Postdoc offer 2025- CEMEF

starting at january 2025

Deep learning for the modelling of thermodynamic coupling in additive manufacturing

Gildas Guillemot, David Ryckelynck, Charles-André Gandin

Thermodynamic coupling is essential for modelling mater transformation taking place in forming processes. Its introduction in finite element tools applying at the scale of the processes yet remains limited, justifying the development of alternative methods.

The physical metallurgy modules of the library PhysalurgY (PY https://physalurgy.cemef.mines-paristech.fr/) are coupled with the CALPHAD methodology (CALculation of PHase Diagram) thanks to the call of thermodynamic databases. They give a multicomponent description of the phases found in industrial alloys. The kinetics of phase transformations are computed and should serve as entry to the simulations of forming processes by the finite element method.

Optimization of the call to the CALPHAD method was so far based on multi-field tabs deduced from PhysalurgY, reaching a good precision for sufficiently small tabulation steps. However, tabulations become heavy due to the number of input and output variables, as well as to the multidimensional interpolations.

We propose to develop a module of neural network as part of the PhysalurgY library (PY\ANNE), making use of the progress of recent deep learning methodologies [1, 2]. It should be sufficiently versatile to design input and output fields according the physical metallurgy module considered. The first application will be on solid state precipitation (module PY\PREC) [3]. The on-going PhD work of Ducottet aims at simulating the precipitation for a temperature history deduced for laser powder-bed fusion additive manufacturing [4]. The metallurgical evolution must account for the temperature evolution deduced from finite element simulations using the FusalurgY (FY) tool named MACRO-PBF [5]. The use of the neural network PY\ANNE will permit direct integration of PY\PREC in FY\MACRO-PBF. The combination of the modules PY\PREC and PY\ANNE could be useful for coupling with other software developed in the context of the lab, such as FORGE or THERCAST.

Expected skills: Python programming language, knowledge in supervised learning and metallurgy

Location : Mines PARIS PSL, CEMEF, Sophia Antipolis

Salary : 2950 euros brut

Supervisors :

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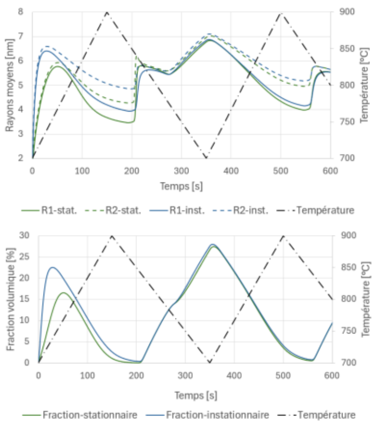
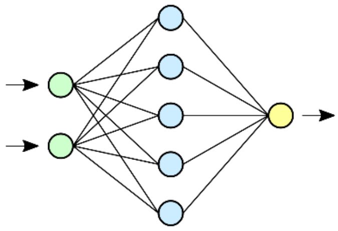
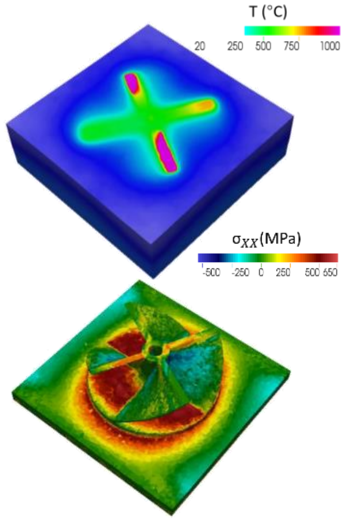
PY\PREC **PY\ANNE** **FY\MACRO-PBF**







[1] D. Marchand, A. Jain, A. Glensk, and W. A. Curtin, *Machine learning for metallurgy I. A neural-network potential for Al-Cu*, Physical Review Materials 4 (2020) 103601.

[2] C. Capdevila, F.G. Caballero, C. García De Andrés, *Determination of Ms temperature in steels: A Bayesian neural network model*, 42 (2002) 894.

[3] G. Guillemot, Ch.-A. Gandin, *An analytical model with interaction between species for growth and dissolution of precipitates*, Acta Materialia 134 (2017) 375.

[4] S. Ducottet, *Modélisation numérique du traitement thermique et de la précipitation à l'état solide en fabrication additive dans les superalliages base nickel*, PhD project, 1st year report (2024).

[5] Y. Zhang, Ch.-A. Gandin, M. Bellet, *Finite Element Modeling of Powder Bed Fusion at Part Scale by a Super-Layer Deposition Method Based on Level Set and Mesh Adaptation*, 144 (2022) 051001-1.

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