*Journal for Multiscale Computational Engineering*, 11 (3) vii (2013)

# SPECIAL ISSUE

# MODEL REDUCTION APPROACHES IN MULTISCALE MODELING OF HETEROGENEOUS MATERIALS

***Guest Editor***

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## PREFACE

Multiscale computational modeling has seen tremendous progress in the past couple of decades as evidenced by an ever-increasing number of journal publications, thematic conferences, and workshops on the topic. One key bottleneck that has not yet been adequately addressed is that despite continuous developments in computational modeling and simulation, the computational costs accrued in multiscale simulations remain significant, and have so far limited the potential impact of multiscale models and methods in engineering industry and applications beyond academia. Reduced order modeling ameliorates this tremendous computational burden by eliminating degrees of freedom from the computational problem, as appropriate, to attain computational efficiencies rivaling traditional single scale computations, and has been identified as a key area of further research in recent technical workshops and conferences. The purpose of this special issue is to provide the state of the art in reduced order modeling approaches for evaluation of mechanics problems that involve multiple scales. The contributions in this special issue focus on modeling the response of heterogeneous materials within both stochastic and deterministic settings. With this special issue, we also attempted to identify those areas that need further research in addition to establishing the current state of progress in reduced order modeling approaches.

The manuscripts in this special issue address a range of solid mechanics problems concerning model reduction in the context of multiscale modeling. The variety of the model reduction methods advocated by the manuscripts indicate the multitude of approaches one can take to reduce the computational burden depending on the underlying physical characteristics of the problem. This variety also points to the significant body of research that remains to be undertaken to understand and form the balance between computational tractability and model fidelity in multiscale computational modeling of heterogeneous materials.

Sparks and Oskay propose a method to identify the optimal reduced order models that can best capture the failure response of heterogeneous materials at a given model order. They employ the Eigendeformation-based reduced order homogenization method as the model reduction approach, which is based on concurrent nonlinear computational homogenization. Yvonnet et al. propose a nonconcurrent reduced order approach for modeling deformation response of heterogeneous materials with hyperelastic constituents. The primary idea is the numerical construction of the constitutive response (via defining a numerical hyperelastic potential) for the homogenized domain based on off-line computations defined over the representative volume element (RVE). The six-dimensional (for 3D problems) strain space is interrogated using the reduced database model to construct the homogenized hyperelastic potential. Deng and Chen propose the atomistic field theory (AFT), a new coarse graining method at the atomistic scale that has the capability to accurately predict dynamic fracture. They show that the atomistic features of the crack propagation can be captured by the AFT method, while providing nearly two orders of magnitude computational efficiency. Gal et al. provide an extended finite element model for inclusion-reinforced matrices that develop a distinct interphase region. Their model eliminates the need to resolve the interphase region, the thickness of which may be orders of magnitude

1543–1649/13/$35.00 

smaller than the characteristic size of the RVE. This approach is important in modeling the behavior of concrete and other cement based-composites, which are well known to exhibit an interfacial transition zone. The accuracy characteristics of the reduced order multiscale models are often degraded around fracture process zones and high stress gradients. Kerfriden et al. describe a new computational methodology to objectively differentiate between the problem subdomains at which model reduction approaches can be applied, and the fracture process zones that may require full resolution. They investigate stochastic fracture problems in materials with random inclusions. Bogdanor et al. propose a stochastic calibration and uncertainty quantification methodology to describe damage evolution in heterogeneous materials. The proposed approach addresses two important research questions relevant to the reduced order modeling of heterogeneous materials. They provide promising approaches for calibration of the multiscale model parameters, and for quantification of various sources and types of uncertainty such as material parameter variability, as well as the modeling errors due to discretization, model reduction, and others.

Despite the increasing research activity in the past few years, model reduction methods for multiscale modeling of heterogeneous materials continues to be a young field and is likely to remain a fertile field of research for quite some time in the future. This special issue addresses some of the critical questions surrounding reduced order modeling of heterogeneous material systems, and poses additional questions that need to be answered in the near future. The guest editor would like to thank the authors for their valuable contributions, all the reviewers for their assessments of the manuscripts, and Professor Jacob Fish, the editor in chief, for allowing the publication of this special issue in the *International Journal for Multiscale Computational Engineering*.

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