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HUB is Where the Heart Is

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THE NETWORK FOR COMPUTATIONAL NANOTECHNOLOGY (NCN) is a six-university initiative that was established in 2002 to connect those who develop simulation tools with those who use them. The NCN currently addresses three science themes, nanoelectronics, nano-electrical-mechanical systems (NEMS) and nanofluidics, and nanomedicine, but is expanding its coverage into other areas of nanotechnology. The NCN’s strategy to serve and engage the nanotechnology community centers on a unique, science gateway, www.nanoHUB.org, offering online simulation services for research, education, and collaboration and a new way to publish research and instructional materials. The NCN’s primary goal is to lower barriers for the use of simulations in emerging fields of study.

At the nanoHUB Web site (Figure 1), users log on, access state-of-the-art simulation software, run interactive
graphical or batch simulations, and view the results online. There is no need to download, install, support, or maintain sophisticated software and tremendous computing resources are provided freely and transparently. Users do not need to worry about accounts or how to access specific machines. The nanoHUB is also a resource for cross-disciplinary education by hosting online tutorials, short courses, and full courses. Over 60,000 people make use of the nanoHUB each year; about one-half of the nanoHUB users are outside of the United States.

SIMULATION STATION

The nanoHUB is compared to the successful Open Courseware Initiative from MIT, but the nanoHUB is more than a repository for course materials. As of March 2008, users can access over 70 interactive graphical tools, launch jobs, and visualize and analyze the results, all via any Web browser. The NCN’s emphasis on usability has produced a clean interface that makes it easy to use powerful research tools. Simulation jobs can be dispatched to national computational resources, including the National Science Foundation TeraGrid and the Open Science Grid. The nanoHUB middleware hides the complexity of grid computing, handling authentication, authorization, file transfer, and visualization, and letting the user focus on research.

This ease of use also helps educators bring simulation tools to the classroom. Rather than spending precious time on arcane issues of computer use, faculty can focus directly on the science they are trying to teach, bypassing the mire of grid computing and focusing instead on the physics they are trying to teach.

At its core, the nanoHUB is a Web site built with many familiar open source packages—the Apache Web server, PHP Web scripting, the Joomla content management system, and a MySQL database for storing content and usage statistics. Then nanoHUB middleware builds upon that infrastructure to create an environment in which researchers, educators, and students can access tools and share information.

The signature service of the nanoHUB is its ability to deliver interactive graphical simulation tools through an ordinary Web browser. In the world of portals and cyber-environments, this capability is unique. Unlike a portal, the tools in a hub are interactive (Figure 2); you can zoom in on a graph, rotate the image of a molecule, probe isosurfaces of a three-dimensional volume—all in real time, without having to wait for a Web page to refresh (Figure 3). Users do not have to reserve time on a supercomputer or wait for a batch job to engage.

A key aspect of the nanoHUB middleware is that simulation programs are deployed to the Web as interactive applications without having to change any of their code. The nanoHUB infrastructure includes a tool execution and delivery mechanism based on Virtual Network Computing. Tools with a graphical user interface can be installed on the nanoHUB and deployed within a few hours. For legacy tools and other codes without a graphical interface, an interface can be quickly created with the associated Rappture toolkit. The Rappture interface helps set up jobs and visualize results. The jobs can be dispatched to the TeraGrid, the Open Science Grid,
and other participating cluster resources via Condor. Using this architecture, the nanoHUB has brought over 80 different simulation tools online in less than three years, with 80 more tools under development (Figure 4).

**ONLINE PRESENTATIONS**

For users to make the most of the tools on a hub, they need to understand the underlying science and the limitations of each tool. Alongside the tools, the nanoHUB features a series of online presentations, which are PowerPoint slides combined with voice and animation. Listening to a presentation on a hub is much like being in the room during a standard seminar. But unlike a seminar, the material is available 24/7, and you can skip through the talk by browsing the table of contents or searching for important keywords. The online presentations are delivered in a very compact format using Flash, which is installed on 98% of the world’s internet-enabled desktops. Unlike streaming video, the Flash format can be viewed over a dial-up connection, so presentations can reach places where network bandwidth is limited. Online presentations can also be distributed as podcasts, so users can access them on-the-go via their video or audio iPod. Some presentations are designed to teach the underlying theory of the simulation tools on the nanoHUB. Others are tutorials and short and full online courses on a variety of nanotechnology topics (Figure 5). A large collection of research seminars allows nanoHUB users to keep up with the latest advances in nanoscience and technology.

**A VIRTUAL ORGANIZATION**

The nanoHUB is a place where researchers and educators can meet to accomplish real work. The nanoHUB offers integrated, online Web meetings, support for collaborative software development, event calendars, and many other services designed to connect researchers and build a community. Over 200 software projects are hosted on the development site nanoFORGE.org, and the new ability to share interactive sessions among users facilitates collaborative software development and makes it easy for instructors to help students with simulation homework. A “nanoHUB Answers” section allows users to ask questions that other nanoHUB users answer—a step toward building a worldwide community of collaborators. Users are encouraged to be uploaders of resources on the...
nanoHUB. See “Contribute” on the nanoHUB main page for instructions on how to contribute your own software and other resources to the nanoHUB.

**NANOELECTRONICS AND THE NANOHUB**

The nanoHUB evolved from an initiative that began with electronic devices. That history is still reflected in the nanoHUB site. Although other areas are now growing, the nanoHUB’s resources for nanoelectronics are especially strong. Users visiting the nanoHUB site should look for the “Nanoelectronics” link on the main page for an introduction to the nanoelectronics resources. There, users will find a list of recommended simulation tools for education and research as well as recommended tutorials and courses. Nanoelectronics tools include standard tools for semiconductor devices, such as Padre and Prophet, which were developed at Bell Laboratories and the Schrödinger-Poisson solver for MOS capacitors, and Schred, developed at Arizona State University. Also included are tools for new nanoelectronics technologies such as carbon nanotube electronics, semiconductor nanowires, bio-sensors, and carbon nanotube composites.

In addition to simulation tools, the “Electronics from the Bottom Up” educational initiative seeks to bring new approaches to the education of engineers in electronic devices and materials. For those looking to use simulation in the classroom, see the list of recommended tools and suggested homework assignments from Gerhard Klimeck.

**TRENDS AND FUTURE DIRECTIONS**

The nanoHUB resource base continues to grow rapidly (Figure 6) as it serves a rapidly expanding population of users from throughout the world. The nanoHUB is becoming an increasingly vital resource for the international community of students, faculty, and professionals. With more than 60,000 users each year and more than 3.5 million hits per month, the nanoHUB is an excellent vehicle for engaging the global nanotechnology community.

To serve the global population, we expect to see the NCN/nanoHUB become an international network and are seeking partners as we take the first steps in that direction. We believe that the HUB model being pioneered by the NCN is one that can serve many scientific and engineering disciplines.

To meet that need, the HUBzero organization has been created to develop and disseminate the underlying nanoHUB infrastructure as an open source platform. We encourage readers to visit the nanoHUB, make use of the resources there and even become a nanoHUB contributor. Also, don’t forget to use the “Give Us Feedback” link to tell us how you use the nanoHUB and to pass along your suggestions. All nanoHUB services are free; just sign up and join the nanoHUB community.

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**FIGURE 5** Prof. Mark Ratner’s lecture, “A Gentle Introduction to Nanotechnology,” is available for view online or it can be downloaded as a podcast.

**FIGURE 6** The nanoHUB is a worldwide community of students, faculty, and professionals. The total number of annualized users has grown dramatically in the past few years.