10^{-2}	regression	2.96e1	3.90e1	3.32e1
Burgers	10^{-1}	interpolation	8.72e-1	6.82e-1	7.85e-1
Burgers	10^{-1}	regression	1.81e1	5.42e1	3.74e1
Burgers	1	interpolation	3.67e-1	6.48e-1	5.02e-1
Burgers	1	regression	3.31e-1	5.53e-1	4.33e-1
Burgers	10	interpolation	3.52e-1	4.92e-1	4.12e-1
Burgers	10	regression	3.34e-1	4.53e-1	3.83e-1
Cavity	0	interpolation	failed	failed	failed
Cavity	0	regression	failed	failed	failed
Cavity	10^{-6}	interpolation	failed	failed	failed
Cavity	10^{-6}	regression	failed	failed	failed
Cavity	10^{-5}	interpolation	9.98e3	1.09e4	1.05e4
Cavity	10^{-5}	regression	2.14e-1	2.83e-1	2.5e-1
Cavity	10^{-4}	interpolation	9.98e3	1.09e4	1.05e4
Cavity	10^{-4}	regression	2.14e-1	2.83e-1	2.5e-1
Cavity	10^{-3}	interpolation	9.98e3	1.07e4	1.03e4
Cavity	10^{-3}	regression	2.14e-1	2.82e-1	2.5e-1
Cavity	10^{-2}	interpolation	1.01e4	1.2e4	1.11e4
Cavity	10^{-2}	regression	1.95e-1	2.56e-1	2.27e-1
Cavity	10^{-1}	interpolation	4.29e-2	3.90e-2	4.11e-2
Cavity	10^{-1}	regression	9.56e3	1.03e4	1.08e4

Continued on next page

Equation	λ	Method	Error $[0, T]$	Error $[T, 2T]$	Error $[0, 2T]$
Cavity	1	interpolation	$4.01e-2$	$3.88e-2$	$3.95e-2$
Cavity	1	regression	$8.35e-2$	$9.60e-2$	$9.00e-2$
Cavity	10	interpolation	$2.21e-1$	$1.51e-1$	$1.96e-1$
Cavity	10	regression	$2.37e-1$	$1.66e-1$	$2.08e-1$

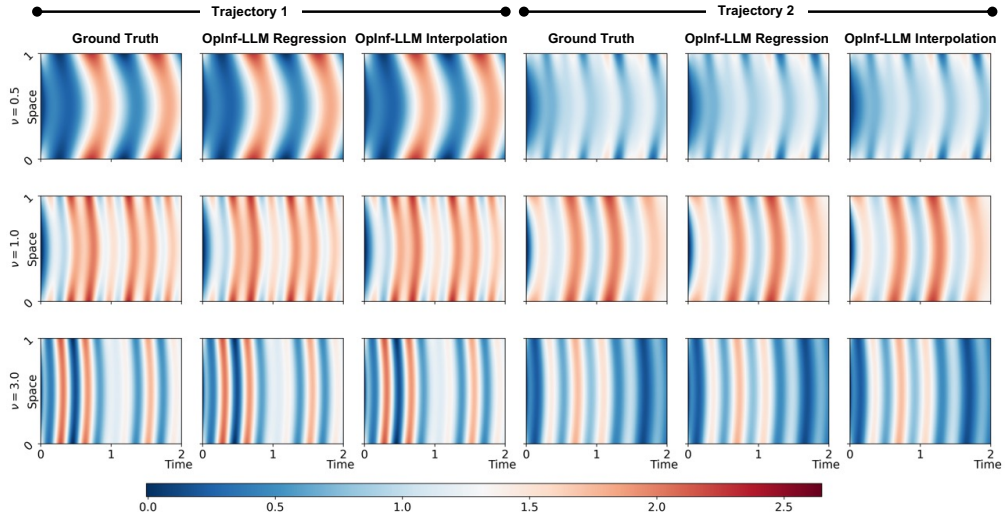


Figure 5: Heat equation predictions of different ν .

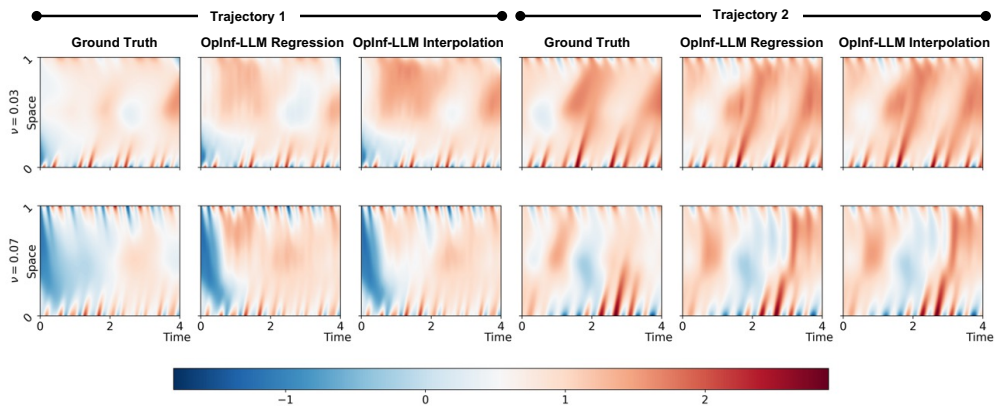


Figure 6: Burgers' equation predictions of different ν .

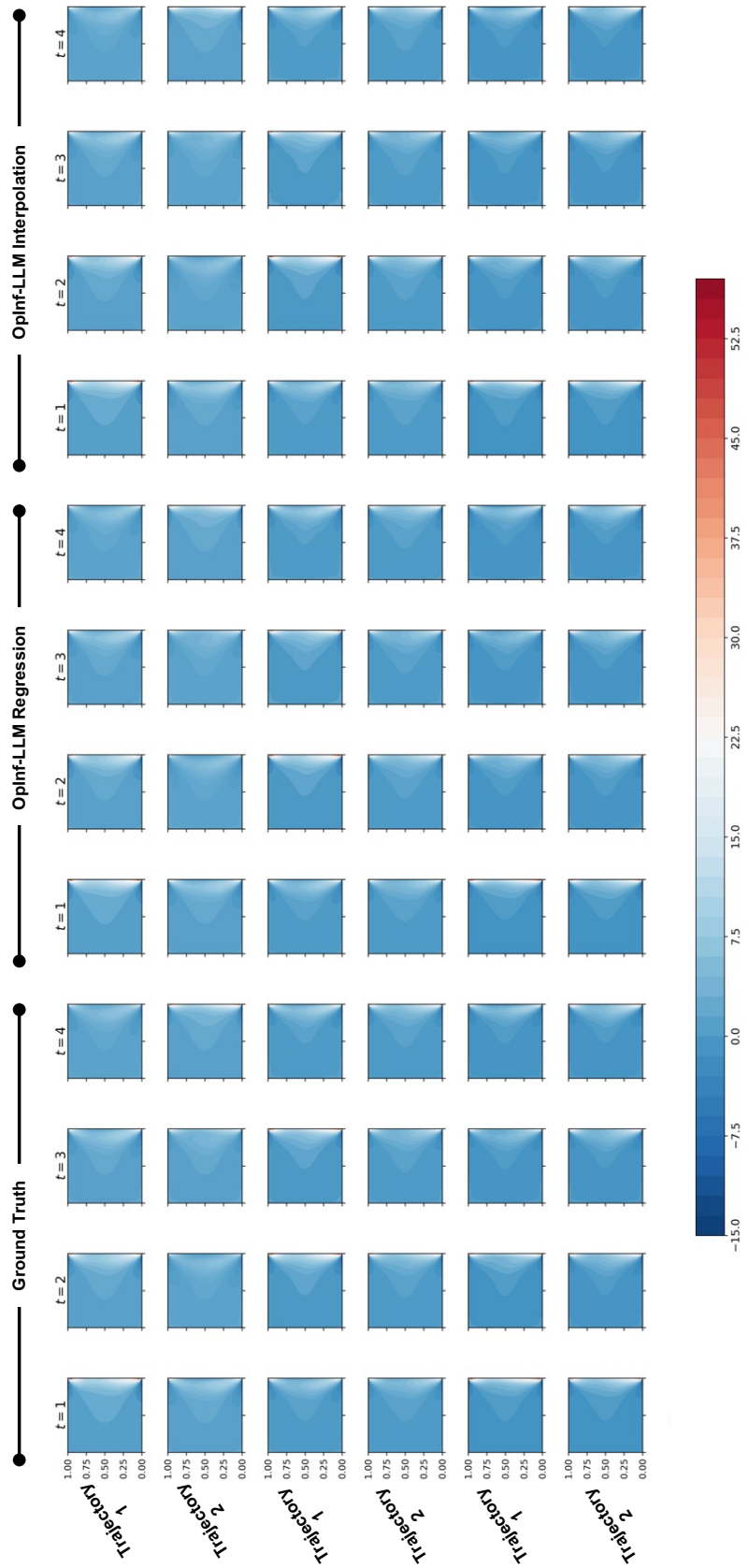


Figure 7: Cavity results across Reynolds numbers.

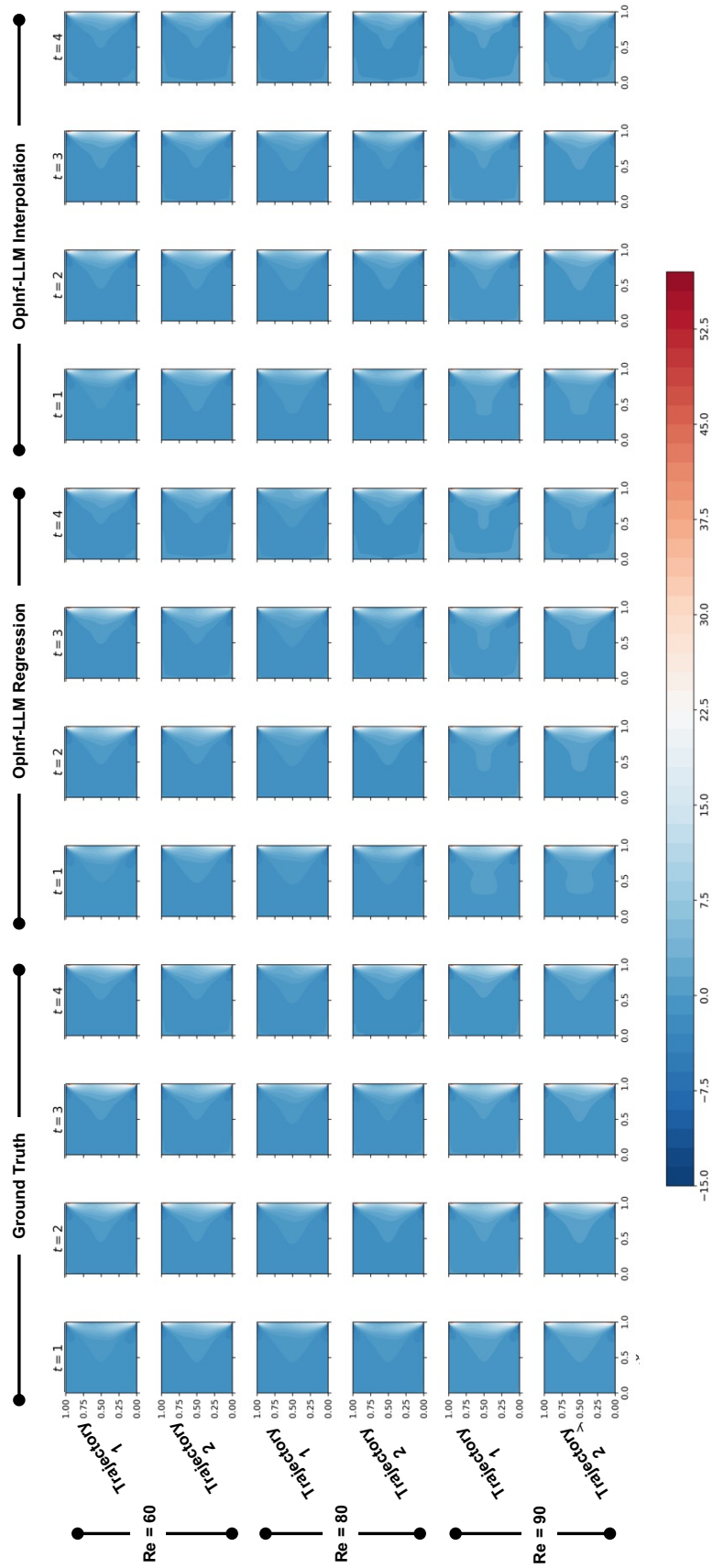


Figure 8: Cavity results across Reynolds numbers.