Nanotechnology institutions

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nanoHUB.org: cloud-based services for nanoscale modeling, simulation, and education

Abstract: nanoHUB.org is arguably one of the most successful science gateways funded by the National Science Foundation (NSF). It is the cyberinfrastructure that supports the Network for Computational Nanotechnology (NCN), currently serving over 240,000 users annually in 172 countries worldwide. It features a range of resources including seminars, online courses, short courses, full-fledged tool-powered curricula, and over 260 online simulations and modeling tools. nanoHUB functions as a scientific cloud where users cannot only design and run their tools but also provide a worldwide audience access to these tools with no installation or minimal infrastructural requirements on the users’ part.

Keywords: computational modeling; nanotechnology; science gateways; simulations.

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1 Introduction

The Network for Computational Nanotechnology (NCN) is a National Science Foundation (NSF) infrastructure and research network established in September 2002. Our mission is to support the National Nanotechnology Initiative (NNI) by creating and operating an ever-evolving cyber platform for sharing simulation and education resources [1]. Our mission is embodied in nanoHUB.org and driven by pioneering research, education, outreach, and support for the nanotechnology community formation and growth [2]. Our early experimentation with online simulation for the nanotechnology community has turned into a robust, production-level infrastructure used by a global community. From an initial user base of about 1,000 users, nanoHUB.org has grown to support more than 240,000 users annually. For the 12-month period ending October 31, 2012, nanoHUB.org supported 242,105 users in 172 countries with materials for research and education (Figure 1). Of those users, 12,510 ran about 402,000 simulation jobs with over 260 available simulation tools [3]. The growth in the nanoHUB user base over the past 9 years is shown in Figure 2. Over 940 citations in the literature are evidence of research usage, and 14,521 students identified in 761 formal classes at 189 institutions are evidence of the site’s direct use in education. In 6 years of tracking the availability of all functionality on the site, nanoHUB full uptime exceeds 99% with ongoing efforts in place to continue to improve.

1.1 Global presence

The use of nanoHUB resources is truly global, with 27% of our total users coming from the United States, 39% from Asia, and 23% from Europe. We continue to see growth from a variety of worldwide locations, including significant growth in South America, Africa, and Australia. About 92% of our users are affiliated with an academic institution.

The use of simulation tools shows a slightly different picture: 49% of the simulation users are in the United States running 65% of all nanoHUB simulations. We believe that this is, in part, due to the effect of network delay on the user experience with interactive simulations. We have initiated collaboration with partners in Colombia who will host a mirror nanoHUB site, dedicated to simulations for users in South America.

1.2 Broad US Presence

In the United States, our users represent about 21% of all 7,073 US.edu domains. Considering the very broad
spectrum of the institutions represented by the set of organizations with a .edu domain, we believe that 21% represents a very strong presence for the quite specialized nanotechnology research area.

1.3 Presence at US universities

We have been tracking nanoHUB use at members of the U.S. News and World Report’s list of Top 50 Engineering Schools. Since 2007, nanoHUB has delivered “and more” content – lectures, seminars, online courses, and other such learning material to users in all of the Top 50 Engineering Schools (Figure 3). Almost all of these schools ran simulations on nanoHUB in a recent 12-month period, accounting for nearly 24% of our worldwide simulation users. The Top 50 Engineering Schools account for about 50% of our US-based simulation users. Since achieving use in all 50 schools in 2006, our number of users at these schools has continued to increase each year. Similarly, while our reach to the top chemistry and physics schools has necessarily reached a plateau, the number of our users continues to grow each year.

In 1970, the Carnegie Commission on Higher Education developed a classification system to serve as a framework for comparing institutions. There are three classifications within doctorate-granting institutions: Research Universities – very high research activities (RU/VH), Research Universities – high research activity (RU/H), and Doctoral/Research Universities (DRU). The nanoHUB usage for institutions classified as RU/VH, RU/H, DRU, as well as Minority Serving Institutions (MSI) are depicted in Figure 4. We have reached 100% of the RU/VH schools and 95% of the RU/H institutions. nanoHUB clearly has a strong reach into the top research institutions. While our total number of institutions briefly declined slightly in both the DRU and minority-serving areas, in the past year, usage has stayed relatively steady at DRU institutions and grown at minority-serving institutions. Changes in the number of institutions served can be the result of faculty who use nanoHUB moving from one institution to another or courses utilizing
We are still reaching more than 35 institutions in both classifications, and we have stayed relatively steady, reaching 25% of all MSI institutions that grant degrees in STEM fields.

1.4 Diversity of the nanoHUB user community

Four years ago, we began to report data on the diversity of the nanoHUB user base and tracked the usage at various minority-serving institutions. Most of the diversity data, such as gender, Hispanic origin, or African American origin, are from information volunteered at the time of user registration. Some nanoHUB users choose not to reveal this demographic information. Cumulative numbers indicate that 4.8% declined to report gender, 14.2% declined to report on Hispanic origin, and 15.3% declined to report on racial background. Adjusting for these reporting rates, our nanoHUB user diversity is 18% female, 79% Hispanic, and 3.3% African American. Our Hispanic user base is showing growth due to our increased educational involvement with typically Hispanic groups from UT El Paso and UT Pan American.
Through self-identification and through mapping to IP addresses, we can also try to extract the usage at minority-serving institutions. For the 449 Minority Institutions listed by the US Department of Education (Listing available at http://www.ed.gov/about/offices/list/ocr/edlite-minorityinst.html), including 90 Historically Black Colleges and Universities (HBCU), and 215 High Hispanic Enrollment institutions, we measure cumulative nanoHUB use at rates of 18%, 34%, and 23%, respectively. Last year, these rates were at 16%, 30%, and 22%, indicating a continued increase in our reach for these institutions.

2 Educational infrastructure

2.1 Tool-powered curricula

We have received feedback from some users that the sheer volume of the nanoHUB content is overwhelming. The participants of our first educational workshop in 2009 noted the same concern. They wanted to see a focal point for their course interest where they could find the appropriate content in one single page. Our concept of tool-powered curricula, as a one-stop-shop for tools related to a particular educational topic, was well received by the workshop participants.

Over the first several years of tool-powered curricula, we deployed five such integrated single tools that host multiple individual tools within a single environment (Figure 5). NCN@Berkeley (NCN nodes at partner institutions are referred to as NCN@University) demonstrated the integration of a set of tools into a single nanoHUB application to form a one-stop shop for a nano course taught at Berkeley; this tool is now known as MIT Atomic Scale Modeling Toolkit. Subsequently, we focused on existing classes that could be augmented immediately by online simulation if teachers and students had a single computational resource with all the necessary tools combined into a single tool. ABACUS, focused on the teaching and learning of semiconductor device fundamentals, serves such a user community [4]. Homework and project assignments are available in an associated, living document wiki page that undergoes continuous improvement. Our current set of tool-powered curricula includes the original five: ABACUS, AQME [5], UCB_COMPNANO, ANTSY, and ACUTE as well as: QC-Lab, CNDO, NSOPTICS, and NUITNS. Over 11,491 users have used the tool-powered curricula.

2.2 Presence on iTunes U

Prior to 2009, users could access an iTunes application to read RSS feeds on nanoHUB.org, resulting in about
1,500 users and 19,000 downloads. On March 31, 2009, we made a presentation about nanoHUB.org to John Couch, vice president for education, Apple, Inc., and won his support for access to iTunes U. Since that time, nanoHUB has continued to see traffic referred from iTunes U, and we continue to deploy our introductory and most highly rated content for download. As of May 31, 2012, nanoHUB tracks have been downloaded from iTunes U 40,795 times and nanoHUB’s iTunes U site has received nearly 900 unique users since its inception (Figure 6). One of the most popular nanoHUB downloads from iTunes is ECE 606 Solid State Devices course developed at Purdue University (Prof. Ashraf Alam), which consistently makes up over 10% of downloads from our iTunes U site.

2.3 Presence on Wikipedia

Wikipedia continues to grow its content and user base in the education and the research community. Wikipedia hosts nearly 4 million articles in English and is the sixth most visited website in the world, according to Alexa, which provides free web metrics. We have benefited from the huge user base exploring Wikipedia to drive web traffic to nanoHUB. We have found that we must make meaningful contributions to Wikipedia to help make it better if we are to use it as a vehicle to drive traffic to nanoHUB. Our first course of action was to find compelling images to add to existing content. Next, we realized that some Wikipedia pages drive significant daily traffic and began to focus on such pages. In fact, our top 10 Wikipedia articles referred over 35% of all Wikipedia-driven traffic to nanoHUB.org. The next part of the plan was to ask our NCN@University sites to place nanoHUB links and content into their areas of expertise. To date, over 89 Wikipedia articles link back to nanoHUB.org. Add to that 30 animated images from nanoHUB tools, and it is easy to see why, in the last year alone, we have been able to nearly double cumulative visitors to nanoHUB from Wikipedia from about 37,000 to over 61,000 as of May 2012 (Figure 7).
3 Ensuring quality and defined level of service

With over 260 tools, nanoHUB.org hosts more online simulation tools than any other science gateway, anywhere. That quantity supports the rapid development of the field, but quality tools are the foundation for significant scientific progress. Several years ago, we identified a limited list of supported tools that we believe produce the strongest results and for which we commit the following level of service: 1) monitoring support tickets, questions, and wish lists, providing a response within one business day; 2) fixing simple bugs within a week; and 3) moving long-term projects and tool improvement requests to a public wish list.

Every one of the large NCN@University programs maintains their own list of supported tools. Each nanoHUB tool is displayed on the site along with the numbers of its users, community-contributed reviews and questions, classroom usage, and citations in the literature. As a distinction, supported tools receive a gold badge followed by “NCN Supported.” The set of 45 NCN-supported tools have served 67% of the nanoHUB simulation users; 61% of the nanoHUB simulation users use community-supported tools (Figure 8). We also rank the expertise level needed to operate every tool. We have defined a five-level system: 0) K-12; 1) Freshmen/Sophomore; 2) Juniors/Seniors; 3) Master’s students; 4) PhD/experts. Users can browse nanoHUB tools by pre-selecting their experience level and focus on the most suitable tools for themselves.

3.1 nanoHUB taxonomy for courses and nanoelectronics courses

nanoHUB currently hosts over 3000 content items, which makes item-by-item browsing almost impossible. In response to user feedback, we created a taxonomy of nanoHUB content that guides both our strategic decision-making and users’ browsing. We developed such browsable taxonomies for two different, yet highly valuable, content categories. We identified 43 different full courses, short courses, and tool-powered curricula as primary targets for the taxonomies.

The courses are categorized by audience level ranging from freshmen to PhD on one axis and topical categories such as electronics, materials, photonics, and chemistry on the other (Figure 9A). Some of the courses cover multiple audience levels as indicated by their horizontal extent. The size of the circle for the resource corresponds to the number of online lectures comprising the course. The colors of the symbols reinforce the color coding of the
Figure 7  nanoHUB benefits significantly from a large and strong presence on Wikipedia. A significant amount of nanoHUB traffic is driven from users arriving on nanoHUB content in Wikipedia.

Figure 8  Over 61% of nanoHUB tool users utilize community-supported tools. However, the 45 NCN-supported tools have served over 67% of all nanoHUB simulation tool users.
target audience we use with the tools. The users on the website can hover the mouse over a course icon and read a brief description of the course, and they can click on the icon to jump to the course resource.

The nanoelectronics simulation tools need to be described with additional characteristics. We put in place a solution that maps the tools into different device types, such as MOSFETs, nanowires, quantum dots, and different theoretical treatments such as drift diffusion, Monte Carlo, and quantum transport (Figure 9B). The required expertise level to operate the tool is indicated by the color scheme of the expertise ranking that we use, in general, for all the tools. By hovering over the tool with the mouse, the users can read a brief synopsis of the tool and also jump to the tool directly.

3.2 External university networks relying on nanoHUB – viral use

Historically, we have tracked the classroom usage of nanoHUB.org through the registration information and follow-up inquiries. As our user base and usage continues...
to grow, tracking classroom usage becomes tedious and more difficult to perform manually. To make the process scalable, we began work on an algorithm-based analysis of user activity that automatically detects emergent, voluntary classroom use as well as research use of nanoHUB.org, using raw usage data to identify organized subsets of coordinated behavior that can be identified as distinct types of use. Through this analysis, we were able to identify 14,521 students in 761 courses at 189 institutions over the course of nanoHUB’s existence. Our user flow analysis methodology shows great promise for automatically identifying and documenting classroom and other types of use and utilizing these data to better understand details about classroom use of nanoHUB, such as class size, tools used, resource consumption, usage intensity, and usage patterns. Classroom use varies slightly from semester to semester and year to year. Step-like patterns are evident in the behavior of users identified as coordinated classroom users, reasonably corresponding to typical activity throughout the semester (Figure 10). A dissimilar behavior is seen in users identified as researchers or self-study users, who generally show a slow decay in activity over time.

4 Research impact in brief

Four years ago, we began charting citation network maps to address the question of whether nanoHUB can indeed be used for research. The documented citations and their extent into the non-NCN-affiliated nano community exceed those of any other science gateway we are aware of [6]. Next the question arose: “Is it good research?” Over the past several years, we have begun to address that question by asking: “Are the papers that cite nanoHUB subsequently cited by other authors?” We have refined our approach to both collecting citations and to mining the Google Scholar service to obtain the secondary citations to the nanoHUB citations, such that we are regularly updating both. Collecting the secondary citation counts allow us to calculate nanoHUB’s h-index as a measure of impact. Let us imagine nanoHUB as the author of the 940 papers citing nanoHUB. We have found over 5400

![Figure 10](image-url) Step-like patterns are evident in the behavior of users identified as coordinated classroom users, reasonably corresponding to typical activity throughout the semester.

![Figure 11](image-url) nanoHUB’s h-index is computed as 41 (based on Google Scholar) showing tremendous research impact.
citations to these 940 primary papers such that the h-index is 41 (Figure 11). That means 41 of the primary papers have at least 41 citations. In comparison, a researcher might expect to have an h-index, on average, equal to the number of years spent working in their field after receiving their PhD. nanoHUB’s h-index is more closely related to the US National Academy of Engineering Members with PhD’s granted in 1980 and 1983 (represented by AM1 and AM2, respectively, in Figure 11) than to that of the PhD graduates (2001 Grad and 2000 Grad in Figure 11) close to the year nanoHUB was formed.

5 Conclusion

By bringing tools and content to one common place for the nanotechnology community, nanoHUB is facilitating migration of tool use from the originating nanotechnology subdomain community to the broader scientific community. This collaborative effort enables work that would not have occurred otherwise or perhaps even been possible. nanoHUB continues to broaden its reach through continued growth of resources and by impacting new communities.

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References


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