Bridging scales in Titanium alloys

Postodctoral position

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The European Commission has established a target of reducing greenhouse gas (GHG) emissions of the European Union by over 80% by 2050, in comparison to 1990 levels. Additionally, the Commission aims to achieve carbon neutrality by that same year. In the aeronautics industry, one of the ways to achieve these objectives is to reduce the weight of structures, thereby reducing fuel consumption.

In this context and due to its lightweight, titanium alloys emerge as a material with a huge potential. Depending on its composition and manufacturing process, a rather wide range of mechanical properties can be obtained which means that Titanium alloys could potentially replace multiple steel components in quest of weight reduction.

As for all other materials, its properties are the consequence of its microstructure. However the biphasic (α/β) nature of the material and its phase fraction evolution at different temperatures makes it difficult to develop numerical models that could be used to predict both its microstructural evolution and associated mechanical properties. Furthermore, the microstructure of titanium alloys is complex and evolves over large span of length scales, starting from milimeter size β grains in the raw material, all the way to fine microstructures containing micrometric α grains and laths.

There is a large number of homogenization schemes that are used to study materials presenting a multiscale nature. However most of these schemes are limited to the computation of the equivalent mean response of the material at the mesoscopic scale, which is the used to fit a phenomenological law. The fitted phenomenological law is then used at the macroscopic scale and in this way the multiscale simulation is carried out. The drawback of these approaches is that when the macroscopic simulation induces local stress states that have not been studied at the mesoscopic scale, then the fitted constitutive law is nothing more than an extrapolation of the mesoscopic behavior. For materials displaying strong non linear behavior, this extrapolation can lead to large error.

The aim of the project is to develop and explore different homogenization techniques in order to describe the mechanical behavior of titanium alloys. The different homogenization techniques that will be explored include self-consistent approaches that will be compared to fully coupled multilevel macrocroscopic/mesoscopic scheme developped in the context of FE^2 or FE/FFT approaches.

Numerical modeling

The project is divided into two main stages, each one of them aiming at limiting the impact of the main drawbacks of multilevel approaches, namely excessive computational time and large memory footprint.

The first stage consists in replacing the lower scale full-field finite element model by a FFT-based full-field model. This is possible thanks to the length scale separation previously mentioned that allows to assume periodic boundary conditions at the mesoscopic scale.

Using FFT-based mesoscopic models allows to significantly reduce the computational time since these methods take advantage of the efficiency of the Fast-Fourier Transform. Another advantage of FFT-based methods is that, in contrast to finite elements, the condition number of the system is not degraded as the discretization size is reduced (mesh refinement).
The second stage of the project consists in using machine-learning (ML) techniques in order to tackle the second limitation: large memory usage requirements. We are planning to use an autoencoder in order to train a model that would be able to pack the 3D data into an abstract condensed data set.
This comptacted data will be stored and unpack when the computations at the mesoscale level are required. The challenge consists in generating a training database that is rich enough so that it could be representative of the possible topology and internal variables history. Then using this database, a physically-based autoencoder will be developped in order to limit the data degradation during the packing/unpacking process.

Candidate profile

The candidate must hold PhD degree in computational mechanics, high performance computing, material science, or a closely related field. The candidate should demonstrate a strong interest in numerical modeling and programming within a high-performance modeling environment.

Partners

The project is being conducted as part of a academic/industrial collaborative work carried out within the *Continuum* consortium. The consortium is formed by Safran, Airbus, Aubert&Duval and Timet and three academic teams at Chimie ParisTech, Institute Pprime and CEMEF MINES Paris.