Network for Computational Nanotechnology

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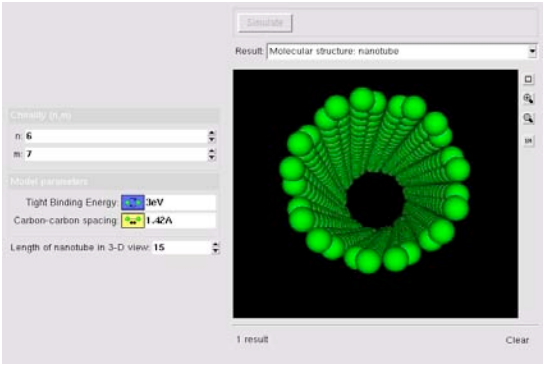
PIs: **Mark Lundstrom and Gerhard Klimeck**
Purdue University
Morgan State University, Northwestern University, Stanford University, University of Florida, University of Illinois at Urbana-Champaign, University of Texas at El Paso

The Network for Computational Nanotechnology (NCN) is a multi-university initiative that was established to create a resource for nanoscience and nanotechnology - on-line services for research, education and collaboration. The NCN's cyberinfrastructure delivers online simulation, courses, tutorials, services for collaboration, and more. It is an example of a new paradigm in science that some are calling service-oriented science [1]. The NCN's objective is to put theory, simulation, experimental and computational research, and education together with cyberinfrastructure in a way that has impact on the development of nanotechnology as a new engineering discipline. This overview of the NCN emphasizes the nanoHUB (www.nanohub.org), the NCN science gateway, and briefly mentions NCN programs in research and education.

The nanoHUB provides unique educational resources, collaborative services, and delivers simulation, visualization, and high-performance computing services on-line. The nanoHUB's signature service is online simulation. Experience in many fields has demonstrated the power of simulation, when software leaves the domain of the computational experts and is placed in the hands of users with real problems to solve. The need to acquire, install, and maintain software is, however, a barrier to its use — especially in new fields where commercial packages are not available. The NCN's goal is to dramatically lower the barrier to the pervasive use of simulations in research and education. Through a partnership with the NSF's middleware initiative, the NCN is deploying In VIGO, middleware that relies on the concept of virtualization, which allows systems of virtual machines, networks, and storage to be constructed on top of heterogeneous collections of hardware [2]. In-VIGO insulates the user from the challenges of traditional grid computing. Users log on, access state-of-the-art simulation software, run interactive graphical or batch simulations, and view the results online, with no need to download, install, support, and maintain sophisticated software. From the user's perspective, they have access to a vast network of machines, all exactly configured to their needs, and launching a job "just works." Computing resources are provided transparently without the need for users to worry about accounts or how



CNTBands, a simple software tool that treats the electronic and physical structure of carbon nanotubes. This tool used Rappture to make a batch application graphical and interactive and suitable for use in the classroom.

to access specific machines. Supporting material such as manuals, example simulations, online tutorials, etc., are also available.

Lowering barriers to the use of simulation involves ready access to tools through a web browser, but *usability* of the software itself is also a key factor. Typical scientific applications are designed with one user in mind: the developer. To engage a larger class of users, however, these scientific codes have to be more than "accessible" or "downloadable" over the web. They have to be usable interactively through an intuitive user interface. A tool that can execute in a few seconds should be interactive and allow the users to ask "what if?" questions. Even the tools that will require significant compute time to execute should be user friendly; simulation set-up as well as the data exploration should be interactive. No additional external tools should be needed to do the scientific work of problem setup and data exploration.

Graphical user interfaces (GUIs) are essential, but they are the last thing that a typical scientist wants to deal with. To address this need, the NCN developing a scripting approach to GUI development that enables rapid wrapping of legacy codes and their custom I/O routines and at the same time offer a full set of I/O routines that generate a GUI automatically. Dr. Michael McLennan of the NCN leads the development of this scripting platform, Rappture. Rappture is more than a package for rapidly building GUI's, it is also part of NCN's longer-term vision for a powerful scripting platform to support the rapid development of high-quality software in emerging research fields. Rappture allows C, C++, even Matlab solvers to be scripted together with new modules to rapidly develop software for new problems.

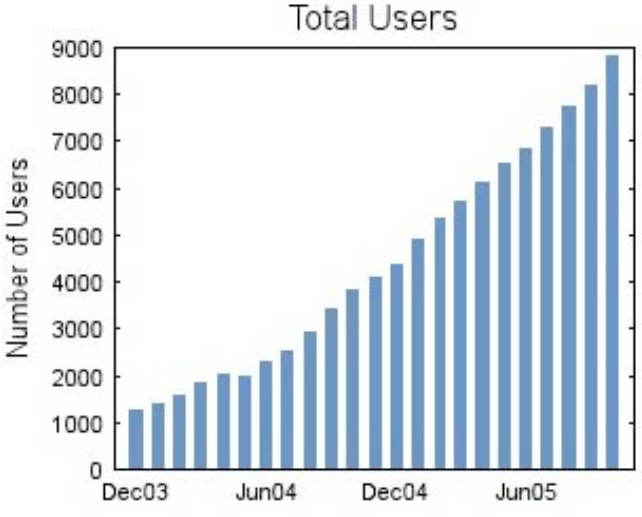
Although online simulation is its signature service, the nanoHUB is **more than simulation tools and services**. Users can access the following services are the nanoHUB:

online:

- simulation
- courses
- seminars and tutorials
- learning modules
- collaborative services

The NCN's educational resources include an innovative nanocurriculum, online courses, lecture, seminars, and tutorials as well as self-paced learning modules that include live simulations as an integral component. Workshops, forums, discussion, and debates also knit the community together. Users may identify themselves as students, researchers, or educators and see resources specifically designed for them. If they request materials on specific topics, the relevant materials are collected, organized, and presented to them. The portal is designed so that users can readily access a growing set of resources that includes a set of collaborative tools to facilitate online seminars, research group meetings, project management, and collaborative software development. Users are encouraged to be "uploaders" as well as "downloaders" of resources to encourage the development of a shared resource built by and serving for the nanoscience and technology community.

The NCN's ultimate objective is not to build infrastructure, but to show how new cyberinfrastructure can have an impact in the field of nanotechnology. To drive the development of its infrastructure to meet the real needs of researchers, educators, students, and professionals, the NCN addresses three sub-fields of nanotechnology – nanoelectronics, nanoelectromechanical systems (NEMS), and nanoelectronics and NEMS devices for nanomedicine. Each NCN science theme is developing new theory, new simulation approaches, and new public domain software while working closely with experimentalists and educators. By focusing on these three fields, we intend to develop infrastructure that will serve the broader nanoscience and technology community as well.



The nanoHUB user community is rapidly growing. Much of the use is for online simulation, but online seminars, courses, and other services are also popular.

In summary, the NCN is addressing the challenges of nanotechnology by developing the theory and simulation approaches to treat devices from the bottom up. It is addressing the software and computing challenge through Rappture, a scripting infrastructure for rapidly developing high quality scientific software and for making them graphical and interactive. The NCN is lowering the barriers to the pervasive use of simulation in the emerging field of nanotechnology by providing ready access to these friendly, interactive simulation tools through the Internet and removing the need to download, install, and support software. The NCN is also creating a collaborative community of students, faculty, and professionals that interact through its unique, web-based infrastructure. NCN educational initiatives, workshops and meetings, the NCN are playing an active role in the NNI. We believe that the NCN is a demonstration of the impact that a well-crafted program in theory, modeling, and simulation can have in exploratory research. We also believe that it is a demonstration of the value cyberinfrastructure in facilitating research, education, and collaboration and a model for the emerging concept of service-oriented science.

[1] Ian Foster, "Service-Oriented Science," *Science*, **308**, May 6, 2005.

[2] J.A.B. Fortes, R.J. Figueiredo, and M.S. Lundstrom, "Virtual Computing Infrastructures for Nanoelectronics Simulation," *Proc. IEEE*, **93**, pp. 1839-1847, 2005.