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nanoHUB.org: A Gateway to Undergraduate Simulation-Based Research in Materials Science and Related Fields

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ABSTRACT

Our future engineers and scientists will likely be required to use advanced simulations to solve many of tomorrow's challenges in nanotechnology. To prepare students to meet this need, the Network for Computational Nanotechnology (NCN) provides simulation-focused research experiences for undergraduates at an early point in their educational path, to increase the likelihood that they will ultimately complete a doctoral program. The NCN summer research program currently serves over 20 undergraduate students per year who are recruited nationwide, and selected by NCN and the faculty for aptitude in their chosen field within STEM, as well as complementary skills such as coding and written communication. Under the guidance of graduate student and faculty mentors, undergraduates modify or build nanoHUB simulation tools for exploring interdisciplinary problems in materials science and engineering, and related fields. While the summer projects exist within an overarching research context, the specific tasks that NCN undergraduate students engage in range from modifying existing tools to building new tools for nanoHUB and using them to conduct original research. Simulation tool development takes place within nanoHUB, using nanoHUB's workspace, computational clusters, and additional training and educational resources. One objective of the program is for the students to publish their simulation tools on nanoHUB. These tools can be accessed and executed freely from around the world using a standard web-browser, and students can remain engaged with their work beyond the summer and into their careers. In this work, we will describe the NCN model for undergraduate summer research. We believe that our model is one that can be adopted by other universities, and will discuss the potential for others to engage undergraduate students in simulation-based research using free nanoHUB resources.

INTRODUCTION

Experimentally relevant computation and simulation is playing an ever-increasing role in interdisciplinary STEM research; thus, future engineers and scientists will likely be required to use advanced simulations to solve many of tomorrow's challenges. For example, computational simulations are expected to play a critical role in the Materials Genome Initiative [1], and computational nanotechnology is an important area with significant funding from a broad consortium of research-oriented organizations including federal agencies, companies, and non-profits [2].

Despite the importance of computation and simulation in research, faculty in this area face a dearth of well-trained, diverse graduate student applicants [3]. As the *Chronicle of Higher Education* recently noted, " 'Fewer qualified applicants are choosing to enroll in critical fields like engineering, math and computer science,' Ms. Stewart said. 'We have to try to understand why that's happening and what we can do to reverse it.'" [3]. To prepare more students to meet this need, the Network for Computational Nanotechnology (NCN) provides simulation-focused research experiences for undergraduates at an early point in their educational path. NCN is an NSF-funded project that developed and operates nanoHUB.org, an open-access science gateway for cloud-based simulation tools and resources for research and education in nanoscale science and technology [4]. In this paper we describe the summer research experience at NCN, summarized by a program logic model, and focus on the unique aspects of the program that relate to nanoHUB. Then we consider the student experiences, followed by some data quantifying their views on research and graduate schools. We conclude by summarizing recent changes, and presenting future opportunities for improvement of this program, as well as opportunities for extension and collaboration using this model with other research sites.

DESCRIPTION OF THE SUMMER RESEARCH EXPERIENCE

The NCN summer research program is now in its 10th year, and has had the advantage of association with the College of Engineering's Summer Undergraduate Research Fellowship (SURF) program at Purdue University since 2008. SURF serves about 150 undergraduate students per year, oversees the administrative process and provides student training and enrichment activities including an end-of-summer SURF symposium and preparation to enable students to publish their work as a Purdue research publication in Purdue ePubs, the *Journal of Purdue Undergraduate Research*, or a discipline-appropriate research journal.

NCN-SURF currently serves around 20 undergraduate students per year who are recruited from the SURF applicants and selected by NCN staff and faculty for aptitude in their chosen field within STEM, as well as for complementary skills such as coding and written communication. Under the guidance of graduate student mentors and faculty advisers, the undergraduate students modify or build nanoHUB simulation tools for exploring interdisciplinary problems in materials science and engineering, and other related fields.

The simulation tool development takes place within nanoHUB, using nanoHUB's workspace (web-delivered full-fledged Linux workstations), extensive computational clusters, and additional training and educational resources. One objective of the NCN-SURF program is for students to publish their simulation tools on nanoHUB. The published tools can be accessed and executed freely from around the world using a standard web-browser; thus students can remain engaged with their work beyond the summer and into their careers.

<u>NCN Summer Undergraduate Research Program Logic Model</u>

The NCN summer undergraduate research program has evolved over time, and to better visualize its objectives, the approaches taken to meet these objectives, and best methods for assessment, we created a program logic model [5-7], shown in Figure 1. Reading the columns from left to right, this model first shows the resources available to us in creating the summer program, then the activities planned to meet our objectives, the outputs expected at the end of the summer as a result of these activities, and finally the short term and long term outcomes we hope to achieve for the students and their mentors.

Some elements of the NCN-SURF program logic model will be common to many research experiences for undergraduates (REUs); this paper will focus on those elements that may not be as common across all REUs, which are highlighted in Figure 1: the nanoHUB infrastructure, the Rappture training bootcamp, and the nanoHUB tool publication process.

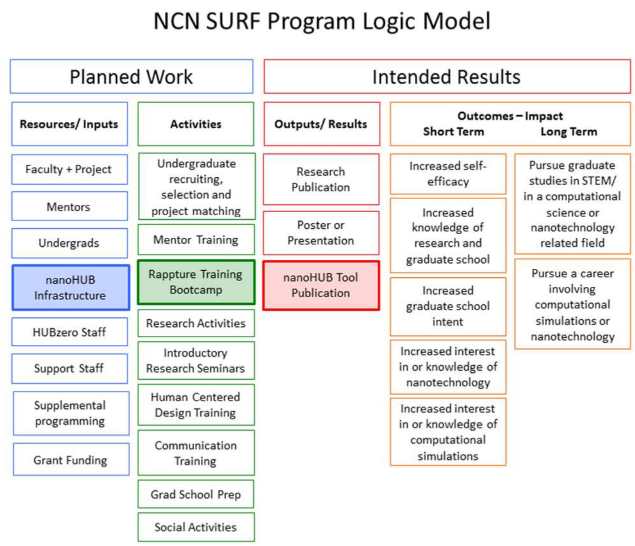

Figure 1. NCN-SURF Program Logic Model. Particularly unique aspects relating to computational nanotechnology are highlighted: the nanoHUB infrastructure, the Rappture training bootcamp, and the tool publication process.

A key component enabling our research program is the nanoHUB cyberinfrastructure. nanoHUB was established to provide a platform to disseminate research code to a global audience [4]. nanoHUB now serves over 300,000 annual users with both simulation tools and a wide variety of supporting material in a virtual environment with low entry thresholds [8]. nanoHUB is built on the HUBzero® open-source software platform and is a production-level infrastructure running on multiple dedicated web servers and utilizing several local execution hosts as well as high-performance computing (HPC) resources transparent to the user [9].

The nanoHUB infrastructure includes a virtual Linux desktop called *Workspace*, which is accessed through an Internet browser. Students can use *Workspace* as a program development environment for new simulation tools, where they can program, compile and run code, use Subversion (SVN) for version control, and access NCN's Rappture toolkit. The Rappture toolkit makes it easier to prepare simulation code to run on nanoHUB by generating user-friendly graphical user interfaces (GUIs) for code written in a wide range of languages, including C/C++, Fortran, Octave, Java, Python and Tcl [9]. In other words, Rappture creates a GUI that can wrap around traditional simulation code and input/output processes, allowing more intuitive user interaction with the simulation and lowering the barriers to learning to use simulations.

At the beginning of the summer, NCN-SURF students participate in an intensive 3-day Rappture bootcamp training session where they learn how to use Rappture to create interactive GUIs. Additional Rappture help sessions are provided later in the summer. The Rappture bootcamp is taught by members of the HUBzero team, a group of over 20 IT professionals who support a variety of HUBs, including nanoHUB, that are based on the HUBzero platform.

In order to facilitate student access to the Rappture training material, a course on creating nanoHUB tools, based on the Rappture bootcamp, was created and deployed on nanoHUB and is openly available [10]. This course contains Rappture coding problems and solutions. Additionally, the accompanying lectures were video-recorded, and are available to view on nanoHUB [11].

Following Rappture training, each student works on a research project with a graduate student mentor and faculty advisor. The specific tasks that students engage in range from using Rappture to add user friendly GUIs to existing simulation tools, to verifying tools and building new tools for nanoHUB and using them to conduct original research. One objective of the NCN-SURF program is for the students to publish their simulation tools on nanoHUB, in addition to presenting their research at the SURF symposium. Publishing these tools can immediately benefit research among nanoHUB users worldwide, and can also rapidly impact education [12]. In our program, the faculty-mentor-student teams work together to define a problem that will fit in the short summer time frame. Several examples are provided in the next section.

Examples of Student Research

NCN SURF students have worked on projects that are often multidisciplinary in nature, and that include a wide range of fields including physics, materials science, electrical engineering, and mechanical engineering. In addition to the underlying science, they often learn the approximations and applications of simulation, especially when working directly on nanoHUB tools. A list of simulation tools published by NCN SURF students can be found on the NCN SURF webpage [13]. There have been over 35 simulation tools built by the students in the last 5 years, but here we highlight just a few.

For example, a student with a background on electrical engineering developed usage examples for a Bayesian calibration tool in his undergraduate studies. The tool uses the Bayes theorem to obtain the most likely distribution of unknown model parameters from experimental data and prior knowledge [14]. One of these examples, currently deployed in the tool, involves obtaining minority carrier lifetimes from Haynes-Shockley experiments.

Another NCN SURF student developed a simulation tool called S4sim that simulates the interaction of light with layered materials [15]. The tool was based on command-line code written by Victor Liu and Shanhui Fan at Stanford University [16]; the NCN summer student created a GUI that makes it easier for users to select materials and specify the layer geometry. After creating the GUI, the undergraduate researcher validated the solver by running simulations and comparing to previously published research. This simulation tool has now been run over 10,000 times by users from all over the world, and was used in research on selective absorption and emission of metasurfaces presented in Symposium L (metamaterials) of the Fall 2014 MRS Symposium, and published in *Optics Express* [17].

A third student's project this past summer was to build a numerical tool for modeling thin-film solar cells: a timely topic, given the new efficiency records recently set in these systems [18]. There is a pressing need to combine detailed models of both wave optics and electronic transport in a self-consistent way to accurately predict the behavior of high-performance thin-film cells. The SURF student wrote the S-matrix optical code, integrated it with an existing tool on nanoHUB.org called ADEPT 2.0 that provided a detailed electronic model, updated the GUI on nanoHUB, and validated the tool against existing code, showing that the new combined approach is more accurate for thin-film solar cells [19].

A fourth student's project this past summer was to build a numerical tool for modeling the performance of rare earth-based thermal emitters for thermophotonic (TPX) applications. TPX has the potential to efficiently convert heat to electricity by using metamaterial and/or photonic crystal layers to enhance the naturally favorable emission properties of rare earths. This thermal emission is then captured by a photovoltaic diode in a process known as thermophotonics [20]. The student was able to create a detailed graphical user interface which spoke to virtually every nuance of the multilayer structures that could be used for thermophotonics, and also devised multiple graphical output formats to aid in comprehension of the variables controlling performance. The tool allowed her to find improved designs both for erbium aluminum garnet and samarium-doped glass, with heat-to-electricity efficiencies of up to 38.5% [21].

Finally, another pair of students worked on *ab initio* electronic structure calculations of small molecules and crystals and created a nanoHUB tool designed for the community to share, analyze and explore such calculations.

ASSESSMENT

An underlying goal in investing in NCN-SURF is to provide students with computational modeling experience related to nanotechnology in a way that contributes to their pursuit of careers in these areas. Social Cognitive Career Theory [22] is a model developed by psychologists to explain the personal, contextual, and experiential factors that contribute to career-choice. One of the personal factors that contributes to career choice is domain-specific self-efficacy, or students' personal belief in their capability to perform tasks in the research area. Self-efficacy is developed through successful performance, affirmation from others, observing others who are successful, and experiencing positive emotions [23]. Specifically, NCN-SURF provides a learning experience that can increase students' self-efficacy in computational modeling and nanotechnology. Throughout the research and tool-development process, students receive peer and mentor support including feedback and positive enforcement to work through challenges to successful completion. Additionally, they see that peers and more experienced researchers also struggle with their designs prior to being successful.

Assessment of students' short-term outcomes was performed through open coding analysis of group interviews and written surveys given to the undergraduate students. 18 undergraduate students responded to the survey. Key results are reported in Figure 2, which shows that the program had a positive impact on the knowledge of, and interest in, computational science, nanotechnology and graduate school for a majority of the NCN SURF students.

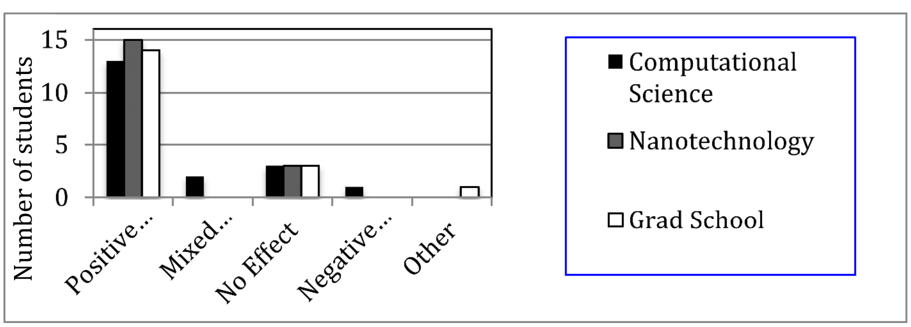

Figure 2. NCN-SURF survey results showing the effect of the program on students' knowledge or interest in computational science (black), nanotechnology (striped) and plans to attend graduate school (white).

DISCUSSION

The survey results and discussions with the NCN-SURF students show that they had an overall positive experience in this program. Most students reported positive gains in knowledge or interest in computational science or nanotechnology, and increased interest in or determination to go to graduate school as a result of the program (Figure 2). A couple of students reported already having high interest in nanotechnology or in simulations, and that the program did not affect their level of interest.

Comparing this year's program with last year's program, two related changes were made in the recruiting process that seem to have had positive results: first, it was made clear to students up-front that they will be coding a lot; and recruitment focused more on students with previous coding experience.

Some changes planned for the next implementation include developing more team projects, earlier matching of students with research projects by specific areas of interest, increased recruiting outside of Purdue (particularly of underrepresented groups) to improve diversity, and clearer communication of the program goals to NCN-SURF students, mentors and faculty advisers—development of their understanding of the basic physics, the role of simulation in research, simulation methods, and ultimately, creating a GUI and publishing a tool.

Our current assessment does not probe their learning gains, but we believe that the process of creating user interfaces, tutorials or examples for a simulation tool forces students to understand details of the model in a way that running pre-existing control files may not touch on as deeply. The process requires students to think about how the model works, how parameters feed into the results of the model, and which parameters will be of greatest interest to practitioners in the field.

Through training exercises and discussions, students are reminded to think of the needs of future users of their simulation tools. They are also aware that publication of their tool will make it accessible to users world-wide. These aspects of the project give it real-world validity and students know that their work will have measureable future impact in terms of numbers of users and simulation runs. Seeing the impact of their work should increase the students' self-efficacy.

One perspective on our REU model is that students are working on a GUI development project that has a fairly well-defined scope and should have a high success rate, with over 35 simulation tools published on nanoHUB in the last five years [13]. The students' work is also closely associated with a research project, which by contrast may have more depth and uncertainty in outcomes. In this way, students should have a high success rate for their piece of the project, giving them positive reinforcement of their efforts, while also being exposed to and participating in the research process.

CONCLUSIONS

Through NCN's summer research program, students gain valuable research experience, mentoring, and peer support that contribute to both their educational and career development. We believe that our model for introducing students to research involving computational simulations is one that can be adopted by other universities, using the free nanoHUB cyberinfrastructure and associated resources. Instructions for creating simulation tools for publication on nanoHUB can be found in our simulations and computational science group [24].

The nanoHUB infrastructure is available to other programs that would like to use it to introduce undergraduate students to research involving computational science.

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