

The Center for Research Computing proudly presents...

## ***Cyberinfrastructure for nanoHUB.org and Beyond***

### **Michael McLennan**

Senior Research Scientist, Purdue University

<http://www.nanohub.org/>

**Friday, December 7, 2007 + 2:00 – 3:00 p.m.**

**131 DeBartolo Hall**

Michael McLennan is the software architect for the Network for Computational Nanotechnology and the nanoHUB.org web site. His latest project is the Rappture Toolkit, a package which accelerates the creation of simulation tools for scientific modeling, available as open source at <http://rappture.org>.

Dr. McLennan has a long history of software development for nanotechnology simulation. He received a Ph.D. in 1990 from Purdue University for his dissertation on dissipative quantum mechanical electron transport in semiconductor heterostructure devices. He blended his expertise in physics with a love of software when he joined Bell Labs in 1992 to work on tools for semiconductor device and process simulation. He is co-author of *Effective Tcl/Tk Programming* and *Tcl/Tk Tools*. He also developed [incr Tcl], an object-oriented extension of Tcl, which has been used by thousands of developers worldwide on projects ranging from the TiVo digital video recorder to the Mars Pathfinder. Dr. McLennan joined Cadence Design Systems in 1998 as a Software Architect for their SimVision visualization and debugging environment. In 2004, he became a Senior Research Scientist at Purdue University and began his work on nanoHUB.



Figure 1 – nanoHUB.org offers “online simulation and more” for over 26,000 users worldwide.

### **ABSTRACT**

The Network for Computational Nanotechnology (NCN) was established in 2002 by the NSF with a mission to create, deploy, and operate a national resource for theory, modeling, and simulation in nanotechnology, to connect users in research, education, design, and manufacturing. To support that mission, the NCN created a web site at nanoHUB.org with a supporting cyberinfrastructure that allows users to upload and access various kinds of resources for research and education. During the past 5 years, the use of this site has grown exponentially. In the 12-month period from October 2006 to September 2007, more than 26,000 users accessed nanoHUB to view a collection of seminars, tutorials, animations, publications, and simulation tools submitted by more than 390 contributors from all over the world.

What sets nanoHUB apart from other science gateways or web portals is its unique approach for accessing simulation tools. Instead of using web forms to access batch mode simulations, nanoHUB offers instant access to any graphical user interface via a thin client running within a web browser. Any tool running on Linux with a graphical interface—including commercial tools such as Matlab or ANSYS—can be deployed as-is within hours on nanoHUB. Each application pops up within the user's web browser, but actually runs on a machine within the nanoHUB cluster where it has access to national Grid computing facilities, including the TeraGrid and the Open Science Grid.

Other projects are beginning to adopt the nanoHUB software to create a "hub" for their own scientific domain. The Rosen Center for Advanced Computing now has a team dedicated to creating new hubs for pharmacy, thermal transport, global engineering education, and other very diverse applications. This talk will start with a live demonstration of nanoHUB and show how it can be used to support collaborative research and educational activities for nanotechnology development. The software architecture and its unique implications will be explored, and applications in other domains will be discussed.

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