Hierarchical Computational Methods for Cross-disciplinary Multiscale Dynamics

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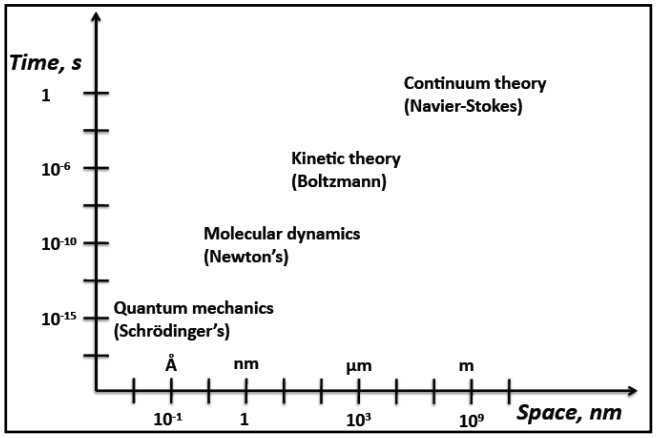
Overview

A wide gamut of natural phenomena, scientific processes and engineering applications are governed by physical, chemical and biological mechanisms that span from the atomic level (nano) to the meso-micro-continuum scales. The construction of an exhaustive knowledgebase and design paradigms in thrust areas such as, but not limited to, energy conversion and storage, genetics to tissue mechanics, micro/nano flows, cardiovascular dynamics, strength of materials etc., requires efficient and integrated modeling coupling molecular information with the macroscopic dynamics. The anisotropy and non-linearity of the constitutive properties are governed by the molecular kinetics, while the realizable scale applications follow mesoscopic/ continuum mechanics relations. The computational study of these problems necessitates the development and implementation of hierarchical tools and mathematical methods.



This course will provide researchers across various scientific disciplines engaged with multiscale problems a broad exposure to analytical and numerical techniques that cohesively describe scientific phenomena across length scales. The resource demanding expensive computations at the finest grid and for large molecular systems require high performance computing. A "top-down" strategy will be adopted and the course structure will be distributed as:

- (***Module-A***) Parallel computing, GPU and multiscale information extraction and processing
- (***Module-B***) Multiscale constitutive model, lower-order and entropy based modeling
- (***Module-C***) Molecular dynamics and Monte-Carlo simulations of material structure and transport behavior at the nanoscale

The uniqueness of this course offering lies on its interdisciplinary character by bridging the disciplinary boundaries of engineering, sciences and biology. Subtle synergies that exist between, for e.g., chemists, biologists and engineers, will be encouraged by the cross-fertilization of ideas between multi-disciplinary participants.

Modules	**A: High performance computing and information science : October 14 – 'October 15** **B: Continuum-to-micro scale modeling techniques : October 16 – October 18** **C: Micro-to-nano scale modeling techniques : October 19 – October 22** **Number of participants for the course will be limited to fifty.**
You Should Attend If.....	• You are a practicing engineer or R&D scientist from industry or research labs working in the field of materials and mechanics. • You are computational scientists from industry or research labs interested in application of high performance computing applications and architectures. • You are a student or faculty from academic institution interested in multi-scale dynamics, computational methods and analytical techniques.
Fees	The participation fees for taking the course is as follows: **Participants from abroad : US $500** **Industry/ Research Organizations: Any two modules: INR 20000 ; all modules: INR 30000** **Academic Institutions: Faculties: INR 5000; Students and Project Staffs: INR 1000** The above fee include all instructional materials, computer use for tutorials and assignments, laboratory equipment usage charges, 24 hr free internet facility. The participants will be provided with accommodation on payment basis.

The Faculty

Dr. Ganesh Balasubramanian is in the faculty of Mechanical Engineering Department at Iowa State University, USA. His research interests include Nanoscale transport phenomena, surface modifications through photoswitchable polymers, development and implementation of multiscale computation techniques, improving performance of thermoelectric materials, predicting mechanical properties of soft matter and synthetic (bio)materials, identifying potential long-term thermal storage materials and the related mechanisms, designing novel curriculum for teaching emerging technologies

Dr. Somnath Roy is an Assistant Professor of Indian Institute of Technology Patna. His research interest is turbulence, mixing, dynamic systems, moving boundary flow simulation, high performance computing using cluster and GPGPUs.

Dr. Somnath Sarangi is an Associate Professor of Indian Institute of Technology Patna. His research interest is continuum mechanics, non-linear dynamics and fluid structure interactions.

Course Co-ordinator

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