Foreword

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The recent times have seen a surge in the interest and research efforts in multi-scale computational modeling of structure–material interactions for predicting deformation and failure. To address state of the art topics and major issues in this emerging field, an IUTAM symposium was held on Integrated Computational Structure–Material Modeling of Deformation and Failure under Extreme Conditions in Baltimore, MD on June 20–22, 2016. This special issue in Computational Mechanics, entitled “Integrated Structure–material Modeling” has directly resulted from discussions that ensued at this symposium.

The IUTAM symposium brought together experts in the complementary fields of Computational and Experimental Mechanics and Materials Science to discuss multidisciplinary approaches for integrating structure–material modeling and simulations, material characterization and experiments to predict non-homogeneous deformation and failure in heterogeneous materials. The technical focus was on the understanding and prediction of extreme and rare events e.g. fatigue, failure, impact, blast, etc. in material response through physics-based modeling at multiple spatial and temporal scales for a range of material classes including metals, ceramics and composites. The symposium consisted of four thematic parts, viz. (1) physics-based

multi-scale model development; (2) multi-scale data acquisition, characterization and experiments at different scales; (3) probabilistic modeling and uncertainty quantification and (4) structure–material integration and design. Various methods of coupling multiple scales in regions of homogeneous and localized deformation, leading to localization, damage and failure were discussed. In addition, uncertainty characterization of material structure, uncertainty identification in material properties and mapping material structure uncertainty to structural performance were discussed as essential ingredients of a robust modeling process.

This symposium also had an agenda for special discussions on identifying opportunity trends and future needs along the lines of the technical themes. Some of the discussion points are itemized next.

- Future trends within the experimental sciences community, viz. ability of instrumentation to get both high spatial resolution and rapid time resolution and capabilities to reach 3D spatial information need to be consolidated.
- It is critical to supplement experimental observations with other methods such as advanced physical theory and first principle techniques.
- Data science is an opportunity area for this field since we must access many different types of information and combine them to give a physical picture of damage and failure events.
- Models currently in use are often phenomenological in nature to varying degrees, and uncertainty exists in that state of phenomenology and inherently in the degree of physicality in the parameter sets. Statistical quantification should be better accomplished.
- Physical basis of models can lower uncertainly level and systematic quantification of parameter uncertainty

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should be used. Reduction of parameters in models is a related goal.

- Artificial intelligence techniques will likely be used more extensively in the future to learn from large data sets or combine different data sets in a disciplined way. The next 10 years should see rapid growth in this direction, implementing better ways of attributing datasets properly is important.
- The community should do a better job in how code development, code maintenance and code distribution is currently done. The Mechanics of Materials community should begin borrowing more from other communities in how codes are written (to some extent this is happening with some of the national initiatives). The animation or graphics design communities use computing extensively.
- Code robustness for general applications is a very important consideration, which is generally not reported upon in published articles and yet has critical practical implications.
- Porting or writing codes for new hardware architectures is a serious issue and requires a great deal of resources to achieve.
- In industry where survivability relies on making a successful structural component, which is acceptable to a customer at an agreeable price, product specifications, quality standards, and design criteria are very important. These are always quantifiable and are necessary to the design engineer. How does one talk about these engineering quantities in the context of the mechanisms of behavior and challenging statistical responses?
- When discussing lifecycle response of structural materials, we should also account for the aging of materials as an important issue under extreme environmental conditions.
- From an industry perspective, an envisioned workforce of the future that is a bit more diverse and actually is a bit more capable with many of these advanced experimental and computational tools is needed. In that way industry can either use these advanced tools or understand them to the point where they can frame the right questions so that we can actually use these tools in the design process.

- Bringing together new technology as being discussed here will determine the rate of change within industry, government, and academia.

This special issue in Computational Mechanics, entitled “Integrated Structure–material Modeling” contains fourteen papers that address some of the breadth in the above stated goals of the IUTAM symposium. Topics covered in this special issue include: evolution of adiabatic shear bands, shock-induced phase transition, probabilistic modeling of composite structures, multi-time-domain methods for crystal plasticity modeling of twin evolution, uncertainty aggregation for structure/material performance, mixed parallel strategy for coupled multi-scale problems, effect of microstructure on deformation of titanium, shear-band modeling with gradient plasticity, ductile crack propagation in polycrystalline microstructure with XFEM, hydraulic fracture in shale rock, microstructural evolution in copper grain boundary structures due to femtosecond laser processing, shear bands in mechanical behavior of magnesium alloys, concurrent multiscale modeling of localization behavior, hydraulic fractures from perforated horizontal wellbore, etc. The contributions point to the collaboration necessary between experiments, theory, and simulations to address the challenges and opportunity rich areas of material and structural behavior and failure. This collection of work illustrates an exciting future for technological advancement and the demonstrated need for it from our government and industrial partners.

We, the guest editors of this special issue, would like to thank all the authors who contributed to this special issue. We also express our appreciation to the editor-in-chief of Computational Mechanics, Professor Peter Wriggers, for his encouragement and enthusiastic help with the preparation of this collection of works.