

Modeling and Simulations at Nanoscale and Nanostructures

Overview

Computational nanoengineering is highly interdisciplinary with a potential to enhance nanotechnology field from an empirical science to a quantitative engineering field. Relevant modeling and simulations at nanoscale and nanostructures provides an enabling computational microscope that images, and analyses enhancing the understanding at such low length scales.

This course focuses on molecular/atomistic modeling methods relevant to nanoscale; introduce principles, theoretical and foundational backgrounds; introduce selected academic/scientific atomistic/molecular dynamics modeling analysis codes via illustrative applications of relevance to crystalline, amorphous, and bio material systems. The purpose is to introduce underlying principles and basis, associated computational methods for defined physical quantities, caveats and limitations to learn best practices and applications of nanoscale modeling and simulation. In addition, this course through examples discusses recent modeling and simulation applications from our research for understanding material interactions, interfaces, deformation and failure; property predictions of relevance to polymeric composites; cementitious materials, nanoscale layered metallic composites, bio systems and biosensor applications to stimulate research motivation.

This course is based on a semester long graduate level course developed and currently taught by Prof. Mohan. Course attendees will learn through lectures; interactive, web-based hands on nanomodeling analysis and/or applications; introductory hands on exercise using an open source molecular modeling analysis via examples - if possible to coordinate installation and computer facilities with the host institution.

Modules	A: Modeling and Simulation at Nanoscale and Nanostructures: March 7 – March 11, 2016 Number of participants for the course will be limited to forty.
You Should Attend If...	<ul style="list-style-type: none"> ▪ You are an engineer or research scientist or a technical professional in engineering disciplines (mechanics and materials, mechanical engineering, material science, nanotechnology, civil engineering, applied mechanics, metallurgy, nanoscience and nanoengineering etc.) interested in modeling and simulation at nanoscale; methods and applications of relevance in mechanics, material sciences and bio systems. ▪ You are a physical, chemical, biological, and mathematical scientist or a professional from these science disciplines interested in nanoscale modeling. ▪ You are a student or faculty from academic institutions interested in learning how to do research in this field; and for applications in mechanics, material sciences and bio systems. <i>Students should be at least in their final year of undergraduate study in engineering, sciences, or graduate students.</i> ▪ <i>Fundamental knowledge of computational methods and modeling; computer skills is preferred for all attendees but not necessary.</i>
Fees	<p>The participation fees for taking the course is as follows: Participants from abroad : US\$ 100 Industry/ Research Organizations: ₹ 5000 Academic Institutions: ₹ 2000 Students (including Research Scholars): ₹ 1000</p> <p>The above fee includes all instructional materials, computer use for tutorials and assignments, laboratory equipment usage charges, 24 hrs free internet facility. The participants will be provided with accommodation on payment basis subject to availability.</p> <p>All course registrations will processed via the national GIAN portal (gian.iitkgp.ac.in), where a Rs 500/- one-time fee is payable in addition to the above amount.</p> <p>Registration fee can be directly deposited through NEFT to the designated account as given below or can be sent in the form of demand draft (D.D.) drawn on any nationalized bank in favour of "GIAN-MSNN 2016" payable at Allahabad.</p> <p>Account Name: GIAN-MSNN 2016. Account No.: 718400301000187. Bank: Vijaya Bank, MNNIT Branch, Allahabad- 211004, U.P. IFSC Code: VJIB0007184.</p>

The Faculty



Dr. Ram Mohan is Professor of Nanoengineering, at Joint School of Nanoscience and Nanoengineering (JSNN), North Carolina A&T State University, Greensboro, NC, USA, and is a faculty as Adjunct Professor of Nanoscience at JSNN. He leads as the Project Director and Principal Investigator of the US Army funded center for hierarchical and multi-scale materials. He currently has more than 120 peer reviewed journal articles, book chapters and conference proceedings to his credit. In 2012, Dr. Mohan was awarded the Senior Researcher of Excellence at North Carolina A&T State University. He also serves as the Track Chair for Materials: Genetics to Structures track at the 2014, 2015, and 2016 ASME conference and exposition.



Dr. Anuj Jain is Professor in the Department of Applied Mechanics at Motilal Nehru National Institute of Technology Allahabad, India. He has taught Computational Material Science course at PG level. His research interests include development of nanoferrites for various applications.



Dr. Abhishek Kumar is Assistant Professor in the Department of Applied Mechanics at Motilal Nehru National Institute of Technology Allahabad, India. His research interest includes nanomaterials, coatings and mechanical behaviour of materials.

Course coordinator(s)

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