

## CONTEXT AND GOALS OF THE PHD

### FINITE ELEMENT MODELING OF HOT ISOSTATIC PRESSING AT THE MESOSCOPIC SCALE

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.

Because of opportunities that powder metallurgy (PM) processes offer in both technical and economic points of view, these processes are increasingly used in industries for the manufacture of complex shaped parts for many applications. PM technologies, which allow the production of near-net-shape densified metal or ceramic parts with controlled microstructure, are very diverse but Hot Isostatic Pressing (HIP) appears as the key process when large complex parts, such like nuclear plant components (pipes, valves, impellers...), are required. The modeling of the powder densification during HIP and the prediction of the final microstructure through numerical simulation is an open and complex research problem. It is not easy to answer to seemingly simple questions like: is full densification achieved everywhere in the part? Will the as-HIPed shape allow to achieve the component? Did the powder microstructure lead to a satisfactory dense material which will exhibit good properties? What if I change the HIP parameters (pressure, temperature, time) or the powder production process? Indeed, theories that provide quantitatively correct predictions of local heterogeneities observed during densification of the granular packing, as well as theories able to predict the final polycrystalline grain size distribution, have long been sought to fill a critical link in our ability to model HIP process from start to finish. To date, such theories do not exist. In this context, 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 and the RealMotion ANR Industrial Chair are dedicated to this topic at the service of major industrial companies.

In terms of microscale modeling, the present project aims at developing advanced numerical techniques for taking into account, in 2D/3D simulation context, all the key physical phenomena that take place during HIP process from start to finish. Within a parallel computing context, simulations will be firstly based on a level-set interface capturing technique in a FE framework and Eulerian formalism [1,2]. Combined with an anisotropic mesh adaptation strategy, this numerical approach will be used to describe with accuracy the granular packing geometry, particle interface evolution, grain interface evolution but also the second phase particle populations and their evolution. Such simulations in a context of a new front-tracking methodology will also be considered [3]. The developments will be validated thanks to pre-existing experimental and numerical data concerning the evolution of particle/grain boundary interfaces available in CEA Grenoble.

These numerical developments will also be integrated in an extension of the DIGIMU<sup>®</sup> software dedicated to HIP process modeling at the mesoscopic scale.

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## PARTNERS



## KEYWORDS

HIP process - Digital twins - HPC - Computational Metallurgy - Interface networks

## CANDIDATE PROFILE AND SKILLS

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

## OFFER

The 3-year PhD will take place in CEMEF, an internationally-recognized research laboratory of MINES ParisTech located in Sophia-Antipolis, on the French Riviera. It offers a dynamic research environment, exhaustive training opportunities and a strong link with the industry. Annual gross salary: about 27.7k€. She/He will join the Metallurgy  $\mu$ Structure Rheology (MSR) and the Computational Solid Mechanics (CSM) research teams under the supervision of Prof. M. Bernacki, Dr D. Pino Muñoz, and E. Rigal from CEA Grenoble.

[1] E. Rigal, N. Bouquet, M. Bernacki, and F. Bernard. *Etablissement et évolution des interfaces lors du soudage diffusion. In Journées annuelles de la SF2M, Matériaux et conversion d'énergie, 2015.*

[2] A. Zouaghi, M. Bellet, Y. Bienvenu, G. Perrin, D. Cédacat, and M. Bernacki. *Modélisation de la phase de compaction du procédé CIC à l'échelle mésoscopique. Proceedings of the 20ème Congrès Français de Mécanique, 2011.*

[3] S. Florez, K. Alvarado, D. Pino Muñoz and M. Bernacki. *Computer Methods in Applied Mechanics and Engineering, 367:113107, 2020.*