Second Workshop on Physics Enhancing Machine Learning in Applied Mechanics

20 November 2023
Institute of Physics, London, UK and Online

Programme and Abstract Book

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DATA-CENTRIC ENGINEERING ROLLS ROYCE SIEMENS IOP Institute of Physics

Welcome to the second Workshop on Physics Enhancing Machine Learning in Applied Mechanics!

The ambition of the Institute of Physics Applied Mechanics group is to widening participation and facilitate exchange of knowledge in applied mechanics: from experiments to models and including approaches that combine physics-knowledge with machine learning strategies. This 1-day workshop is part of the activities organised by the Institute of Physics Applied Mechanics group and this year is co-sponsored by the journal Data-Centric Engineering, Siemens, and Rolls-Royce. Thanks to the support of the Institute of Physics (IOP), to the sponsors and to the outstanding invited speakers (who agreed to contribute to the workshop without a refund for travel expenses), this workshop is organised with a free registration for in-person attendance of sixty people and unlimited online participation. Moreover, thanks to the generosity of Data-Centric Engineering (DCE), five DCE travel grants were awarded to early career researchers to facilitate their in-person participation.

The workshop features two outstanding keynote speakers who are driving the development of methods for enhancing machine learning in applied mechanics by embedding physics-knowledge. Moreover, this edition of the workshop features two speakers from industry and one from the UK's national institute for data science and artificial intelligence, providing invaluable inputs to current and future challenges on the application of physics-enhanced machine learning techniques. These speakers are at various stages of their career and cover a broad range of applications. I am beyond thankful to Eleni, Youngsoo, Shiva, Onur and Zack for accepting the invitation to contribute. Undoubtedly, they helped in attracting the overwhelming number of high-quality contributions for Session II of this workshop. I am extremely happy to report that this session consists of five early career researchers and one early career academic!

It would have been impossible to organise this workshop without the excellent management skills of Claire Garland (IOP). Claire is without any doubt the most fantastic event manager with whom I have ever worked. Thank you, Claire! I would also like to personally thank: Andrew Hyde (from Data-Centric Engineering) for his immediate enthusiastic reaction in sponsoring again this event, and Onur Atak (from Siemens) and Adrian Jones and Soph Patsias (from Rolls-Royce) for their precious help in setting up these new sponsorships.

As of today, we know that sixty people will participate in-person and 191 will join the event online. These numbers are well-above the target we initially set. On behalf of the IOP Applied Mechanics group, I would like to thank each person that has registered to the workshop and will join the exciting discussions in this rapidly evolving field where physics-knowledge is more than ever extremely important!

Dr Alice Cicirello
Chair of the workshop and co-opted member of the Institute of Physics Applied Mechanics group
17/11/2023

Programme

09:00 Registration and coffee

09:30 Welcome on behalf of the IOP Applied Mechanics group and structure of the day
Dr Alice Cicirello (University of Cambridge, UK)

09:40 A brief introduction to Physics Enhancing Machine Learning in solid mechanics
Dr Alice Cicirello (University of Cambridge, UK)

SESSION I

10:00 Keynote 1: Physics Enhanced Machine Learning for dynamics: at the nexus of data and models
Professor Eleni Chatzi (ETH, Switzerland)

11:00 Coffee Break

11:30 Keynote 2 (remote): Physics-guided interpretable data-driven simulations
Dr Youngsoo Choi (Lawrence Livermore National Laboratory, USA)

12:30 Lunch Break

SESSION II – CONTRIBUTED TALKS

13:30 Differentiable programming for mesh-free fluid control
Roussel Desmond Nzoyem (University of Bristol, UK)

13:50 A frame-invariant physically recurrent neural network for microscale analysis of rate and path-dependent heterogeneous materials
Ms. Marina Maia, F P Van der Meer and I B C M Rocha (TU Delft, The Netherlands)

14:10 A frame-invariant physically recurrent neural network for microscale analysis of rate and path-dependent heterogeneous materials
Mr Andreas Ioakim[1]**,** Szymon Gres[2], Michael Döhler[3], Luke J. Prendergast[1], and Eleni Chatzi[2]
([1]University of Nottingham, UK [2]ETH Zürich, Switzerland, [3] Univ. Gustave Eiffel, France)

14:30 Coffee Break

15:00 Normalising Flows and Nonlinear Normal Modes
Lawrence Bull[1], Nikolaos Dervilis[2], Tina Dardeno[2], and Keith Worden[2] ([1]University of Cambridge, UK, [2]University of Sheffield, UK)

15:20 Gaussian Process Port-Hamiltonian Systems
Thomas Beckers (Vanderbilt University, USA**)**

15:40 Integrating Physics in Graph Neural Networks for Interaction Modeling
Vinay Sharma, Keivan Faghih Niresi and Olga Fink (EPFL, Switzerland**)**

16:00 Tea Break

SESSION III: TALKS FROM INDUSTRIES AND RESEARCH CENTRES

16:30 Generative AI supporting preliminary engineering design
Babu Shiva (Rolls-Royce, UK)

17:00 An Industrial Perspective to Machine Learning and Physics for Simulation and Digital Twiw
Atak Onur (Siemens, UK**)**

17:30 Physics - informed machine learning: a critique towards robust generalization and interpretability
Zack Xuereb Conti (The Alan Turing Institute, UK)

18:00 **Drinks reception sponsored by DCE, Rolls Royce and Siemens**

Keynote I: Physics Enhanced Machine Learning for dynamics: at the nexus of data and models

Eleni Chatzi (ETH, Switzerland)

Modern engineering structures form complex - often interconnected - assemblies that operate under highly varying loads and adverse environments. To ensure a resource-efficient, safe and resilient operation of such systems, it is imperative to understand their performance as-is; a task which can be effectuated through Structural Health Monitoring (SHM). This talk elaborates on use of monitoring and twinning technologies as a means to recast our engineering approach into one that regards structures and infrastructures as animate cyber-physical systems. We offer a view to fusing data and models via physics-enhanced machine learning schemes for modelling dynamical systems. We discuss the spectrum of such schemes as this unfolds from white to grey to black-box representations, which pose different requirements in terms of availability of physics and data. An optimal balance is sought with the aim to faithfully represent structures across their operational envelop, to reliably predict their performance under future stressors, and to advise on preventive and remedial actions at both the unit and fleet (system) level. We exemplify such a hybrid approach toward establishing closed-loop twin representations on a number of use cases drawing from civil, wind energy and aerospace structures.

Keynote II: Physics-guided interpretable data-driven simulations

Youngsoo Choi (Lawrence Livermore National Laboratory, USA)

A computationally demanding physical simulation often presents a significant impediment to scientific and technological progress. Fortunately, recent advancements in machine learning (ML) and artificial intelligence have given rise to data-driven methods that can expedite these simulations. For instance, a well-trained 2D convolutional deep neural network can provide a 100,000-fold acceleration in solving complex problems like Richtmyer-Meshkov instability. However, conventional black-box ML models lack the integration of fundamental physics principles, such as the conservation of mass, momentum, and energy. Consequently, they often run afoul of critical physical laws, raising concerns among physicists. These models attempt to compensate for the absence of physics information by relying on vast amounts of data. Additionally, they suffer from various drawbacks, including a lack of structure-preservation, computationally intensive training phases, reduced interpretability, and susceptibility to extrapolation issues. To address these shortcomings, we propose an approach that incorporates physics into the data-driven framework. This integration occurs at different stages of the modeling process, including the sampling and model-building phases. A physics-informed greedy sampling procedure minimizes the necessary training data while maintaining target accuracy. A physics-guided data-driven model not only preserves the underlying physical structure more effectively but also demonstrates greater robustness in extrapolation compared to traditional black-box ML models. We will showcase numerical results in areas such as hydrodynamics, particle transport, plasma physics, pore-collapse, and 3D printing to highlight the efficacy of these data-driven approaches. The advantages of these methods will also become apparent in multi-query decision-making applications, such as design optimization.

Contributed Talks:

Differentiable programming for mesh-free fluid control

Roussel Desmond Nzoyem (University of Bristol, UK)

The field of Optimal Control under Partial Differential Equations (PDE) constraints is rapidly changing under the influence of Deep Learning and the accompanying automatic differentiation libraries. Novel techniques like Physics-Informed Neural Networks (PINNs) and Differentiable Programming (DP) are to be contrasted with established numerical schemes like Direct-Adjoint Looping (DAL). We present a comprehensive comparison of DAL, PINN, and DP using a general-purpose mesh-free differentiable PDE solver based on Radial Basis Functions. Under Laplace and Navier-Stokes equations, we found DP to be extremely effective as it produces the most accurate gradients; thriving even when DAL fails and PINNs struggle. Additionally, we provide a detailed benchmark highlighting the limited conditions under which any of those methods can be efficiently used. Our work provides a guide to Optimal Control practitioners and connects them further to the Deep Learning community.

A frame-invariant physically recurrent neural network for microscale analysis of rate and path-dependent heterogeneous materials

F P van der Meer, **Ms. Marina Maia**, I B C M Rocha (Delft University of Technology, Netherlands)

Machine learning techniques have shown great potential for reducing the computational cost of finite element-based numerical analysis. In multiscale applications, so-called surrogate models are widely used to replace the FE problem at the microscale. By doing so, the main computational bottleneck of the method is alleviated and significant speed-up can be achieved. However, applying these models to materials with history-dependence comes with challenges. Two well-known problems in one of the most popular methods, Recurrent Neural Networks, are their poor extrapolation properties and their data-hungry nature.

The alternative explored here benefits from the physics-based knowledge embedded in traditional constitutive models to address those problems. This work builds on previous developments and extends the Physically Recurrent Neural Network (PRNN) to deal with path and rate-dependent heterogeneous materials in a 3D finite strain framework. For that, a new architecture is conceived. In this setting, polar decomposition is applied to the deformation gradient, and the network is used to learn the mapping between stretch and stress. Finally, the stresses in the global coordinate frame are retrieved based on the principle of material objectivity.

In the network, we encode the homogenized stretch tensor into a set of deformation gradients passed to a set of fictitious material points where the stress is computed using the same material models as in the micromodel. As a result, not only stresses are obtained, but also internal variables that are updated at every load step according to the physics-based assumptions in the microscale constitutive models. Finally, a decoder is applied to obtain a homogenized stress from the local stresses in the material points. For the numerical examples, we consider a composite micromodel with rate dependent plasticity for the matrix and hyperelasticity for the fibers. The extrapolation properties are tested considering loading scenarios unseen during training, including cyclic loading and relaxation.

CMA-ES Optimization in Dynamic Soil-Structure Interaction

Andreas Ioakim[1], Szymon Gres[2], Michael Döhler[3], Luke J. Prendergast[1], and Eleni Chatzi[2] ([1]University of Nottingham, UK [2]ETH Zürich, Switzerland, [3]Univ. Gustave Eiffel, France)

In the context of the workshop, which seeks to explore advanced techniques that merge physics knowledge with machine learning in applied mechanics, this works delves into an application of the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) for uncertainty quantification in dynamic soil-structure interaction (DSSI).

Our focus revolves around the prediction of crucial soil-pile parameters, with a special emphasis on the embedded length of foundation piles, mobilized soil mass, and stiffness. Accurate estimation of these parameters is pivotal for modelling foundation behaviour but is often a challenging task.

The key highlight of our work is the adaptation of the CMA-ES optimization method to tackle uncertainties related to estimation of foundation parameters. Specifically, it encompasses the embedded length, mobilized soil mass, and stiffness of foundation piles, leveraging data from dynamic lateral loading.

This presentation aligns with the workshop's theme by emphasizing the critical role of the CMA-ES method in addressing the limitations and challenges in the integration of physics knowledge with stochastic model updating. We aim to demonstrate the efficacy of the CMA-ES method in predicting the distribution of soil-pile parameters, highlighting its potential for enhanced modelling, forecasting, and understanding the sources of uncertainty within the context of DSSI.

Normalising Flows and Nonlinear Normal Modes

Lawrence Bull[1], Tina Dardeno[2], Nikolaos Dervilis[2], and Keith Worden[2] ([1]University of Cambridge, UK [2]University of Sheffield, UK)

In the context of dynamic decoupling problems, engineering dynamics has long held modal analysis as an exemplar. The method allows the exact decomposition of linear multi-degree-of-freedom (MDOF) systems into single-degree-of-freedom (SDOF) oscillators, thus simplifying the analysis of complex dynamic systems. However, modal analysis is a linear theory; if applied to nonlinear systems, the decoupling property (among others) is lost. We propose an alternative approach for nonlinear systems, utilising a physics-informed autoencoder. The modal transformation embeds measured data from nonlinear systems into a latent space where the log-likelihood of a linear state-space model is maximised. We build the encoder with normalising flows, and estimate the transformation alongside the latent states and parameters of the linear representation (in a combined inference). We incorporate physics by imposing inductive biases on latent space: firstly, using a (generic) state space approximation (Kalman filter) and secondly by constraining the structure of that model to sample SDOF oscillators, reflecting predefined ordinary differential equations, which enable modal analysis.

Gaussian Process Port-Hamiltonian Systems

Thomas Beckers (Vanderbilt University, Nashville, USA)

Data-driven approaches achieve remarkable results for modeling and control of nonlinear electromechanical systems based on collected data. However, these models often neglect basic physical principles which determine the behavior of any real-world system. This omission is unfavorable in two ways: The models are not as data-efficient as they could be by incorporating physical prior knowledge, and the model itself might not be physically correct and hence lack trustworthiness. In this talk, I will present Gaussian Process Port-Hamiltonian systems (GP-PHS) as a physics-constrained, nonparametric Bayesian learning approach. Gaussian processes are a powerful and flexible machine learning tool that has gained significant attention in recent years. GPs provide a probabilistic framework for modeling complex functions based on noisy observations, enabling not only predictions but also uncertainty quantification.

GP-PHS have many favorable properties that make them highly interesting for modeling and control of electromechanical systems. In contrast to many physics-informed techniques that impose physics by penalty, the proposed data-driven model is physically correct by design. The Bayesian nature of GP-PHS uses collected data to form a distribution over all possible Port-Hamiltonian systems instead of a single-point estimate. Due to the underlying physics model, sampling from a GP-PHS model generates passive dynamics with respect to designated inputs and outputs. As the proposed approach preserves the compositional nature of Port-Hamiltonian systems and allows us to quantify the uncertainty of the model, robust energy-shaping control methods are exploited to achieve safe control of electromechanical systems with partially unknown dynamics.

Integrating Physics in Graph Neural Networks for Interaction Modeling

Keivan Faghih Niresi, **Vinay Sharma**, and Olga Fink (EPFL, Switzerland)

Graph Neural Networks (GNNs) have recently shown efficacy in capturing interactions within complex systems. However, purely data-driven GNNs require extensive data and may struggle with unfamiliar configurations. Introducing physics into GNNs improves learning with less data, reduces long-term prediction errors in case of trajectory rollout generation, and enhances adaptability to novel configurations.

In this study, we present two effective approaches for integrating physics into GNNs. The first approach enriches the input dimension of the graph with information extracted from underlying physics equations, while the second approach embeds physical inductive bias into the GNNs' message-passing scheme, specifically tailoring it for dynamic predictions.

In the first approach focused on district heating networks (DHNs), we demonstrate the beneficial role of physics in compensating for limited input data. Here, we apply physics-enhanced GNNs to estimate soft sensors i.e., pressures and temperatures solely based on mass flow rate (physical sensors). By incorporating fluid flow equations, losses in essential water state variables (temperature and pressure) are calculated and added as nodes in the DHN graph, enriching the input space. Primarily focused on enhancing the input space, this approach maintains versatility, allowing either spectral or spatial graph convolutional layers without any constraints.

The second approach, applied to spring-mass systems, incorporates a physics-informed message-passing scheme into the GNN architecture. This inclusion aims to address the challenges encountered by purely data-driven GNNs concerning error accumulation during trajectory rollouts and generalization to configurations not seen before. By conceptualizing the message-passing scheme as forward-time stepping and treating scalar and vector features distinctly, we achieve enhanced generalization and stable error accumulation over extended trajectory rollouts. Collectively, our studies underscore the importance of integrating physics in GNNs to enhance accuracy and interpretability, establishing the effectiveness of physics-informed GNNs for soft sensor modeling and complex interaction learning.

Talks from Industries and Research Centres:

Generative AI supporting preliminary engineering design

Babu Shiva (Rolls Royce, UK)

Many engineering solutions require technologies that rely on specialised know-how and knowledge of physics mechanisms underpinning their design and operation. As the world moves towards a digital era, current surrogate model approaches are either not fit for processing large databases, or unsuitable to deal directly with data typically deriving from computer-based analyses such as geometry representations and field quantities (e.g., stress, displacements, temperature, etc.). At the same time there is a need for enhanced design space exploration capabilities overcoming the limitations from parametric models, enabling the assessment of innovative design concepts through more free-form geometry modelling approaches. Conditional Generative Adversarial Networks are amongst the AI tools emerging for engineering design applications. This presentation provides an overview of the work conducted by Rolls-Royce and academic partners for the adoption of recent advances in deep learning to engineering applications by introducing a physics enhanced observational bias to the input dataset to train machine learning models, offering a semi-instant alternative to costly design simulations otherwise required for the assessment of possible design candidates.

An Industrial Perspective to Machine Learning and Physics for Simulation and Digital Twin

Atak Onur (Siemens, UK)

AI and Machine Learning is transforming our world at an incredibly rapid phase. These innovative trends are steadily gaining momentum and also significantly influencing our engineering fields. While such techniques truly unlock new frontiers in the engineering field, their pure data-driven nature should be carefully treated. This aspect needs special attention as we move forward and correct positioning of ML methods and their variants are key in this sense.

With a focus on an industrial perspective, this presentation will explore the application of Machine Learning methods in the context of Simulation and Digital Twin. It will emphasize the crucial integration of physics into these models, while referencing an overview of acceleration and Reduced Order Modelling (ROM) techniques. It will also explore different aspects of bringing physics knowledge to the fore, e.g. as part of real world measurement data, as well as part of constraining the ML architectures for efficient learning.

Physics - informed machine learning : a critique towards robust generalization and interpretability

Zack Xuereb Conti (The Alan Turing Institute, UK)

The applied engineering world needs a machine learning that a) can generalize robustly with less dependence on representation in the data, and b) whose model structure holds an acceptable degree of physical interpretation. Often, these criteria are not easily met with in traditional machine learning methods, especially when applied to real-world systems where external factors and unknown phenomena bias the observations.

In response, Physics-informed machine learning is a rapidly emerging topic where centuries of scientific knowledge and understanding are fused with data-driven strategies to model a variety of systems. There already exists a growing body of work on this topic, where different bias strategies are adopted to represent and incorporate knowledge from mechanistic models across a variety of machine learning frameworks. Predominantly, contributions so far focus on reducing the data-cost whereas less focus on preserving physical interpretability of the learned model.

In this phase of emergence, it is crucial to inquire critically and discuss openly the pertinent criteria for modeling real-world systems, with in the current landscape of Physics - informed machine learning. These include model generalization and domain transfer, preservation of structural attributes, and model validation. With this, we seek to propose a research direction where the "Physics" in Physics-informed machine learning, could be leveraged more fundamentally.

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