14th World Congress on Computational Mechanics (WCCM XIV)
8th European Congress on Computational Methods in Applied Science and Engineering (ECCOMAS 2020)
July 19- 24, 2020, Paris, France

COMPUTATIONAL MULTI-SCALE MODELING AND DESIGN OF NEW ENGINEERING MATERIALS

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Key words: New engineering materials, Multiscale modelling, Meta- and nanomaterials.

ABSTRACT

Many envisaged advances in engineering and science are based on the development of a wide range of advanced materials. The concept of digital material representation and metamaterials (artificially designed materials displaying exotic properties) constitutes a paradigm of this requirement. Computational mechanics contributes to solving crucial challenges in this area, by an application of numerical tools to the micro/meso and nano/micro scales and design of materials with morphologies at low scales satisfying properties at the macro scale. This minisymposium is devoted to discuss recent advances in modelling of advanced engineering materials in problems that involve two or more scale lengths. The topics of interest are:

I) **Advanced multi-scale material modelling**: i) Basis of multiscale techniques, such as Monte Carlo, Cellular Automata, Molecular Dynamics, Front tracking approaches, Mesh free and particle methods, etc ii) Computational homogenization including FE^2, Fast Fourier Transform-based homogenization and transformation field analysis, iii) Molecular and ab initio methods, iv) Reduced and Hyper-reduced order modelling techniques, v) Application of these approaches in an industrial context through software package integration, vi) Computing costs of multiscale modelling, applications of High Performance Computing.

II) **Multi-scale material-design**: i) Computational techniques for multi-scale design of the materials morphology and topology, inverse material design methods, design of materials with heterogeneous microstructures using stochastic models, inverse approach and optimization for stochastic variables; ii) multi-scale material design, oriented to specific applications in engineering; iii) Manufacturability issues in computational material design.