PhD position

AI-driven surrogate approaches for microstructure-aware structural modeling

Context and project description

The present PhD proposal is part of the project **AMMETIS**[1] (AI-assisted Simulations of Microstructure driven MEchanical properties from high Throughput and multiscale analysIS), in the framework of **PEPR DIADEM**[2], which aims to develop an advanced characterization platform for innovative materials by combining advanced experimental techniques, physics-based mesoscopic modeling, and artificial intelligence. Within this context, high-throughput experiments and large-scale numerical simulations will generate rich datasets describing the relationship between microstructure, deformation mechanisms, and mechanical response.

While physics-based simulations involving advanced mesoscopic crystal plasticity provide powerful predictive capabilities, they remain computationally expensive when applied to realistic microstructures and large-scale structural analyses. A key challenge is therefore to develop efficient surrogate models capable of rapidly predicting macroscopic mechanical properties directly from microstructural descriptors while preserving the underlying physical mechanisms.

The objective of this PhD project is to develop AI-based surrogate models for microstructure-aware macroscopic mechanical behavior by leveraging the large datasets generated within the AMMETIS project. These datasets will combine information from high-resolution experiments (HR-DIC, HR-EBSD, nanoindentation mapping) and large-scale numerical simulations performed using advanced FFT-based crystal plasticity platform.

Different machine learning strategies will be explored to capture the complex relationships between microstructural features and mechanical responses. In particular, the project will investigate deep learning architectures capable of learning microstructure-property mappings, including convolutional neural networks for microstructure image analysis, graph-based representations of microstructures, physics-oriented microstructure descriptors discovery based on the use of RRAE (rank reduction autoencoders) and neural operator approaches designed to approximate the solution of complex mechanical problems [1-3]. Special attention will be devoted to the integration of physics-informed constraints in the learning process to ensure robustness, interpretability, and extrapolation capabilities of the trained models [4,5].

The resulting surrogate models will enable fast prediction of effective mechanical properties and deformation fields for complex microstructures, thereby providing an efficient bridge between mesoscale simulations and structural-scale applications. These tools will significantly accelerate the

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[1] https://www.pepr-diadem.fr/projet/ammetis-2/
[2] https://www.pepr-diadem.fr/

exploration of microstructure-property relationships and will open new perspectives for the design and optimization of advanced structural materials.

Required skills

- Master's degree (or equivalent) in Mechanical Engineering, Materials Science, Applied Mathematics, Data Science or Computational Mechanics.
- Solid background in continuum mechanics and numerical modeling
- Strong interest in machine learning and scientific computing
- Experience with numerical methods for PDEs and data-driven modeling
- Programming skills in Python and machine learning packages such as PyTorch and TensorFlow
- Scientific curiosity and critical thinking
- Ability to work in interdisciplinary environments
- Motivation for collaborative academic-industrial research

Starting date, duration and location of the PhD

The PhD position is available starting in September 2026 (flexible date). The research will be conducted primarily at PIMM (Laboratoire Procédés et Ingénierie en Mécanique et Matériaux), Paris, in collaboration with LEM3 (Laboratoire d'Études des Microstructures et de Mécanique des Matériaux). The duration of the PhD is three years, with a gross salary of around €2300 per month.

Application

Applications (including a CV, transcripts of Master's years 1 and 2 (or equivalent), a cover letter describing the candidate's interests and skills related to the proposed PhD topic, the contact details of two academic referees, and, if possible, two letters of recommendation, all compiled into a single PDF file) should be sent to:

- Francisco Chinesta (francisco.chinesta@ensam.eu)
- Sebastian Rodriguez (sebastian.rodriguez_iturra@ensam.eu)
- Duc-Vinh Nguyen (duc-vinh.nguyen@ensam.eu)
- Mohamed Jebahi (mohamed.jebahi@ensam.eu)

References

[1] Chinesta F., Cueto E., Abisset E., Duval J. L., El Khaldi, F. (2020). Virtual, Digital and Hybrid Twins. A new paradigm in data-based engineering and engineered data. Archives of Computational Methods in Engineering. 27, 105–134.

[2] Chinesta F., Cueto E. (2022). Empowering Engineering with Data, Machine Learning and Artificial Intelligence: A Short Introductive Review. Advanced Modeling and Simulation in Engineering Sciences, Adv. Model. and Simul. in Eng. Sci. 9, 21

[3] Cueto, E., Chinesta, F. Thermodynamics of Learning Physical Phenomena. Arch Computat Methods Eng 30, 4653–4666 (2023).

[4] Nguyen, D. V., Jebahi, M., & Chinesta, F. (2024). Spatio-temporal physics-informed neural networks to solve boundary value problems for classical and gradient-enhanced continua. *Mechanics of Materials*, *198*.

[5] Nguyen, D.-V., Jebahi, M., & Chinesta, F. (2026). Wavelet-based enrichment for physics informed neural networks to approximate localized and heterogeneous solutions in solid mechanics. *Computer Methods in Applied Mechanics and Engineering*, *452*, 118768.