

**Scientific Machine Learning for Dynamical Systems:  
Theory and Applications  
to Fluid Flow and Ocean Ecosystem Modeling**

by

Abhinav Gupta

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**Abstract**

Complex dynamical models are used for prediction in many domains, and are useful to mitigate many of the grand challenges being faced by humanity, such as climate change, food security, and sustainability. However, because of computational costs, complexity of real-world phenomena, and limited understanding of the underlying processes involved, models are invariably approximate. The missing dynamics can manifest in the form of unresolved scales, inexact processes, or omitted variables; as the neglected and unresolved terms become important, the utility of model predictions diminishes. To address these challenges, we develop and apply novel scientific machine learning methods to learn unknown and discover missing dynamics in models of dynamical systems.

In our Bayesian approach, we develop an innovative stochastic partial differential equation (PDE) - based model learning theory and framework for high-dimensional coupled biogeochemical-physical models. The framework only uses sparse observations to learn rigorously within and outside of the model space as well as in that of the states and parameters. It employs Dynamically Orthogonal (DO) differential equations for adaptive reduced-order stochastic evolution, and the Gaussian Mixture Model-DO (GMM-DO) filter for simultaneous nonlinear inference in the augmented space of state variables, parameters, and model equations. A first novelty is the Bayesian learning among compatible and embedded candidate models enabled by parameter estimation with special stochastic parameters. A second is the principled Bayesian discovery of new model functions empowered by stochastic piecewise polynomial approximation theory. Our new methodology not only seamlessly and rigorously discriminates between existing models, but also extrapolates out of the space of models to discover newer ones. In all cases, the results are generalizable and interpretable, and associated with probability distributions for all learned quantities. To showcase and quantify the learning performance, we complete both identical-twin

and real-world data experiments in a multidisciplinary setting, for both filtering forward and smoothing backward in time. Motivated by active coastal ecosystems and fisheries, our identical-twin experiments consist of lower-trophic-level marine ecosystem and fish models in a two-dimensional idealized domain with flow past a seamount representing upwelling due to a sill or strait. Experiments have varying levels of complexities due to different learning objectives and flow and ecosystem dynamics. We find that even when the advection is chaotic or stochastic from uncertain nonhydrostatic variable-density Boussinesq flows, our framework successfully discriminates among existing ecosystem candidate models and discovers new ones in the absence of prior knowledge, along with simultaneous state and parameter estimation. Our framework demonstrates interdisciplinary learning and crucially provides probability distributions for each learned quantity including the learned model functions. In the real-world data experiments, we configure a one-dimensional coupled physical-biological-carbonate model to simulate the state conditions encountered by a research cruise in the Gulf of Maine region in August, 2012. Using the observed ocean acidification data, we learn and discover a salinity based forcing term for the total alkalinity ( $TA$ ) equation to account for changes in  $TA$  due to advection of water masses of different salinity caused by precipitation, riverine input, and other oceanographic processes. Simultaneously, we also estimate the multidisciplinary states and an uncertain parameter. Additionally, we develop new theory and techniques to improve uncertainty quantification using the DO methodology in multidisciplinary settings, so as to accurately handle stochastic boundary conditions, complex geometries, and the advection terms, and to augment the DO subspace as and when needed to capture the effects of the truncated modes accurately. Further, we discuss mutual-information-based observation planning to determine what, when, and where to measure to best achieve our learning objectives in resource-constrained environments.

Next, motivated by the presence of inherent delays in real-world systems and the Mori-Zwanzig formulation, we develop a novel delay-differential-equations-based deep learning framework to learn time-delayed closure parameterizations for missing dynamics. We find that our neural closure models increase the long-term predictive capabilities of existing models, and require smaller networks when using non-Markovian over Markovian closures. They efficiently represent truncated modes in reduced-order-models, capture effects of subgrid-scale processes, and augment the simplification of complex physical-biogeochemical models. To empower our neural closure models framework with generalizability and interpretability, we further develop neural partial delay differential equations theory that augments low-fidelity models in their original PDE forms with both Markovian and non-Markovian closure terms parameterized with neural networks (NNs). For the first time, the melding of low-fidelity model and NNs with time-delays in the continuous spatiotemporal space followed by numerical discretization automatically provides interpretability and allows for generalizability to computational grid resolution, boundary conditions, initial conditions, and problem specific parameters. We derive the adjoint equations in the continuous form, thus, allowing implementation of our new methods across differentiable and non-differentiable computational physics codes, different machine learning frameworks, and also non-uniformly-spaced spatiotemporal training data. We also show

that there exists an optimal amount of past information to incorporate, and provide methodology to learn it from data during the training process. Computational advantages associated with our frameworks are analyzed and discussed. Applications of our new Bayesian learning and neural closure modeling are not limited to the shown fluid and ocean experiments, but can be extended to other fields such as control theory, robotics, pharmacokinetic-pharmacodynamics, chemistry, economics, and biological regulatory systems.

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Om Bhūr Bhuvah Svah  
Tat Saviturvareṇyam  
Bhargo Devasya Dhīmahi  
Dhiyo Yonah Prachodayāt

---

*Gayatri Mantra*  
*Rig Veda 3.62.10*

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