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An Exploratory Study of Engineering and Science Students' Perceptions of nanoHUB.org Simulations*

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This study examined how science and engineering students with different academic level perceived and experienced computational simulation tools for nanotechnology in terms of learning outcomes, evidence of learning, pedagogical approaches, and ease of use. The simulation tools used in this study are part of the research and learning resources in nanoHUB.org. Data were collected by anonymous and optional online survey questionnaire given to 312 science and engineering students with access to nanoHUB.org. The quantitative and qualitative analyses showed that overall, graduate and undergraduate students reported positive experiences of nanoHUB.org simulation tools and their uses. However, differences were observed in the way undergraduate students reacted to the computational simulations as compared with graduate students. Possible explanations for these differences and suggestions to close this differential gap were also discussed. Potential explanations for these differences are that undergraduate students may have not fully developed graphical literacy skills, may lack the prior knowledge required at the time they interact with the tools, or tools may be too complex. Suggestions to overcome some of these difficulties include the development of well integrated curricular materials, the application of frameworks for technology-enhanced support for inquiry learning, and the use of just-in-time instructional supports together with the simulation tools.

Keywords: computational simulations; nanoHUB.org; engineering education; cyber-enabled learning

1. Introduction

Computational science has been described as the third leg of the 21st century's methodologies of science, complementing the traditional areas of theory and physical experimentation [1]. Because computational simulations can provide science and engineering students with tools that enable them to do things they could not do in the real world [2], they have also become a critical element of learning experiences [3]. The purpose of this study was to investigate how undergraduate and graduate students in science and engineering perceived their experiences with computational simulations as learning tools.

Benefits of computer simulations on student learning have been widely recognized. For example, educational benefits provided by simulations include: (a) an opportunity to study abstract and complex physical phenomena that involve many variables [4]; (b) the ability to see and, in some ways, manipulate phenomena that is not possible with other tools [5]; (c) an environment that approximates, simplifies, or hypothetically creates reality [6]; (d) the ability to change the time-scale of real processes [6]; (e) a cost savings that results from using the simulation instead of lab equipment [7]; and (f) a safe environment in which to experiment [7]. Other educational benefits inherent to any computer-based tool include: (a) increased opportunities for frequent practice [5]; (b) immediate feedback [5]; (c) the ability to serve the need of individualization [8] and learner-centeredness [9]; and, perhaps, (d) the ability to deliver highly motivational instruction [8]. Simulation tools that are web-based can also provide students with access to the tool at a time and place they find convenient.

Although progress has been made on research that examines students' learning with computer simulations, less progress has been made toward understanding how students perceive the usefulness of computational simulation tools for their current and future learning. Computational simulations, as different from computer simulations, have been developed as research tools for use by experts that are subsequently incorporated into undergraduate and/or graduate courses in science and engineering [10–12]. Computer simulations, on the other hand, have been used for educational purposes in both formal and informal learning environments. These

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simulations have been described as 'working representation[s] of reality; used in training to represent devices and processes and may be low or high in terms of physical or functional fidelity' [13, p. 318]. Within educational contexts, Alessi [14] suggested that a computer simulation is 'any program which incorporates an interactive model (one which can be repeatedly changed and rerun) and where the learning objective is for students to understand that model, whether through discovery, experimentation, demonstration, or other methods' (p. 177). Computational simulation tools used by the participants of this study, however, were originally developed for use by subject-matter experts as research tools, and then implemented in a classroom setting. Unlike computer simulations originally developed for instruction, the tools used in this study are based on mathematical models that require extensive calculations executed on supercomputers or distributed computer platforms. These tools were developed by expert researchers to use to analyze and solve scientific and engineering problems. These tools might therefore be referred to as computational simulations, which have been defined as working representations of reality that are used to represent physical phenomena, devices, and/or processes based on mathematical models and numerical solution techniques executed on supercomputers or distributed-computing platforms [3]. This study was motivated by the significant increase in recent years in the use of computational simulation tools by both researchers and students to increase their understanding of nanotechnology.

A cyberinfrastructure that provides freely-available online computational simulation tools for nanotechnology education is called nanoHUB.org The Network for Computational Nanotechnology (NCN) developed this cyberinfrastructure designed to support nanoscience and nanotechnology research through online computational simulation tools and training that have served to over 200,000 users annually [15]. The mission of the NCN is to design, construct, deploy, and operate national cyber-resources for nanotechnology theory, modeling, and simulation that are closely linked to experimental research and education [15]. The NCN mission is embodied in nanoHUB.org, a web portal that hosts approximately 240 computational simulation tools. The nanoHUB.org initially focused on the development of nanotechnology from basic science to manufacturing through theory, exploratory simulation, and cyber-infrastructure. Recently, the portal has also become an educational source for facilitating the teaching and learning of nanotechnology-related concepts and theory by incorporating 3279 user-contributed resources such as course materials, lectures, podcast, learning materials, seminars, tutorials and user groups. nanoHUB interactive computational simulation tools are accessible from web browsers and run via a middleware-enabled distributed computing network. nanoHUB resources have been provided by approximately 940 member contributors in the science and engineering community and its content has been used by 14,000 students in over 760 formal classes in over 100 institutions [15]. There is no need to download, install, support, or maintain sophisticated software or additional procedures to access specific machines. The end user, therefore, has access not only to the user interface and the computational resources necessary to run it but also to the scientific and engineering community responsible for its maintenance. An example of a computational simulation tool interface is shown in Fig. 1.

The library of computational resources and learning materials on nanoHUB.org continues to grow as well as its usage for research and education. Strachan and colleagues [16] provide a recent and detailed description of usage metrics of computational simulation tools on the nanoHUB.org for research and education. This significant increase in use of cyber-enabled resources for education raises, among others, questions such as: (a) how users perceive the use of computational simulation tools for education (b) how these tools are being used for educational purposes and (c) how effective these tools can be in supporting student learning in nanotechnology related concepts. Our research agenda attempts to provide understanding to these three questions. For instance, preliminary studies on *how* computational simulation tools have been

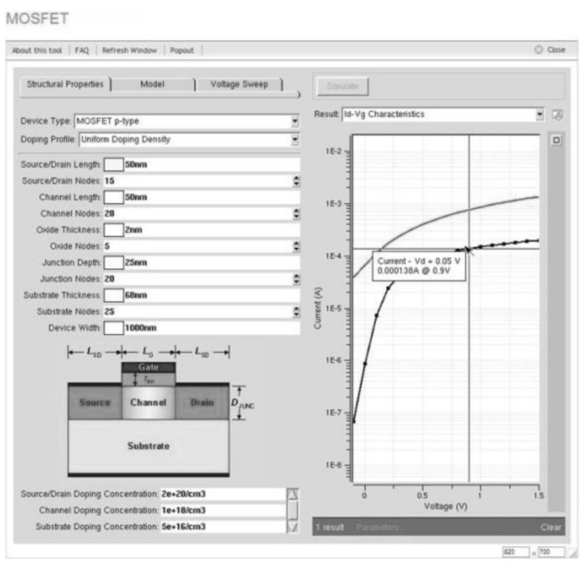

Fig. 1. MOSFET simulation tool interface.

used by instructors have been reported in [3] and in another article on student views and challenges of their instructors uses of computational simulations in nanotechnology in this special issue [17]. We have also identified the effectiveness of computational simulation tools for conceptual understanding of plastic deformation of materials at the atomic level [18]. This exploratory study focuses on a higher level aiming to identify student *perceptions* of the use of these tools in their learning. The research questions of this study are:

- How do students perceive and experience the ease of use and usefulness of nanoHUB.org simulation tools for their learning?
- Are there any differences on students' perceptions and ease of use of computational simulation tools for learning according to their academic level (i.e. graduate and undergraduate levels)?

2. Theoretical framework

The theoretical framework that provided a rationale of this study and guided its design is based elements of the technology acceptance model [19], adoption and diffusion of innovation model [20], and affordances [21]. Understanding students' ease of use and perceptions of these tools is an important research endeavor that can suggest technology acceptance [22, 23]. The perceived attributes of an innovation, in this case computational simulation tools, are one important explanation of the rate of adoption of an innovation [20]. That is, the individuals' perceptions of the attributes of an innovation affect its rate of adoption. As discussed by Rogers [20], in the persuasion stage of the innovation-decision process, individuals form a favorable or unfavorable attitude toward the innovation. Rogers defined attitude as a relatively enduring organization of an individual's beliefs about an object that predisposes his or her actions [20]. It is at the persuasion stage that a general perception of the innovation is developed and consequently may lead to adoption or rejection of the innovation. Therefore, it is important of identify what are students perceptions of computational simulation tools as well as their expectations of what it is possible to accomplish with a specific technology; that is their affordances. The definition of 'affordance' adopted for this study builds on Gibson [21] description of 'affordance' as the perceived and actual properties of a thing; in particular it refers to functional properties that define how such things could potentially be used. One can argue that identifying potential computational simulation tools' affordances for learning as conceived and experienced by learners is a necessary initial step in order to incorporate them successfully in their life-long learning process.

3. Conceptual framework

The conceptual framework for this study provides an organizational framework for the findings of the study. The conceptual framework used to make sense of our findings is an educational tool known as understanding by design [24, 25]. Understanding by design is a way of thinking about curricular design and implementation that emphasizes a set of tools and practices that consist of three stages: (a) identifying the desired learning outcomes (the content of the lesson), (b) determining the acceptable evidence of learning (the method of assessing learning), and (c) planning the experiences and instructional approach (or pedagogy). We used understanding by design as a framework for the design of the study because it encompasses all elements that should be involved in any instructional intervention.

The goal of this study was to identify science and engineering students' perceptions of nanoHUB.org simulation tools developed in terms of (a) students' opinions of the relevance of using the simulation tools as related to their learning experience and the learning outcomes that can be accomplished with the simulation tools, (b) their observations of their perceived gained knowledge accomplished by using this tools and (c) their views of how these tools actually guided and helped them during their learning process. By identifying their perceptions of the computational simulation tools in terms of the understanding by design framework we may infer their potential adoption or rejection of these tools and identify ways to better support these learners in their future learning endeavors. Understanding by design therefore provided a framework upon which to build the design of the study, the methods of analysis, and the reporting of results. In specific, this study built upon the unique characteristics of the nanoHUB.org simulation tools and the advantages simulation tools may provide to explore how science and engineering students with different academic level perceive and experience nanoHUB.org simulation tools in terms of learning outcomes, evidence of learning and pedagogical approach.

4. Method

4.1 Participants

The participants in this study included 314 students in 20 different courses from a total of nine different universities who used learning activities available through the nanoHUB.org portal. The sample

Table 1. Summary of participants by discipline and academic level

	Academic level		
Discipline	**Undergraduate**	**Graduate**	**Total**
Electrical engineering	49	158	207
Materials engineering	54	27	81
Physics	0	14	14
Mechanical Engineering	0	10	10
Total	**103**	**209**	**312**

population included students with majors in materials, mechanical, electrical and computer engineering, and physics. Table 1 depicts number of participants by discipline and academic level. Women represented slightly less than one-quarter (23%) of the sample population.

4.2 Data collection

The data were collected for this study through an online survey instrument. As noted previously, Wiggins and McTighe's [24, 25] approach to understanding by design was used to develop the survey questions. Each of the three stages of backward design—learning outcomes, evidence of learning, and pedagogical approach—was used as guidance to identify students' perceptions of constructs we wanted to measure. A fourth construct—ease of use—was included in the design process to identify if students perceived the interface was limiting their learning experiences. At least two questions were created to measure students' perceptions or ease of use for each of the four constructs, as shown in Table 2. The survey instrument also included three-open ended questions that gave students an opportunity to provide their comments.

The development of the survey went through an iterative process of refinement where questions were added, deleted, or refined as we considered necessary. For example, in the pilot study, we changed the question 'Do you have a nanoHUB account? (Yes, No)' to 'Have you used nanoHUB simulation tools in the past? (Yes, No)' since data were collected at the end of the academic term and by then it was obvious that students were required to create an account to complete the course assignments. Also, in this process of refinement the scale of the survey

Table 2. Survey questions categorized by construct

Construct	#	Question ID	Survey question
Learning outcomes—to identify students' opinions of the relevance of using the simulation tools as related to their learning experience and the learning outcomes that can be accomplished with the simulation tools.			
Learning outcomes	1	Positive experience	Using nanoHUB.org is a very positive experience.
	2	Tools relevant to interests	nanoHUB.org simulation tools are highly relevant to my areas of interest.
	3	Supported my course goals	nanoHUB.org simulations supported my goals and expectations for the course.
Evidence of the learning—to identify students' observations of their perceived gained knowledge accomplished by using computational. simulation tools			
Evidence of the learning	4	Comprehend better	I can comprehend concepts better by using the nanoHUB.org simulations compared to lectures and readings only.
	5	Able interpret output	I do not have trouble interpreting the output of the nanoHUB.org simulation(s).
Pedagogical approach—to identify students' views of how computational simulation tools guided and helped them during their learning process.			
Pedagogical approach	6	Able to approach problems	I feel confident in my ability to use concepts embedded in these tools to approach new problems.
	7	Guide thinking	When I use nanoHUB.org simulation tools I generate questions that guide my thinking.
	8	Engaging compared to	Using the nanoHUB.org made this course a lot more engaging for me compared to courses that only use lectures, homework and readings.
Ease of Use—to identify how students' perceived the easiness or intuitiveness of using computational simulation tools.			
Ease of use	9	Easy to use	nanoHUB.org is easy to use.
	10	Intuitive to use	nanoHUB.org simulation tools are very intuitive to use.

changed. Specifically, in our pilot study, survey, students responded to each question (where appropriate) on a scale from one to five corresponding to the categories of strongly agree, agree, undecided, disagree, and strongly disagree. In the next iteration we decided to change the scale from five options to four because we noticed many students responded 'undecided' to many of the questions; therefore we changed the scale to four possible options because wanted the students to be more decisive in their responses. As a result, for the surveys collected afterwards, students responded to the same questions on a scale from one to four corresponding to strongly agree, agree, disagree, and strongly disagree. For the questions in which students responded 'undecided', the response was considered as missing data so our statistical analyses would be more consistent changing the scale from five to four responses. Also, as already mentioned, through the multiple iterations of the survey instrument, new questions were added and others deleted. However, the data reported as part of this study consists of survey questions that were consistently asked in all iterations.

4.3 Validity and reliability of the survey instrument

The survey instrument was validated by two researchers who independently categorized each question according to the four constructs being studied using the following criteria.

- Learning outcomes (content): To what extent did the simulation tools support the goals of the course and how relevant were they to the students' areas of interest?
- Evidence of the learning (assessment): To what extent did students report having learned with (and from) the simulation tools? E.g., did the simulations tools lead to improvements in their understanding of concepts from the course, their ability to interpret the output, and/or their ability to transfer their knowledge to new situations?
- Pedagogical approach (pedagogy): To what extent did students find the simulation tools helped them learn? E.g., did the simulation tools help guide their thinking or increase their tendency to be engaged with the tasks with which they were confronted?
- Ease of use aspects: How easy and intuitive did the students feel the tools were to use?

The percentage of agreement for the classification of the survey questions was 90%. However, after discussing the discrepancies both of the researchers came to an agreement. Reliability testing within constructs was conducted using Cronbach's alpha (a) coefficient [26]. The number of items and the Cronbach's a coefficient for each of the four categories in the survey, as depicted in Table 2, can be summarized as follows: learning outcomes (a = 0.82), evidence of learning (a = 0.37), pedagogical approach (a = 0.69), ease of use (a = 0.81).

4.4 Implementation of nanoHUB.org in the classroom

All instructors known to have incorporated nanoHUB simulation tools in the classroom were contacted and 19 of a total population of 20 responded to email, phone calls, or personal conversations. The most common instructional approach instructors described following was to first introduce (in class) the governing physical principles defining the behavior of a device, material, or phenomenon together with a demonstration of how to use the simulation tool. They then asked their students to apply these principles with homework assignments, projects, or lab sessions that used the simulation tools. Most of the instructors who taught undergraduate courses were limited their use of the nanoHUB simulations to one or two occasions during the academic term, whereas instructors who taught graduate courses were more likely to use the tools more frequently, and more intensively, throughout the term. Seven of the 11 undergraduate courses but four of the graduate courses, for example, used the simulation tools either once or twice during the academic term, whereas three of the graduate courses used between three and seven simulations and five graduate courses used eight simulations tools during a single academic term. In total, 29 different simulation tools were used within the 20 surveyed courses as depicted in Table 3.

As shown on Table 2, graduate students utilized more simulation tools than undergraduate students did. Looking closer at all simulation tools utilized, they all had the following commonalities: (a) had a graphical user interface where input parameters were introduced through typing or selecting values and (b) had as an output either a graph or a visualization.

4.5 Procedures

The data upon which this study is based were collected from surveys administered at the end of the academic term during the Fall 2006, 2007, 2008 and 2009 and Spring 2008, 2009 and 2010 semesters. The survey was anonymous and voluntary; students were free to respond any of the questions and they could stop responding to the survey at any time.

4.6 Quantitative data analysis

Multiple levels of analysis were conducted for this study. The first level of analysis involved the use of descriptive statistics to identify students' perceptions of the simulation tools. The sample population

Table 3. nanoHUB simulation tools used as part of undergraduate (US) and graduate (GS) courses

Tool	http://nanohub.org/resources/	US	GS
Process Lab: Concentration-Dependent Diffusion	1881		1
Process Lab: Defect-coupled Diffusion	1882		1
Process Lab: Oxidation	1879		1
Process Lab: Oxidation Flux	1880		1
FiPy	vkmlpsgg		1
OOF	3363		1
Nano-Materials simulation toolkit	1692	1	2
Micromechanics	3067		3
SCHRED	221		6
SPICE	227	1	1
PN Junction Lab	pntoy	1	4
MOSCAP	451		3
MOSFET	452		5
QuaMC 2D	1092		4
nanoFET	1090		2
nanoMOS	1305		2
CNTFET	1091		3
CNTbands	1838		3
nanoWIRE	2949		2
Quantum Dot Lab	qdot		2
Carrier Statistics Lab	3798	2	
Crystal Viewer	crystal_viewer	1	2
Bandstructure Lab	bandstrlab		4
Periodic Potential Lab	3847		2
PCPBT	pcpbt		1
MESFET	5126		1
BJT	3984		1
FETToy	220		2
Computational Nanoscience toolkit	ucb_compnano/about		1

was divided into different levels, e.g., graduate students (GS) and undergraduate students (US), and the average scores and standard deviations for these levels were calculated. The survey data were coded on a scale from one to four as follows: strongly disagree (1), disagree (2), agree (3) and strongly agree (4).

The second level of analyses focused on identifying patterns in the way graduate students and undergraduates perceived nanoHUB simulation tools as a way to predict how students would respond to each of the items on the survey. This involved the creation of a proportional odds model for the individual survey questions using the student level as the explanatory variable and the answer to the question as the response, while controlling for the number of simulation tools used and the times the instructors reporting used the simulation tools during the academic term. The students' gender was not included in the proportional odds model that was generated because we found that this factor did not have an impact on students' perceptions.

A factor analysis was then conducted to identify items reflected in the variations in the data. This analysis was performed with the goal of explaining potential experiences that may cause differences on students' perceptions. Two factors were identified and each of them was used to transform the data. A single factor was computed using linear combinations for each of the observations and for each of the factors. The computed factors explained 46% and 12% of the variance respectively. Because the two identified factors were found to be independent, ($r = -0.05$) separate ANOVA models were used with the level as the explanatory variable [e.g., graduate students (GS) and undergraduate students (US)] and the newly computed factors as the response for each of the observations. The ANOVA model was used to determine whether there was a significant difference between the two levels (e.g., graduate students versus undergraduate students). A Tukey multiple comparison procedure was used to control the Type I error rate when comparing the graduate student (GS) and undergraduate student (US) populations. The assumptions of the model were independent, normally distributed residuals with constant variance; standard diagnostic checks were used to validate these assumptions.

The fourth level of quantitative analysis involved a study of correlations among students' responses within each of the two levels (GS and US).

4.7 Qualitative data analysis

The last stage of data analysis involved a qualitative analysis of students' responses to open-ended questions which was done to provide additional insight into the students' perceptions of their experiences with the nanoHUB.org simulations. One of the open-ended questions asked what could be done to make nanoHUB simulations more useful for students' learning in their courses. Another question asked students how the nanoHUB simulations might have helped them in their learning, and the last question on the survey asked for students' general comments.

Constant comparison approaches were used to analyze the qualitative data [27]. To compare students' statements, we first grouped similar statements. After the bits were separated into initial categories, each statement compared within other statements in the same category. For example, if a student responded: 'add more detailed instructions' or 'add more documentation on what the input and output parameters mean,' we coded these statements in the category 'Add tutorials, help functions, more information, more transparency.' Statements that required further differentiation were divided up into separate subcategories. We then compared observations within each category or subcategory, looking for similarities or differences within the data [28]. Following this process of including and excluding observations the categories became more precise. At the end, the data were quantified by computing frequencies of occurrence of comments within a given category that were then turned into percentages [29].

5. Results

5.1 Analysis of answers to individual questions and comparisons among groups

An analysis of the mean, standard deviation and sample size for the 209 graduate students and 103 undergraduate students for whom data were collected is shown in Table 4. As noted previously, the 10 survey questions that were analyzed were grouped into four categories: learning outcomes, evidence of learning, pedagogical approach, and ease of use.

Learning Outcomes. Survey items grouped into this category focused on the general experience(s) of the students, whether the students thought the simulation tools were relevant to their areas of interest, and their level of satisfaction. Both graduate and undergraduate students seemed to consider the use of nanoHUB.org simulations as a positive experience, and that these tools supported their goals and expectations for the course. Both groups also viewed the simulations as relevant to their areas of interest.

The proportional odds model for this construct can be summarized as follows. The probability that students would perceive the nanoHUB simulation tools as a positive experience was 0.989 for undergraduates and 0.989 for graduate students, which suggests that there were no significant differences between undergraduate and graduate students' perceptions of finding using nanoHUB simulation tools as a positive experience. The probability that undergraduate students would consider the tools relevant to their areas of interest as 0.933, while for graduate students it was 0.938, which, once again, suggests that there were no significant differences between the undergraduate and graduate students' perceptions of the relevance of the computer simulation tools. And the probability that undergraduate students would perceive the nanoHUB simulations tools as supporting their expectations for the course was 0.982 and the probability for graduate students was 0.973.

As depicted on Table 5, the number of simulation tools used during the academic term and the frequency with which these tools were used had an impact on students' perceptions of the tools as a positive experience. Similarly, the frequency with which tools were used also had an impact on students' perceptions that the tools were relevant to their areas of interest.

Evidence of Learning. Both the graduate students and the undergraduates reacted positively to the survey item that probed whether the nanoHUB.org simulations improved their understanding of the concepts being modeled with the simulations. Both groups also responded positively to their

Table 4. Mean, standard deviation, and sample size per each question for graduate (GS) and undergraduate (US) students

	Mean		Std. Deviation		Sample size	
Question ID	**US**	**GS**	**US**	**GS**	**US**	**GS**
Positive experience	3.24	3.46	0.59	0.59	100	209
Tools relevant to interests	2.90	3.18	0.78	0.66	101	207
Supported my course goals	3.06	3.30	0.67	0.61	94	187
Comprehend better	3.01	3.24	0.77	0.64	103	209
Able interpret output	2.62	2.95	0.76	0.59	100	203
Able to approach problems	2.80	3.10	0.63	0.65	94	187
Guide thinking	2.79	3.11	0.64	0.65	103	205
Engaging compared to	2.86	3.19	0.71	0.62	102	208
Easy to use	2.96	3.31	0.56	0.58	101	207
Intuitive to use	2.86	3.16	0.69	0.61	101	207

ability to identify ways in which they might transfer their knowledge to practical situations and approach new problems. Neither group of students reported having trouble interpreting the output of the simulation tools.

The proportional odds model for this construct provided the following results. The probabilities that students would perceive that using nanoHUB simulation tools would improve their understanding of the concepts upon which these simulations were based were 0.887 for the undergraduate students and 0.921 for the graduate students, respectively. Probabilities for the students' perception of their ability to interpret the output of the simulation tools were 0.845 for the undergraduates and 0.878 for the graduate students. Probabilities for students' perceptions of their confidence in their ability to use concepts embedded in the simulation tools to approach new problems were 0.961 for the undergraduates and 0.962 for graduate students.

Both the number of simulation tools used in the academic term and the frequency of use of such tools had a significant impact on how students perceived their ability to interpret the output of the simulation tool. Likewise, the frequency of use of the simulation tools had an impact on students' confidence in their ability to transfer concepts learned with the tools to practical situations (see Table 5).

Instructional Approach. Items in this category focused on whether the students perceived the simulation tools as useful in helping them learn. The undergraduate and graduate students reported positive responses to using nanoHUB.org simulation tools to generate questions that guided their thinking, and also positively reported that using the nanoHUB.org made the course more engaging for them compared to courses that only use lectures, homework, and readings.

The proportional odds model for this construct provided the following results. Probabilities that students would perceive the use of nanoHUB simulation tools as helping to guide their thinking were 0.916 for undergraduate students and 0.941 for graduate students. Probabilities of students' perceptions that courses that used the simulation tools were more engaging were 0.941 for undergraduate students and 0.948 for graduate students.

Ease of Use. The graduate and undergraduate students reported positive perceptions of nanoHUB.org simulations as both intuitive and easy to use. The proportional odds model provided the following results. Probabilities that students would find the nanoHUB simulation tools easy to use were 0.956 for undergraduates and 0.979 for graduate students. And probabilities that students would perceive nanoHUB simulation tools as intuitive to use were 0.934 for undergraduates and 0.945 for graduate students.

The students' academic level, the number of tools used in the academic term, and the frequency with which they were used, as shown in Table 5, all had a significant impact on students' perceptions of the simulation tools as easy to use. Also, the number of tools used in the academic term and the frequency with which those tools were used had a significant effect on students' perception of the simulation tools as intuitive to use.

5.2 Differences between graduate students and undergraduate students

The two factors identified in the factor analysis of survey item responses were named 'perceived ease of use' and 'perceived relevance and learning.' Factor 1 was named 'perceived ease of use' because it encompassed statements describing the ease with which students could employ a particular simulation tool and the intuitive aspects of interpreting the output of the simulation tool.

Factor 2 was named 'perceived relevance and

Table 5. Summary of impact of number of tools used in the academic term, frequency of use in the academic term, and academic level on student perception by category

			Number of tools used		Frequency of use		Academic level	
Construct	**#**	**Question ID**	**F**	**p**	**F**	**p**	**F**	**p**
Learning outcomes	1	Positive experience	4.97	0.0022	11.43	<0.0001		
	2	Tools relevant to interests			4.88	0.0082		
	3	Supported my course goals						
Evidence of the learning	4	Comprehend better						
	5	Able interpret output	4.32	0.0053	21.22	<0.0001		
Pedagogical approach	6	Able to approach problems			3.43	0.0339		
	7	Guide thinking						
	8	Engaging compared to						
Ease of use	9	Easy to use	5.72	0.0008	8.74	0.0002	4.18	0.0417
	10	Intuitive to use	3.41	0.0180	7.15	0.0009		

learning' because it included items related to students' perceptions of simulation tools as relevant to their areas of interest and their level of satisfaction with the tools. It also included items focused on how students perceived simulation tools as useful for their learning process and their perceived ability to transfer what they learned to practical situations.

ANOVA results revealed a significant difference between undergraduate students and graduate students ($F = 31.92$, $p < 0.0001$) for the factor 'perceived ease of use'; while no significant difference was found for the 'perceived relevance and learning' factor ($F = 1.94$, $p = 0.165$).

5.3 Relationships between responses to different questions

A correlation analysis was carried out to examine patterns in the relationship among answers students' gave to individual questions in the survey (see Table 6). Four questions had the most frequent and strongest correlations among survey items regardless of whether the students were undergraduate or graduate students. Three of these items (1, 2 and 3) related to the learning outcomes category, while the fourth one related to instructional approach.

Items that strongly correlated to students' perceptions of the nanoHUB.org simulations as a positive experience probed relevance to their areas of interest ($r = 0.58$), whether the simulations supported their goals and expectations for the course ($r = 0.62$), and the perception that computer simulations made the course more engaging ($r = 0.53$). Items strongly correlated to students' perceptions that the simulation tools supported their goals and expectations of the course examined the relevance of the nanoHUB tools ($r = 0.60$) and the extent to which courses that used these tools were engaging ($r = 0.55$). Additional items that were strongly correlated were students' perceptions of the simulation tools as easy to use and as intuitive to use ($r = 0.68$).

Correlation analyses that were performed within each of the two academic levels (US and GS) provided results that were remarkably similar to those shown in Table 6.

5.4 Analysis of the open-ended responses

Qualitative analysis of the open-ended responses to the survey was done to provide additional insight into students' perceptions of the simulation tools. In total, 510 responses were obtained to the three open-ended questions. The percentage of the responses from graduate students (67%) and undergraduate students (33%) mirrored the distribution of students in the sample population. Most of the comments (90%) could be grouped into two emergent themes that were labeled 'transformative aspects' (54%) and 'operational aspects' (36%).

Transformative aspects. Transformative aspects are features of the simulation tools that supported students' transformative processes, i.e., aspects of the simulation tools that students perceived enhanced or inhibited their learning. Of the total, 160 (31%) comments were related to students' perceptions of identifying the simulations as useful tools for their learning. From those 160 comments 58% were from the graduate students and 42% were from the undergraduate students. Overall, graduate and undergraduate students perceived the simulation tools as very useful for their learning. In particular, students mentioned that the simulation tools helped them to understand concepts, understand relationships between parameters in the simulation, identify practical application of concepts learned in class, generate new ideas and understand topics taught in other courses, facilitate mathematical calculations, and so on. In the following statement, for example, a graduate student described how the simulation tool helped him/her identify relationships between parameters: 'The ability to see clearly how a change in parameters would affect the properties of a system was helpful in making certain relationships clear. This is a very nice set of tools to have when analytic descriptions of problems are hard to come by'.

Students commented that the most useful part of

Table 6. Correlations between Survey Items

		Question #								
#	**Question ID**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
1	Positive experience									
2	Tools relevant to interests	0.55								
3	Supported my course goals	0.53	0.62							
4	Comprehend better	0.41	0.50	0.50						
5	Able interpret output	0.44	0.32	0.35	0.27					
6	Able to approach problems	0.52	0.5	0.46	0.49	0.28				
7	Guide thinking	0.10	0.23	0.26	0.24	–0.02	0.14			
8	Engaging compared to	0.47	0.60	0.58	0.47	0.27	0.45	0.25		
9	Easy to use	0.35	0.33	0.47	0.44	0.21	0.38	0.38	0.34	
10	Intuitive to use	0.38	0.37	0.39	0.36	0.23	0.35	0.34	0.39	0.68

the simulation tool in their learning was ability to the visualize concepts. For instance, an undergraduate student responded: 'I really liked using the nanoHUB simulator to actually visualize the material learned in class. It made learning about semiconductors a lot easier to comprehend, not only at a single point in the semiconductor, but throughout the entire length'.

A small group of students who were primarily graduate students commented on the simulation tools as an interesting and even motivating experience. One graduate student, for example, noted: 'The simulation tool helped me a lot and it also made me to gain interest in this subject.' Comments describing difficulties with the simulations were infrequent (4%) and more likely to come from undergraduates. These students reported that the output of the simulation was hard to interpret, or, in some assignments where programming was a requirement, that it was hard to complete the assignment.

Students suggested ways in which nanoHUB simulation tools could be more useful for their learning. In 17% of the comments students mentioned they wanted to have more support or scaffolding associated with the simulation tools. In particular, they wanted to have more tutorials, more help functions, and overall better documentation. The information they wanted ranged from theoretical aspects such as worked examples or lectures to operational aspects such as tutorials.

One graduate student noted, for example: 'I think it's often times not apparent what set of assumptions are being made when the computations are being performed, so when a result differs from how you computed it in another fashion (using another package/program), it is hard to know why.'

Another student commented, 'Provide explanations of what might happen when each parameter changes.' Graduate students sometimes suggested that simulation tools should provide more flexibility and more functionality. These students wanted to be able to add more parameters to the simulation tool, add more materials or devices, add more simulation tools, and even allow the manipulation of the simulation programming codes. 'It would be very helpful if the simulations could include some additional parameters we can play with.' A few students (3%) noted that they would like their professors to use the simulation tools more often and also during class time.

Operational aspects. Operational aspects are those features of the simulation tools that relate to students' operational processes, e.g., the technical aspects required to operate the simulation tools. Students' comments related to these aspects focused on performance, access and ease of use. Some students (11%) reported not having any problems related to operational aspects and found the simulations useful. For example a graduate student commented: 'I thought nanoHUB is as useful as can be' and an undergraduate student mentioned: 'I don't see anything wrong with it.' In contrast, a group of students (13%) that majority whom were graduate students suggested improving the performance of the simulation tools. In particular, students wanted the simulations to perform faster: 'Speed up the interface, include more options, provide more information about job submission, run time, number of processors, etc.' Some students (9%) also made comments related to aspects of ease of use. For example, they wanted to have better access to the simulation tools and better interfaces for users and developers: 'Make Rappture more flexible to allow for greater customization by developers. This would in effect allow the developers to create tools that are much more user friendly.' Other students (2%) suggested improving navigation and searching capabilities.

6. Discussion

6.1 How do students with different academic level perceive and experience the usefulness of nanoHUB.org simulation tools for their learning?

In summary, graduate and undergraduate students acknowledged the value of nanoHUB simulation tools for their learning by agreeing with statements on a survey related to positive experiences using the tools. This conclusion is supported by the results of the proportional odds model that showed high probabilities between survey items of students' perceiving nanoHUB simulation tools and their overall use as positive experiences for their learning. For example, similarities found across both groups were the strong correlations between students' perceptions of using the simulation tools as a positive experience with supporting their goals and expectations of courses. In addition, their positive perspectives were also correlated with their areas of interest. These findings are also supported by the result of the factor analysis and the ANOVA that reported no significant differences in students' relevance and learning perceptions (factor 2). Finally, from the open ended responses, we could identify that most of the comments students made were related to how useful the simulation tools were for their learning.

6.2 Are there any differences on students' perceptions according to their level of expertise (e.g., graduate and undergraduate levels)?

Differences were noted in students' perceptions when the two levels of students were compared (i.e., graduate and undergraduate students). For example, undergraduate students showed a moderately positive attitude toward their ability to interpret the outputs of the simulation tools. This finding is supported by undergraduate students' open-ended responses where 10% of all undergraduate students reported having difficulties in this regard.

Interesting findings resulted from the factor analysis and the ANOVA such as significant differences between graduates and undergraduates in what we identified as ease of use perceptions (factor 1). Here, the frequency of use of the tools in the academic term as well as the number of tools used, had an impact on students' perceptions in this factor. The difference on students' perceptions *could* be explained by considering that the undergraduate students may not have fully developed graphical literacy skills necessary to reason with the data outputted by the computational simulations. Another potential reason for this difference may be students, lack the prior knowledge required to appropriately interact with the simulation tools. From the evidence of the learning we identified that another important factor relates to students' perceptions on how the tools can assist them in their learning process. For example, undergraduate students' could see the value of using simulation tools but may have encountered some cognitive overload as the simulation may be too complex and task may not be well integrated. Focusing on the pedagogical approach and considering the analysis of the undergraduate students open ended responses and the results of the proportional odds model, possible explanations of these students' differences in their perceptions of the simulation tools may derive from students' inexperience with simulation tools in general and nanoHUB in particular.

Njoo and de Jong [30] pointed out two difficulties for incorporating simulations into educational contexts: exploratory learning processes may be too difficult for learners, and/or students may not use exploratory skills even though they possess them. In addition, Bodemer et al. [31] suggested that learners may lack the declarative and/or procedural prerequisite knowledge for benefitting from using the simulation tools.

This study highlighted students' needs for more scaffolding through their learning process. Researchers have emphasized that inquiry learning, in order to be successful, needs adequate but not intrusive scaffolding [2, 30, 32–35]—e.g. in a just-in-time base [36]. Free exploration without any support, has been shown not to benefit learners [35, 37]. Davies [38] pointed out that simulations do not operate in isolation but in conjunction with the learning environment as a whole. What has been found to be effective for learners are the kind of learning experiences that accompany the simulations, such as designing instructional assignments [39]. For example, by asking students to generate their own or design assignments for other students [40], or by having students use simulations before formal instruction [41].

These novice learners may need additional supports to develop their learning process for skills that graduate students have already developed. These additional supports could take the form of introductory materials and guidance in the concepts, anticipated simulation results, and meaning of the results. Additional research is needed to better understand what exact needs undergraduate students have and how additional supports for learning can be provided. These supports could be provided by/embedded in the nanoHUB.org.

6.3 Implications for instruction

The major implications of this study are focused on the design of effective instructional interventions that will consider ways to support students' transformative processes, regulative processes, and operational processes [30]. Transformative processes involve the basic inductive and deductive processes operations of analysis, hypothesis generation, testing the hypothesis and evaluation [30, 42]. These processes can be supported with the development of curricular materials and scaffolding that appropriately orchestrate the use of computational simulations together with the learning outcomes, evidence of the learning, and pedagogical approaches. Instructors should be aware that as important as the simulations tools is the method of instruction.

Regulative processes include the strategic decision in controlling the inquiry process [42] through planning, verifying, and monitoring [30]. To support regulative processes Quintana et al. [42] suggested organizing the task in steps or provide useful boundaries to learners such as embedding expert guidance together with the simulation learning environment and reducing cognitive demands by automating non-salient tasks. Quintana et al. also recommended providing reminders and guidance to learners facilitating planning, monitoring, and articulation in order to help learners to conduct reflection through their inquiry process.

Operational processes refer to processes involved in operating the simulation [30], and any other technology involved as part of a learning task (e.g. chat tools, text editors, etc.). For example, Clariana and Strobel [43] argued that by increasing the amount and complexity of the simulation output will result in increasing learners' cognitive load. Finally, to support operational processes, and other aspects related to the interface design, general principles of multimedia for learning can be adopted [see 44].

Today, technological advances such as nanoHUB.org allow not only the merging of method and media [45], but also provide capabilities that could integrate adequate supports for transformative, regulative, and operational processes that without technology would not be possible [2]. Utilizing the capabilities of a particular medium together with appropriate methods may influence learners representation and processing of information resulting in more or different learning [46]. Frameworks for technology enhanced support for inquiry learning [see 42, 47, 48] provide useful guidelines for supporting transformative, regulative, and operational processes. For example, by applying the backward design model [24] it could be identified what is the required prior knowledge students should know. Then, undergraduate students could be provided with the required prior knowledge by bridging prior conceptions [42] and providing expert guidance [42]. Also, students' cognitive load could be reduced by pre-training them [44] on how to use the simulation tools so they can easily adapt to the learning curve to operate the interface.

6.4 Limitations of the study

This study had the following limitations. In its design, this study has the limitation that it measures student self-reporting measures of their perceptions of their use of computational simulation tools and not direct measures of learning and engagement. However, as mentioned earlier, understanding student perceptions are also an important construct to identify that can suggest technology acceptance of technology for learning purposes.

In its implementation, this study has limitations because there were not enough details obtained about how and why the simulation tools were integrated in the courses and the kinds of assignments and activities students were asked to do. Also, there was not enough information obtained to describe the response rate due to the voluntary nature of the survey and limited access and information about the courses that were surveyed. Therefore, there is not enough evidence to be able to report the response rate.

7. Summary

The results of this study identify the potential of nanoHUB simulations as learning tools that graduate and undergraduate students value as part of their learning experience, particularly when it relates to their goals and interests. Graduate and undergraduate students reported positive experiences of nanoHUB.org simulation tools and their uses; however, minor differences were identified. For example, undergraduate students showed a moderate positive attitude toward their ability to interpret the outputs of the simulation tools. Also, significant differences were found between graduates and undergraduates in their perceptions of ease of use where graduate students' perceptions were more positive. Potential explanations for these differences could be that: (a) undergraduate students may have not fully developed graphical literacy skills or have developed enough experience using simulation tools, (b) students may lack the prior knowledge required at the time they interact with the tool and (c) tools may be too complex. Suggestions to overcome some of these difficulties were centered on ways to effectively support students' transformative processes, regulative processes, and operational processes by taking advantage of technological advances such as nanoHUB.org. These ways include the development of well integrated and effective curricular materials, the application of frameworks for technology-enhanced support for inquiry learning, and the use of just-in-time instructional supports together with the simulation tools.

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