# CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

## TRIP REPORT

**SUBJECT**: The 15th National Congress of Theoretical and Applied Mechanics
Project # 20.06002.01.342
AI # 20.06002.01.342.606

**DATE/PLACE:** June 25–30, 2006
Boulder, Colorado

**AUTHOR:** Fernando Ferrante

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**PERSONS PRESENT:**

Attendance at the 15th National Congress of Theoretical and Applied Mechanics was estimated at 2,000 participants during the opening lecture on June 25, 2006. These included academic, industry, and government agency researchers in wide-ranging areas of computational mechanics.

**BACKGROUND AND PURPOSE OF TRIP:**

The event is part of quadrennial congresses organized by the U.S. National Committee on Theoretical and Applied Mechanics, which is a member of the International Union of Theoretical and Applied Mechanics. Current member societies of U.S. National Committee on Theoretical and Applied Mechanics are: Acoustical Society of America, American Institute of Aeronautics and Astronautics, American Institute of Chemical Engineers, American Mathematical Society, American Physical Society, American Society of Testing and Materials, American Society of Civil Engineers, American Society of Mechanical Engineers, Society of Experimental Mechanics, Society for Industrial and Applied Mathematics, Society of Naval Architects and Marine Engineers, Society of Engineering Science, and Society of Rheology.

The technical program consisted of four plenary lectures and 130 sessions organized in 60 mini-symposia with over 600 papers accepted for presentation. The conference proceedings will be published in book form in a few months.

Specific purposes for attending the meeting were to

- Present a paper titled Micromechanical Analysis of Random Non-Homogeneous Composites Using Moving-Window Generalized Method of Cells in the mini-symposium Probabilistic Mechanics and Uncertainty

- Fulfill an invitation to attend a meeting of the Probabilistic Methods Committee, comprising several members from academia and industry organizations committed to advancing probabilistic analysis and the treatment of uncertainty in engineering applications

- Attend technical sessions on various topics outlined in the next section

**SUMMARY OF PERTINENT POINTS:**

The theme of this year's congress was Mechanics in Emerging Technologies, with an emphasis on analytical, experimental, and computational mechanics techniques covering several topics involving new technologies and applied mechanics. The mini-symposia were divided into seven overarching topics: solid/structural mechanics, mechanics of materials, inverse/probabilistic mechanics, device/applications, fluid mechanics, biomechanics, and unique topics in mechanics. Developments in nanomechanics and biomaterials were focused on as two of the prime areas where computational mechanics has thrived in recent years.

The four plenary lectures highlighted the theme of the congress, presenting different perspectives for the current state of emerging technologies in both academia and in government research organizations. The first plenary lecture was given by Dr. J. Pazik (replacing Dr. S. Walker, who was unable to attend) from the Office of Naval Research in Arlington, Virginia. Dr. Pazik discussed current and future mechanics research for national defense projects, emphasizing the need for active engagement from the computational mechanics community in solving some of the complex research issues involved in several advanced naval applications.

The second plenary lecture was given by Dr. S. Bull, the director of the Science and Technology division at the National Renewable Energy Laboratory, which is maintained by the U.S. Department of Energy. Dr. Bull described current efforts in solar, wind and biomass energy renewal taking place at the National Renewable Energy Laboratory. He compared the worldwide advances made in recycling energy and warned that the technological achievements in the United States have not yet achieved their goals for a more efficient and environmentally committed energy policy. In particular, Dr. Bull indicated that despite significant advances in biomass energy production, coal, oil, and nuclear-based technologies continue to be short-term solutions for national energy needs.

Dr. M. Roukes, the director of the Kavli Nanoscience Laboratory at the California Institute of Technology in Pasadena, California, presented the third plenary lecture. He focused on the state of nanotechnology research and current opportunities for the computational mechanics community. This included an overview of the state-of-the-art nanodevices being developed and the challenges that remain for further industrial and commercial implementation in this field. Several common areas of interest between the nanomechanics research groups and the wider computational mechanics communities were highlighted, with an invitation to further explore applications at the nanoscale.

The last plenary lecture was delivered by Prof. S. Kim from Purdue University, who described his interests in fluids and hydrodynamic problems at the microscale. By incorporating his own personal experience in the pharmaceutical industry, Prof. Kim presented new advances for research and development projects in the field of pharmaceutical informatics.

Due to the large number of concurrent sessions taking place in each mini-symposia, only a brief outline of the most pertinent points of the sessions attended by the author will be discussed below. However, a full description of the congress organization and the abstracts for all papers scheduled to be presented are available at http://usnctam06.colorado.edu.

A recurrent theme of the mechanics of materials presentations was the development of accurate multiscale approaches to model heterogeneous materials. For example, C. McVeigh from Northwestern University presented a decomposition of the physical and mathematical representation of the composite at the individual scale of deformation in terms of its kinematic response and constitutive behavior. This is intended to capture the overall contributions to the material deformation at the microscale, nanoscale, and atomistic level using a representative volume element approach.

On a similar vein, S. Gonella presented another multiscale modeling approach applied to the simulation of wave propagation in damaged periodic media. In this case, the problem of detecting localized damage for the application of an efficient non-destructive evaluation technique is promoted through the use of meshes with different refinement levels. A coarse mesh is implemented to capture the macroscopic behavior of the structure, while a refined mesh is applied to the discontinuity regions. However, any spurious effects in the analysis due to the use of coarse refinement must be bridged accordingly with the finer mesh sizes. A simple example was shown, where the computational cost was effectively reduced using a coarser mesh with local refinement for a homogenized periodic material to capture microstructural effects and localized discontinuities.

I. Idiart from the École Polytechnique in France introduced multiscale modeling to characterize microstructure evolution and instability development in random porous media. In this work, a homogenization technique is derived by extrapolating the effective behavior of nonlinear composites from linear assumptions derived using variational principles. Examples included a demonstration of the effects of microstructural evolution on the macroscopic instabilities in porous materials under finite strains and how this approach can be applied to the modeling of deformations during processing techniques.

A. Muliana introduced interesting generalizations of a micromechanical method based on the homogenization scheme where traction continuity and displacement compatibility between adjacent volume elements are satisfied in an average sense. This approach is applied to the derivation of the effective properties of polymers reinforced with solid spherical particles, with extensions into time-dependent behavior modeling and three-dimensional microstructural characterization.

A combined research effort between several academic and government institutions on three-dimensional microstructural characterization using digital imaging was presented by A. Rollett of the Food and Drug Administration. This effort resulted in the development of a set of tools to create three-dimensional digital microstructure images coupled with an interface to computational solid mechanics finite element modeling. The approach allows for the simulation of morphology characteristics such as grain size, shape, and texture via statistical information gathered from experimental results. Examples illustrated some applications of the framework to commercial aluminum alloys and two-phase materials in areas such as fatigue crack initiation and deformation during material processing.

J. Spowart of the Air Force Research Laboratory presented a study of spatial anisotropy in discontinuously reinforced aluminum and other metal-matrix composites. The approach he developed was aimed at characterizing the effect of higher-order random microstructural features in predicting the constitutive behavior of the composite. The spatial homogeneity of a discontinuously reinforced aluminum sample is decoupled into two length scale parameters that refer to the axial and transverse directions. By using an elasto-plastic finite element routine, the effect of these length scales on the tensile strength, yield strength, and strain-hardening rates were quantified. Interestingly, observations of the microstructural randomness effects on the post-yielding behavior of the samples led to the conclusion that controlling the spatial homogeneity of the reinforcement in the aluminum matrix results in improved performance of the material without any loss in the ductility capabilities of the discontinuously reinforced aluminum.

Another session of interest included a review of the World Trade Center towers collapse with the presentation of three consecutive papers on the subject. The renowned Prof. Z. Bazant of Northwestern University reviewed the rapid progressive collapse failure mode assumed for the towers. Through the use of simple physical formulations, Prof. Bazant described a methodology for tracking the collapse of the World Trade Center towers from the critical floors where impact occurred to the lower and higher portions of the structure. An inverse initial boundary value problem was then applied based on the displacement history observed in actual footage of the collapse to obtain information on the energy dissipation of the progressive failure of individual floors. This was followed by a presentation by F. Sadek of the National Institute of Standards and Technology on the conclusions reached by the National Institute of Standards and Technology after an investigation of the possible causes that triggered the collapse of the towers. This presentation reviewed the complex finite element models used to track the spread of the jet fuel and subsequent ignition of the fire that crucially contributed to the failure mode of both buildings. The session was concluded with a presentation by Prof. L. Esparragoza who introduced alternative formulations of the possible World Trade Center collapse resulting in a lively discussion of the material from all three presentations.

The sessions on probabilistic mechanics encompassed several papers on diverse fields of applications. L. Tan from Johns Hopkins University introduced a technique for characterizing microstructural evolution during the deformation of crystalline structures in ductile metals. The microscopic grains are modeled as polygons with random orientation and size, which can be controlled through the use of a so-called orientation distribution function to capture the statistical information of the material. The changes in the orientation distribution function content during deformation are tracked via an analytical plasticity model for single crystalline inclusions in an equivalent homogeneous medium.

S. Wojtkiewicz of the University of Minnesota presented an approach to improve the efficiency of large computational models where the uncertainty is localized to smaller regions of the problem to be solved. The formulation utilizes linear algebra techniques for low-rank matrix updates and other mathematical tools and was exemplified for dynamic systems. The approach couples a small number of full runs with a solution updating routine involving subsets of the larger problem where uncertainty is present.

J. Zhao of the Sikorsky Aircraft Company described a framework for coupling structural health monitoring of aircraft propulsion systems with uncertainty modeling and propagation. This work was performed for the Defense Advanced Research Projects Agency and provided an interesting overview of the challenges involved in combining multi-disciplinary topics such as data collection, signal processing, network optimization, and life prediction models within a probabilistic context. The discussion included a glimpse of the complexities involved in verification and validation efforts for uncertainty models used in advanced government agencies projects.

The author of this report presented the paper Micromechanical Analysis of Random Non-Homogeneous Composites Using Moving-Window Generalized Method of Cells in one of the mini-symposia dedicated to probabilistic mechanics issues (see abstract attached). The exposition of the work performed at Johns Hopkins University previous to joining Southwest Research Institute was well received, eliciting several interesting and constructive questions on the methodology and results.

The author of this report also attended an official meeting of the Probabilistic Mechanics Committee. Committee chair, Prof. R. Ghanem from the University of Southern California presided over the meeting which included Prof. R. Corotis from the University of Colorado at Boulder, Prof. S. Arwade from Johns Hopkins University, Prof. S. Wojtkiewicz from the University of Minnesota (previously with Sandia National Laboratories), Dr. F. Xu from Stevens Institute of Technology, and Dr. J. Shi from ABAQUS, Inc. Although absent from this meeting, Dr. L. Huyse from Division 18 of Southwest Research Institute is schedule to become the chair of the Probabilistic Methods Committee in the coming months. Prof. L. Graham-Brady extended an invitation to the author of this report to apply for Probabilistic Methods Committee membership.

**CONCLUSIONS:**

The participation in the 15$^{th}$ National Congress of Theoretical and Applied Mechanics was a highly beneficial way to interact with researchers in the probabilistic mechanics community as well as in the wider computational mechanics research environment. Exposure to presentations on academic, industrial, and government agency projects provided an excellent overview of current leading edge research and potential areas of further development for researchers in all fields involved.

**PROBLEMS ENCOUNTERED:**

None.

**PENDING ACTIONS:**

None.

**RECOMMENDATIONS:**

Continued involvement in current and future activities of the U.S. National Committee on Theoretical and Applied Mechanics and its associated member societies is highly recommended.

**SIGNATURE:**

7-31-2006

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Sitakanta Mohanty, Assistant Director
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## ATTACHMENT

# MICROMECHANICAL ANALYSIS OF RANDOM NON-HOMOGENEOUS COMPOSITES USING MOVING-WINDOW GMC

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The analysis of composite materials with random microstructures usually assumes that homogenized or equivalent effective properties can be used to represent the average material behavior, while neglecting localized variation due to spatial randomness in composition. When local extreme effects arise, this assumption will not be adequate for the accurate prediction of failure mechanisms such as plastic yielding or crack initiation. In such cases, a probabilistic approach can be used to include such effects [1]. In the case of non-homogeneous composites, this is augmented by the fact that the probabilistic information (i.e. mean and/or probability density function) can vary between different spatial locations. Since such materials exhibit compositional heterogeneity as well as statistically inhomogeneous phase distribution (i.e. gradients), it becomes even more difficult to accurately ascertain where extreme phenomena may arise.

An analysis approach that accounts for the microstructural variation in a probabilistic framework is presented. The technique involves digital image analysis and a computational micromechanics model titled the Moving-Window Generalized Method of Cells (MW-GMC) [2]. The Generalized Method of Cells approach differentiates from traditional Finite Element Methods (FEMs) in the sense that it assumes average continuity of displacements and tractions, instead of only point-wise displacement continuity. This approximate formulation provides a computationally efficient and accurate way of deriving the material properties at any given location by defining a repeating volume-element unit cell (or window) as a representation of a periodic microstructure, from which local fields of the effective material properties can be generated [3].

By applying the micromechanics approach to both digitally generated samples (using probabilistic algorithms) and actual images of non-homogeneous composites under a finite element application, an investigation of the method's effectiveness is provided. In this context, its accuracy and computational efficiency are compared to brute-force finite element analysis of a full sample. The sensitivity of the resulting local stress distributions with respect to window size is investigated for two-dimensional images generated using a probabilistic framework that incorporates the simulation of non-Gaussian, non-stationary samples [4].

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**Keywords:** micromechanics, composites, characterization