The rapid advances in nanotechnology, nanomaterials and nanomechanics offer huge potentials in national defense, homeland security, and private industry. An emphasis on nanoscale entities will make our manufacturing technologies and infrastructure more sustainable in terms of reduced energy usage and environmental pollution. Recent advances in the research community on this topic have stimulated ever-broader research activities in science and engineering devoted to their development and their applications.

With the confluence of interest in nanotechnology, availability of experimental tools to synthesize and characterize systems in the nanometer scale, and computational tools widely accessible to model microscale systems by coupled continuum/molecular/quantum mechanics, we are poised to unravel the traditional gap between the atomic and the macroscopic world in mechanics and materials. This in turn opens up new opportunities in education and research.

Over the past three decades, we have acquired new tools and techniques to synthesize nanoscale objects and to learn their many incredible properties. Today's high-resolution electron microscopes can routinely see individual atoms. Scanning probe techniques allow us to manipulate atoms one at a time. Advanced materials synthesis provides the technology to tailor-design systems from as small as molecules to structures as large as the fuselage of a plane. We now have the technology to detect single molecules, bacteria or virus particles. We can make protective coatings more wear-resistant than diamond and fabricate alloys and composites stronger than ever before.

Advances in the synthesis of nanoscale materials have stimulated ever-broader research activities in science and engineering devoted entirely to these materials and their applications. This is due in large part to the combination of their expected structural perfection, small size, low density, high stiffness, high strength and excellent electronic properties. As a result, nanoscale materials may find use in a wide range of applications in material reinforcement, field emission panel display, chemical sensing, drug delivery, nanoelectronics and tailor-designed materials. Nanoscale devices have great potential as sensors and as medical diagnostic and delivery systems.

In most of these applications, nanoscale materials will be used in conjunction with other components that are larger, and have different response times, thus operating at different time and length scales. Single scale methods such as “ab initio” quantum mechanical methods or molecular dynamics (MD) will have difficulty in analyzing such hybrid structures due to the limitations in terms of the time and length scales that each method is confined to. Because of the availability of accurate interatomic potentials for a range of materials, classical MD simulations have become prominent as a tool for elucidating complex physical phenomena. However, the length and time scales that can be probed using MD are still fairly limited. For the study of nanoscale mechanics and materials, we must model up to a scale of several microns, consisting of billions of atoms, which is too large for MD simulations to-date. Hence, we need to develop multiscale approaches for this class of problems. One possible approach that can be applied to many problems is to use MD only in localized regions in which the atomic-scale dynamics are important, and a continuum simulation method, such as the finite element or meshfree method, everywhere else. This general approach has been taken by several different groups using methods that have had varying degrees of success. In particular, these methods do not satisfactorily address the issue of disparate time scales in the two regions, and provide a rather simplified treatment of the interface between the atomistic and continuum regimes.

Current research in engineering is just beginning to impact molecular scale mechanics and materials and would benefit from interaction with basic sciences. For solids, research in the area of plasticity and damage has experienced some success in advancing microscale component design. Development of carbon nanotubes is also an area in which nano scale research has clearly played a major role. Other areas of opportunities include nano composites and nano alloys. For fluids, coupling physics phenomena at the nanoscale is crucial in designing components at the microscale. Electrophoresis and electro-osmotic flows coupled with particulate motion in a liquid have been important research areas that have had great impact in the homeland security area. Microfluidic devices often comprise components that couple chemistry, and even electrochemistry, with fluid motion. Once the physics-based models are determined for the solids and fluids, computational approaches will need to be employed or developed to capture the coupled physics phenomena.

The material presented in this talk informs researchers and educators about specific fundamental concepts and tools in nano mechanics and materials, including solids and fluids. It is envisioned that this work will serve as a starting point from which interested researchers may jump into and contribute to the emerging field of computational nanotechnology.

The talk’s outline is given by the following. We first review the fundamentals of classical molecular dynamic simulations, such as the Lagrangian and Hamiltonian formulations, and the structure of interatomic potential functions. We then inform the reader on the relevant quantum mechanical approaches and explains the energetic link between the quantum and classical systems. We will outline the intrinsic limitations of molecular dynamic simulations and emphasize the necessity in developing the coupled multiscale methods and reviews available multiscale approaches: hierarchical and concurrent coupling of the atomistic and continuum simulations (with the emphasis on the bridging scale method), multiscale boundary conditions and multiple scale fluidics. We conclude the talk by discussing future research needs in multiple-scale analysis, and the impact the current research has on the graduate curriculum at Northwestern.