www.nanohub.purdue.edu

The nanoHUB is a web-based system that is placing a rapidly-growing suite of nanoelectronic simulation tools in the hands of experimentalists, students, and educators while providing them with manuals, examples, tutorials, short courses, and discussion forums. Users 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. Since going on-line in January 2001, the nanoHUB has attracted an international base of users. It is a working demonstration of a utility computing system that allows users to access and use specialized software and hardware resources via a web-based computing portal.

Success in nanotechnology will require that experimentalists and computational experts work hand-in-hand. Computational chemistry and electronic device design are examples of how computer tools developed by theorists and computational scientists can play an important role in the development of a field. Putting tools in the hands of experimentalists and designers was the crucial factor in this success. The impact of computational nanotechnology will be similarly enhanced if those with problems to solve do the simulations themselves. Advanced simulations, however, frequently run on specialized machines, are often difficult to port to other machines, and must be supported, maintained, and upgraded. Users need easy access to manuals, tutorials, examples, short courses, and consultation with experts. Typical users also find it difficult to transition to supercomputers when the size of their problem exceeds the capacity of their personal computer, so on-demand, high-performance computing services must be provided. The nanoHUB is designed both to allow users to operate simulation tools and to provide the additional support that they require.

The current content of the nanoHUB reflects its founders' interests in nanoelectronics:

1) "Full quantum" nanoMOS simulations are being used to examine silicon transistors of the type that might be manufactured in a decade or so.
2) Huckel_IV simulates the current vs. voltage characteristics of a single molecule.
3) Supriyo Datta's tutorial, "Resistance of a Molecule," includes a set of exercises that can be run on the nanoHUB.
4) Users share approaches to use and modify nanoHUB simulation tools with other users in a set of nanoHUB Forums.
5) A 2-day short course, "Electronic Device Simulation at the nano/molecular Scale," is available on-line, and all of the computer exercises can be done on the nanoHUB.

As the nanoHUB evolves, the simulation tools and resources will grow to address the broader nanotechnology community.

The nanoHUB is powered by PUNCH, a network-computing platform that began as the thesis research of one of Prof. Fortes's Ph.D. students, Nirav Kapadia. Since 1995, when that project began, PUNCH has served as a testbed for research in decentralized computing since while operating 24 hours a day serving the real needs of users. It is a working demonstration of a new paradigm that may revolutionize the way in which computing services are delivered by using computational grids to distribute and deliver computing services to users anytime, anywhere. Increasingly, users will access and operate specialized software via Web-based computing portals. PUNCH, an example of such a system of the future, brings together technologies for Internet computing and turns the World Wide Web into a distributed computing portal. It decouples the computing environment perceived by users from the underlying physical infrastructure, thus turning individual computing systems into interchangeable parts. Users access and run programs via standard Web browsers. Applications are installed essentially without modification. Machines, data, applications, and other computing services are located at different sites and managed by different entities. PUNCH provides a network operating system, logical user accounts, a virtual file system service that can access remote data on-demand, and an active yellow pages service that can manage resources spread across administrative domains. Together, these capabilities allow PUNCH to manage and broker resources among end users, application providers, and data centers and compute cycle farms. Extensive documentation is available on the PUNCH web site, www.punch.purdue.edu.

Experience with the nanoHUB and PUNCH over the past several years has demonstrated that web-based computing is not only viable, but often preferred. The nanoHUB's services and capabilities are now rapidly expanding. The operation and support of PUNCH and the nanoHUB has moved out of the research lab to Purdue University's computing support organization, (ITaP - Information Technology at Purdue), where the university will use it to support its strategic initiative in nanotechnology. The nanoHUB will also support the research and educational mission of a six-university Institute for Nanoelectronics and Computing funded by NASA and led by Purdue. Development of In-VIGO, a second-generation network computing platform that will be more flexible, configurable, and grid-compatible has also been launched at the University of Florida. A number of related initiatives is also planned, and the nanoHUB team is seeking partners in the US and abroad to expand the set of simulation tools, services, and resources that are offered. Interested parties should contact Prof. Mark Lundstrom (lundstro@purdue.edu).

What they say about the nanoHUB and PUNCH:

Mark Lundstrom, Scifres Distinguished Professor of Electrical and Computer Engineering and director of the nanoHUB initiative:

> *"When we started this project in 1994, I expected it to be a part-time effort by one student. Today, we support thousands of users in dozens of countries. The nanoHUB and PUNCH continue to grow because they meet the real needs of real users."*

Supriyo Datta, Thomas Duncan Distinguished Professor of Electrical and Computer Engineering and Director of the NASA/Purdue Institute for Nanoelectronics and Computing:

> *"With little effort on our part, we can make our simulation tools available to our colleagues. And with essentially no effort on their part, our colleagues can be running molecular electronics simulations."*

Karl Hess, Swanland Professor of Electrical and Computer Engineering, Beckman Institute, University of Illinois:

> *"The nanoHUB is a great resource. When my students need to do a computation, it's the first place they look for anything from a quick calculation to an independent study project."*

Jose Fortes, Bell South Eminent Scholar, and Director of the Advanced Computer and Information Services Laboratory at the University of Florida:

> *"As a computer engineer, this project has provided me with a global testbed where we can explore approaches for grid-computing systems of the future."*

Nirav Kapadia, lead developer of the PUNCH system and Chief Scientist at Cantiga Systems:

> *"PUNCH is a new approach to computing that lets users focus on their applications and data and tap compute power just as easily as they use electricity today."*

Jim Bottum, Chief Information Officer, Purdue University:

> *"PUNCH is an enabling technology with applications far broader than computational science. Computational grids are coming, and when they do, systems like PUNCH will harness them for users."*