Post-doctorate offer in modelling and machine learning for material science

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Post-doctorate title: *Development of a new multi-scale approach combining the phase field model and recurrent neuron networks*

Keywords: Machine Learning, Recurrent Neural Network, Phase Field Model, Phase field Crystal, Multi-Scale Modelling, Structural transformation, Material science.

Host laboratory: Groupe de Physique des Matériaux (GPM), UMR 6634, Université de Rouen-Normandie.

Supervisors: Gilles Demange (Maître de Conférences, GPM), Helena Zapolsky (Professeur, GPM).

Starting date: 01/11/2023-01/12/2023

Duration: 1 year (possible extension).

Contact: gilles.demange@univ-rouen.fr

Subject:

The phase field model (PFM) is a powerful and versatile computational tool for the simulation of microstructure evolution in complex materials. Today, the scope of applications of the PFM ranges from solidification and structural transformations at mesoscale [2] (standard PFM) to grain boundary segregation [3] and displacive transformations [4]at atomic scale (phase field crystal -PFC- [5] and quasi-particules -QA- [6] approaches). However, because the system is therein described by a set of continuous field variables that evolve both in space and time, phase field models turn to be computationally expensive and cumbersome to implement. **This significantly curtails the capacity of the PFM to perform quantitative predictions of the microstructure on space and time scales sufficient to connect to the macroscopic properties of the material.**

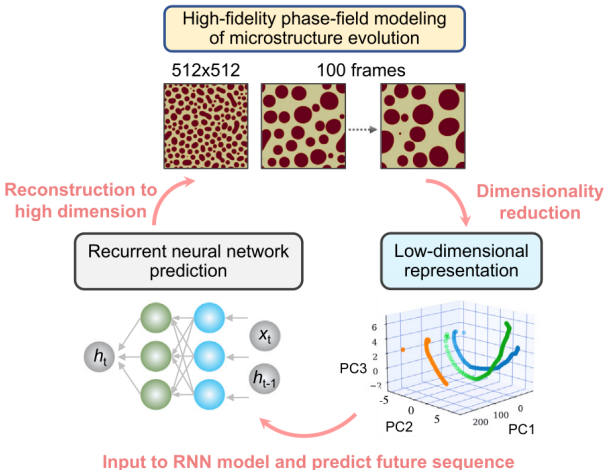

Figure 1: *Accelerated PFM workflow [1].*

Recently, a new strategy has been proposed, that allows to upscale PFM simulations based on a class of history-dependent ML algorithms called Recurrent Neural Network (RNN). RNN demonstrated its ability to learn evolution rules of various dynamics using low dimensionality representation of a large set of microstructure generated by PFM simulations [1, 7]. The trained RNN was then used to extrapolate the evolution of the system to substantially larger space domains, longer times, and new parametric

configurations, yet requiring drastically less computational resources (time and memory) than PFM calculations (see figure 1). However, PFM informed RNN multi-scale models currently remain at the state of proof of concept. **In this context, the central motivation of this project is to develop a new machine learning approach based on the RNN framework, in order to upscale recent 3D high end PFM simulations of specific challenging applications where time and space scale limitations preclude the quantitative connection of materials microstructure with macroscopic properties.** Depending on the progress of the project, the proposed methodology will be applied to the PFC/QA modelling of structural transformations at atomic scale, and/or the dendritic growth of faceted crystals at mesoscale in three dimensions. The project will be organized as follows:

1. The first step of the workflow will be to generate a vast dataset of high fidelity PFM simulations, destined to train and test the RNN procedure. For that purpose, high throughput PFM simulations (standard PFM and/or QA/PFC) will be straightforwardly performed using our pre-existing home-made parallel code on the supercomputer of Normandy (CRIANN).

2. The second step of the procedure will be to project the PFM simulation outputs in a so-called latent space via a dimensionality-reduction method. One ideal candidate will be to compute autocorrelation functions that capture the degree of spatial correlations between locations, and then perform principal component analysis (PCA) on these functions [1]. Features calculation may be performed via the Scikit-Learn python open access library.

3. The third step of the project will be the development of a learning algorithm based on RNN. This will rely on the open-source neurone-network library Keras available on CRIANN.

Expected skills:

1. **General skills in Machine Learning are required.** A previous experience of neural networks would be valuable.

2. **Good programming skills in Python**, or at least in a close language (Julia, C/C++, etc.) is mandatory.

3. Background knowledge in the field of materials and/or condensed matter will be useful.

4. Background knowledge in phase field models (standard PFM, phase field crystal, etc.) will be appreciated.

References

[1] C. Hu *et al.*, Computer Methods in Applied Mechanics and Engineering **397**, 115128 (2022).

[2] I. Steinbach, Modelling and simulation in materials science and engineering **17**, 073001 (2009).

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[7] K. Yang *et al.*, Patterns **2**, 100243 (2021).