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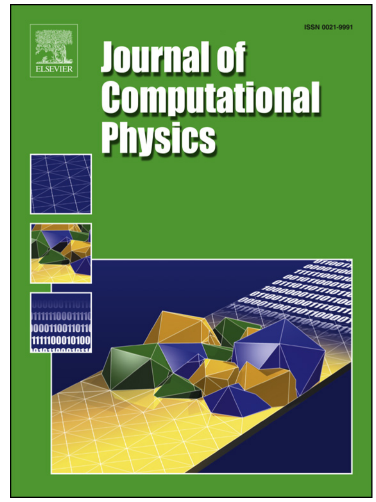

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PII: S0021-9991(16)30578-2
DOI: http://dx.doi.org/10.1016/j.jcp.2016.10.070
Reference: YJCPH 6948

To appear in: *Journal of Computational Physics*

Received date: 8 April 2016
Revised date: 26 September 2016
Accepted date: 31 October 2016

Please cite this article in press as: K. Matouš et al., A review of predictive nonlinear theories for multiscale modeling of heterogeneous materials, *J. Comput. Phys.* (2016), http://dx.doi.org/10.1016/j.jcp.2016.10.070

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A Review of Predictive Nonlinear Theories for Multiscale Modeling of Heterogeneous Materials

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Abstract

Since the beginning of the industrial age, material performance and design have been in the midst of innovation of many disruptive technologies. Today's electronics, space, medical, transportation, and other industries are enriched by development, design and deployment of composite, heterogeneous and multifunctional materials. As a result, materials innovation is now considerably outpaced by other aspects from component design to product cycle. In this article, we review predictive nonlinear theories for multiscale modeling of heterogeneous materials. Deeper attention is given to multiscale modeling in space and to computational homogenization in addressing challenging materials science questions. Moreover, we discuss a state-of-the-art platform in predictive image-based, multiscale modeling with co-designed simulations and experiments that executes on the world's largest supercomputers. Such a modeling framework consists of experimental tools, computational methods, and digital data strategies. Once fully completed, this collaborative and interdisciplinary framework can be the basis of *Virtual Materials Testing* standards and aids in the development of new material formulations. Moreover, it will decrease the time to market of innovative products.

Keywords: Predictive Science, Image-Based Multiscale Modeling, Computational Homogenization, High Performance Computing, Co-designed Simulations and Experiments, Verification and Validation

1. Need for Predictive Multiscale Computational Science and Engineering in Materials Design

Over the past decade, an abundance of new processing conditions from the material science community has ushered development of materials with unique properties. Similarly, design of machine parts pushes material science towards discoveries of materials that are lighter, stronger, thermally and electromagnetically shielded, multifunctional, etc., and the processing conditions that will create them. This constant push and pull between material science, physics/mechanics, and materials design creates the need for predictive modeling tools that accurately describe the physical phenomena at each length and time scale with the resolution required in product design and safety assessment (see Figure 1(a)).

For a long time, development of new materials has been guided by experience and empirical correlations between processing conditions and desired performance [1]. Recently, this ad hoc approach is being challenged by the *Integrated Computational Materials Engineering* (ICME) paradigm [2–5]. ICME combines both bottom-up and top-down modeling and simulation strategies and aims to reduce the time to market of innovative products. It is concerned with multiple spatial and temporal scales of structural hierarchy typical of materials with microstructure. Moreover, it synthesizes information and data from both experiments and simulations across time scales and/or length scales. A report by the National Research Council of the National Academies [3] describes ICME as a transformational discipline for improved competitiveness and national security. It also views it as a grand challenge: "The grand challenge for the field of materials science and engineering is to build an ICME capability for all classes and applications of materials."

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