In situ multimodal experimental testing and simulations in volume for statistical analysis of crystal plasticity

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Establishing microstructure-property relationships is a critical engineering challenge for advanced structural materials. Metals display heterogeneous polycrystalline organization which drives performance, hence the necessity to access to grain and sub-grain scales.

A variety of characterization techniques now allows to reach those levels of details. Primarily recent progress in synchrotron and laboratory X-ray techniques [1] have paved the way to a paradigm shift leading to more and more complex non destructive multimodal in situ experiments producing significantly richer datasets [2]. In particular, Diffraction Contrast Tomography (DCT - developed at ESRF) allows reconstruction of 3D digital grain maps on which simulations can be computed directly [3]. Convergence of complex experimental and numerical techniques lead to wealthy but unconsolidated massive datasets. Thanks to development of data plateforms, concurrent analysis of the modalities is made possible.

This work aims to present on-going deployment effort for users of a in situ X-ray technique involving Near Field DCT and Far Field 3DRXD on PSICHE beamline at synchrotron SOLEIL. In addition we will showcase a new type of methodology combining X-rays with laboratory based techniques (SEM, in situ EBSD) and simulations with the objective to probe microstructure-properties. Actual datasets on titanium samples will be presented in this scope that allow to study the development of polycrystal plasticity during tensile loading. Specifically regarding digital twins, a crystal plasticity finite strain model is implemented within a massively parallel FFT solver framework [4] .Mechanisms of interest include slip activity, stress field and lattice rotation evolution at grain level.

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Image-based digital twins on Nickel-based superalloy fatigue specimens via model order reduction

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Owing to drastic security criteria in the aeronautical industry, manufacturing parts of Safran's aircraft engines are controlled at almost every step of the fabrication process. Aircraft engines performance enhancement is a challenge that induces development of more complex geometries. To maintain mechanical behaviour of critical pieces like high pressure turbine blades, fresh air is injected through the piece and escapes using profiled drillings called Shaped Holes. To withstand such a severe environment, blades are produced via investment casting technology with the third generation Nickel-based single crystal superalloy CMSX4-PLUS **[Wahl and Harris, 2020]**. This process can be the source of some geometrical variabilities, which in turn can affect the lifetime. We present a new approach for lifetime estimation considering real geometries obtained via X-ray Computed Tomography (CT). CT data is used to create FEA-compatible meshes **[Taddei et al, 2004]** and compare their simulated lifetime to experimental results. The lifetime predictions are carried out on typical Shaped Hole drilled on tubular specimens all imaged by CT. The experimental tests consist in low cycle creep-fatigue cycles of uni-axial loadings under a thermal gradient based on the set-up developed in **[Koster et al, 1994]**. An infrared furnace heating while fresh air is injected from either side of the sample generates the thermal loading with wall thermal gradient. A thermo-mechanical digital twin is adjusted on experimental results to simulate the elastoviscoplastic behavior of the Nickel-based single crystal superalloy Fatigue specimen. The mechanical model is a *Meric-Cailletaud* formulation under crystalline plasticity theory **[Meric, 1991]**. The lifetime is predicted with a behavior-uncoupled stress-based model called "*Fat-Flu*" where damaging is computed from a non-linear summation of Creep and Fatigue damaging **[Bonnand, 2006]**. Creep damage is based on a Hayhurst formulation adapted for single crystal with multi axial loading and Fatigue is computed using a Chaboche model. Still, the heavy costs of 3D simulation using a real geometry from CT measurements have led to model order reduction methods for computations speed-up. Hyper Model Order Reduction methods may be used to fasten computations **[Ryckelynck, 2005]**. Interest mechanical fields are reduced with Proper Orthogonal Decomposition (POD) added to mesh reduction technics. To allow such methods, for image-based digital twin, a mesh-morphing algorithm has been developed to compensate mesh morphological scattering of tomography meshes. A digital twin database with a statistical model is assembled to represent the parts' process geometrical variations impact on the lifetime. Thus, the thesis' work aim to create an automatic chain for lifetime prediction with accelerated computations, as shown on Figure 1.

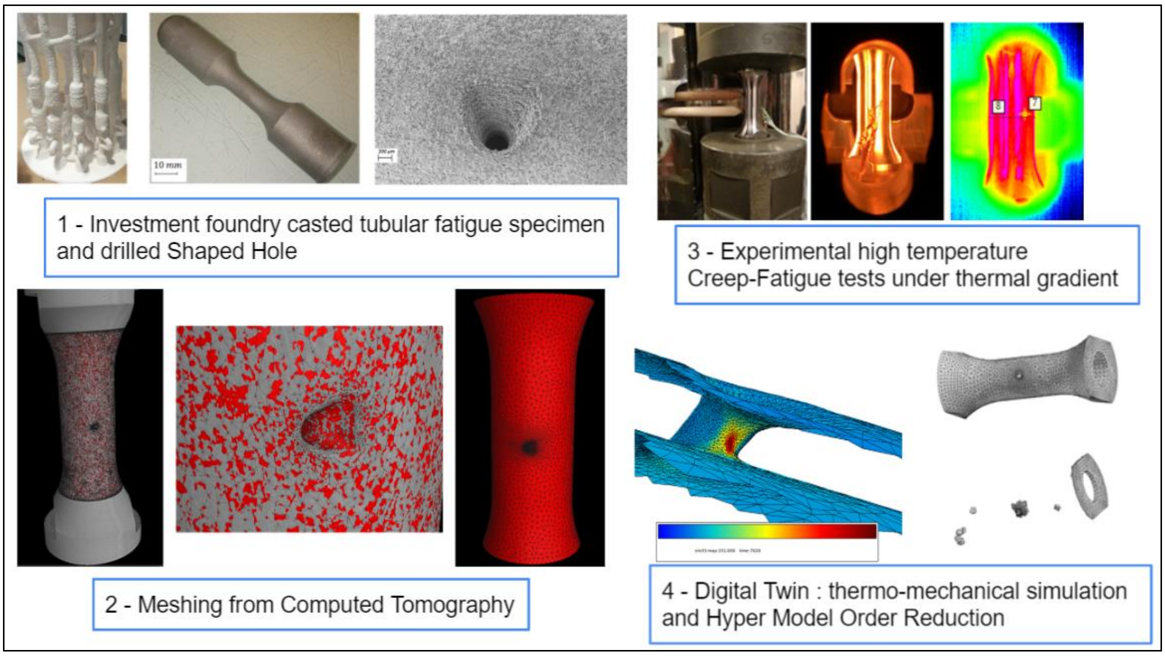

Figure 1 - Lifetime prediction chain using digital twin based on CT scan

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Uncertainty quantification in a mechanical submodel driven by a Wasserstein-GAN

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Abstract

The analysis of parametric and non-parametric uncertainties of very large dynamical systems requires the construction of a stochastic model of said system. Linear approaches relying on random matrix theory Soize (2000) and principal componant analysis can be used when systems undergo low-frequency vibrations. In the case of fast dynamics and wave propagation, we investigate a random generator of boundary conditions for fast submodels by using machine learning. We show that the use of non-linear techniques in machine learning and data-driven methods is highly relevant.

Physics-informed neural networks Raissi et al. (2017) is a possible choice for a data-driven method to replace linear modal analysis. An architecture that support a random component is necessary for the construction of the stochastic model of the physical system for non-parametric uncertainties, since the goal is to learn the underlying probabilistic distribution of uncertainty in the data. Generative Adversarial Networks (GANs) are suited for such applications, where the Wasserstein-GAN with gradient penalty variant Gulrajani et al. (2017) offers improved convergence results for our problem.

The objective of our approach is to train a GAN on data from a finite element method code (Fenics) so as to extract stochastic boundary conditions for faster finite element predictions on a submodel. The submodel and the training data have both the same geometrical support. It is a zone of interest for uncertainty quantification and relevant to engineering purposes. In the exploitation phase, the framework can be viewed as a randomized and parametrized simulation generator on the submodel, which can be used as a Monte Carlo estimator.

Keywords : deep learning, adversarial learning, generative models, submodeling, uncertainty quantification, supervised learning, regression models.

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