

# CIFRE PhD

## CONTEXT AND GOALS OF THE PhD

### AI AND DIGITAL TWINS IN METALLURGY

One of the European Union's objectives in climate change consists of reaching net-zero greenhouse gas emissions by 2050. Such perspective puts the metallic materials industry, as a large contributor to carbon emissions, under tremendous pressure for change and requires the existence of robust computational materials strategies to enhance and design, with a very high confidence degree, new metallic materials technologies with a limited environmental impact. From a more general perspective, the in-use properties and durability of metallic materials are strongly related to their microstructures, which are themselves inherited from the thermo-mechanical treatments.

Hence, understanding and predicting microstructure evolutions are nowadays a key to the competitiveness of industrial companies, with direct economic and societal benefits in all major economic sectors (aerospace, nuclear, renewable energy, naval, defense, and automotive industry).

Multiscale materials modeling, and more precisely simulations at the mesoscopic scale, constitute the most promising numerical framework for the next decades of industrial simulations as it compromises between the versatility and robustness of physically-based models, computation times, and accuracy. The DIGIMU consortium, the RealIMotion ANR Industrial Chair and the DIGIMU software package developed by TRANSVALOR S.A. are dedicated to this topic at the service of major industrial companies like Aperam, ArcelorMittal, Aubert&Duval, Constellium, Framatome and Safran.

In this context, the efficient and robust modeling of evolving interfaces like grain boundary networks is an active research topic, and numerous numerical frameworks exist. In the context of hot metal forming, a new promising front-tracking (FT) method [1,2] was recently developed as illustrated in Fig.1. This PhD will focus on exploring Machine Learning strategies for different applications to enhance the solutions proposed within DIGIMU® for data generation and exploitation. First, 3D representative polycrystalline microstructure reconstruction from 2D data will be explored by GAN based methods [3]. Secondly, use of supervised DNN and Deep Reinforcement Learning will be explored to build fast surrogates on top of high-fidelity simulation data generated by the new developed front tracking method [2]. These tools shall enable the automatic causal interpretation of microstructural singularities such as abnormal grain growth (see Fig 2). The developments will be validated thanks to pre-existing experimental and numerical data concerning the evolution of grain boundary interfaces during recrystallization and related phenomena for different materials. They will also be integrated in the DIGIMU® software.

[1] S. Florez et al., *Computer Methods in Applied Mechanics and Engineering*, 367:113107, 2020.

[2] S. Florez et al., *Statistical behaviour of interfaces subjected to curvature flow and torque effects applied to microstructural evolutions. Acta Materialia*, 222:117459, 2022.

[3] S. Kench, S.J. Cooper, *Generating three-dimensional structures from a two-dimensional slice with generative adversarial network-based dimensionality expansion. Nat Mach Intell*, 3:299-305, 2021.

[4] A. Agnoli et al., *Development of a level set methodology to simulate grain growth in the presence of real secondary phase particles and stored energy - Application to a nickel-base superalloy. Computational Materials Science*, 89:233-241, 2014.

## KEYWORDS

Digital twins - IA - Computational Metallurgy - Interface networks - Front tracking - ToRealMotion algorithms - Mesh based algorithms - Deep learning strategy.

## CANDIDATE PROFILE AND SKILLS

Degree: MSc or MTech in Applied Mathematics, with excellent academic record. Skills: Numerical Modeling, programming, proficiency in English, ability to work within a multi-disciplinary team.

## OFFER

The 3-year Cifre PhD will take place in CEMEF, an internationally-recognized research laboratory of MINES ParisTech and in the TRANSVALOR company. The PhD student will be located in Sophia-Antipolis, on the French Riviera. She/He will join the Metallurgy  $\mu$ Structure Rheology (MSR) CEMEF research team and the Deep Learning & Multiphysics development team from TRANSVALOR under the supervision of Prof. M. Bernacki, Dr. P. De Micheli, and Dr. J. Alves in "Numerical Mathematics, HPC and Data" doctoral speciality. Annual gross salary: about 29.4k€ plus additional benefits from TRANSVALOR S.A.

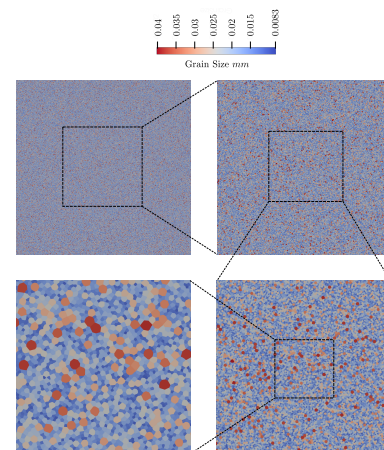


Fig.1. 2D polycrystal composed of 560000 grains - grain growth modeling with FT algorithms [1,2].

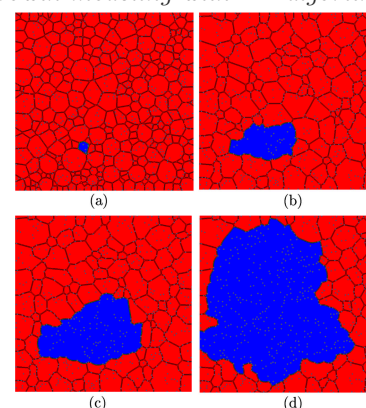


Fig.2. Occurrence of abnormal grain growth for Inconel718 [3].