NATIONAL TECHNICAL UNIVERSITY OF ATHENS
SCHOOL OF CIVIL ENGINEERING
LABORATORY FOR EARTHQUAKE ENGINEERING
DIRECTOR: PROFESSOR CONSTANTINE SPYRAKOS

ΕΘΝΙΚΟ ΜΕΤΣΟΒΙΟ ΠΟΛΥΤΕΧΝΕΙΟ
ΣΧΟΛΗ ΠΟΛΙΤΙΚΩΝ ΜΗΧΑΝΙΚΩΝ
ΕΡΓΑΣΤΗΡΙΟ ΑΝΤΙΣΕΙΣΜΙΚΗΣ ΤΕΧΝΟΛΟΓΙΑΣ
ΔΙΕΥΘΥΝΤΗΣ: ΚΑΘΗΓΗΤΗΣ ΚΩΝ/ΝΟΣ ΣΠΥΡΑΚΟΣ

ΑΝΑΚΟΙΝΩΣΗ ΟΜΙΛΙΑΣ

Την ΠΑΡΑΣΚΕΥΗ 29-05-2015

Computational Modeling at Nanoscale – Materials, Mechanics and Bio Applications

Το Εργαστήριο Αντισεισμικής Τεχνολογίας, ΕΜΠ (LEE-NTUA) σε συνεργασία με την Ερευνητική Ομάδα Ηλεκτρονικά Νανο-υλικά και Διατάξεις και με την Ερευνητική Μονάδα Προηγμένων, Σύνθετων, Νάνο Υλικών και Νανοτεχνολογίας (**R-NanoLab**) έχουν τιμή να σας προσκαλέσουν στην ομιλία που θα πραγματοποιηθεί στο αμφιθέατρο του Εργαστηρίου Αντισεισμικής Τεχνολογίας, της Σχολής Πολιτικών Μηχανικών του ΕΜΠ την **Παρακευή 29 Μαΐου 2015** και ώρα **16:30** από τον καθηγητή κ. Ram Mohan, Professor of Nanoengineering, Joint School of Nanoscience and Nanoengineering, North Carolina A&T State University με τίτλο: **Computational Modeling at Nanoscale – Materials, Mechanics and Bio Applications**. Ακολουθεί σύντομο βιογραφικό σημείωμα του ομιλητή καθώς και περίληψη της ομιλίας.

Πρόσβαση στο Εργαστήριο (http://lee.civil.ntua.gr/images/diafores/map_gr.jpg)

Κωνσταντίνος Σπυράκος

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Dr. Ram Mohan is currently a Professor of nanoengineering. He is also the co-lead of the computational science and engineering research cluster at North Carolina A&T State University. Dr. Mohan currently has nearly 100 peer reviewed journal articles, book chapters and conference proceedings to his credit. He plays an active role in American Society for Mechanical Engineers (ASME) and serves as the chair of the ASME materials processing technical committee. He also serves as the member of the Nanoengineering Council Steering Committee with a focus on nanoengineering in energy and medicine. He is a member of American Society of Aeronautics (AIAA), American Society for Engineering Education (ASEE), Society for Advancement of Materials and Process Engineering (SAMPE), and regularly presents, organizes and conducts seminars and conferences for these professional and engineering organizations. Dr. Mohan has been serving as a regular reviewer for several scientific journals and conferences in his field of research. Over the past several years, he has worked with and his research work has been supported by several federal agencies and industries. He has been an invited and keynote speaker at several international conferences, universities, research laboratories, and industries in US, Europe, India and several other countries. His industrial interactions include Lockheed Martin-Manassas, Boeing-Mesa, Northrop Grumman, Boeing-St. Louis, and Lockheed Martin-Skunk Works.

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ABSTRACT

Computational Modeling at Nanoscale – Materials, Mechanics and Bio Applications

Nanoengineering requires transformational research and technologies in several areas that necessitate understanding of the nanoscale phenomena and processes using direct measurements and simulations. Computational modeling in nanoengineering is highly interdisciplinary built upon mathematical models of associated physical phenomena at nanoscale with a potential to enhance the nanotechnology field from an empirical science to a quantitative engineering field. Computational nanoengineering research thrust area in our group currently focuses on: 1. Multi-scale modeling and mechanics of nanoengineered material systems, 2. Material interactions in nanoengineered polymer composites, 3. Deformation behavior at nanoscale, and, 4. Nano and bio systems and interfaces. In complex material systems, computational modeling provides an enabling computational microscope that images and analyses for enhancing the understanding of their properties and behavior through appropriate mathematical computational material models at different length scales.

This presentation will discuss our work on the computational modeling at the nanoscale level; including brief discussions on the molecular/atomistic modeling methods relevant to nanoscale; commonality that exists at the nanoscale level in the mathematical methods and principles in both engineered materials, mechanics and bio applications, and their multi-scale features. This will be followed by specific discussions of our recent computational nanoscale modeling work in materials, mechanics and bio applications. These include: Materials and Mechanics: Our recent research work on the understanding of material interactions and property predictions in the processing and mechanics of polymer composites will be discussed. Hybrid and nano composites consist of material phases at varying length scales, and include nano material constituents. The behavior of these composites is influenced by the material interactions during processing, and by the damages/defects in the associated constituent nano materials. The role of nano scale modeling based on the molecular material structures to provide an insight into the molecular level interactions that exist, and their influence on the associated composite properties will be discussed. Other areas of our research focusing on the computational modeling of deformation and fracture at nanoscale in bi-metallic nanolayers, material chemistry level modeling of cementitious material systems will be briefly highlighted. Bio Systems: Biomarkers are molecules that correspond with or produced by bio-chemical changes in concentration, physiology and morphology that are detected by suitable aptamer based bio-recognition elements. Our computational modeling study of molecular level interactions that are of relevance to breast cancer peptide-aptamer system will be highlighted.

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