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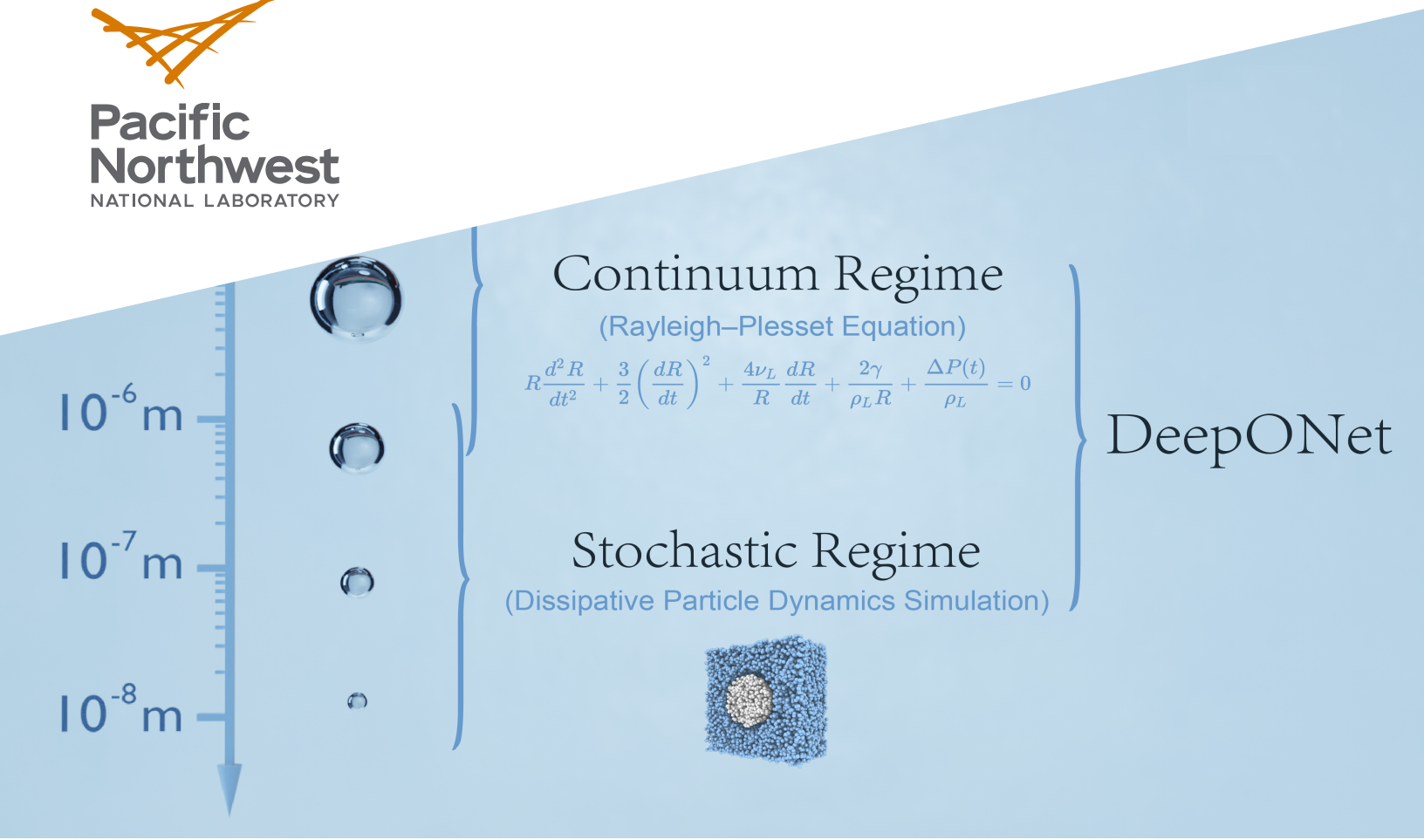

PhILMS: Collaboratory on Mathematics and Physics-Informed Learning Machines for Multiscale and Multiphysics Problems

October 2021

U.S. DEPARTMENT OF ENERGY | Prepared for the U.S. Department of Energy under Contract DE-AC05-76RL01830

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ANNUAL REPORT

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Pacific Northwest National Laboratory
Richland, Washington 99354

Executive Summary

Motivation:

Complex multiphysics systems are governed by the hidden physics of interfaces and inhomogeneous cascades of scales, (e.g., multifunctional materials, subsurface transport, reactive transport), requiring new data-driven multiscale modeling that is accurate, efficient, and easy to implement. In particular, inhomogeneous cascades of scales involve long-range spatiotemporal interactions and often lack proper closure relations to form complete and mathematically well-posed systems of governing equations. Existing multiscale and multiphysics approaches, along with classical integer-order partial differential equations (PDEs) have been ineffective in addressing nonlocal interactions, inhomogeneous cascades of scales, or propagation of uncertainty and stochasticity across scales. These approaches are inadequate for solving *inverse* stochastic multiscale problems, especially in the context of noisy *multifidelity* data. Moreover, existing approaches do not scale well to big systems in real-world applications.

Research Plan:

PhILMs members are developing stochastic, multiscale modeling frameworks in conjunction with emerging deep learning techniques to seamlessly fuse physical laws, including thermodynamics and multifidelity data, for forward and inverse multiscale problems. Our approach is based on a synthesis of physics-based and data-driven tools and approaches, including nonlocal operators, multifidelity data and information fusion, deep neural networks (DNNs), meshfree methods, uncertainty propagation, and stochasticity to simulate complex multiscale systems. Therefore, we are conducting research at the interface of mathematics, physics, data science, and deep learning. With an emphasis on predictability, reproducibility, *and* uncertainty quantification, the PhILMs research plan includes:

- *developing physics-informed learning machines by encoding conservation and thermodynamic laws as well as other prior physical knowledge into deep learning networks and analyzing their mathematical properties;*
- *demonstrating the effectiveness of PhILMs in designing functional materials with tunable properties and extending PhILMs to other U.S. Department of Energy (DOE)-relevant multiscale problems (e.g., combustion, subsurface, and Earth systems)–all exhibiting inhomogeneous scaling cascades;*
- *establishing scientific machine learning (ML) as a new meta-discipline at the interface of computational mathematics, data science, information fusion, and deep learning.*

Our integrated mathematical and computational activities can be classified into four research areas (RA):

1. **RA-I**: partial differential equation (PDE)-based modeling of macroscales
2. **RA-II**: stochastic modeling of mesoscales.
3. **RA-III**: bridging methods to connect the scales.
4. **RA-IV**: deep learning approximations and algorithms to support RA-I to RA-III.

Coordination, Integration, and Evaluation Plan:

We are developing PhILMs by coordinating and assimilating the four research areas. In **RA-I**, we are developing PDE-based, physics-informed neural networks (PINNs) for forward and inverse problems. We also develop appropriate representations and a unified theory for nonlocal calculus. A new exciting area is using DNNs to approximate nonlinear operators. In **RA-II**, we are learning PDEs from molecular simulations, applying operator regression to predict mesoscopic dynamics, and learning effective coarse-grain potentials for energy storage materials. In **RA-III**, we are considering concurrent coupling of heterogeneous domains using conservative PINNs, including nonlocal to local PDEs (e.g., fractional/local), and applying PINNs to learning non-Newtonian fluid dynamics and subsurface transport in porous media. In **RA-IV**, we develop foundational algorithms for optimization, uncertainty quantification, and generative adversarial networks (GANs). We are also developing new methods for data augmentation for faster training and a fundamental new theory for generalization. Ultimately, these advances will be combined with the knowledge and inherent structure of physical laws to develop PINNs for material design, enhancing combustion efficiency, and making predictions for subsurface systems and ice sheets.

In a fashion similar to the PhILMs project's objective of elucidating and integrating activity across different scales of complex multiphysics systems, successfully coordinating the four research areas requires considerable

integration of activities from the six participating institutions. We have established and maintained pair and trio collaborative interactions among the various PhILMs institutions to cultivate an exchange of strengths, ideas, and approaches.

Our evaluation plan defines benchmarks of increasing complexity to measure progress in each research area and calls for annual workshops and mini-symposia. We believe that the documented early adoption of ideas originating in the PhILMs project indicates the viability of our approach. In addition, we have formed a dissemination panel so that our work is presented across all the DOE laboratories to make sure that DOE scientists will be the first who can benefit from our findings. We have also successfully reached out to industrial partners (e.g., Nvidia, Ansys, Cummins, TSI, La Vision, P&G, Anailytica, etc). During the third year, we held regular webinars on Monday afternoons, given by scientists, both external and internal to PhILMs, and attended by all researchers associated with PhILMs at Pacific Northwest National Laboratory (PNNL), Sandia National Laboratories (SNL), Stanford University, Massachusetts Institute of Technology (MIT), University of California, Santa Barbara (UCSB), and Brown University. With speaker permission, recordings of the webinars are shared on the PhILMs website[1].

Highlights of Accomplishments and Outcomes

Research Area I

PDE-Based Modeling of Macroscales: Last year, we emphasized the development of techniques for operator regression, both local and nonlocal. This year, the Sandia team continued developing theory for nonlocal and fractional calculus to facilitate their application in a machine-learning context, including nonlocal kernel networks. The UCSB team developed data-driven methods that allow the solution of PDEs on manifolds. The Brown team, the SNL team, and the PNNL team developed ML tools for simulating the incompressible Navier-Stokes equations, for predicting the evolution of ice sheets, for learning fractional and nonlocal operators for turbulence, for simulating multiphysics subsurface transport (forward and backward in time), and for solving forward and inverse problems with the Boltzmann equation. The Brown team also used PINNs to infer velocity and pressure fields from tomographic data.

Research Area II

Stochastic Modeling of Mesoscales: The data-driven modeling of mesoscales, especially if it is stochastic, benefits from methods that guarantee satisfaction of the laws of thermodynamics. The SNL, Brown, and PNNL teams developed such methods, which are vastly superior to black-box neural models of ordinary differential equations (ODEs). The Brown team built an approach to learning stochastic equations for advection-diffusion reactions from sparse measurements. The PNNL team developed a method for learning potentials that depend on the distance from an interface and applied them to tackle nontrivial solid-liquid interfaces.

Research Area III

Bridging of Methods to Connect the Scales: The Brown and SNL teams developed various methods based on a deep operator network (DeepONet), nonlocal calculus, and data-driven exterior calculus to bridge vastly different scales. The Brown team also combined PINNs with domain decomposition (extended PINN, XPINN) to tackle problems where one PINN is not enough to capture all the details of the solution. The DeepONet was used to propose a framework for simulating multiphysics and multiscale problems (using the composite supervised neural network DeepM&Mnet) and was applied to electroconvection. PINNs and DeepONet were used to solve complex problems involving the prediction of the crack path of a brittle material and constitutive modeling in rheology.

Research Area IV

Statistical Learning and Deep Learning Approximations and Algorithms: Activity in this research area covered various topics. The MIT team developed techniques for learning parameters using dependent data, which is the usual case in applications where data independence is hard to guarantee. The Stanford team (G. Valiant) developed methods for four purposes: (i) more efficient semi-supervised classification, (ii) estimating the cost of misspecification of distributions, (iii) more efficient estimation using collection processes that yield dependent data, and (iv) better calibration of online predictive models. The PNNL team developed a multifidelity framework for DeepONets. The Brown team investigated the generalization properties of PINNs and XPINNs, employed PI-GANs to learn functional priors, introduced a framework for neural networks (NNs) with adaptive activation functions, and proposed an optimization algorithm based on the Caputo fractional derivative. The SNL team developed

[1] https://www.pnnl.gov/projects/PHILMS

a Bayesian operator regression framework using partition-of-unity (POU) NNs and also proposed a multilevel optimization algorithm for PINNs inspired by multigrid constructions. The UCSB team developed a variational autoencoder (VAE) framework to learn parsimonious disentangled representations of nonlinear dynamical systems. The Stanford team (Darve) developed a physics-informed generative model for learning distributions of physical parameters.

Challenges and Implemented Course Corrections

The ongoing pandemic has significantly reduced travel, limiting in person meetings and conference attendance in 2020-2021. However, we have adapted to using technology to communicate virtually, and team members have participated widely in virtual conferences. We note that, while limiting in person interactions, the adaptation to virtual work has increased inclusivity among team members unable to travel.

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PhILMs Progress Report 2020-2021

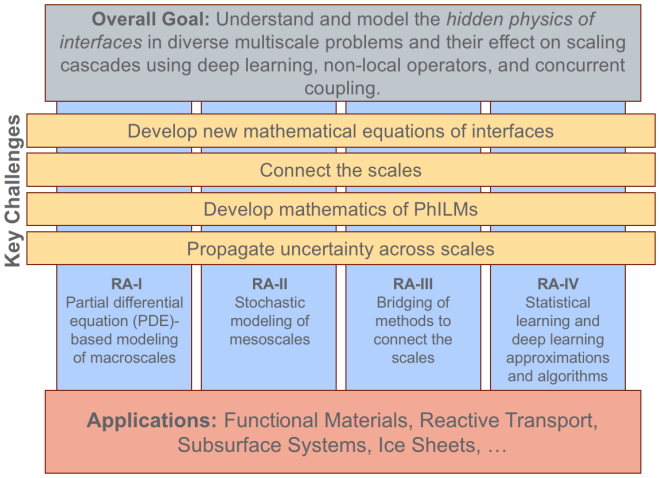


Figure 1: *Overview of the PhILMs proposal:* Relation between the overall goal of PhILMs, the thematic key challenges derived from this goal, and its four research areas motivated by exemplar DOE applications.

Most multiscale problems can be broadly classified into three categories: (i) data-poor but with complete knowledge of the governing physics, (ii) data-rich but with little knowledge of governing physics, and (iii) only moderate data and moderate knowledge of the governing physics. Existing multiscale and multiphysics approaches have been ineffective, especially for the latter two categories, in addressing key scientific challenges, such as inhomogeneous cascades of scales, propagation of uncertainty/stochasticity across scales, and nonlocal interactions. They are inefficient for solving inverse stochastic multiscale problems, especially in the context of noisy multifidelity data. In the Physics-Informed Learning Machines for Multiscale and Multiphysics Problems (PhILMs) project, we address these shortcomings by seamlessly fusing physical laws and multifidelity data, for both forward *and* inverse multiscale and multiphysics problems, with the goals of discovering, modeling, and understanding hidden physics of interfaces and beyond. Our integrated mathematical and computational activities can be classified into the following four research areas (see fig. 1): (RA-I) partial differential equation (PDE)-based modeling of macroscales; (RA-II) stochastic modeling of mesoscales; (RA-III) bridging methods to connect the scales; and (RA-IV) statistical learning and deep learning approximations and algorithms. Physics-informed neural networks (PINNs) are a workhorse tool for the project, and new work in this year has emphasized local and nonlocal approaches, the bridging of scales, and multifidelity (see also [1] by PhILMs members for a review of the field of physics-informed machine learning.) In the following, we summarize research accomplishments, highlights, and current directions from the third year of the project.

1 RA-I: PDE-based Modeling of Macroscales

We continued developing the theory of operator regression, both local and nonlocal, and applied it to problems including incompressible flows, ice-sheet modeling, subsurface transport, and rarefied flows. Sandia National Laboratories (SNL), the University of California, Santa Barbara (UCSB), Brown University, and Pacific Northwest National Laboratory (PNNL) have contributed to topics in Research Area (RA)-I.

1.1 Theoretical Foundations of Nonlocal and Fractional Calculus

Building on PhILMs' continued efforts toward the development of a unified nonlocal and fractional theory to facilitate expressive and seamless modeling, M. D'Elia and M. Gulian (SNL) further advanced the state of the art of nonlocal and fractional analysis. This included (1) developing a rigorous theory for compositions of nonlocal vector calculus operators, using it to prove nonlocal vector calculus identities, and establishing a fractional Helmholtz decomposition in Hölder spaces. (2) Formulating and analyzing an anomalous transport problem characterized by an anisotropic generalization of the fractional Laplacian (FL) that finds application in describing anomalous transport of solutes in the subsurface [2]. (3) Introducing two new models for the variable-order FL operator. The first model stems from the integral formulation of the FL and substitutes the fractional order—usually constant—with a two-point spatial function; this structure allows for efficient and accurate modeling of interfaces [3]. The second is a novel definition based on a natural generalization of the standard Riesz potential and holds for values of the fractional parameter spanning the entire open set $(0, n/2)$, rather than the standard $(0, 1)$ interval. This formulation finds application in the fractional Newtonian gravity theory and it is the result of a SNL-Stanford collaboration together with A. Giusti (ETH Zürich), one of the speakers at the weekly PhILMs seminar. This work provides the groundwork for the development of an ML framework to identify optimal models for the gravitation potential. (4) Continuing the investigation of the relationship between tempered and truncated FL operators by deriving L^p bounds on the difference of the two operators as well as developing a graphics processing unit (GPU)-capable Tensorflow code that trains optimal truncated surrogates for tempered operators and other operators with infinite support. (5) Conducting a thorough literature review on the use of fractional operators in engineering applications; this research effort produced the review paper [4].

1.2 Efficient Continuum-Scale Discretization and Numerical Analysis

In support of ML efforts, we developed numerical methods and analyses relevant to discretization of continuum models, targeting local, meshfree, and nonlocal discretizations for physics spanning transport, solid/fluid mechanics, and electromagnetism [5, 6, 7, 8, 9, 10, 11, 12, 13] . Continuing the previous efforts on the design of coupling methods, M. D'Elia and P. Bochev (SNL) are developing local-to-nonlocal coupling techniques based on our previous work [14] and methods for the treatment of nonlocal (virtual) interfaces in a domain decomposition setting. Our framework [7], based on a finite element tearing and interconnect (FETI) domain decomposition technique, was applied to large-scale problems of 191 million unknowns and 55 billion nonzeros; it outperformed, by factors up to 7×, standard approaches to the distributed numerical solution of meshfree discretizations of PDEs and nonlocal equations. Applications include fracture mechanics, with inclusion of this algorithm in SNL's *Sierra* mechanics code.

1.3 Nonlocal Kernel Networks for PDE Learning and Image Classification

Deep neural networks (DNNs), often required in complex learning tasks such as image classification, are hard to train. M. D'Elia (SNL) in collaboration with Y. Yu (Lehigh University) proposed a novel formulation, inspired by the graph kernel network (GKN) [15], that is stable in the limit of deep layers. This nonlocal kernel network (NKN) stems from the interpretation of the NN as a discrete, nonlocal diffusion reaction problem that, in the limit of infinite layers, is equivalent to a parabolic nonlocal equation, whose stability is analyzed via nonlocal vector calculus [16, 2]. The resemblance to graph neural networks allows NKNs to capture long-range dependencies in the feature space, while the continuous treatment of node-to-node interactions makes NKNs resolution independent. Furthermore, the resemblance with neural ordinary differential equations (ODEs), reinterpreted in a nonlocal sense, and the stable network dynamics between layers allow for generalization of an NKN's optimal parameters from shallow to deep networks. This fact enables the use of shallow-to-deep initialization techniques. NKNs outperform baseline methods in both PDE learning tasks (e.g., they are more accurate and stable than GKNs [15] and the Fourier neural operator [17] when learning Poisson and multidimensional Darcy equations) and image classification tasks (they are more accurate than convolutional neural networks and Nonlocal NNs [18] in cross-resolution classification of the Canadian Institute For Advanced Research's CIFAR10 dataset and the Modified National Institute of Standards and Technology [MNIST] dataset).

1.4 Data-Driven Numerical Methods for Stochastic PDEs on Manifolds

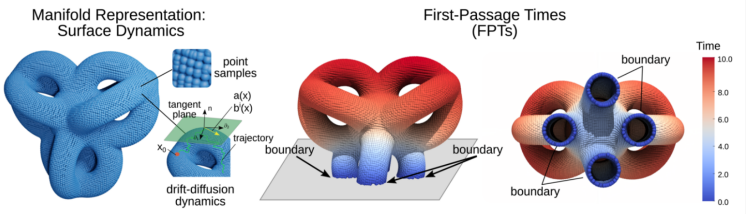


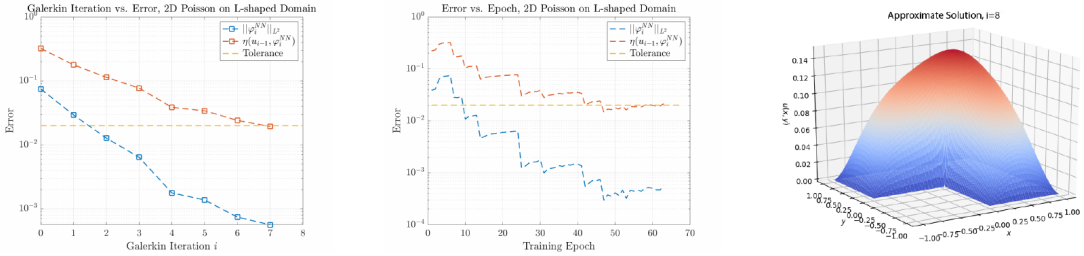
Figure 2: Data-driven numerical methods for PDE Solvers. We use data-driven local regression approaches to develop numerical methods for solving PDEs on manifolds. These are used to develop methods for stochastic differential equations (SDEs) on manifolds for computing first-passage times and other statistics arising in many problems in scientific computation; see [19].

We developed data-driven numerical discretizations for PDEs on manifolds building using generalized moving least squares (GMLS) in [19]. To handle the complications with geometry, local regression problems are solved using GMLS to estimate both the geometric contributions and local field reconstructions to discretize PDEs on general manifolds. This allows for general Ito stochastic processes on manifolds to compute first-passage times and other statistics that arise in many applications in scientific computation. Our work reported in [19] was done in collaboration with P. Kuberry of SNL and graduate student B. Gross of UCSB.

1.5 Galerkin Neural Networks: A Framework for Approximating Variational Equations with Error Control

In [20], we present an approach using NNs to approximate variational equations, based on the adaptive construction of a sequence of finite-dimensional subspaces whose basis functions are realizations of a sequence of NNs. The finite-dimensional subspaces can be used to define a standard Galerkin approximation of the variational equation. This work enjoys several advantages: (i) the sequential nature of the algorithm offers a systematic approach to enhancing the accuracy of a given approximation; (ii) the sequential enhancements provide a useful indicator for

the error that can be used as a criterion for terminating the sequential updates; (iii) the basic approach is to some extent oblivious to the nature of the PDE under consideration; and (iv) some basic theoretical results presented regarding the convergence (or otherwise) of the method form basic guidelines for its application.



(a) (b) (c)

Figure 3: Approximation using Galerkin NNs of Poisson equation in L-shaped domain. Estimated errors after each Galerkin iteration (a) and epoch (b) and approximate solution at eighth iteration (c). Observe that GNN provide good resolution of the singularity.

1.6 NSFnets (Navier-Stokes Flow Nets): PINNs for the Incompressible Navier-Stokes Equations

We employ PINNs, encoding the governing equations directly into the DNN via automatic differentiation (AD), to overcome some of the current limitations for simulating incompressible laminar and turbulent flows. We develop the Navier-Stokes flow nets (NSFnets) [21] by considering two mathematical formulations of the Navier-Stokes equations: the velocity-pressure (VP) formulation and the vorticity-velocity (VV) formulation. The spatial and temporal coordinates are the inputs of the NSFnets, while the instantaneous velocity and pressure fields are the outputs for the VP-NSFnet, and the instantaneous velocity and vorticity fields are the outputs for the VV-NSFnet. This is unsupervised learning, and hence, no labeled data are required beyond boundary and initial conditions and the fluid properties. The residuals of the VP or VV governing equations, together with the initial and boundary conditions, are embedded in the loss function of the NSFnets. No pressure data are provided to the VP-NSFnet, because pressure is a hidden state and is obtained via the incompressibility constraint without extra computational cost. For laminar flow solutions, the VP and the VV formulations have comparable accuracy but their best performance corresponds to different NN architectures. For turbulent channel flow, NSFnets can sustain turbulence at Reynolds number $Re_\tau = 1000$, but because training is expensive, we only consider part of the channel domain and enforce velocity boundary conditions on the subdomain boundaries provided by the direct numerical simulation data base.

1.7 Boosting Ice Sheet Computational Models using DeepONet

Predicting sea level rise is one of the main goals of U.S. Department of Energy (DOE) Earth system modeling efforts. It requires the solution of computationally expensive ice sheet models. Quantifying the uncertainty on the sea level predictions is hindered by the large number of uncertain parameters, such as the sliding coefficient at the base of the ice, and the high cost of the computational models. A team formed by Brown, PNNL, and SNL researchers has been developing a deep operator network (DeepONet) surrogate of the most expensive part of an ice sheet model, the ice velocity solver. The DeepONet takes as inputs two fields, i.e., the thickness of the ice at a given time and the sliding coefficient, and computes the ice velocity field. Preliminary results on a synthetic ice sheet problem are promising and show significant computational savings when the velocity solver is replaced with the DeepONet [1]. The team is also exploring multifidelity approaches to reduce the cost of generating the data and training the DeepONet (see section 4.7). Furthermore, the team is working on a hybrid PINNs/DeepONet surrogate to replace the full dynamical core of ice sheet equations, which would lead to huge computational savings.

1.8 Learning Optimal Nonlocal and Fractional Operators for Turbulence and Anomalous Transport

Based on our previous work [22], M. D'Elia and N. Trask (SNL), in collaboration with Y. Yu (Lehigh), applied nonlocal operator regression to the identification of optimal, nonlocal closure terms for Reynolds-averaged Navier-Stokes models in the context of turbulent flow. In addition, inspired by our previous work on nonlocal PINNs

(nPINNs) [23], M. D'Elia (SNL) in collaboration with G. Karniadakis and E. Kharazmi (Brown) have extended nPINNs to nonlocal kernel learning and are applying this technique to identify the optimal closure terms for Large Eddy Simulation following the model proposed in [24] for the two-point stress–strain-rate correlation. Here, classical gradients are replaced by truncated fractional operators whose fractional orders are identified via PINNs. Preliminary results confirm the findings in [24] and set the foundations for more accurate and potentially cheaper models. Furthermore, by combining nPINNs [23] and the previously developed control volume PINNs (cvPINNs) framework for conservation laws [25], M. D'Elia, M. Gulian, R. Patel, and N. Trask (SNL) in collaboration with A. Tartakovsky (University of Illinois Urbana-Champaign) are using an nPINNs-cvPINNs approach to identify optimal models for anomalous subsurface transport with the ultimate goal of using this technique on field data such as the MAcroDispersion Experiment (MADE) [26] dataset.

1.9 Inferring 3-D Velocity and Pressure Fields from Schlieren Photography via PINNs

Tomographic background oriented Schlieren (Tomo-BOS) imaging measures density or temperature fields in three dimensions using multiple camera BOS projections, and is particularly useful for visualizing instantaneous flow of complex fluid dynamics problems. We propose a new method based on PINNs to infer the full, continuous, three-dimensional (3-D) velocity and pressure fields from snapshots of 3-D temperature fields obtained by Tomo-BOS imaging [27]. The PINNs seamlessly integrate the underlying physics of the observed flow and the visualization data, which enables the inference of latent quantities using limited experimental data. In this hidden fluid mechanics paradigm, we trained the NN by minimizing a loss function composed of a data mismatch term and residual terms associated with the coupled Navier-Stokes and heat transfer equations.

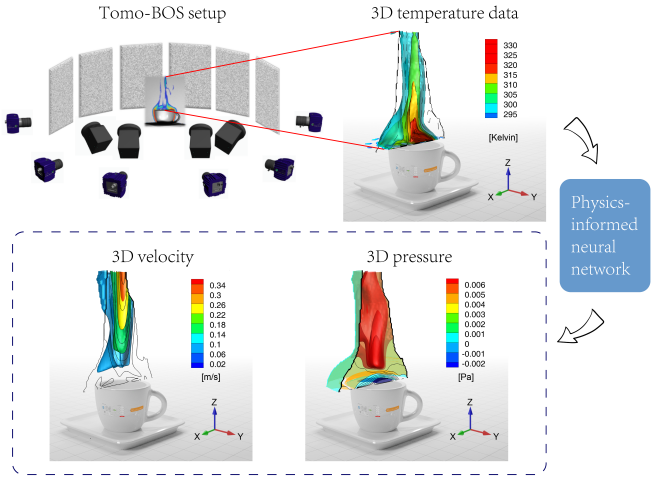


Figure 4: Tomo-BOS/PINN result with temporal downsampling data: BOS temperature, absolute error of temperature, inferred pressure at $z = -21$ mm and $t = 2.96$ s. The training data are sampled with time interval $t = 0.1s$. Although this snapshot is not used in training (it is unseen data for the PINN), the relative L_2-norm error of temperature for this snapshot is 0.362%.

1.10 PINNs for Multiphysics Data Assimilation: Subsurface Transport in Porous Media

We have introduced a meshfree approach based on the PINN method for solving the coupled advection-dispersion equation (ADE) and Darcy flow equation with space-dependent hydraulic conductivity [28]. Thorough investigation was conducted to compare the PINN method and the standard discretization-based numerical solvers for one- and two-dimensional forward Advection-Dispersion Equations (ADEs) with respect to various Péclet numbers (Pe). We found that the PINN method outperforms some conventional discretization-based methods, especially for the problems with large Pe and advection skew to the underlying discretization where instability and/or excessive diffusion can develop if the proper crosswind diffusion is not well represented by the numerical schemes. The PINN method yields desirable results in both cases without producing oscillations at the dispersion front. We have further investigated the performance of a PINN for backward ADE with nonuniform velocity field, which describes essential transport phenomena in porous media.

1.11 PINNs for Solving Forward and Inverse Flow Problems via the Boltzmann-BGK Formulation

The Boltzmann equation with the Bhatnagar-Gross-Krook collision model (Boltzmann-BGK equation) has been widely employed to describe multiscale flows, i.e., from the hydrodynamic limit to free molecular flow. In [29], we employed PINNs to solve forward and inverse problems via the Boltzmann-BGK formulation (PINN-BGK), enabling PINNs to model flows in both the continuum and rarefied regimes. In particular, the PINN-BGK is composed of three subnetworks, i.e., the first for approximating the equilibrium distribution function, the second for approximating the nonequilibrium distribution function, and the third one for encoding the Boltzmann-BGK equation and the corresponding boundary/initial conditions. By minimizing the residuals of the governing equations and the mismatch between the predicted and provided boundary/initial conditions, we can approximate the Boltzmann-BGK equation for both continuum and rarefied flows.

2 RA-II: Stochastic Modeling of Mesoscales

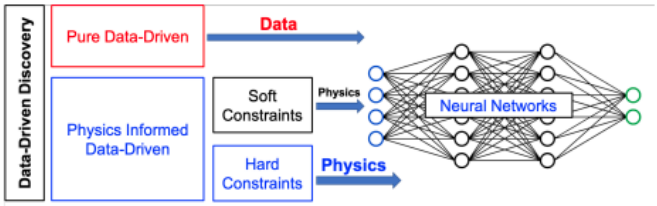


Figure 5: Schematic of the three major approaches in the data-driven discovery of dynamical systems. One is the pure data-driven approach. The other two are the physics-informed data-driven approaches. The second one is based on soft constraints imposed in an associated loss function. The third one directly imposes the underlying physics into NNs by designing novel network architectures.

We continued developing techniques for approximating mesoscale problems, especially through the imposition of hard thermodynamic constraints and necessary statistical attributes, e.g., the fluctuation-dissipation theorem. In addition, we have developed a technique for learning potentials that depend on the distance from an interface. Brown, SNL and PNNL have contributed to topics in RA-II.

2.1 GFINNs: GENERIC Formalism PINNs for Deterministic and Stochastic Dynamical Systems

We propose the General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC)-formalism–informed neural networks (GFINNs) that obey the symmetric degeneracy conditions of the GENERIC formalism [30]. GFINNs comprise two modules, each of which contains two components. We model each component using a NN whose architecture is designed to satisfy the required conditions. The component-wise architecture design provides flexible ways to leverage available physics information into NNs. We prove theoretically that GFINNs are sufficiently expressive to learn the underlying equations, hence establishing the universal approximation theorem. We demonstrate the performance of GFINNs in three simulation problems: gas containers exchanging heat and volume, thermoelastic double pendulum, and the Langevin dynamics. In all the examples, GFINNs outperform existing methods, demonstrating good accuracy in predictions for both deterministic and stochastic systems.

2.2 Developing Distance-Dependent Machine Learning Potential for Solid-Liquid Interface Systems

Solid-liquid interfaces occur in many fields of technology, such as catalysis, electrochemistry, energy storage materials, geochemistry, self-assembly–based biosensors, fluid transport, and biological membranes. To investigate the fluid properties and the interfacial structures, developing a coarse-grained (CG) model as a dissipative particle dynamics (DPD) model is feasible since *ab initio* calculation is usually very expensive at a large scale. We have developed a two-step NN framework that allows construction of an ML CG potential that depends on the distance from the solid-liquid interface. First, a neural network potential was designed to represent the molecular interactions in an octane-wall interfacial system at a CG level. The training data were obtained from atomic-level simulation of an octane-wall interfacial system. Figure 6a and b show that the CG NN potential can reproduce well the force and radial distribution function at the atomic level. The NN potential was integrated into a DPD framework to enable it to also reproduce the diffusion/viscosity properties of molecules by tuning the friction coefficient.

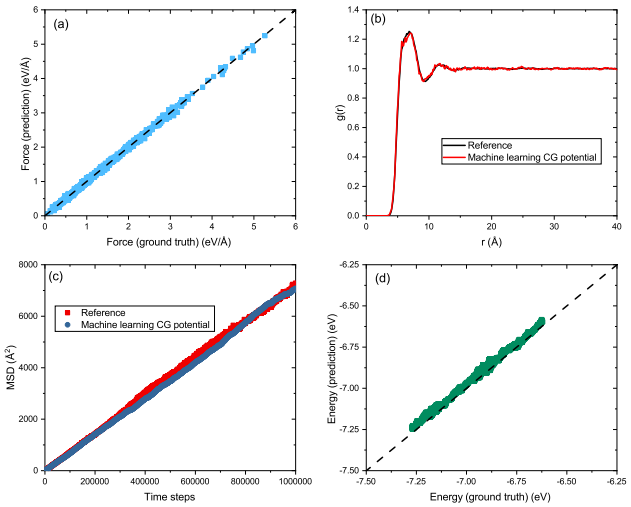


Figure 6: (a) The parity plot of the calculated force in reference and simulation with the NN CG potential simulation. (b) The radial distribution functions between octane molecules in reference and simulation with the NN CG potential. (c) The mean square displacement of octane molecules in reference and simulation with the NN CG potential.(d)The parity plot of the energy in reference and simulation with the distance-dependent NN potential.

As shown in fig. 6c, the mean square displacement obtained by simulation with the NN potential agrees well with reference data at the atomic level. Then we built a second NN to convert the first NN potential to one that is *distance-dependent* to the boundary wall in space using the data generated by the previously trained CG potential.

That means converting the Lagrangian specification to the Eulerian specification for a CG particle in the system. Figure 6d shows that the converted ML potential can reproduce the energy well.

2.3 Learning and Meta-Learning of Stochastic Advection-Diffusion-Reaction Systems from Sparse Measurements

PINNs were recently proposed as an alternative way to solve PDEs. An NN represents the solution while a PDE-induced NN is coupled to the solution NN, and all differential operators are treated using automatic differentiation. Here, we first employ the standard PINN and a stochastic version, sPINN, to solve forward and inverse problems governed by a nonlinear advection-diffusion-reaction equation, assuming we have some sparse measurements of the concentration field at random or preselected locations [31]. Subsequently, we attempt to optimize the hyperparameters of sPINN using Bayesian optimization (meta-learning) and compare the results with the empirically selected hyper-parameters of sPINN.

3 RA-III: Bridging Methods to Connect Scales

We continued developing techniques for bridging vastly different scales using DeepONet, nonlocal calculus, and data-driven exterior calculus. We also developed domain decomposition methods based on PINNs to tackle problems where a single PINN is not enough. DeepONet and PINNs were used to introduce new frameworks to address multiscale and multiphysics applications. Brown and SNL contributed to topics in RA-III.

3.1 Bridging the Micro/Molecular and Continuum Scales with Nonlocal Modeling

Nonlocal models are characterized by integral operators that embed length scales in their definitions. As such, they are preferable to classical PDE models in situations where the system dynamics is affected by the small-scale behavior, yet treating the small scales explicitly would require prohibitive computational cost. However, the kernels in nonlocal operators are difficult to derive from the data that are typically observed for a given physical system, such as laboratory mechanical property tests. Based on PhILMs' previous work [22], M. D'Elia (SNL), in collaboration with Y. Yu (Lehigh) developed a series of algorithms to learn nonlocal constitutive laws from high-fidelity data. This involved extending the basic nonlocal operator regression technique to time-dependent vector functions and to multidimensional problems. The technique was applied to infer a new peridynamic model for highly heterogeneous materials [32] and a linear peridynamic solid model that accurately describes MD displacements [33, 34]. Second, using nonlocally constrained optimization, with constraints on the group wave velocity, we inferred a nonlocal model for wave propagation through materials that feature heterogeneities in their microstructure [35]. All these works are based on the combination of high-fidelity data, ML algorithms, known physics, and nonlocal theory; this guarantees that the resulting model is mathematically well-posed, physically consistent, and generalizes well to settings that are different from the ones used during training, hence enabling transfer learning.

3.2 A Seamless Multiscale Operator Neural Network for Inferring Bubble Dynamics

Modeling multiscale systems from nanoscale to macroscale requires use of both atomic and continuum methods along with bridging different simulation schemes. We have developed a seamless method based on DeepONet, which is a composite DNN (a branch-and-trunk network) for regressing operators. DeepONet provides a robust framework to model physical systems across scales ranging from molecular fluctuations at the nanoscale to traditional continuum descriptions at the microscale and larger. We have demonstrated this approach in a recent paper [36], where we consider bubble growth dynamics in an expansion/compression domain while varying the external pressure. We represent small bubbles of initial size ranging from 100 nm to 10 μm, by a modified Rayleigh-Plesset equation in the continuum regime above 1 μm and by the DPD method for bubbles below 1 μm in the atomic regime. After offline training based on data from both regimes, DeepONet can accurately predict bubble growth on-the-fly (within a fraction of a second) across four orders of magnitude difference in spatial scales and over two orders of magnitude in temporal scales. The results are seamless and can be evaluated over a wide range of parameters and with continuous time variation. This builds on the previous work [37], where we had demonstrated DeepONet for each simulation scheme separately.

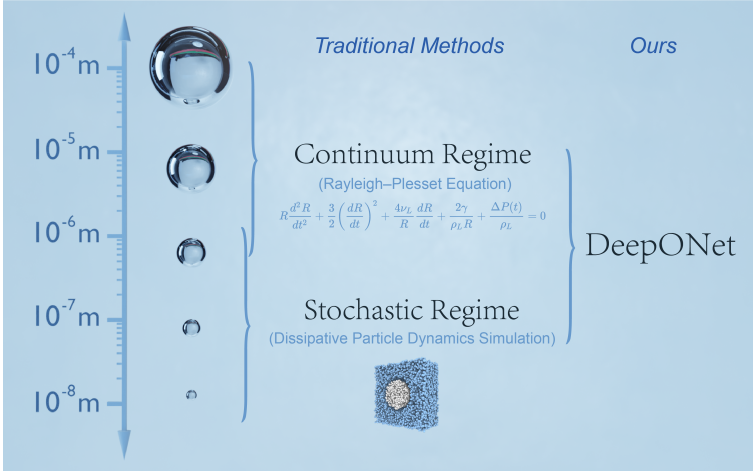


Figure 7: DeepONet can learn both from molecular simulations at the nanoscale as well as at the meso- and macroscales, hence forming an implicit multiscale operator that can simulate multiscale bubble dynamics in a fraction of a second instead of the tens of hours required with traditional solvers, even for a single nanobubble. The input to DeepONet is an arbitrary pressure difference and an initial radius of the bubble and the output is the bubble growth as a function of time.

3.3 Multiscale Electromagnetism: Bridging Quantum/Molecular/Continuum Scales with data-driven exterior calculus

The data-driven exterior calculus (DDEC) (N. Trask) allows learning of continuum models preserving algebraic structure critical for handling electromagnetism [38]. We use the recently developed Spectral Neighbor Analysis Potential (SNAP) methodology [39, 40] to extract an MD model of iron from quantum density functional theory enriched with magnetic spin. This MD model may then be used to train a continuum DDEC model at continuum length scale. In this manner, we extract a data-driven finite element method space that accounts for effects of thermomagnetism, allowing prediction of thermal influence on band gaps necessary for designing radar systems. This work has been selected for external follow-on funding for microelectronic co-design. Additionally, the same framework is being used in a collaboration with Jeffrey Hyman (Los Alamos National Laboratory [LANL]) to learn fracture networks for subsurface flow problems.

3.4 Parallel Physics-Informed Neural Networks via Domain Decomposition

We develop a distributed framework for the PINNs based on two recent extensions, namely conservative PINNs (cPINNs) and extended PINNs (XPINNs), which employ domain decomposition in space and in time-space, respectively. This domain decomposition endows cPINNs and XPINNs with several advantages over the vanilla PINNs, such as parallelization capacity, large representation capacity, efficient hyperparameter tuning, and is particularly effective for multi-scale and multiphysics problems. Here, we present a parallel algorithm for cPINNs and XPINNs constructed with a hybrid programming model described by MPI + X, where X $\in$ {CPUs, GPUs}. The main advantage of cPINN and XPINN over the more classical data and model parallel approaches is the flexibility of optimizing all hyperparameters of each NN separately in each subdomain. We compare the performance of distributed cPINNs and XPINNs for various forward problems, using both weak and strong scalings. Our results indicate that for space domain decomposition, cPINNs are more efficient in terms of communication cost but XPINNs provide greater flexibility as they can also handle time-domain decomposition for any differential equations, and can deal with any arbitrarily shaped complex subdomains. To this end, we also present an application of the parallel XPINN method for solving an inverse diffusion problem with variable conductivity on the United States map, using 10 regions as subdomains.

3.5 A Physics-Informed Variational DeepONet for Predicting the Crack Path in Brittle Materials

Failure trajectories, identifying the probable failure zones, and damage statistics are some of the key quantities of relevance in brittle fracture applications, and they are expensive to obtain with traditional high-fidelity numerical solvers. Therefore, fast and generalizable surrogate models are needed to alleviate the computational burden, but the discontinuous nature of fracture mechanics presents a major challenge to developing such models. We propose a physics-informed variational formulation of DeepONet (V-DeepONet) for brittle fracture analysis [41].

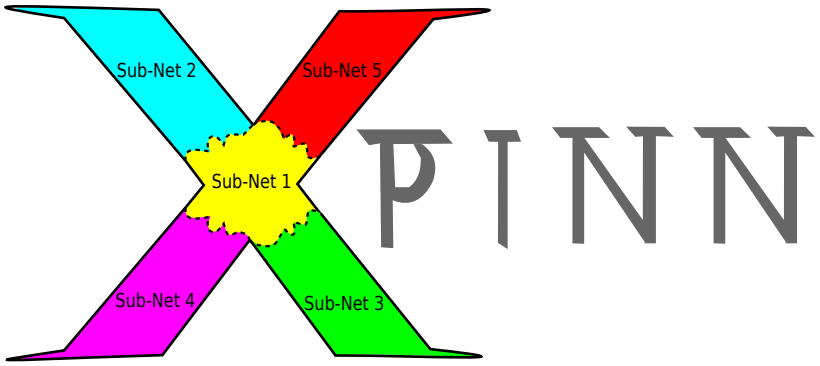


Figure 8: Schematic representation of XPINNs: Irregularly shaped subdomain divisions in 'X'-shaped domain, where sub-net is employed in each subdomain and they are stitched together using the interface conditions.

V-DeepONet is trained to map the initial configuration of the defect to the relevant fields of interests (e.g., damage and displacement fields). Once the network is trained, the entire global solution can be rapidly obtained for any initial crack configuration and loading steps on that domain. While the original DeepONet is solely data-driven, we take a different path to train the V-DeepONet by imposing the governing equations in variational form and we also use some labeled data. We demonstrate the effectiveness of V-DeepONet through two benchmarks of brittle fracture, and we verify its accuracy using results from high-fidelity solvers. Encoding the physical laws and also some data to train the network renders the surrogate model capable of accurately performing both interpolation and extrapolation tasks, considering that fracture modeling is very sensitive to fluctuations.

3.6 DeepM&Mnet: Inferring the Electroconvection Multiphysics Fields Based on Operator Approximation by Neural Networks

Electroconvection is a multiphysics problem involving coupling of the flow field with the electric field as well as the cation and anion concentration fields. Here, we use electroconvection as a benchmark problem to put forward a new data assimilation framework, the DeepM&Mnet [42], for simulating multiphysics and multiscale problems at speeds much faster than standard numerical methods using pre-trained NNs. We first pre-train DeepONets that can predict independently each field, given general inputs from the rest of the fields of the coupled system. DeepONets, which are extremely fast, are used as building blocks in the DeepM&Mnet and form constraints for the multiphysics solution along with some sparse available measurements of any of the fields. We demonstrate the new methodology and document the accuracy of each individual DeepONet, and subsequently we present two different DeepM&Mnet architectures that infer accurately and efficiently 2-D electroconvection fields for unseen electric potentials. The DeepM&Mnet framework is general and can be applied for building any complex multiphysics and multiscale models based on very few measurements using pre-trained DeepONets in a "plug-and-play" mode.

3.7 Data-Driven, Physics-Informed Constitutive Metamodeling of Complex Fluids: A Multifidelity Neural Network (MFNN) framework

In this work [43], we introduce a comprehensive machine-learning algorithm, namely, a multifidelity neural network (MFNN) architecture for data-driven constitutive metamodeling of complex fluids. The physics-based NNs developed here are informed by the underlying rheological constitutive models through the synthetic generation of low-fidelity model-based data points. The performance of these rheologically informed algorithms is thoroughly investigated and compared against classical DNNs. The MFNNs are found to recover the experimentally observed rheology of a multicomponent complex fluid consisting of several different colloidal particles, wormlike micelles, and other oil and aromatic particles. Moreover, the data-driven model is capable of successfully predicting the steady-state shear viscosity of this fluid under a wide range of applied shear rates based on its constituting components. Building upon the demonstrated framework, we present the rheological predictions of a series of multicomponent complex fluids made by DNN and MFNN. We show that by incorporating the appropriate physical intuition into the neural network, the MFNN algorithms capture the role of experiment temperature, the salt concentration added to the mixture, as well as aging within and outside the range of training data parameters. This is made possible by leveraging an abundance of synthetic low-fidelity data that adhere to specific rheological models. In contrast, a purely data-driven DNN is consistently found to predict erroneous rheological behavior.

4 RA-IV: Statistical Learning and Deep Learning Approximations and Algorithms

We continued developing techniques and algorithms to tackle various issues related to inference from data and optimization e.g., lack of independence, misspecification of distributions, noisy data, slow convergence of descent algorithms and training. In addition, methods for learning disentangled representations of nonlinear dynamical systems and physics-informed generative models for learning distributions of physical parameters. Stanford, MIT, Brown, SNL and UCSB contributed to topics in RA-IV.

4.1 Learning from Dependent Data and Statistical Physics

Statistical inference and ML methods commonly assume access to independent observations from the phenomenon of interest. However, the assumption that available data comprise independent observations is too strong. In many applications, variables are observed on nodes of a network, or some spatial or temporal domain, and are dependent. Examples abound in physical systems, epidemiological, geographical, meteorological and financial applications, and dependencies naturally arise in social networks through peer effects, whose study has been recently explored in topics as diverse as criminal activity, welfare participation, school achievement, participation in retirement plans, obesity, etc. Estimating models that combine peer and individual effects to predict behavior has been challenging, and for many standard statistical inference tasks even consistency results are elusive. Is it possible to have a statistical learning theory for dependent data? We develop statistical learning frameworks which extend classical ones to the data dependent setting, wherein training samples and test samples are all jointly sampled from a high-dimensional distribution. Extending works in COLT'19 and STOC'19 from previous cycles, PI Daskalakis and students Yuval Dagan, Nishanth Dikkala (now at Google), Vardis Kandiros, and Surbhi Goel (formerly a PhD at UT Austin, now a postdoctoral researcher at Microsoft Research) we develop a binary classification framework for observations collected on a network or a spatio-temporal domain with dependencies [44]. We model these dependencies in the language of Markov Random Fields and, importantly, allow these dependencies to be substantial, i.e., do not assume that the Markov Random Field capturing these dependencies is in high temperature. As our main contribution we provide algorithms and statistically efficient estimation rates for this model, giving several instantiations of our bounds in logistic regression, sparse logistic regression, and NN settings with dependent data. Our estimation guarantees follow from novel results for estimating the parameters (i.e., external fields and interaction strengths) of Ising models from a single sample, developed in this work and another work with students Dagan, Dikkala, and Kandiros focusing on Ising model estimation, also from this cycle [45].

4.2 Sinkhorn Label Allocation: Semi-Supervised Classification via Annealed Self-Training

Self-training is a standard approach to semi-supervised learning where the learner's own predictions on unlabeled data are used as supervision during training. Work of PhD student Kai Sheng Tai, colleague Peter Bailis, and PI Valiant reinterpreted this label assignment process as an optimal transportation problem between examples and classes, wherein the cost of assigning an example to a class is mediated by the current predictions of the classifier. This formulation facilitates a practical annealing strategy for label assignment and allows for the inclusion of prior knowledge on class proportions via flexible upper bound constraints. The solutions to these assignment problems can be efficiently approximated using Sinkhorn iteration, thus enabling their use in the inner loop of standard stochastic optimization algorithms. We demonstrated the effectiveness of our algorithm on the CIFAR-10, CIFAR-100, and Street View House Number (SVHN) datasets in comparison with FixMatch, a state-of-the-art self-training algorithm. Our code is available via GitHub (see below for a link).

4.3 Quantifying the Cost of Misspecification

Suppose we want to find a probability distribution that models outcomes y given data x. Typically one chooses a parametric family of probability distributions and aims to find the "best" member of this family according to a given loss. If the true distribution of y given x does not belong to this parametric family, this is termed model misspecification. Work with PhD student Annie Marsden, John Duchi, and PI Valiant showed that misspecification can significantly complicate optimization, with regret rates that scale as $\sqrt(n)$ times a problem-specific constant, as opposed to the usual logarithmic regret that is achieved for well specified settings. This work was accepted for a full oral presentation at the International Conference on Artificial Intelligence and Statistics (AISTATS) (fewer than two percent of submissions received this distinction).

4.4 Worst-Case Analysis for Randomly Collected Data

Work with undergraduate researcher Justin Chen, colleague Paul Valiant, and PI Valiant, introduced a framework for statistical estimation that leverages knowledge of a data collection process, in contrast to making distribu-

tional assumptions on the underlying data values. We described a near-optimal estimation algorithm for such settings, via an intriguing connection to the Groethendick Problem. We also applied this framework to several specific commonly encountered data collection processes that are not informally, identically distributed, including importance sampling, snowball sampling, and setting with chronological structure, showing significantly improved estimation error versus standard approaches. This work was accepted for full oral presentation at NeurIPS'20 (fewer than 2% of submissions received this distinction).

4.5 Calibration in Online Prediction

Work with PhD student Mingda Qiao and PI Valiant considered the challenge of producing *calibrated* predictions in a fundamental online setting. In the binary prediction setting, a calibrated predictor has the property that, for each probability value p, out of all the times when the predictor outputs p, roughly a p fraction of the outcomes are 1. (E.g., a calibrated weather prediction has the property that, historically, of the times when the report says "60% chance of rain," it has rained roughly 60% of the time.) Given an arbitrary (even adversarial) binary length n sequence, what is the best calibration error that a predictor can achieve? This problem has been studied since the 1980's, and is still open. In a paper we presented at STOC'21 (the top Computer Science theory conference), we provided the first improvement to the lower bound on this problem since the 1990's. We are currently working on providing a matching (algorithmic) upper bound.

4.6 Learning Functional Priors and Posteriors from Data and Physics

We develop a Bayesian framework based on DNNs to extrapolate in space-time using historical data and to quantify uncertainties arising from both noisy and gappy data in physical problems (fig. 9) [46]. Specifically, the proposed approach has two stages: (1) prior learning and (2) posterior estimation. At the first stage, we employ the physics-informed generative adversarial networks (PI-GANs) to learn a functional prior either from a prescribed function distribution, e.g., Gaussian process, or from historical data and physics. At the second stage, we employ the Hamiltonian Monte Carlo method to estimate the posterior in the latent space of PI-GANs. In addition, we use two approaches to encode the physics: (1) automatic differentiation, used in the PINNs for scenarios with explicitly known PDEs, and (2) operator regression using the deep operator network (DeepONet) for PDE-agnostic scenarios. We then test the proposed method for (1) meta-learning for one-dimensional regression, and forward/inverse PDE problems (combined with PINNs); (2) PDE-agnostic physical problems (combined with DeepONet), e.g., fractional diffusion as well as saturated stochastic (100-dimensional) flows in heterogeneous porous media; and (3) spatial-temporal regression problems, i.e., inference of a marine riser displacement field. The results demonstrate that the proposed approach can provide accurate predictions as well as uncertainty quantification given very limited scattered and noisy data, since historical data could be available to provide informative priors.

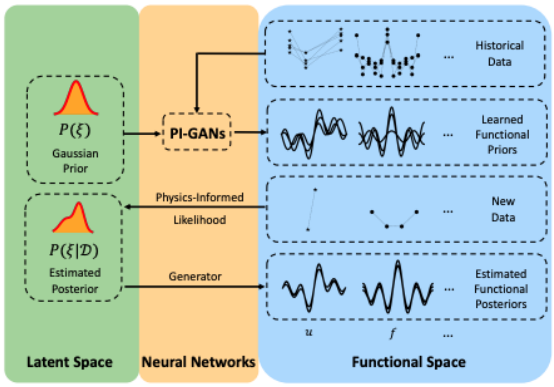


Figure 9: Schematic of learning functional priors and posteriors from data and physics. The "PI" part is based on either PINNs with AD or operator approximation in the form of DeepONet.

4.7 Multifidelity DeepONets

Our work has formulated a multifidelity version of a Deep Operator Network (DeepONet) [47] that can find both linear and nonlinear correlations between high- and low-fidelity data. We consider a system with high-fidelity data $y_h(b)(x) = \mathcal{F}(b, y_l)(x)$, where b are the sensor values, y_l are the low-fidelity data, and x are the sensor locations. This formulation lends itself well to training with a DeepONet, but here we consider two DeepONets, $y_h(b)(x) = \mathcal{F}_l(b, y_l)(x) + \mathcal{F}_{nl}(b, y_l)(x)$, where $\mathcal{F}_l$ captures the linear correlation and $\mathcal{F}_{nl}$ captures the nonlinear correlation between the high-fidelity and low-fidelity data. In doing so, we can find complex correlations between the data, and provide more robust training in cases where the high-fidelity data alone is not sufficient. We note that the low-fidelity data y_l can have different dimensions than the number of sensors, which is advantageous in the case where the low-fidelity data may come directly from simulations or measurements.

4.8 Theory on Generalization of PINNs and XPINNs

Recently, extended PINNs (XPINNs) based on domain decomposition methods have attracted considerable attention because they can effectively model multiscale and multiphysics problems and their parallelization. We have taken an initial step toward understanding how and when XPINNs outperform PINNs. Specifically, for general multi-layer PINNs and XPINNs, we first provide a prior generalization bound via the complexity of the target functions in the PDE problem, and a posterior generalization bound via the posterior matrix norms of the networks after optimization. Moreover, based on our bounds, we analyze the conditions under which XPINNs improve generalization. Concretely, our theory shows that the key building block of XPINN, namely the domain decomposition, introduces a trade-off for generalization. On the one hand, XPINNs decompose the complex PDE solution into several simple parts, which decreases the complexity needed to learn each part and boosts generalization. On the other hand, decomposition leads to less training data being available in each subdomain, and hence such model is typically prone to overfitting and may become less generalizable. Empirically, we choose five PDEs to show when XPINNs perform better than, similar to, or worse than PINNs, hence demonstrating and justifying our new theory.

4.9 Deep Kronecker Neural Networks: A General Framework for Neural Networks with Adaptive Activation Functions

We propose a new type of neural network, Kronecker neural networks (KNNs), that form a general framework for NNs with adaptive activation functions. KNNs employ the Kronecker product, which provides an efficient way of constructing a very wide network while keeping the number of parameters low. Our theoretical analysis reveals that under suitable conditions, KNNs induce a faster decay of the loss than that by the feed-forward networks. This is also empirically verified through a set of computational examples. Furthermore, under certain technical assumptions, we establish global convergence of gradient descent for KNNs. As a specific case, we

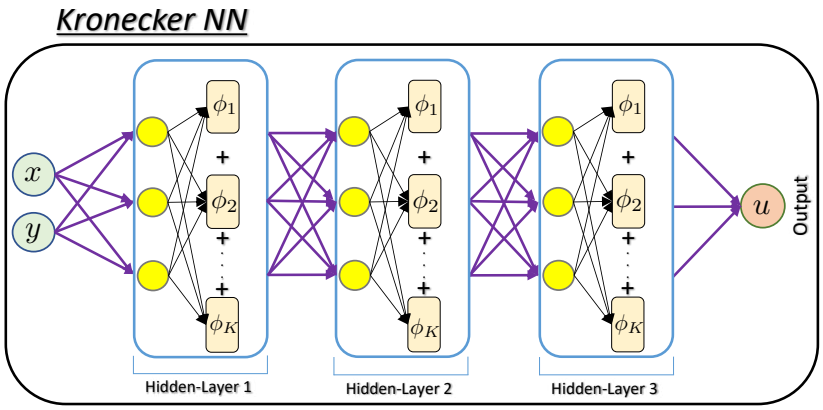


Figure 10: A schematic of a Kronecker NN with all the activation functions learned by the data directly.

propose the *Rowdy* activation function that is designed to get rid of any saturation region by injecting sinusoidal fluctuations, which include trainable parameters. The proposed Rowdy activation function can be employed in any NN architecture like feed-forward NNs, Recurrent NNs, Convolutional NNs, etc. The effectiveness of KNNs with Rowdy activation is demonstrated through various computational experiments including function approximation using feed-forward NNs, solution inference of partial differential equations (PDEs) using the PINNs, and standard deep-learning benchmark problems using convolutional and fully connected NNs.

4.10 Bayesian Operator Regression with POU-nets

Several works from SNL in past year have aimed to realize deep architectures and optimizers which converge, avoiding the optimization error barrier by building a hybrid approach combining deep partitioning with polynomial regression [48, 49]. Incorporating a probabilistic noise model has allowed for Bayesian extensions of this approach and a connection to the well-known "Mixture of Experts" model. This connection allows applications of the expectation maximization training strategy, providing closed-form expressions for optimal polynomial fits which admit a trivially parallel implementation amenable to Message Passing Interface (MPI) or GPU solution. Bayesian

extensions to operator regression provide state-of-the-art accuracy for learning solution operators and measures of uncertainty. Costly look-up tables ubiquitous to production codes suffer from the curse-of-dimensionality and may be replaced by POU-net surrogates. For example, replacing chemical kinetics table in *Fuego*, a production SNL combustion code, has led to a 1000x reduction in memory usage and allows scientists to consider previously intractable dimensions in their chemistry models. These provide a foundation for the newly funded "Beyond Fingerprinting" grand challenge Laboratory Directed Research and Development (LDRD) effort at SNL which aims to develop a digital twin for additive manufacture of weapons system components.

4.11 Multilevel Optimization for PINNs

PINNs have demonstrated a remarkable ability to solve inverse and forward problems for PDEs. However, they suffer from many of the same training challenges as other NN models. SNL (Patel, E.C. Cyr) has developed a strategy to speed up the training of PINNs based on multigrid optimization (MG/OPT) [50] in which a hierarchy of coarser PINNs optimization problems are solved to obtain corrections to the full problem. This approach results in up to 4-5x speedup for cvPINNs/PINNs relative to standard training. Additionally, SNL has begun collaborating with B. Southworth (LANL), S. Gunther (Lawrence Livermore National Laboratory), and J. Schroder (University of New Mexico) to combine the multigrid in time-based layer-parallel training strategy [51] with MG/opt and enable parallel training of PINNs.

4.12 A Caputo Fractional Derivative-Based Algorithm for Optimization

We propose a novel Caputo fractional derivative-based optimization algorithm [52], see fig. 11. Upon defining the Caputo fractional gradient with respect to the Cartesian coordinate, we present a generic Caputo fractional gradient descent (CFGD) method. We prove that the CFGD yields the steepest descent direction of a locally smoothed objective function. The generic CFGD requires three parameters to be specified, and a choice of the parameters yields a version of CFGD. We propose three versions – non-adaptive, adaptive terminal, and adaptive order. By focusing on quadratic objective functions, we provide a convergence analysis. We prove that the non-adaptive CFGD converges to a Tikhonov regularized solution. For the two adaptive versions, we derive error bounds, which show convergence to integer-order stationary point under some conditions. We derive an explicit formula of CFGD for quadratic functions. We computationally found that the adaptive terminal (AT) CFGD mitigates the dependence on the condition number in the rate of convergence and results in significant acceleration over gradient descent (GD). For non-quadratic functions, we develop an efficient implementation of CFGD using the Gauss-Jacobi quadrature, whose computational cost is approximately proportional to the number of the quadrature points and the cost of GD. Our numerical examples show that AT-CFGD results in acceleration over GD, even when a small number of the Gauss-Jacobi quadrature points (including a single point) is used.

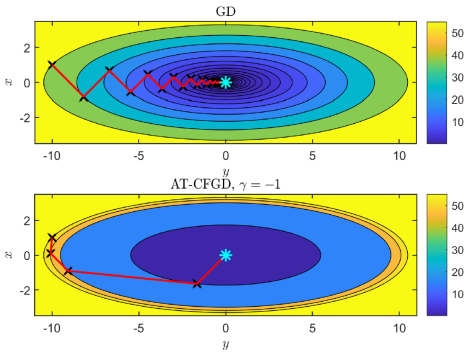


Figure 11: A contour graph of the objective function $f(x, y) = 10x^2 + y^2$ (black) along with trajectories of (top) GD and (bottom) adaptive terminal CFGD.

4.13 Variational Autoencoders (VAE) for Nonlinear Dynamics

We developed methods using variational inference for ways to train DNNs to obtain probabilistic autoencoders incorporating prior knowledge about physical systems. Our resulting VAEs provide methods for learning parsimonious disentangled representations of nonlinear dynamical systems arising in parametric PDE problems and other physical systems; see [53]. We also developed ways to incorporate geometric and topological priors into the latent space allowing for representations with non-Euclidean geometry. This allows for using lower dimensional latent spaces, can improve robustness, and help with mechanistic interpretation of the learned dynamics. We performed systematic studies comparing our nonlinear VAE methods with other dimension reduction techniques, such as proper orthogonal decomposition (POD), dynamic mode decomposition (DMD), and other analytic methods. We showed how our VAE methods can help in capturing nonlinear, dynamical behaviors of the system and robust predictions. We demonstrated our methods on the nonlinear, viscous Burgers equation and a parameterized PDE problem, making comparisons with POD, DMD, and reductions based on Cole-Hopf transformations. We further demonstrated our methods for constrained mechanical systems and the role of using non-Euclidean latent spaces to incorporate geometric / topological priors for the representation of the dynamics.

Method	Dim	0.25s	0.50s	0.75s	1.00s
VAE Nonlinear	2	**4.44e-3**	**5.54e-3**	**6.30e-3**	**7.26e-3**
VAE Linear	2	9.79e-2	1.21e-1	1.17e-1	1.23e-1
DMD	3	2.21e-1	1.79e-1	1.56e-1	1.49e-1
POD	3	3.24e-1	4.28e-1	4.87e-1	5.41e-1
Cole-Hopf-2	2	5.18e-1	4.17e-1	3.40e-1	1.33e-1
Cole-Hopf-4	4	5.78e-1	6.33e-2	9.14e-3	1.58e-3
Cole-Hopf-6	6	1.48e-1	2.55e-3	9.25e-5	7.47e-6

γ	0.00s	0.25s	0.50s	0.75s	1.00s
0.00	1.600e-01	6.906e-03	1.715e-01	3.566e-01	5.551e-01
0.50	1.383e-02	1.209e-02	1.013e-02	9.756e-03	1.070e-02
2.00	1.337e-02	1.303e-02	9.202e-03	8.878e-03	1.118e-02

β	0.00s	0.25s	0.50s	0.75s	1.00s
0.00	1.292e-02	1.173e-02	1.073e-02	1.062e-02	1.114e-02
0.50	1.190e-02	1.126e-02	1.072e-02	1.153e-02	1.274e-02
1.00	1.289e-02	1.193e-02	7.903e-03	7.883e-03	9.705e-03
4.00	1.836e-02	1.677e-02	8.987e-03	8.395e-03	8.894e-03

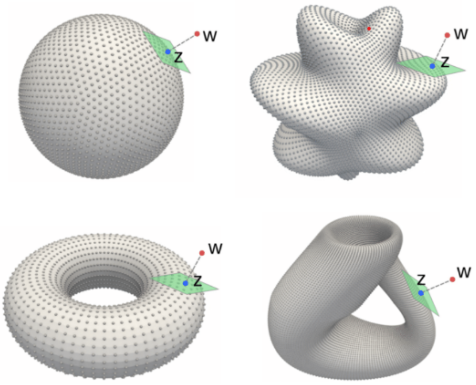


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Figure 12: Variational autoencoders for learning dynamics of physical systems. The methods allow use of non-Euclidean latent spaces for parsimonious representations. Shown are the reconstruction errors given the dimension of the latent spaces; for more details see [53]

4.14 PhysGNN: Training Generative Neural Networks with Physics Knowledge

We consider how to incorporate physics knowledge into training generative NNs for learning distributions of physical parameters. Unlike traditional deep generative NNs [54, 55, 56, 57] that are directly trained to represent data distribution, our physics generative neural networks (PhysGNNs) are trained to represent underlying distributions of physical parameters by imposing physical constraints on the final layer outputs of the generative NNs. In doing so, we can generalize deep generative models to solve a wide variety of physical problems. Physical constraints are usually described by PDEs and solved by numerical solvers such as finite element analysis [58]. We require that the numerical PDE model is differentiable so that the gradients can be calculated by AD [59, 60, 61] and the coupled system of PDEs and generative NNs can be trained by minimizing the loss function using GD methods. One challenge in implementing AD is back-propagating the gradient through *implicit* numerical PDE solvers. We derived an efficient algorithm based on the implicit function theorem, which fits into the reverse-mode AD framework. This algorithm allows us to couple generative NNs and both explicit and implicit numerical PDE solvers, making PhysGNN applicable to most physical equations and problems for modeling distributions of underlying physical parameters.

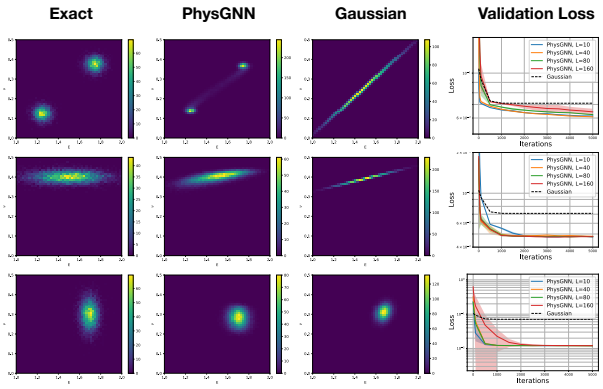

Figure 13: Training results for a linear elasticity problem. For plots on the left panel, E is on the x-axis while ν is on the y-axis. L is the latent vector dimension. Each row is a different case. In the "Validation Loss" plots, we show the validation loss (calculated using newly generated samples) for different latent vector dimensions. We also show a one standard deviation bound for each case.

5 Integration and Outreach

Dissemination and outreach have been hampered by the pandemic. However, we have leveraged electronic means for dissemination along with our existing broad, professional networks to communicate the results of PhILMs and have many examples of external adoption of PhILMs capabilities by laboratories, universities, and industry, as depicted in fig. 14.

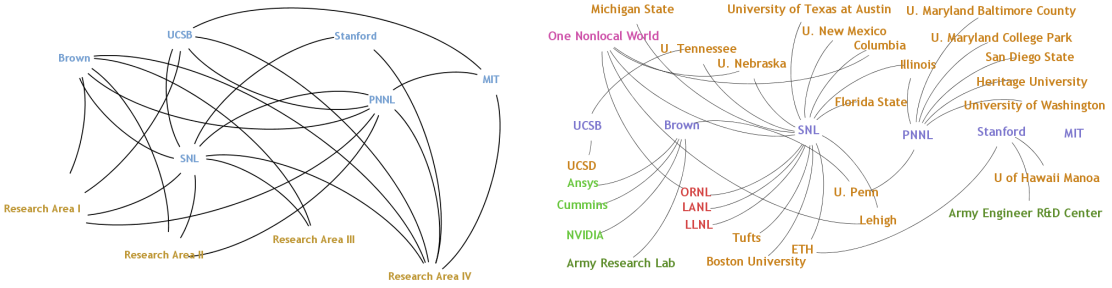

Figure 14: A schematic of internal and external collaborations.

5.1 Early Career Advancement

(1) K. Lee finished his postdoctoral work at Sandia and is a tenure-track professor in Computer Science at Arizona State University. (2) R. Patel finished his postdoctoral work at Sandia supporting PhILMs and transitioned to permanent staff, where he will continue to support PhILMs and other projects. (3) M. Gulian completed his appointment as Sandia's John von Neumann Postdoctoral Fellow in Computational Science, where part of his time supported PhILMs, and has transitioned to permanent staff where he will continue to support PhILMs and other Scientific Machine Learning (SciML) projects. (4) M. D'Elia was promoted to Principal Member of the Technical Staff. (5) N. Trask served as PhD co-advisor for Quang Ha at Boston University, who has defended and has taken a position with Mathworks. (6) L. Lu graduated from Brown and finished his MIT postdoctorate before starting a tenure-track position at the University of Pennsylvania. (7) Q. He finished his postdoctoral research at PNNL and is a tenure-track professor in Mechanical Engineering at San Diego State University. (8) J. Chen graduated from Stanford and is beginning work toward a PhD at MIT. (9) K. S. Tai received his PhD in September 2021.

5.2 Interns Mentored

One key form of outreach is mentoring interns, particularly from historically underrepresented groups. PI Karniadakis and his postdoctoral students supervised four interns this summer, working on topics related to physics-informed ML and its applications. Here we describe the specific activities of two female interns from underrepresented groups: The first one, Anna Diaz from Heritage University, worked on data fusion methods in application to ocean acidification at Brown. She presented her work at the Leadership Alliance Virtual National Symposium. She focused on the marine ecosystem and the global environment affected by ocean acidification. She noted that high-quality data is expensive, and that more accurate and timely predictions of sea temperature at regional and local scales might better help resource management and economic planning. She employed the multifidelity Gaussian processes regression model to assimilate sea surface temperature/PH/salinity in Boston Harbor, Massachusetts, with different resolutions or fidelities, (e.g., satellite data [low fidelity], *in situ* data [high fidelity]), and hence enhance the prediction accuracy over that from modeling with high-fidelity data only. Jessica Turner is an undergraduate in the Department of Computer Science, University of Maryland, Baltimore County. During the internship, she mainly used Fourier transforms as a tool to analyze how NNs learn. In particular, she applied fast Fourier transforms to identify the features learned by a NN for function approximation, and showed that the

NNs generally learn the low frequencies of a function at the beginning of training and then fit the high frequencies at the end. She also participated in the 2021 Leadership Alliance Virtual National Symposium, and gave a presentation titled, "How Neural Networks learn."

A. Howard (PNNL) mentored a Graduate Education for Minorities (GEM) PhD Intern, Justin Peterkin. The GEM fellowship "promotes the participation of underrepresented groups in post-graduate science." Justin worked on learning continuum-scale equations for fluid-solid flows. Justin is currently a PhD student in the Physics Department at University of Maryland, College Park.

M. D'Elia (SNL) mentored Yiming Fan (Lehigh) and Hayley Olson (University of Nebraska) via the National Science Foundation Mathematical Sciences Graduate Internship (MSGI) Program and Huaiqian You (Lehigh) via the SNL long-term internship program. M. Parks (SNL) mentored Nicole Buczkowski (U. Nebraska) via a National Science Foundation Non-Academic Research Internships for Graduate Students (INTERN) Award. N. Trask is mentoring Huansheng Chen (Lehigh) through the National Science Foundation INTERN program.

5.3 Dissemination

PhILMs team members authored 126 journal articles, peer-reviewed conference papers, and technical reports in the last year. In addition, PhILMs members have contributed to panels and boards across a wide range of topics designed to increase the participation of students in science, technology, engineering and mathematics (STEM) fields. Among these, M. D'Elia served on the Research Experiences for Undergraduates/Research Experience for Teachers (REU/RET) panel on Careers in Data Science held at Emory University. M. Parks was a panelist on the *Atypical Ph.D. Journeys in Computing and Data Science* career development panel discussion at Boston University held on December 3, 2020. P. Atzberger worked with Santa Barbara Partners in Education, which includes visiting local junior high and high schools to give presentations in classes and to facilitate discussions on topics in mathematics, computation, and related application areas. He served on a panel on "networking with applied mathematicians" for the student chapter of the Association of Women in Mathematics at UCSB, and participated in events for the First-Generation Students Opening New Doors to Accelerating Success (ONDAS) Center. In addition, M. D'Elia co-founded the One Nonlocal World Project [62], an online platform where people working on nonlocal problems can regularly check for updates on nonlocal modeling, analysis, and computation.

5.4 PhILMs External University Collaborations

M. D'Elia has ongoing collaboration with O. Burkovska [63] and P. Seleson [62] at Oak Ridge National Laboratory; G. Capodaglio at LANL [6]; M. Zayernouri at Michigan State [4]; T. Mengesha at the University of Tennessee, Knoxville; J. Scott at Columbia; M. Gunzburger at Florida State [6]; Y. Yu at Lehigh [22, 33, 35, 15]; and J. Foster at the University of Texas at Austin [7, 32]. N. Trask has ongoing collaborations with X. Hu (Tufts University), J. Hyman and H. Viswanathan (LANL), P. Barbone (Boston University), J. Foster (University of Texas), Y. Bazilevs (Brown), Y. Yue and J. Jaworski (Lehigh). A. Howard and P. Stinis have ongoing collaboration with Q. He (San Diego State University.)

5.5 PhILMs Industrial Collaborations and Technology Adoption

PINNs have become now the main tool for industry to merge data and mathematical modeling. The PI has worked closely with industrial partners to promote development and dissemination of the new tools of PhILMs. Nvidia has implemented PINNs in their parallel code SimNet and Ansys have been exploring creative uses of DeepOnet. Cummins has been using PINNs for truck engine specific models and online parameter estimation. Proctor and Gamble (P&G) have been using multifidelity modeling for inferring the viscosity of new variants of their shampoos.

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A Presentations and Publications

The PhILMs team measures its success, in part, on its fundamental contributions to the scientific literature, as well as the generation and dissemination of algorithms and open-source software. A publications list also is available online at `https://www.pnnl.gov/projects/philms/publications`.

A.1 Publications

1. Ainsworth, M. & Dong, J. Galerkin Neural Networks: A Framework for Approximating Variational Equations with Error Control. *SIAM J. Sci. Comput.* **43,** A2474–A2501 (2021)

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A.1.1 Peer-Reviewed Conference Proceedings

1. Chen, J. Y., Valiant, G. & Valiant, P. *Worst-Case Analysis for Randomly Collected Data* in *NeurIPS* (2020)

2. Christia, F., Curry, M. J., Daskalakis, C., Demaine, E. D., Dickerson, J. P., Hajiaghayi, M., Hesterberg, A., Knittel, M. & Milliff, A. *Scalable Equilibrium Computation in Multi-agent Influence Games on Networks* in *Proceedings of the 35th AAAI Conference on Artificial Intelligence* (2021)

3. Dagan, Y., Daskalakis, C., Dikkala, N. & Kandiros, A. V. *Learning Ising models from one or multiple samples* in *Proceedings of the 53rd Annual ACM SIGACT Symposium on Theory of Computing (STOC)* (2021)

4. Daskalakis, C., Skoulakis, S. & Zampetakis, M. *The complexity of constrained min-max optimization* in *Proceedings of the 53rd Annual ACM SIGACT Symposium on Theory of Computing (STOC)* (2021)

5. Daskalakis, C., Fishelson, M. & Golowich, N. *Near-Optimal No-Regret Learning in General Games* in *Proceedings of the 35th Annual Conference on Neural Information Processing Systems (NeurIPS)* (2021)

6. Daskalakis, C., Stefanou, P., Yao, R. & Zampetakis, E. *Efficient Truncated Linear Regression with Unknown Noise Variance* in *Proceedings of the 35th Annual Conference on Neural Information Processing Systems (NeurIPS)* (2021)

7. Daskalakis, C., Kontonis, V., Tzamos, C. & Zampetakis, E. *A Statistical Taylor Theorem and Extrapolation of Truncated Densities* in *Proceedings of the 34th Annual Conference on Learning Theory (COLT)* (2021)

8. Daskalakis, C. & Pan, Q. *Sample-optimal and efficient learning of tree Ising models* in *Proceedings of the 53rd Annual ACM SIGACT Symposium on Theory of Computing (STOC)* (2021)

9. Diakonikolas, J., Daskalakis, C. & Jordan, M. I. *Efficient Methods for Structured Nonconvex-Nonconcave Min-Max Optimization* in *Proceedings of the 24th International Conference on Artificial Intelligence and Statistics (AISTATS)* (2021)

10. Ding, M., Daskalakis, C. & Feizi, S. *GANs with Conditional Independence Graphs: On Subadditivity of Probability Divergences* in *Proceedings of the 24th International Conference on Artificial Intelligence and Statistics (AISTATS)* (2021)

11. Fan, T., Xu Kailai Pathak, J. & Darve, E. *Solving Inverse Problems in Steady State Navier-Stokes Equations using Deep Neural Networks.* in *AAAI 2020 Fall Symposium on Physics-Guided AI to Accelerate Scientific Discovery (PGAI-AAAI-20)* (2020)

12. Hu, X., Huang, A., Trask, N. & Brissette, C. *Greedy Fiedler Spectral Partitioning for Data-driven Discrete Exterior Calculus* Accepted in AAAI Spring Symposium: MLPS. 2021

13. Kandiros, V., Dagan, Y., Dikkala, N., Goel, S. & Daskalakis, C. *Statistical Estimation from Dependent Data* in *Proceedings of the 38th International Conference on Machine Learning (ICML)* (2021)

14. Lopez, R. & Atzberger, P. J. Variational Autoencoders for Learning Nonlinear Dynamics of Physical Systems. *accepted AAAI-MLPS Proceedings.* arXiv: `2012.03448 [cs.LG]` (2021)

15. Marsden, A., Duchi, J. C. & Valiant, G. *Misspecification in Prediction Problems and Robustness via Improper Learning* in *The 24th International Conference on Artificial Intelligence and Statistics, AISTATS 2021, April 13-15, 2021, Virtual Event* **130** (PMLR, 2021), 2161–2169. `http://proceedings.mlr.press/v130/marsden21a.html`

16. Qiao, M. & Valiant, G. *Exponential Weights Algorithms for Selective Learning* in *Conference on Learning Theory* (2021), 3833–3858

17. Qiao, M. & Valiant, G. *Stronger calibration lower bounds via sidestepping* in *Proceedings of the 53rd Annual ACM SIGACT Symposium on Theory of Computing* (2021), 456–466

18. Tai, K. S., Bailis, P. & Valiant, G. *Sinkhorn Label Allocation: Semi-Supervised Classification via Annealed Self-Training* in *International Conference on Machine Learning (ICML)* (2021)

19. Xu, K. & Darve, E. *ADCME: Learning Spatially-varying Physical Fields using Deep Neural Networks.* in *3rd Workshop on Machine Learning and the Physical Sciences, Workshop at the 34th Conference on Neural Information Processing Systems* (2020)

20. Xu, K. & Darve, E. *Data-Driven Inverse Modeling with Incomplete Observations.* in *AAAI 2020 Spring Symposium on Combining Artificial Intelligence and Machine Learning with Physical Sciences* (2020)

21. Xu, K. & Darve, E. *Calibrating Multivariate Lévy Processes with Neural Networks* in *Proceedings of The First Mathematical and Scientific Machine Learning Conference* (eds Lu, J. & Ward, R.) **107** (PMLR, 2020), 207–220. `https://proceedings.mlr.press/v107/xu20a.html`

22. You, H., Yu, Y., Silling, S. & D'Elia, M. *Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws* Accepted in AAAI Spring Symposium: MLPS. 2021

A.2 Conferences and Workshops

A.2.1 Invited Presentations

The PI (G. Karniadakis) has given close to 50 invited presentations to national laboratories, industry, universities, and conferences. He was one of the main organizers of the Digital Twins conference in San Diego (September 2021) and the AmeriMech symposium (October 2021), sponsored by the U.S. National Committee for Theoretical and Applied Mechanics. A subset is listed below:

Karniadakis GE. "Physics-Informed Neural Networks PINNs and DeepONet: Theory and Applications,"

- *Siemens Inc., USA*
- *Hitachi Inc, USA*
- *Bosch Inc., USA*
- *University of Cambridge, UK*
- *AMD Inc., UK*
- Plenary Talk in 10th Workshop on Parallel-in-Time Integration.

Invited presentations by other members of the PhILMs collaborative are listed here.

P. J. Atzberger, "Stochastic Immersed Boundary Methods," Courant Institute, New York University, New York, NY, April 2021.

P. J. Atzberger, "Machine Learning for investigating dynamics of physical systems," PhILMs, DOE, May 2021.

P. Bochev, "Development of Data-driven Radiation-aware Device Compact Models for Circuit Simulations." *Machine Learning and Deep Learning Conference*, July 2020. Virtual.

P. Bochev, "Development of Data-driven Radiation-aware Device Compact Models for Circuit Simulations." Invited talk at the Society of Engineering Science (SES) *57th Annual Technical Meeting, Eringen Medal Symposium*. September 28-30, 2020. Virtual.

P. Bochev, "Hybrid analytic-numerical compact models for radiation-induced photocurrent effects." *A symposium in honor of Jackie Chen's selection as a 2020 DOE Office of Science Distinguished Scientist Fellow*, Sandia National Laboratories, May 26, 2021. Virtual.

P. Bochev, "Computational mathematics careers in national labs: an inside perspective." STEM Talk, Casper College, WY November 19, 2020. Virtual.

P. Bochev "What does a computational mathematician do in a national lab?." Society for Industrial and Applied Mathematics (SIAM)/Career talk, Virginia Tech, December 2, 2020. Virtual.

C. Daskalakis. "Three ways Machine Learning fails and what these have to do with Game Theory and Economics," *SET Seminar in Economic Theory*, October 2020, held virtually. (Invited Talk)

C. Daskalakis. "Equilibrium Computation and the Foundations of Deep Learning," *One World Mathematical Game Theory Seminar*, online seminar part of One World Series, October 2020, held virtually. (Invited Talk)

C. Daskalakis. "Robust Mechanism Design: Multiple Items, Dependent Distributions, and Distribution Shifts," *CMU Economic Theory Seminar*, November 2020, held virtually. (Invited Talk)

C. Daskalakis. "Equilibrium Computation and the Foundations of Deep Learning," *NYU and ETH MaD+ (math and data plus) seminar*, November 2020, held virtually. (Invited Talk)

C. Daskalakis. "Equilibrium Computation, GANs and the foundations of Deep Learning," *16th Conference on Web and Internet Economics*, December 2020, held virtually. (Plenary talk)

C. Daskalakis. "Learning Ising Models from one, ten or a thousand samples," *High-Dimensional Learning and Testing Workshop at Simons Institute for Theory of Computing*, December 2020, held virtually. (Invited Talk)

C. Daskalakis. "Equilibrium Computation, GANs and the foundations of Deep Learning," *National Technical University of Athens, Greece*, January 2021, held virtually. (Invited Talk)

C. Daskalakis. "Equilibrium Computation, GANs and the foundations of Deep Learning," *Virtual Seminar Series on Games, Decisions and Networks*, January 2021, held virtually. (Invited Talk)

C. Daskalakis. "Equilibrium Computation and the Foundations of Deep Learning," *AAAI Workshop on Reinforcement Learning in Games*, February 2021, held virtually. (Invited Talk)

C. Daskalakis. "Three ways Machine Learning fails and what to do about them," *NYIT School of Architecture and Design*, February 2021, held virtually. (Public Lecture)

C. Daskalakis. "Equilibrium Computation and the Foundations of Deep Learning," *32nd International Conference on Algorithmic Learning Theory (ALT)*, March 2021, held virtually. (Plenary Talk)

C. Daskalakis. "How AI fails, and why it matters," *Greek Scientists Society Symposium*, March 2021, held virtually. (Public Lecture)

C. Daskalakis. "The Revolution of Tomorrow and the moral implications of Artificial Intelligence," *Hellenic Innovation Network and Greek Consulate in Boston webinar*, March 2021, held virtually. (Panel Discussion)

C. Daskalakis. "How does Artificial Intelligence fail and what can we do about it?," *Athens Science Virtual Festival*, April 2021, held virtually. (Public Lecture)

C. Daskalakis. "Robust (ML + MD) = Learned Mechanisms," *Google Market Algorithms Workshop*, May 2021, held virtually. (Invited Talk)

C. Daskalakis. "How Long Until Truly Intelligent Machines?," *University of Crete*, May 2021, held virtually. (Public Lecture)

C. Daskalakis. "Equilibrium Computation and the Foundations of Deep Learning," *University of Washington,* May 2021, held virtually. (Invited Talk)

C. Daskalakis. "From von Neumann to Machine Learning: Equilibrium Computation and the Foundations of Deep Learning," *John von Neumann Lecture, University of Zurich and ETH*, June 2021, held virtually. (Public Talk)

C. Daskalakis. "Equilibrium Computation and Deep Learning," *CVPR conference*, June 2021, held virtually. (Keynote Talk)

C. Daskalakis. "Min-Max Optimization: from von Neumann to Deep Learning, Nash and Wilson," *Stony Brook Game Theory Festival*, July 2021, held virtually. (Plenary Talk)

C. Daskalakis. "Min-Max Optimization: from von Neumann to Deep Learning," *Conference on Research on Economic Theory and Econometrics*, July 2021, Naxos, Greece. (Plenary Talk)

C. Daskalakis. "Equilibrium Computation and Machine Learning," *Congress of the Game Theory Society*, July 2021, held virtually. (Semi-Plenary Talk)

C. Daskalakis. "Min-Max Optimization: from von Neumann to Deep Learning," *Symposium on Fundamentals of Computation Theory*, September 2021, held virtually. (Plenary Talk)

M. D'Elia, "A unified theoretical and computational nonlocal framework: generalized vector calculus and machine-learnt nonlocal models." *SIAM TX-LA Section*. October 17-18, 2020. Virtual.

M. D'Elia, "A unified, data-driven framework for the identification of nonlocal models: ALGORITHMS & APPLICATIONS." *Engineering Sciences Seminar at Sandia National Laboratories*. December 10, 2020. Virtual.

M. D'Elia, "A unified theoretical and computational nonlocal framework." *Mathematics Department Colloquium at MODEMAT, Ecuador*. December 15, 2020. Virtual.

M. D'Elia, "Challenges in nonlocal modeling: nonlocal boundary conditions and nonlocal interfaces." *WCCM-ECCOMAS 2020*. January 11-15, 2021. Virtual.

M. D'Elia, "Data driven learning of nonlocal models: from MD to continuum mechanics." *New Mexico Machine Learning in Material Science Symposium*. February 23, 2021. Virtual.

M. D'Elia, "A general framework for Nonlocal Domain Decomposition." *SIAM CSE 21*. March 3, 2021. Virtual.

M. D'Elia, "Data driven learning of nonlocal models." *Computing and Mathematical Science Colloquium at the California Institute of Technology*. March 10, 2021. Virtual.

M. D'Elia, "Data driven learning of nonlocal models." *CNA seminar at Carnegie Mellon University*. March 16, 2021. Virtual.

M. D'Elia, "Data driven learning of nonlocal models." *AAAI 2021 Spring Symposium on Combining Artificial Intelligence and Machine Learning with Physics Sciences*. March 22-24, 2021. Virtual.

M. D'Elia, "Data driven learning of nonlocal models." *Mathematics Department Colloquium at Florida State University*. March 26, 2021. Virtual.

M. D'Elia, "Data driven learning of nonlocal models." *The 50th John H. Barrett Memorial Lectures*. May 17-19, 2021. Virtual. (Keynote)

M. D'Elia, "A new variable-order fractional Laplacian." *SIAM MS 21*. May 17-28, 2021. Virtual.

M. D'Elia, "Addressing micro-scale interfaces via nonlocal models using machine learning." *Coupled Problems 21*. June 14-16, 2021. Virtual.

M. D'Elia, "Data driven learning of nonlocal models." *ALOP Workshop, Nonlocal Models: Analysis, Optimization, and Implementation*. July 12-14, 2021. Virtual. (Plenary)

M. D'Elia, "A unified theory of fractional and nonlocal calculus." *INdAM workshop on Fractional Differential Equations: Modeling, Discretization, and Numerical Solvers*. July 12-14, 2021. Virtual. (Plenary)

M. D'Elia, "Being a mathematician at a national laboratory." *REU/RET Panel on Careers in Data Science at the Emory University*. July 19, 2021. Virtual. (Plenary)

M. D'Elia, "Data driven learning of nonlocal models." *SIAM AN 21*. July 22, 2021. Virtual.
M. D'Elia, "Data driven learning of nonlocal models." *16th U.S. National Congress on Computational Mechanics*. July 28, 2021. Virtual.
M. D'Elia, "Data driven learning of nonlocal models." *DDPS Seminar at Lawrence Livermore National Laboratory*. July 30, 2021. Virtual.
M. D'Elia, "Data-driven learning of nonlocal models: bridging scales with nonlocality." *Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology* September 2021. Virtual.
M. D'Elia, "Data-driven learning of nonlocal models: bridging scales with nonlocality." *Machine learning in heterogeneous porous materials, AmeriMech Symposium Series*. October 4-6, 2021. Virtual.
M. Gulian, "Data-driven learning of nonlocal physics from high-fidelity synthetic data." CONFERENCIA IFIP TC7 2021. August 30, 2021. Virtual.
M. Gulian, "Analysis of Anisotropic Nonlocal Diffusion Models: Well-posedness of Fractional Problems for Anomalous Transport." SIAM MS 21. May 26, 2021. Virtual.
M. Gulian, "A block coordinate descent optimizer for classification problems exploiting convexity." AAAI-MLPS, March 3, 2021. Virtual.
M. Gulian, "Robust architectures, initialization, and training for deep neural networks via the adaptive basis interpretation," SIAM SEAS, September 18, 2021. Virtual.
A. Howard, "Nonlocal models for modeling multiphase fluids," Arizona State University, Tempe, AZ, 2021. Virtual.
A. Howard, "Nonlocal models for modeling multiphase fluids," San Diego State University, San Diego, CA, 2021. Virtual.
A. Howard, "Nonlocal models for modeling multiphase fluids," University of Washington, Seattle, WA, 2021. Virtual.
M. Parks, "nPINNS: Nonlocal Physics-Informed Neural Networks." *16th U.S. National Congress on Computational Mechanics*, Chicago, Illinois (virtual), July 29, 2021.
M. Parks, "Computational Aspects of Nonlocal Models." Center for Nonlinear Analysis, Department of Mathematical Sciences, Mellon College of Sciences, Carnegie Mellon University, Virtual, April 13, 2021.
M. Parks, "nPINNS: Nonlocal Physics-Informed Neural Networks," One Nonlocal World, Virtual, January 23, 2021.
M. Perego, "Modeling land ice with deep operator networks." *SIAM Southeastern Atlantic Section Conference*. Sept 19, 2021. Virtual.
R. Patel, "PDE discovery with machine learning," *University of New Mexico Applied Math Seminar*, November 2020. Virtual.
R. Patel, "Control volume PINNs: a method for solving inverse problems with hyperbolic PDEs," *Brown University CRUNCH Seminar*, January 2021. Virtual.
R. Patel, "A Physics-Informed Operator Regression Framework for Extracting Data-Driven Continuum Models," *SIAM Conference on Computational Science and Engineering*, March 2021. Virtual.
R. Patel, "Modal operator regression for extracting nonlocal continuum models," *16th U.S. National Congress on Computational Mechanics*, July 2021. Virtual.
N. Trask, "A data-driven exterior calculus for model discovery." *RPI engineering webinar* 9/30/21. Virtual.
N. Trask, "A data-driven exterior calculus for model discovery." *Princeton Plasma Physics Laboratory Webinar* 11/16/2020. Virtual.
N. Trask, "ASCR physics-informed machine learning at SNL." *Presentation to DOE Office of AI* 12/10/2020. Virtual.
N. Trask, "Designing convergent and structure preserving architectures for SciML." *UTEP Department Webinar* 2/26/2021. Virtual.
N. Trask, "A data-driven exterior calculus for model discovery." *SIAM CSE* 3/01/2021. Virtual.
N. Trask, "Designing convergent and structure preserving architectures for SciML." *One World ML virtual webinar* 3/03/2021. Virtual.
N. Trask, "Physics-informed ML tutorial for Northwestern engineering." *Northwestern Engineering colloquium* 3/05/2021. Virtual.
N. Trask, "A data-driven exterior calculus for model discovery." *USACM UQ Webinar* 3/18/21. Virtual.
N. Trask, "Making physics-informed ML work." *Los Alamos invited machine learning webinar* 3/17/2021. Virtual.
N. Trask, "Partition of unity networks: deep hp-approximation." *AAAI-MLPS virtual meeting* 3/17/2021. Virtual.

N. Trask, "Structure preservation and mathematical foundations for scientific machine learning." *CIS External Review* 3/24/2021 . Virtual.

N. Trask, "Structure preserving architectures for SciML." *CRUNCH webinar, Brown University* 6/07/2021. Virtual.

N. Trask, "Structure preserving machine learning for high-consequence engineering and science applications." *New Research Ideas Forum (SNL)* 6/17/2021. Virtual.

N. Trask, "A data-driven exterior calculus for model discovery." *USACM* 7/27/2021. Virtual.

N. Trask, "Discovery of structure-preserving finite element spaces for multiscale." *Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology i* 9/27/2021. Virtual.

G. Valiant. "Charting the Landscape of Memory/Data Tradeoffs in Continuous Optimization: A Survey of Open Problems," *Simons Institute for Theory of Computing, workshop on Rigorous Evidence for Information-Computation Trade-offs*, September 2021.

G. Valiant. "Estimation and Learning Beyond the IID Setting," *Workshop MHC2020: Mixtures, Hidden Markov Models and Clustering*, June 2021.

G. Valiant. "Statistical Challenges in the Federated Setting," *New Problems and Perspectives on Sampling, Learning, and Memory*, April 2021.

G. Valiant. "Statistical Challenges in the Federated Setting," *Federated Learning One World Seminar (FLOW)*, November 2020.

G. Valiant. "Worst-Case Analysis for Randomly Collected Data," *University of Wisconsin, Madison, invited talk*, October 2020.

A.2.2 Organized Conferences and Workshops

Organized minisymposium: A. Biswas, M. Parks, and P. Radu, "Nonlocal Operators and Machine Learning in Multiscale Modeling," *Mechanistic Machine Learning and Digital Twins for Computational Science*, San Diego, CA, September 2021.

Organized minisymposium: A. Biswas, M. Parks, and P. Radu, "Nonlocal Models in Continuum Mechanics: Mathematical, Computational, Machine Learning Aspects," *16th U.S. National Congress on Computational Mechanics*, Chicago, IL, July 2021.

Organized minisymposium: P. Bochev, P. Kuberry, B. Paskaleva, "Data Driven Approaches for Circuit Design and Analysis," *Mechanistic Machine Learning and Digital Twins for Computational Science*, San Diego, CA, September 2021.

Organized symposium: E. Darve, J. H. Lee, *AAAI 2020 Spring Symposium Series, Combining Artificial Intelligence and Machine Learning with Physical Sciences*, 2020. (14 speakers)
`https://sites.google.com/view/aaai-mlps/aaai-mlps-2020/program-2020`

Organized symposium: E. Darve, *AAAI 2021 Spring Symposium on Combining Artificial Intelligence and Machine Learning with Physics Sciences*, March 2021.
`https://sites.google.com/view/aaai-mlps/program?authuser=0`

Co-organizer and scientific committee member: E. Darve, *1st IACM conference for machine learning and digital twins for computational science and engineering*, September 2021.

Organized conference: M. D'Elia, Q. Du, P. Radu, P. Seleson, X. Tian, Y. Yu, *One Nonlocal World Opening Event*, Virtual, January 2021.

Organized conference: M. D'Elia, Q. Du, E. Madenci, P. Radu, P. Seleson, S. Silling, X. Tian, Y. Yu, *Nonlocal Codes, A One Nonlocal World Project event*, Virtual, December 2021.

Organized conference: M. D'Elia, G. Rozza, M. Gunzburger, *RAMSES: Reduced order models; Approximation theory; Machine learning; Surrogates, Emulators and Simulators*, SISSA, Trieste, Italy, (hybrid) December 2021.

Organized minisymposium: M. D'Elia, N. Trask, Y. Yu "Identifying constitutive behavior and dynamics via physics-informed machine learning," *Mechanistic Machine Learning and Digital Twins for Computational Science*, San Diego, CA, September 2021.

Organized minisymposium: M. D'Elia, P. Seleson, " Local-to-Nonlocal and Nonlocal-to-Nonlocal Coupling Methods: Advances in Coupling Techniques and Treatment of Interfaces in Nonlocal Mechanics and Diffusion," *16th U.S. National Congress on Computational Mechanics*, Chicago, IL, July 2021.

Organized minisymposium: M. D'Elia, P. Seleson, " Local-to-Nonlocal and Nonlocal-to-Nonlocal Coupling Methods: Advances in Coupling Techniques and Treatment of Interfaces in Nonlocal Mechanics and Diffusion," *SIAM Conference on Mathematical Aspects of Material Science*, Bilbao, Spain, July 2021.

Organized minisymposium (invited session): M. D'Elia, " Nonlocal interface problems for the simulation of heterogeneous materials and media," *Coupled Problems 2021*, Chia Laguna, Italy, June 2021

Organized minisymposium: M. D'Elia, C. Glusa, "Model learning and optimization for nonlocal models," *SIAM Conference on Computational Science and Engineering*, Fort Worth, TX, March 2021.

Organized minisymposium: M. D'Elia, P. Seleson, Y. Yu "Nonlocal models in computational Science and Engineering," *SIAM Conference on Computational Science and Engineering*, Fort Worth, TX, March 2021.

Organized minisymposium: M. D'Elia, P. Seleson, "Computational aspects of nonlocal models," *WCCM, World Congress on Computational Mechanics*, Paris, France, January 2021.

Organized minisymposium: Q. He, P. Gao, A. Howard, J. Li, "Integration of Models, Data and Artificial Intelligence for Energy and Power Systems," *Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology (MMLDT-CSET Conference)*,September 2021, San Diego, CA.

Organized minisymposium: N. Trask, R. Patel, N. Nelson, "Machine Learning for Surrogate Model and Operator Discovery," *SIAM Conference on Computational Science and Engineering*, Fort Worth, TX, March 2021.

A.2.3 Contributed Presentations and Posters

P. J. Atzberger and R. Lopez. "Variational Autoencoders with Manifold Latent Spaces for Learning Nonlinear Dynamics," *SMB*, June 2021.

P. J. Atzberger and R. Lopez. "Variational Autoencoders for Learning Nonlinear Dynamics of Physical Systems," *Workshop on Mathematical Machine Learning and Application*, Penn. State University Park, PA, December 2020. Virtual.

P. J. Atzberger "Tutorial on using USER-SELM for fluctuating hydrodynamics models in LAMMPS," *LAMMPS Workshop*, break-out session, August 2021.

P. J. Atzberger "USER-MLMOD Package: Machine Learning Methods for Data-Driven Models in LAMMPS," *LAMMPS Workshop*, August 2021.

P. J. Atzberger "Variational Autoencoders with Manifold Latent Spaces for Learning Nonlinear Dynamics," *Sandia Machine Learning and Deep Learning Workshop 2021 (MLDL2021)*, July 2021.

P. J. Atzberger "Surface Fluctuating Hydrodynamics Methods for the Drift-Diffusion Dynamics of Particles and Microstructures within Lipid Bilayer Membranes," 16th U.S. National Congress on Computational Mechanics (USNCCM16), July 2021.

E. Darve, "Machine learning for inverse modeling in mechanics," *Artificial Intelligence for Robust Engineering & Science, AIRES 2: Machine Learning for Robust Digital Twins*, January 2021.

E. Darve, "Deep Neural Networks for Inverse Modeling," *SIAM/CAIMS Annual Meeting (AN20) July 2021, Virtual conference*

M. D'Elia "Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws," *Workshop on Mathematical Machine Learning and Application*, December 14-16, 2020. Virtual.

T. Fan, K. Xu, J. Pathak, and E. Darve, "Solving Inverse Problems in Steady-State Navier-Stokes Equations using Physics Constrained Machine Learning," *World Congress in Computational Mechanics (WCCM)—European Community on Computational Methods in Applied Sciences (ECCOMAS) Joint Congress*

T. Fan, K. Xu, J. Pathak, and E. Darve, "Solving Inverse Problems in Steady-State Navier-Stokes Equations using Deep Neural Networks," *AAAI Fall 2020 Symposium on Physics-Guided AI to Accelerate Scientific Discovery*, Aug. 2020.

M. Gulian, "A Unified Theory of Fractional, Nonlocal, and Weighted Nonlocal Vector Calculus." *One Nonlocal World*, Virtual Poster Presentation, January 22, 2021. Virtual.

A. Howard, "Learning a non-local model for non-Newtonian fluid rheology." *Nonlocal World*, Virtual Poster Presentation, January 22, 2021. Virtual.

A. D. Jagtap, Extended Physics-Informed Neural Networks (XPINNs): A Generalized Space-Time Domain Decomposition Based Deep Learning Framework for Nonlinear Partial Differential Equations, *AAAI 2021 Spring Symposium on Combining Artificial Intelligence and Machine Learning in Physics Sciences*, Stanford University, Palo Alto, California, USA, March 22, 2021 (Virtual Conference).

XH Meng, "Multi-fidelity Bayesian neural networks for inverse PDE problems with noisy data," *SIAM Annual Meeting (AN21)*, July 19-23, 2021 (Virtual Conference).

XH Meng, "Multi-fidelity Bayesian neural networks for inverse PDE problems with noisy data," *16th U.S. Association for Computational Mechanics*, July 25-29, 2021 (Virtual Conference).

R. Patel, "Learning continuum-scale models from micro-scale dynamics via Operator Regression," *14th World Congress in Computational Mechanics*, January 2021. Virtual.

R. Patel, "Multiscale training for Physics-informed Neural Networks," *20th Copper Mountain Conference on Multigrid Methods*, March 2021. Virtual.

K. Xu and E. F. Darve, "ADCME: A General Framework of Machine Learning for Computational Engineering," *SIAM Conference on Computational Science and Engineering (CSE21)*, March 2021, Virtual conference

K. Xu, E. Darve, "ADCME—Machine Learning for Computational Engineering," *Berkeley/Stanford CompFest,* 2020

K. Xu and E. Darve, "Data-Driven Inverse Modeling and Deep Learning with Incomplete Observations," *14th World Congress on Computational Mechanics (WCCM) meeting*, Paris, France

A.3 Software

The PhILMs team has released numerous software packages, listed below. We expand on some of the software pages in this section.

`ADCME`: Automatic Differentiation Library for Computational and Mathematical Engineering
`https://github.com/kailaix/ADCME.jl`

`AdFem.jl`: Inverse Modeling with the Finite Element Method,
`https://github.com/kailaix/AdFem.jl/`

`ADSeismic.jl`: Inverse Problems in Earthquake Location/Source-Time Function, FWI, Rupture Process,
`https://github.com/kailaix/ADSeismic.jl`

`cvPINNs`: `github.com/rgp62/cvpinns`

`DeepXDE`: A deep learning library for solving differential equations,
`https://github.com/lululxvi/deepxde`

`FwiFlow.jl`: Seismic Inversion, Two-phase Flow, Coupled seismic and flow equations,
`https://github.com/lidongzh/FwiFlow.jl`

`MOR-Physics`: `github.com/rgp62/MOR-Physics`

`pyPCGA`: Python library for principal component geostatistical approach,
`https://github.com/jonghyunharrylee/pyPCGA`

`SinkhornSSL`: Software for semi-supervised learning, based on our International Conference on Machine Learning (ICML) paper *Sinkhorn Label Allocation: Semi-Supervised Classification via Annealed Self-Training*.
`https://github.com/stanford-futuredata/sinkhorn-label-allocation`

`USER-MLMOD`: `https://arxiv.org/abs/2107.14362`

`USER-SELM`: Fluctuating hydrodynamics simulations in LAMMPS,
`http://mango-selm.org/`

A.3.1 DeepXDE: A Deep Learning Library for Solving Differential Equations

Deep learning has achieved remarkable success in diverse applications; however, its use in solving partial differential equations (PDEs) has emerged only recently. Here, we present an overview of physics-informed neural networks (PINNs), which embed a PDE into the loss of the neural network using automatic differentiation. The PINN algorithm is simple, and it can be applied to different types of PDEs, including integro-differential equations, fractional PDEs, and stochastic PDEs. Moreover, from the implementation point of view, PINNs solve inverse problems as easily as forward problems. We propose a new residual-based adaptive refinement method to improve the training efficiency of PINNs. For pedagogical reasons, we compare the PINN algorithm to a standard finite element method. We also present a Python library for PINNs, DeepXDE, which is designed to serve both as an education tool to be used in the classroom as well as a research tool for solving problems in computational science and engineering. Specifically, DeepXDE can solve forward problems given initial and boundary conditions, as well as inverse problems given some extra measurements. DeepXDE supports complex-geometry domains based on the technique of constructive solid geometry, and enables the user code to be compact, resembling closely the mathematical formulation (fig. 15). We introduce the usage of DeepXDE and its customizability, and we also demonstrate the capability of PINNs and the user-friendliness of DeepXDE for five different examples. More broadly, DeepXDE contributes to the more rapid development of the emerging Scientific Machine Learning field.

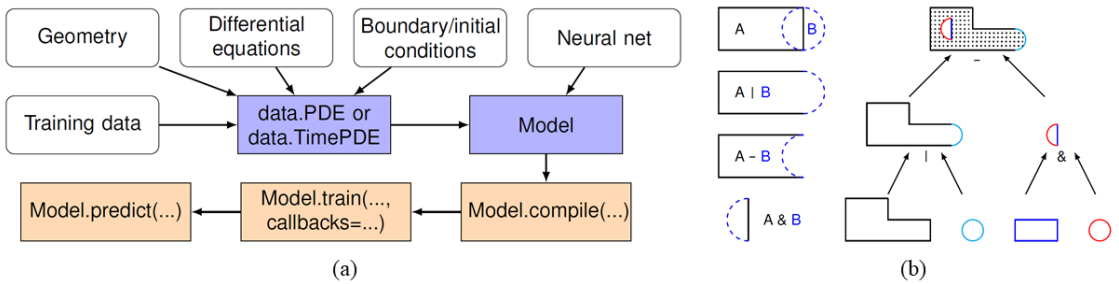


Figure 15: Schematic of DeepXDE. (a) Flowchart of DeepXDE. The white boxes define the PDE problem and the training hyperparameters. The blue boxes combine the PDE problem and training hyperparameters in the white boxes. The orange boxes are the three steps (from right to left) to solve the PDE. (b) Examples of constructive solid geometry in 2-D. (left) A and B represent the rectangle and circle, respectively. The union $A|B$, difference $A - B$, and intersection $A\&B$ are constructed from A and B. (right) A complex geometry (top) is constructed from a polygon, a rectangle and two circles (bottom) through the union, difference, and intersection operations. This capability is included in the module geometry of DeepXDE.

A.3.2 LAMMPS MD Package: USER-SELM: Fluctuating Hydrodynamics Simulations

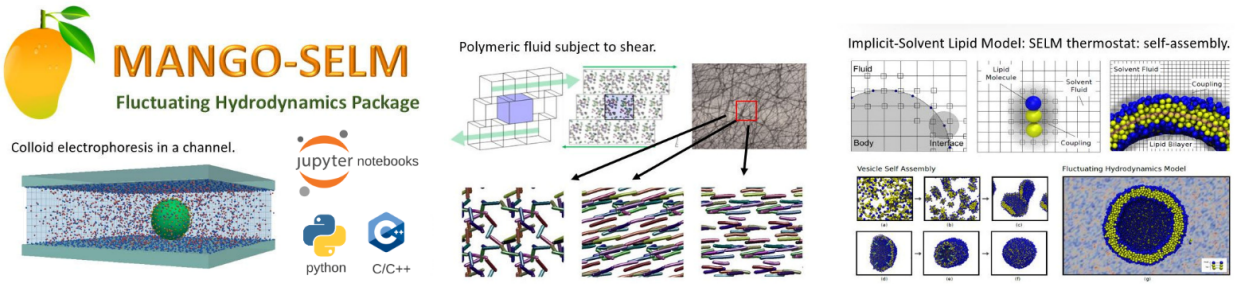
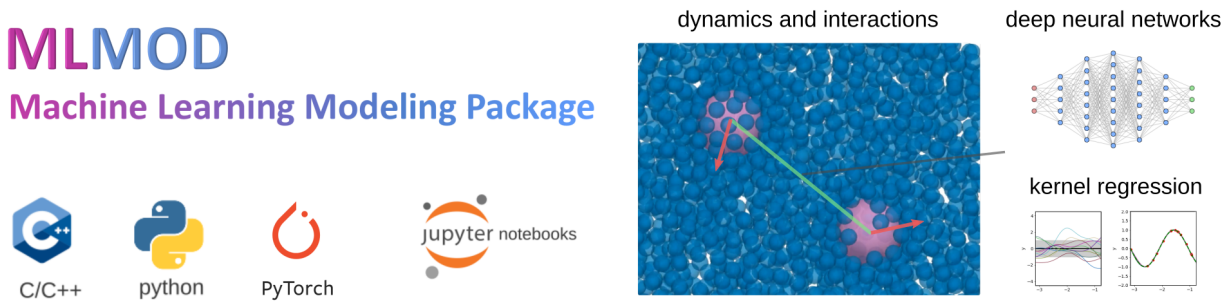


Figure 16: The USER-SELM package provides fluctuating hydrodynamics capabilities for the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) for simulating fluid-structure interactions subject to thermal fluctuations based on stochastic continuum fields (stochastic partial differential equations). Python interfaces and other new implementations were developed to facilitate easier modeling in LAMMPS and better integration with machine learning approaches.

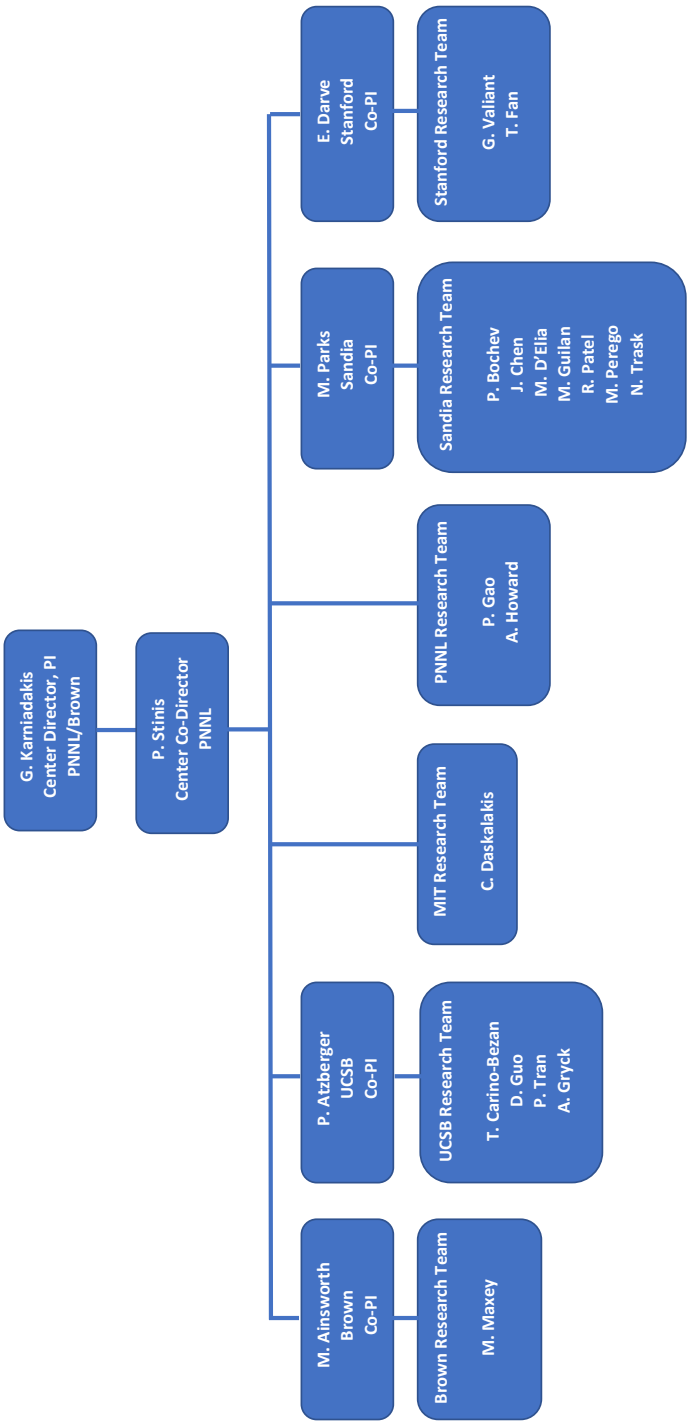
The USER-SELM package provides fluctuating hydrodynamics capabilities for LAMMPS for simulating fluid-structure interactions subject to thermal fluctuations based on stochastic continuum fields (stochastic partial differential equations). The package provides a variety of time-step integrators for different physical regimes for implicit-solvent coarse-grained simulations, stochastic immersed boundary methods, and other stochastic Eulerian Lagrangian methods (SELMs). The C++ back-end of the package was greatly reworked to operate with the LAMMPS shear functionality to facilitate rheological studies of complex fluids and soft materials, and for better integration with machine learning methods. An interface was developed for using a SELM package from Python and within Jupyter notebooks. This new release was accompanied by new tutorial videos, example scripts, and notebooks, as shown on the webpage `http://mango-selm.org/`. This work was also presented as an extended session as part of the 2021 LAMMPS Workshop: `https://www.lammps.org/workshops/Aug21/`.

A.3.3 LAMMPS MD Package: USER-MLMOD



For machine learning (ML) modeling (MOD) in LAMMPS, we developed a new package called USER-MLMOD to provide ways to deploy ML models in SELM and other simulations. This includes deep neural network representations for microstructure interactions and dynamics, as well as functionality related to our variational autoencoder methods for learning nonlinear dynamics. This package allows our learned models to be used (i) as time-step integrators, (ii) for interactions within LAMMPS, and (ii) to compute quantities of interest. This facilitates the practical use of our learned reduced-order models in application domain simulations. Our package is developed in C++ and interfaces with ML libraries. This work was presented at the 2021 LAMMPS Workshop. For more details, see Atzberger, P. J. MLMOD Package: Machine Learning Methods for Data-Driven Modeling in LAMMPS. *arXiv*. arXiv: `2107.14362 [cs.LG]` (2021).

B Organization Chart



C Work Responsibilities and Timelines

Research Area I: PDE-Based Modeling of Macroscales (Lead: Ainsworth-Brown; co-PIs: Parks, D'Elia, Trask, Bochev-SNL; Karniadakis, Stinis–PNNL; C. Li, Maxey–Brown; Atzberger–UCSB; Darve–Stanford; Daskalakis–MIT)

Year 4: Integrate the advances in RA-III and RA-IV. Develop diverse machine learning frameworks for multiscale and multiphysics problems in exemplar applications, specifically subsurface reactive transport and ice sheets. Combine nonlocal and fractional operators with PINNs and their extensions to discover (stochastic) closures in the exemplar applications. Compare the approximation properties of extensions of scalable PINNs and meshfree, high-order methods for multiphysics problems at the macroscale. Study the ability of Bayesian PINNs to quantify uncertainty in long-term predictions in geophysical applications and validate it using historical data.

Research Area II: Stochastic Modeling of Mesoscales (Lead: Stinis–PNNL; co-PIs: Atzberger–UCSB; Stinis, Howard, Gao–PNNL; Trask, Parks-SNL; Kharazmi, Meng, Maxey–Brown; Darve–Stanford)

Year 4: Integrate the advances in RA-I and RA-IV; synthesize and scale up peptoids to achieve desired properties and functionality at the macroscale. Employ the Mori-Zwanzig–derived mDPD to study nucleation in soft materials and obtain phase diagrams. Evaluate the ability of recurrent neural networks to deal with multiple time scales in realistic soft material applications. In collaboration with RA-I, use fractional operators to represent nonlocal interactions (arising from aggressive coarse-graining) in scaled-up functional materials and other systems.

Research Area III: Bridging Methods to Connect the Scales (Lead: Bochev-SNL; co-PIs: Chen, Trask, D'Elia, Perego, Parks-SNL; Ainsworth, Kharazmi, Meng–Brown; Howard, Gao, Karniadakis–PNNL; Atzberger–UCSB; Daskalakis–MIT; Darve, Valiant–Stanford)

Year 4: Integrate the advances in RA-I, RA-II, and RA-IV. Apply active learning and upscaling to peptoids and direct numerical simulation in combustion and examine accuracy and cost; validation using data from PNNL and SNL, respectively. Apply active learning and domain decomposition to subsurface reactive transport and ice sheets and examine feasibility and scaling up from laboratory scales to field scales. Validation with existing (classical) solvers and partial data available at PNNL and SNL.

Research Area IV: Statistical Learning (Lead: Darve–Stanford; co-PIs: Valiant–Stanford; Daskalakis–MIT; Karniadakis, Stinis–PNNL; Parks, Trask, Bochev–SNL; Atzberger–UCSB; Ainsworth, Kharazmi, Meng–Brown)

Year 4: Develop the next generation of PINNs and DeepONets for continuum- and molecular-based physical systems, including multiscale and multiphysics NN frameworks. Systematically study the findings of RA-I–III and incorporate lessons learned into the new deep learning architectures and the stochastic gradient descent (SGD) and DNN algorithms. Develop and finalize information-theoretic approaches for designing *a priori* PhILMs with a specific number of layers and neurons and document accuracy bounds. Provide practical guidelines on learnability and generalization in DNNs.

D Abbreviations

- AD: automatic differentiation
- ADE: advection-dispersion equation
- AISTATS: International Conference on Artificial Intelligence and Statistics
- BGK: Bhatnagar-Gross-Krook
- BOS: background oriented Schlieren
- CFGD: Caputo fractional gradient descent
- CG: coarse-grained
- cPINN: conservative PINN
- cvPINN: control volume PINN
- DDEC: data-driven exterior calculus
- DNN: deep neural network
- DOE: Department of Energy
- DPD: dissipative particle dynamics
- FL: fractional Laplacian
- GAN: generative adversarial network
- GD: gradient descent
- GENERIC: General Equation for Non-Equilibrium Reversible-Irreversible Coupling
- GFINN: GENERIC formalism informed neural networks
- GMLS: generalized moving least squares
- GPU: graphics processing unit
- KNN: Kronecker neural network
- LAMMPS: Large-scale Atomic/Molecular Massively Parallel Simulator
- LANL: Los Alamos National Laboratory
- MD: molecular dynamics
- MFNN: multifidelity neural network
- MIT: Massachusetts Institute of Technology
- ML: machine learning
- MPI: Message Passing Interface
- NKN: nonlocal kernel network
- NN: neural network
- nPINN: nonlocal PINN
- NSF: National Science Foundation

- ODE: ordinary differential equation
- PDE: partial differential equation
- PhILMs: Physics-Informed Learning Machines for Multiscale and Multiphysics Problems
- PhysGNN: physics generative neural network
- PI: principal investigator
- PI-GAN: physics-informed generative adversarial network:
- PINN: physics-informed neural network
- PNNL: Pacific Northwest National Laboratory
- POU: partition of unity
- RA: Research Area
- SciML: Scientific Machine Learning
- SDE: stochastic differential equations
- SELM: stochastic Eulerian Lagrangian method
- SIAM: Society for Industrial and Applied Mathematics
- UCSB: University of California, Santa Barbara
- VAE: variational autoencoder
- VP: velocity-pressure
- VV: vorticity-velocity
- XPINN: extended PINN

Pacific Northwest National Laboratory

902 Battelle Boulevard
P.O. Box 999
Richland, WA 99354
1-888-375-PNNL (7665)

www.pnnl.gov