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nanoHUB.org: Advancing Education and  
Research in Nanotechnology

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# nanoHUB.org: Advancing Education and Research in Nanotechnology

*Through the Network for Computational Nanotechnology Web site, nanoHUB.org, tens of thousands of users from 172 countries collaborate, share resources, and solve real nanotechnology problems. The authors share their experiences in developing and using the site's unique cyberinfrastructure.*

In 2002, the US National Science Foundation established a university network, called the Network for Computational Nanotechnology (NCN), to support the National Nanotechnology Initiative. This initiative provides a multi-agency framework in support of US government investments in fundamental nanoscale phenomena research and the translation of new understanding to new technology. NCN aimed to further these goals in three ways: bringing computational tools online, making the tools easy to use, and educating users about the tools and nanoscience.

Along the way, NCN has created a unique cyberinfrastructure to support its Web site, nanoHUB.org, where researchers, educators, and professionals have been collaborating, sharing resources, and solving nanotechnology problems. In 2007, nanoHUB.org served more than 56,000 users from 172 countries. In this article, we share our experiences in developing and using this cyberinfrastructure, particularly in an educational context.

## Developing nanoHUB.org

NCN chose to focus initially on nanoelectronics, nanoelectromechanical systems, and devices for biology and medicine for three reasons: these areas are developing rapidly, no curricula have been fully established, and nanoelectronics has

a history of sharing simulation tools, such as the Simulation Program with Integrated Circuit Emphasis (SPICE).<sup>1</sup> The goal was to encourage the development of many tools, tutorials, podcasts, animations, publications, lecture notes, and homework assignments, which we refer to collectively as “resources.” To achieve this, we needed an infrastructure that would make it easy for a worldwide community of content contributors to upload and share their resources, receive feedback, and make improvements. All of this had to happen in a self-serve fashion, with very little intervention by NCN staff, so that it could scale to serve a very large community.

nanoHUB.org hosts nearly 1,000 resources, including 87 simulation tools (see Figure 1). Many of our resources are published under a Creative Commons 2.5 license (<http://creativecommons.org/licenses/by-nc-sa/2.5/>), letting others create derivative works. NCN staff review contributed content for appropriateness, completeness, and basic functioning, and we encourage users to rate and comment on all resources. Roughly 27

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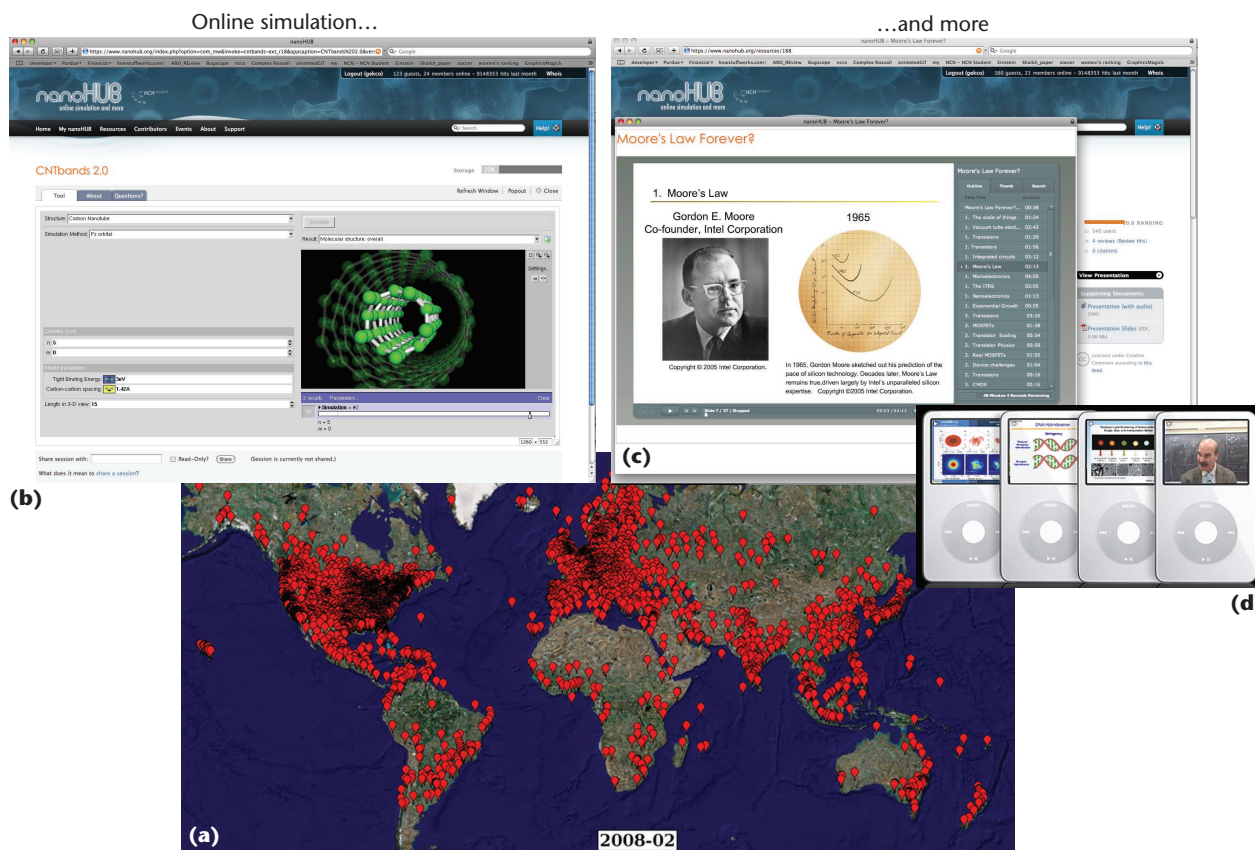


Figure 1. nanoHUB.org provides online simulation and more to a global following. (a) More than 56,000 users in 2007 accessed its resources, including (b) simulations and (c) Flash-based tutorials. Many tutorials are also available as (d) iTunes podcasts, which have attracted more than 6,800 users.

percent of the content has received ratings (using a five-star scale), and 46 percent of the ratings have associated comments. Content with many favorable ratings tends to bubble up in search results, whereas content with poor ratings is harder to find. To date, NCN has pursued tool quality by engaging selected research groups for tool development. NCN member sites have encouraged the majority of other content, such as research seminars, tutorials, short courses, homework exercises, and animations.

The nanoHUB.org user community grew from 1,000 users in 2002 to more than 56,000 in 2007. Some 5,800 registered users logged in and ran more than 240,000 simulation jobs in 2007. We identify unregistered users by IP address and count them only if they aren't a Web-crawling robot and if they download a resource or spend more than 15 minutes browsing the site. Roughly 85 percent of our registered users and 91 percent of unregistered users are affiliated with an educational institution. nanoHUB.org has users

at all Top 50 US engineering schools<sup>2</sup> and more than 14 percent of all .edu domains. (See [www.nanoHUB.org/usage](http://www.nanoHUB.org/usage) for additional usage details, updated monthly.)

### Cyberinfrastructure

nanoHUB.org simulation tools aren't the batch-mode services common on the Web; rather, they're intuitive, interactive graphical tools that make it easy for users to learn and explore. Users can launch simulations from their Web browser simply by clicking the "Simulate" button and can change any parameter, launch another simulation, and quickly compare results. About one-third of the nanoHUB.org tools deliver results in less than 10 seconds, about one-half in less than one minute. Computationally demanding simulation jobs dispatch to grid computing resources, including the NSF TeraGrid ([www.teragrid.org](http://www.teragrid.org)), Open Science Grid ([www.opensciencegrid.org](http://www.opensciencegrid.org)), and virtual clusters powered by Violin software.<sup>3</sup> Intensive volume rendering and flow-visualization tasks dis-

patch seamlessly to a specialized rendering cluster.<sup>4</sup> nanoHUB.org middleware hides grid computing's complexity, handling authentication, authorization, file transfer, and visualization, and letting the user focus on conducting experiments and learning new concepts. Irrespective of the computation time, users can set up and analyze their numerical experiments' results interactively in a friendly GUI without installing any software. nanoHUB.org can achieve such ease of use for numerous tools because of its unique cyberinfrastructure.

nanoHUB.org is built on the open source LAMP (Linux, Apache, MySQL, and PHP) platform<sup>5</sup> and the Joomla (www.joomla.org) content management system. Launching a tool session invokes a Joomla component that we developed. The component then communicates with our middleware to launch a tool session on a cluster of available machines and emits a Web page containing a virtual network computing applet<sup>6</sup> that connects back to the live tool session. To users, it appears that a simple Java applet is running in their Web browser—and indeed it is—but nanoHUB.org is serving the tool (which could be a community code consisting of a few hundred thousand lines of source code developed in tens of person years) and the computing cycles from a much more sophisticated platform, which can scale to handle very large jobs (such as memory-intensive jobs that require large amounts of RAM or highly parallel jobs that might require many CPUs).

To drastically reduce the programmer hours needed to create friendly GUIs to a wide variety of powerful simulation codes, NCN created an open source toolkit called Rappture (*Rapid Application Infrastructure*; <http://rappture.org>). Rappture-based tools are ordinary applications that run on Windows, Mac OS X, and Linux platforms, irrespective of any Web deployment. Coupled with our unique middleware, however, nanoHUB.org delivers them via any Java-enabled browser; no extra work is required to deploy a powerful Linux-based tool online. Not only is the resulting tool easy to use, but it's also easy to develop, typically by graduate students deeply involved with the underlying theory code or undergraduate students working in a team with expert graduate students.

Rappture programmers describe the input parameters and output results for a simulation code as a hierarchy of data objects in an XML file ([www.w3.org/XML](http://www.w3.org/XML)). Rappture reads that file and generates a GUI automatically, producing a tool such as the one in Figure 2. Each input and output has a description that pops up when users mouse

over its associated control. The GUI can include embedded notes in HTML format, with links to tutorials and documentation. Rappture recognizes various output types and automatically invokes the appropriate visualization engine. In the past three years, more than 200 developers have used Rappture on more than 190 projects. Typical projects have required a few days of programmer time to create the Rappture interface that readied a raw simulation code for nanoHUB.org deployment.

Rappture also provides a consistent and accessible presentation, which is extremely important in an educational setting. Instructors interested in constructing a coherent sequence of learning experiences for students need a common interface for all the tools. For example, the design project for a course might require the synthesis of results from several simulation tools. With a consistent interface, learners will apply their intellectual energy to investigating their questions rather than to learning new interfaces.

### Role in Education

Early on, NCN identified users at academic institutions—both educators and researchers—as our target audience and set out to meet their needs. Many educators and students don't have administrator privileges to install software on their computers. For tools to be used in the classroom, they must be available on all platforms, including Windows, Mac OS X, and Linux, without user-based installation. They must be easy to use and time efficient. They should have integrated visualization capabilities so that, with minimal effort, students can generate, view, compare, and capture many different results for further use. The tools must have supporting materials so that students can jump quickly from a result to a seminar that explains underlying concepts. As the Science Environment for Ecological Knowledge and SciDesign projects in this issue show (see p. 28), tools alone are insufficient for community adoption; a rich set of resources supporting tool use is necessary. Web-based resources such as nanoHUB.org can provide anytime, anywhere support to distributed educational initiatives, such as Ohio's inter-institution undergraduate minor in computational science (see p. 12). They can also level the field for access by users from diverse backgrounds and institutions who want to gain experience with HPC, such as the experience reported in this issue by David Joiner and colleagues (see p. 40).

Experienced computational scientists in nanoscience, and their graduate students, can advance their learning through nanoHUB.org resources

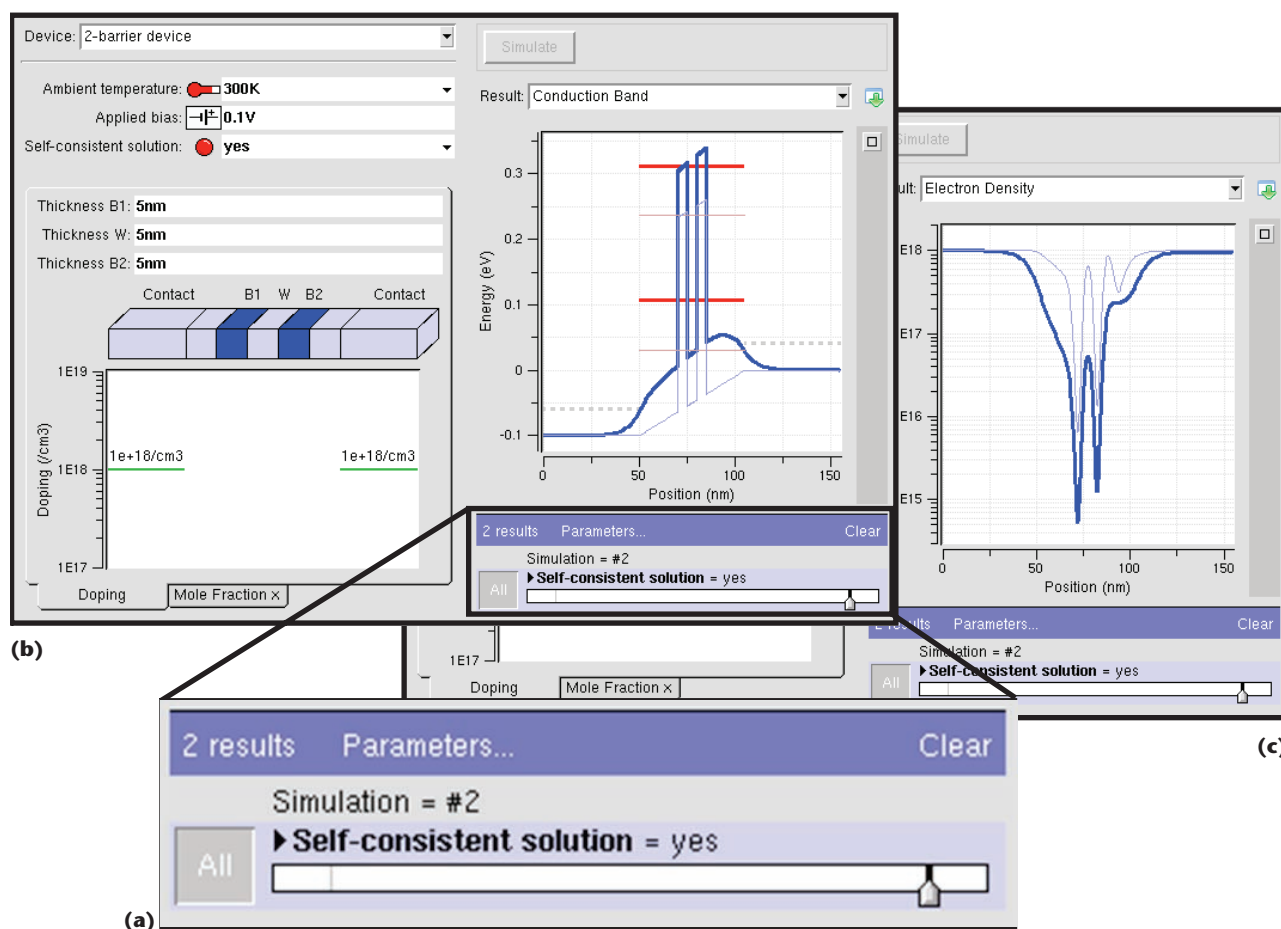


Figure 2. Instant GUI. Rappture generates the GUI for a tool on the basis of a description of its inputs and outputs. Users can change any input parameter, run simulations, and compare results with (a) intuitive sliders or data overlay. This example compares the (b) conduction band edge and (c) charge distribution in a resonant tunneling diode<sup>7</sup> for a simple linear potential drop and a charge self-consistent potential.

with little additional pedagogical support. Based on resource ratings and comments, users can successfully leverage their prior knowledge to comprehend the new content knowledge and conduct research with the simulations tools. In this way, the available resources are helping to educate the nanotechnology research community and to conduct research.

Graduate students new to nanoscience and computational inquiry require more guidance through formal educational settings. Multiple pedagogical approaches can involve using simulation tools to support student learning in the classroom, for both homework assignments and design projects. Each of these uses has a slightly different use model.

### Classroom Learning

For classroom demonstrations, instructors can run

the tool sessions live, projecting on a screen so that students can follow along. With its integrated visualization capabilities, nanoHUB.org becomes a vivid whiteboard of sorts for instructors, as Figure 3 shows. They can demonstrate their own thought processes as they run experiments and interpret results. Instructors can pose “What if?” questions to students, ask them to generate predictions, and then provide explanations while examining the results. This *cognitive apprenticeship* lets instructors assume the mentor role, introducing students to the discipline and its methods.<sup>8</sup>

If live simulation runs would take too much time, instructors can easily prepare any number of runs before class because closing a Web browser doesn’t close tool sessions. Tools remain active and, upon reconnecting to nanoHUB.org, show on the users’ “My nanoHUB” page under the “My Sessions” heading. Clicking on a session



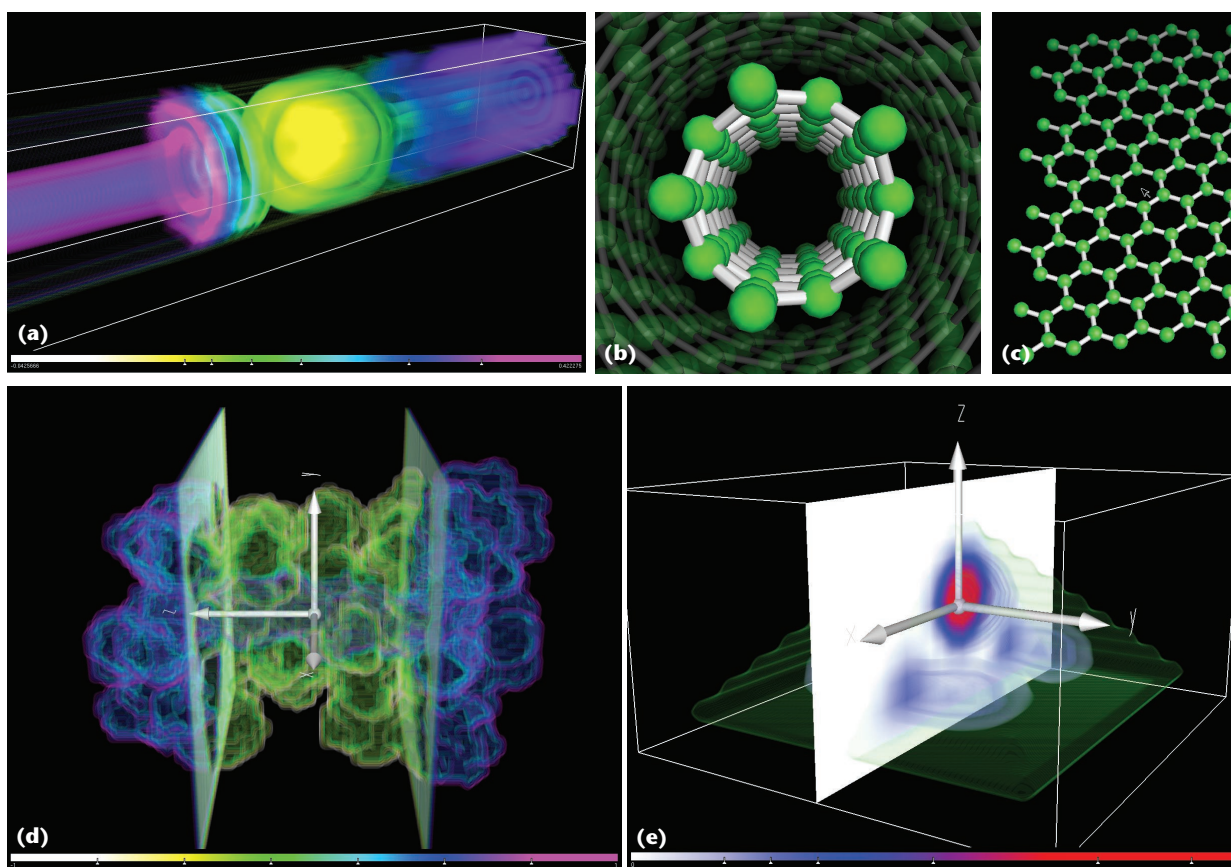


Figure 3. 3D nanoHUB.org simulation images. (a) An electrostatic potential from NanoWire,<sup>9</sup> (b) (5, 0) and (10, 2) carbon nanotubes in CNTbands,<sup>10</sup> (c) A (10, 2)B Carbon Nano Ribbon in CNTbands, (d) a Gramicidin in BioMOCA,<sup>11</sup> and (e) an eigenstate in Quantum Dot Lab.<sup>12</sup> Users can rotate, zoom, insert cut planes, as in (e), and interactively manipulate all images. Users can download the images with a simple click of a button.

name quickly revives the tool session. So, instructors can present examples smoothly to maintain engaging classroom dynamics with students.

### Homework Assignments

For homework assignments, students use the tools to explore the relationships between input and output parameters. They can compare the results of an analytical solution calculated by hand to the numerical results obtained from nanoHUB.org, or they can seek to understand input and output relationship trends. Through these methods, learners can begin to unpack the black-box simulation model and notice subtle changes in its characteristics. These experiences develop students' ability to systematically investigate questions rather than use trial-and-error strategies.

### Design Projects

Design projects provide students with the opportunity to synthesize everything they've learned

from the smaller investigations conducted in the homework problems. Students often work in teams and must share their tool sessions with each other and with the instructor to work out problems. Users can share any nanoHUB.org tool session by entering the nanoHUB.org login name for one or more users (with equal security privileges) and clicking the "Share" button.

### Feedback

NCN faculty are investigating our resources' benefits for educating a wide range of learners and examining how experts use nanoHUB.org resources to build new knowledge. Toward that end, NCN developed a short student survey to provide an initial glimpse into how students perceive the utility and usability of nanoHUB.org resources in their courses and for their future goals.

NCN recently surveyed more than 100 graduate students in electrical engineering, bioengineering, and material sciences courses. These

students agree that the tools are accessible and the graphical outputs are easy to interpret. In addition, they report that their interaction with the simulations facilitates their own question generation and self-exploration to generate new knowledge. They also agree that simulations help them comprehend nano concepts better than lectures and readings do.<sup>13</sup> Most encouraging are students' reports that these tools align with their interests, and they anticipate using these resources in their own research. Therefore, these introductions to nanoscience through expert-level tools have a positive impact in advancing the research community. Continuing work will focus on how learners develop their ability to think and reason with the tools relative to the way experts use the tools.

Undergraduate students surveyed reported experiences in their courses similar to the graduate students' experiences. We have reports from 100 students using nanoHUB.org in chemistry and nanodevices. They agree that demonstrations

at the molecular and atomic levels.<sup>14</sup> Further research is under way.

### For Education, Research, or Both

Early on, NCN tried to classify tools as being for education or for research, but we learned that with ready access and nanoHUB.org's ease of use, the distinction isn't clear. For example, CNTbands<sup>10</sup> was created for classroom use and provides a simple density of states, dispersion calculation, and 3D visualization of various carbon nanotubes, yet scientific literature has cited it five times ([www.nanohub.org/tools/cntbands-ext/#citations](http://www.nanohub.org/tools/cntbands-ext/#citations)) for its use in research. A Stanford University student began using the Resonant Tunneling Diodes simulator in a nanotechnology class taught by H.-S. P. Wong in 2005 and went on to use that tool in his own research project.<sup>15</sup> Schred,<sup>16</sup> a 1D Schrödinger-Poisson Solver for Silicon devices, also has 80 citations in the research literature, which indicates serious research use, yet instructors have repeatedly used it in the classroom. Overall, scientific literature has cited nanoHUB.org and its tools more than 265 times ([www.nanohub.org/citations](http://www.nanohub.org/citations)), and roughly 60 percent of these citations are from authors unaffiliated with the NCN. NCN has received many testimonials from professors about nanoHUB.org's usefulness in education and research (<http://nanohub.org/about/quotes>). Even tutorial materials have been cited.<sup>17,18</sup> Researchers are recognizing nanoHUB.org as a new way of publishing.

***Most encouraging are students' reports that these tools align with their interests, and they anticipate using these resources in their own research.***

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with simulations helped their comprehension of the concepts more than traditional lectures and readings. They found the resources easy to use and accessible. However, undergraduates were split on their perception of simulations as "highly relevant to my area of interest," and response variance was quite large. Related to this response is their perception of their ability to interpret tool results and generate their own questions. These results could be because undergraduate courses are less specialized than graduate courses and that these students need more instruction on how to use these tools to support inquiry.

Undergraduate students are still developing the foundational technology and information literacy skills necessary to comprehend the assignments and tools appropriate for graduate students. Therefore, new learning modules and instructional approaches are needed to accommodate the possibly wide variance of undergraduate learners' ability to reason with the tools—for example, we see great potential in visualizations to develop learners' mental representations of system behav-

**A**s we continue to make improvements, nanoHUB.org remains a work in progress. By developing our cyberinfrastructure in close collaboration with users—especially professors and their students—NCN maintains contact with community needs and values.

nanoHUB.org is changing how users and developers in research and education alike access and use simulation tools and associated material. The underlying cyberinfrastructure is now a generic package called HUBzero (<http://hubzero.org>). We believe the "HUB" concept is transferable to many engineering and science disciplines, and we're actively deploying new HUBs for discovery and learning. The HUB concept will greatly expand the user base for modeling and simulation, and open new possibilities for many people who would otherwise avoid computing. We plan an open source software release of HUBzero for fall 2009.



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