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# AI Seminar: Physics-Informed Machine Learning

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# Today's Paper

Karniadakis, G.E., Kevrekidis, I.G., Lu, L. et al. Physics-informed machine learning. *Nat Rev Phys* **3**, 422–440 (2021). https://doi.org/10.1038/s42254-021-00314-5

# Outline

- What is Physics-Informed Machine Learning?
- How to Embed Physics in ML
- Merits of Physics-Informed Learning
- State-of-art Applications/Works
- Current Limitations
- Future Directions
- Reference

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# What is Physics-Informed Machine Learning?

# What is Physics-Informed Machine Learning?

- Predictions in ML may be physically inconsistent or implausible, owing to extrapolation or observational biases that may lead to poor generalization performance.
- There is a pressing need for integrating fundamental physical laws and domain knowledge by 'teaching' ML models about governing physical rules.
- Provide strong theoretical constraints and inductive biases on top of the observational ones.

# What is Physics-Informed Machine Learning?

- Physics-informed learning
  - defined as the process by which prior knowledge stemming from our observational, empirical, physical or mathematical understanding of the world can be leveraged to improve the performance of a learning algorithm.
- Physics-informed neural networks
  - neural networks that are trained to solve supervised learning tasks while respecting any given laws of physics described by general nonlinear partial differential equations.

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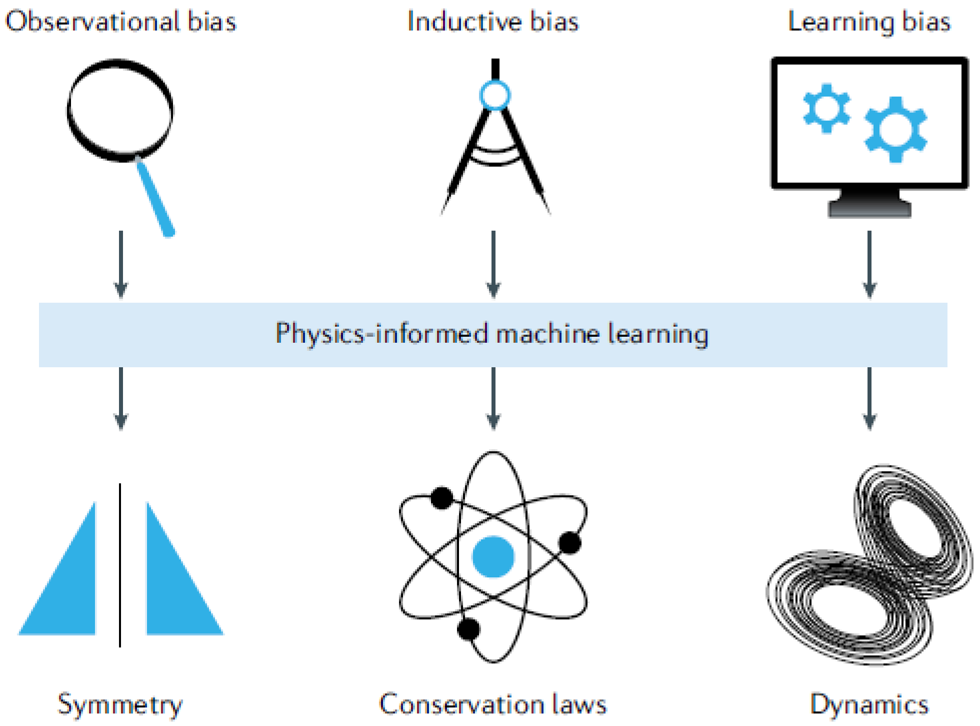
# How to Embed Physics in ML

# How to Embed Physics in ML

- There are currently three pathways that can be followed separately or concurrently to accelerate training and enhance generalization of ML models by embedding physics in them.
  - Observational biases
  - Inductive biases
  - Learning bias



# Observational Biases

- Observational biases can be introduced directly through data that embody the underlying physics or carefully crafted data augmentation procedures.
- These observational data ought to reflect the underlying physical principles that dictate their generation, and can be used as a weak mechanism for embedding these principles into an ML model during its training phase.
- A large volume of data is typically necessary to reinforce these biases and generate predictions that respect certain symmetries and conservation laws. → Data acquisition could be difficult in real case.

# Inductive Biases

- Inductive biases correspond to prior assumptions that can be incorporated by tailored interventions(干預) to an ML model architecture, such that the predictions sought are guaranteed to implicitly satisfy a set of given physical laws.
- Designing specialized NN architectures that implicitly embed any prior knowledge and inductive biases associated with a given predictive task. (e.g. CNN, GNN)
- Such approaches are currently limited to tasks that are characterized by relatively simple and well-defined physics or symmetry groups, and often require craftsmanship and elaborate implementations.
- Moreover, their extension to more complex tasks is challenging, as the underlying invariances or conservation laws that characterize many physical systems are often poorly understood or hard to implicitly encode in a neural architecture.

# Learning Bias

- Learning biases can be introduced by appropriate choice of loss functions, constraints and inference algorithms (soft penalty) that can modulate the training phase of an ML model to explicitly favor convergence towards solutions that obey the underlying physics.
- The flexibility of soft penalty constraints allows one to incorporate more general instantiations of domain-specific knowledge into ML models.

# Others

- Hybrid approaches
  - Combined these different method together.
  - Several methods have been proposed to learn operators that describe physical phenomena.
  - DeepONets have been demonstrated as a powerful tool to learn nonlinear operators in a supervised data-driven manner.
  - Combining DeepONets with physics encoded by PINNs, it is possible to accomplish real-time accurate predictions with extrapolation in multi-physics applications such as electro-convection(對流) and hyper-sonics.
- Connections to kernel methods
- Connections to classical numerical methods

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# Merits of Physics-Informed Learning

# Incomplete Models and Imperfect Data

- Physics-informed learning can easily combine both information from physics and scattered noisy data, even when both are imperfect.
- Recent research demonstrated that it is possible to find meaningful solutions even when, because of smoothness or regularity inherent in the PINN formulation, the problem is not perfectly well posed.
- Moreover, compared with the traditional numerical methods, physics-informed learning is mesh-free and thus can easily handle irregular problems.

# Strong Generalization in Small Data Regime

- Physics-informed learning has the advantage of strong generalization in the small data regime.
- By enforcing or embedding physics, deep learning models are effectively constrained on a lower-dimensional manifold, and thus can be trained with a small amount of data.
- Physics-informed learning is capable of extrapolation, not only interpolation: that is, it can perform spatial extrapolation in boundary-value problems.

# Understanding Deep Learning

- Physical principles are also being used to provide theoretical insight and elucidate the inner mechanisms behind the surprising effectiveness of deep learning.
- For example, inspired by the successful density matrix renormalization group algorithm developed in physics, ref. proposed a framework for applying quantum-inspired tensor networks to multi-class supervised learning tasks, which introduces considerable savings in computational cost.

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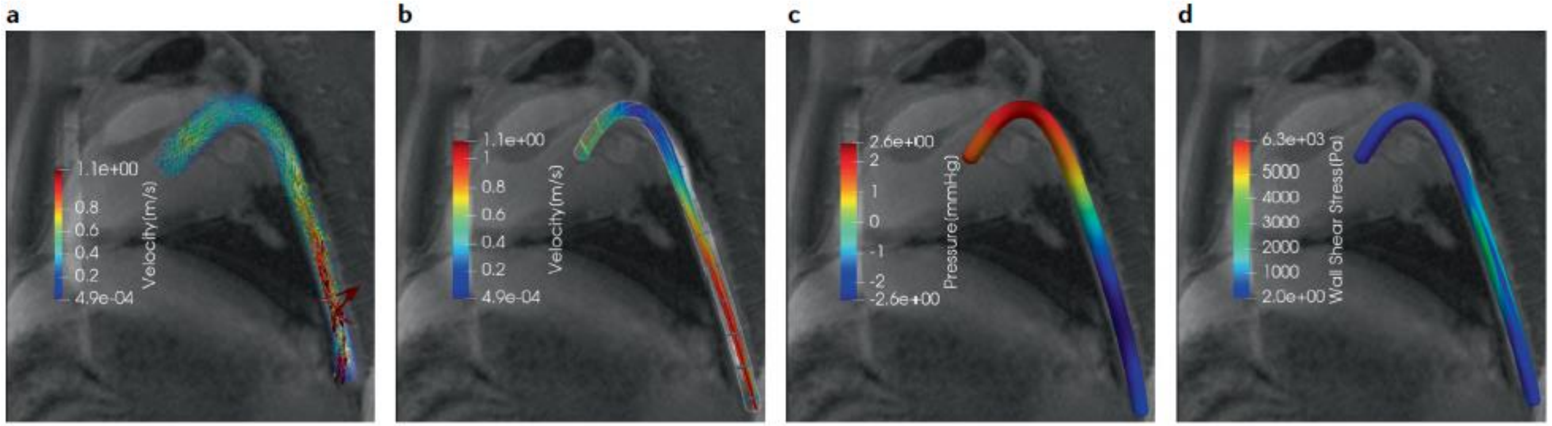
# State-of-art Applications/Works

# Physics-informed Deep Learning for 4d-flow MRI

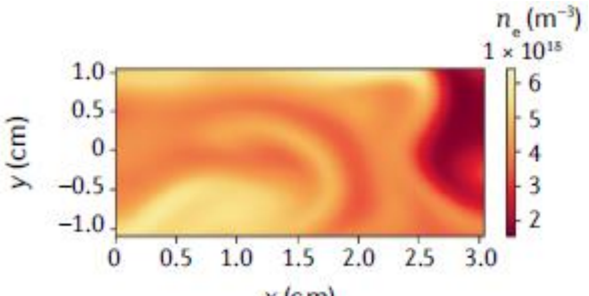
- Construct DNNs that are constrained by the Navier–Stokes equations in order to effectively de-noise MRI data and yield physically consistent reconstructions of the underlying velocity and pressure fields that ensure conservation of mass and momentum at an arbitrarily high spatial and temporal resolution.
- PINNs failed to predict the complex pattern in MRI. (for example, due to high-vorticity regions, turbulent bursts through a stenosis, tortuous branched vessels)



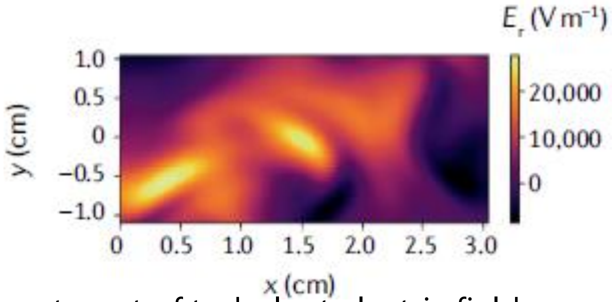

(a). snapshot of in-vivo 4D-flow MRI measurements (b). PINN reconstruction of velocity field (c). PINN reconstruction of pressure field (d). PINN reconstruction of wall shear stress

# Uncovering Edge Plasma Dynamics via Deep Learning from Partial Observations

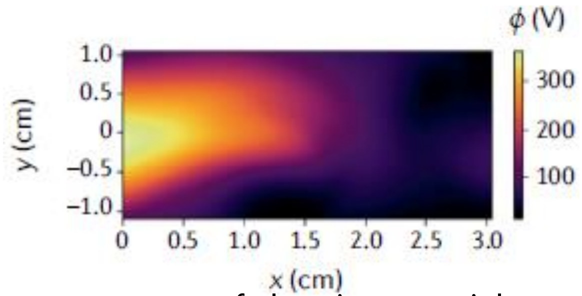
- PINNs can accurately learn turbulent field dynamics consistent with the drift-reduced Braginskii two-fluid theory from just partial observations of a synthetic plasma, for plasma diagnosis and model validation in challenging thermonuclear environments.



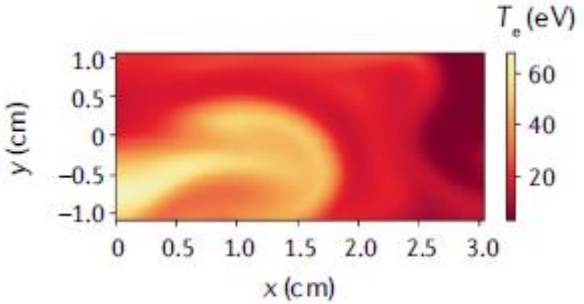
plasma's electron density



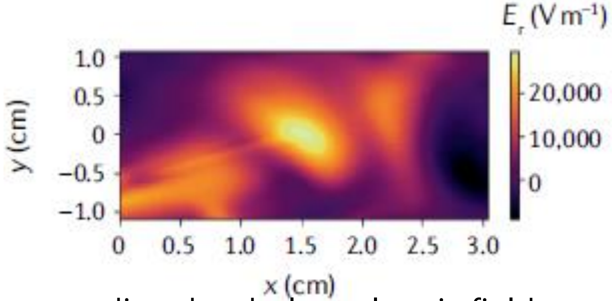
target of turbulent electric field



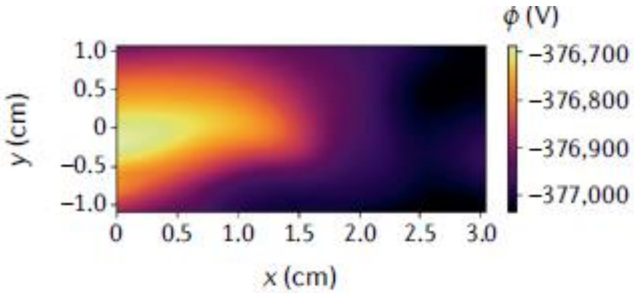
target of electric potential



plasma's temperature



predicted turbulent electric field



predicted electric potential

# Application to Material Sciences

- In ref, the authors introduced an optimized PINN trained to identify and precisely characterize a surface breaking crack in a metal plate.
- The PINN was supervised with realistic ultrasonic surface acoustic wave data acquired at a frequency of 5 MHz and physically informed by the acoustic wave equation, with the unknown wave speed function represented as an NN.
- A key element in training was the use of adaptive activation functions, which introduced new trainable hyper-parameters and substantially accelerated convergence even in the presence of significant noise in the data.

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# Current Limitations

# Multiscale and Multiphysics Problems

- Fully connected NNs have difficulty learning high-frequency functions, a phenomenon referred to in the literature as the ‘F- principle’ or ‘spectral bias’.
- High-frequency features in the target solution generally result in steep gradients, and thus PINN models often struggle to penalize accurately the PDE residuals. As a consequence, for multiscale problems, the networks struggle to learn high-frequency components and often may fail to train.
- Develop new techniques to aid the network learning, such as domain decomposition, Fourier features and multiscale DNN.

# New Algorithms and Computational Frameworks

- Physics-informed ML models often involve training large-scale NNs with complicated loss functions, which generally consist of multiple terms and thus are highly non-convex optimization problems. The terms in the loss function may compete with each other during training. Consequently, the training process may not be robust and sufficiently stable, and thus convergence to the global minimum cannot be guaranteed.
- For example, REFs found a discrepancy in the convergence rate of different components in a PINN loss function, leading to vanishing back-propagated gradients.
- To resolve this issue, one needs to develop more robust NN architectures and training algorithms for diverse applications.

# Data Generation and Benchmarks

- In the ML community dealing with imaging, speech and natural language processing problems, the use of standard benchmarks is very common in order to assess algorithm improvement, reproducibility of results, and expected computational cost.
- The UCI Machine Learning Repository is a collection of databases and data generators.
- However, in many different applications in physics and chemistry, full-field data are required, which cannot be obtained experimentally and which tax computational resources heavily both in terms of time and memory.
- Careful consideration should be given to how to make these data publicly available, how to curate such valuable data, and how to include the physical models and all parameters required for the generation of these databases.
- In addition, it will take a concerted (齊心協力的) effort by researchers to design meaningful benchmarks that test accuracy and speed-up of the new proposed physics-informed algorithms

# New Mathematics

- Despite the empirical success of physics-informed learning models, little is known about the theoretical foundation of such constrained NNs. A new theory is required to rigorously analyze the capabilities and limitations of physics-informed learning (for example, the learning capacity of NNs).
- The first mathematical analysis for PINNs in solving forward problems appeared in ref. Specifically, ref. analyzed the second-order linear elliptic and parabolic type PDEs and proved the consistency of results.
- In general, NNs are trained by gradient-based optimization methods, and a new theory should be developed to better understand their training dynamics (gradient descent, stochastic gradient descent, Adam and so on).

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# Future Directions

# Digital Twins

- Questions to be addressed
  - Observational data can be scarce and noisy, are often characterized by vastly heterogeneous data modalities (images, time series, lab tests, historical data, clinical records and so on), and may not be directly available for certain quantities of interest.
  - Physics-based computational models heavily rely on tedious pre-processing and calibration procedures (such as mesh generation or calibration of initial and boundary conditions) that typically have a considerable cost, hampering their use in real-time decision making settings.
  - Physical models of many complex natural systems are, at best, 'partially' known as conservation laws, and do not provide a closed system of equations unless appropriate constitutive laws are postulated.
- Thanks to its natural capability of blending physical models and data as well as the use of automatic differentiation that removes the need for mesh generation, physics-informed learning is well placed to become an enabling catalyst in the emerging era of digital twins.

'Digital twins', a concept first put forth by General Electric to describe the digital copy of an engine manufactured in their factories, are now becoming a reality in a number of industries. By assimilating real measurements to calibrate computational models, a digital twin aims to replicate the behavior of a living or non-living physical entity in silico.

# Data and Model Transformations, Fusion and Interpretability

- As the interactions between physics-based modelling and ML intensify, one will encounter situations in which different researchers arrive at different data-driven models of the same phenomenon, even if they use the same training data.
- The importance of building ML-based transformations between predictive models, models at different fidelities, and theories.
- Test how far these transformations generalize: for what range of observations an ML model can be mapped to a different ML model, or to a physical model, and what the generalization limit is, beyond which they cannot be transformed or calibrated to each other.

# Searching for Intrinsic Variables and Emergent, Useful Representations

- Most of the current physics-informed ML methods follow this paradigm:
  - First define a set of (humanly interpretable) observables/variables → collect data → formulate the physics completely or incompletely using a 'reasonable' dictionary of operators based on the chosen observables → finally apply the learning algorithm of choice.
- An emerging paradigm fueled by advances in ML is to use observations and learning methods to automatically determine good/intrinsic variables and to also find useful or informative physical model formulations.
- Moreover, instead of collecting data from experiments first and then performing the learning algorithm, it becomes important to integrate both in an active learning framework.

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# Q & A

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