

# Network for Computational Nanotechnology - A Strategic Plan for Global Knowledge Transfer in Research and Education

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**Abstract**—The Network for Computational Nanotechnology (NCN) manages the science gateway nanoHUB.org, recognized as the world’s largest nanotechnology user facility, with over 2800 research and teaching resources in use by over 180,000 users annually. Resources consist of 220 simulation tools and nearly 2600 other content items ranging from podcasts of lectures to first time user guides for simulation tools to complete sets of university course materials. Simulation tools developed for research have been found to be used in the classroom and simple classroom tools are being used by researchers. With a global community spread across 172 countries, nanoHUB.org facilitates fast knowledge transfer across countries, disciplines, and communities. NCN follows a carefully planned strategy to lower barriers to this knowledge transfer and the growth and success of the site validates this strategy.

## I. INTRODUCTION

THE Network for Computational Nanotechnology (NCN) is a highly successful virtual organization that was founded in 2002 on the premise that computational tools were seriously underutilized in such emerging fields of science and engineering as nanotechnology. In the context of this paper, a virtual organization is defined as “a group of individuals whose members and resources may be dispersed geographically and institutionally, yet who function as a coherent unit through the use of cyberinfrastructure (CI).” [1] NCN was established as a virtual organization to foster, expand, and support the community of researchers using modeling and simulation tools for nanoscale engineering and science research and education. Figure 1 illustrates how NCN functions as a virtual organization.

The establishment of NCN must be seen in the larger context of a major intellectual and societal paradigm shift that is referred to as the “progressive convergence” [2] – namely, the confluence of nanotechnology, biotechnology, information technology, and cognitive science. In the context of this progressive convergence, it is widely understood that the combination of nanotechnology and information

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technology will drive innovation in other areas of engineering and science. However, at the time NCN was formed, computational tools were not used heavily for research into nanoscale phenomena. Where such tools existed, they were mostly rudimentary in nature and difficult for individual researchers to easily adopt or use. nanoHUB.org was created as the cyberinfrastructure that would support the community of researchers being fostered by the NCN virtual organization.

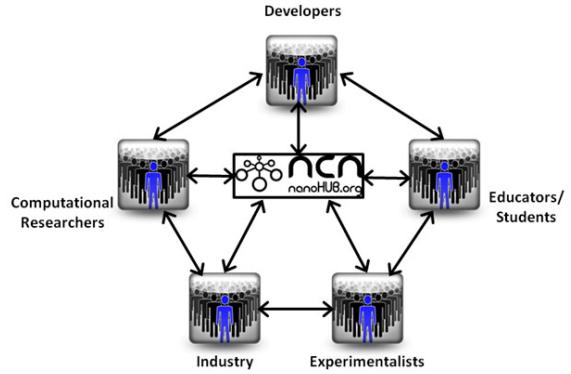


Figure 1. The NCN Virtual Organization

The fundamental premise behind the development of nanoHUB.org was that the full impact of computation comes when simulation tools move beyond the domain of computation experts and become essential tools for the broad community of those with experiments to analyze, devices to design, manufacturing processes to develop, and students to educate. In essence, through nanoHUB.org, NCN’s primary vision and contribution is the complete democratization of computation for the purpose of furthering research and education in nanoscale engineering and science. Branscomb and Kahin [3] point out that “the democratization of computing over the past fifteen years has lead to an extremely competitive market for software applications that integrate an increasingly complex set of functions while remaining highly reliable.” (p. 5). Through nanoHUB.org, NCN is indeed creating a market place – more collaborative than competitive – for the use of software to address some of the major computational problems in nanoscale engineering and science. For example, work at NCN has resulted in the scaling of the research code OMEN almost perfectly to 221,400 cores (Figure 2) on the world’s fastest supercomputer (Jaguar at Oak Ridge) in order to answer fundamental questions of

carrier transport at the nanometer-scale. OMEN and its earlier prototypes as well as the related engine NEMO now power several applications on nanoHUB.org with 108,413 simulations run by the user community using OMEN/NEMO powered tools through December 2010.

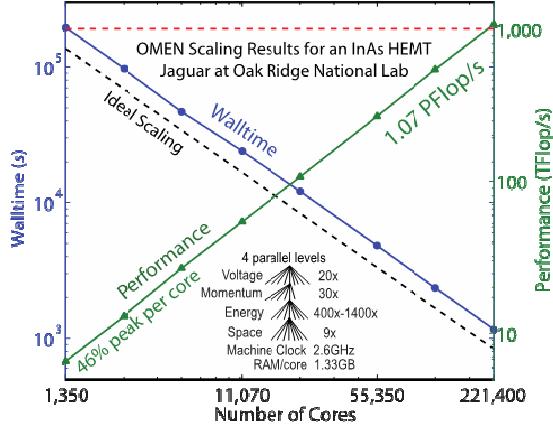


Figure 2. OMEN - a nanoHUB.org petascale application

The semiconductor industry is an example of the impact of widely used simulation tools: widespread end-to-end modeling of complex systems with software originally developed in the research community has led to today's industry success. Still, the process of translating basic nanoscience into applied nanotechnology is in its infancy. Growth will be accelerated by widely sharing newly developed computational tools within the nanotechnology research and development community.

Within this context, we address the major knowledge gap that exists in how a virtual organization focused on an engineering discipline can be successfully formed and developed to foster a large community of researchers. We address the fundamental question of how to go about setting up a vision and goal for an engineering cyber-environment. Furthermore, we address how to determine when the virtual organization is beginning to fulfill its goals.

The mission of NCN is to support the National Nanotechnology Initiative (NNI) by designing, constructing, deploying, and operating a national cyber-resource for nanotechnology theory, modeling and simulation which can be used for both research and education. Our mission is embodied in nanoHUB.org and driven by pioneering research, education, outreach, and support for community formation and growth. nanoHUB.org lowers the barriers to knowledge transfer between teams of researchers and blurs the line between research and education. Much more than a simple website, nanoHUB.org currently provides access to over 2800 resources including 220 simulation tools and a vast array of lectures, full length courses, and other materials, with new resources being continually added. The science gateway nanoHUB.org is recognized as the world's largest nanotechnology user facility, serving over 180,000 users annually with 10,667 users running 388,936 simulation jobs in the last year (September 2010-August 2011)[4].

nanoHUB.org utilizes an underlying infrastructure known as HUBzero®, which was extracted from nanoHUB.org to create an infrastructure capable of supporting a variety of other scientific HUBs [5]. The HUBzero platform allows users to access computational tools directly through a web browser and run simulations using computational resources based at Purdue University and across powerful grid resources on which NCN maintains community accounts.

The U.S. National Science Foundation (NSF) recently released a revised strategic plan [6] which emphasizes collaboration both across disciplines and globally, and recognizes the key role that cyberinfrastructure plays in all areas of science and engineering as well as science, technology, engineering, and math (STEM) education. With users across multiple disciplines in 172 countries and proven use in both research and education [7]-[9], NCN and nanoHUB.org strive to play an important role in this exciting future.

## II. CORE VALUES AND GOALS

### A. Core Values

NCN adheres to core values which support our mission and guide our decisions and actions. These values, in turn, have led us to develop success criteria for establishing a thriving community within a science gateway such as nanoHUB.org. The values which drive our mission are as follows:

- Widespread use of computation for theory, modeling, and simulation;
- Peer review of scholarly endeavors;
- Availability of information and tools for discovery and learning;
- Support of discovery and learning by all;
- Partnership to build a vibrant community of scholarship;
- Ethical conduct and respect towards participants in the community we foster.

Our experience has shown that the culture of a community emerges from the daily actions of its members. With its cyber-resources and by the design of its cyberinfrastructure, NCN encourages actions that will build a scholarly culture characterized by:

- A philosophy of sharing the tools of discovery;
- An ease of collaboration among members of the community;
- A strong connection between research and education.

NCN unites a diverse community by sharing research and educational resources via leading-edge cyberinfrastructure, leading to new modes of discovery, innovation, learning, and engagement. The end result is to accelerate the transformation of nanoscience to nanotechnology through innovative theory, modeling, and simulation, all tightly linked to experimental research and to education.

### B. Goals

In order to fulfill our mission and support our core values, we focus on the following goals:

- Become an essential resource for the nanoscience and

nanotechnology community worldwide;

- Lower the barriers to the widespread use of simulation for nanotechnology;
- Develop high quality simulation tools quickly for this fast-moving field;
- Enable research that addresses key challenges that are tightly linked to experimental work through theory and simulation;
- Disseminate the results of our work and engage the broader nanotechnology community through universally available web technology;
- Transform nanotechnology education and workforce development to increase the number and diversity of engaged faculty and students and to equip them to be critical, effective simulation users;
- Create and operate cyberinfrastructure that delivers services for simulation, education, and collaboration efficiently and robustly;
- Provide professional leadership that bridges disciplines and connects communities to identify challenges and move the nanotechnology field ahead.

The unique and unifying NCN goal is to achieve the above objectives within our innovative science gateway, nanoHUB.org.

### III. SUCCESS CRITERIA

Over nearly ten years of existence, NCN has defined a clear set of success criteria for a science gateway site serving a large user community effectively. The vision for a science gateway is to employ fundamental science and engineering to drive basic research and invention which then facilitates applied research and innovation leading to impact. The transition from basic research to application can be a difficult and slow process, but a vibrant and active scientific community utilizing resources that speed technology transfer is an asset to the process.

A successful science gateway site begins with outstanding science that meets the needs of a broad community. This tenet is fairly easy to grasp for most science gateway projects, but beyond acquiring content, the next step can be difficult. For many sites, a large effort in terms of time and resources is put toward developing a single tool or a few resources. NCN promotes an open source, collaborative philosophy within the computational community, and engages experimentalists and educators by developing research and delivery programs that meet their needs. NCN uses a strategy that involves leveraging research by working within a set of seven academic partner institutions as well as several partnerships with industry. Each partner institution capitalizes on the strengths of their local scientific community and encourages and facilitates transfer of simulation codes as well as educational materials to nanoHUB.org which are then available to the global nanotechnology community.

In order to thrive, a science gateway site requires a commitment to dissemination from the community it serves. The seven partners in NCN take the lead in content generation

and deployment on nanoHUB.org, but significant content contribution also comes from outside the network. It can be difficult to convince faculty and researchers to release teaching materials and codes to the community at large when the benefits are not clearly defined. Faculty who have utilized nanoHUB.org to deploy simulation code and learning material have not only found that they reach a large audience, but that their research results disseminate quickly into their scientific community. Usage statistics are freely available to each contributor, allowing them to easily show proof of impact. This has assisted faculty contributors in proposal submission and positively impacted promotion and tenure decisions. The large amount of quality content available on nanoHUB.org is a direct result of contributors understanding the benefits both to themselves and to the scientific community.

NCN develops and deploys resources on nanoHUB.org to guide and support instructors in creating effective learning experiences based on the literature on how people learn. We hold workshops to give instructors hands-on experience in developing outcomes-based learning experiences using the most effective approaches with nanoHUB.org. We work with instructors in developing new methods to create educational research opportunities, facilitating better understanding of learning issues and identifying opportunities for innovative pedagogical methods using nanoHUB.org. By working closely with undergraduate instructors we engage more undergraduate students in modeling and simulation.

A key to success for a science gateway site is to understand and respond to the needs and behaviors of its users. nanoHUB.org lowers as many barriers as possible, allowing the user fast and easy access to the resources they need. Our browser-based interface eliminates the problem of software installation for which users may not have the time, experience, or permission to install locally. We understand that users may have limited experience and time constraints that require them to be able to utilize tools "out of the box," without spending time reading manuals or working through a time-consuming learning curve. The user needs immediate access and instant feedback with a smooth and transparent transition to high performance computing resources when needed. Users benefit from the ability to visualize and compare results as they work.

Science gateways must be supported by an underlying technology or platform that is simple and completely reliable with adequate funding dedicated specifically to operation. nanoHUB.org experienced 99.6% uptime last year.

In order to grow, the site must facilitate technology transfer, making the process easy and painless for contributors and providing necessary encouragement to recruit new contributors. At NCN, each of the seven partner institutions employs a site lead, whose function is to facilitate content creation and provide support for contributors.

One of the most important parts of success is to be able to measure and objectively report impact. At NCN, we focus carefully on gathering, understanding, and disseminating

statistics related to access, use, and impact of our site. We can use these statistics to show impact for our site as a whole, as well as incentivize participation by providing usage statistics to contributors for their own content. NCN continually assesses the access, use, community interaction, and impact of nanoHUB.org and makes these assessment data openly available. We continue to enlarge our efforts in meaningful impact assessment. nanoHUB.org functions as a role model in opening access to impact data and will continue to lead the way for cyber-enabled virtual organizations who report their performance to the public. The gathering and use of statistics is a powerful tool for a science gateway site to concretely show that it is fulfilling its mission.

#### IV. SUCCESS METRICS

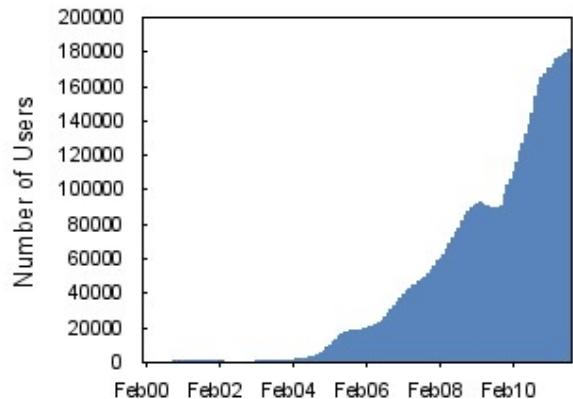
Success metrics provide us with quantitative verification of whether our strategic plan is effective in meeting our goals as a science gateway site. Table 1 provides usage statistics for nanoHUB.org for the period from September 2010 through August 2011.

**Table 1. nanoHUB.org Usage, Sept 2010-Aug 2011**

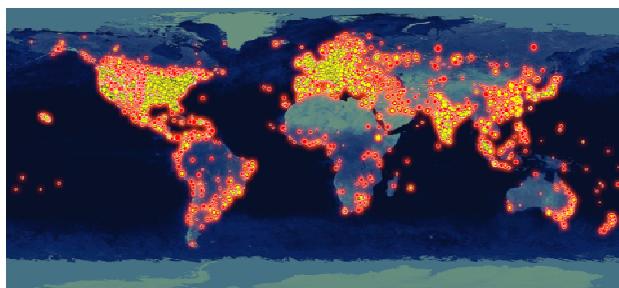
Total Users	181,106
Simulation Users	10,667
Interactive Users	51,598
Download Users	158,966
Simulation Runs	388,926
Domains Served	13,608
Visitors	387,733

We are careful in how we define users in order to avoid inflated counts and to eliminate or significantly reduce counting of web crawlers. A *visitor* to the site is conservatively defined as a unique IP address. To be counted as a *user*, a visitor must either be a registered user who has logged in, an interactive user (defined as a non-registered user with a unique IP address and an active session on the site lasting at least 15 minutes), or a download user (defined as an non-registered user with a unique IP address who downloads a piece of content such as a PDF or podcast).

We have seen the use of nanoHUB.org grow steadily since its inception. Figure 3 shows the growth in usage from the beginning of nanoHUB.org to the present. Figure 4 gives a different view, illustrating the use of both simulation tools (shown in yellow) and other content (shown in red) worldwide. nanoHUB.org is clearly a widely used, global resource.



**Figure 3. nanoHUB.org Annualized Usage**



**Figure 4. Cumulative nanoHUB.org Usage Worldwide**

#### V. CONCLUSION

A science gateway site such as nanoHUB.org is an ever-evolving entity. Careful and continual assessment provides feedback on impact as well as providing direction for improving the site and the user and contributor experience. In managing nanoHUB.org for nearly ten years, the Network for Computational Nanotechnology has developed and tested goals and strategies for success and a variety of usage data validates the strength of the strategies put in place. Because fields such as nanotechnology and cyberinfrastructure evolve rapidly, it is necessary for organizations such as NCN to adapt and re-examine its strategies to make certain that nanoHUB.org continues to be at the leading edge.

#### ACKNOWLEDGMENT

Mark S. Lundstrom founded nanoHUB.org in 1998. In 2005, Michael McLennan created the Rappture Toolkit and Rick Kennel wrote the scalable middle ware of HUBzero that, respectively, enable and power interactive nanoHUB simulations. The Network for Computational Nanotechnology (NCN) manages nanoHUB.org, and works in conjunction with NCN partners at Purdue University, Norfolk State University, Northwestern University, Massachusetts Institute of Technology, the Department of Energy Molecular Foundry, University of California, Berkeley, University of Illinois at Urbana-Champaign, and the University of Texas at El Paso.

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