

## **PREFACE: COMPUTATIONAL MULTISCALE MODELLING AND DESIGN OF NEW ENGINEERING MATERIALS**

This special issue of the *International Journal for Multiscale Computational Engineering* (IJMCE) is dedicated to the minisymposium “Computational Multi-Scale Modelling and Design of New Engineering Materials,” organized within the World Congress on Computational Mechanics, WCCM 2018, in New York. The issue contains seven papers selected from those presented during this symposium.

The World Congress on Computational Mechanics (WCCM) brings together our scientific communities and identifies emerging research trends and issues. Such contacts are important for establishing cooperative research activities. The objective of the “Computational Multi-Scale Modelling and Design of New Engineering Materials” minisymposium was to discuss recent progress in the design of advanced engineering materials and single-layer materials with regard to problems that consider two or more length scales, with emphasis on metamaterials and nanomaterials. The fact that many presently envisaged advances in engineering and science are based on the development of a wide range of advanced materials that are designed using various modelling techniques was the motivation for the organization of the minisymposium. The modern 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 contributes to solving crucial challenges in this area by exploring the application of numerical tools to the micro/meso and nano/micro scale modelling and design of materials with morphologies and topologies at low scales satisfying preconceived optimal properties at the macro-structure scale. The nature of this kind of problem, intimately related to well-defined material length scales, suggests placing these tools around computational multiscale modelling methods and optimal design techniques. All these aspects were discussed during the objective minisymposium at the WCCM.

A total of 28 papers were presented during the minisymposium, and after evaluation of the presentations, 12 authors were invited to submit extended versions of their papers to this special issue of the *International Journal for Multiscale Computational Engineering*. After the usual peer review procedure for IJMCE, seven articles were accepted for publication.

These articles focus on topics connected with widely understood applications of multiscale methods in modelling of materials, as well as atomistic and molecular approaches. The papers also deal with the RVE approach, the homogenization-based topology optimization algorithm, various phenomenological models, the Mori-Tanaka scheme, and molecular simulations in lower dimensional scales. Subsequent papers describe selected applications of multiscale modelling techniques, including the numerical homogenization of heterogeneous materials and the design of metamaterials with periodic microarchitectures. One paper shows application of the Mori-Tanaka finite element method for numerical homogenization and modelling of composite materials. Problems of computational efficiency are addressed in the paper describing the methodology for efficient performance of multiscale modelling methods in heterogeneous hardware infrastructures.

The following papers are dedicated to the modelling behaviors of particular advanced materials, including simulations of laser-assisted tube bending of Inconel 718 and the modelling of single-layered MoS<sub>2</sub> using energy minimization and molecular dynamics with Stillinger-Weber, REBO, and ReaxFF potentials. The last paper focuses on the mathematical aspects of the solution of a delayed differential equation describing the evolution of an internal variable in the micro scale. Analytical and numerical solutions are described, and the stability and existence of these solutions are proved in the paper. The papers also address a variety of advanced materials, including steels and nonferrous metals alloys as well as graphenelike polymorphs.

The guest editors of this issue express their thanks to the authors of the papers for their contributions. Particular thanks are directed to the reviewers for their hard work in reviewing the submitted papers and for help in

maintaining the high publication standards of IJMCE. It is our hope that this special issue of the *International Journal for Multiscale Computational Engineering* will be a source of inspiration for the readers in their scientific work.

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