EDITORIAL OF THE SPECIAL ISSUE
"ADVANCES IN COMPUTATIONAL MATERIALS SCIENCE"

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Computational mechanics has developed over the last several decades as a powerful discipline driven by the need to perform predictions of the mechanical behavior of systems and materials while avoiding extensive and costly experimentation. Today modeling is an intrinsic component of industrial design and a necessary part of any research program. Modeling is central to the development of new products, the prediction of the life range of existing products and the exploration of physical mechanisms that control deformation.

Modeling and simulation applied to materials science forms the broader and rapidly evolving body of Computational materials science. Within this sub-field, methods are developed to investigate physical processes taking place on multiple scales and to predict system-scale material behavior based on the integration of these processes. Traditionally, single scale models have been developed, mostly based on the formalism of continuum mechanics. This led to the creation and subsequent implementation and commercialization of multipurpose codes based on the Finite element method, which are now used broadly in industry and research. Beginning in late 1990's, attention has been given to the development of methods and models that account for and integrate physics taking place on multiple scales. This acknowledges the fact that the macroscopic material behavior is dictated by phenomena taking place on all scales from the atomistic to the continuum system scale. These include complex processes such as the evolution of the meso- and micro-structure of the material during loading, the strong interaction of crystalline defects such as dislocations, precipitates and point defects, non-linear effects in the core of dislocations etc. In principle, if these phenomena could be accounted for and their effective influence could be predicted, the macroscopic constitutive behavior of materials could be also predicted, which would lead to the creation of new, exceptional materials. While this perspective is fascinating, the current state-of-the-art falls short from attaining this goal. Most multiscale methods developed to date integrate two material scales and focus on a small number of physical processes. The key missing component is accounting for the meso-scale, *i.e*. for the scale at which large populations of defects – such as dislocations – interact in highly non-linear ways to create the net behavior observed macroscopically – such

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as plastic deformation. Similar problems exist in heat transfer, diffusion and coupled physical phenomena such as thermo-mechanics. It is acknowledged today that these models and methods have to include stochasticity and uncertainty quantification as an intrinsic component.

This special issue bring together several articles that cover a range of topics in mechanics and materials modeling. The set of problems addressed is necessarily limited and the contributions do not present a comprehensive review of existing methods. However, they demonstrate computational tools and methods applicable to several currently important engineering problems. The trends in the respective areas emerge from the discussion.

Referring to the atomistic scale, the article by Ciobanu presents a review of the current state of the art of two-dimensional materials, the associated modeling and computational methods and relevant physics. This field developed very fast over the last few years, with many types of 2D structures (beyond graphene) and associated superlattices being investigated. Novel electronic and mechanical properties are observed in these structures due to their small dimensionality and presence of reconstructed free edges. The computational methods used are either atomistic – in cases in which empirical potential exist – and, more often, quantum mechanical. This article entices the reader to dwell deeper in this emerging area.

The article by Zhang and Bobaru presents an overview of the relatively new method of peridynamics. This versatile method makes use of concepts commonly employed in discrete models of matter to reformulate the balance equations of the continuum. The method is applied to the prediction of fatigue crack growth in a plate with notches and complex geometry. This application is one of the most demanding for any model and the results presented in this article are of great interest.

The article by Stuparu *et al*. presents an application of the newly developed XFEM method, in conjunction with cohesive elements, to the prediction of crack growth leading to the failure of single-lap joints. The XFEM technique allows the representation of cracks and other discontinuities on meshes which are not conforming to the manifold over which the field is discontinuous. Cohesive zone models have also been used for a long time to represent crack growth. This method presents the drawback that cracks can only advance along planes where such special elements are pre-defined. The combination of the two techniques offers attractive advantages which are explored in this article.

The article by Picu *et al*. explores the design space of highly heterogeneous materials with the aim to identify stochastic microstructures that may lead to interesting macroscopic properties, beyond those that can be obtained from periodic micro-structures composed from few constituents. This work underlies the need for a stochastic approach to materials modeling and opens an interesting perspective on how material stochasticity can be used to create systems with unusual properties.

The article by Sorohan *et al*. presents a component of a multiscale method applied to cellular materials. When performing large scale simulations of structures composed from cellular materials it is impractical to represent the actual geometry of the microstructure. The usual approach is to use smaller scale models in which the microstructure is explicitly represented in order to calibrate the elastic constants of an orthotropic continuum, which is then used in larger scale models. This article presents an elegant method to perform this calibration using modal analysis. The method can be applied to other types of structures and hence is of broad interest.

Nastasescu and Marzavan use the method of Smooth particle hydrodynamics to solve the particularly challenging problem of modeling an underwater explosion, including the interaction with submerged structures. This method has roots in both discrete and continuum formulations and has been used with great success in a wide variety of applications. The present article demonstrates the versatility of the method and is expected to stimulate its further use.

The challenges posed to the researcher by problems in mechanics and materials are tremendous. The future of the field depends on the close collaboration of experimentalists, theorists and computational scientists. We hope that this volume will stimulate the interest in these methods and foster future developments.

The guest editors,

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