Delft University of Technology
Purdue University

Project: Adjoint-consistent deep learning for surrogate modeling of partial differential equations

Supervisor(s):
Alexander Heinlein (Numerical Analysis, EEMCS)
Romit Maulik (Mechanical Engineering, Purdue University)

November 12, 2025

Topic

Approximating solutions to partial differential equations (PDEs) with neural networks has seen a dramatic rise over the past decade [2]. A key driver of this growth is the demand for fast surrogate models that accelerate the computation of quantities of interest [4]. Such surrogates can bypass the high computational cost of classical numerical solvers, especially for multiscale problems such as turbulent flows [11], weather forecasting [8], or reservoir simulations [5]; see figure 1 for the porosity field in groundwater flow. Operator learning provides a framework for surrogate modeling that learns parametric solution operators mapping between function spaces (for example, from initial and boundary conditions to the solution space) [3]. Neural operator models have already shown promising results for surrogate modeling across various scientific domains [7].

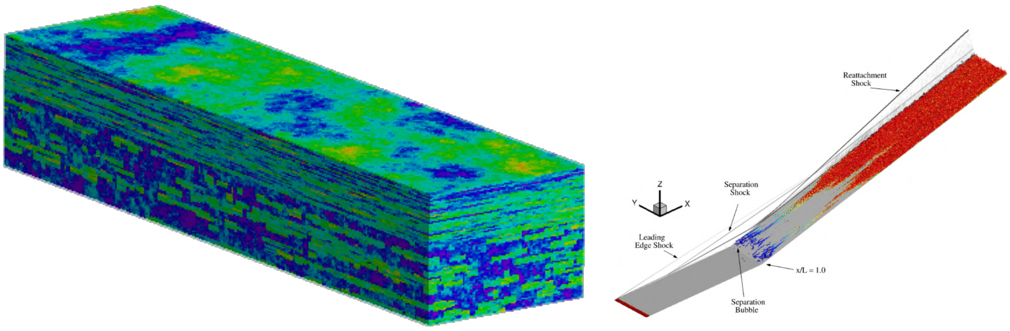

Figure 1: Exemplary multiscale problem in groundwater flow: porosity field of Model 2 from the SPE10 benchmark; cf. [6] and a Mach 7.7 Transitional Shock-Boundary Layer Interaction [1].

For many applications involving optimization, gradients of the solution operator are essential. They enable inverse modeling, where one seeks optimal initial conditions or parameters consistent with observed data [9, 10]. Traditionally, PDE-constrained optimization has been used for such problems, but solving a PDE and its adjoint incurs high computational costs at every iteration. Neural network surrogates, being lightweight and differentiable, allow adjoints to be efficiently computed via automatic differentiation (AD) [7].

However, while neural operators can accurately approximate the forward model, their ability to approximate the adjoint remains unclear, especially since adjoint data from numerical solvers are rarely available. This motivates our central research question: how can we design neural operators that yield accurate approximations for both the forward and adjoint operators? Furthermore, if the adjoint cannot be directly approximated, how can such surrogates still be used reliably in inverse problems?

We aim to introduce formal adjoint-consistency conditions in training, ensuring that gradients of a scalar loss with respect to model parameters match those derived from the discrete adjoint of a numerical forward model. To this end, our surrogates will incorporate discrete structure similar to that of numerically discretized PDEs. The discrete adjoint can then be compared to the AD-based gradient via an augmented loss function. Specifically, we define a discretized forward model

$$F_h(u_h, \theta) = 0,$$

yielding an objective function

$$J_h(u_h, \theta),$$

and a discrete adjoint

$$\frac{\partial F_h}{\partial u_h} \lambda = \frac{\partial J_h}{\partial u_h}.$$

We then enforce consistency by penalizing discrepancies between

$$\nabla_\theta J_h = \frac{\partial J_h}{\partial \theta} - \lambda^T \frac{\partial F_h}{\partial \theta}$$

and gradients from automatic differentiation. Embedding this structure into neural training, we hypothesize that such surrogates will yield accurate AD-based derivatives for inverse problems. In this project, we will explore this for optimizing turbulent flows using a deep neural operator, without access to ground-truth adjoints.

Contact

Are you interested or do you have any questions? Send an email to Alexander Heinlein (a.heinlein@tudelft.nl) and/or Romit Maulik (rmaulik@purdue.edu).

References

[1] S. Ahmed, M. Schuabb, L. Duan, R. Singh, T. Toki, and C. Scalo. Direct numerical simulation and subfilter scale analysis for a hypersonic transitional shock-boundary layer interaction. In *AIAA AVIATION FORUM AND ASCEND 2025*, page 3429, 2025.

[2] C. Beck, M. Hutzenthaler, A. Jentzen, and B. Kuckuck. An overview on deep learning-based approximation methods for partial differential equations. *arXiv preprint arXiv:2012.12348*, 2020.

[3] N. Boullé and A. Townsend. A mathematical guide to operator learning. *arXiv preprint arXiv:2312.14688*, 2023.

[4] S. L. Brunton and J. N. Kutz. Promising directions of machine learning for partial differential equations. *Nature Computational Science*, 4(7):483–494, 2024.

[5] A. Chandra, M. Koch, S. Pawar, A. Panda, K. Azizzadenesheli, J. Snippe, F. O. Alpak, F. Hariri, C. Etienam, P. Devarakota, A. Anandkumar, and D. Hohl. Accelerating Porous Media Flow Simulations With Fourier Neural Operators: An Application to Geologic Storage of CO_2. *Advanced Theory and Simulations*, page e00747, Sept. 2025. ISSN 2513-0390, 2513-0390. doi: 10.1002/adts.202500747. URL https://advanced.onlinelibrary.wiley.com/doi/10.1002/adts.202500747.

[6] M. A. Christie and M. J. Blunt. Tenth spe comparative solution project: A comparison of upscaling techniques. In *SPE Reservoir Simulation Symposium*, Houston, Texas, USA, Feb. 2001. Society of Petroleum Engineers. doi: 10.2118/66599-MS. URL https://doi.org/10.2118/66599-MS. SPE-66599-MS.

[7] Z. Li, N. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. Stuart, and A. Anandkumar. Fourier neural operator for parametric partial differential equations. *arXiv preprint arXiv:2010.08895*, 2020.

[8] I. Price, A. Sanchez-Gonzalez, F. Alet, T. R. Andersson, A. El-Kadi, D. Masters, T. Ewalds, J. Stott, S. Mohamed, P. Battaglia, et al. Probabilistic weather forecasting with machine learning. *Nature*, 637 (8044):84–90, 2025.

[9] S. A. Renganathan, R. Maulik, and V. Rao. Machine learning for nonintrusive model order reduction of the parametric inviscid transonic flow past an airfoil. *Physics of Fluids*, 32(4), 2020.

[10] S. A. Renganathan, R. Maulik, and J. Ahuja. Enhanced data efficiency using deep neural networks and gaussian processes for aerodynamic design optimization. *Aerospace Science and Technology*, 111:106522, 2021.

[11] R. Wang, K. Kashinath, M. Mustafa, A. Albert, and R. Yu. Towards physics-informed deep learning for turbulent flow prediction. In *Proceedings of the 26th ACM SIGKDD international conference on knowledge discovery & data mining*, pages 1457–1466, 2020.