

Differential Data-Physics Fusion for Solving PDEs

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1. INTRODUCTION & OBJECTIVE

Physical systems are governed by the laws of physics, which are often expressed as Partial Differential Equations (PDEs). The study of PDEs is well-established, with techniques such as Finite Element Methods (FEM), Finite Difference Methods (FDM), and Finite Volume Methods (FVM) widely accessible. However, these established physical laws are frequently derived from specific assumptions and approximations. An alternative approach involves utilizing data-driven methods where recent advancements in neural operators [1] have demonstrated their effectiveness in learning complex nonlinear partial differential equations (PDEs). However, purely data-driven models have certain limitations: (a) they often lack interpretability, (b) they require large amounts of data, and (c) they may struggle to generalize beyond the training domain. To overcome these challenges, a potential solution resides in data-physics fusion, where data-driven models are employed to learn the missing physics and thus acts as model corrector.

In this research work, our objective is to develop a novel hybrid framework that combines neural operators with conventional physics-based models. The proposed framework combines the principles of differentiable physics [2] with the recently introduced Wavelet Neural Operator (WNO) [1]. It utilises WNO's capacity to learn from data while maintaining the interpretability and generalisation of physics-based solvers. The salient features of the proposed framework are as follows:

- **Physics-WNO Integration:** The proposed framework introduces an innovative approach that integrates the Wavelet Neural Operator (WNO) with a low-fidelity physics model directly within the governing equation. This in-equation augmentation enhances generalization compared to extrusive augmentation methods.
- **End-to-End Training:** The approach supports end-to-end training, which ensures computational efficiency during the training phase.
- **Differentiable Physics:** The framework incorporates a differentiable physics solver [2] into the WNO. This integration allows the model to be trained using the backpropagation algorithm, eliminating the need for numerical approximations during the training process.
- **In-Equation Augmentation:** The proposed framework also emphasizes the augmentation of WNO with a low-fidelity physics model within the governing equation itself, offering superior generalization capabilities compared to extrusive augmentation methods.

Method	Cases	Proposed	WNO only	Known physics
		(Er-1)	(Er-1)	(Er-1)
Burgers	Only Diffusion	0.4624	11.0227	2.916
	Missing Diffusion	0.118	15.667	0.505
Allen Cahn	Only Diffusion	0.1583	72.033	2.6089
	Missing Diffusion	0.0011	28.6927	0.1046
Burgers' 2D	Only Diffusion	0.0010	0.1148	0.2258
Smoke-plume	Inexact Buoyancy	0.00399	0.3605	0.3881

Table 1. The prediction errors (Er-1: Mean square error (MSE)) for the different examples obtained using the proposed approach, WNO only (data-driven WNO), and known physics. MSE is computed by taking all 100 test samples for all spatial locations up to 100 time steps in all example cases.

2. RESULTS & HIGHLIGHTS OF IMPORTANT POINTS

In this research, we assess the performance of the proposed framework using a series of benchmark problems with multiple cases to evaluate the framework's effectiveness in handling various scenarios and complexities, one of which is shown here. For illustrative purposes, a synthetic low-fidelity physics model was created by omitting certain portions of the PDE. The solutions produced by the proposed framework are compared with the ground truth to assess accuracy as shown in Fig 1. Particularly, we demonstrate the extrapolation and generalization capabilities of the proposed framework. For quantitative assessment, mean squared error (MSE) values were calculated for all benchmark examples, comparing the performance of different models relative to the ground truth, as shown in Table 1.

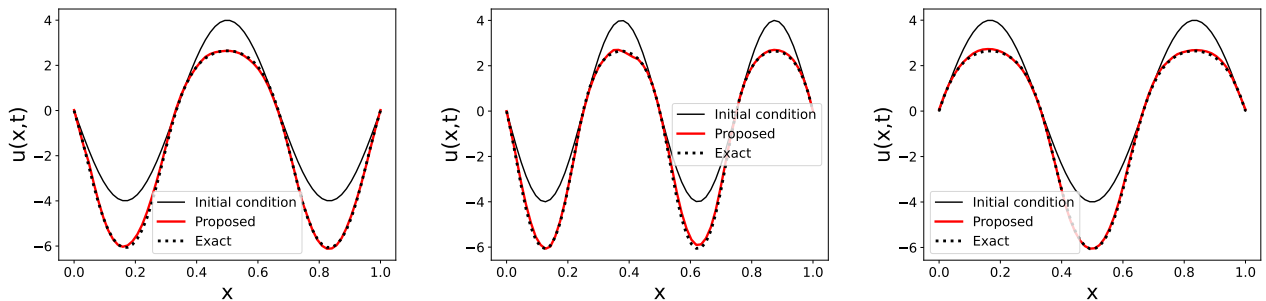


Figure 1. Comparison of predictions from the proposed approach with the ground truth for the Nagumo equation for the case with missing cubic term in the known equation, tested across three different initial conditions (three columns), with $t > t_{train}$) to demonstrate the extrapolative capabilities

REFERENCES

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- [2] K. Um, R. Brand, Y. R. Fei, P. Holl, and N. Thuerey, "Solver-in-the-loop: Learning from differentiable physics to interact with iterative pde-solvers," *Advances in Neural Information Processing Systems*, vol. 33, pp. 6111–6122, 2020