Doctoral Dissertation
Doctoral Program in Mechanical Engineering (35th Cycle)

Data driven and physics based methods to assess the mechanical response of advanced materials

From experiments to efficient predictions

By

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Abstract

This PhD thesis pioneers an innovative approach, merging physics-based models with data science techniques to efficiently define and predict the mechanical properties of advanced materials. Focusing on composite materials and additive manufactured metals with intricate microstructures, we aim to bridge the gap between microstructural features and material properties, vital for enhancing the design of advanced materials.

Traditional Machine Learning (ML) approaches often prioritize accuracy over physics compliance. In response, this thesis introduces the concept of Mechanistic Data Science (MDS), which combines the predictive power of ML with the grounding in physics laws. At its core, MDS integrates physics knowledge with advanced machine learning methods, offering a solution to a longstanding challenge: efficiently predicting the mechanical properties of complex materials with intricate microstructures. While the objective is clear—to establish a link between microstructural features and material properties—the true achievement lies in the methodology itself. The thesis unfolds in a series of interconnected chapters, each contributing to the overarching goal.

A Physics-Informed Neural Network (PINN) with a customized architecture is developed to learn the constitutive behaviour of orthotropic materials from the distributed strain measurements acquired with the Digital Image Correlation (DIC). Being the Neural Network (NN) a universal approximator, the proposed architecture can learn arbitrary constitutive models avoiding the definition of parametric models and defining the constitutive properties of the materials from the experimental data. With the proposed approach the full elastic constitutive model of an orthotropic material can be defined with a single test, and different damaging

laws can be inferred using the same architecture. The model is validated on artificial data - i.e., generated with a Finite Element Model (FEM) - and later applied to experimental data. This PINN approach eliminates the need for defining parametric models, allowing for rapid characterization of material properties.

Moving forward, the thesis combines DIC data with microstructural reconstructions from Fiber Reinforced Polymer (FRP) samples to characterize composite material stiffness, accounting for manufacturing-induced defects and fiber misalignment. This information contributes to the development of a Stochastic Volume Element (SVE), a mesoscale representation of the FRP, which have a microstructure sampled from the experimental reconstructions and variable material properties statistically calibrated from the experiments. When the SVE is integrated into a multiscale Finite Element Model (FEM), offers a unique capability to provide probabilistic predictions of structural responses.

The thesis further extends the application of MDS to predict the crushing behavior of origami-shaped carbon FRP structures at the part scale, optimizing design processes with a significant reduction in computational cost. The model evaluates the crushing force and the absorbed energy of the thin-walled structure by preserving the physics relationship between the two quantities, which is governed by the energy conservation law. The good accuracy of the method and the reduced computational cost, permit to perform an optimization study of the origami tube with a full exploration of the design space reducing the optimization time by 30 times. The results of the PINN are compared with the FEM, showing a remarkable accuracy of the surrogate model.

The final chapter focuses on the fatigue response of aluminium alloys produced through Additive Manufacturing (AM). By combining experimental observations of manufacturing parameters with a damage-tolerant model developed by Murakami, a customized Neural Network (NN) architecture is employed. This chapter demonstrates remarkable accuracy in predicting the fatigue response, offering designers a potent tool to assess the influence of manufacturing processes on material properties and avoid impractical experimental investigations.

The MDS methods presented in this thesis puts its roots in the governing laws of the mechanics, leveraging on the increasing data that are nowadays available thanks to innovative experimental techniques (e.g., micro-CT, DIC) and shared database, or can be reliably generated through experimentally calibrated models (e.g., FEM).

In summary, this thesis showcases the novel MDS framework, effectively combining empirical and theoretical knowledge with abundant data to advance materials science and design. While the abstracted methodology connects various chapters, it is the transformative potential of MDS that unites these diverse investigations, paving the way for future research to refine and expand upon this innovative approach.