

Master thesis proposal

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

Keywords : Phase transformations, Phase-field models, Partial differential equations, PINNs, Neural operators

SCIENTIFIC DESCRIPTION :

This project is an interdisciplinary collaboration between experts on phase-field and multiscale modeling of metallurgical phase transformations from **Institut Jean Lamour (IJL)** – Benoît Appolaire and Miha Založnik – and experts on partial differential equations (PDEs) and PDE control theory from **Institut Élie Cartan de Lorraine (IECL)** – Ludovick Gagnon.

Phase transformations play an important role in elaboration of metal materials because they determine the structure and, consequently, the properties of the material. The properties of the product depend on the final phases, their size and shape.

Phase-field models that describe phase transformations in materials [Kur21,Tou22] are formulated by **reaction-diffusion PDEs**. This description is such that it couples the phase transformations to external fields (temperature, chemical composition, stresses, liquid flow, etc.).

Today, such PDEs are generally solved numerically with classical discretization methods (finite difference, finite element, Fourier spectral, etc.). The multi-scale and nonlinear nature of phase transformation models, however, requires fine space and time discretizations, leading to long computation times and costly simulations. These times are prohibitive for scaling up to the process level and for conducting extensive parametric studies. Recently developed **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 employ surrogate models based on neural networks (NN).

Most NN training processes in literature are data-driven [Din24], requiring substantial datasets and frequently resulting in instability in long-term predictions. Such approaches also suffer from limited generalization – ability to predict results that are outside the parameter range of the training set. Better generalization properties are provided by **Physics Informed Neural Network (PINN)** type approaches [Kar21]. PINNs are trained to satisfy the governing physical equations by minimizing the residuals of the PDEs. Plain vanilla PINNs pose several challenges: need for large number of collocation points, difficulties in achieving convergence, and long training times [Mat24]. Also, a new PINN needs to be constructed for different boundary and initial conditions, limiting their applicability.

A more practical approach is to design NNs that take initial and boundary conditions as inputs, giving rise to so-called neural operators that learn the numerical scheme directly. Phase-field models offer another advantage: they can be formulated as a variational problem, involving the minimization of a functional. This is leveraged by the **Deep Ritz method** [Yu18], a NN-based technique that uses deep learning to approximate solutions by minimizing an energy functional rather than directly solving the PDEs as in PINNs. This strategy has been shown to be more efficient for highly nonlinear PDEs [Mat24,Hua25].

We recently employed a Deep Ritz approach in a **novel Reaction-Diffusion neural operator** architecture [Hua25] for phase-field equations. We have shown that this architecture outperforms standard NN models for the Allen-Cahn equation as well as for a model of dendritic solidification [Kar98], applicable in conditions of **metallurgical processes**. The objective of the master thesis will be to leverage this approach by fine tuning of its parameters and of the training strategy in order to achieve the best possible accuracy and generality of the predictions.



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Objectives and impact

The objectives of the Master thesis are to extend the developed approaches in two ways:

- to improve the better 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 NN models, enabling them to make robust out-of-distribution predictions.

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

References

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Methods: Our NN implementations employ the *JAX* framework alongside the *Equinox* library. We use different NN architectures: standard architectures, such as multi-layer perceptrons, FNO (Fourier neural operator), UNet, as well as custom developed Reaction-Diffusion Neural Operators (RDNO) [Hua25]. For benchmarking we use in-house phase-field model codes solved by a Fourier spectral scheme.

Budget description and use: Full internship stipend (*gratification de stage*) and travel expenses for the participation in the DIADEM Summer School 2026 for one student.

Requirements for applicants:

- 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.

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