By Carie Windham

The nanoHUB: Community and Collaboration

In 2002, when Purdue University researchers merged the six-year-old Purdue University Network Computing Hubs (PUNCH) with the mission of the NSF's Network for Computational Nanotechnology (NCN), scientists saw, from the beginning, a new frontier for computational science. What would happen, they wondered, if researchers in the field of nanotechnology (the study of particles 25,000 times smaller than the width of a human hair) could harness the power of grid computing to provide a single entry point to scientific tools, discoveries, and research on the Web without forcing the user to download a single piece of code?

The fruits of that marriage became the nanoHUB (http://www.nanohub.org/), a Science Gateway[1] for researchers, faculty, and students in nanotechnology. Taking advantage of PUNCH's extensive cyberinfrastructure and later that of TeraGrid—which employs supercomputers and data storage at nine partner sites—the nanoHUB portal enables users to access scientific tools for research, demonstration, and collaboration. It also serves as a resource for nanotechnology workshops, lectures, and curricula. Users can run experiments, brush up on nanotechnology research, or download a series of undergraduate lectures meant to explain the science at a level appropriate for novices. For the thousands of students, faculty, and researchers who have logged in since the portal launched, the nanoHUB has become a virtual toolkit for understanding how scientists are leveraging nanotechnology to manipulate and understand matter and how even students can conduct experiments and add to the academic discourse.

The Site

Although the site has the look and feel of any multimedia portal—with links to simulations, lectures, and seminars and a personal user panel for organizing the tools, content, and exercises that a user needs most—it acts like a menu in a sit-down restaurant. Just as diners pick an entrée from the menu and eat at their tables, users of nanoHUB choose a tool or simulation to run on their own computers. And just as restaurant-goers usually do not venture into the kitchen to see the inner workings of the meal-production process, nanoHUB users likewise never see the complex system of supercomputers and data-storage devices that host and store the content they access. What they *do* see on their menu is a virtual toolkit of applications and learning resources:

- *Industry-Level Tools*: The initial focus of the nanoHUB was to provide researchers access to computational tools for simulation. Today, the portal features more than fifty high-performance tools that allow users to enter their own data and parameters to run scientific experiments on their desktop. A user might explore the placement of atoms within a carbon nanotube, for example, by entering different variables in the nanoHUB simulation and then observing differences in the molecular structure. The simulated tube, in the molecular view, resembles a cylinder of marbles. Depending on the variables entered, the marbles may appear to line up in rows or cascade like spirals down the tube. To help navigate the science behind each simulation, users can click on tool descriptions or interactive demos as they access the resource.
- *Learning Modules*: Using Macromedia Breeze, learning modules group seminars, quizzes, and exercises in one- to two-hour sequences to teach specific content, such as the fundamentals of nanoelectronics. Each module begins with an abstract explaining the module's learning goals and a list of downloads relevant to the module. An individual module might contain a series of lectures, each available for individual download, presented as narrated slides using Breeze. In addition to lectures, students can access simulations that allow them to walk through the lesson and quiz-like exercises that test learning outcomes and assess their progress. Modules are built in XML to ensure compatibility so that faculty and contributors can upload individual modules to course management systems or national repositories.
- *Teaching Tools*: Faculty can dig into a treasure trove of predesigned teaching tools meant to reinforce nanotechnology concepts in the classroom. There are homework exercises that correspond to specific lectures, PowerPoint presentations to teach individual concepts, and exercises designed to guide students through content. A homework assignment designed to teach electronic transport, for example, provides ten word-problems that guide students through a nanoHUB simulator meant to demonstrate high-field transport in bulk silicon.
- *Lecture Series*: As with the individual learning modules, students and faculty

can access entire courses, provided as a series of lectures with corresponding lecture notes and suggestions for textbooks and readings. Lectures are available as narrated slides using Breeze, and notes are available for download using Adobe PDF.

- *Presentations and Seminars*: Users can also access individual online presentations and seminars, which introduce key concepts or key fields within nanotechnology. Like lectures, the presentations are created by scholars in the field and are presented as slides with audio using Breeze. In a presentation on nanowires and nanotubes, for example, the Purdue researcher Tim Sands defines nanotechnology terminology and introduces basic concepts such as the electronic structure of solids and the relationship between size and properties in nanomaterials.
- *Animations*: Faculty can search for animations to demonstrate key concepts using Flash-technology and cartoon-like drawings and characters for use in the classroom or after class on an individual student's computer. Two cartoon-like children named Laura and Martin, for example, define a nanometer by shrinking Martin to the size of a pinhead (entering the milliworld), then to the size of a red blood cell (entering the microworld), and then finally to the nanometer. An animation demonstrating semiconductors and transistors, on the other hand, feels like a video game as users use their 3D "Do-It-Yourself Kits" to make silicon atoms and crystals.
- *Scholarship*: The nanoHUB is also a repository for current research in nanotechnology, providing access to scholarly articles and materials gathered at nationwide workshops and conferences. Without leaving their desktops, users can browse video tutorials from a molecular conduction workshop held at Northwestern University in July 2004.
- *Downloads*: Users can browse for podcasts or download nanotechnology programs to run on their computers. They can also download source code or datasets. These services differ from the vast majority of nanoHUB offerings, which appear as applets in the user window and require no additional downloads.
- *Collaboration*: Within the nanoHUB structure, various tools enable collaboration among users. Faculty or students can create user groups within the hub to share content. They can reserve online meeting rooms and meet virtually using Breeze meeting software. Researchers can also use individual workspaces to run computation tools, develop new tools, and deploy new tools on the nanoHUB.

The Users

Since the portal's formal launch in 2003, the nanoHUB site has recorded more than 44,000 visitors, growing from roughly 1,300 users in 2003 to more than 19,000 in 2006. In 2007, user figures reached an all-time high: more than 1,000 national and international researchers each month, representing a fivefold increase since February 2004.[2]

Each month, the majority of users (typically more than 90 percent) come from academia: students, faculty, and staff. Private industry represents the next-highest group of users, though the numbers rarely top 10 percent of total usage in a given month. Still-smaller numbers of K–12 educators and individuals from government agencies, national laboratories, and the military are logging in. The site does not differentiate between student and faculty logins, so although it is easy to tell where people are coming from, it is difficult to determine who they are.[3]

The Value

Within higher education, the site serves three purposes: as a scientific repository; as a tool for sharing information; and as a resource for teaching and learning.

As a scientific repository, the nanoHUB stores scholarly papers, conference proceedings, cutting-edge tools, and presentations narrated by scholars in the field. For the field of nanoscience, it provides a "Google-like" entry point for research inquiries.

As a tool for sharing information, the nanoHUB allows users to upload their own tools, research, and course content to collaborate with others, giving individual researchers the ability to spread their science and giving faculty members the chance to learn from and take advantage of the expertise of others. In addition, users can share their own data from running experiments, perhaps pointing out scientific anomalies or searching for help with sessions run amok.

As a resource for teaching and learning, the nanoHUB is both content provider and online laboratory. Faculty can look for simulations, homework exercises, course modules, or narrated presentations. Students can search for presentations, podcasts, animations, or online courses to better understand nanotechnology concepts. And the tools serve as hands-on opportunities for students to try their hand at running experiments with real machines and real data, opening new opportunities for authentic learning.

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Within the fields of both nanotechnology and cyberinfrastructure,[4] the nanoHUB is revolutionizing the way that scholars access and share scientific resources and also is changing the way faculty and students use the Web for teaching and learning. With its unique and intuitive design, the nanoHUB holds numerous valuable benefits for students, educators, and researchers in higher education.

Notes

1. "Science Gateway" is the TeraGrid term for a user interface that accesses TeraGrid resources, granting the user access to the tools and capabilities of the grid through discipline-specific portals.
2. Phillip Fiorini, "Discovery Park's nanoHUB Site Draws Record Simulation Traffic, Advances Nanotech Research," *Purdue University News*, February 23, 2007, <http://news.uns.purdue.edu/x/2007a/070223KlimeckNanohub.html>.
3. Current usage statistics, broken down by time or type of user, can be found on the nanoHUB site at <http://www.nanohub.org/about/usage/>.
4. EDUCAUSE Learning Initiative (ELI), "7 Things You Should Know about . . . Cyberinfrastructure," August 2007, <http:/www.educause.edu/ir/library/pdf/ELI7028.pdf>.

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