



Associazione Italiana di Aeronautica e Astronautica  
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Member of:  
International Astronautical  
Foundation (IAF)  
International Council of  
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# AIDAA Educational Series and Academy Introduction to Theory-Guided Machine Learning and Its Applications to Multi- Physics Problems in Engineering

*25-27 June 2024*

## **Overview and General Information:**

Problems of interest in science and engineering are often multi-physics, with complexities stemming from the interactions of various mechanisms, and inherent uncertainties and variabilities. In an industrial setting, we frequently aim to conduct optimization tasks in such complex and high-dimensional domains. For example, the 3D printing of thermoplastics involves heat and mass transfers, where the material undergoes thermo-chemical and thermo-mechanical changes along with several phase transformations. Evaluating the performance of the material under such conditions is challenging due to the complexities of the underlying multi-physics problem, as well as noise/errors in measurements, process uncertainties, and material variabilities. To evaluate or conduct optimization tasks, current practices often rely on methods such as Design of Experiments (DoE), and/or numerical methods.

In the recent decade, the application of data-driven and machine learning (ML) methods has also been explored with varying degrees of success. However, ML methods have been shown to suffer from a variety of shortcomings, including brittleness outside of their training zones. More recently, different families of data-driven methods have evolved to address the complexities of such multi-physics problems, including theory-guided machine learning (TGML), also referred to as scientific AI or physics-informed ML. TGML represents a merger between science-based methods, including finite element (FE) analysis, and ML techniques to overcome the challenges associated with theory-agnostic ML methods in physical domains.

## **Learning Objectives:**

This course aims to introduce participants to TGML and its applications. First, a short overview of theory-agnostic ML methods, including Neural Networks (NN) for large datasets and Gaussian Process Regression (GPR) for small datasets, will be given. Simple engineering applications including heat transfer will be demonstrated. Next, TGML and its notable techniques will be introduced, with examples provided. A combination of experimental data and numerical data will be used to train ML models. Python programming with built-in libraries will be employed to develop ML codes during the course. Participants can follow the instructor to develop codes using Python on their own machines. Python codes and example datasets will be provided as well.

## **Dates and schedule:**

25, 26, and 27 June from 9.00-12.30 PM, CEST

25 June 2024

- Why use Machine Learning (ML) for multi-physics problems?
- Why physics-informed or theory-guided ML?
- Quick introduction to Python coding used in the course.
- Simple demonstration: OFAT (One-Factor-At-A-Time) vs. DOE (Design of Experiments) vs. Iterative ML
- Overview of traditional ML methods, with example Python codes:
  - Deterministic methods: Neural Networks (NN)
  - Probabilistic methods: Gaussian Process Regression (GPR)
  - Ensemble methods: Decision Tree
  - Dimensionality reduction methods: Principal Component Analysis (PCA)

26 June 2024

- Introduction to physics-informed or theory-guided ML.
- Case Study I with Python coding: Heat transfer analysis during curing of a polymeric material in an oven
  - Physics: convection + conduction + polymerization
  - Method: Neural Networks with physics-based transformations
- Case Study II with Python coding: Outlier and noise detection in mechanical tests
  - Physics: failure of composite materials
  - Method: Robust Principal Component Analysis (RPCA) with physics-based transformation

27 June 2024

- Case Study III with Python coding: Kinetics discovery from test data
  - Physics: rate of chemical reactions
  - Method: SINDy (Sparse Identification of Nonlinear Dynamics)
- Case Study IV with Python coding: 3D printing
  - Physics: convection + conduction + flow + surface tension + failure
  - Method: Ensemble methods with FE simulation-based data transformation
- Tentative Case Study V with Python coding: Failure of adhesive bonding
  - Physics: residual stresses + hydrothermal stresses + failure
  - Method: Gaussian Process Regression in physics-informed domains

## Speakers' bio

**Navid Zobeiry** is an Assistant Professor at the Materials Science and Engineering Department of the University of Washington, USA. He is also an Adjunct Professor at the Aeronautics & Astronautics Department, University of Washington; a member of the Scientific Advisory Committee of the Advanced Composites Center (ACC), University of Washington; and an Affiliate Faculty at the Boeing Advanced Research Center (BARC), University of Washington. He earned a PhD in Civil Engineering at the University of British Columbia. He is the Technical committee vice-chair of the American Society of Mechanical Engineers (ASME), Aerospace Materials; Technical committee member of the American Society for Composites (ASC); and member of the Scientific Committee for the Italian Association of Aeronautics and Astronautics (AIDAA).

## Registration and Contacts

### Course Code:

This course is part of the 2023 institutional activity for AIDAA members. The **registration** requires the purchase of one of the packages described here <http://www.aidaa.it/package-list/>, and the completion of the online form.

**Course platform:** Webex, a link will be sent via email as the registration is complete.

At the end of each course, **attendance certificates** will be sent to participants via email.

For further info, please, contact [academy@aidaa.it](mailto:academy@aidaa.it)

## Figures

