Integrating Physics-Based Modeling with Machine Learning: A Survey

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Abstract

In this manuscript, we provide a structured and comprehensive overview of techniques to integrate machine learning with physics-based modeling. First, we provide a summary of application areas for which these approaches have been applied. Then, we describe classes of methodologies used to construct physics-guided machine learning models and hybrid physics-machine learning frameworks from a machine learning standpoint. With this foundation, we then provide a systematic organization of these existing techniques and discuss ideas for future research.

1 Introduction

Machine learning (ML) models, which have already found tremendous success in commercial applications, are beginning to play an important role in advancing scientific discovery in domains traditionally dominated by physics-based models [Karpatne *et al.*, 2017a]. The use of ML models is particularly promising in scientific problems involving processes that are not completely understood, or where it is computationally infeasible to run physics-based models at desired resolutions in space and time. However, the application of even the state-of-the-art black box ML models has often met with limited success in scientific domains due to their large data requirements, inability to produce physically consistent results, and their lack of generalizability to out of sample scenarios. Given that neither an ML-only nor a scientific knowledge-only approach can be considered sufficient for complex scientific and engineering applications, the research community is beginning to explore the continuum between physics-based and ML models, where both scientific knowledge and data are integrated in a synergistic manner. This paradigm is fundamentally different from mainstream practices in the ML community for making use of domain-specific knowledge, albeit in subservient roles, e.g., feature engineering or post-processing. In contrast to these practices that can only work with simpler forms of heuristics and constraints, this approach explores a deeper coupling of ML methods with scientific knowledge.

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Even though the idea of integrating physics and ML models has picked up momentum just in the last few years, there is already a vast amount of work on this topic. This work is being pursued in diverse disciplines (e.g., climate science, turbulence modeling, material discovery, quantum chemistry, biomedical science, biomarker discovery, and hydrology). Also, it is being performed in the context of diverse objectives specific to these applications. Early results in isolated and relatively simple scenarios have been promising, and the expectations are rising for this paradigm to accelerate scientific discovery and help address some of the biggest challenges that are facing humanity in terms of climate, health, and food security.

The goal of this survey is to bring these exciting developments to the ML community, to make them aware of the progress that has been made, and the gaps and opportunities that exist for advancing research in this promising direction. To enable this, we organize the paper as follows. Section 2 describes different objectives that can be achieved through combinations of physics and machine learning. Then, Section 3 discusses ML methods that researchers are using to achieve these objectives. Table 1 categorizes the work surveyed in this paper by objective and approach. We hope that this survey will also be valuable for physical scientists who are interested in exploring the use of ML to enhance modeling in their respective disciplines. Please note that while the focus of this survey is largely on physics-based models, the ideas carry over to a wide range of scientific disciplines.

2 Objectives of Physics-ML Integration

2.1 Improving predictions beyond that of state-of-the-art physical models

Physics-based models are used extensively to model engineering and environmental systems. Even though these models are based on known physical laws, in most cases, they are necessarily approximations of reality due to incomplete knowledge of certain processes, which introduces bias. In addition, they often contain a large number of parameters whose values must be estimated with the help of limited observed data, degrading their performance further, especially due to heterogeneity in the underlying processes in both space and time. The limitations of physics-based models cut across discipline boundaries and are well known in the scientific community.

Given that ML models can automatically extract complex relationships from data, they appear promising for scientific problems with physical processes that are not fully understood by researchers, but for which data of adequate quality and quantity is available. However, the notion of black-box application of ML has met with limited success in scientific domains since ML approaches are prone to false discoveries due to non-stationary relationships among the variables that are difficult to capture from limited observation data. Hence, there is an interest in combining elements of physics-based modeling with state-of-the-art ML models to leverage their complementary strengths. The objective is to develop innovative integrated physics-ML models to better capture the dynamics in scientific systems and advance the understanding of underlying physical processes. Effective representation of physical processes requires the development of novel abstractions and architectures that can simulate these processes that may be evolving and interacting at multiple scales.

2.2 Parameterization

Complex physics-based models (e.g., simulations in climate, weather, turbulence modeling, astrophysics) are often capable of capturing physical reality more precisely than simpler models, as they may simulate physical processes at higher spatial and temporal resolution (e.g., cloud physics in climate models). However, they often require a prohibitively high computational cost to run. In such cases, specific complex dynamical processes are replaced by simplified physical approximations that are described by parameters, whose values are estimated from observed data. This is known as *parameterization*.

The failure to correctly identify parameter values can make the model less robust when generalized to different scenarios. Errors that result from imperfect parameterization can also feed into other components of the entire physics-based model and deteriorate the modeling of important physical processes. Hence, there is a great interest in ML models to learn new parameterizations directly from high-resolution model simulations [Schneider *et al.*, 2017]. Specifically, the ML model is trained on a high-resolution model in which the physical process desired is resolved and can be substituted into a coarser resolution model as a more accurate parameterization for processes of interest [Goldstein *et al.*, 2014; Chan and Elsheikh, 2017; Gentine *et al.*, 2018].

2.3 Forward Solving Partial Differential Equations

In many physical systems, governing equations are known but direct numerical solutions of partial differential equations (PDEs) using common methods like the Finite Elements Method or the Finite Difference Method [Fish and Belytschko, 2007] are prohibitively expensive. In such cases, traditional methods are not ideal or sometimes even possible. A common technique is to use an ML model as a surrogate for the solution to reduce computation time [Lagaris *et al.*, 1998]. More recently with the advancement of computational power, neural networks models have shown success in approximating solutions across different kinds of physics-based PDEs [Arsenault *et al.*, 2014; Rudd and Ferrari, 2015; Khoo *et al.*, 2019]. As a step further, deep neural networks models in particular have shown success in approximating solutions across high dimensional physics-based PDEs previously inaccessible by ML [Han *et al.*, 2018]. However, slow convergence in training, limited applicability to many complex systems, and reduced accuracy due to unawareness of physical laws can prove problematic.

2.4 Inverse Modeling

The forward modeling of a physical system uses the physical parameters of the system (e.g., mass, temperature, charge, physical dimensions or structure) to predict the next state of the system or its effects (outputs). In contrast, inverse modeling uses the (possibly noisy) output of a system to infer the physical parameters. A well-known example of inverse modeling is the use of x-ray images from a CT scan to create a 3D image reflecting the structure of part of a person's body.

Inverse problems are traditionally solved using regularized regression techniques. Data-driven methods have seen success in inverse problems in remote sensing of surface properties [Dawson *et al.*, 1992], photonics [Pilozzi *et al.*, 2018], and medical imaging [Lunz *et al.*, 2018] among many others. Recently, novel algorithms using deep learning and neural networks have been applied to inverse problems. While still in their infancy, these techniques exhibit strong performance for applications like computerized tomography [Chen *et al.*, 2017], seismic processing [Vamaraju and Sen, 2019], or various sparse data problems.

However, there are noted challenges in inverse modeling particularly in small sample size and paucity of ground-truth label scenarios [Karpatne *et al.*, 2018]. The integration of prior physical knowledge is common in current approaches to the inverse problem, and its integration into inverse problem ML applications has the potential to improve data efficiency and increase its ability to solve ill-posed inverse problems.

2.5 Discovering Governing Equations

When the governing equations of a dynamical system are known, they allow for forecasting, control, and the analysis of system stability and bifurcations. However, many complex dynamic systems have no formal analytic descriptions (e.g., neuroscience, cell biology, finance, epidemiology). Often in these cases, data is abundant but the underlying governing equations remain elusive.

Advances in ML for the discovery of these governing equations has become an active research area with rich potential to integrate principles from applied mathematics and physics with modern ML methods. Data-driven discovery of governing equations has recently been pioneered by [Bongard and Lipson, 2007; Schmidt and Lipson, 2009] where they apply symbolic regression to differences between computed derivatives and analytic derivatives to determine underlying dynamical systems. More recently, [Brunton *et al.*, 2016; Rudy *et al.*, 2017] uses sparse regression built on a dictionary of functions and partial derivatives to construct governing equations.

3 Physics-ML Methods

3.1 Physics-Guided Learning

Scientific problems often exhibit a high degree of complexity due to relationships between many physical variables varying across space and time at different scales simultaneously. Standard ML models can fail to capture such relationships directly from data, especially when provided with limited observation data. This is one reason for their failure to generalize to scenarios not encountered in training data. In the following, we discuss a number of ways researchers are beginning to incorporate physical knowledge into the learning process such that ML models can capture generalizable dynamic patterns consistent with established physical laws.

Physics-based loss to improve predictions

One of the most common techniques to make ML models consistent with physical laws is to incorporate physical constraints into the loss function of ML models as follows [Karpatne *et al.*, 2017a],

$$\text{Loss} = \text{Loss}_{\text{TRN}}(Y_{\text{true}}, Y_{\text{pred}}) + \lambda R(W) + \text{Loss}_{\text{PHY}}(Y_{\text{pred}}) \quad (1)$$

where the training loss Loss_{TRN} measures a supervised error (e.g., RMSE or cross-entropy) between true labels Y_{true} and predicted labels Y_{pred}, and λ is a hyper-parameter to control the weight of model complexity loss $R(W)$. These first two terms are the standard loss of ML models. The addition of physics-based loss Loss_{PHY} aims to ensure consistency with physical laws. An added benefit is that training can include unlabeled data by omitting Loss_{TRN}.

In the context of complex natural systems, physics-based losses have shown great success in improving prediction ability. A number of researchers [Karpatne *et al.*, 2017b; Muralidhar *et al.*, 2018] have studied how to incorporate monotonic physical relationships as constraints in loss functions for a neural network (NN). In the context of lake temperature modeling, [Karpatne *et al.*, 2017b] includes an additional physics-based penalty that ensures denser water predictions remain at lower depths, a known monotonic relationship. [Jia *et al.*, 2019; Read *et al.*, 2019] further extended this work to capture even more complex and general physical relationships that happen on a temporal scale. Specifically, they use a physics-based penalty for energy conservation in the loss function to ensure the lake thermal energy gain across time is consistent with the net thermodynamic fluxes going in and out of the lake. Other work in parameterization [Beucler *et al.*, 2019] has also shown it is possible to enforce energy conservation laws in emulating cloud processes.

Another strand of work incorporating loss function alterations is in solving PDEs, in which adherence to the governing equations is enforced in the loss function. In [Raissi *et al.*, 2019a], this concept is developed and shown to create data-efficient spatiotemporal function approximators to both solve and find parameters of basic PDEs like Burgers Equation or the Schrodinger Equation. In [Raissi *et al.*, 2019b], this is extended to cover inverse modeling problems for quantities of interest in vortex induced vibrations. Beyond a simple feed-forward network, [Zhu *et al.*, 2019] proposes an encoder-decoder for predicting transient PDEs with governing PDE constraints, which was further extended to deep auto-regressive dense encoder-decoders with a Bayesian framework using stochastic weight averaging to quantify uncertainty in [Geneva and Zabaras, 2020].

Certain aspects of dynamical systems modeling have also shown promise in informing loss functions for improved prediction beyond that of the physics model. In [Erichson *et al.*, 2019], they penalize autoencoders based on physically-meaningful stability measures in dynamical systems for improved prediction of fluid flow and sea surface temperature. They showed an improved mapping of past states to future states in both modeling scenarios in addition to improved generalizability to new data.

Though these loss functions are mostly seen in common variants of neural networks, they can also be seen in architectures like echo state networks [Doan *et al.*, 2019]. In this work they find integrating the physics-based loss from the governing equations in a Lorenz system, a commonly studied system in dynamical systems, strongly improves the echo state network's time-accurate prediction of the system and also reduces convergence time.

Auxiliary Task in Multi-Task Learning Multi-task learning frameworks allow for multiple learning tasks to be solved at the same time, ideally while exploiting commonalities and differences across tasks. This can result in improved learning efficiency and predictions for one or more of the tasks. Therefore, another way to implement physics-based learning constraints is to use an auxiliary task in a multi-task learning framework. This is shown to be successful in computer vision [Zhang *et al.*, 2014], but a physics-based analogue would be to have an auxiliary task representing consistency with physics-based principles. In this paradigm, a task-constrained loss function can be formulated to allow errors of related tasks to be back-propagated jointly to improve model generalization. Early work in computational chemistry showed that a NN could be trained to predict energy by constructing a loss function that had penalties for both inaccuracy *and* inaccurate energy derivatives with respect to time as determined by the surrounding energy force field [Pukrittayakamee *et al.*, 2009]. Then in particle physics, [de Oliveira *et al.*, 2017] uses an additional task for the discriminator network in a generative adversarial network (GAN) to satisfy certain properties of particle interaction for the production of jet images of particle energy.

Physics-Guided Initialization Since many ML models require an initial choice of model parameters before training, researchers have explored different ways to physically inform a model starting state. Poor initialization can cause models to anchor in local minima, which is especially true for deep neural networks. *Transfer learning* can effectively tackle this issue, where the pre-trained models from a related task are fine-tuned with limited training data to fit the desired task. One way to harness physics-based modeling knowledge is to use the physics-based model's simulated data to pre-train the ML model, which also alleviates data paucity issues.

Jia *et al.* extensively discusses this strategy [Jia *et al.*, 2019]. They pre-train their Physics-Guided Recurrent Neural Network (PGRNN) models for lake temperature modeling on simulated data generated from a physics-based model and fine tune the NN with little observed data. They show that pre-training, even using data from a physical model with an incorrect set of parameters, can still significantly reduce the training data needed for a quality model. In addition, [Read *et al.*, 2019] show that such models are able to generalize better to unseen scenarios than pure physics-based models.

3.2 Physics-Guided Design of Architecture

Although the physics-based loss in the previous section helps constrain the search space of neural networks during training, the neural network architecture is often still a black box. There are usually no architectural properties to implicitly encode physical consistency or other desired physical properties. A recent research direction has been to construct new ML architectures for the tasks defined in Section 2 with this in mind.

Intermediate Physical Variables

One way to embed well-known physical principles into NN design is to ascribe physical meaning for certain neurons in the NN by computing physically relevant intermediate variables in the neural pathway from inputs to outputs. In lake temperature modeling, [Daw *et al.*, 2019] incorporates a physical intermediate variable as part of a monotonicity-preserving structure in the LSTM architecture as shown in Figure 1. This model produces physically consistent predictions in addition to appending a dropout layer to quantify uncertainty. In [Muralidhar *et al.*, 2018], a similar approach is taken to insert physics-constrained variables as the intermediate variables in the convolutional neural network (CNN) architecture and achieve significant improvement over state-of-the-art physics-based models on the problem of predicting drag force on particle suspensions in moving fluids.

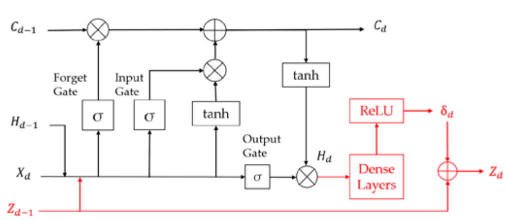

Figure 1: Monotonicity-preserving LSTM Architecture. Components in red represent novel physics-informed innovations in LSTM. The following link contains the code for this paper: https://github.com/arkadaw9/PGNN [Daw *et al.*, 2019]

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An additional benefit of adding physically relevant intermediate variables in an ML architecture is that they can help extract physically meaningful hidden representation that can be interpreted by domain scientists. This is particularly valuable, as standard deep learning models are limited in their interpretability since they can only extract abstract hidden variables using highly complex connected structure. This is further exacerbated given the randomness involved in the optimization process.

Encoding invariances

Common neural network design paradigms like the RNN and CNN have revolutionized the ability of ML algorithms by implicitly encoding time invariance into the RNN architecture and spatial translation, rotation, and scale invariance into the CNN. In the same way, scientific modeling tasks may require other invariances based on physical laws. In turbulence modeling and fluid dynamics, recent work defines a *tensor basis neural network* to embed the fundamental principle of rotational invariance into a NN [Ling *et al.*, 2016] for improved prediction accuracy. This solves a key problem in ML models for turbulence modeling because without rotational invariance, the model evaluated on identical flows with axes defined in other directions could yield different predictions. This work alters the NN architecture by adding a higher-order multiplicative layer that ensures the prediction lies on a rotationally invariant tensor basis. Additionally, in [Anderson *et al.*, 2019], a rotationally covariant neural network architecture is shown to learn the behavior and properties of complex many-body physical systems in molecular dynamics.

Architectural modifications in the context of solving PDEs

Architecture modifications are also seen extensively in dynamical systems research involving differential equations. In [Chen *et al.*, 2018a], a continuous depth neural network based on the Residual Network [He *et al.*, 2016], is proposed for solving ordinary differential equations. They change the traditionally discretized neuron layer depths into continuous equivalents such that hidden states can be parameterized by differential equations in continuous time. Then, in pioneering work by [Ruthotto and Haber, 2018], three variations of CNNs are proposed for solving PDEs. Each variation uses mathematical theories to guide the design of the CNN based on fundamental properties of the PDEs. Multiple types of modifications are made, including adding symmetry layers to guarantee stability expressed by the PDEs and layers that convert inputs to kinematic eigenvalues that satisfy certain physical properties. They define a parabolic CNN inspired by anisotropic filtering, a hyperbolic CNN based on Hamiltonian systems, and a second order hyperbolic CNN. Hyperbolic CNNs were found to preserve the energy in the system as intended, which set them apart from parabolic CNNs that smooth the output data, reducing the energy. In a similar application, [Chang *et al.*, 2019] uses principles from the stability properties of differential equations in dynamical systems modeling to guide the design of gating mechanism and activation functions in an RNN.

Physics-Guided Neural Architecture Search

Currently employed architectures primarily have been developed manually by human experts, which can be a time-consuming and error-prone process. Because of this, there is growing interest in automated neural architecture search methods [Elsken *et al.*, 2018]. Though outside of the objectives defined in Section 2, a young but promising direction in ML architecture design is to embed prior physical knowledge into neural architecture searches. In [Ba *et al.*, 2019a], physically meaningful input nodes and physical operations between nodes are added to the neural architecture search space for the search algorithm to discover more ideal physics-guided machine learning architectures.

3.3 Residual modeling

The oldest and most common approach for directly addressing the imperfection of physics-based models in the scientific community is residual modeling, where an ML model (usually linear regression) learns to predict the errors, or residuals, made by a physics-based model [Forssell and Lindskog, 1997]. The key concept is to learn biases of the physical model (relative to observations) and use it to make corrections to the physical model's predictions. As an example, in [Kani and Elsheikh, 2017] a physics-driven "deep residual recurrent neural network (DR-RNN)" is proposed to find the residual minimiser of numerically discretized PDEs. Their architecture involves a stacked RNN embedded with the dynamical structure of the PDEs such that each layer of the NN solves a layer of the residual equations. They showed DR-RNN to sharply reduce both computational cost and time discretization error of the reduced order modeling framework. Recently, researchers have begun to use ML models more sophisticated than regression [Wan *et al.*, 2018] for residual modeling. However, one key limitation in residual modeling is the physics-based constraints (like in Section 3.1) are hard to enforce because such approaches model the errors instead of the physical quantities physics-based problems.

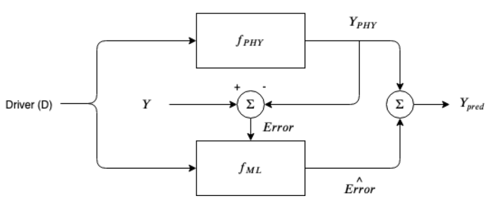

Figure 2: Machine Learning model f_{ML} trained to model the error made by Physics model f_{PHY}

More recently, a key area in which residual modeling has been applied is in reduced order models (ROMs) of dynamical systems. ROMs of dynamical systems are simplified versions of high fidelity, PDE-based numerical simulations that are much cheaper computationally. Usually, this involves techniques like principal components analysis to project governing equations onto a low-dimensional subspace spanned by basis functions [Kerschen *et al.*, 2005]. After reducing model complexity, an ML model can be used to model the residual due to the truncation. ROM methods were created in response to the problem of many detailed simulations being too expensive to be used in various engineering tasks including design optimization and real-time decision support. In [San and Maulik, 2018], a simple NN used to model the error due to the model reduction is shown to sharply reduce high error regions when applied to Bousinessq equations. Also, in [Wan *et al.*, 2018], an RNN is used to model the residual between a ROM for prediction of extreme weather events and the available data projected to a reduced-order space.

3.4 Hybrid Physics-ML Models

Residual modeling is just one way to combine physics-based models with ML where both are operating simultaneously. We will call a generalized version of this *Hybrid Physics-ML Models*.

One straightforward method to combine physics-based and ML models is to feed the output of a physics-based model as input to an ML model. [Karpatne *et al.*, 2017b] showed that using the output of a physics-based model as one feature in an ML model along with inputs used to drive the physics-based model for lake temperature modeling can improve predictions. Visualization of this method is shown in Figure 3.

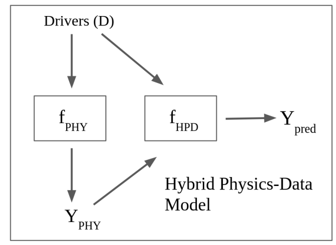

Figure 3: Diagram of a hybrid physics-ML model [Karpatne *et al.*, 2017b]

Another variant of hybrid physics-data models is to use an ML model to predict intermediate quantities in a physics-based model. Recent work in fluid dynamics [Parish and Duraisamy, 2016] proposes a NN to estimate variables in the closure model to account for missing physics to improve predictions of discrepency of RANS solvers. They show this correction to traditional turbulence models results in convincing improvements of predictions. In [Hamilton *et al.*, 2017], a subset of the mechanistic model's equations are replaced with data-driven nonparametric methods to improve prediction beyond the baseline process model. Then, in [Zhang *et al.*, 2018], a physics-based solving architecture for power system state estimation embeds a deep learning model in place of traditional predicting and optimization techniques.

Hybrid models for parameterization take a similar form, where complex physical processes are too difficult or expensive for numerical process models to simulate and an ML model can be substituted. In geodynamics modeling, [Goldstein *et al.*, 2014] showed that an ML model for oscillatory flow ripples can be substituted into an established model for geologic material being moved by fluid flow. They showed that the hybrid model was able to capture dynamics previously absent from the model, which led to the discovery of two new observed pattern modes in the geology.

In another class of hybrid frameworks, the overall prediction is a weighted sum of predictions from a physical model and an ML model, where the weights depend on prediction circumstance. For example, oftentimes in physics-based models long-range interactions are more easily modeled by existing physics equations (e.g. gravity) than more stochastic short-range interactions (e.g. quantum mechanics). Hybrid frameworks have been used to adaptively combine ML predictions for short-range processes and physics model predictions for long-range processes for applications in chemical reactivity [Yao *et al.*, 2018] and seismic activity prediction [Paolucci *et al.*, 2018]. Estimator quality at a given time and location can also be used to determine whether a prediction comes from the physical model or the ML model, which was shown in [Chen *et al.*, 2018b] for air pollution estimation and in [Vlachas *et al.*, 2018] for dynamical system forecasting more generally.

Moreover, in inverse modeling, there is a growing use of hybrid models that first use physics-based models to perform the direct inversion, then use deep learning models to further refine the inverse model's predictions. Multiple works have shown an effective application for this in computed tomography (CT) reconstructions [Jin *et al.*, 2017; Bubba *et al.*, 2019]. Another common technique in inverse modeling of images (e.g. medical imaging, particle physics imaging), is the use of CNNs as *deep image priors* [Ulyanov *et al.*, 2018]. In [Senouf *et al.*, 2019], they embed both a CNN that serves as the image prior for a physics-based forward model for MRIs to exploit data and prior knowledge simultaneously.

4 Discussion, Future Directions and Concluding Remarks

Given the current deluge of sensor data and advances in ML methods amidst pressing environmental and physical modeling problems facing scientists, we envision the merging of principles from ML and physics to play an invaluable role in the future of scientific modeling. Although both physics-based modeling and ML are rapidly advancing fields, knowledge integration for mutual gain requires clear lines of communication between disciplines. Currently, most of the diverse set of techniques for bringing ML and physical knowledge together have been developed in isolated applications by researchers working in distinct disciplines.

In this survey, we reviewed a number of techniques for integrating physics-based knowledge with machine learning. We classified these methodologies into four categories; Physics-Guided Learning, Physics-Guided Design of Architecture, Residual Modeling, and Hybrid Physics-ML Modeling. From the early results reported in some of the papers, we can see that the incorporation of prior physics-based knowledge can alleviate some of the most significant problems with black box ML approaches: the requirement of large datasets, inconsistency with physical laws, and the struggle to extrapolate to unseen scenarios [Read *et al.*, 2019]. This increase in data efficiency and physical consistency serves to benefit several application specific research objectives including inverse modeling, parameterization, discovery of governing equations, and solving PDEs.

From Table 1, it is easy to see that a large amount of research has been done in the context of developing integrated physics and ML models that are able to improve predictions beyond that can be obtained using the state of the art physical models (row 1 in Table 1). Also note that many boxes in the Table 1 are empty, many of which represent opportunities for future work. For example, combining ML and physics models for better parameterizations is increasingly being used in domains like climate science and weather forecasting [Krasnopolsky and Fox-Rabinovitz, 2006], but most of these works have relied on simple ML models. Furthermore, principles from super-resolution frameworks are beginning to be applied to downscaling to create higher resolution climate predictions [Vandal *et al.*, 2017]. All of these approaches can benefit from more powerful approaches listed here (e.g., physics based loss, intermediate physics variables, etc).

Two emerging research directions in Physics-ML integration not previously mentioned in this survey include efforts in uncertainty quantification (UQ) and data generation. State-of-the-art physics-based models for simulating real systems are often characterized by vast numbers of input parameters, and quantifying uncertainty of these models using traditional methods like Monte Carlo is usually infeasible due to the thousands or millions of forward model evaluations needed to obtain convergent statistics. ML models, especially when augmented with physics-based knowledge, can serve as surrogate models for faster evaluation of uncertainty [Yang and Perdikaris, 2019a]. For data generation, generative ML models can be used in a manner similar to simulations by physics-based models. Using generative models as opposed to physical simulation often incurs certain benefits, including reduced computation time and being able to represent complex data spaces without knowing the entire topology. Furthermore, generative models are often used as representations of solution spaces to complex physical and dynamical systems. Many of the approaches discussed in this work can apply to generative models as well [Shah *et al.*, 2019]. More works in uncertainty quantification and data generation can be found in Table 1.

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[Beucler *et al.*, 2019] T Beucler, S Rasp, M Pritchard, and P Gentine. Achieving conservation of energy in neural net-

Table 1: Table of literature classified by objective and method

	Basic ML	Physics-Guided Learning	Physics-Guided Architecture	Residual Model	Hybrid Model
Improve prediction beyond physics model	[Yi and Prybutok, 1996] [Brown *et al.*, 2008] [Ham *et al.*, 2019]	[Pukrittayakamee *et al.*, 2009] [Karpatne *et al.*, 2017b] [Muralidhar *et al.*, 2018] [Doan *et al.*, 2019] [Erichson *et al.*, 2019] [Jia *et al.*, 2019] [Liu and Wang, 2019] [Muralidhar *et al.*, 2019] [Read *et al.*, 2019] [Zhang *et al.*, 2019] [Hu *et al.*, 2020]	[Ling *et al.*, 2016] [Baseman *et al.*, 2018] [Sturmfels *et al.*, 2018] [Anderson *et al.*, 2019] [Ba *et al.*, 2019b] [Muralidhar *et al.*, 2018] [Muralidhar *et al.*, 2019] [Park and Park, 2019] [Sadoughi and Hu, 2019] [Hu *et al.*, 2020]	[Xu and Valocchi, 2015] [Wang *et al.*, 2017] [San and Maulik, 2018] [Wan *et al.*, 2018] [Liu and Wang, 2019]	[Goldstein *et al.*, 2014] [Grover *et al.*, 2015] [Sadowski *et al.*, 2016] [Hamilton *et al.*, 2017] [Karpatne *et al.*, 2017b] [Solle *et al.*, 2017] [Chen *et al.*, 2018b] [Long *et al.*, 2018] [Paolucci *et al.*, 2018] [Yao *et al.*, 2018] [Zhang *et al.*, 2018] [Vlachas *et al.*, 2018] [Yang *et al.*, 2019b]
Parameterization	[Krasnopolsky and Fox-Rabinovitz, 2006] [Goldstein *et al.*, 2014] [Chan and Elsheikh, 2017] [Gentine *et al.*, 2018] [O'Gorman and Dwyer, 2018] [Rasp *et al.*, 2018] [Bolton and Zanna, 2019]	[Beucler *et al.*, 2019]	[Beucler *et al.*, 2019]		[Zhang *et al.*, 2018]
Uncertainty quantification	[Xu and Valocchi, 2015] [Lakshminarayanan *et al.*, 2017] [Yang and Perdikaris, 2019b]	[Wu *et al.*, 2016] [Yang and Perdikaris, 2018] [Yang and Perdikaris, 2019a] [Zhu *et al.*, 2019] [Geneva and Zabaras, 2020]	[Daw *et al.*, 2019]		[Dong *et al.*, 2016]
Inverse modeling	[Dawson *et al.*, 1992] [Chen *et al.*, 2017] [Lunz *et al.*, 2018] [Pilozzi *et al.*, 2018]	[Biswas *et al.*, 2019] [Raissi *et al.*, 2019b]			[Parish and Duraisamy, 2016] [Hamilton *et al.*, 2017] [Jin *et al.*, 2017] [Bubba *et al.*, 2019] [Senouf *et al.*, 2019]
Discover Governing Equations	[Bongard and Lipson, 2007] [Schmidt and Lipson, 2009] [Brunton *et al.*, 2016] [Mangan *et al.*, 2016] [Rudy *et al.*, 2017]	[Raissi *et al.*, 2017a]			
Solve PDEs	[Arsenault *et al.*, 2014] [Rudd and Ferrari, 2015] [Han *et al.*, 2018] [Sirignano and Spiliopoulos, 2018] [Khoo *et al.*, 2019]	[Raissi *et al.*, 2017b] [Sharma *et al.*, 2018] [Yang *et al.*, 2018] [Yang and Perdikaris, 2018] [de Bezenac *et al.*, 2019] [Meng *et al.*, 2019] [Raissi *et al.*, 2019a] [Shah *et al.*, 2019] [Zhu *et al.*, 2019] [Geneva and Zabaras, 2020] [Karumuri *et al.*, 2020] [Wu *et al.*, 2020]	[Chen *et al.*, 2018a] [Ruthotto and Haber, 2018] [Chang *et al.*, 2019] [de Bezenac *et al.*, 2019] [Mattheakis *et al.*, 2019] [Yang *et al.*, 2019a]		
Data Generation	[Klein and Manning, 2003] [Denton *et al.*, 2015] [Oord *et al.*, 2016]	[de Oliveira *et al.*, 2017] [Bode *et al.*, 2019] [Kim *et al.*, 2019] [Yang *et al.*, 2019c] [Zheng *et al.*, 2019]	[Chen and Fuge, 2018] [Shah *et al.*, 2019]		

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