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***Abstract* — The ABACUS and AQME on-line tools and their associated wiki pages form one-stop shops for educators and students of existing university courses. They are geared towards courses like "introduction to Semiconductor Devices" and "Quantum Mechanics for Engineers". The service is free to anyone and no software installation is required on the user's computer. All simulations, including advanced visualization are performed at a remote computer. The tools have been deployed on nanoHUB.org in August 2008 and haven already been used by over 700 users. This paper describes nanoHUB educational tool user requirements and the motivation for and some details about these new tools. Usage patterns and future planned assessment are discussed. The concepts of "NCN supported" and "Community Supported" tools are discussed.**

Keywords: education, semiconductor, quantum mechanics, simulation, web-based, cyberinfrastructure

INTRODUCTION - MOTIVATION

We observe in our practice as Electrical Engineering faculty members that few Electrical Engineering students who take courses such as semiconductor device fundamentals gain or retain any interest in the field of semiconductor devices. Such courses are often the first contact a student has with semiconductor devices and should lead in a continuation of a study of nanoelectronic devices. Although there seems to be some general excitement about nanotechnology and nanoelectronics, the transition from US undergraduates into a PhD program in nanoelectronics is relatively small. We also observe that most industrial semiconductor device and circuit design is driven by computer-aided design, which is typically not reflected in semiconductor introductory classes. We hypothesize here that interactive, simulation-driven learning may be more appealing and intuitive to a generation of students who have grown up with interactive video games and artificial worlds where "What if?" scenarios can be played out. To encourage the use and exploration of more interactive learning scenarios at the undergraduate and graduate level, we have assembled a set of tools that faculty members and students can freely and easily access on nanoHUB.org. The two toolsets we introduce here are geared towards "Introduction to Semiconductor Devices" and "Quantum Mechanics for Electrical Engineers."

SAMPLING THE "WHAT IF?" SCENARIOS

In a traditional "*Introduction to Semiconductor Devices*" class, students might be confronted with questions like:

- How does a Silicon crystal look from different angles? What is the crystal orientation at which we have the highest or the lowest density of atoms at the surface?
- What is bandstructure? What is an effective mass?
- What happens to the bandstructure if atoms are getting closer? What is a bi-axial distortion?
- What is a carrier distribution? What is its thermal dependence?
- What does doping do in a semiconductor?
- What is drift and diffusion?
- What is the effect of degenerate doping in a PN junction?
- What is a bi-polar junction transistor?
- What is a MOS capacitor?
- What is a MOSFET? And how does it operate?

In an "Introduction to Nanoelectronic Devices" or "Quantum Mechanics for Electrical Engineers" class a teacher might want to convey the first quantum mechanical concepts such as:

- What is a confined state? In 1D, 2D, and 3D?
- What is resonant tunneling?
- What is an artificial atom?
- What is the relationship between different confinement types and the resulting Eigenstate spectrum?
- What happens if the MOSFET channel is getting shorter?

All of these questions can indeed be answered with existing tools one can find on "the web." But downloading software alone would not be enough for optimal learning in these classes; some additional requirements must be met for students to begin to answering these questions.

REQUIREMENTS

Within the operation of nanoHUB.org over the past six years, we have identified a set of minimal requirements that are essential for classrooms that use

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software for students to engage these critical preparatory questions. The tools must:

- fit into an existing curriculum
- need to run in the web browser, eliminating the need for user-level software installation
- create a user-friendly environment for setting up the problem and displaying the results
- run fast (seconds to minutes)
- offer prepared homework or project assignments
- use validated simulation engines
- be available reliably 24/7/365.
- provide open and free account sign-up and access.
- supply a defined level of support.

With over 99.5% operational uptime in the year 2008, nanoHUB.org demonstrates operational reliability and now provides over 140 simulation tools that are used by over 7,100 users for over 400,000 simulations within 12 months of April 2008 to March 2009 alone. However, faculty members and students have also mentioned that it was hard to find “the right tool.” We have therefore implemented the concept of tool assemblies within tool-powered curricula [1]. In this paper we discuss two of these curricula, ABACUS [2] and AQME [3] in some detail; see screen splashes in Fig. 1 with prototypical “What if?” questions).

ABACUS

ABACUS (Assembly of Basic Applications for the Coordinated Understanding of Semiconductors) [2] is geared towards the teaching of semiconductor device fundamentals taught in most Electrical Engineering programs that cover solid state devices. ABACUS consists of 10 individual nanoHUB.org tools: crystal viewer, periodic potential lab, finite potential barrier lab, bandstructure lab, carrier statistics lab, drift diffusion lab, PN junction lab, bipolar transistor lab, MOScap, and MOSFET.

A community Wiki page [2] which guides teachers and students through the different tools and provides sample homework and project assignments augments the ABACUS tool. The Wiki page is a live document for all users of the tool, and the page is continually supported and updated by the authors of this paper. The community can suggest improvements and upload additional exercises and assignments.

AQME

AQME (Advancing Quantum Mechanics for Engineers) [3] is geared towards the introduction of quantum mechanical issues to electrical engineers. It consists of 10 different tools: piecewise constant potential lab, bound states lab, periodic potential lab, bandstructure lab, Schred, 1dhetero, quantum dot lab,

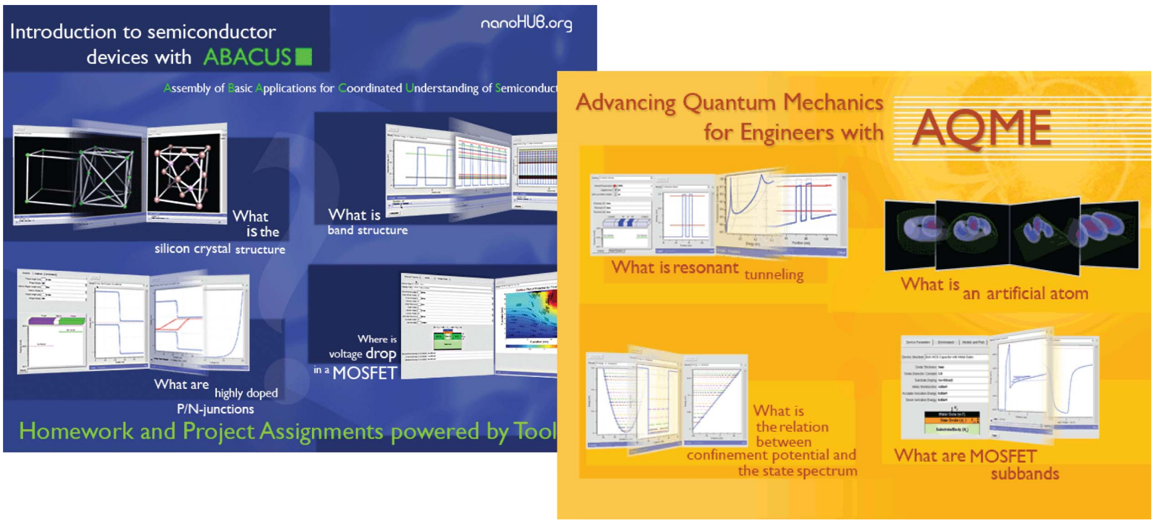

Figure 1: ABACUS and AQME screen splashes with prototypical “What If?” questions.

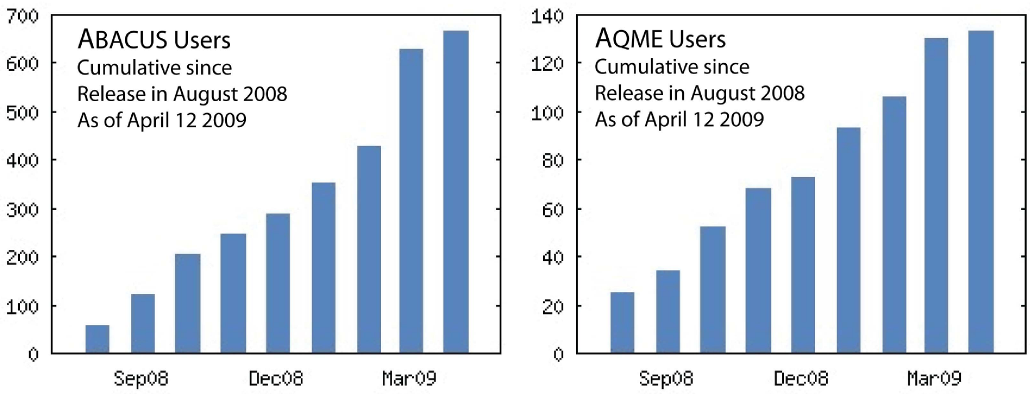

Figure 2: Cumulative number of ABACUS and AQME users since the tool releases in August 2008.

resonant tunneling diode lab, bulk Monte Carlo lab, and Coulomb Blockade lab. Also AQME is supported by a Wiki page that continues to be supported by the authors of this paper.

USAGE ANALYSIS AND ASSESSMENT

ABACUS has seen a significant growth in user numbers since its release in August 2008. Over 660 users have run over 4,600 simulations until April 12 2009. With nanoHUB's philosophy of free and open access, we enable any instructor, teaching assistant, and student to utilize tools such as ABACUS for education. Faculty members do not need to register their classes in any formal sense to use nanoHub. During account sign-up, nanoHUB asks for a reason the account is being requested, but this is an optional question. Since only a few individuals have answered that field, we can only approximate classroom usage; however, through investigation of the sign-up logs and through an analysis of clustered usage at certain IP address domains, we have been able to identify at least 15 institutions at which at least one class uses ABACUS.

For teachers interested in all of the nanoHUB.org usage statistics, they are available online [4]. The usage of each tool is measured and flows into the overall tool ranking, which also factors in user ratings and the tool support level.

nanoHUB.org in general and ABACUS in particular are undergoing a formal assessment of their usefulness in the classroom. An assessment expert in the Purdue College of Engineering, Dr. Diane Beaudin is assessing nanoHUB in terms of access, use, and impact, through available nanoHUB statistics and nanoHUB user surveys.

An educational team comprised of three Professors at Purdue's School of Engineering Education is beginning to study the effect of nanoHUB on the learning experience of students. The team is also beginning to devise, through surveys and user interviews, recommended methodologies in this new online teaching environment.

Two independently NSF-funded efforts in the program of Virtual Organizations as Sociotechnical Systems (VOSS) are beginning to study and assess virtual organizations in general, and nanoHUB with its very large user base in particular. The Purdue-based NCN assessment team is using surveys, user interviews, and usage patterns to measure the success and the problems with our educational tool initiative.

OPEN COMMUNITY AND RAPID TOOL DEPLOYMENT

The novel nanoHUB.org middleware and **R**apid **app**lication infrastruc**ture** *Rappture* [5,6] have enabled deployment of over 140 tools to the nanotechnology community in less than four years. A key ingredient to the large number of available tools is that the nanoHUB.org software team has invented an infrastructure and software environment that lets scientific tool developers deploy their own codes rapidly without handing them over to some other web developer who knows nothing about the science code. *Rappture* enables scientific users to create beautiful, interactive graphical user interfaces (GUIs) and helps them manage their data in a hierarchical form that documents provenance. Graduate and even undergraduate students can create their first-cut GUIs in a few days. *Rappture* can deal with legacy applications that cannot or must not get changed through a scripted wrapper approach and it can be fully integrated as an I/O library in active software projects. *Rappture* supports standard compiled and interpreted languages such as (C, C++, FORTRAN, F90, Matlab, phython, tcl, perl, and ruby). I/O of a tool are described in an XML file and the GUI is automatically generated in a standard Linux environment. nanoHUB.org provides the development environment online to its users through its advanced middleware. The bottom line is that a research team with a code that they want to share with the community does not have to rewrite the code to be deployed on the web; this means the code does not have to leave their control. The whole software deployment process has been formalized [7], much like the inverse of an Amazon.com shopping experience and requires little nanoHUB.org staff intervention.

nanoHUB.org is truly open to the contributions from the community. The over 140 tools are being used by over 7,100 simulation users for over 400,000 simulations within the past 12 months (April 08-March 09). nanoHUB.org is considered the shining example of a Science Gateway which enables others to conduct simulation-based endeavours in research and education [6,8].

DEFINED LEVELS of SUPPORT

After public presentations about nanoHUB.org, one of the first or second questions we are asked is usually: "How do you ensure quality of *all* these tools and how do you support them?"

Since nanoHUB.org is designed in the spirit of research and educational support through online simulation, everyone in the community is encouraged to contribute tools and seminars to the Nanoscience and Nanotechnology community! However, as a central cyberinfrastructure provider, we are faced with issues of "Quality Control" and "Software Support". We therefore take a two-pronged approach to tackle the issues of "Quality Control" and "Software Support": We distinguish between two different sets of tools:

1) contributed tools:
   supported solely by the tool contributor. nanoHUB.org puts processes and infrastructure in place that makes the tracking of bugs, questions, and improvement requests as automated as possible. We request that the tool authors provide enough supplemental materials to their tools such as scientific heritage, tool validation, tool limitation discussions, tutorials, and even possibly usage scenarios (homework or project assignments).
2) NCN supported tools:
   nanoHUB.org is operated by the Network for Computational Nanotechnology (NCN) which consists of several university nodes. Each of the major four nodes at Purdue, Northwestern, U. of Illinois, and UC Berkeley has identified a short

list of tools they will support with a defined level of service that is common to all [9]. The level of service assures:

- monitoring of support tickets, questions, and wishlists, and responses provided within one business day.
- fixing simple bugs within a week.
- moving long-term projects and any reported tool improvement requests to a public wish list.

ABACUS and all of its 10 constituent tools are part of the NCN@Purdue-supported tool list [10] which contains 17 tools altogether, including education- and research-focused tools.

We are still developing the software on the nanoHUB backend which streamlines the triage process for filed tickets, posted questions, and wishlists and to route them to the appropriate persons. Right now we are able to inform software developers automatically about posted questions on their tools. Soon we will automatically route support tickets and wishes for tool improvements. As this management process matures we are planning to roll out the concept of "NCN certified tools" where authors will be asked to subscribe to a higher level of support similar to the "NCN supported tools," rather than their best effort.

With all of these questions of support we still want to emphasize that there is value in the dissemination of "hot off the press" research tools to be shared amongst collaborators, with the understanding that some of these tools will break and that they are meant for a limited set of users. The concepts of "NCN supported" or "NCN certified" tools will ultimately help distinguish between tools and also guide user expectation.

OUTLOOK and SUMMARY

We have briefly described two tool sets ABACUS and AQME in our tool-powered curriculum [1] on nanoHUB.org. Several other tool sets such as the Berkeley Computational Nanoscience Class, ANTSY (Assembly for Nanotechnology Survey Courses), ACUTE (Assembly for Computational Electronics), and a Freshman Chemistry course have been deployed or are under development. nanoHUB.org is a work in progress and we would like to encourage the community to provide feedback and to contribute.

ACKNOWLEDGMENTS

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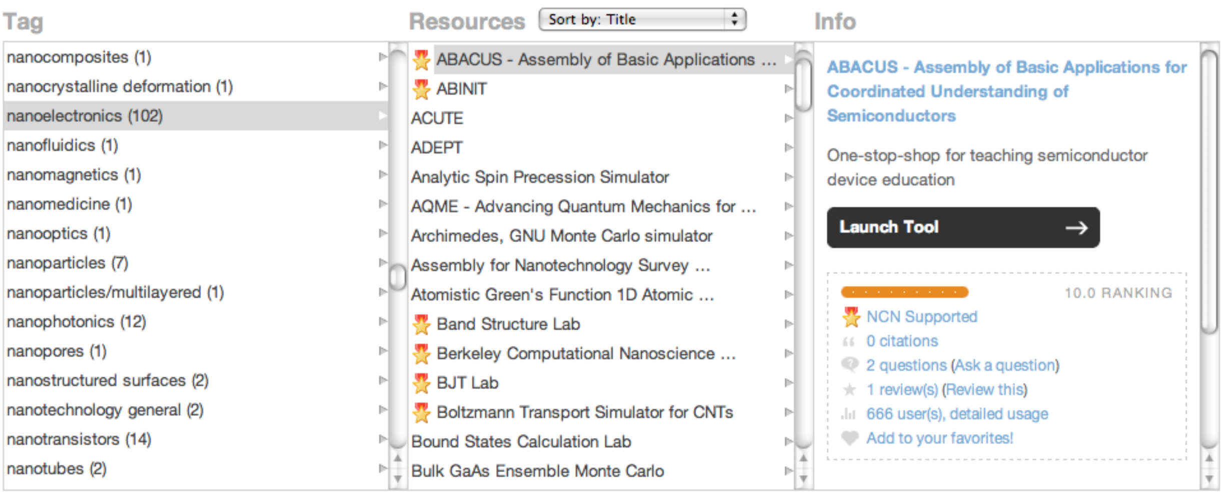

Figure 3: nanoHUB.org tool browser by author and community driven tags. NCN Supported are indicated by a medal icon. Each tool is characterized by its number of citations in the literature, posted questions, reviews, and users.