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COMPUTATIONAL MULTI-SCALE MODELING AND DESIGN OF NEW ENGINEERING MATERIALS

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ABSTRACT

Many presently envisaged advances in engineering and science are based on the development of a wide range of advanced materials. The modernly coined concept of "metamaterials" i.e.: those artificially designed materials displaying exotic mechanical, optical, electrical, acoustic or thermal properties, among others, constitutes a paradigm of this requirement. Computational mechanics can contribute to solving crucial challenges in this area, by exploring the application of numerical tools to the micro/meso and nano/micro scales modeling and design of materials with morphologies and topologies at low scales satisfying pre-conceived optimal properties at the macro-structure scale. The nature of this kind of problem, intimately related to well-defined material length scales, suggests placing this tools around computational multi-scale modelling methods and optimal design techniques.
This minisymposium is devoted to discuss recent advances in computational modeling and design of advanced engineering materials and single layer materials, in problems that consider two or more scale lengths, with special emphasis in metamaterials and nanomaterials. The main focus of the MS are computational multiscale-based material design techniques, but manufacturability aspects for the obtained design, possibly based on the use of additive manufacturing techniques, are also considered very relevant.
Typical topics of interest for the minisymposium are:

I) ADVANCED MULTI-SCALE MATERIAL MODELING

- Computational homogenization techniques: FE2 homogenization techniques, Fast Fourier Transform-based homogenization, transformation field analysis (TFA), etc.
- Multi-scale analysis and assessment of new engineering materials in mechanical, acoustic, thermal problems, etc.
- Computational techniques based on molecular and ab initio methods.
- Reduced and Hyper-reduced order modeling (ROM/HPROM) techniques in multi-scale material analysis.

II) MULTI-SCALE MATERIAL-DESIGN

1) Computational techniques for multi-scale design of the material's morphology and topology.

- Density based topology design methods (SIMP).
- Topological derivative-based methods.
- Inverse material design methods.
- Free material optimization (FMO) techniques.
- Computational intelligent techniques for material design.
- Other.

2) Computational techniques for multi-scale material design, oriented to specific applications.

- Acoustic applications (phononic materials, local-resonant materials, band gap design, Bragg-scattering, acoustic cloaking, etc.).
- Mechanical applications (ultra-light/ultra-stiff materials, micro-buckling material design, shock absorbing materials, etc.).
- Thermal applications (heat-flux handling, inverse-flux concentrators, etc.).
- Other applications in engineering (optical etc..).

III) MANUFACTURABILITY ISSUES IN COMPUTATIONAL MATERIAL DESIGN

- Manufacture feasibility issues in computational micro/meso-scale topology material design (numerical filters, perimeter control etc).
- Other.