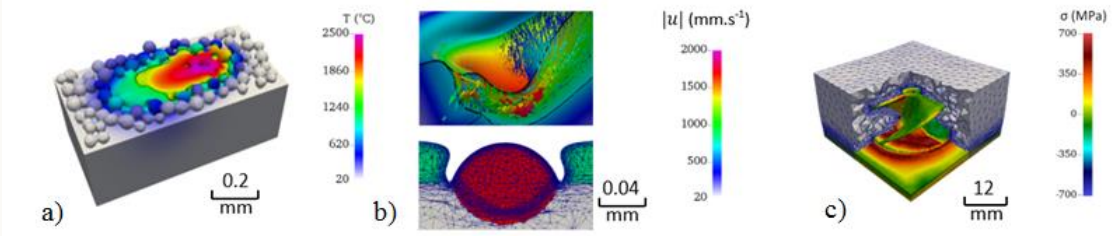
TITLE	**GRain structure based Anisotropic Mechanical behaviour for laser beam MElting simulation at part scale by reduced-order model**
Project acronym	**GRAMME**
Global objective of work	GRAMME project aims at developing an efficient and relevant coupling strategy in laser powder bed fusion (LPBF) process modelling between microstructure development and anisotropic mechanical behaviour at part scale during and after construction. An efficient computational platform based on model-order reduction and experimental validations will be established by the end of the project to meet this objective.
Context	LPBF is one of the typical powder-bed fusion additive manufacturing (AM) techniques, which can fabricate quasi-fully dense near net-shape components from metallic powders. As a result, great interest is received from both industries and academics. However, during the AM process, the extremely high temperature gradients (10 °C μm^{-1} ~ 20 °C μm^{-1}) and cooling rates (10^5 ~ 10^8 K s^{-1}) [1] lead to solidification of the melt pool in form of columnar dendrites oriented along the building direction and rather equiaxed grain shapes at the section perpendicular to the building direction [2]. This anisotropic microstructure leads to different mechanical properties in the construction and scan directions. The associated anisotropic mechanical behaviour may induce unpredictable distortion or damage for thin-walled structures during the process [3]. So the control of the anisotropic grain microstructure and its associated mechanical behaviour is still a big challenge to master LPBF processes, especially when complex part shape is to be developed. In order to minimize costly trial and error approaches by repeated experiments, numerical methods have been introduced and continuously developed to model the thermal and mechanical response of materials during and after the construction process. In the team Metallurgy, Mechanics, Structures & Solidification (2MS) at the Centre de Mise en Forme des Matériaux (CEMEF), MINES ParisTech, three-scale numerical models of LPBF process have been established in a unified framework of 3D finite element (FE) / level-set (LS) formulations (Fig. 1). The first model was proposed by Chen et al. [4] at meso-scale for LPBF processing of alumina to capture melt pool hydrodynamics, track formation and associated local stress during processing. It was extended by Queva et al. to account for vaporization effects for IN718 and Ti-6Al-4V [5] (Fig. 1b). The same FE/LS formulation was adapted at the micro-scale defined by the explicitly described powder particles [6] (Fig. 1a). This could potentially be used to simulate more accurately porosity formation by lack of fusion and to investigate the influence of powder granulometry on melt pool formation and surface roughness. Finally, the FE/LS strategy has been extended to macro-scale simulations without considering melt pool nor hydrodynamics, providing a description of heat flow and mechanical behaviour at the scale of the whole part [7] (Fig. 1c). Recently, the fraction of layer [7], layer by layer and super-layer [8] methods have been developed to reduce computational cost.  Fig. 1 Three-scale models developed at CEMEF (IN718): a) Particle-scale model: temperature distribution, b) Meso-scale model: fluid flow in melt pool, c) Macro-scale model: stress distribution.

Detailed presentation with figure(s)

The purpose of GRAMME project is to develop a numerical platform for optimizing the LPBF process by coupling the description of the development of the solidification grain structure and its anisotropic mechanical behaviour at part scale. A FE heat flow model at part scale will be coupled to predict the grain structure predicted by Cellular Automaton (CA) method [9]. Anisotropic elastic-viscoplastic laws will be tested and adapted to different grain structures for the mechanical analysis during and after the construction process. The prediction of microstructure, distortion and residual stresses will be validated by experiments through manufacturing of simple parts before final application to complex parts. As a by-product of the study, a benchmark exercise concerning the prediction of grain structure, distortion and residual stresses, with clear and detailed input process parameters, online measurements and post-process characterization measurements, will be developed and released to the relevant academic community. To reduce computational cost for non-linear mechanical simulations, the reduced-order model will be applied for both validation and demonstration parts [10].

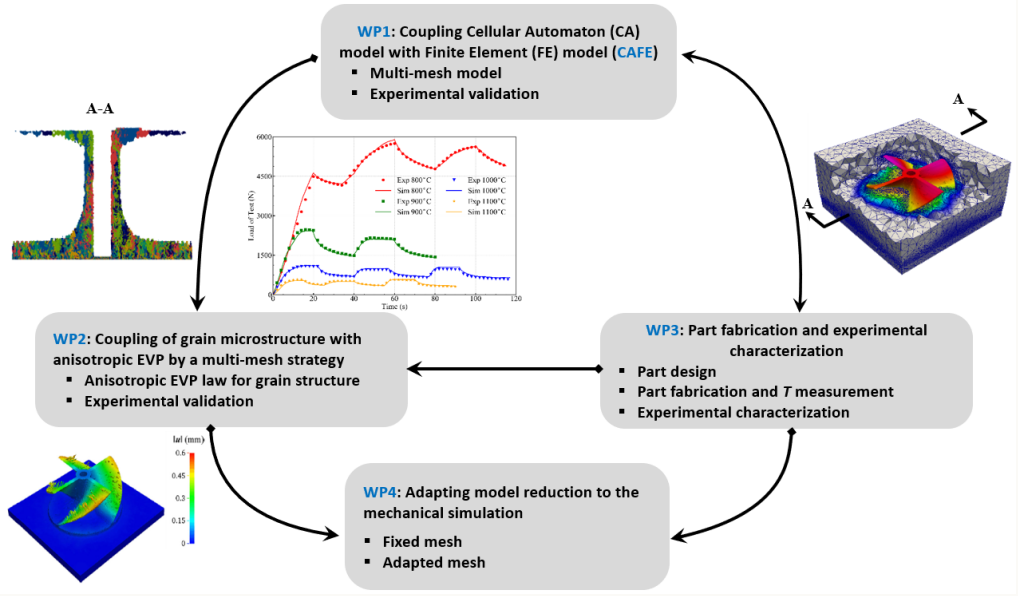


Fig. 2 Schematics of thermo-metallurgical-mechanical model interactions

This project is a central research field at CEMEF, i.e. Material Forming. The coupling work between Metallurgy and Mechanics is also one of the essential tasks of the research group 2MS. The main research works will be structured in four work packages (WPs, Fig.2):

- WP1: Coupling the cellular automaton (CA) model with the finite element (FE) heat flow.
- WP2: Coupling the description of the grain structure with anisotropic elastic-viscoplastic laws.
- WP3: Part fabrication and experimental characterization.
- WP4: Adapting model-order reduction to the mechanical simulation of the LPBF process.

This project is mainly led by Yancheng ZHANG, who is permanent Associate Professor in MINES ParisTech, CEMEF. The recruited Ph.D. student will be co-supervised by three senior researchers within group 2MS at CEMEF. The CAFE method in WP1 will be developed in collaboration with Gildas Guillemot, Associate Professor, and Charles-André Gandin, CNRS senior researcher. The anisotropic plasticity and experimental characterization will be collaborated with Michel Bellet, Professor.

All the numerical simulations will be performed within the C++ library **CimLib** developed in the laboratory CEMEF, in which a first application of the CAFE model for AM-LPBF is currently being achieved in the PhD work of Théophile Camus (defense planned in 2022) in the 2MS team (Fig. 2, grain structure at section A-A). The PhD student will adapt and extend the existing numerical developments in this library and specifically its application to LPBF simulations. The characterization of anisotropic laws will benefit from one on-going PhD work funded by CSC

	and SAFRAN. Specimens for validation of the numerical model will be printed at CMAT (Centre des Matériaux, Mines ParisTech Evry) with the help of Jean-Dominique Bartout (senior engineer from CMAT) and Christophe Colin (senior researcher). Moreover, in-situ temperature measurements are planned by InfraRed imaging of the surface being printed, and by embedded thermocouples through interrupted constructions. The team 2MS will use the computational resources and experimental facilities available at CEMEF for numerical simulation and for the other characterizations (microstructure, residual stresses, distortions). [1] Y. Zhang, G. Guillemot, C.-A. Gandin, M. Bellet. Comptes Rendus Mecanique 346 (11) (2018): 1055-1071 (cover page). [2] K. Kunze, T. Etter, J. Grässlin, V. Shklover. Materials Science and Engineering: A, 620 (2015): 213-222. [3] M. Ni, C. Chen, X. Wang, P. Wang, R. Li, X. Zhang, K. Zhou. Materials Science and Engineering: A 701(2017): 344-351. [4] Q. Chen, G. Guillemot, C.-A. Gandin, M. Bellet. Additive Manufacturing 16 (2017): 124–137. [5] A. Queva, G. Guillemot, C. Moriconi, C. Metton, M. Bellet. Additive Manufacturing 35 (2020): 101249. [6] Y. Shan, Q. Chen, J. Yu, M. Bellet, Y. Zhang. Planned to submit to "Applied Physics B" (2021). [7] Y. Zhang, G. Guillemot, M. Bernacki, M. Bellet. Computer Methods in Applied Mechanics and Engineering 331 (2018): 514–535. [8] Y. Zhang, C.-A. Gandin, M. Bellet, submitted to Journal of Manufacturing Science and Engineering (2021). [9] S. Chen, G. Guillemot, Ch.-A. Gandin, Acta Materialia 115 (2016) 448-467. [10] Y. Zhang, A. Combescure, A. Gravouil. Finite Elements in Analysis and Design 102-103 (2015): 37–51.
Tools	Numerical development is based on the parallel finite element library CimLib®; Fabrication and characterization of additive manufactured specimens will benefit from available apparatus within CMAT (part fabrication by the machine CONCEPTLASER M2 and temperature measurement) and CEMEF (measurements of crystal texture orientation by Scanning Electron Microscopy with Electron Back Scattered Diffraction, distortion and residual stress).
Key-words	Grain structure, Anisotropic plasticity, Thermo-mechanical modelling, Model-order reduction, Laser beam melting
Project type/ cooperation	The GRAMME project has been selected in July 2021 within the framework of the JCJC program (Jeune chercheur, Jeune chercheuse) of ANR (Agence Nationale de la Recherche). Gross monthly salary of 1827.55 euros.
Skills, abilities requested	Engineer/Master student in the field of computational mechanics, or applied mathematics. Strong knowledge of finite element method, solid mechanics and programming (C++) skills, good English level and basic knowledge of metallurgy are required.
Location	CEMEF (Sophia Antipolis), MINES ParisTech, PSL Research University.
CEMEF team(s)	2MS
Expected starting date	September or October 2022 (3 years)
Supervisor(s)	Yancheng ZHANG, Gildas GUILLEMOT, Michel BELLET, Charles-André GANDIN
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