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ABSTRACT

Recent applications of machine learning, in particular deep learning, motivate the need to address the generalizability of the statistical inference approaches in physical sciences. In this Letter, we introduce a modular physics guided machine learning framework to improve the accuracy of such data-driven predictive engines. The chief idea in our approach is to augment the knowledge of the simplified theories with the underlying learning process. To emphasize their physical importance, our architecture consists of adding certain features at intermediate layers rather than in the input layer. To demonstrate our approach, we select a canonical airfoil aerodynamic problem with the enhancement of the potential flow theory. We include the features obtained by a panel method that can be computed efficiently for an unseen configuration in our training procedure. By addressing the generalizability concerns, our results suggest that the proposed feature enhancement approach can be effectively used in many scientific machine learning applications, especially for the systems where we can use a theoretical, empirical, or simplified model to guide the learning module.

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Advanced machine learning (ML) models such as deep neural networks are powerful tools for finding patterns in complicated datasets. However, as these *universal approximators*^{1–4} become complex, the number of trainable parameters (weights) quickly explodes, adversely affecting their interpretability and hence their trustworthiness. Using these models in combination with other traditional models compromises the trustworthiness of the overall system. While such techniques have been emerging in both scientific computing and ML fields,^{5–27} they offer many opportunities to fuse topics in domain-specific knowledge, numerical linear algebra, and theoretical computer science²⁸ toward improving the generalizability of these models. In this Letter, we focus on a modular approach for improving generalizability by augmenting input features with simplified physics-based models or theories. By the term of *generalizability*, we refer to the performance of the learning engine for unseen configurations. Such new situations are pervasive in scientific applications. In many cases, there is a grand challenge in making

accurate predictions using data-driven methods based strictly on statistical inference. For example, in fluid mechanics, potential flow and boundary layer theories often provide simplistic models pertaining to a certain level of approximations. A remaining task is how to combine these models for making more generalizable learning architectures. Therefore, our approach provides intermediate features based on approximate physics to statistical models that can relate or fulfill the gap between these simplified theories and more accurate models (i.e., experimental or high fidelity computational fluid dynamics simulation datasets).

A wide variety of engineering tasks, such as optimal control, design optimization, and uncertainty quantification, requires the prediction of the quantity of interest in real-time. In such scenarios, the partial differential equation (PDE) based discretization methods are not feasible as they can take days or weeks to simulate different configurations. Reduced order models (ROMs) are the state-of-the-art models that construct the basis from the past data and then

solve the governing equations after projecting them on the low-dimensional manifold.^{29–31} The main limitation of such projection based intrusive ROMs is that it requires a complete description of the dynamics of the system, and often, this information is unavailable or inadequate for the desired application. Recently, model-free prediction using machine learning has proven successful for many physical systems.^{32–34} One of the main challenges with these non-intrusive models is the prediction for unseen data and their interpretation. Even though probabilistic machine learning methods such as Bayesian neural networks can give the uncertainty bound on the predicted state,^{10,35} the generalizability of non-intrusive models is not on par with physics-based models. On the other hand, the simplified models such as the lumped-capacitance model for heat transfer analysis and Blasius boundary layer model in fluid mechanics are highly generalizable to different conditions. Therefore, it is important to leverage the knowledge of physical systems into learning, and to this end, we make progress toward physics guided machine learning (PGML) by embedding features from simplified physical models into the neural network architecture. The proposed framework is flexible enough to be applied to many physical systems, and it has great potential in scientific machine learning.

We now introduce different components of the physics guided machine learning (PGML) framework as depicted in Fig. 1(a). In supervised machine learning, the input vector $\mathbf{x} \in \mathbb{R}^m$ is fed to the machine learning model (for example, the neural network in our case), and the mapping from the input vector to output vector $\mathbf{y} \in \mathbb{R}^n$ is learned through training. The neural network is trained to learn the function F_θ , parameterized by θ , that includes the weights and biases of each neuron. The function F_θ should be such that it approximates the known labels and the cost function is minimized. Usually, for the regression problems, the cost function is the mean squared error between true and predicted output, i.e., $C(\mathbf{x}, \theta) = \|\mathbf{y} - F_\theta(\mathbf{x})\|_2$. The weights and biases of the neural network are optimized using any gradient-descent algorithm such as stochastic gradient descent. In the PGML framework, the neural network is augmented with the output of the simplified physics-based model. The features extracted from simplified physics-based models can be either combined with input features or they can be merged

into hidden layers along with latent variables. During the training, the PGML framework is provided with $(\mathbf{x}, G(\mathbf{x}))$, where G is the model based on simplified theories for the problem at hand, and the parameters θ are optimized based on the true output \mathbf{y} . The features from the simplified model G can also be fed at an intermediate hidden layer along with learned latent representation.

The PGML framework allows us to extract the knowledge from the simplified physics-based model and combine it with the latent variables of the system discovered by the neural network at intermediate hidden layers. This information from the physics-based model assists the neural network in constraining its output to a manifold of physically realizable models. It encourages the neural network to learn the physically consistent representation of the quantity of interest drawn from complex distributions, such as pressure and velocity field of fluid simulations. Another advantage of the PGML framework is that it brings interpretability to otherwise black-box models. We highlight here that the PGML framework allows us to incorporate the physics of the problem even during the prediction stage, and not just the training as in the case of approaches such as regularization based on governing equations.

In a nutshell, we highlight that there might be a handful of simplified models (e.g., similarity solutions, lumped parameter models, zone models, and zero or one-dimensional models) to approximate or describe the underlying physical processes in many disciplines. For example, in aerodynamics, the use of simplistic panel methods is a proven approach for analysis of inviscid flow over bodies, especially for a smaller angle of attacks where the potential flow theory becomes valid. The execution time for these simplified models is significantly smaller compared to the run time needed for full-fledged computational fluid dynamics (CFD) simulations. Therefore, in the PGML method, we propose to fuse the knowledge coming from such simplified theories in a statistical inference architecture. This is accomplished by a feature enhancement procedure as described in Fig. 1(b). Specifically, it constitutes a predictor–corrector philosophy where we first run a simplified theory (computationally less demanding) to estimate an intermediate prediction as an input for the overall ML architecture. We then estimate the quantity of interest based on the enhancement procedure abstracted by $G(\mathbf{x})$. We hypothesize that the predictive performance and generalizability of

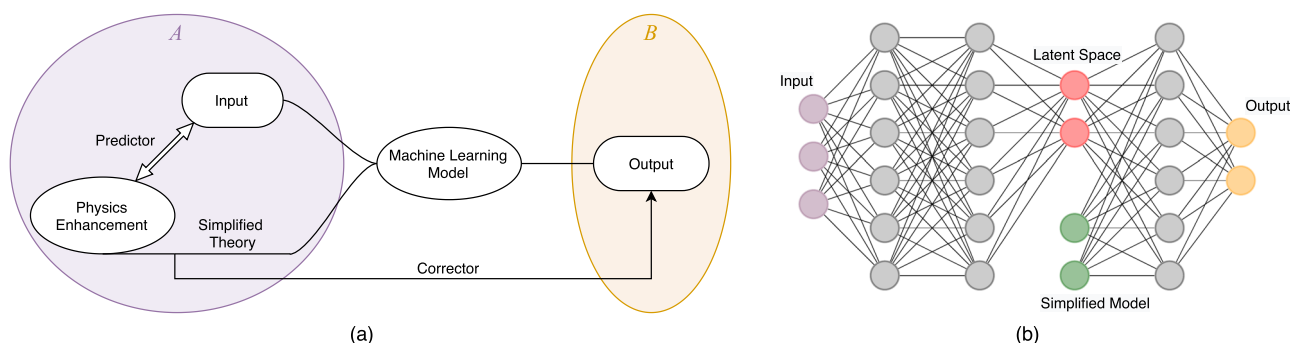


FIG. 1. Physics guided machine learning (PGML) framework to train a learning engine between processes A and B: (a) a conceptual PGML framework, which shows different ways of incorporating physics into machine learning models. The physics can be incorporated using feature enhancement of the ML model based on the domain knowledge, embedding simplified theories directly into ML models, and corrector approach in which the output of the ML model is constrained using the governing equations of the system, and (b) an overview of the typical neural network architecture for the PGML framework.

statistical inference will be significantly improved by the involvement of $G(\mathbf{x})$ as illustrated with the aerodynamic performance prediction task.

Results and Discussion—We demonstrate the PGML framework using the aerodynamic performance prediction task. This is a problem relevant to many applications, such as predictive control³⁶ and design optimization.³⁷ The prediction of flow around an airfoil is a high-dimensional, multiscale, and nonlinear problem that can be solved using high-fidelity methods such as computational fluid dynamics (CFD). However, these methods are computationally intractable as the design space exploration increases. In certain flow regimes, the simplified methods such as panel codes come with a non-negligible difference between the actual dynamics and approximate models for real-world problems. The full-order CFD simulations typically take extensive computational run time, thus limiting their use in many inverse modeling methodologies that require a model run to be performed in each iteration. To overcome these challenges, combining CFD models with machine learning to build a data-driven surrogate model is gaining widespread popularity.^{38–40} In this example, we exploit the relevant physics-based features from panel methods through the PGML framework to enhance the generalizability of data-driven surrogate models.

The training data for the neural network are generated using a series of numerical simulations. The main goal of this work is to demonstrate how a simplified model can be used in the PGML framework, and therefore, to reduce the computational complexity, we utilize XFOIL⁴¹ for the aerodynamic analysis of different airfoils instead of full CFD simulation to get the most accurate results for the forces on the airfoil. The lift coefficient data were obtained for different Reynolds numbers between 1×10^6 and 4×10^6 and several angles of attacks in the range of -20 to $+20$. A total of 168 sets of two-dimensional airfoil geometry were generated for training the neural network. This includes NACA 4-digit, NACA210, NACA220, and NACA250 series, and each airfoil is represented by 201 points. The maximum thickness of all airfoils in the training dataset was between 6% and 18% of the chord length. We use the NACA23012 and NACA23024 airfoil geometry as the test dataset to evaluate the predictive capability of the trained neural network. The simplified model used to generate the physics-based feature corresponds to the Hess–Smith panel method⁴² based on potential flow theory. We highlight that our testing airfoils are selected not only from a different NACA230 series (i.e., not used in the training dataset) but also the maximum thickness of 24% is well beyond the thickness ratio limit included in our training dataset.

The neural network architecture used in this study has four hidden layers with 20 neurons in each hidden layer. The physical parameters, i.e., the Reynolds number and the angle of attack, are concatenated at the third hidden layer along with the latent variables at that layer. In the PGML model, we augment the latent variables at the third layer with the lift coefficient and the pressure drag coefficient predicted by the panel method along with physical parameters of the flow (i.e., the Reynolds number and angle of attack). Therefore, the third layer of the PGML neural network has 24 latent variables. The representative neural network for the PGML framework to predict the aerodynamic forces on an airfoil is displayed in Fig. 2. We utilize an ensemble of neural networks to quantify the predictive uncertainty.^{43–45} In this method, a small number of neural networks are trained from different initialization and the variance

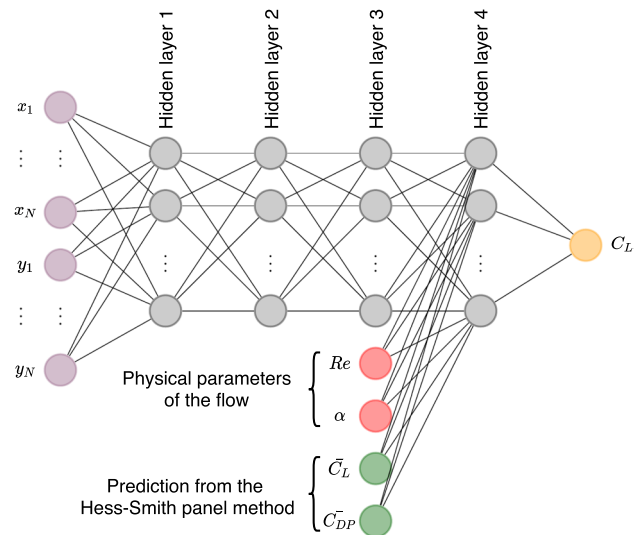


FIG. 2. The representative neural network architecture of the PGML framework used in this study for the aerodynamic force prediction task. The latent variables at the third hidden layers are augmented with the physical parameters of the flow (i.e., the Reynolds number and angle of attack) and the prediction from the Hess–Smith panel method (i.e., lift coefficient and pressure drag coefficient denoted as \bar{C}_L and \bar{C}_{DP} , respectively).

of the ensemble’s prediction is interpreted as the epistemic uncertainty. This method is appealing due to its simplicity, scalability, and strong empirical results of the uncertainty estimate that are as good as the Bayesian neural networks.⁴⁵ We train multiple neural network models using different values of the initial weights and biases. The weights and biases of each model are initialized using the Glorot uniform initializer, and different random seed numbers are used to ensure that the different values of weights and biases are assigned for each model. The ensemble of all these models indicates the model uncertainty estimate of the predicted lift coefficient. Figure 3 shows the actual and predicted lift coefficients for the NACA23012 and NACA23024 airfoil geometry. The reference *True* performance is obtained by XFOIL. The ML corresponds to a simple feed-forward neural network that uses the airfoil x and y coordinates as the input features, and the physical parameters of the flow are concatenated at the third hidden layer along with the latent variables at that layer.

As shown in Fig. 3, we can see that the uncertainty in the prediction of the lift coefficient by the PGML model is less than the ML model for both NACA23012 and NACA23024 airfoils. The proposed PGML framework provides significantly more accurate predictions with reduced uncertainty for the angle of attacks between -10° and $+10^\circ$. This further illustrates the viability of the proposed PGML framework since the physics embedding considered here employs constant source panels and a single vortex to approximate the potential flow around the airfoil. We can also notice that the uncertainty is higher for the angle of attacks outside the range of -10° to $+10^\circ$. This finding is not surprising as the Hess–Smith panel method is a proven method for analysis of inviscid flow over airfoil for the smaller angle of attacks regime. We highlight that the maximum thickness of an airfoil included in the training dataset is 18% of the chord length. Therefore, the uncertainty in the prediction of the

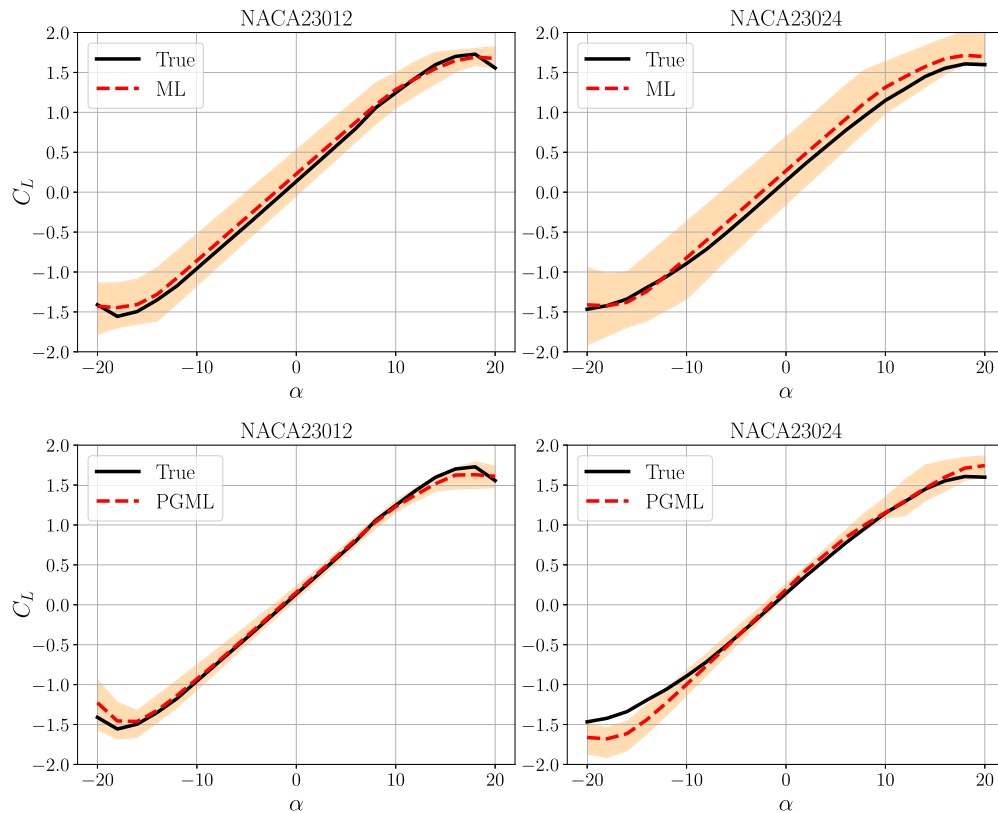


FIG. 3. Actual vs predicted lift coefficient (C_L) for NACA23012 and NACA23024 airfoils at $Re = 3 \times 10^6$ using ML and PGML framework. The dashed red curve represents the average of the predicted lift coefficient by all ML models (i.e., testing runs with different initialization seeds). Both airfoil geometries were not included in the training. Here, we note that there is a significant reduction of uncertainty in performance when we use the proposed PGML framework, especially for the smaller angle of attacks where the embedded simplistic physics-based model is valid. The physics embedding in these tests is based on the utilization of the Hess–Smith panel method, which is limited mostly for the angle of attacks between -10° and $+10^\circ$, which further verifies the success of the proposed PGML framework.

lift coefficient by the ML model is higher for the NACA23024 airfoil compared to the NACA23012 airfoil. The inclusion of physics-based features from the panel method in the PGML model leads to a reduction in this uncertainty estimate. These results clearly show the advantage of augmenting the neural network model with simplified theories and the potential of the PGML framework for physical systems. One of the important caveats with any neural network is its design and the hyperparameters. The neural architecture search and hyperparameter optimization are important processes for the success of the PGML framework. If the network is shallow, then it has less expressive capabilities and that deteriorates the prediction. On the other hand, if the neural network architecture is very deep and there are no sufficient training data, then the network fits the training data very well. However, its generalizability is reduced and this is usually indicated by an increase in the loss of the validation dataset after a few iterations of the training. Some of the strategies to mitigate overfitting issues in the deep neural network are using L_1/L_2 regularization, applying dropout, early stopping, data augmentation, and k -fold cross-validation. Overall, our findings suggest that the absorption of physical information into ML methods improves the modeling uncertainty of the ML architectures.

Concluding Remarks—The data-driven models derived from the data collected from satellite measurements, internet of things (IoT) devices, and numerical simulation are increasingly being applied for scientific applications in fluid dynamics. While these data-driven models are successful, it might be vital to complement them with physical laws that have been studied for many decades. To this end, physics-informed machine learning approaches, such as embedding soft and hard constraints designed based on governing laws of the physical system, have been proposed.^{9,10,17,18} In this work, we illustrated how physics-based models derived from simplified approximations of the physical system can be coupled within data-driven models such as neural networks. The PGML framework introduced in this study allows us to take advantage of the generalizability of physics-based simplistic models and the robustness of data-driven models. We demonstrated the proof-of-concept for the aerodynamic performance analysis of airfoil geometry. The physics-based features computed from the simplistic panel method are coupled with the latent representation learned at the intermediate layers of the neural network. The inclusion of these physics-based features assists the neural network model in reducing the uncertainty of the lift coefficient prediction. Therefore, the PGML

framework is successful in improving the generalizability of data-driven models.

Additionally, the PGML framework will also be useful for physical systems where the data are scarce. For example, the generation of training data is computationally expensive when dealing with larger problems, such as the optimization of a wind farm layout⁴⁶ or the shape optimization of a three-dimensional wing.⁴⁷ The simplified models such as the actuator disk theory can be used along with a velocity field generated from few high-fidelity numerical simulations to build a physics-guided neural network-based surrogate model of the wind farm that can be coupled with any optimization algorithm. Another area where the PGML framework may bear huge potential is the digital twin technologies for physical systems,⁴⁸ where the digital replica of the physical system is built for tasks, such as real-time control, efficient operation, and accurate forecast of maintenance schedules. In the present study, we started with XFOIL to assess the feasibility of the proposed framework. Despite its simplicity, this is the first step toward demonstrating the PGML framework for problems in fluid dynamics. In our future work, we plan to extend the PGML approach to complex and high-dimensional problems such as prediction of terrain induced atmospheric boundary layer flows or flows around bluff bodies immersed in fluid to illustrate the true capability of the PGML framework.

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DATA AVAILABILITY

The data that support the findings of this study are available within the article. Implementation details and Python scripts can be accessed from the Github repository.⁴⁹

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