

PREFACE: MULTISCALE COMPUTATIONAL ANALYSIS OF COMPLEX MATERIALS

Complex materials play an essential role in many applications, ranging from turbine blades, car chassis, computer and cell phone cases, battery systems, and stretchable and wearable electronics to biomedical applications. Those materials often operate and must maintain their high performance in harsh environments. The advancement of computational methods at multiple scales opens new possibilities for the design of such complex materials and the optimization of their intrinsic properties under extreme events. The bridging of different length and time scales, though, still represents an area of active research with many unresolved challenges. For example, material degradation is considered as a typical multiscale process, controlled by nanoscale defects, highly affecting the macroscopic material response.

In order to discuss the methods of modeling of multiphysics aspects of complex materials behavior, the International Symposium on Multiscale Computational Analysis of Complex Materials was organized on August 29–31, 2017, at the Technical University of Denmark/DTU, Copenhagen. The symposium topics included multiscale multiphysics modeling of materials; computational materials science; micromechanics of materials; scale bridging and homogenization; materials under extreme environments; hierarchical, biological, and natural materials; and nanomaterials. Several selected papers from this symposium are presented in this issue of the *International Journal for Multiscale Computational Engineering*.

In the paper “A Damage Particle Method for Smeared Modeling of Brittle Fracture,” by Jiun-Shyan Chen (University of California, San Diego), a new damage particle method based on the smeared fracture modeling approach is presented which allows the capturing of moving strong discontinuities. This work was presented at the symposium as a keynote presentation in the Multiscale Composites session.

The paper “A Multi-Scale/Multi-Domain Model for the Failure Analysis of Masonry Walls,” by Professor Patrizia Trovalusci (University of Roma, Italy) and her colleagues, was a keynote presentation in the Structured Materials session. In this paper, a novel multiscale/multidomain approach for nonlinear analysis of masonries is presented.

In the Porous and Granular Materials session, the paper by Professor Waiching Sun (Columbia University), “An Adaptive Reduced-Dimensional Discrete Element Model for Dynamic Responses of Granular Materials with High-Frequency Noises,” was presented. In this paper, a dimensional-reduction framework based on proper orthogonal decomposition (POD) for nondissipative explicit dynamic discrete element method (DEM) simulations is presented. The approach allows faster and more efficient discrete element simulations.

Several presentations were made in the Crystalline Materials session at the symposium. In the paper “Modelling Plastic Deformation of Nano/Submicron-Sized Tungsten Pillars Under Compression” by Shuozhi Xu (University of California, Santa Barbara), coarse-grained atomistic simulations via the concurrent atomistic-continuum (CAC) method are performed to investigate compressive deformation of nano/submicron-sized pillars in body-centered cubic (BCC) tungsten. This work is the first attempt to simulate BCC systems using the CAC method and highlights the significance of the surface roughness in the deformation of the samples.

An important direction of computational mechanics of materials is multifunctional materials, e.g., with electrical, sensing functionality and high mechanical performance. In this area, two papers were selected for this issue. In the paper “Variationally Consistent Computational Homogenization of Micro-Electro-Mechanics at Finite Deformations,” by Professor Marc-Andre Keip and colleagues (University of Stuttgart, Germany), a variationally consistent approach of computational homogenization to large-deformation microelectromechanics is presented. A phase-field model for microstructure evolution in ferroelectrics is linked to an electromechanical macrocontinuum. Krzysztof Grabowski and colleagues from AGH University of Science and Technology, Poland, developed a multiscale model to predict mechanical properties of carbon nanotube reinforced sensing composites in their paper “Multiscale Model-Based Sensitivity Analysis of Mechanical Response of CNT/Polymer for Strain Sensing.”

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FIG. 1: Presentations at MCACM Symposium. Top row: Jacob Fish (Columbia), Ole Sigmund and Lars Mikkelsen (DTU), Christian Linder (Stanford), John Hutchinson (Harvard), Jose E. Andrade (Caltech). Middle row: Bent Sørensen (DTU), Emilio Martínez-Pañeda (DTU), Jiun-Shyan (JS) Chen (UC San Diego), Christian Niordson (DTU), Siegfried Schmauder (Stuttgart), and Leon Mishnaevsky, Jr. (DTU). Bottom row: William Curtin (EPF Lausanne), Ricardo Lebensohn (Los Alamos), Alexander Hartmaier (Ruhr Bochum).

Guest Editors and Symposium Chairmen:

Leon Mishnaevsky, Jr.
Senior Researcher, Dr. habil,
Technical University of Denmark

Christian Linder
Professor, Stanford University

WaiChing (Steve) Sun
Professor, Columbia University