Northwest Consortium for Multiscale Mathematics and Applications – *"Educational Strategies and Critical Problems in the Thermo-mechanics of Materials"*

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Summary

The Northwest Consortium for Multiscale Mathematics has been developing an integrated multiscale approach to the study of critical problems in the thermo-mechanical properties of materials. These problems require new formalism to mathematically and computationally represent and link the physics describing discrete phenomena taking place at the atomic level with that of the macroscopic continuum. The disparity between the current practice of simulation and these new multiscale formalisms necessitate educational strategies to bring advances in multiscale mathematics into the graduate school classroom through the development of new curricula, textbooks, educational software, and summer programs.

The Northwest Consortium for Multiscale Mathematics has been developing mathematical and computational solutions for multiscale simulation of materials. There exists a critical need to reconcile phenomena that take place at the atomic level of organization with that of the macroscopic; the different size and time scales form an 'information' hierarchy that influences the properties and behaviors of a material. New mathematical and computational methods are required to break free of the restrictions of conventional single scale formalisms towards a more predictive model of nature. The consortium has taken approaches such as:

- Homogenization
- Lattice-continuum models
- Coarse-graining of dislocation mechanics
- Microstructural characterization
- Discrete particle dynamics
- Multiple and dynamically-grained computational simulation

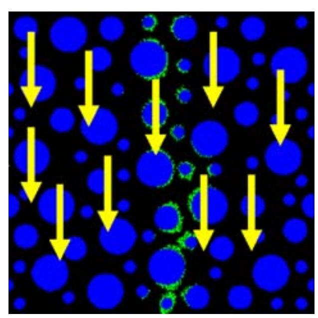

Figure 1. Multifractals are used to characterize the heterogeneity of material microstructural features such as the two-point correlation measure.

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High performance computation for material science problems, such as the thermomechanical property of plasticity, has been intractable due to the limitations imposed by single scale methods. The challenge of this effort is to accurately model the properties and size effects at the interface between levels of description. Although a number of theories have been proposed, none has been able to predict size effects in a general way, and none has incorporated interface energies.

Recent developments have resulted in a new method to combine discrete dislocation dynamics with a mesoscopic continuum model that includes more accurate representations of interfaces. These models are used to identify size-scaleable definitions for the improved representative volume element. Preliminary results on high performance computing architectures are underway for validation and benchmarking.

At the mesoscale, multifractals have been applied to improve the representation of microstructural characteristics, such as grain size, impurities, and porosity, which provide information linking the composition and processing of a material to its properties and performance (Figure 1). Current approaches do not scale well, limiting their value for simulations over increasing orders of magnitude in size and time scales. We developed software for extracting the probability distribution from a microstructural image and applied these algorithms to a number of sample datasets. Current work focuses on expanding the applicability and scalability of this approach on high performance computing architectures.

The efforts of this project have also resulted in a number of new educational resources including:

- New course offered Winter 2006, "Fractal Computing" at Washington State University/Tri-Cities
- New course will be offered Fall 2006, "Multiscale Modeling in Thermomechanics of Materials" at Washington State University/Pullman
- Seminar series in multiscale modeling of materials at Washington State University/Pullman as a core graduate curriculum requirement
- Seminar series and workgroup on Multifractal Representation and Multiscale Computing at PNNL.
- Progress on the development of three books: "Multiscale Mathematics and Computation", "Multifractals: Step-By-Step", and "Homogenization".

In addition, this program organized the "Multiscale Mathematics in Material Science" workshop, May 25-30 2006 as the starting point for the FY2007 (and ongoing) summer school on Multiscale Modeling and Computation. The motivation for the workshop was twofold: to discuss the state of critical multiscale problems in material science and to determine how we might use their fundamental scientific, mathematical, and computational elements in the DOE-sponsored summer school, multiscale materials book, and supporting software repository. Approximately sixty researchers and students from universities, DOE and other federal research labs participated. A report summarizing this event, as well as streaming video from the individual talks, are available online*.

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* http://matscimultiscale2006.pnl.gov