SPECIAL ISSUE

On Advances in Multiscale and Multiphysics Methods

Guest Editors
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PREFACE

The last decade has witnessed significant advances in the development of complex material systems and devices that are starting to bring profound impact to engineering applications. Examples of such include multifunctional nanocomposites, self-assembled bio- and nanostructures, smart materials that can sense and actuate, self-healing materials, quantum dots, thin films, and many others. To understand and fully utilize the underlying mechanisms for advanced functionality and superior properties, the development of modeling and simulation tools necessitates close integration across many science and engineering disciplines. For instance, understanding how mechanical deformation affects the electronic properties of nanomaterials requires substantial knowledge in both continuum mechanics and electronic band structures and coupling mechanisms. Another common research theme is the multiple spatial and temporal scales involved in the particular engineering applications of these material systems and devices. As significant progress is being made in the areas of synthesis and fabrication, many challenges remain in advancing a truly seamless simulation-based design and analysis approach.

Motivated by these challenges, a symposium titled Multiscale Methods and Applications to Nano- and Bio-Mechanics and Materials was organized as part of the 8th World Congress on Computational Mechanics (WCCM). The major goal of this symposium was to directly address the challenges by providing a forum for researchers to exchange their ideas. A total of 15 presentations (including three keynote speeches) covering state-of-the-art developments were made and a wide range of topics was covered. In light of the presentations made at the symposium, we organized this special issue on advances in multiscale and multiphysics methods for the *International Journal for Multiscale Computational Engineering*. A total of eight papers were collected for this special issue and they can be divided into two groups based on their themes. The first group centered on the exciting applications of a wide spectrum of simulation tools in the area of nano- and biomechanics of materials. Wu, Wang, Cohen, and Ge discussed the use of both molecular modeling and reduction approaches in understanding the mechanics of normal and sickle hemoglobin. The interfacial mechanics of polymer systems reinforced by functionalized carbon nanotubes were studied by Qian, He, and Shi using a molecular mechanics approach. Voskoboynikov presented a hybrid method for analyzing the mageto-optical response of semiconductor systems. This multiscale approach is featured by coupled electrodynamic and quantum mechanical representation. Shen and Chen developed a classical molecular dynamics approach to study the failure mechanism in low-dimensional nanoscale hierarchical structures with an emphasis on the effects of size and imperfection. Using a density-functional-based first-principles method, Pan, Yang, Zhang, and Hu presented a study on the stability and elastic properties of boron nanotubes under different temperatures.

The second group of papers explored recent developments in the field of modeling methodology. Wang and Tang reformulated the multitransmitting approach developed earlier and demonstrate that the new method shows significant improvement in reducing the spurious reflections at the numerical interface. Ma, Gao, and Reddy presented a theoretical framework on the nonclassical

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Reddy–Levinson (R-L) beam model by incorporating the microstructural effects. The results are important for applications in which the length scale effect is significant and the classical elasticity theory needs to be modified. Finally, Aubertin, Rethore, and de Borst proposed a method for modeling dynamic crack propagation by coupling the method of molecular dynamics with an extended finite element method. They have developed a so-called "MD box" concept for the purpose of coupling and shown that this approach is effective in removing spurious reflection and achieving energy conservation.

In summary, the collection of papers in this special issue represents continuing interest in integrating modeling and simulation with new developments in material and device synthesis and fabrication. These new developments, along with phenomena that are observed to be beyond and sometimes contradictory to the predictions based on classical theories, necessitate the reformulation of many basic methodology and simulation concepts. With this in mind, it is hoped that publication of this special issue will contribute to the field of multiscale and multiphysics methodologies by prompting new ideas and findings.

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