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NUMERICAL METHODS FOR MULTISCALE MATERIALS MODELLING

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ABSTRACT

Numerical modelling of material’s behaviour under processing and/or exploitation conditions is widely used in industry and research. Several methods based on phenomological material models are commonly used to describe deformation, thermomechanical or heat treatment processes of materials. In the last decade such phenomelogical models are replaced or improved by more physical and chemistry based models (e.g. crystal plasticity, phase field, Cellular Automata, Molecular Dynamics, ab initio, …) to describe phenomena operating at different length and time scales. These approaches more often include also explicit representation of material structure during modelling. Numerous experimental techniques are now available for obtaining even high resolution 3D images of material microstructures. They provide a very accurate representation of heterogeneous materials with complex microstructure but lead to a large amount of data. Incorporating microstructure information in more physical based models and developing efficient computational methods represent a challenge in multi-scale analysis of heterogeneous materials.

The aim of this mini-symposium is to address this challenge by discussing recent advances in numerical methods for physically based multiscale material modeling.

Researchers addressing following topics are invited to submit their contribution to this multiscale materials modelling mini-symposium:

- New computational mechanics tools based on materials physics in order to predict more accurately material properties (e.g. efficient solvers for microstructure-based simulation, like Lippman-Schwinger (FFT, SLS,…), model reduction methods (POD, PGD), …).
- Alternative multi scale methods: e.g. combination of the CA-FE method, MC-FE, Phase field finite element, Level set finite element, Crystal plasticity finite element, etc.
- Theoretical basis of various numerical methods for multi-scale analysis techniques, such as Homogenization Method (HM), Monte Carlo (MC) method, Cellular Automata (CA) method, Molecular Dynamics (MD), Dislocation Dynamics (DD), etc.
- Multiscale approaches based on the mesh free and other particle methods.
- Algorithms to generate efficient models from microstructural images: segmentation, advanced voxel-based mesh (smoothing, …), FE immersion.
- Algorithms to generate statistical representative volume element (RVE).
- Morphology analysis tools, RVE size determination, ….
- Microstructure-based materials processing models combined with high-accuracy material characterization methods (EBSD, TEM, …).
- Multiscale methods involving uncertainties.
- Multiscale computational optimization approaches in design of engineering materials.
- Applications of the multiscale modelling to existing and future industrial problems such as melting, casting, welding, laser treatment, joining, forming, semi-solid metalworking, highly filled material processing, injection moulding, blow or compression moulding, sintering, and others.
- Materials: alloys, plastics, composites, functionally graded materials, concrete.