Third Physics-Enhancing Machine Learning workshop: Mechanics & Materials

27 November 2024
Institute of Physics, London, UK

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DATA-CENTRIC ENGINEERING SIEMENS IOP Institute of Physics

Welcome to the third Workshop on Physics Enhancing Machine Learning: mechanics and materials (27/11/2024)!

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 Digital Industries Software and the IOP Materials and Characterisation Group.

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, we were able to offer a number of travel awards to early career researchers to facilitate their in-person participation.

The workshop features speakers are at various stages of their career and from all around the world, and cover a broad range of applications. Two outstanding keynote speakers, Marta D'Elia and Iuri Rocha, are driving the development of methods for enhancing machine learning in applied mechanics and materials by embedding physics-knowledge. Undoubtedly, they helped in attracting the overwhelming number of high-quality contributions for this workshop.
This edition of the workshop features a session dedicated to real-world applications covering Nuclear, Wind Turbines and Materials Applications. These talks will provide invaluable inputs to current and future challenges on the application of physics-enhanced machine learning techniques. Moreover, 18 Lightning talks will address fundamental approaches, real-world applications and will also describe new benchmarks.

Also this year, the excellent management skills of Claire Garland (IOP) made the difference in organising this workshop. Without any doubts, Claire is the most efficient 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) for their precious help in setting up these new sponsorships.

As of today, we know that sixty people will participate in-person and more than 250 will join the event online. These numbers set a new record for this workshop, whose community is grooving each year. Most importantly, they show the importance of Physics for enhancing Machine Learning, and Machine Learning for enhancing Physics, both in academia and industry. 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
21/11/2024

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Programme

08:30	Registration and Coffee
09:00	Welcome on behalf of the IOP Applied Mechanics Group and structure of the day **Alice Cicirello**, University of Cambridge
09:10	A brief introduction to Physics Enhancing Machine Learning in solid mechanics and materials **Alice Cicirello**, University of Cambridge
	Lightning Talks – Session I
09:30	Separable Physics-Informed Neural Networks for inverse quantification of material properties **Damien Bonnet-Eymard,** KU Leuven
09:37	Discovering Partially Known Ordinary Differential Equations: a Case Study on the Cellulose Degradation **Kateryna Morozovska,** KTH Royal Institute of Technology
09:44	A robust multi-level data-driven Bayesian approach for stochastic model identification of complex nonlinear systems **Michael McGurk,** University of Strathclyde
09:51	A study of maximum spreading ratio at zero impact velocity of mixed oils with Bayesian Optimisation **Qianrong Liu**, University of Birmingham
09:58	Scour Depth Monitoring of Pile Foundations with a Data-Driven Model Updating Framework **Andreas Ioakim,** University of Nottingham
10:05	Physics-informed data-driven modelling of the precipitation hardening of 6XXX series Aluminium alloys **Amir Alizadeh**, Brunel University London
10:12	Data Generation and Physics-Informed Strategies for Machine-Learned Force Fields in Molecular Dynamics **Saffron Luxford**, University of Nottingham
10:19	Machine Learning and DFT Integration: Development of Quantum Chemically Accurate Density Functionals with the QM9 Data Set **Ali Kemal Havare**, Toros University
10:26	Physics Enhanced Capsule Robot: Pathway to Advancing Early Disease Diagnosis **Kenneth Afebu,** University of Exeter
10:32	Coffee Break

	Lightning Talks – Session II
11:00	A benchmark for Physics-Enhanced Machine Learning research in SHM **Francesca Marafini,** University of Florence
11:07	A Functional Ontology of Physics-Enhanced Machine Learning **Marcus Haywood-Alexander,** ETH Zurich
11:14	Disentanglement by Backpropagation with Physics-Informed Variational Autoencoder **Ioannis Koune,** Technical University of Delft
11:21	Heteroscedastic change-point Gaussian processes **Matthew Jones**, University of Sheffield
11:28	Modelling a Nonlinear Oscillator from Experimental Data using Lagrangian Neural Networks **Alan Xavier**, Imperial College London
11:35	Physics-Informed Holomorphic Neural Networks (PIHNNs) with applications to linear elasticity **Matteo Calafà**, Aarhus University
11:42	Pre-trained physics-informed deep learning-based reduced order models for nonlinear parametrized PDEs **Andrea Manzoni**, Politecnico Di Milano
11:49	Physics-Informed Machine Learning for the Bearing Monitoring of a long Highway Viaduct with Displacement Transducers **Enrico Cianci**, Politecnico di Torino
11:56	Virtual sensing and impact force estimation on an operating ferry quay via Gaussian process latent force model **Luigi Sibille**, NTNU
12:03	Efficient Wind Farm Monitoring with Multi-Task Learning **Simon Brealy**, University of Sheffield
12:07	Lunch
13:00	Keynote I: Hybrid surrogate modeling for multiscale simulations with Physically Recurrent Neural Networks **Iuri Rocha**, TU Delft
	Session: Real-world applications of PEML
13:45	Machine learning in action: case studies across nuclear applications **Caroline Shenton-Taylor**, University of Surrey
14:05	The Language of Hyperelastic Materials **Georgios Kissas**, ETHZ
14:25	Gaussian Processes for input-modeling in virtual sensing of wind turbine blades **Silvia Vettori**, Siemens
14:45	Tea break
15:15	Keynote II: On the use of Graph and Point networks in scientific applications (ONLINE) **Marta D'Elia**, ICME, Stanford

16:00	**Interactive session about challenges, opportunities, future trends** **(For in-person attendees only)**
17:00	Drinks and Pizza
18:30	Depart

A brief introduction to Physics Enhancing Machine Learning in solid mechanics and materials

Alice Cicirello[1]
[1]University of Cambridge, UK

Physics-Enhanced Machine Learning (PEML), also known as Scientific Machine Learning, is a natural evolution of Machine Learning (ML) for guiding high-consequence decision making in engineering applications by developing hybrid physics-data models and tackling ML issues such (i) poor generalization performance and physically inconsistent/implausible predictions; (ii) inability of accounting for and quantifying the different sources/types of uncertainties; (iii) inability of providing explainable and interpretable inferences. PEML strategies are critical for (i) informing the physics describing the underlying dynamical system to be able to analyze, control and predict the wide range of behaviours of the real-world system; (ii) providing fast and accurate solutions of hybrid physics-data models, including governing equations, reduced order models, prediction, forecasting and simulation models. During this lecture, PEML will be introduced and three broad groups of PEML approaches will be discussed: physics-guided, physics-encoded and physics-informed. More info can be found here: https://arxiv.org/abs/2405.05987

Lightning talks - Session I

Separable Physics-Informed Neural Networks for inverse quantification of material properties

Damien Bonnet-Eymard[1]
[1]KU Leuven, Belgium

In the past decade, advancements in full-field measurement techniques like digital image correlation (DIC) have fundamentally transformed material testing. This progress opens the way to material testing 2.0, an era where experiments are tailored to extract the most information from materials. Traditional inverse quantification methods, such as the Virtual Fields Method (VFM) and Finite Element Method Updating (FEMU), have been used to derive material properties from full-field data. However, these techniques can struggle with complex material behaviors or geometries.

Recently, Physics-Informed Neural Networks (PINNs) have emerged as a promising alternative, especially suited for reconstructing hidden information. Despite their potential, PINNs can be slow to converge and computationally demanding, limiting their practical application. To overcome these hurdles, a new architecture called Separable Physics-Informed Neural Networks (SPINNs) has recently been introduced.

In this study, we demonstrate how Separable Physics-Informed Neural Networks (SPINNs) can be applied to recover elasticity properties from simulated Digital Image Correlation (DIC) data. These measurements are generated using either analytical solutions or finite element models, and possibly corrupted with noise. We compare the performance of SPINNs to other existing inverse quantification techniques. The accompanying figure shows a side-loaded plate example, where SPINN is used to perform both field reconstruction (displacement and stress) and inverse quantification of the elasticity parameters simultaneously.

Discovering Partially Known Ordinary Differential Equations: a Case Study on the Cellulose Degradation

Federica Bragone[1], Kateryna Morozovska[1], Tor Laneryd[2], Khemraj Shukla[3], and Stefano Markidis[1]
[1]KTH Royal Institute of Technology, Stockholm, Sweden, [2]Hitachi Energy, Sweden, [3]Brown University, USA

The degree of polymerization (DP) is one of the methods for estimating the aging of polymer-based insulation systems, such as cellulose insulation in power components. The main degradation mechanisms in polymers are hydrolysis, pyrolysis, and oxidation. These mechanisms combined cause a reduction of the DP. However, data availability for these types of problems is usually scarce. This study analyzes insulation aging using cellulose degradation data from power transformers, modeled with ordinary differential equations (ODEs), in this case, Ekenstam ODE. A modification of the Ekenstam ODE is given by Emsley's system of ODEs, where the rate constant expressed by the Arrhenius equation decreases in time with the new formulation. We recover the governing equations of the degradation system using Physics-Informed Neural Networks (PINNs) and symbolic regression. We propose some techniques to help discover the equations that model the DP degradation. PINNs can help find better parameters and functions given observed field data. Using synthetic data and DP measurements, they can infer unknown parameters like the activation energy and the pre-exponential factor of the Arrhenius equation in the Ekenstam kinetic model.

Moreover, we can also employ a combination of PINNs with symbolic regression to discover an unknown function of a system of equations. We assume the form of the ODE describing the DP degradation and the rate constant at which the initial reaction rate deteriorates in Emsley's system of ODEs to be unknown. We employ PINNs with an extra network to approximate the values of the unknown function while estimating the unknown parameter. Finally, we rediscover the unknown function using symbolic regression.

The resulting model allows for discovering unknown parameters from the limited data set. For the discovery of the function, the results lead to other equation forms that would require additional experimental tests and field data collection to validate.

A robust multi-level data-driven Bayesian approach for stochastic model identification of complex nonlinear systems

Michael McGurk[1], and Jie Yuan[2]
[1]University of Strathclyde, UK [2]University of Southampton, UK

This work presents a robust, multi-level data-driven Bayesian framework designed to significantly enhance the computational efficiency of stochastic model identification for complex nonlinear systems, particularly in scenarios where experimental data is limited. Traditional Bayesian model identification typically relies on building a single, highly accurate data-driven model; however, this approach is often computationally prohibitive for complex systems. In response, we introduce a multi-fidelity data-driven model structure refined iteratively via a multi-level Bayesian approach, which dramatically reduces the sampling demands associated with high-fidelity, nonlinear simulations.

Key to this framework is the incorporation of physics-enhanced machine learning techniques. Specifically, the framework integrates epistemic uncertainties from the multi-fidelity data-driven models directly into the multi-level Bayesian model, an innovative step that enhances the robustness and predictive power of probabilistic response assessments. By factoring in these uncertainties, the framework supports an uncertainty-informed model identification process that adapts dynamically to data limitations while maintaining high accuracy. This is particularly valuable for high-stakes applications in which accurate probabilistic modeling is required but data acquisition is costly or constrained.

To validate the framework, a nonlinear aerofoil aeroelastic test case incorporating limit-cycle oscillation (LCO) experimental data from two configurations is employed. The attached figure shows the probabilistic bifurcation diagram that was produced with the resulting model predictions in the second configuration. Results show that this multi-level, data-driven Bayesian approach achieves a substantial 76% reduction in the number of high-fidelity simulation runs required, while delivering parameter estimations with only a 2% deviation from the traditional single-level Bayesian approach. This improvement underscores the efficacy of the physics-informed, multi-fidelity Bayesian framework in providing efficient, accurate, and robust model identification for complex nonlinear systems, setting a new standard for data-driven uncertainty quantification in computationally intensive applications.

A study of maximum spreading ratio at zero impact velocity of mixed oils with Bayesian Optimisation

Qianrong Liu[1,2], Chao Jiang[2], Tugce Caykara[1], Miqing Li[2], and Zhenyu Zhang[1]
[1]School of Chemical Engineering, University of Birmingham, UK, [2]School of Computer Science, University of Birmingham, UK

Drop impact is a common and important phenomenon in both industrial and healthcare settings. It has been shown that dynamic wetting plays an important role in the spreading at low velocity. The maximum spreading ratio at zero impact velocity (beta zero) of different droplets depends on the balance between kinetic energy, capillary energy, and viscous dissipation. However, designing formulations requires great deal of resources, time, and cost to find maximum beta zero. Thus, a machine learning algorithm such as Bayesian Optimisation (BO) would be extremely valuable, which could predict the next most likely formulation conditions for optimal performance. In the present work, BO was introduced to investigate the maximum spreading ratio of formulations such as mixed oils to improve the performance while being cost effective. A lab-on-a-chip setup was utilised to mix different ratios of jojoba oil and castor oil to obtain the beta zero. The adjustment and control of the mixing ratio was set by the BO algorithm and Elveflow pressure controller by using five initial jojoba oil /castor oil ratios of 0.59, 0.50, 0.44, 0.40, and 0.33. The results showed that the predicted ratio, 0.61, resulted in highest value within all ratios studied by two runs. We evidence that BO algorithm offers a great potential to efficiently predict the optimal ratio of mixed oils in order to obtain maximum spreading ratio at zero impact velocity.

Scour Depth Monitoring of Pile Foundations with a Data-Driven Model Updating Framework

Andreas Ioakim[1], Szymon Greś[2], and Luke Prendergast[1]
[1]University of Nottingham, UK, [2]Aalborg University, Denmark

This work introduces a data-driven model updating framework for scour monitoring in laterally loaded piles, specifically designed to minimize discrepancies between numerical models and real pile foundations while addressing data biases. The framework integrates both scour depth and soil mass and stiffness profile estimation, leveraging output-only data to accurately estimate critical operational parameters essential for robust structural health monitoring (SHM) and reliable performance assessment of pile foundations. By combining modal parameter estimations with a stochastic optimization approach, the model iteratively refines model parameters, enhancing generalization across diverse real-world conditions. Validated through an experimental case, this framework demonstrates a robust approach to scour monitoring, underscoring its potential to advance physics-enhanced machine learning-based SHM techniques in geotechnical engineering.

Physics-informed data-driven modelling of the precipitation hardening of 6XXX series Aluminum alloys

Amir Alizadeh[1], and Hamid Assadi[1]
[1]Brunel University London, UK

A Multiphysics system that contains numerous unknown variables with intertwined interrelationships bring new challenges to conventional frameworks for modelling digital twins. The ill-defined dynamics between these variables necessitate using data-driven methods such as the neural networks [1]. However, purely data-driven methods require extensive training data and lack physical interpretability for the end user. On the other hand, purely physics-based models of such engineering systems result in an extremely complicated model with lots of fitting parameters [2], [3], thus difficult model calibration. Taking the physics-based model of the precipitation hardening of 6XXX aluminum, called the Kampmann-Wagner Numerical (KWN) [4], a novel architectural variant of physics-informed neural networks (PINN), [5] combines theoretical physics-based constraints and experimental data to calibrate multiple fitting parameters. This variant removes the need for training a large number of neural network's weights, provides a better physical interpretability of the predictions, and automatically learns the physical free parameters.

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Data Generation and Physics-Informed Strategies for Machine-Learned Force Fields in Molecular Dynamics

Saffron Luxford[1]
[1]University of Nottingham, UK

Machine-learned force fields (MLFFs) are advancing molecular dynamics simulations by offering greater accuracy and adaptability compared to traditional force fields. However, the effectiveness of MLFFs depends on the quality and scale of the datasets used for training [1], with significant challenges in data curation, scalability, and computational costs. Overcoming these challenges is crucial for advancing molecular dynamic simulations, with significant implications for high-temperature superconductors, ferroelectrics, and energy technologies. This talk explores the theoretical underpinnings and challenges in the generation of datasets for MLFFs, with a focus on the need for accurate, diverse, and computationally feasible data that capture critical structural and dynamic features, and the integration of physics-informed methods with MLFFs [2] to enhance dataset robustness. These methods can improve generalisation and accuracy in simulations of complex materials, paving the way for practical applications in superconductor design and broader material innovations.

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Machine Learning and DFT Integration: Development of Quantum Chemically Accurate Density Functionals with the QM9 Data Set

Ali Kemal Havare[1], Evrim Ersin Kangal[2], and Merve Ozcan[2]
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[2]Erdemli School of Applied Technology and Management, Computer Technology and Information Systems, Mersin University, Turkey

Density Functional Theory (DFT) is a theoretical computational method widely used to understand the quantum mechanical properties of atoms and molecules. When combined with machine learning, DFT enables improved and faster analyses, especially in the fields of materials science and chemistry. Integrating DFT with machine learning is an effective approach to enhance model accuracy and ensure physical consistency. By reproducing DFT energies for a variety of molecular geometries, machine learning can be employed to achieve improved accuracy, allowing for the construction of quantum chemically accurate density functionals.

The QM9 dataset contains a variety of chemical and physical properties of organic molecules, generated through hybrid DFT calculations. The dataset includes properties such as molecular energy, dipole moment, polarizability, and HOMO/LUMO energy levels, and is frequently used to train and test machine learning algorithms. The QM9 database, comprising 134,000 small molecules, is widely used in machine learning research, particularly in materials and molecular design. This dataset is especially valuable for predicting molecular structures and properties in materials science using hybrid DFT.

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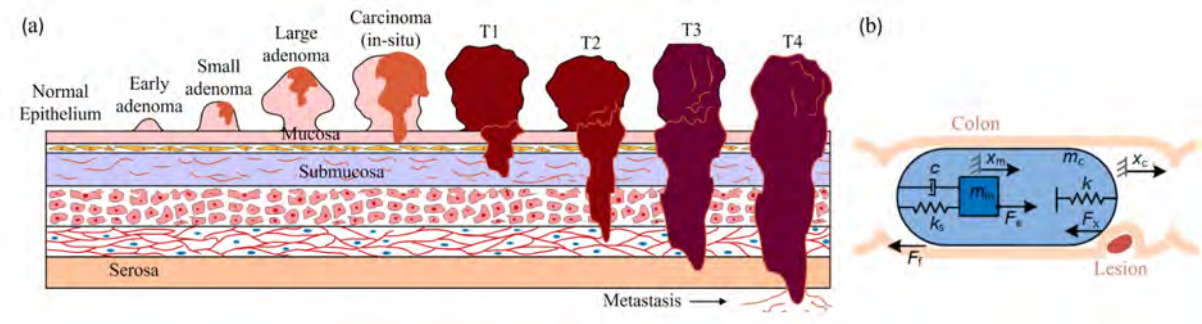
Physics Enhanced Capsule Robot: Pathway to Advancing Early Disease Diagnosis

Kenneth Afebu[1], Evangelos Papatheou[1], Yang Liu[1], Shyam Prasad[2]
[1]University of Exeter, UK, [2]Royal Devon University Healthcare NHS Foundation Trust, UK

Recent progress in microelectronics, soft and smart materials, and micro-fabrication technologies has led to increased research and development of small-scale robots (at millimetre and micrometre scales) for biomedical applications, especially early disease diagnosis.

With early diagnosis being crucial to timely intervention and treatment outcomes, efforts are constantly aimed at developing sophisticated small-scale robots that can aid early disease diagnosis and improve patients' survival. With majority of these robots relying on visual examination, results are often impaired by the intuition and experience of the clinician. For diseases like bowel cancer, this often results in high-miss rate of precancerous polyps which are difficult-to-visualise. As an alternative, current studies explores the use of the dynamical responses of the robot for sensing its surrounding tissues rather than the visual feedbacks. This innovative approach aims to aid early diagnosis of sometimes hard-to-visualise disease like bowel cancer, which often set off with biomechanical changes of infected tissues (Fig. 1a).

To demonstrate this, dynamic signals from a vibration-assisted robotic capsule travelling and encountering lesions in the bowel (Fig. 1b) was investigated. With no established hypothetical relationship for mapping capsule dynamics to tissue biomechanics, a data-driven approach involving two-stage machine learning (ML) was adopted. Firstly, supervised regression models were trained to predict tissue stiffnesses from the capsule's dynamical signals. Secondly, unsupervised classification was performed on the predicted stiffnesses using K-means clustering. This way, precancerous tissues were well separated from their benign counterparts, achieving > 97 % accuracy for both simulation and experiment. However, these results were, characterised with wide and sporadically varying confidence intervals, indicating a high degree of uncertainty in the models' predictions.
As future works, we are proposing to incorporate the physics governing the motion and interaction of the capsule in the bowel into the models (i.e., physics-enhanced) to improve their reliability and precision.



(a) Schematic depiction of adenoma-carcinoma progression sequence and subsequent primary tumour stages and (b) the vibration assisted robotic capsule traverses the bowel and encounters a lesion. The capsule consists of a permanent magnet mm excited by an external sinusoidal magnetic force F_e interacting with the main body of the capsule via a connecting spring k_s, a damper c, and an impact spring k

Lightning talks - Session II

A benchmark for Physics-Enhanced Machine Learning research in SHM

Francesca Marafini[1], Giacomo Zini[1], Alberto Barontini[1], Nuno Mendes[2], Alice Cicirello[3], Michele Betti[1], and Gianni Bartoli[1]
[1]University of Florence, Italy, [2]Universidade do Minho, Portugal, [3]University of Cambridge, UK

This work presents a synthetic Structural Health Monitoring (SHM) benchmark dataset that simulates structural response under environmental and operational variabilities, sensor faults, and both fast- and slow-varying damage. Developed as a comprehensive resource, it includes acceleration and displacement measurements generated using parallel computing on a fixed-fixed steel beam. While for the dynamic response the beam is modelled as a Single Degree of Freedom (SDOF), the static data generation is carried out according to the Euler-Bernoulli theory. The conditions replicated are chosen to be as realistic as possible, including dynamic and static loads and temperature-dependent stiffness variations. The benchmark provides controlled conditions for validating and testing data-driven SHM methods.

The dataset is well-suited for Physics-Enhanced Machine Learning (PEML) research because it offers a structured, realistic environment to test models that integrate physics principles with machine learning. PEML models could incorporate physical constraints related to the temperature-dependent material properties, such as expected frequency shifts due to temperature variations, or to load-dependent deflections due to the operational load variability. These physical principles help PEML models distinguish between environmental or operational variability and true damage-related signals in SHM applications. Each effect can be simulated separately or overlapped, providing a controlled testing ground for PEML methods to evaluate the reliability and interpretability of damage identification results, considering each variability singularly detangled and jointly with the rest. Additionally, by including both fast- and slow-varying damage scenarios alongside sensor malfunction data, the dataset supports the development of models that can accurately differentiate true structural degradation from sensor anomalies. This setup also allows PEML models to quantify uncertainties in their predictions, enhancing the explainability and robustness of damage detection and characterisation within SHM datasets.

A Functional Ontology of Physics-Enhanced Machine Learning

Marcus Haywood-Alexander[1], and Eleni Chatzi[1]
[1]ETH Zurich, Zürich, Switzerland

Physics-enhanced machine learning aims to improve the capability and reduce the shortcomings of data- or physics-only methods. Naturally, there exist many different motivations and schemes within the broad-scoping genre of PEML, and, recently, classification of such schemes has matured beyond the description of a one-dimensional spectrum, to a two-dimensional spectrum of physics and data [1, 2], or even a three-dimensional representation accounting for the involved model/algorithmic complexity [3]. These spectra can provide a high-level classification of PEML schemes, however, often more low-level details are required to make the most appropriate selection. Beyond simply physics and data, selection includes consideration of characteristics such as; data domain, downstream task, prior knowledge, as well as their interdependent relationships. Ontologies provide a schematic approach to objectively defining an intricate system of concepts, and by including interdependencies between objects, objective reasoning can be delivered. This talk delivers an ontological framework designed to provide a structured and comprehensive description of PEML methodologies. The proposed ontology leverages principles from both the machine learning and physics domains to support decision-making processes by offering insights into the compatibility of various machine learning techniques with specific physical phenomena, allowing researchers to select the most appropriate schemes for specific datasets, available prior knowledge, and the overarching objectives.

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Disentanglement by Backpropagation with Physics-Informed Variational Autoencoder

Ioannis Koune[1], and Alice Cicirello[2]
[1]Delft University of Technology, Delft, Netherlands, [2]University of Cambridge, UK

The existence of unobserved damage and the variability in environmental and operational conditions can have a significant influence on the measured response of a structure, posing a challenge for data-driven machine learning techniques aimed at system identification, damage detection and structural response prediction. Furthermore these techniques might suffer from poor generalization to previously unseen conditions, particularly when limited noisy data is available. On the other hand, accounting explicitly for these influences in physics-based models is often infeasible due to lack of domain knowledge or due to cost and time constraints. We introduce a physics-informed variational autoencoder architecture for disentangled representation learning with the aim of computing the posterior distribution over uncertain latent variables of a physics-based model of an engineering structure, and predicting the structural response in the presence of multiple unknown confounding sources in the measurements. To this end the latent space of the autoencoder is augmented with a set of physically meaningful latent variables that allow for domain knowledge in the form of prior distributions to be included, and the decoder is formulated as a combination of a physics-based and a data-driven model. We propose a regularization method, which utilizes observables that can not be directly included in the physics-based model, to constrain the excess flexibility of the data driven components and prevent them from overriding the known physics. This ensures that the physical meaning of the latent variables is preserved, and allows the model to disentangle features of the input signal and separate the known physics from unknown influences.

Heteroscedastic change-point Gaussian processes

Daniel Pitchforth[1], Matthew Jones[1], Samuel Gibson, and Elizabeth Cross
[1]University of Sheffield, UK

Balancing the relative contribution of data and physics within a physics-informed model is an important consideration to make when embedding knowledge into data-driven learners. Often, the type of physics that is included represents basic, fundamental laws, that will not always be valid across all areas in which we want to make predictions. In these scenarios, if the physics component dominates, then there is potential for this prior structure to negatively influence overall model performance. Conversely, in regions where it is known that the prior knowledge sufficiently captures the overall behaviour of interested, then an under utilisation of the physics can limit the advantages of physics-informed models.

This talk will present a methodology for balancing the reliance of physics and data through the development of physics-informed change point kernels. Within a Gaussian process framework, a kernel structure is constructed that allows the contribution of the physics to be adjusted according to how well it characterises the overall process being modelled. It is also demonstrated how change-point kernels can be used within a heteroscedastic setting, where input-dependent noise can be accounted for; a common occurrence in change-point models.

Modelling a Nonlinear Oscillator from Experimental Data using Lagrangian Neural Networks

Alan Xavier[1], and Ludovic Renson[1]
[1]Imperial College London, UK

Accurately modelling the dynamic behaviour of nonlinear structures is challenging due to the wide range of potential nonlinearities and dynamic phenomena that they can exhibit. Physics-guided machine learning (PGML) has emerged as an attractive way to combine prior knowledge with data to solve a wide range of complex, nonlinear problems in science and engineering. Lagrangian Neural Networks (LNNs) are a particular PGML approach that models nonlinear systems' Lagrangian functions using artificial neural networks (NNs). The Euler-Lagrange equation is then reconstructed through automatic differentiation (AD) to derive the equations of motion, enforcing physical consistency during training.

In this work, we use LNNs to model the nonlinear vibrations of mechanical structures. We now explore the applicability of our methodology to a nonlinear oscillator from experimental data. We analyse the physical consistency of the trained model and interpret the identified stiffness and damping nonlinearities from the partial derivatives of the potential energy and dissipation functions.

Physics-Informed Holomorphic Neural Networks (PIHNNs) with applications to linear elasticity

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We introduce Physics-Informed Holomorphic Neural Networks (PIHNNs [1]), an innovative approach for solving boundary value problems characterized by solutions expressible through holomorphic functions. We focus on plane linear elasticity, where the Kolosov-Muskhelishvili representation can be leveraged to develop complex-valued neural networks capable of fulfilling stress and displacement boundary conditions while inherently satisfying the governing equations. The network architecture is carefully designed to ensure that approximations respect the Cauchy-Riemann conditions through specific choices of layers and activation functions. Additionally, we propose a novel weight initialization technique to address the challenge of vanishing or exploding gradients during training. Compared to standard Physics-Informed Neural Networks (PINNs), this inductive bias offers several advantages, including more efficient training — requiring evaluations only on the domain's boundary — lower memory requirements due to a reduced number of training points, and the smoothness of the learned solution.

[1] Calafà, Matteo, et al. "Physics-Informed Holomorphic Neural Networks (PIHNNs): Solving 2D linear elasticity problems." Computer Methods in Applied Mechanics and Engineering 432 (2024): 117406.

Pre-trained physics-informed deep learning-based reduced order models for nonlinear parametrized PDEs

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Among several recently proposed data-driven Reduced Order Models (ROMs), the coupling of Proper Orthogonal Decompositions (POD) and deep learning-based ROMs (DL-ROMs) has proved to be a successful strategy to construct non-intrusive, highly accurate, surrogates for the real time solution of parametric nonlinear time-dependent PDEs. Inexpensive to evaluate, POD-DL-ROMs are also relatively fast to train, thanks to their limited complexity. However, POD-DL-ROMs account for the physical laws governing the problem at hand only through the training data, that are usually obtained through a full order model (FOM) relying on a high-fidelity discretization of the underlying equations. Moreover, the accuracy of POD-DL-ROMs strongly depends on the amount of available data. In this talk we describe a recent, major extension of POD-DL-ROMs by enforcing the fulfillment of the governing physical laws in the training process - that is, by making them physics-informed - to compensate for possible scarce and/or unavailable data and improve the overall reliability. To do that, we first complement POD-DL- ROMs with a trunk net architecture, endowing them with the ability to compute the problem's solution at every point in the spatial domain, and ultimately enabling a seamless computation of the physics-based loss by means of the strong continuous formulation. Then, we introduce an efficient training strategy that limits the notorious computational burden entailed by a physics-informed training phase. In particular, we take advantage of the few available data to develop a low-cost pre-training procedure; then, we fine-tune the architecture in order to further improve the prediction reliability. Accuracy and efficiency of the resulting pre-trained physics-informed DL-ROMs (PTPI-DL-ROMs) are then assessed on a set of test cases ranging from non-affinely parametrized advection-diffusion-reaction equations, to nonlinear problems like the Navier-Stokes equations for fluid flows.

Physics-Informed Machine Learning for the Bearing Monitoring of a long Highway Viaduct with Displacement Transducers

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In the field of Structural Health Monitoring (SHM) for bridges, effective damage detection is often complicated by environmental and operational variability. Factors such as temperature, traffic loads, wind, and dry friction between structural components significantly influence data, making it essential to differentiate normal responses from anomalous behaviour. The aim is thus to create a predictive model that isolates these normal responses, establishing a baseline that highlights only displacements linked to structural anomalies.
The research focuses on developing a static monitoring technique using displacement and temperature sensors to assess the longitudinal movements of a bridge deck. A predictive model is built to detect anomalies, with temperature as the primary independent variable, supplemented by time to capture both daily and seasonal movement cycles. These temperature-related movements are chosen for their major influence on bearing displacements and ease of monitoring, enabling the capture of the non-linear relationship between temperature and displacement.

Machine Learning regression techniques, specifically Gaussian Process Regression and Support Vector Machine Regression, are employed to model the structure's thermal response and accurately predict expected displacements. In addition to these conventional Black-box models, the study introduces a Physics-Informed Machine Learning (PIML) approach, or Grey-box model, which integrates engineering knowledge of the bridge behaviour. This hybrid approach improves both predictive accuracy and interpretability, making it a reliable tool for bridges' maintenance decision-making.

To validate the models, an Early Warning System based on displacement thresholds is implemented. Simulated damage scenarios, such as bearing device failures, assess the models' capabilities in distinguishing anomalous displacements from environmental effects. The comparative analysis shows that Grey-box models outperform Black-box ones in accuracy and robustness, confirming the value of PIML-based modelling for enhanced anomaly detection. This approach supports proactive maintenance and extends the lifespan of critical structures, ensuring higher infrastructure resilience and safety.

Virtual sensing and impact force estimation on an operating ferry quay via Gaussian process latent force model

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Vibrational structural health monitoring has gained widespread popularity in the recent decades, driven by its capacity to provide accurate and valuable information about the structural behavior of operating infrastructures. Despite the critical importance of ferry quays, which offer essential access to healthcare and goods in coastal regions, limited research has been conducted to understand their dynamic response during ferry impacts, which are believed to be a major contributor to structural degradation. This study investigates the application of a Gaussian process latent force model (GPLFM) to simultaneously estimate the structural response and ferry impact force on an operating ferry quay. The physics-enhanced machine learning algorithm combines physical information with a data-driven Gaussian process used to model the acting force. The posterior inference of the input and states is performed by means of a Kalman filter and a Rauch-Tung-Striebel smoother in an augmented state-space model. The GPLFM has demonstrated better accuracy and stability compared to other methodologies in different case studies, including virtual sensing of strain response in offshore wind turbines and friction force estimation on a single-storey frame with a brass-to-steel. In this work, a finite element model (FEM) of the ferry quay is combined with measured data collected from six sensors, comprising four accelerometers and two LVDTs. The virtual sensing approach is validated by comparing acceleration response estimated at a location that is not included in the identification model with data recorded from a fifth accelerometer. The identified force is validated through simulations using the FEM model of the structure. The results indicate that the GPLFM can accurately estimate the joint input-state space even with a limited number of sensors and without prior knowledge about the acting force.

Efficient Wind Farm Monitoring with Multi-Task Learning

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The offshore wind sector is currently going through a rapid expansion globally, with the UK specifically planning to quadruple the current 15GW of capacity by the end of the decade. With this, the total expenditure on operations and maintenance (O&M) will continue to rise, which typically represents around 40% of the lifecycle costs of a 1GW wind farm. Online monitoring of wind farms is commonly employed as part of O&M strategies, using data from instruments fitted throughout the turbines; gaining the maximum possible insight from this data is therefore of interest to help minimise O&M costs, and maximise the economic viability of offshore wind farms.Transfer Learning (TL) is a machine learning technique, which enables sharing of information between machines. Multi-Task Learning (MTL) is one such flavour of TL, whereby a model is trained on all machines simultaneously, to improve predictive inference on each individual machine via shared parameters. A commonly used approach to MTL, is the use of hierarchical Bayesian models, which can pool information across machines though population-level parameters, whilst accounting for machine-specific nuances through machine-level parameters. By pooling information in this way, these models can better handle machines with limited data, and produce robust, probabilistic predictions.

In this work we initially developed a hierarchical Bayesian model, applied to the task of wind turbine power prediction—a commonly modelled parameter for assessing the health of wind turbines. This model, when applied to isolated wind turbines, was found to produce spatial correlations in model parameters across the wind farm. This motivated the incorporation of a “metamodel”, which aimed to learn this spatial correlation in turbine-level parameters through population-level “meta” parameters. Using this adapted model structure, the metamodel can make power predictions using turbine spatial coordinates alone, allowing us to predict the behaviour of previously unobserved turbines. The results show that the model significantly outperforms a range of benchmark models both in terms of model mean prediction and uncertainty. This novel modelling approach could be applied in situations where there are likely to be spatial correlations in a population of structures (such as in wind farms), and where data is difficult or expensive to obtain—including from real physical sensors or physics-based simulations. It could also be used as a justification to reduce the need (and associated costs) for sensors on every turbine, as is done currently in the industry.

Keynote I

Hybrid surrogate modeling for multiscale simulations with Physically Recurrent Neural Networks

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Modeling material behavior across the scales is essential in improving our understanding of how complex materials behave and how they can be better designed. A popular approach for multiscale modeling is FE2 (also known as Computational Homogenization), consisting in nesting lower-scale FEM models at each macroscopic material point and therefore simulating material behavior at two scales concurrently. However, although FE2 is a powerful approach, it is extremely computationally expensive due to the need to solve a very large number of micromodels.

Machine learning-based surrogate models are a popular approach for accelerating FE2. For strain path dependent material behavior, recurrent neural networks such as LSTM or GRU are the current models of choice. However, although RNNs can be fast and accurate surrogates when properly trained, they often need an inordinate amount of data for training and their predictions lack interpretability. Here we present Physically Recurrent Neural Networks (PRNNs), an alternative surrogate modeling approach that directly tackles these two drawbacks. The key idea behind PRNNs is to build a hybrid data-physics model where classical constitutive models are embedded in an encoder-decoder neural network architecture in a completely intact way. By leaving the embedded models untouched, the task to be learned by the network shifts from reproducing complex time-dependent constitutive patterns we can already explain with our decades-old physical models to the much simpler one of combining the response of a number of real constitutive models undergoing different strain histories.

This keynote includes a gentle introduction to PRNNs, a comparison against state-of-the-art RNNs for 2D elastoplastic micromodels, and our latest work on extending PRNNs to 3D anisotropic micromodels under large strains and a combination thermoviscoplasticity and hyperelasticity. We also showcase our PRNNs on a real-life validation case involving reproducing off-axis loading experiments on thermoplastic composite coupons and show how the networks can extrapolate not only to unseen strain paths, temperatures and strain rates but also successfully transfer to different sets of material properties while only seeing a single one during training.

Real-World applications of PEML

Machine learning in action: case studies across nuclear applications

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Machine learning is driving advancements across the nuclear community, encompassing both defence and civil applications. This talk will highlight recent research case studies, including using neural networks in the areas of nuclear security and nuclear decommissioning. Additionally, the talk explores the role of machine learning within radiation detection, including jewellery beads, communication fibres, and compact discs as dosimeters.

Beyond the technical applications, the talk presents an initiative to create a dedicated framework for supporting Artificial Intelligence (AI) across the nuclear industry. Through promoting best practices, this new Nuclear AI centre aims to support the development of AI-driven solutions, researchers working within the field, and guide policy and regulation in a rapidly evolving landscape.

The Language of Hyperelastic Materials

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The automated discovery of constitutive laws forms an emerging research area, that focuses on automatically obtaining symbolic expressions describing the constitutive behavior of solid materials from experimental data. Existing symbolic/sparse regression methods rely on the availability of libraries of material models, which are typically hand-designed by a human expert using known models as reference or deploy generative algorithms with exponential complexity which are only practicable for very simple expressions. In this talk, we present a novel approach to constitutive law discovery relying on formal grammars as an automated and systematic tool to generate constitutive law expressions. Compliance with physics constraints is partly enforced a priori and partly empirically checked a posteriori. We deploy the approach for two tasks: i) Automatically generating a library of valid constitutive laws for hyperelastic isotropic materials; ii) Performing data-driven discovery of hyperelastic material models from displacement data affected by different noise levels. For the task of automatic library generation, we demonstrate the flexibility and efficiency of the proposed methodology in avoiding hand-crafted features and human intervention. For the data-driven discovery task, we demonstrate the accuracy, robustness and significant generalizability of the proposed methodology.

Gaussian Processes for input-modeling in virtual sensing of wind turbine blades

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Data assimilation techniques foresee the integration of both model-based and data-driven information to construct predictive tools that can be used for real-time monitoring of structural components such as wind turbine blades. These strategies are often employed for Virtual Sensing (VS) implementation, i.e., to infer system responses or unknown loads in dynamic environments.

Among these techniques, Kalman-based filters are usually employed to address the task of joint input-state prediction by using data to reduce uncertainties associated with the limitations of mechanistic models, which are then leveraged to enhance the available data and deepen understanding of the system's dynamic behavior.

These advanced methodologies are particularly useful in addressing the challenges of identifying structural properties and loading conditions in wind turbine infrastructure. They support the dynamic characterization of wind turbine blades during pre-installation testing and can also be applied in real-time in the field.

Assumptions about the nature of loading sources are critical for ensuring reliability of the VS estimated quantities. A Gaussian Process Latent Force Model (GPLFM) approach is hereby implemented to construct flexible data-driven a priori models for the unknown inputs, which are then coupled with a combined deterministic-stochastic state-space model of the structural component under study for Kalman-based input-state estimation.

The performance of the implemented framework has been evaluated for VS through laboratory testing a small-scale wind turbine blade. This case study enabled an assessment of the method performance and an exploration of various Gaussian Process (GP) kernels, offering valuable insights into their suitability for developing a Gaussian Process Latent Force Model (GPLFM) for input-state estimation.

Keynote II

On the use of Graph and Point networks in scientific applications

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In the context of scientific and industrial applications, one often has to deal with unstructured space-time data obtained from numerical simulations. The data can be either in the form of a mesh or a point cloud. In this context, graph neural networks (GNNs) have proved to be effective tools to reproduce the behavior of simulated data; however, depending on the physical nature of the datasets, variations of vanilla GNNs have to be considered to ensure accurate results. Furthermore, when only a point cloud is available, one can also consider a graph-free approach by building a "point network" that doesn't require connectivity information.

In this presentation we focus on particle-accelerator simulations; a computationally demanding class of problems for which rapid design and real-time control are challenging. We propose a machine learning-based surrogate model that leverages both graph and point networks to predict particle-accelerator behavior across different machine settings. Our model is trained on high-fidelity simulations of electron beam acceleration, capturing complex, nonlinear interactions among macroparticles distributed across several initial state dimensions and machine parameters. Our initial results show the model’s capacity for accurate, one-shot tracking of electron beams at downstream observation points, outperforming baseline graph convolutional networks. This framework accommodates key symmetries inherent in particle distributions, enhancing stability and interpretability. We also mention our ongoing work focused on extending these methods to autoregressive tracking across multiple timesteps. This research offers a powerful approach to reducing computational demands in particle-accelerator simulations, contributing to advancements in real-time optimization and control.

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