The nanoHUB:
A Science Gateway for the Computational Nanotechnology Community

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1. The Network for Computational Nanotechnology (NCN)

The NCN was launched in September 2002 with a mission to create a network to serve the National Nanotechnology Initiative by providing live simulations and related services online. The NCN has a vision to be the place where theory, experiment, and computation meet and help move nanoscience to nanotechnology. By "place" we mean a cyber-environment that offers online services to users from the community. We define science gateways as an integrated ecosystem of infrastructure, middleware, educational and content aggregation tools that will provide the primary means for conducting science in a specific field. Furthermore, ideally the cyber-services offered by the science gateways should be available to the larger community through traditional media such as the web, and also through emerging mobile platforms such as PDAs and cell phones. The "network" in NCN refers to both the computer network that will be most visible to the nanotechnology community nation- and worldwide as well as the network of people who comprise the NCN. We use the term "computing" in NCN broadly to mean theory (which often involves computation), simulation (which is focused on scientific problems and engineering applications), and computation (which involves algorithms and software). The NCN was established to connect theory, simulation, and computation to the broader community of experimentalists, educators, and students. The major outcomes of this initiative will be:

- **Research** that re-invents electronic and electromechanical device engineering from the bottom up and connects such devices to living systems.
- Innovative (bottom-up) approaches to **education**.
- **Leadership** through meetings, workshops, debates, and forums that bring people together, identify challenges, and move the field ahead.
- **Software** that addresses new challenges and sets the stage for nanotechnology CAD.
- Increased numbers and **diversity** of students and faculty engaged in nanotechnology.
- A **cyberinfrastructure** that connects people, disseminates unique educational resources, and delivers simulation, visualization, and high-performance computing services online.

The defining deliverable for NCN is its web site, www.nanoHUB.org. Our goal is that nanoHUB.org becomes the 'first stop' within our areas of focus (nanoelectronics, nano-electromechanical systems and nano-biology) for students, educators, and researchers in academia and industry. The nanoHUB will also serve as a real-world testbed for a new paradigm in computing. Users will be able to access and run live simulations without the need to acquire, install, support, and maintain software. But nanoHUB.org will be more than an online simulation service. In addition to software tools and services, our plan is that the nanoHUB provides online training and tutorials, short courses and full courses that present material in innovative ways, learning modules, seminars by leading researchers, forums and debates, and collaboration services.

Indeed, the nanoHUB origins stem from the deployment of applications for web-based computing. We now have an improved philosophy for what a nanoHUB service is; we see an application not as a standalone program but as an integrated package that encapsulates knowledge on a specific topic. As such, applications are much more meaningful when presented with additional web content in support of the NCN mission, including a nanotechnology curriculum complete with courses, tutorials, and seminars, as well as other documentation, the nanoHUB gateway aims at serving these services to the nanotechnology community.

We believe that a really useful and significant infrastructure can only be achieved as a *result* of a synergistic effort that involves leading researchers and educators in nanotechnology, as well as computer scientists and professionals in numerical analysis, software engineering, middleware, and cyberinfrastructure. This synergistic effort is essential to define and create a truly unique and useful infrastructure. The activities of this diverse set of participants will in turn enrich the infrastructure.

2. The nanoHUB infrastructure

Because we cannot define in advance exactly what the most useful content for nanoHUB.org to host will be, we designed the NCN to include a tight link to leading researchers and educators. New simulation tools will be the key resource that the NCN brings to the community. We aim to bring new capabilities to the field and to develop the community codes that lead the next generation of CAD tools for engineers and researchers in nanoelectronics, NEMS, and nano-bio. These new simulation tools must be designed by researchers actively engaged in the field, assisted by computational experts and by software professionals.

The nanoHUB is designed to provide much more than simulation tools and services. The faculty and students in the research themes must also develop these resources. As resources are developed, they will be evaluated and refined so that a package of high-quality resources results. Examples of the content currently being developed by NCN faculty are: online tutorials, online courses, course modules that make use of simulation, toy models that illustrate key concepts, online debates and scripts that illustrate key approaches.

To most people, www.nanohub.org "is" the NCN. It is therefore important, that our web presence and cyberinfrastructure be a very high priority. The overall NCN infrastructure consists of five components:

1) The nanoHUB, www.nanohub.org,
2) The middleware that delivers the nanoHUB's simulation services (In-VIGO)
3) Software applications for live, online operation (download as open source)
4) Educational modules
5) Access to computational resources for general users.

2.1 Web-Site Content Management

During the NCN's first two years, we defined and deployed a web presence for the NCN that consists of two parts. The first is the NCN home page, which contains program specific information, such as our vision and mission, and our people, programs, and events. The second component is the nanoHUB where NCN nanoscience and nanotechnology content is hosted. The nanoHUB in particular is a site that is expected to grow in content significantly. The content will have to be contributed remotely from different individuals and organization. The site content must be managed by distributed remote administration, rather than being an accumulation of documents, managed by a single administrator. After much experimentation, we selected Mambo, an open source content management system that provides the required capabilities for the NCN. A critical component of the selection of a portal system has been the ability to manage the site with multiple remote contributors and access to system source code. The nanoHUB, in its previous version, was tool-centric. The nanoHUB was a great resource for potential users who knew of a particular application, knew of its installation on the nanoHUB, and also partly knew how to use it. However we also need to serve users in a more theme-oriented sense, where potential users come in with the desire to model carbon nanotubes (CNTs), without knowing in detail what tools we have for CNTs, We have redesigned the nanoHUB to serve a larger class of users, by making it theme-oriented according to scientific topics such as CNTs, molecular electronics etc., and user role-oriented such as Educator, Researcher. Then we can serve the users information about these themes that may consist of seminars, tutorials, classes, and simulation tools that are relevant to their interest. Therefore, a content database-driven approach was needed for the nanoHUB.

2.2 Middleware for Online Simulation

To deliver computational services through the Internet, the nanoHUB makes use of grid-computing middleware. Web-based delivery of computing services is a topic of considerable current interest in academia and industry. It is not the NCN's mission to develop such middleware, which is an expensive undertaking best done by computer scientists, engineers, and professionals. Our middleware strategy is to leverage existing efforts in the field. We plan to serve as a testbed for middleware research by deploying, extending, hardening, and supporting a system that meets the real-world needs of the nanotechnology community. During the NCN's first year, we transitioned our first-generation system, PUNCH [1], to a production environment supported by Purdue's central IT organization (ITaP). PUNCH was one of the earliest systems for web enabling of applications. It was created before many of today's standards (e.g. Apache), but it demonstrates the promise of computing online. During the NCN's second year, our partners at the University of Florida deployed a second-generation network-computing system, In-VIGO [2] and demonstrated it with NCN applications. In-VIGO is now being deployed to support the nanoHUB and is being integrated with Condor-G to access remote computational resources [3]. In-VIGO middleware builds on virtualization technology to 1) offer a home directory to users through a virtual file system, 2) Allow users to run applications on resources where they do not have physical accounts through shadow accounts, 3) Provide a computing environment to anonymous users using virtual machine isolation and 4) Rapidly deploy applications within the In-VIGO framework through a set of API and a service-based description of the application logic.

2.3 Rapid Application Prototyping

The nanoHUB philosophy is that all online applications must be easily accessible to the user on the nanoHUB in a graphical user interface (GUI). One could possibly argue that the more advanced the user is, the less sophisticated the user interface needs to be and the more computation time will be required. However, tight integration of simulator input and simple visualization of the output is actually essential on all levels of education, research, development, and discovery. The Rapid Application Infrastructure toolkit (Rappture) is geared to enable the simple creation of user-friendly GUIs for legacy and new applications without significantly increased burden on the application development. The idea is to use a reusable I/O description germane to most simulation tools and to provide application developers with a very simple API.

The Rappture toolkit solves the problem detailed above by providing the basic infrastructure for a large class of scientific applications, letting scientists focus on their core algorithm. It does so in a language-neutral fashion, so scientists can access Rappture in a variety of programming environments, including Fortran and Python, and in the near future, C/C++ and MATLAB®. Instead of inventing their own input/output, scientists declare the parameters associated with their tool by using Rappture objects, such as `number`, `string`, and `choice`. For device structures, they use geometric objects, such as `box`, `sphere`, and `plane`, and they use `fields` to add material parameters and doping profiles. For output, they use composite objects, such as `curve` and `table`. All physical simulation tools that we are aware of require three fundamental classes of input that map naturally to the various Rappture objects: 1) topology, 2) material or incident properties in the topology, and 3) algorithm directives. These categories map to all the tools we are currently hosting or plan to host; for example, in circuits (1-connections, 2-device properties, 3-simulation targets), device simulation (1-structure, 2-materials, 3-simulation targets), and molecules (1-structure, 2-atom description, 3-simulation targets).

The Rappture toolkit extracts a description of all parameters from their program, along with hints, such as default values, minimum/maximum values, pop-up help information, and so forth. Then, it generates a Graphical User Interface (GUI) for their tool automatically. Rappture generates the GUI dynamically, each time they run their tool, based on the information available at that point. So if they make any changes to their program, Rappture will detect their changes and adjust the GUI accordingly the next time they run their tool.

2.4 Educational Applications

Elements of the nanoHUB content can in principle provide a tremendous resource for educators of a wide K-20 audience. However, the content needs to be packaged and delivered to the audience so it can indeed be used in the classroom. Furthermore, the content needs to be easily adoptable and interoperable with already available course management systems and educational resource repositories. E-Learning specifications handle the formal processes of content management and content description. Learning Modules, in our context, are defined as highly interoperable, reusable, and standard-compliant sequence of digital assets. They have varying granularity ranging from simple voiced presentations to ones that include quizzes, feedback, and access to online simulations. The standards used in the nanoHUB are IMS [not an acronym] and Shareable Content Object Reference Model (SCORM v1.2), which are currently being considered by IEEE for release as e-learning standards. Conformance to e-learning standards enables nanoHUB learning modules to be disseminated through compliant course management systems such as WebCT, Blackboard, and Sakai. Such dissemination significantly increases potential positive impact within the day-to-day classroom curricula.

The relatively simple educational simulation tools will immediately benefit from Rappture, as we can begin to migrate codes with rapid execution times into a user-friendly educational tool. These educational applications are integrated into educational modules that explain the science, demonstrate the tool usage, provide exercises, and quizzes with appropriate feedback. These educational modules are then announced on sites like MERLOT [4], which catalog and host educational modules nationwide. Online simulation capabilities specifically tailored to education are being tightly integrated with the new curriculum development. Learning Modules couple the NCN nanocurriculum tightly to online simulation and provide a much needed layer of contextualized content aggregation. These learning modules, hosted on the nanoHUB, break down the elements of the curriculum into smaller components with tightly integrated simulation exercises. Learning modules consist of PowerPoint presentations with voice-over, lecture videos on the nanoscience and the use of the tools, links to the online tools, quizzes, homework problems, and problem solutions. Learning modules are described with a formal xml-based IEEE standard meta-language. Adherence to such an educational module description standard allow us to post these module descriptions at other web-sites such as MERLOT and allow us to integrate these modules into online class management systems.

Learning modules developed for the nanoHUB are wrapped in XML-based metadata descriptors and contain a wide range of content, such as voiced presentations by experts, quizzes, and links to appropriate online simulation tools. For example, the "Introduction to Nanofluidics" module on the nanoHUB is a full-fledged learning module that leverages NCN expertise in the area of nanofluidics and links to the online simulation tools provided on the nanoHUB. Similar modules on Molecular Electronics and other areas are under development. These learning modules allow students to learn using real-world, authentic tools and datasets – thus enabling educators to adopt more hands-on pedagogies, such as problem-based and inquiry-based learning, in ways that were not feasible before.

2.5 Computational Resources

As the nanoHUB becomes more popular will hopefully reach the point where our local resources can no longer cover all requests for computation. We developed a strategy to address the anticipated need for increased compute power. The model that is being pursued is to leverage contribution of computational cycles by other centers or partners. One step in the direction of distributed remote computing is our partnership with the NSF TeraGrid project. Purdue's selection as the nanotechnology "science gateway" for the TeraGrid will provide the NCN with access to high-performance computing resources on the TeraGrid. We have already the use of the TeraGrid for at least one NCN application that requires significant compute time, NEMO3D [5]. The In-VIGO middleware is being developed to tie the nanoHUB to the TeraGrid resources and work is underway within TeraGrid to put the policies in place to let a community such as the nanoHUB to use the nation's resource. The NCN now has a community allocation which delegates to the NCN PI the ability to add users and also makes the NCN accountable for the allocation usage through the nanoHUB.

2.6 Real Users and Real Usage

The Purdue University Simulation Hubs (PUNCH) has delivered batch-oriented online simulation since 1995. The primary use has been in education for homework assignments. Use for research has been growing as more mature simulation tools have been deployed. Simulation user numbers have been level around 800-1000 annual users. The simulation load fluctuates significantly throughout the year with cycles in the semesters. The total number of simulations runs in the past 12 months exceeded 71,000 performed by over 1,100 users. With the deployment of interactive applications and interactive educational modules we expect that the simulation usage number will grow significantly beyond the students that "have to" use the tools for homeworks. The complete redesign of the nanoHUB enabled users to access content more effectively and enabled us to deploy more content rapidly. This redesign appears to have paid off in the total user numbers of the nanoHUB. The total user numbers rose from

2,000 to over 6,600 in the last year. It is our strategy to grow the simulation user numbers through better service as discussed above.

3. Conclusions

The nanoHUB is serving as a science gateway for users interested in educational and research applications. The services are provided to real users with real usage. Users can use the facility without installation of any software. The overall usage number has begun to grow spontaneously after a deployment of value added nanotechnology content. The nanoHUB team is pursuing the deployment of a new middleware (In-VIGO) which provides access to more computational resources and enables deployment of interactive applications. With these interactive applications we believe we will be able to grow the online simulation user numbers as well and provide high quality services to the nanotechnology community.

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