NSF Network for Computational Nanotechnology

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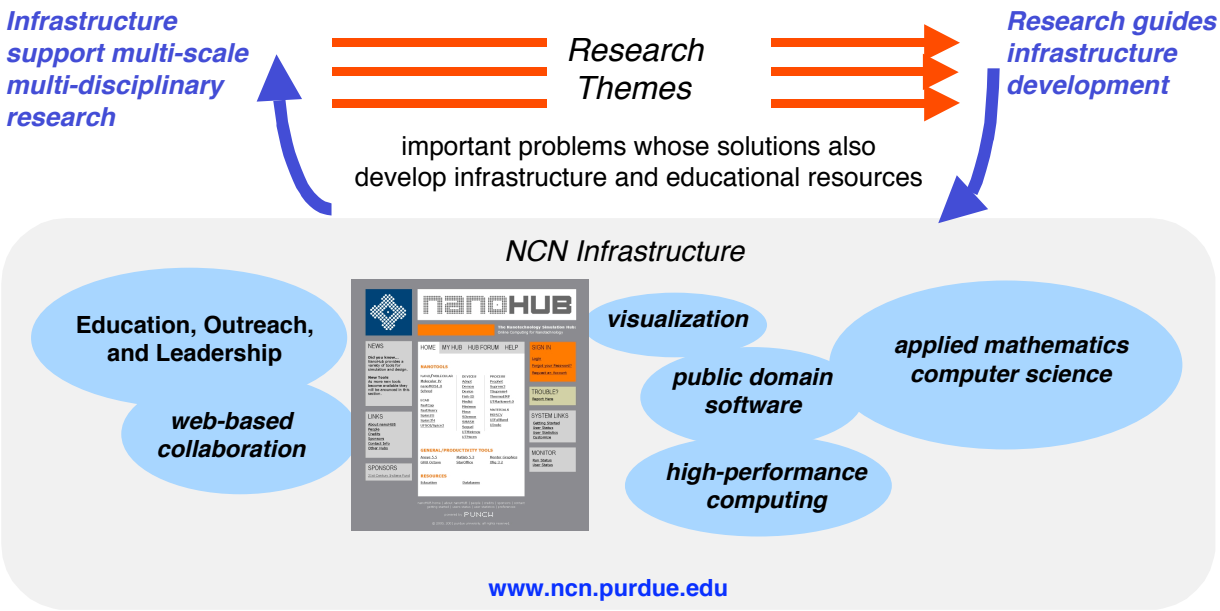
Vision and Mission: Turning the promise of nanoscience into practical nanotechnologies will require: 1) integrating knowledge, concepts, and techniques covering many different spatial and temporal scales, 2) close interactions between experimentalists, theorists, and computational experts from many different disciplines, and 3) restructuring engineering curricula to complement traditional macroscopic approaches with a microscopic viewpoint. The Network for Computational Nanotechnology (NCN) was established to help address these challenges through theory and computation. Our mission is to:

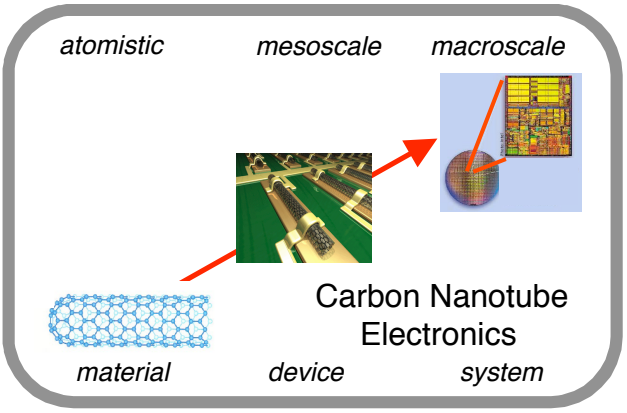
- Address key research challenges through theory and computation – research that begins at the atomistic level, proceeds to the system scale, and is tightly linked to experimental work.
- Create and support a cyber-infrastructure that facilitates collaboration and provides ready access to simulation services, high-performance computing, visualization, and public-domain software.
- Educate students and professionals in the use of new software tools and approaches, and develop new courses and course modules using simulation to provide "hands-on" experiences to students at all levels.

The NCN's three-fold mission of research, infrastructure, and education is a synergistic process in which the infrastructure will attract leading experts and educators into the network, while their activities in turn will enrich the infrastructure.



Research Themes: The NCN focuses on three research themes, ***nanoelectronics***, ***nanoelectromechanics***, and ***nanobioelectronics***, which cover a broad subset of nanoscience yet have sufficient synergy to provide the overall focus that is essential to success. The specific projects and participants within these themes will evolve over time and new themes involving new topics, investigators, and institutions may be added through leveraged support.

Research Projects: The NCN supports a special kind of research for which initial scientific groundwork has established prospects for significant technological impact. We address problems for which the theory does not exist and needs to be worked out as new numerical methods and large-scale computing approaches are developed. We support projects that are ready for a coordinated, multi-disciplinary attack and that can only be solved by an interdisciplinary team that works closely together and with collaborating experimentalists. Each project begins at the atomistic scale, and proceeds to the macroscale of integrated nanosystems.



Carbon nanotube electronics, the first project in the nanoelectronics theme, is led by Datta (Purdue) and will study nanotube/metal and insulator interfaces (Cho, Stanford), device design (Lundstrom, Purdue), carrier-phonon coupling (Leburton, Illinois), chemical sensors (Ratner, Northwestern) and circuit and system issues (Roy, Purdue). Applied mathematicians (Sameh, Purdue and Golub, Stanford) will develop numerical algorithms for quantum transport equations. The work is tightly linked to experimental studies (Dai, Stanford and McEuen, Cornell). In addition to addressing critical research challenges, this project will produce public domain software for tight binding molecular dynamics and NEGF simulation of quantum transport.

The development of a suite of ***computational prototyping tools and approaches for NEMS*** is the first project in the NEMS theme. Atomistic, device, circuit, and system issues will be explored using a suite of computational design tools based on fine-grained and coarse-grained multiscale approaches (Sinnott, Florida), continuum approaches (Aluru, Illinois), and reduced-order and circuit-level approaches (Dutton, Stanford). The initial focus of this team, led by Dutton, will be on carbon nanotube structures where the experimental knowledge base is rapidly expanding. The software resulting from this approach will impact a variety of other structural and material nanoscale problems.

Transport in artificial and natural ion channels is the first project in the nano/bio theme. Hess (Illinois) will lead an effort to study ion transport in naturally occurring nanoscale channels and to understand how elementary devices function and how complex systems are assembled. The objective is to understand how artificial structures that duplicate properties of biological systems at the nanoscale can be realized. Ravaioli (Illinois) will develop transport solvers using approaches from semiconductor transport, and Murthy (Purdue) will couple microscopic thermal-fluid simulation to continuum scale simulations. Schatz (Northwestern) will focus on the chemistry of ion-channel interactions. A bottom up approach, will establish a simulation capability for a specific problem and then extend it for wet/dry systems more generally.

Infrastructure: Prospects for success in nanotechnology will be enhanced if CAD tools can be developed and made available to experimentalists and to system designers so that those with problems to solve can do the simulations themselves. In addition to doing research that matters, therefore, the NCN also has a mission to develop and support a ***computational user facility*** that provides simulation services remotely through the WWW. NCN projects develop theory, numerical approaches, and software tools that fill critical needs for nanotechnology. These software tools, and the educational resources to facilitate their use by others, contribute to a growing infrastructure that will support the NCN and the broader nanotechnology community.

The NCN delivers computational services through the nanoHUB (www.nanohub.purdue.edu), which allows users to access computer programs, run simulations, and view results via standard Web browsers – without needing to install and support software. Researchers share simulation tools, educators create computer labs with state-of-the-art modeling tools, and students access educational modules that bring abstract concepts to life. As research projects mature, a growing library of tools and approaches will be made available to researchers, educators, and students. The nanoHUB is one part of a developing cyberinfrastructure that will deliver simulation and educational services and facilitate collaborative research.

Education and Outreach: The NCN's educational mission is inspire and educate the young people who will realize the promise of nanoscience as well as to equip practicing professionals to contribute to this new field. To achieve these objectives, the NCN will: a) develop short courses for graduate students and professionals on new software tools and approaches; b) create research experiences for students at all levels; c) recruit students and underrepresented populations; d) create new course modules that make use of simulation; and e) organize workshops and meetings. Advanced on-line technologies will ensure the maximum impact for these activities.

Summary: The NCN's research will produce new knowledge, approaches, algorithms, and public-domain software that will help realize the promise of nanoscience. It will also provide a concrete context for developing new ways to educate a new generation of students. Research and education will also guide the development of an infrastructure whose impact will be felt for years to come by making theorists and computational scientists more effective and by providing unique simulation services and educational resources to users worldwide. We aim to add a new dimension to the intellectual networking that drives the research and education enterprise of our nation.