Appendix 9: Purdue University/Network for Computational Nanotechnology Profile

I. Description

Institutions: Purdue University, Northwestern University, Morgan State University, Stanford University, University of Florida, University of Illinois, and the University of Texas at El Paso
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II. Research Agenda

Research Focus: The NCN is comprised of research themes on nanoelectronics, NEMS/nanofluidics, and nanobioelectronics – and a cross-cutting computational theme. These research themes cover a broad subset of nanoscience while providing the focus and synergy that are essential to success. The key intellectual challenge for the NCN is to develop both the engineering science and software tools necessary to understand and design nanoscale devices at the atomistic level and to relate atomistic structure to macro-scale system performance. The nanobioelectronics theme serves as an intellectual testbed in which the new knowledge and software tools developed in the nanoelectronics and NEMS/nanofluidics themes are used to explore specific devices for applications in medicine and biology. The NCN requires that each research project produce outstanding science, and also i) develop public-domain software, ii) create unique educational resources, and iii) play a visible leadership role in its field. Through this process, a growing set of software tools, design approaches, and educational resources are being made available to the nanotechnology community. To deliver these resources and services to the broader community, the NCN is developing and deploying a unique cyberinfrastructure, the nanoHUB. The NCN intends to serve as a model for other communities and actively seeks partnerships to expand the scope of its activities beyond its three science themes.

NCN Description: The Network for Computational Nanotechnology (NCN) is a multi-university initiative that was launched in September 2002 to create a unique, web-based infrastructure to serve researchers, educators, and students. NCN research, education, and outreach programs drive the development of its infrastructure. The NCN web site, www.nanohub.org, is a "science gateway" that hosts collaborative tools and delivers unique educational resources such as online courses, learning modules, lectures, and seminars. Its signature service is online simulation, visualization, and high-performance computing. We intend for the NCN to be an example of the role that theory and simulation can play in emerging fields of research, of how effective simulation can be in education, and of how innovative cyberinfrastructure can serve a community of researchers, educators, and students. In the process of this work, we will create a new generation of software tools and a web-based infrastructure of services that will become an essential component of the research and education enterprise.

III. Education Activities within the University

Description of activities
NCN is collaborating with the National Center for Learning and Teaching in Nanoscale Science and Engineering to support the development of teaching modules for grades 7-16. In particular, NCN is providing expertise, development and resources for interactive and simulation based material that can be integrated in the NCLT modules.

Program staff and expertise
Umberto Ravaioli (NCN investigator at Illinois) is member of the NCLT leadership team and heads the educational software development group, including Prof. Richard Braatz (Chemical and Environmental Engineering, Illinois) with several graduate students, undergraduate students, and researchers. U. Ravaioli has co-directed the educational effort of NCN, including the organization of two Summer Schools on nanotechnology themes in 2004 and 2005.

Goals and objectives
The NCLT has a varied set of objectives in the establishment of a methodology to introduce and evaluate educational material in nanotechnology in grades 7-16, to promote teachers' professional development and to develop educational curricula for future educators in nanotechnology. The goal of NCN is to interact with the NCLT to provide content and interactive software to pursue all of these educational tasks.

Target audience (educational levels, number of students at each level, etc.)
The primary audience for current development is now at the high school level, but activities will be broadened at a second stage to cover middle school as well as college level students. Teachers professional development is also a priority for NCLT which can be facilitate by NCN contributions.

Current activities
Development of advanced Java Applets, FLASH animations, graphical user interfaces for simulations, educational videogame framework.

Nano S&E content focus
Present focus is on the basic issues of scale and geometry which are fundamental in the understanding of any nanoscale phenomena. Simulations developed at NCN will be very valuable to provide compelling and practical application to illustrate important science and engineering concepts at all levels. The development of the Rappture framework at NCN has in particular the potential to make advanced research simulation tools accessible to a wide audience, by making available efficient interactive graphical interfaces.

IV. Education Activities Outside the University

Description of Activities
The Network for Computational Nanotechnology (NCN) has adopted a new pedagogically sound content-aggregation strategy for the nanoHUB that uses learning modules as the delivery mechanism. Learning modules offer an ideal methodology to bundle voiced lectures, PowerPoint presentations, scientific papers, and most importantly online simulation tools into a single coherent standard-compliant package. The learning modules developed by NCN adopt the Shareable Content Object Reference Model Version 1.2. This ensures that nanoHUB content can interoperate with other compliant course management systems such as Sakai and WebCT Vista. The learning module development process leverages the discovery work on-going within the NCN in an effective manner. Each learning module contains presentations, exercises,

and examples, designed by NCN scientists working on that particular area. For example, the Introduction Molecular Conduction learning module begins with a talk by Dr. Supriyo Datta – a well-known expert in this area. The most important characteristic of a learning module is the ability to provide students access to serious simulation tools within the context of their learning. The Introduction to Molecular Conduction learning module requires students to actively use the MolCToy simulation tool to complete exercises and assignments. One other area of learning that the learning module addresses is assessment. By definition, a learning module should provide students with *measurable* learning objectives. The learning modules include a quiz that includes appropriate feedback. The next challenge that NCN is tackling is to provide reliable score tracking and reporting services. Also, we want to facilitate the measurement of learning impact as part of each learning module. To this end, we are now experimenting with the integration of course management systems (in our case we are focusing on an open-source system called Sakai) with the nanoHUB. To provide better dissemination of the nanoHUB content, we are in the final phases of announcing a partnership with MERLOT (http://www.merlot.org) - an online repository for educational content.

Program Staff and Expertise
Drs. Krishna Madhavan and Mike McLennan lead the development of learning modules on the nanoHUB under the supervision of the NCN Technical Director Dr. Gerhard Klimeck and Director Dr. Mark Lundstrom. The development of all content aspects requires input from NCN PIs engaged in research. To this end, the nanoHUB maintains continuous communication with content area experts.

Goals and Objectives
The primary goal of the learning module development effort is to act as the direct conduit of research content to educators and learners. Furthermore, we want learners to interact with NCN research content at their own pace. Learning modules are ideal for self-paced learning. The allow students to focus on the use of simulation tools within the broader context of the topical area they are trying to learn.

Target Audience
Primarily undergraduate, graduate, and expert users. But, learning modules can also be designed to target K-12 levels.

V. Education Outreach Materials

Description of Activities
We have developed a museum exhibit entitled, *Nanotechnology: The Science of Making Things smaller*. The exhibit was designed and built by a team of undergraduate students and faculty. The exhibit has several components. There are posters at the start of the exhibit to emphasize how nanostructures are built from the ground up, and the idea is illustrated by the use of the popular LEGO bricks. Maintaining this LEGO theme, there is a scanning probe microscope (SPM) made out of LEGOs that is used to scan LEGO landscapes. This LEGO SPM duplicates in many ways the operation of a real scanning probe microscope. There are hands on workbenches with activities that illustrate some of the basic principles underlying nanotechnology. There are two kiosks that run cartoon animations on various aspects of nanotechnology. These animations can be viewed at www.nanohub.org. There is a kiosk that displays rotating renditions of nanostructures such as carbon nanotubes, bucky balls, and DNA. There is a wall of nano-art that consists of 18 framed scanning probe micrographs of actual carbon nanotubes, quantum corrals, atomic surfaces, etc. There are models of nanostructures such as carbon nanotubes, bucky balls, and DNA that hang above the exhibit. Finally there are take home brochures and bookmarks that provide more information to guide the students' study of Nanotechnology on the web.

The exhibit premiered at the Children's Museum of Oak Ridge, TN, where it was on view from April 2, 2005 through May 31, 2005. The next stop for the exhibit is the National Inventors' Hall of Fame in Akron, Ohio, where it will be displayed from November 1, 2005 through August 31, 2006.

Goals and Objectives
The primary goal of the museum exhibit is to introduce middle school children to the fascinating and rapidly changing field of Nanotechnology.

Target Audience
Primarily middle-school children, but all ages should find the exhibit entertaining and educational.