


Northeastern University
College of Engineering
Civil and Environmental Engineering

Physics Informed Machine Learning Part I: Different Strategies to Incorporate Physics into Engineering Problems

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01/28/2024

IMAC XLII

Physics-Based Approaches vs. Data-Driven Strategies

Physics-based strategies most popular approaches used to characterize complex phenomena focusing on the use of mathematical models to describe the physical laws and principles governing the behavior of a dynamic system.

- interpretable and generalizable to systems with similar characteristics
- flexibility to incorporate prior knowledge and constraints into the model

- often have large and time-varying modeling errors
- heavy computational burden
- complex dynamics

Data-driven strategies has seen remarkable advancements due to the abundance of data and computing resources. These methods utilize data to learn the system dynamics and control without the need for an explicit model.

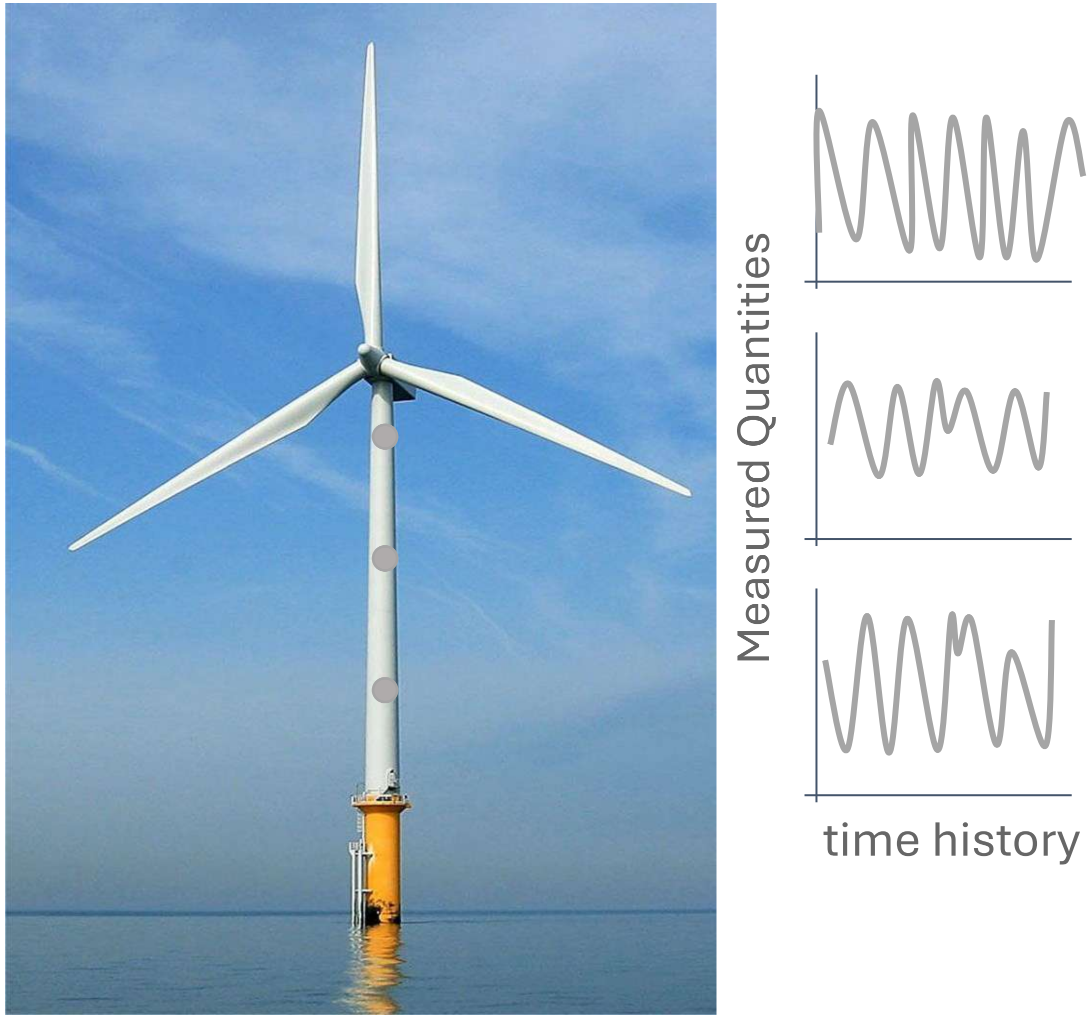
- flexible, adaptive, and scalable
- handle uncertainties and disturbances in the data

- can limitedly represent only the datasets they were trained to learn, without any flexibility or inference capability towards unseen conditions
- low level of interpretability and explainability.

Going Hybrid

What if the physics become to complicated?

What if we don't have enough meaningful data?

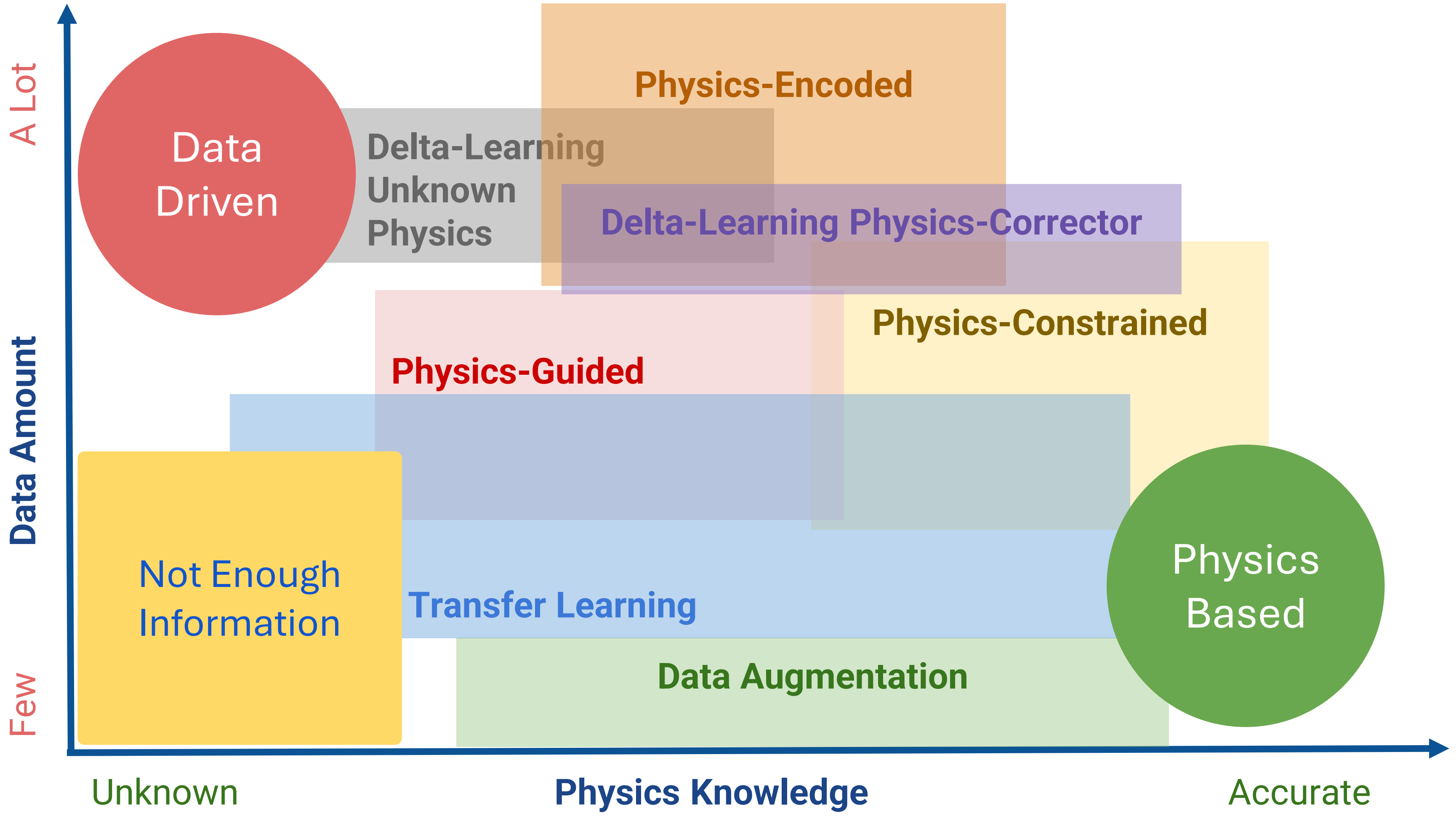


When and How?

Strategies

Variety of strategies classified according to three major characteristics:

1. the **amount** and **quality** of **data** that is utilized to describe a given model
2. the **strategy** chosen to incorporate the physics into the problem
3. the level of **physical knowledge** and understanding representing the phenomena of interest



Literature first!

REVIEWS

Check for updates

Physics-informed machine learning

George Em Karniadakis[1,2], Ioannis G. Kevrekidis[3,4], Lu Lu[5], Paris Perdikaris[6], Sifan Wang[7] and Liu Yang[1]

Abstract | Despite great progress in simulating multiphysics problems using the numerical discretization of partial differential equations (PDEs), one still cannot seamlessly incorporate noisy data into existing algorithms, mesh generation remains complex, and high-dimensional problems governed by parameterized PDEs cannot be tackled. Moreover, solving inverse problems with hidden physics is often prohibitively expensive and requires different formulations and elaborate computer codes. Machine learning has emerged as a promising alternative, but training deep neural networks requires big data, not always available for scientific problems. Instead, such networks can be trained from additional information obtained by enforcing the physical laws (for example, at random points in the continuous space-time domain). Such physics-informed learning integrates (noisy) data and mathematical models, and implements them through neural networks or other kernel-based regression networks. Moreover, it may be possible to design specialized network architectures that automatically satisfy some of the physical invariants for better accuracy, faster training and improved generalization. Here, we review some of the prevailing trends in embedding physics into machine learning, present some of the current capabilities and limitations and discuss diverse applications of physics-informed learning both for forward and inverse problems, including discovering hidden physics and tackling high-dimensional problems.

Table 1 | **Major software libraries specifically designed for physics-informed machine learning**

Software name	Usage	Language	Backend	Ref.
DeepXDE	Solver	Python	TensorFlow	154
SimNet	Solver	Python	TensorFlow	155
PyDEns	Solver	Python	TensorFlow	156
NeuroDiffEq	Solver	Python	PyTorch	157
NeuralPDE	Solver	Julia	Julia	158
SciANN	Wrapper	Python	TensorFlow	159
ADCME	Wrapper	Julia	TensorFlow	160
GPyTorch	Wrapper	Python	PyTorch	161
Neural Tangents	Wrapper	Python	JAX	162

Karniadakis, G.E., Kevrekidis, I.G., Lu, L. *et al.* Physics-informed machine learning. *Nat Rev Phys* **3**, 422–440 (2021).

Structural and Multidisciplinary Optimization (2022) 65:354
https://doi.org/10.1007/s00158-022-03425-4

REVIEW PAPER

Check for updates

A comprehensive review of digital twin — part 1: modeling and twinning enabling technologies

Adam Thelen[1] · Xiaoge Zhang[2] · Olga Fink[3] · Yan Lu[4] · Sayan Ghosh[5] · Byeng D. Youn[6] · Michael D. Todd[7] · Sankaran Mahadevan[8] · Chao Hu[1,10] · Zhen Hu[9]

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Thelen, Adam, Xiaoge Zhang, Olga Fink, Yan Lu, Sayan Ghosh, Byeng D. Youn, Michael D. Todd, Sankaran Mahadevan, Chao Hu, and Zhen Hu. "A comprehensive review of digital twin—part 1: modeling and twinning enabling technologies." *Structural and Multidisciplinary Optimization* 65, no. 12 (2022): 354.

Data-Centric Engineering (2023), 1–33
doi:XX.XXXX/dce.XXXX.X

CAMBRIDGE UNIVERSITY PRESS

SURVEY PAPER

arXiv [cs.LG] 1 Nov 2023

Discussing the Spectra of Physics-Enhanced Machine Learning via a Survey on Structural Mechanics Applications

Marcus Haywood-Alexander[1]*, Wei Liu[2,3], Kiran Bacsa[1,3], Zhilu Lai[4,5] and Eleni Chatzi[1,3]

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[2]Department of Industrial Systems Engineering and Management, National University of Singapore, Singapore
[3]Future Resilient Systems, Singapore-ETH Centre, Singapore
[4]Internet of Things Thrust, HKUST(GZ), Guangzhou, People's Republic of China
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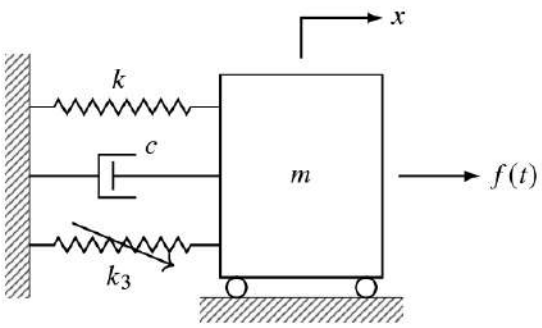
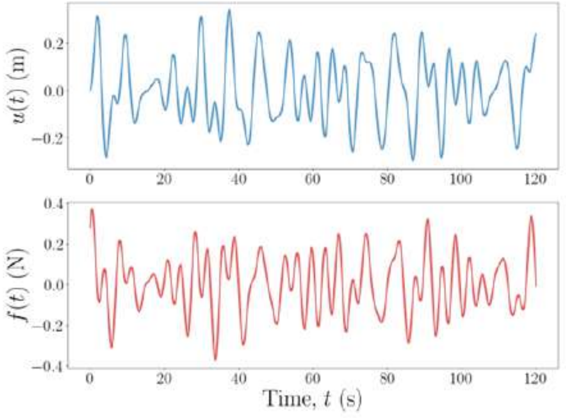
Received xx xxx xxxx

Keywords: physics enhanced, physics-based, physics-guided, physics-encoded, data driven, hybrid learning, structural mechanics

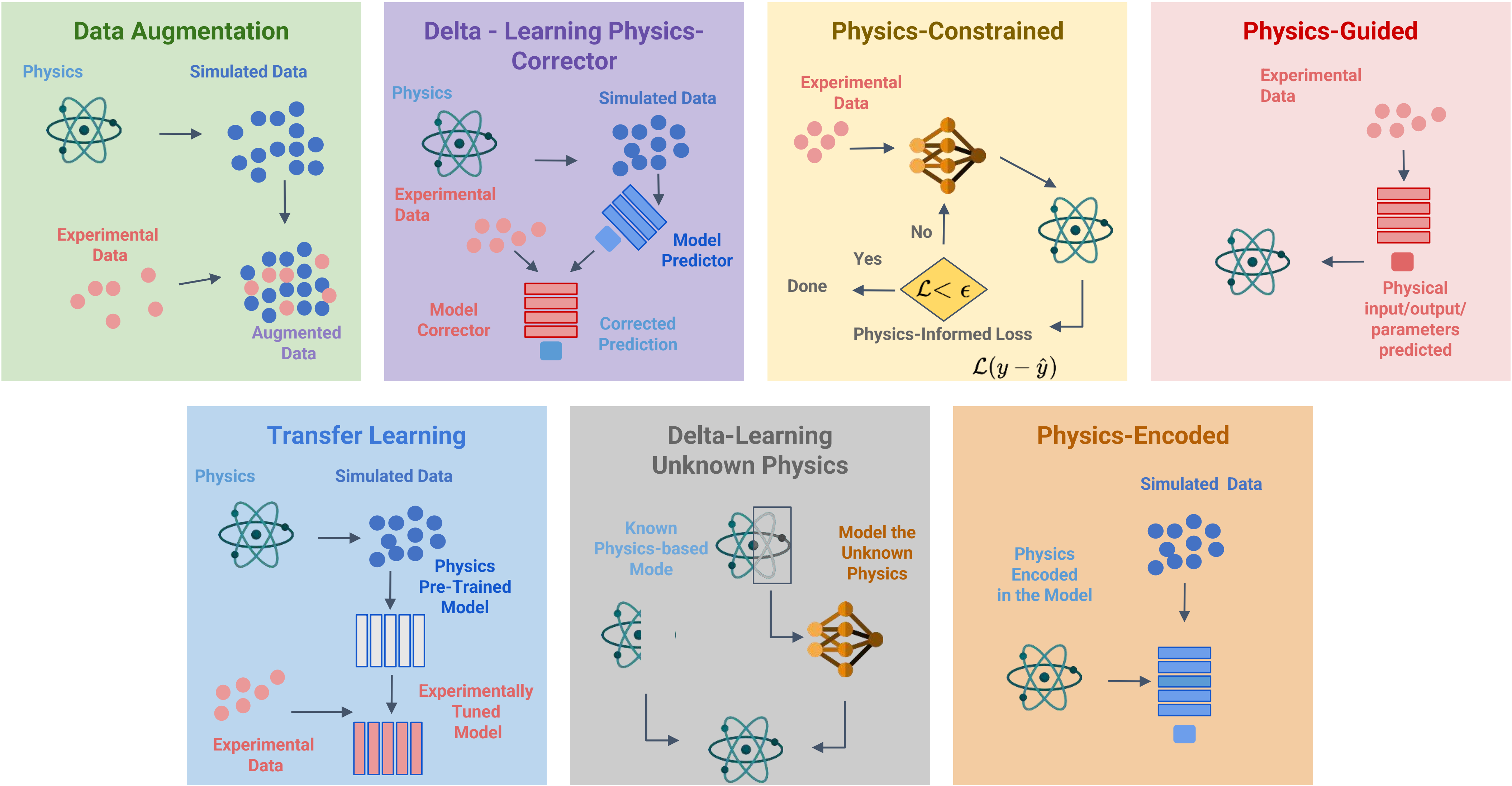




Haywood-Alexander, Marcus, Wei Liu, Kiran Bacsa, Zhilu Lai, and Eleni Chatzi. "Discussing the Spectra of Physics-Enhanced Machine Learning via a Survey on Structural Mechanics Applications." *arXiv preprint arXiv:2310.20425* (2023).

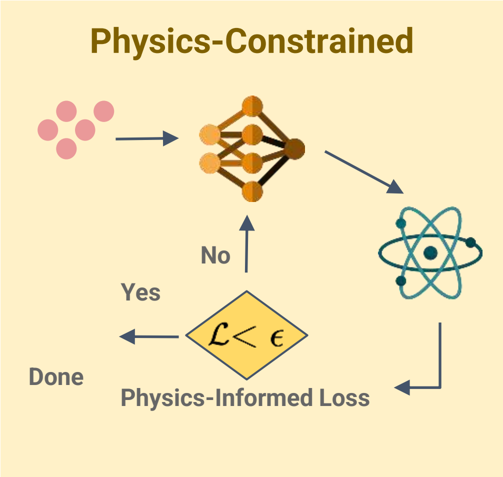
Strategies

Strategies



Karniadakis, G.E., Kevrekidis, I.G., Lu, L. *et al.* Physics-informed machine learning. *Nat Rev Phys* **3**, 422–440 (2021).

1. Physics-Constrained



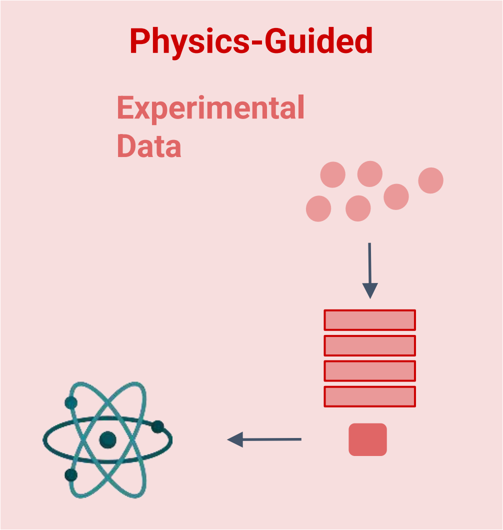
This approach is centered around the **strict enforcement** of physical laws on models (physically consistent)

Physics-constrained neural networks are the most popular implementation of this strategy

GitHub

https://github.com/ARTS-Laboratory/Physics-Informed-Machine-Learning-Example/tree/demonstration

2. Physics Guided



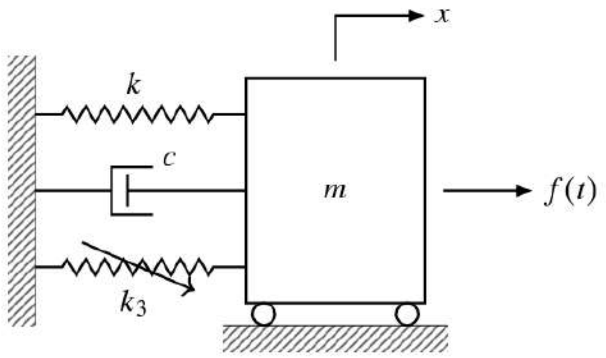
Domain-specific physical knowledge into the machine learning process, but rather than enforcing strict constraints, it uses this knowledge as a **guide**

Learning algorithms are employed to capture the discrepancy between an explicitly defined model based on prior knowledge and the true system from which data is attained. The goal is to fine-tune the overall model's parameters (i.e. the prior and model) in a way that the physical prior knowledge steers the training process toward the desired direction.

- Incorporating Prior Knowledge: Prior knowledge on the physics of the system is integrated into the network architecture, or as part of the model
- Capturing Discrepancy: Deep learning models excel in learning from data,even when this contradicts prior knowledge.

Haywood-Alexander, Marcus, Wei Liu, Kiran Bacsa, Zhilu Lai, and Eleni Chatzi. "Discussing the Spectra of Physics-Enhanced Machine Learning via a Survey on Structural Mechanics Applications." *arXiv preprint arXiv:2310.20425* (2023).

2. Physics Guided



Physics-guided Deep Markov Model (PgDMM) for inferring the characteristics and latent structure of nonlinear dynamical systems from measurement data.

Introduce a physical prior model into the DMM to guide the training process: simplified linear model that excludes the cubic term

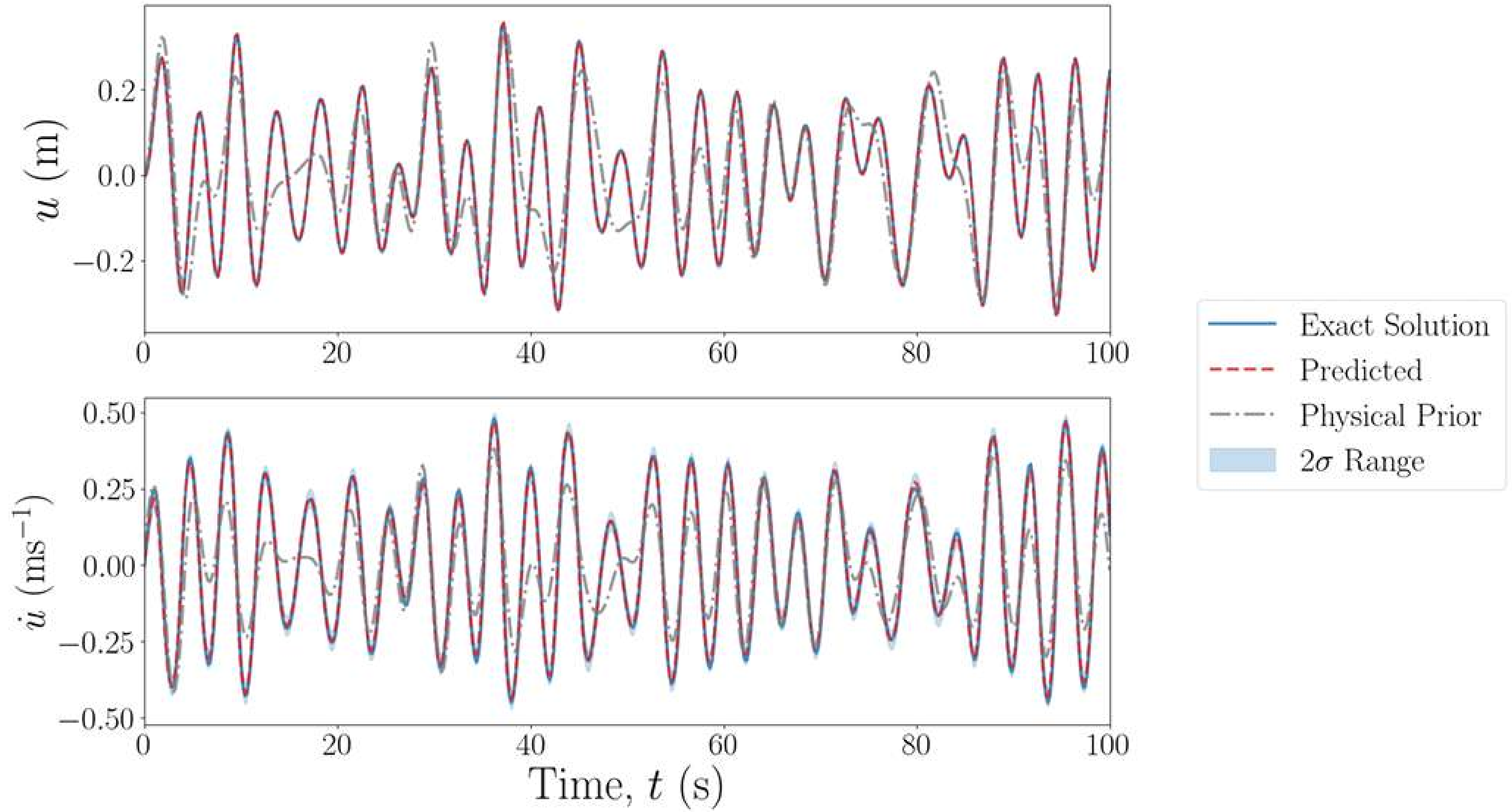
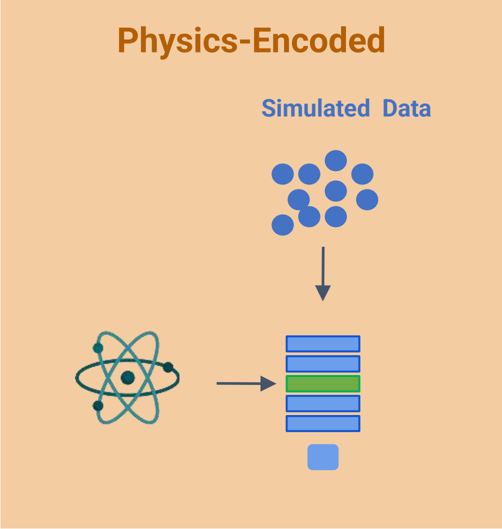


Figure 5. *Predictions vs exact solutions of displacement (top) and velocity (bottom) using the PgDMM applied to the working example. Displacement is assume to be the only measurement. The gray dash-dot line is the physical prior model and the blue bounding boxes represent the estimated 2σ range.*

Haywood-Alexander, Marcus, Wei Liu, Kiran Bacsa, Zhilu Lai, and Eleni Chatzi. "Discussing the Spectra of Physics-Enhanced Machine Learning via a Survey on Structural Mechanics Applications." *arXiv preprint arXiv:2310.20425* (2023).

3. Physics Encoded

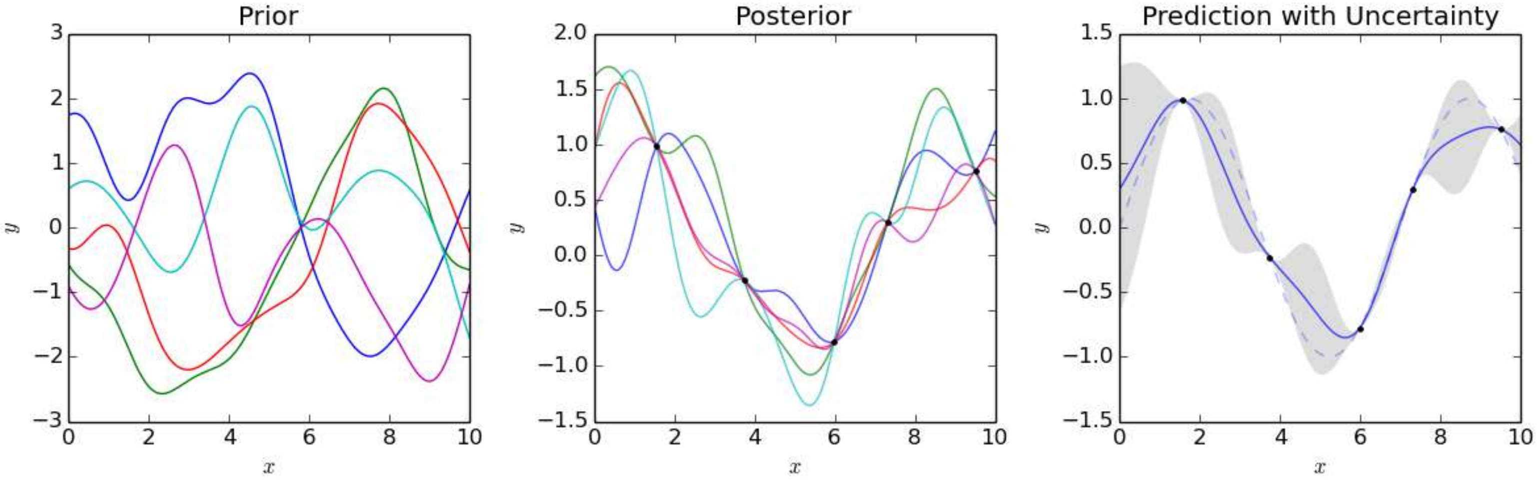


Physics-Encoded ML a framework that embeds physical knowledge into the architecture or design of machine learning models

Via selection of operators, kernels, or transforms such as convolutional layers and recurrent layers (**physics-inspired layers** or modules)

Constrained Gaussian Process uses prior knowledge to modify the kernel function, the likelihood function, or the posterior distribution of the GP model.

$$f(\mathbf{X}) \sim \mathcal{GP}(m(\mathbf{x}), K(\mathbf{x}, \mathbf{x}'))$$



Cross, E.J. and Rogers, T.J.(2021). Physics-derived covariance functions for machine learning in structural dynamics. IFACPapersOnLine,54(7):168–173 (https://drg-greybox.github.io/publications/).

3. Physics Encoded

Duffing Oscillator

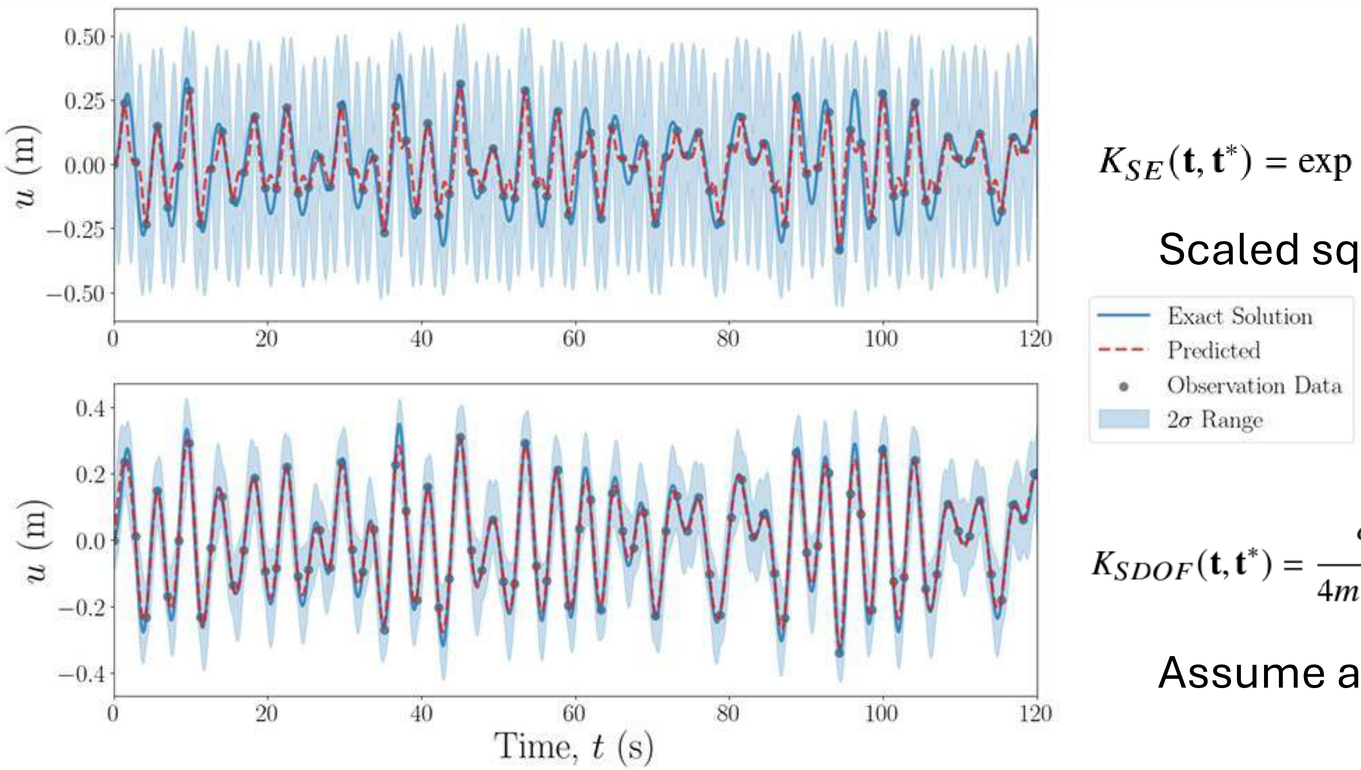
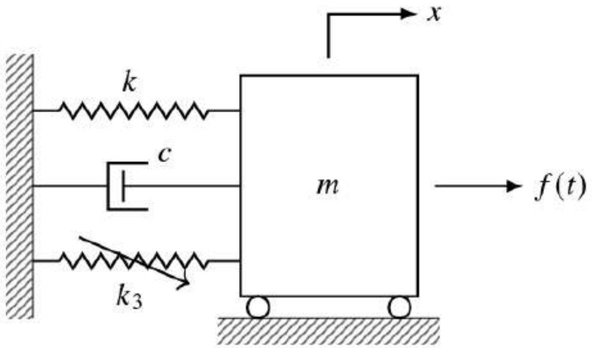


Figure 10. Predicted vs exact solutions of displacement estimation using a GP applied to a subsample of the working example, with (top) no physics embedded and (bottom) constrained GP. The blue bounding boxes represent the estimated 2σ range.



$$K_{SE}(\mathbf{t}, \mathbf{t}^*) = \exp\left(-\frac{1}{2l^2}(\mathbf{t}-\mathbf{t}^*)^T(\mathbf{t}-\mathbf{t}^*)\right)$$

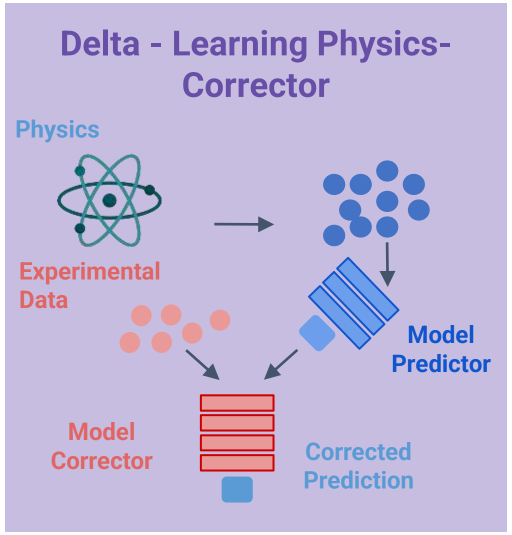
Scaled squared-exponential kernel

$$K_{SDOF}(\mathbf{t}, \mathbf{t}^*) = \frac{\sigma_f^2}{4m^2\zeta\omega_n^3} e^{-\zeta\omega_n|\tau|}\left(\cos(\omega_d\tau) + \frac{\zeta\omega_n}{\omega_d}\sin(\omega_d|\tau|)\right), \quad \tau = \mathbf{t}-\mathbf{t}^*$$

Assume a Gaussian white noise force input kernel

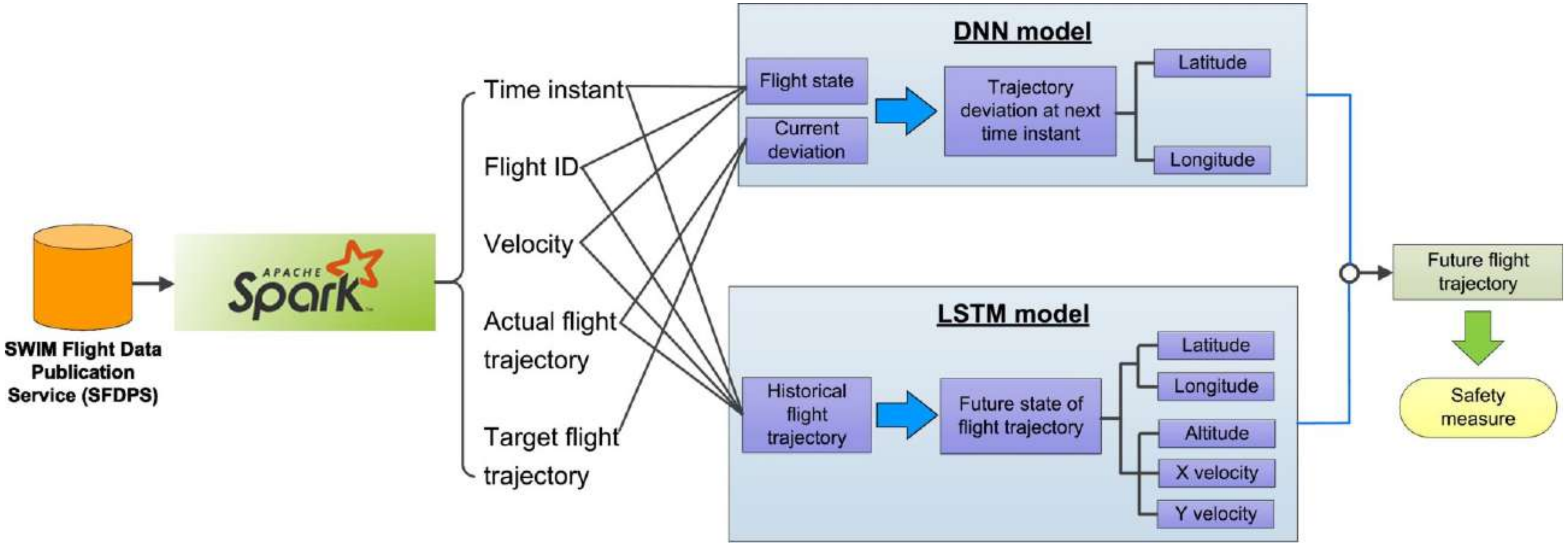
Haywood-Alexander, Marcus, Wei Liu, Kiran Bacsa, Zhilu Lai, and Eleni Chatzi. "Discussing the Spectra of Physics-Enhanced Machine Learning via a Survey on Structural Mechanics Applications." *arXiv preprint arXiv:2310.20425* (2023).

4. Delta – Learning Physics-Corrector



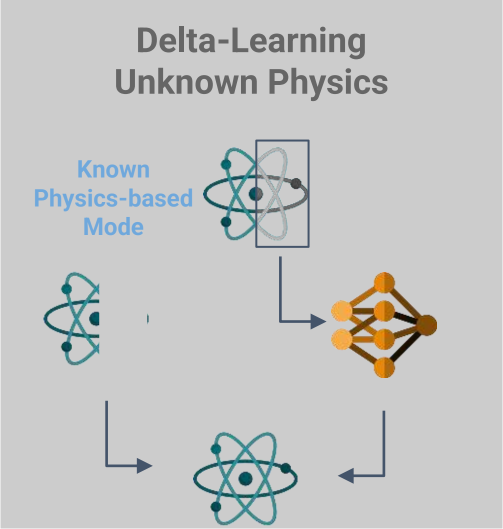
Represents the set of strategies where the **residuals** between physics and data-driven ML model are used to **update** the prediction

- Use a physics-based model to generate training data for an ML model
- The predictions of this physics-trained model will be used to inform a second ML model together with experimental data to learn the **residuals**
- The final predictions are the sum of the initial predictions and residuals to compensate for **missing physics**



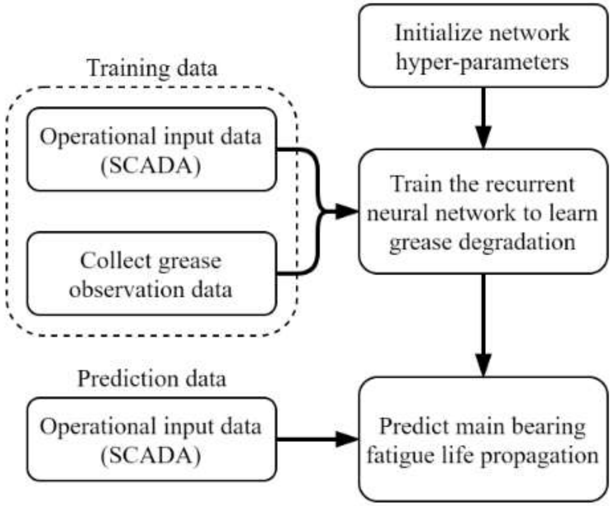
Zhang X, Mahadevan S (2020) Bayesian neural networks for flight trajectory prediction and safety assessment. Decis Support Syst 131:113246

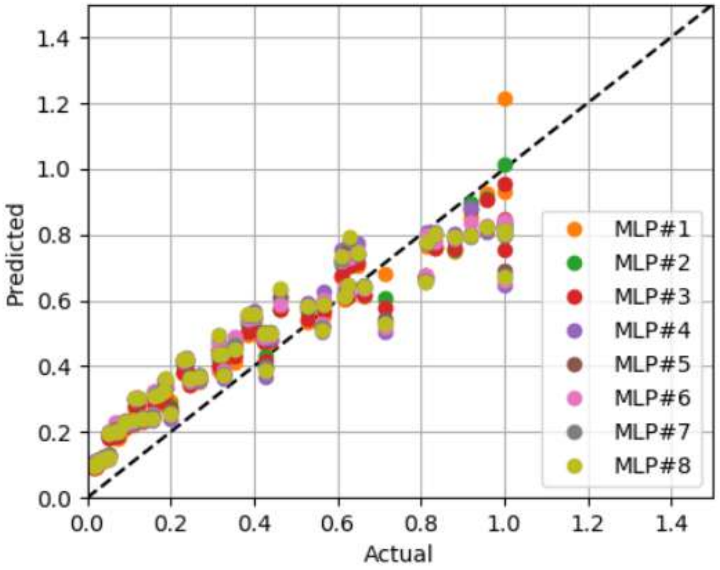
5. Delta – Learning Unknown Physics



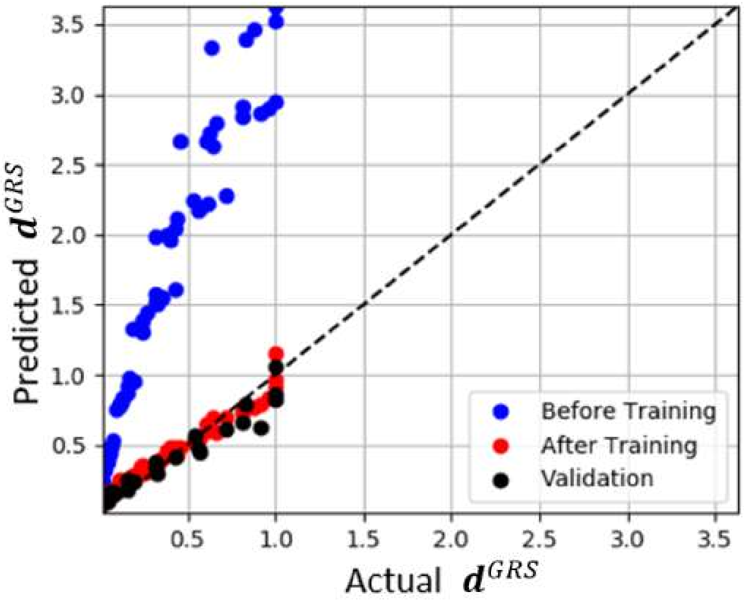
Represents the set of strategies where a data-driven ML model is used as a **surrogate** to learn and **recover the unmodeled physics**

The result is a cumulative damage model where the physics-informed layers are used to model the relatively well-understood physics (L10 fatigue life) and the data-driven layers account for the hard to model components (i.e., grease degradation).



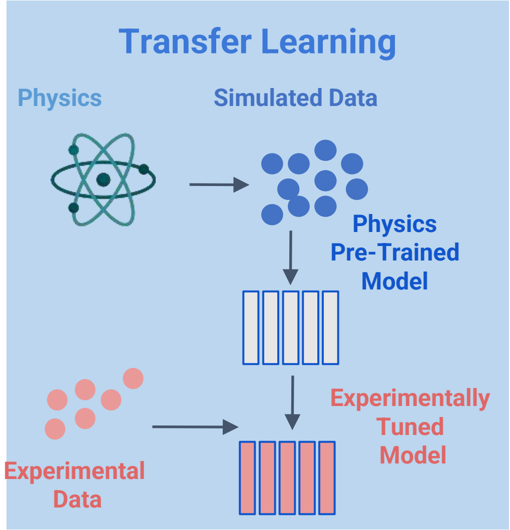


(a) Cross-validation predictions vs. actual grease damage.



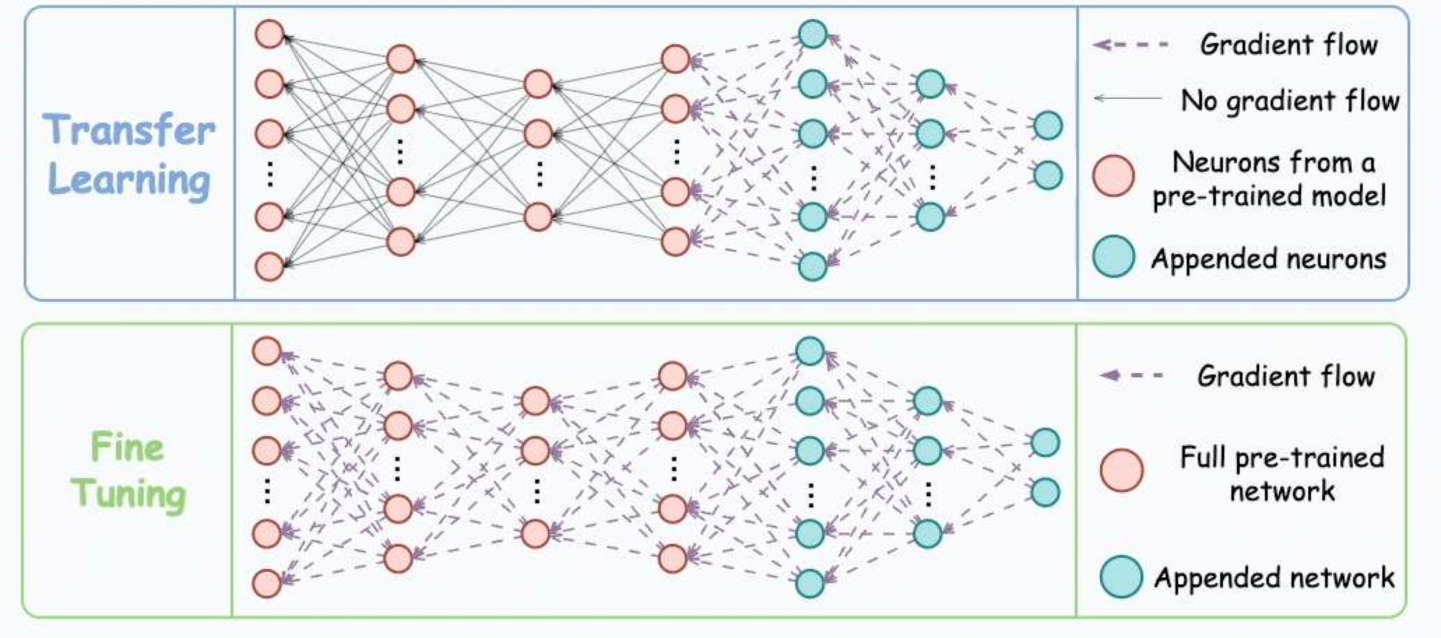
Yucesan YA, Viana FA (2020) A physics-informed neural network for wind turbine main bearing fatigue. Int J Progn Health Manag.

6. Transfer Learning



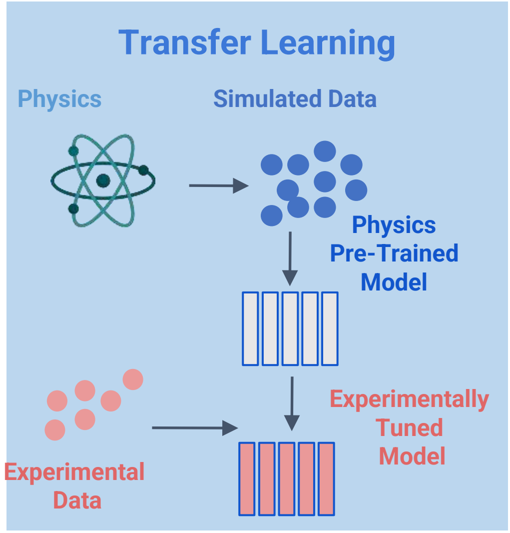
Strategies focused on using a model already trained on one problem to help solve another problem that is similar but not the same

This strategy can save time and resources by using **existing models** instead of training new ones and can also improve the performance of models when there is not enough data for the new problem.



By pre-training the ML model on the synthetic data, the model can learn general and robust features and representations that capture the **underlying physical** mechanisms.

6. Transfer Learning

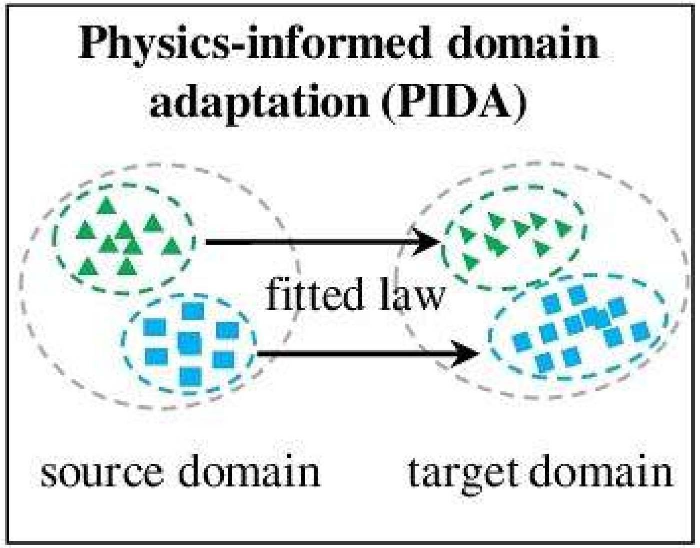


Strategies focused on using a model already trained on one problem to help solve another problem that is similar but not the same

This strategy can save time and resources by using **existing models** instead of training new ones and can also improve the performance of models when there is not enough data for the new problem.

Physics-informed domain adaptation is a technique that combines **physics-based models** with **machine learning** to improve the accuracy of predictions in **new or unseen environments**. The goal is to **adapt** a model trained on one domain to another domain with different characteristics, such as different physical properties or environmental conditions.

Physical laws governing the **domain shifts** and use a small amount of source-domain and target-domain data to fit the physical law.



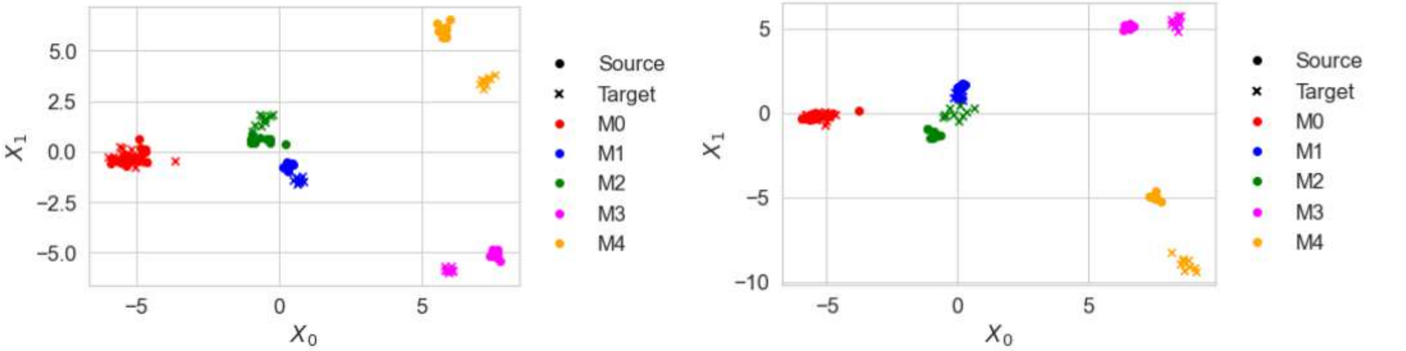
6. Physics-Informed Transfer Learning

Transfer learning can be used to leverage information across related domains. The authors proposes utilizing the Modal Assurance Criterion (MAC) between modes of healthy structures as a measure of data similarity to identify features that minimize conditional distribution shift.

Transfer feature criterion that incorporates MAC-discrepancy into a feature selection criterion to address the challenge of selecting features with high cross-domain similarity.

$$\mathcal{L} = -\frac{1}{n_s}\sum_{n=1}^{n_s} L(f_s(\mathbf{x}_{s,i}), y_s) + \lambda d_{\mathrm{MAC}}(\Phi_s, \Phi_t) - \mu C$$

Figure 1. The experimental setup to perform modal testing on a metal (right) and composite (left) blade simultaneously.



(a) (b)

Figure 5. PCA visualisation of the TFC-selected frequencies, corresponding to the fourth and fifth modes, for M→C (panel (a)) and C→M (panel (b)), representing 66% and 64% of the variance respectively.

Poole, Jack, Paul Gardner, Andrew J. Hughes, Richard S. Mills, Thomas A. Dardeno, and Nikos Dervilis. "Physics-Informed Transfer Learning in PBSHM: A Case Study on Experimental Helicopter Blades." *STRUCTURAL HEALTH MONITORING* (2023).

6. Physics-Informed Transfer Learning

Graphical domain is presented as an objective way of assessing structural similarity, with distance metrics utilised for assessing data-space similarities.

Knowledge transfer is performed using a branch of transfer learning called **domain adaptation**.

The authors demonstrates a methodology for transferring knowledge within a heterogeneous population (a group of non-identical structures).

Transfer localisation labels from a Gnat aircraft wing to an unlabelled Piper Tomahawk aircraft wing dataset, resulting in 100% classification accuracy

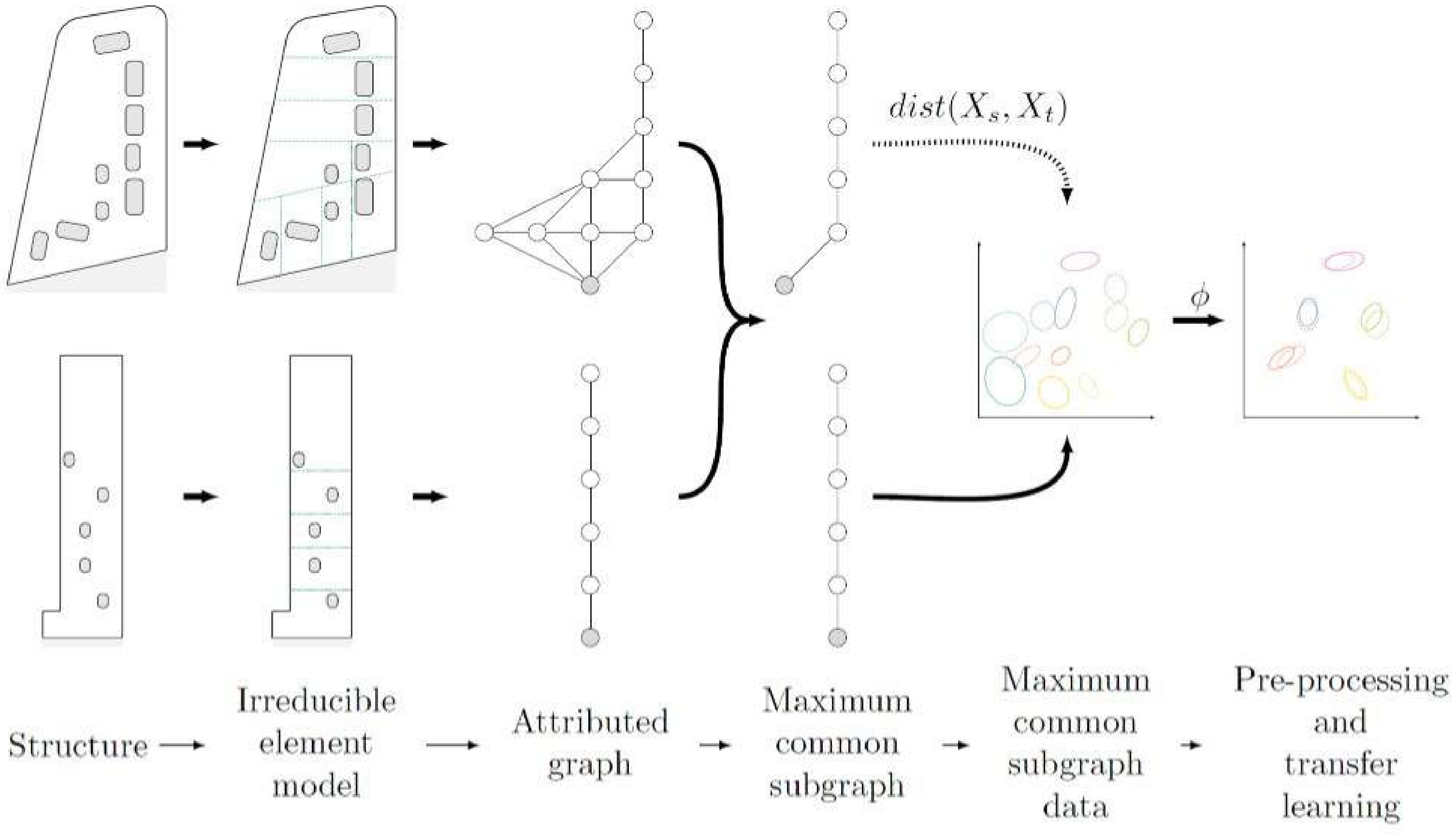
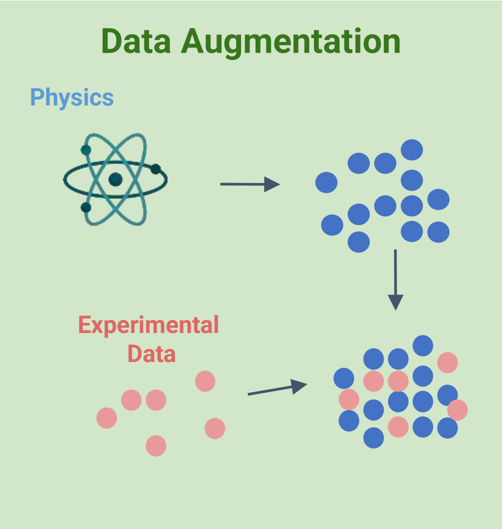


Fig. 5. Schematic overview of the population-based methodology.

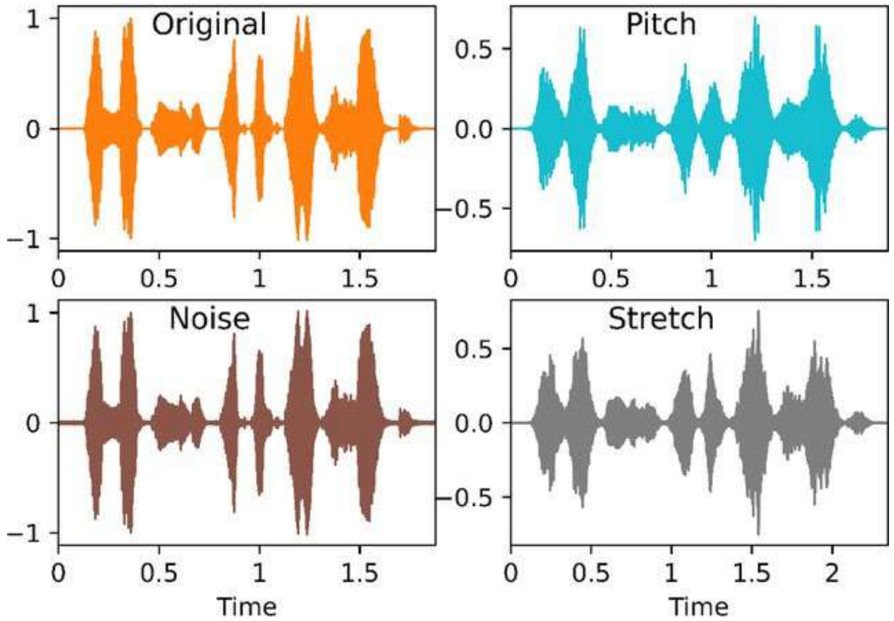
Gardner, P., L. A. Bull, J. Gosliga, J. Poole, N. Dervilis, and K. Worden. "A population-based SHM methodology for heterogeneous structures: Transferring damage localisation knowledge between different aircraft wings." *Mechanical Systems and Signal Processing* 172 (2022): 108918.

7. Data Augmentation



Set of techniques to artificially increase the amount of data by generating new data points from existing data.

Improve the performance and generalization of machine learning models, especially when the original **data is insufficient** or noisy.



When an accurate and robust knowledge of the first principle is available, it is possible to leverage this information and run **first-principle simulations** to generate data at various states and operating conditions of a physical system.

7. Data Augmentation

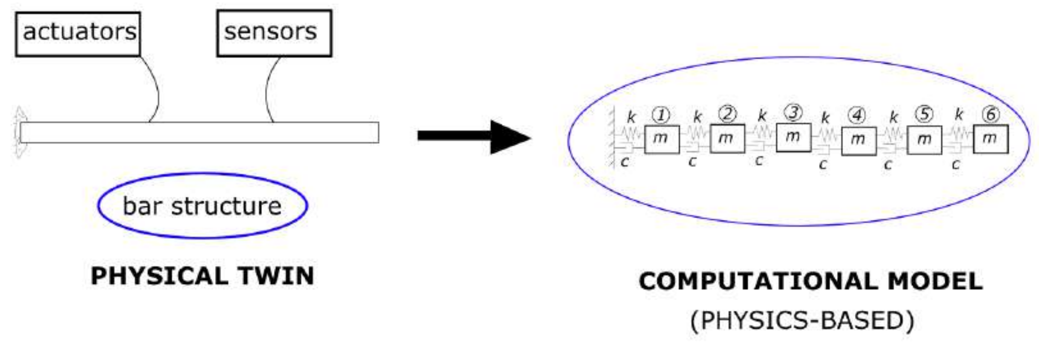


Fig. 2. Sketch of the physical twin and the corresponding physics-based computational model.

The authors generated different damage scenarios using first-principle simulations to augment a training dataset for an ML classifier used for damage detection of a bar structure.

Ritto T, Rochinha F (2021) Digital twin, physics-based model, and machine learning applied to damage detection in structures. Mech Syst Signal Process 155:107614

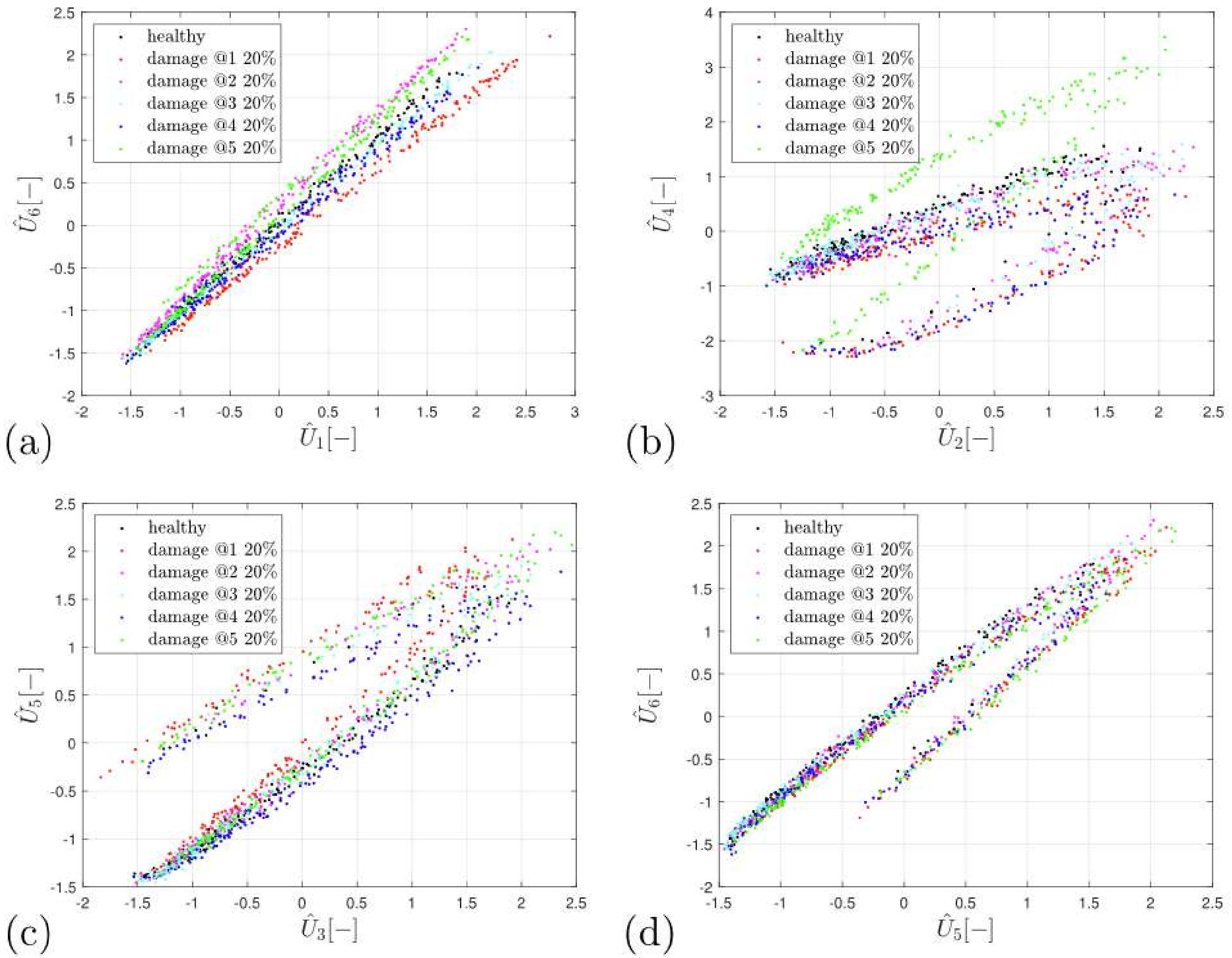


Fig. 8. Training data generated with the stochastic digital twin with excitation frequency of 3800 Hz. Responses at DOFs (a) #1 and #6, (b) #2 and #4, (c) #3 and #5, (d) #5 and #6.

Open Challenges

Open Questions and Challenges

Generalization
How well do the integrated models generalize?

Uncertainty Quantification
Incorporating physical laws and constraints into machine learning models can make the quantification of the uncertainty for the integrated model a challenge

Scalability
Are the integrated models scalable to large datasets? Is it computationally more efficient?

Interpretability and explainability
Machine learning models are often considered as black boxes, making it difficult to interpret and explain their predictions. Is their introduction helping?

Data quality
How integrated models perform in the case of changes in measurements data quality and unbalanced datasets

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Questions?