18 March 2025

PhD contract offer

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

General information

Workplace: Nancy, France
Type of contract: PhD contract funded by the ENACT AI Cluster
Contract period: 36 months
Application deadline: 20 April 2025
Expected date of employment: October 2025
Proportion of work: Full time
Remuneration: 2200 € gross per month until 31/12/2025 and 2300 € gross per month from 1/1/2026
Desired level of education: Master's degree in mathematics, physics or engineering

This PhD offer is a collaborative project of IJL and IECL and is provided by the ENACT AI Cluster and its partners. Find all ENACT PhD offers and actions on https://cluster-ia-enact.ai/

Project description

Background

Phase transformations play an important role in elaboration of metal materials because they determine the structure and, consequently, the properties of the material. They occur, for example, during the additive manufacturing (3D printing) of a metal part. First, the molten liquid metal transforms to a crystalline solid structure and then further phase transformations occur in solid state. The properties of the part depend on the final phases, their size and shape.

Phase-field models that describe these phase transformations are formulated by reaction-diffusion partial differential equations (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.

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, requiring substantial datasets and suffering from limited generalization – ability to predict results that are outside the parameter range of the training set.

Better generalization is provided by Physics Informed Neural Network (PINN) type approaches. PINNs are trained to satisfy the governing physical equations by minimizing the residuals of the PDEs. A particularly practical approach of this type, that avoids some of the pitfalls of plain vanilla PINNs, are *neural operators* that learn the numerical scheme directly. Phase-field models offer another advantage: they can be formulated as a variational problem and can be solved by by minimizing an energy functional rather than directly solving the PDEs. This strategy, leveraged by the Deep Ritz deep learning method, has been shown to be more efficient for highly nonlinear PDEs.

We recently developed a novel Reaction-Diffusion neural operator architecture for phase-field equations employing the Deep Ritz approach. We have shown that this architecture outperforms standard NN models for certain phase-field models (Allen-Cahn, dendritic solidification).

Objectives of the PhD

The objectives of the PhD thesis are to extend the developed approaches to:

- achieve better accuracy of the PDE solution approximations with a suitable or more sophisticated neural network architecture;
- achieve better generality of the NN models in order to obtain robust out-of-distribution predictions;
- extend the Deep Ritz NN approaches to further phase-field models including other multiphysics couplings;
- develop NN approaches for sharp-interface formulations of phase transformations, such as the Stefan problem;
- develop similar NN approaches for phenomenological phase transformation models that can simulate larger spatial and temporal scales, such as the Grain Envelope Model for dendritic solidification.

Work environment

The PhD student will work under the supervision of an interdisciplinary team in materials science (Institut Jean Lamour – IJL) and mathematics (Institut Élie Cartan de Lorraine – IECL): Dr. Miha Založnik, expert on solidification modeling, Ludovick Gagnon, expert on Partial Differential Equations, Prof. Benoît Appolaire, expert on phase-field modeling in materials. She/he will be part of the *Solidification* and *Microstructures and Stresses* groups of IJL and the *Partial Differential Equations* group of IECL.

Skills

The funding is open to excellent students from physics, applied mathematics, mechanical/chemical /process engineering or other disciplines. We are looking for candidates with:

- Master's degree in a relevant discipline.
- Solid background in numerical methods and machine learning.
- Good computer programming skills.
- Proficiency in technical report writing and presentation.
- Excellent capacity for teamwork, sense of initiative, and ability to work in a multidisciplinary environment.
- Fluent in English, some knowledge of French is beneficial

Constraints and risks

The position is in a sector relating to the protection of scientific and technical potential. It therefore requires, in accordance with the regulations, that your arrival be authorized by the competent authority of the Ministry of Higher Education, Research and Innovation.

About Institut Jean Lamour and Institut Élie Cartan

The **Institut Jean Lamour (IJL)** is a joint research unit of CNRS and Université de Lorraine. Focused on materials and processes science and engineering, it covers materials, metallurgy, plasmas, surfaces, nanomaterials and electronics. The IJL has 263 permanent staff (30 researchers, 134 teacher-researchers, 99 IT-BIATSS) and 394 non-permanent staff (182 doctoral students, 62 post-doctoral students/contractual researchers and more than 150 trainees), of 45 different nationalities. Partnerships exist with 150 companies and our research groups collaborate with more than 30 countries throughout the world. Its exceptional instrumental platforms are spread over 4 sites; the main one is located on Artem campus in Nancy.

Specializing in a wide range of pure and applied mathematical disciplines, the **Institut Élie Cartan de Lorraine (IECL)** is one of France's largest mathematics laboratories. It has hosted world-renowned mathematicians such as Jean Leray, Jean Dieudonné, Laurent Schwartz (Fields Medal 1950), Jean-Pierre Serre (Fields Medal 1954), Alexander Grothendieck (Fields Medal 1966) and Jacques-Louis Lions.The **Partial differential equations (PDE) team** is one of the four research groups of the IECL. It gathers around 30 permanent researchers in different aspects of the PDEs, from theoretical research to numerical analysis and scientific computing. Recent developments in scientific computing at IECL has led to numerous industrial collaborations

Application

To apply, send us a short statement of your interests, your CV, and full academic transcripts of the last two years of your master's studies. The deadline for application is 20 April 2025.

Eligible applicants will be interviewed by an ad hoc committee after receipt of the application. The selected candidate will be interviewed in May 2025 by a committee of the funding body – the ENACT AI cluster (https://cluster-ia-enact.ai). The notification on funding will be communicated in early June.

Institut Jean Lamour (IJL) falls under a Zone à régime restrictif (ZRR). The selected applicants will be subject to a Security Clearance check, required for employment at IJL.

Contacts:

Dr. Miha Založnik
Institut Jean Lamour
Email: miha.zaloznik@univ-lorraine.fr

Dr. Ludovick Gagnon
Institut Élie Cartan de Lorraine
Email: ludovick.gagnon@inria.fr