Master thesis proposal

AI-Driven Neural Operators for Modeling of Phase Transformations in Materials

Background

Phase transformations play a crucial role in the elaboration of metal materials. They determine the material's structure, which, in turn, influences the properties of the final product. **Phase-field models** that describe phase transformations in materials are formulated by **reaction-diffusion partial differential equations (PDEs)**. These models couple phase transformations to external fields such as temperature, chemical composition, stresses, and liquid flow.

Today, such PDEs are generally solved numerically with classical discretization methods (finite difference, finite element, spectral, etc.). Novel **artificial intelligence methods for approximating solutions of PDEs** have the potential to be much faster and thus to revolutionize the modeling of phase transformations. These methods provide *surrogate models* based on neural networks (NNs). Usually, data-driven supervised learning is used to train the NNs. However, such approaches require large datasets and struggle with predictions beyond the parameter range they were trained on (*out of distribution*).

To enhance performance, we combine two cutting-edge concepts: **Physics-Informed** (PI) unsupervised learning, which trains a surrogate model to satisfy the governing equations without requiring data, and **Neural Operators** (NO), NNs that directly learn the numerical scheme approximating the governing equations. The resulting PINOs (Physics-Informed Neural Operators) require less training resources and can be used for out-of-distribution predictions, making them a powerful surrogate for solving PDEs efficiently.

We recently developed a novel custom PINO approach for phase-field models, employing a bespoke Reaction-Diffusion NN architecture. The objective of the master thesis is to leverage this approach by fine tuning of its parameters and of the training strategy to achieve the best possible accuracy and generality of the predictions.

Objectives and impact

The objective of the Master thesis is to extend the developed approaches in two ways.

- To improve the accuracy of the PDE solution approximations by fine-tuning a dedicated neural network architecture.
- To explore training strategies and neural network architectures to enhance the generality of the PINO models, enabling them to make robust out-of-distribution predictions.

The student will also be able to participate in the DIADEM Summer School 2026.

Internship location

Institut Jean Lamour (IJL) and **Institut Élie Cartan de Lorraine (IECL),** Nancy, France

Funded by PEPR DIADEM, this project is an interdisciplinary collaboration of experts on multiscale modeling of metallurgical phase transformations (IJL) and experts on PDEs and control theory (IECL).

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Requirements for applicants

- Last year master student in a relevant discipline (applied mathematics, engineering, materials science…)
- Solid background in numerical methods and machine learning.
- Good computer programming skills.
- Proficiency in technical report writing and presentation.
- Excellent capacity for teamwork and ability to work in a multidisciplinary environment.
- Fluent in English, some knowledge of French is beneficial.

How to apply

Send us your CV and a motivation letter by email.

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The position is open until filled. Eligible applicants will be interviewed by an ad hoc committee after receipt of the application.