Abstract:
With concentrated efforts from the material science community to develop new multifunctional materials using unique processing conditions, the need for modeling tools that accurately describe the physical phenomena at each length scale has only further been emphasized. For example, additive manufacturing and shock synthesis lead to unique material morphologies that need to be understood for reliable engineering analysis and product safety assessments. Considering these material complexities, Direct Numerical Modeling (DNM) is accessible only for moderate system sizes. Thus, a multiscale strategy must recognize that just a relatively small part of the material will typically be instantaneously exposed to rapid material transformations. Macroscopic constitutive models obtained from homogenization, of the complex but slowly varying microstructure, may adequately describe the rest of the material. Nonlinear model reduction, pattern recognition and data-mining are a key to future on-the-fly modeling and rapid decision making. To address these challenges, we present an image-based (data-driven) multiscale framework for modeling the chemo-thermo-mechanical behavior of heterogeneous materials while capturing the large range of spatial and temporal scales. This integrated computational approach for predicting the behavior of complex heterogeneous systems combines macro- and micro-continuum representations with statistical techniques, nonlinear model reduction and high-performance computing. Our approach exploits the instantaneous localization knowledge to decide where more advanced computations are required. Simulations involving this wide range of scales, $O(10^6)$ from nm to mm, and billions of computational cells are inherently expensive, requiring use of high-performance computing. Therefore, we have developed a hierarchically parallel high-performance computational framework that executes on hundreds of thousands of processing cores with exceptional scaling performance. Any serious attempt to model a heterogeneous system must also include a strategy for constructing a complex computational domain. This work follows the concept of data-driven (image-based) modeling. We will delineate a procedure based on topology optimization and machine learning to construct a Representative Unit Cell (RUC) with the same statistics (n-point probability functions) to that of the original material. Our imaging sources come from microcomputed tomography (micro-CT), focused ion beam (FIB) sectioning, and advanced photon source nano-tomography at the Argonne National Laboratory. We show that high-performance DNM of these statistically meaningful RUCs coupled on-the-fly to a macroscopic domain is possible. Therefore, well-resolved microstructure-statistics-property (MSP) relationships can be obtained. Finally, the integrated V&V/UQ program with co-designed simulations and experiments provides a platform for computational model verification, validation and propagation of uncertainties.

Bio:
Dr. Matouš is a College of Engineering Associate Professor of Computational Mechanics in the Aerospace and Mechanical Engineering Department at the University of Notre Dame. Dr. Matouš is also a Director of the Center for Shock Wave-processing of Advanced Reactive Materials (C-SWARM) that has been established as one of six NNSA’s center of Excellence whose primary focus is on the emerging field of predictive science. He received his M.S. and Ph.D. in the Theoretical & Applied Mechanics from the Czech Technical University in Prague. Dr. Matouš’s interests are in the area of predictive computational science and engineering at multiple spatial and temporal scales including multi-physics interactions, the development of advanced numerical methods and high-performance parallel computing. His research focuses on the interplay between applied mathematics, computer/computational science and physics/materials science. Moreover, he leads a research program in image-based (data-driven) modeling of heterogeneous materials focusing on co-designed simulations and experiments based on statistically representative analysis. He has authored or co-authored more than hundred and fifty journal and/or conference proceedings articles and abstracts. He is involved in several interdisciplinary research programs with funding from various agencies and private companies. Dr. Matouš received the Rector’s Award for the best Ph.D. students from the Czech Technical University in Prague. Two articles from Dr. Matouš’s group have been featured on Science Direct Top 25 Hottest Articles in their respective engineering areas. One of his papers appeared as the cover article in Proceedings of the Royal Society A. He is a member of ASME, SES, USACM, EUROMECH, and IACM. Dr. Matouš is a Fellow of ASME. Dr. Matouš serves as an Associate Editor of the Journal of Computational Physics and International Journal for Multiscale Computational Engineering.