NCN

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NSF Network for Computational Nanotechnology

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Morgan State University, Northwestern University, Purdue, Stanford University, University of Florida, University of Illinois at Urbana-Champaign, University of Texas at El Paso

Vision and Mission: The Network for Computational Nanotechnology (NCN) has a mission to create an environment where theorists, experimentalists, and computational experts collaborate on significant problems in nanotechnology. In the process, NCN research teams are producing new algorithms, approaches, and software tools with capabilities not yet available commercially. Our vision is to connect theory, experiment, and computation in a way that makes a difference to the future of nanotechnology — both in research and education. The NCN is tightly linked to experimental programs in nanotechnology and to information technology research that is developing next-generation cyber-infrastructures. The NCN team has a track record of research that influences the agenda of experimentalists. Equally strong is its commitment to engaging the community through workshops that set research agendas, to novel educational initiatives, and to putting the latest, research-grade software tools in the hands of students and users with problems to solve. The nanoHUB, a web-based computational user facility with a global user base, is an example of that commitment.

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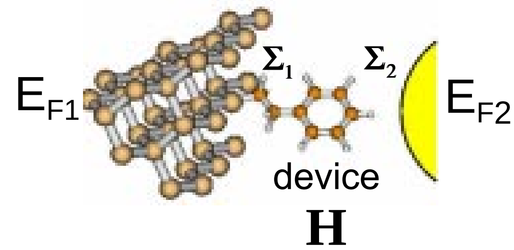
The NCN links theory and computation to experimental work and couples this all to a unique infrastructure that serves the NNI. Our vision is to make a difference in moving the promise of nanoscience towards new technologies.

Research: The NCN's approach to research flows from a commitment to connect experiment, theory, and computation in a new way. The focus is applied, but long term. Each project has clear objectives, a three-year duration, and a mission to advance the field. We choose projects that are ready for a coordinated, multi-disciplinary attack. Sufficient science must have been done so that a promise of significant, new technologies has been identified. A team of experts with complementary skills and interests addresses outstanding scientific questions as well as important technological issues. The team begins with atomistic treatments of materials and connects them to mesoscopic descriptions of devices, and finally to the macroscopic description of integrated nanosystems. In the process of addressing these problems, the teams wrestle with the challenges of connecting length and time scales and crossing disciplinary boundaries. Each project also includes significant computational challenges, and an applied mathematician or computer scientist to address those challenges. The fields that the NCN addresses, i) nanoelectronics, ii) NEMS, and iii) nano-bioelectronics. are broad but with sufficient focus so that they can benefit from synergies. We aim to develop the understanding, approaches, and simulation tools that will allow engineers to design new nanoelectronic and NEMS technologies. Ultimately we see these three themes merging with the goal of connecting dry electronic and mechanical nanosystems to wet biological nanosystems.



$$\mathbf{G}^R = \left[E\mathbf{I} - \mathbf{H} - \mathbf{\Sigma}_1 - \mathbf{\Sigma}_2 - \mathbf{\Sigma}_S\right]^{-1}$$

NCN researchers led by Datta developed new techniques to simulate electronics conduction through molecules on silicon. This group predicted that such devices would display novel electronic characteristics (negative differential conductance) that were recently confirmed experimentally.

The vision of the NCN's **nanoelectronics** research is to understand conduction at the molecular scale and to develop the approaches and tools to simulate molecular electronics. The two projects underway, carbon nanotube electronics and one that treats molecules on silicon are developing simulation tools that range from toy models that provide insight, to empirical models that may become CAD tools of the future, to *ab initio* simulations that provide insight into critical problem. The development of a suite of computational prototyping tools and approaches for ***NEMS*** is the first project in the NEMS theme. NEMS research requires a multidisciplinary approach because of the presence of several physical domains – e.g. mechanics, electrostatics, fluidics, biology, chemistry, and of several forces (Coulomb, van der Waals, bonding). Atomistic, device, circuit, and system issues are being explored using a suite of computational design tools based on fine-grained and coarse-grained multiscale approaches, continuum approaches, and reduced-order and circuit-level approaches. The initial focus is on carbon nanotube and silicon structures where the experimental knowledge base is rapidly expanding, but the software resulting from this approach will impact a variety of other structural and material nanoscale problems. Researchers in the **nano-bio** project are examining the possibility of adapting well-developed methods for carrier transport in semiconductors to new problems in biology. Transport in artificial and natural ion channels is the first problem being addressed. The objective is to understand how natural biological channels function, how artificial structures that duplicate properties of biological systems at the nanoscale might be realized. Applications such as DNA sequencing via artificial nanopores are being explored. Simulation capabilities for specific problems like this will be developed and then extended for wet/dry systems more generally. The NCN also supports smaller efforts with a seed project flavor. Research on ***grid computing middleware*** connects the NCN to a larger effort that is working to develop the NCN's next-generation distributed computing environment. Work on ***visualization*** aims to bring the latest approaches of visualization experts to current problems in nanotechnology.

Integrated Problem Solving and Discovery:

The NCN is led by researchers known for working "close to the problem" – using theory and computation to develop a deep understanding of problems, explain new experiments, and propose new ones. Our work has demonstrated that the results and insights from this type of research can play a significant role in a field, but it is important to keep the focus on the problem. High-level problem solving platforms such as Matlab® have been especially effective in this type of work, where the objective is to develop a theoretical understanding of a problem, formulate it mathematically, and then establish the basic computational approaches. The next step is best taken by experts in computation who begin with an identified approach (i.e. a set of equations) and develop the algorithms, parallel implementations, and performance assessment necessary to solve large-scale problems. By connecting those whose interest is close to the problem with those whose interests are closer to the solution, we believe that the NCN can provide a unique, vertically integrated ability to solve important problems through computation – problems that could not have been solved without the contributions of computer scientists. Finally, we plan to turn this research on theory and simulation into robust community codes that can serve as the basis for nanotechnology CAD .

Education:

The NCN educational program aims to: i) facilitate the application of computation in nanotechnology, ii) encourage the use of simulation by educators and experimentalists, and iii) attract young people to careers in nanoscience. A Summer School on Computational Nanotechnology trains users to operate specific, new software tools and educates them on the underlying theory and numerical approaches. A "software boot camp" teaches computing and software engineering fundamentals to new graduate students. Web-based technologies are used so that these courses and short courses are captured as a permanent educational resource – available to students at any time from anywhere. Finally, in a partnership with the NASA-funded Institute for Nanoelectronics and Computing, the NCN operates a Summer Institute that includes NCN short courses, NCN sponsored workshops, and outreach programs to undergraduates and to pre-college students.

Web-based 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 facility that provides simulation services remotely through the WWW. The **nanoHUB** (www.nanohub.purdue.edu), allows users to access computer programs, run simulations, and view results via standard Web browsers – without needing to install and support software. The nanoHUB is one part of a developing cyberinfrastructure that will deliver simulation and educational services and facilitate collaborative research.

Summary: The NCN's research is producing new knowledge, approaches, algorithms, and public-domain software that will help realize the promise of nanoscience. It is also providing a concrete context for developing new ways to educate a new generation of students. Research and education 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.