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By Alejandra de Jesus Magana de Leon

Entitled Professors' and Students' Perceptions and Experiences of Computational Simulations as Learning Tools.

For the degree of Doctor of Philosophy

Is approved by the final examining committee:

Sean P. Brophy, Ph.D. Co- Chair	George M. Bodner, Ph.D. Co- Chair
Ruth A. Streveler, Ph.D.	Mark S. Lundstrom, Ph.D.

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For the degree of Doctor of Philosophy

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PROFESSORS' AND STUDENTS' PERCEPTIONS AND EXPERIENCES OF COMPUTATIONAL SIMULATIONS AS LEARNING TOOLS

A Dissertation
Submitted to the Faculty
of
Purdue University
by
Alejandra de Jesus Magana de Leon

In Partial Fulfillment of the
Requirements for the Degree
of
Doctor of Philosophy

August 2009
Purdue University
West Lafayette, Indiana

Bedřichovi – za jeho pomoc, trpělivost a lásku.
Jsem velice po*ž*ehnána a sťastná, *ž*e jsem s Tebou.

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Most importantly, I would like to thank my husband Bedrich and my little ones Carmen and Daniel, for all the time you had to give up so I can finish my dissertation work. I love you.

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APPENDICES

ABSTRACT

Magana de Leon, Alejandra de Jesus. Ph.D., Purdue University, August, 2009. Professors' and Students' Perceptions and Experiences of Computational Simulations as Learning Tools. Major Professors: Sean P. Brophy and George M. Bodner.

Computational simulations are becoming a critical component of scientific and engineering research, and now are becoming an important component for learning. This dissertation provides findings from a multifaceted research study exploring the ways computational simulations have been perceived and experienced as learning tools by instructors and students. Three studies were designed with an increasing focus on the aspects of learning and instructing with computational simulation tools. Study One used a student survey with undergraduate and graduate students whose instructors enhanced their teaching using online computational tools. Results of this survey were used to identify students' perceptions and experiences with these simulations as learning tools. The results provided both an evaluation of the instructional design and an indicator of which instructors were selected in Study Two.

Study Two used a phenomenographic research design resulting in a two dimensional outcome space with six qualitatively different ways instructors perceived their learning outcomes associated with using simulation tools as part of students' learning experiences. Results from this work provide a framework for identifying major learning objectives to promote learning with computational simulation tools.

Study Three used a grounded theory methodology to expand on instructors' learning objectives to include their perceptions of formative assessment and pedagogy. These perceptions were compared and contrasted with students' perceptions associated with learning with computational tools. The study is organized around three phases and analyzed as a collection of case studies focused on the instructors and their students' perceptions and experiences of computational simulations as learning tools. This third study resulted in a model for using computational simulations as learning tools. This model indicates the potential of integrating the computational simulation tools into formal learning experiences in terms of content, formative assessment and pedagogy.

These three studies capture the complexity of learning environments that adopt computational simulations as learning tools in graduate engineering education. The results of these studies have implications in the areas of engineering and science education, simulation-based learning environments development, and instructional design.

CHAPTER I

INTRODUCTION: COMPUTATIONAL SIMULATIONS AS LEARNING TOOLS

Background of the Problem

Simulations can provide both a critical element of learning experiences and serve as the basis for computational science (Sabelli, et. al, 2005). Opportunities exist to use simulations as both a tool for experts and a learning environment for novices. This raises the question: What needs to be done to accomplish this duality of a simulation resource? To report my exploration of this question I have organized the document into four major sections. First I provide the background of the problem by describing the context for this study. This description defines key terms and ideas that helped me characterize and at the same time delimit the scope of the study. Second, I identify the researchable problem, present the results of the initial study, and outline the research questions. Third, I review the literature related to scientific discovery and the underlying cognitive processes of scientific thinking, describe the processes involved in scientific discovery, and tie those to scientific inquiry learning. Finally, based on the literature review I discuss the rationale and significance of the study and describe in detail the research design.

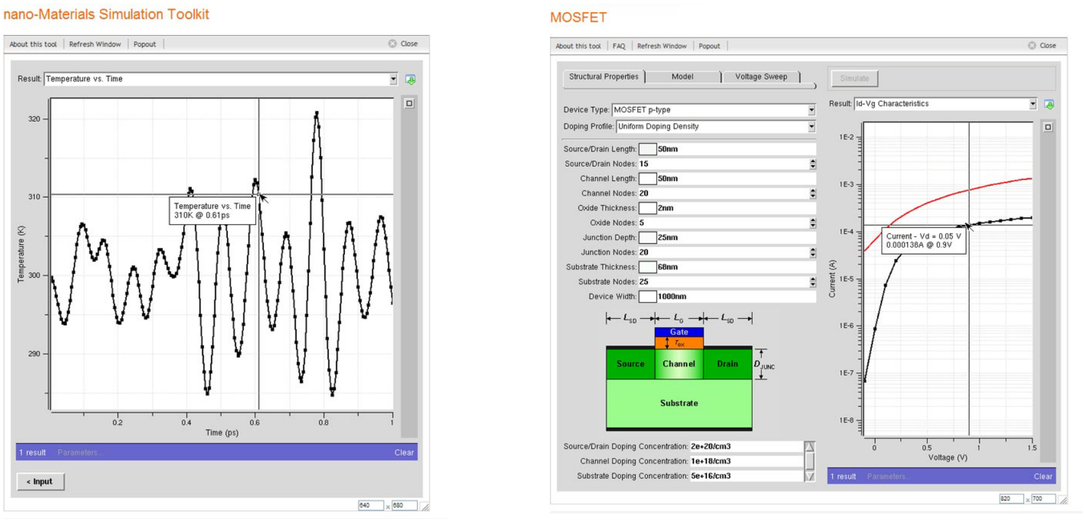
Network for Computational Nanotechnology

As a response to the goals of the National Nanotechnology Initiative, the Network for Computational Nanotechnology (NCN) developed an infrastructure network to help transform nanoscience to nanotechnology through online simulation and training. 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 (Lundstrom, Adams, Klimeck, McLennan, & Potrawski, 2008). The NCN mission is embodied in nanoHUB.org, a web portal that delivered high-end, research quality, online simulations and tutorials to over 89,000 users in 2008 (Lundstrom et al., 2008). These users included professionals, researchers, experimentalists, professors, and undergraduate and graduate students who, as a community of practice, collaborate and learn by sharing ideas, finding solutions, and building innovations in nanotechnology. The nanoHUB.org initially focused on pioneering the development of nanotechnology from science to manufacturing through innovative theory, exploratory simulation, and novel cyber-infrastructure. Recently, the portal has also become an educational source in nanotechnology-related concepts and theory by incorporating resources such as: online presentations, courses, learning modules, podcasts, animations, and teaching materials among others.

nanoHUB.org

The nanoHUB.org provides research-quality simulations that experts in nanoscience commonly use to build knowledge in their field. NanoHUB.org leverages an advanced cyber-infrastructure and middleware tools to provide seamless access to these simulations. As described on the nanoHUB.org website, key characteristics of the nanoHUB.org simulation tools that make them good resources for incorporation into classroom environments are: a) they were produced by researchers in the NCN focus areas, b) they are easily accessed online from a web browser powered by a highly sophisticated architecture that taps into national grid resources, and c) they provide a consistent interactive graphical user interface known as Rappture, which makes esoteric computational models approachable to non-experts. Rappture is a toolkit that allows the incorporation of a friendly graphical user interface with the simulation tools in the nanoHUB.org (McLennan, 2005) (See Figure 1.1).

The nanoHUB.org continues to grow the library of computational resources and learning materials. Specifically, recent years have seen an increase in investigators and graduate students accessing these resources in an attempt to increase their understanding of nanotechnology. My goal is to investigate how these experts use the nanoHUB.org for their own continued learning and how the nanoHUB.org can be integrated into formal and informal learning environments.



Result: Temperature vs. Time

Temperature vs. Time
310K @ 0.61ps

640 × 680

Device Type: MOSFET p-type
Doping Profile: Uniform Doping Density
Source/Drain Length: 50nm
Source/Drain Nodes: 15
Channel Length: 50nm
Channel Nodes: 20
Oxide Thickness: 2nm
Oxide Nodes: 5
Junction Depth: 25nm
Junction Nodes: 20
Substrate Thickness: 68nm
Substrate Nodes: 25
Device Width: 1000nm
Source/Drain Doping Concentration: 2e+20/cm3
Channel Doping Concentration: 1e+18/cm3
Substrate Doping Concentration: 5e+16/cm3

Result: Id-Vg Characteristics

Current - Vd = 0.05 V
0.000138A @ 0.9V

820 × 700

Figure 1.1a: nano-Materials simulation toolkit

Figure 1.1b: MOSFET

Figure 1.1: Samples of interfaces of nanoHUB.org simulation tools

This work will test the conjecture that the nanoHUB.org resource supports learners' goals and expectations for learning in graduate engineering courses. Towards the goal of identifying how these tools can be effectively used in a learning environment my initial research goal involved identifying professors' instructional goals, their approaches, and the students' perceptions of using the nanoHUB.org's simulation tools.

To characterize and focus on a particular type of simulation —i.e. computational simulations— and to identify how its use relates to instruction and learning, I would like to now define and describe some key terms and ideas.

What is a model?

Experts use visual imagery such as models, graphs, symbols, and other representational systems, to help them represent, comprehend, and facilitate achieving solutions to problems (Lehrer & Schauble, 2000; Nersessian, 1992). Because of the strong relationship between models and simulations, Mayer (1992) defined a model as a representation that involves visualizing the principle-based mechanism between interacting components that represent the functionality or operation of a portion of the natural world. This visualization can concretize phenomena that are not directly observable. For the case of building and using simulations, a model is referred to as the mathematics and/or logic rules that reflects the causal relationships that govern a specific situation (Reigeluth & Schwartz, 1989) and that are constructed from variables, relations, and (possibly) conditions (de Jong et al., 2005).

How experts use models as a tool to think with?

Nersessian (1992) argued that experts use models and simulations to construct mental representations and simulations that can be used to comprehend a system. She also argued that operating on these mental representations requires the construction of analogical models and inferring through analogical reasoning. Nersessian suggested that "these techniques involve a process of abstracting from phenomena or existing representations and creating a schematic or idealized model to reason with and quantify" (p. 65, 1992). Sabelli et al. (2005) noted that the addition of computer visualization to the simulation of complex phenomena allows for a visual exploration of the phenomena and overcomes the limits of models. Furthermore, Sabelli described simulations as the third-leg in this century's methodologies of science, arguing that theory and physical experimentation, by themselves, no longer suffice.

What is a simulation?

A simulation can be many things, ranging from a physical model that can be manipulated to a computational model. This section focuses on defining one class of simulation. Cannon-Bowers and Bowers (2007) defined simulations as "a working representation of reality; used in training to represent devices and processes and may be low or high in terms of physical or functional fidelity (p. 318)." In an educational context, Alessi (2002) proposed that simulations are "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)." Winn (2002) alleged that simulations, as different from reifications, do not create an accurate facsimile of real objects or events. Instead, Winn defined reification as computer-created virtual learning environments that allow students to perceive and experience phenomena that they cannot experience in the real world. For this study, my definition of simulation includes the definition of reification. Based on these definitions, I define computational simulations as working representation(s) of reality; used in training, research, and education to represent physical phenomena, devices, and/or processes through mathematical models and numerical solution techniques using computers. These computational simulations are used as tools to analyze and solve scientific and engineering problems.

Alessi (2002) distinguished between "building" simulations and "using" simulations. This distinction was well-described by Clariana and Strobel (2007) who argued that building simulations refers to computer software modeling tools designed to build and run dynamic models, while using simulations involves the use of computer software tools designed under others' own understanding of a model that allow users to manipulate its processes or variables and observe the output results (R. B. Clariana, 1989; Reigeluth & Schwartz, 1989). Alessi (2000) made clear that educational simulations cannot be divided cleanly into the categories of using or building simulations; instead, they form a continuum. Alessi described this continuum with one end emphasizing the use of simulations and the other end emphasizing building simulations or models (p.179).

What are "building" simulation tools?

Building simulation tools --also known as model-building simulation tools--, exist when the learner interacts with the simulation, and also builds a model and programs it along with the user interface (Alessi, 2002). According to Clariana and Strobel (2007), when learners build simulations they are able to change the attributes of variables, change the agents that are part of the system, design different subsystems, and design different functionalities of that subsystem. In addition to change and design systems and subsystems, when learners build simulations they can also use them for what Penner (2005) called "synthetic modeling." According to Penner, synthetic modeling, as opposed to testing theories or other types of experimentation, is used when we want to reproduce a phenomenon of interest by means of simulation, game, or other technology.

What are "using" simulation tools?

Using simulation tools can further be divided into two subcategories: scientific discovery learning simulations (de Jong & van Joolingen, 1998) and laboratory simulations (Alessi, 2002). According to Alessi (2002) and de Jong and van Joolingen (1998), scientific discovery learning simulations are also known as model-exploration simulations. Scientific discovery learning simulations contain models of specific concepts, facts, and principles. The ultimate purpose of this type of simulation is to allow learners to explore and develop an understanding of those models (Clariana & Strobel, 2007).

Model exploration is conducted when learners test an input-output relationship (Du Boulay, O'Shea, & Monk, 1999). Model exploration simulations have the following characteristics: a) the software simulations are purpose/domain specific (Cannon-Bowers & Bowers, 2007; Clariana & Strobel, 2007), b) the software simulation does not allow the learner to alter the system's underlying model (Cannon-Bowers & Bowers, 2007; Clariana & Strobel, 2007) unless it has predetermined options, c) the software simulations request input parameters from the learner (Cannon-Bowers & Bowers, 2007), and d) the simulation tool displays some sort of output (Cannon-Bowers & Bowers, 2007; Clariana & Strobel, 2007). These types of simulations include a black-box model in which the calculations are hidden to the user and the relationships between variables must be inferred (Alessi, 2000; Resnick, Berg, & Eisenberg, 2000).

What are laboratory simulation tools?

According to Alessi (2002), laboratory simulations allow learners to perform experiments as they would do in a laboratory, for example, by using a physical device such as a measurement tool. This particular type of simulation also includes a black-box model. However, in this case the main purpose of the laboratory learning experience is not focused on inferring the relationships between variables, but something else, such as doing a titration, determining an unknown substance, or comparing accelerations of objects Falling.

What kind of knowledge do simulations affect?

Alessi (2002) alleged that simulation tools mainly affect two types of knowledge; declarative knowledge and procedural knowledge. According to Smith and Ragan (2005), declarative knowledge requires a learner to recall and understand facts, lists, names, or organized information. Procedural knowledge involves the application of defined steps or procedures including algorithms, rules of thumb and/or heuristics. Depending on the learning goal, the instructor or the designer may select the type of simulation to use, either building or using simulations. However researchers recommended a combination of both, since instruction of complex learning environments such as engineering, involves multiple and often different types of learning goals (Alessi, 2002; de Jong & van Joolingen, 2007).

Alessi (2002) described the relationship between "building" versus "using" simulations and declarative versus procedural learning as follows "(1) when learning goals are primarily procedural (flying an airplane, doing a titration) the learners use simulations built by other people; (2) When learners are building simulations the goals are primarily declarative (p.182)." Alessi emphasized the importance of directionality in the above mentioned statements. When the goals are procedural the learners generally use simulations, but the converse is not the case. Alessi argued that when learners use simulations the goal is usually procedural when the goal is a procedure itself. In cases where learners build the simulations the knowledge being learned is usually declarative and the converse is not the case. That is, when learning declarative knowledge does not require building simulations. As a result: a) learners rarely learn procedures by building simulations, and b) using simulations are not only applied to learning procedural knowledge, but also declarative knowledge, although exceptions to these generalizations may exist.

What are potential benefits of simulation use in educational contexts?

Simulations, in educational contexts have been used for inquiry learning. According to Pizzini et al. (Roth, 1993), inquiry learning involves activities such as:

> (a) the identification of problems and solutions and the testing of these solutions; (b) the design and students' own procedures and data analyses; (c) the formulation of new questions based on previous claims and solutions; (d) the development of questions based on prior knowledge; (e) the linking of experience to activities, science concepts, and science principles; and (f) the sharing and discussing of procedures, products, and solutions. Problem solving is an inherent feature of open inquiry and an important issue in the training of scientists and engineers. (p.166)

Simulations in this context provide unique educational benefits. They provide students with: a) an opportunity to study abstract and complex physical phenomena involving many variables (Dede, Salzman, Loftin, & Sprague, 1999), b) the ability to see and, in a certain way manipulate phenomena that is not possible with any other tools (Zacharia, 2007), c) an environment that approximates, simplifies, or hypothetically creates reality (de Jong, 1991), d) the ability to change the time-scale of real processes (de Jong, 1991), e) a cost savings from using the simulation instead of lab equipment (Cannon-Bowers & Bowers, 2007), f) a safe environment to experiment (Cannon-Bowers & Bowers), and so on. Other educational benefits inherent to any computer-based tool are: a) increased opportunities for frequent practice (Zacharia, 2007), b) immediate feedback (Zacharia, 2007), c) ability to serve the need of individualization (Reigeluth & Schwartz, 1989) and learner-centeredness (Milrad, Spector, & Davidsen, 2000), and perhaps even d) highly motivational instruction (Reigeluth & Schwartz, 1989). In addition, if the simulation tools are web based, they can provide the students access at any time and from any place.

In educational contexts, studies, such as those conducted by Williamson and Abraham (1995), have shown that the use of computer-interactive animation technology and dynamic, three-dimensional presentations can lead to significant improvements in students' understanding of the concept in question. They argued that this increased understanding may be due to the superiority of the formation of more expert-like dynamic mental models.

What are potential challenges of simulation use in educational contexts?

Njoo and de Jong (1993) pointed out two difficulties encountered when 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. (2005) suggested that learners may lack declarative and/or procedural pre-requisite knowledge. Another difficulty in the case of building simulations results from the complexity of the modeling task (Clariana and Strobel, 2007). However, researchers have emphasized that inquiry learning, in order to be successful, needs adequate but not intrusive scaffolding (de Jong & van Joolingen, 2007; Mayer, 2004; Njoo & de Jong, 1993; Reid, J, & Chen, 2003; van Joolingen, de Jong, & Dimitrakopoulout, 2007; Winn, 2002)—e.g. in a just-in-time base (Hulshof & de

Jong, 2006). Free exploration without any support, has been shown not to benefit learners (van Joolingen et al., 2007; Veermans, van Joolingen, & de Jong, 2006). Davies (2002) 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 (Swaak & de Jong, 2001). For example, by asking students to generate their own or design assignments for other students (Vreman-de Olde & de Jong, 2004), or by having students use simulations before formal instruction (Hargrave & Kenton, 2000).

Windschitl and Andre (1998) conducted an experimental study to investigate how different conditions can enhance conceptual change. They compared two different instructional conditions. In the confirmatory simulation condition, students completed prescribed steps following written instructions that led to the responses of the questions posed. In the exploratory simulation condition, students used a thematic instructional guide to hypothesize and test possible answers to the same questions. They found that when prior computer experience and pretest scores were statistically controlled, students in the exploratory simulation group demonstrated a greater degree of conceptual change in two of the six alternative conceptions than the students exposed to the confirmatory simulation condition. The authors argued that since the goal of the instruction was conceptual change, a constructivist use of simulation would facilitate the conceptual change. Therefore, depending on the goal, we need to include appropriate methods of instruction that would help learners to attain that goal (de Jong, 1991).

Identification of the Problem

Researchers have agreed that studies related to the use of computer simulations for inquiry learning have not demonstrated compelling evidence of their effectiveness in science and engineering domains (Njoo & de Jong, 1993; Winn, 2002). Most of these studies have employed quantitative research methods of inquiry. Therefore these studies may not have taken into account the interaction of different variables that usually take place in complex learning environments, such as the influence of students' expectations of the task or the effect of direct instruction. From a research design point of view these studies lack ecological validity; from a practical point of view, there is a lack of practical application of previous findings (Winn 2002). Therefore the problem this study addresses is to document different qualitative ways in which students and instructors perceive and use simulation tools in a naturalistic learning environments.

For exploratory purposes, an initial study was conducted in order to measure what students in different engineering courses perceive about nanoHUB.org simulations as part of instruction. The survey data were collected with two main intentions: a) monitoring the usage of the nanoHUB.org and b) assessing instructors' incorporation of the tool(s) as part of their course.

Study One

The data included in this proposal were collected from surveys given during the Fall 2006, Fall 2007, and spring 2008 semesters. The participants in this study included students from 16 different courses at nine different universities. The population consisted of approximately 190 graduate students and 360 undergraduate students who used nanoHUB.org as part of their learning activities. The students were asked to participate in a voluntary Likert-scale survey focused on:

- How students perceive simulation tools as useful for their learning,
- How students thought the simulation tools were relevant to their areas of interest and their level of satisfaction, and
- Usability aspects - in particular, how intuitive the tools are.

The survey used for all of the students is displayed below.

Opening Statement:

The purpose of this survey is to identify if resources at the nanoHUB are useful as learning tools. Your participation in this survey is anonymous and strictly voluntary. Completing the survey has no relation to your grade and you may stop at any time.

Category: General information

1. Please indicate your gender

○ Female
○ Male

2. Have you used nanoHUB simulation tools in the past?

○ Yes

○ No

3. Please write the name of the course in which you are currently enrolled and for which you are completing this survey.

4. How often do you visit nanoHUB in this course?

○ Frequently, out of my own interest

○ Every once in a while out of my own interest

○ Only when my professor request me to access/use a nanoHUB resource

5. In my course, nanoHUB is…
(check all that apply)
☐ used to listen to lectures and seminars
☐ used for running simulations to test given hypotheses and refine them
☐ used for running simulations to understand the underlying model
☐ used to generate new hypothesis by testing data through the simulations
☐ used for building models and test them in the simulations
☐ used to extend models already implemented
☐ used for running simulations as a black-box to perform experiments as I would in a lab
☐ tightly integrated with almost all aspects of what is taught
☐ used from time to time with various concepts
☐ used as part of homework assignments
☐ Optional
☐ Other (please specify)

6. Which simulation tools do you use in your course? Please list all the tools you use and please separate each with a comma.

Category: Educational Content

7. Using nanoHUB is a very positive experience

○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

8. nanoHUB simulations supported my goals and expectations for the course

○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

9. I will continue to use nanoHUB after I am done with this course (check all that apply)

☐ Only if I am required to do so as part of a course
☐ I will use it to develop technology
☐ I will use it to conduct research
☐ I will become a contributor
☐ I will probably not use it again

10. nanoHUB simulation tools are highly relevant to my areas of interest

○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

11. This course is highly relevant to my areas of interest

○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree
○ I don't have an area of interest clearly identified yet

12. How would you describe your areas of interest in relation to nanoHUB?

Category: Evidence of the Learning

13. I can comprehend concepts better by using he nanoHUB simulation tools compared to lectures and readings only

○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

14. The assignment(s) related to nanoHUB simulation(s) increased my awareness of practical applications of these concepts

○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

15. I feel very confident with my ability to use nanoHUB simulation tools to approach new problems

○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

16. I have trouble interpreting the output of the nanoHUB simulation(s)

○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

17. I expect that my performance for this class is going to be:

○ Very good
○ Good
○ Not so good
○ Poor

Category: Instructional Approach

18. When I use nanoHUB simulation tools I generate questions that guide my thinking
○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

19. Using the nanoHUB simulations made this course a lot more engaging for me compared to courses that only use lectures, homework, and readings
○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

20. My initial strategy for deciding what input parameter(s) change was:
○ Randomly selected input parameters until the output parameters were close to the solution.
○ Randomly select input parameters to understand relationship with output parameters
○ Carefully selected values for input parameters because I knew the relationship between the input and output
○ Identified output parameters I knew needed to change, then selected input parameters I think relate to those outputs.
○ Selected values for the inputs parameters based on similar problems I have solved.

21. My final strategy that took me to the solution was:
○ Randomly selected input parameters until the output parameters were close to the solution.
○ Randomly select input parameters to understand relationship with output parameters
○ Carefully selected values for input parameters because I knew the relationship between the input and output
○ Identified output parameters I knew needed to change, then selected input parameters I think relate to those outputs.
○ Selected values for the inputs parameters based on similar problems I have solved.

22. The simulation tool helped me to identify phenomena I could not investigate with any other tool

○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

23. I feel very confident with my ability to use concepts embedded in1these tools to approach new problems

○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

Category: Educational Advantages and Disadvantages

24. How did the simulation tool help you the most during your *learning process*?

25. How did this simulation tool inhibit your *learning process*?

26. What can we do to make nanoHUB more useful for your learning in this course?

Category: Usability

27. nanoHUB is easy to use
○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

28. nanoHUB simulations are very intuitive to use
○ Strongly Agree
○ Agree
○ Disagree
○ Strongly Disagree

29. Other comments

For the purpose of analyzing the results of this initial study, three groups were formed: graduate students (n=189), freshmen undergraduate students (n=338), and undergraduate students (n=24).

For the survey collected in the Fall 2006 semester, students responded on a scale from one to five: strongly agree, agree, undecided, disagree, and strongly disagree to each statement in the survey. A senior researcher and I decided to change the scale in 2007 because we wanted the students to be more selective in their responses. For the survey collected in Fall of 2007 and spring of 2008, students responded on a scale from one to four: strongly agree, agree, disagree, and strongly disagree to each question. The average scores for the two versions of the survey were assigned in the following way:

Table 1.1: Average scores for the student survey data

Response	**Fall 2006**	**Fall 2007**	**Spring 2008**
Strongly agree	4	4	4
Agree	3	3	3
Undecided	2.5	n/a	n/a
Disagree	2	2	2
Strongly disagree	1	1	1

My interpretations of students' responses to the questions were as follows: strongly positive, positive, negative, or strongly negative respectively. For the case of questions with multiple responses, the number of responses was divided by the number of participants.

The results of data analysis of this initial study served four main purposes: (1) to provide an initial indicator of students' perceptions of the professors' incorporation of simulation tools in the learning experiences; (2) to focus on the design of our guiding interview protocol with professors; (3) to identify differences in groups according to graduate and undergraduate levels; and (4) to identify potential instructor participants for the qualitative portion of this study. Descriptive statistics were used to analyze the surveys. A summary of the students' responses to the survey are shown in Figure 1.2.

Wiggins and McTighe's backward design (1997) was used as a framework for organizing the survey results. Wiggins and McTighe's backward design process (p.9) is composed of three main stages: a) identifying the desired *learning outcomes* -- the *content* of the lesson, b) determining the acceptable *evidence of learning* also called the *assessment* method, and c) planning the experiences and *instructional approach* or *pedagogy. Usability* aspects were also analyzed. The results from this initial study are detailed below.

Learning Outcomes. This section focuses on the general experience students had, whether students thought the simulation tools were relevant to their areas of interest, and their level of satisfaction. Graduate students and undergraduate students considered the nanoHUB.org as a positive experience as well as being relevant to their areas of interest. These two groups of students had also responded positively to the idea that the nanoHUB.org simulations supported their goals and expectations for the course. In general, freshmen undergraduate students reported negative responses in this area. These students did not consider using the nanoHUB.org as a positive learning experience, and they did not consider it relevant to their areas of interest. Freshmen undergraduate students did not consider that nanoHUB.org simulations supportive of their goals and expectations for the course.

In the final semester in which data were collected (spring 2008), a new question in the area of learning outcomes was added. I asked students whether they considered the course as highly relevant to their areas of interest. From the five groups of students who responded to this version, the three groups of graduate students and the two groups of undergraduate students considered the courses whose instructors incorporated the nanoHUB.org simulations as highly relevant to their areas of interest.

Evidence of Learning. This section focuses on how students perceive simulation tools as useful for their learning and how they may transfer it to practical situations. Graduate students and undergraduate students were positive in perceiving that using the nanoHUB.org simulations allowed them to comprehend the concepts better in comparison to students who only had access to lectures and readings. There was also a positive tendency in the responses of students' awareness to their ability identify ways to transfer their knowledge to practical situations and inconclusive responses of students not having trouble interpreting the output of the tool. Students were also ambiguous in their responses related to their level of confidence in their ability to use the concepts embedded in the simulation tools to approach new problems.

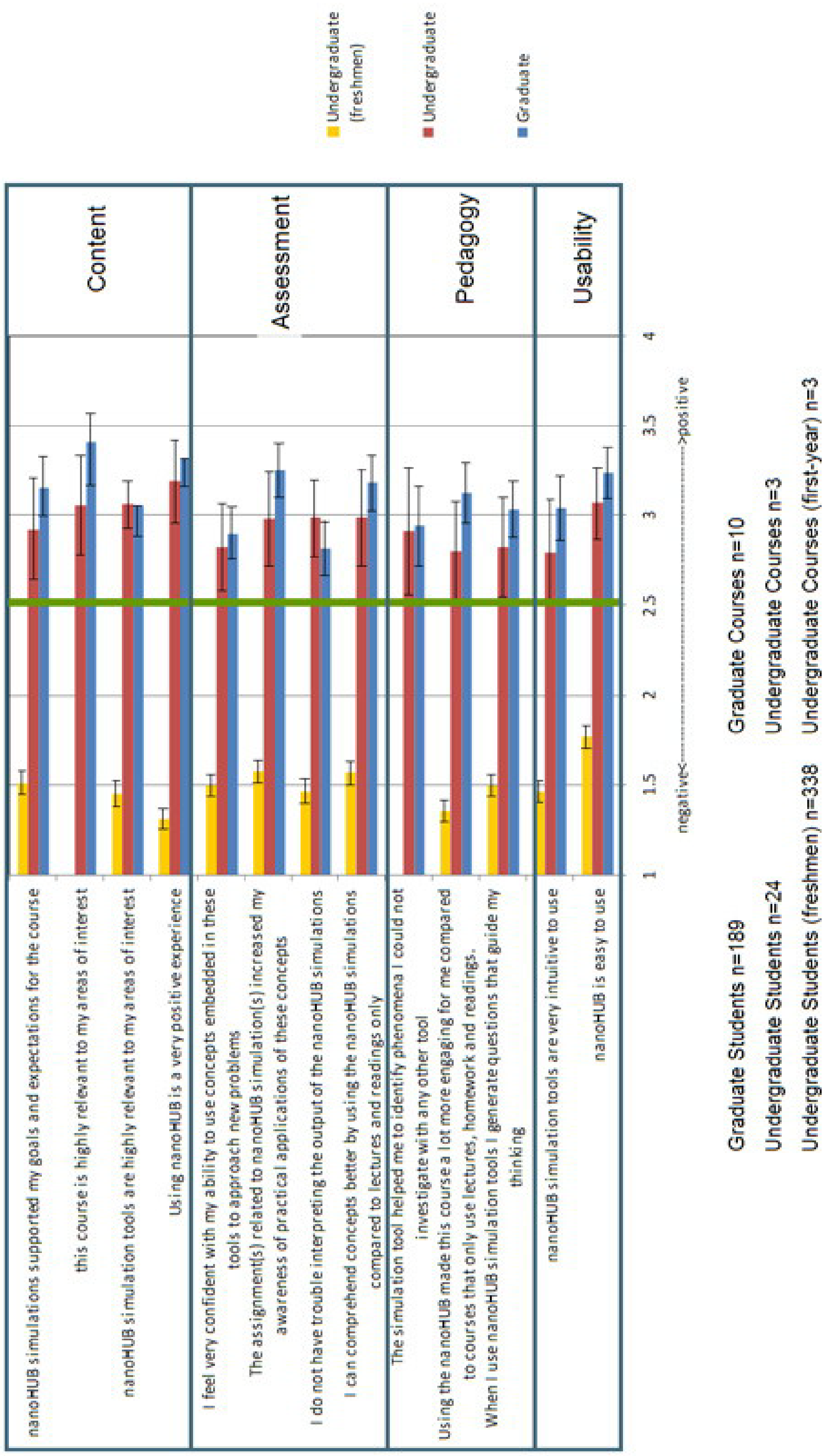


Figure 1.2: Summary of responses from the student survey

Freshmen undergraduate students reported negative responses to the questions related to being able to comprehend the concepts better by using the nanoHUB.org simulation tools compared to lectures and readings only, as well as negative responses to not having trouble interpreting the output of the simulation tools. Also, these students reported negative responses in their ability to use the concepts embedded in the tools to approach new problems, as well as a way to increase their awareness to identify practical applications of these concepts.

Instructional Approach. This section focuses on identifying whether the simulation tools were a useful and engaging tool for their learning. The 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 a lot more engaging for them compared to courses that only use lectures, homework, and readings. Undergraduate students had inconclusive responses that using nanoHUB.org simulation tools helped them generate questions that guided their thinking, and that using the nanoHUB.org made the course a lot more engaging for them compared to courses that only use lectures, homework, and readings. In contrast, freshmen undergraduate students reported negative responses to using nanoHUB.org simulation tools to generate questions that guided their thinking, and also negatively reported that using the nanoHUB.org made the course a lot more engaging for them compared to courses that only use lectures, homework, and readings.

In the spring 2008 another new question in the area of *instructional approach* was added. I asked students if the simulation tools helped them identify phenomena they could not investigate with any other tool. From the five groups of students who responded to this version, the three groups of graduate students and the two groups of undergraduate students considered the simulation tools helped them identify phenomena they could not investigate with any other tool.

Usability. The graduate students reported that nanoHUB.org simulations are very intuitive as well as easy to use. The undergraduate students reported that nanoHUB.org tools are easy to use and ambiguously rated the tools as very intuitive to use. The undergraduate students disagreed that nanoHUB.org is intuitive to use, but they did consider it somewhat easy to use.

Looking closer at the data I noted that the frequency with which students used the tools was not directly related to the students' ability to understand (r=0.52) and apply (r=0.64) the concepts (See Figure 1.3).

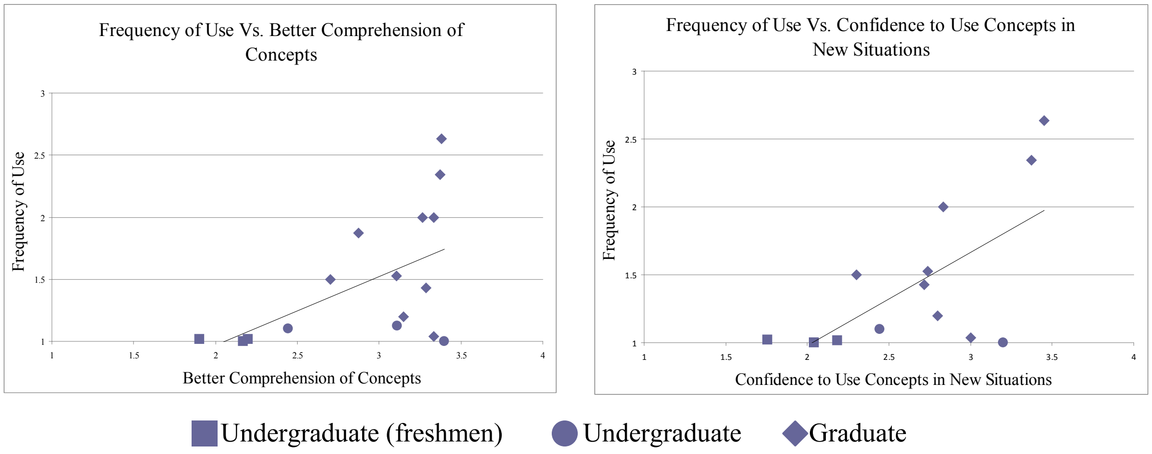


Figure 1.3: Correlation frequency of use between confidence to apply and comprehend concepts

In contrast, I found a correlation between how students, in general, considered nanoHUB.org as being relevant to their areas of interest and how they perceived it as engaging (r=0.84) and useful to comprehend (r=0.87) the concepts better (see Figure 1.4).

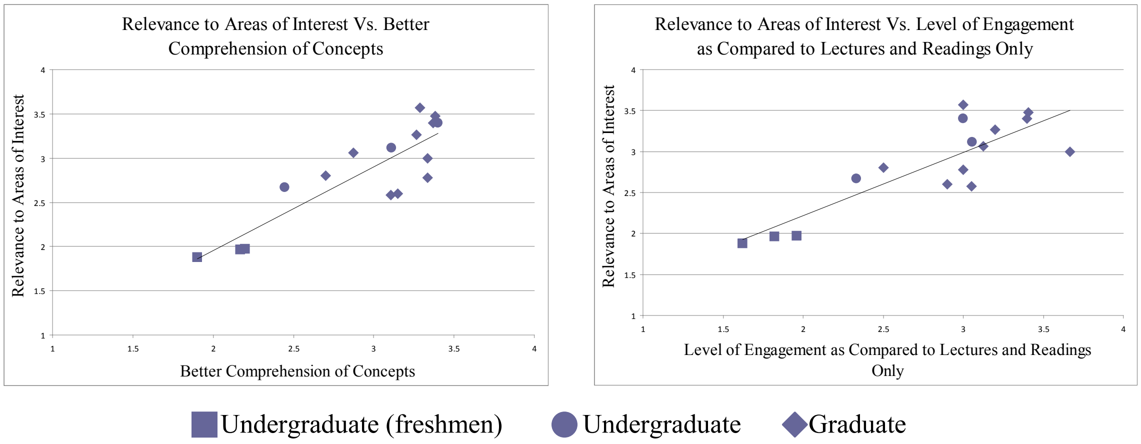


Figure 1.4: Correlation of relevance to students' areas of interest with level of comprehension and level of engagement.

I identified a correlation between the students' ability to interpret the output without trouble with their ability to comprehend the concepts better by using the tools compared to lectures and readings only (r=0.86). I also identified a correlation between students that considered nanoHUB.org as a tool to help them generate questions that guide their thinking with their ability to comprehend concepts better by using the tools compared to lectures and reading only (r=0.91). Finally, I identified a correlation with students' ability to comprehend the concepts better by using the tools to increase their awareness of practical applications of such concepts (r=0.96) (see Figure 1.5).

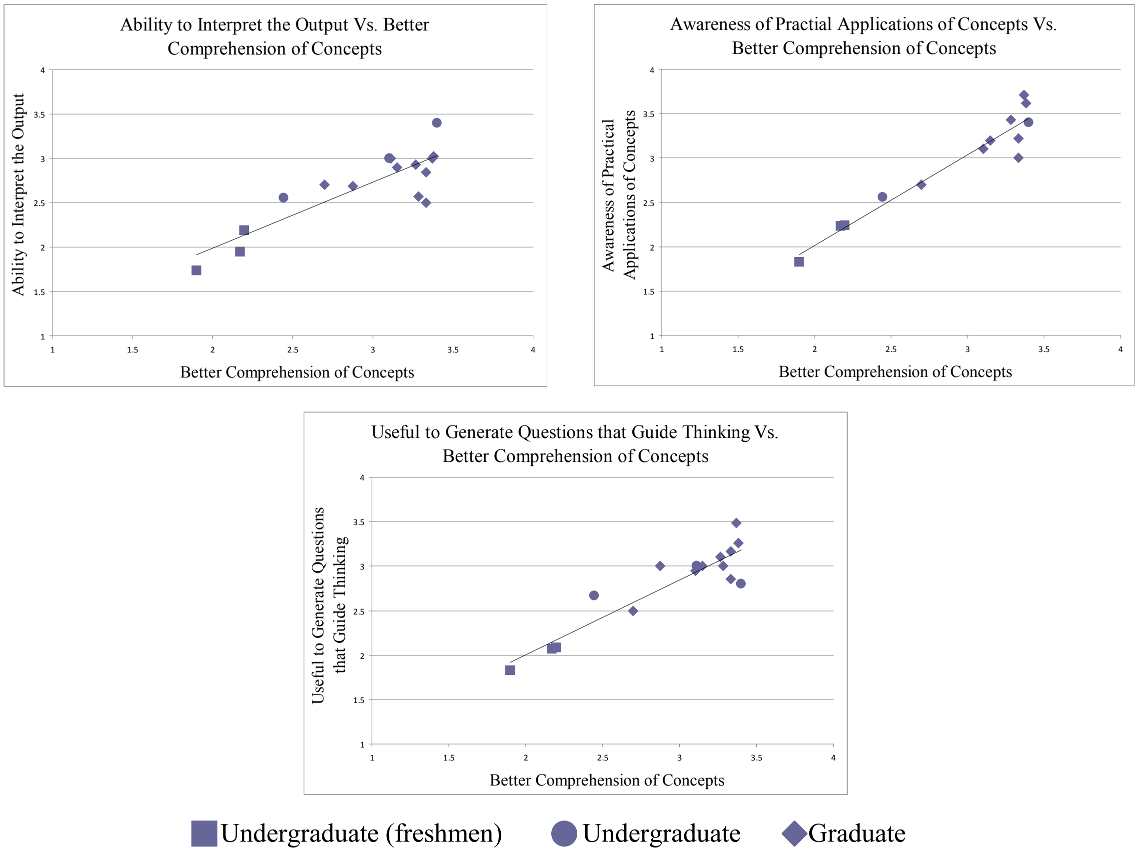


Figure 1.5: Correlation of better comprehension of concepts and students' ability to interpret the output, awareness of practical applications of concepts, and usefulness to guide students' thinking.

There were two open-ended questions in the student survey. Students were asked what could be done to make nanoHUB.org more useful for their learning and other general comments. More than 400 responses were collected. The data were not quantified rigorously from these responses; however I will discuss some general suggestions and concerns students posed. In some responses students asked for more theoretical background before and while using the simulation tools. While graduate students were more specific in their requests, undergraduate students made suggestions about making it "easy to use" and "easy to understand". Students who made such comments needed more information about what the input and output parameters mean, how the graphs connect to theory, and more transparency on what the simulation is actually doing. Some suggestions made by students include accompanying the simulations with materials focused more on the theory and less on the technical aspects; materials such as animations, videos, tutorials, explanations of the input parameters, and worked examples. Students also suggested different ways in which the tools could be used. For example, design assignments in a context of solving a real challenge and the ability to solve the assignments in collaborative groups.

Sample responses of graduate students:

> "Have a description of what the output means for users. Sometimes I don't understand what to I am looking after I put in the input information"
>
> "Make some parametric plots which students can use during theoretical learning. Basic plots can be also for students who do not feel comfortable with advanced topics."
>
> "Reasons for the behavior of wave forms in the graph will help students to understand still better"
>
> "Tutorials on using the different tools would be helpful. I didn't always know how to interpret the results, and a little guided learning would be nice."

Sample responses of undergraduate students:

> "I need to better understand what the results actually mean rather than just seeing random numbers whose purpose I have no idea."
>
> "The actual site nanoHUB and its tools are very interesting to someone who has knowledge of how to use them. As somebody with little knowledge, though, it was very difficult to understand what my results meant. I do see the significance in having the tool available, however…"

> "I don't think nanoHUB can really be made more useful; I think professors can do a better job of utilizing it to support their classes."
>
> "The main problem was that the nanoHUB activities really didn't connect that well with the main concepts of the class. They were interesting, just not well integrated with the rest of the class."
>
> "There needs to be more explanation of the calculations. I feel as If I am running an experiment and simply copying down numbers. There is no understanding involvement."
>
> "Explain how to use it beforehand and show its purpose in class. When a student is just told what to do, they do not understand exactly why they are doing it."
>
> "…the instructions on how to use the programs are all very clear, however, most of the time I end up with a string of data that has no meaning or relevance to whatever we are doing."

From the above data I was able to identify differences in the way students perceived the nanoHUB simulation tools. In general, according to this initial survey, graduate students reported more positive experiences with nanoHUB simulations than undergraduate students did. I decided then to focus the following studies on investigating the most well-perceived uses of simulation tools first. That is, from the graduate courses whose students answered the survey positively, we invited the instructors to participate in a semester-long study where results are reported as part of this dissertation. This study focused on gaining a deeper level of understanding and detail of individual variation and collective similarities in the perception and experience of the nanoHUB.org simulation tools in the context of engineering graduate courses.

Purpose of the Study and Guiding Research Questions

The specific aim of this dissertation study was to provide holistic and meaningful descriptions of experiences and perceptions of nanoHUB.org simulations as learning tools in graduate courses related to nanoscience concepts. Therefore, the focus of this study was not only to describe how professors perceive and experience their use of such tools, but also to identify students' perceptions of the simulation tools and their reactions to their instructor’s uses of them. Consequently, the guiding research questions for this study were:

1. What are instructors’ perceptions and experiences of using simulation tools as part of their instructional practice?
2. What are students’ perceptions and experiences of using simulation tools?
3. What are students’ reactions to professors’ goals and instructional approaches of using simulation tools?

Because the use of computational simulations for understanding and building models has been used by experts to guide their thinking in scientific discovery processes, I considered it important to identify what it means to “think scientifically” and how this relates to scientific discovery learning. Therefore, for conducting this study I adopted a cognitive information processing perspective in which the most important source of knowledge is reason. The following section identifies scientific thinking processes that inform and support scientific discovery processes. I also identify the role of models and modeling and how scientific discovery processes relates to scientific inquiry learning.

CHAPTER II

LITERATURE REVIEW AND THEORETICAL FRAMEWORK

In educational research, the use of computer simulations has mostly been explored as pedagogical tools for scientific inquiry learning. Theories of scientific inquiry learning are usually based on theories of scientific discovery (de Jong & van Joolingen, 1998, p. 180). With the goal of gaining a deeper understanding of how experts conduct scientific experimentation that may result in scientific discovery I felt beneficial to identify and review studies and theories of scientific discovery, scientific thinking, and scientific discovery processes. By reviewing these, I intended to make a connection between the ways experts conduct their scientific activities and how these activities have influenced educational methods for inquiry learning.

Scientific Discovery

Langely, Simon, Bradshaw and Zytkow (1987) described *discovery* as a moment of climax in the scientific progress that is accompanied by a process of verification. Similarly, Zachos, Hick, Doane and Sargent (2000) defined it as the successful result of building and testing conceptualizations of the world through empirical inquiry. Langley and his colleagues also argued that it is possible to identify the processes that lead to those discoveries. Furthermore, they proposed that these processes can be described and modeled and that these processes can be identified as better or worse, more efficient or less efficient, etc. Other labels that have been given to scientific discovery are scientific reasoning and/or scientific thinking (Zimmerman, 2000). However, I would like to distinguish between scientific discovery as the moment of climax of scientific progress, the process of scientific discovery as the processes or steps followed during scientific experimentation, and scientific thinking as the mental processes used when reasoning during scientific activities such as gathering data, formulating explanatory models of the data, testing hypothesis, and so on (Dunbar & Fugelsang, 2005). The relationship between these ideas is summarized in Figure 2.1.

Scientific Thinking

Scientific discovery has been conceptualized as including reasoning processes as well as problem-solving skills (Zimmerman, 2000). Focusing on the reasoning processes first, I refered to these processes as scientific thinking. Dunbar (1999) identified analogical reasoning, attending to unexpected findings, experimental design, and distributed reasoning as key components of contemporary scientific thinking in generating new models. Together with these key components and processes, Dunbar identified other reasoning processes such as causal reasoning, generalization and deduction, and visual reasoning. I will briefly discuss analogical reasoning, causal reasoning, inductive and deductive reasoning, and distributed reasoning as key reasoning processes in scientific discovery.

Analogical reasoning

Analogies are a fundamental cognitive mechanism that people use to map processes by identifying relevant information from a more familiar domain to a less familiar one (Mason, 2004). The powerful role of analogies in enabling people to communicate, explore, and infer about novel phenomena, as well as to transfer learning across subject domains has been well recognized (Gentner & Markman, 1997). While analogizing is a sophisticated process used in applying creative discovery processes, similarity is, as described by Gentner and Markman, (1997) a brute perceptual process. Gentner (1983) defined an analogy as "a device for conveying that two situations or domains share relational structure despite arbitrary degrees of difference in the objects that make up the domains. This promoting of relations over objects makes analogy a useful mental process, for physical objects are normally highly salient in human processing" (as cited in Gentner and Markman, 1997, p.46). Dunbar (1999) alleged that scientists use analogies when they have the goals of formulating a hypothesis, designing an experiment, fixing an experiment, or explaining a result. Dunbar and his colleagues also identified that different types of analogies are used by scientists when they have specific goals. For example, when the goal is to explain a concept, distant analogies are used. In contrast, when the goal is to design and fix experiments, local analogies are used. Local analogies are drawn from very similar experiments (e.g. same organisms), while distant analogies are drawn from concepts in other related domains.

Causal reasoning

Jonassen and Ionas (2008) defined causal reasoning as the ability to make predictions, implications, inferences, and explanations. They proposed that causal reasoning is based on causal propositions; namely concepts that are connected by associative and dynamic relationships. According to Jonassen and Ionas: a) making predictions involves reasoning from a description of an initial condition(s) or state(s) to the possible effect(s) that may result from those states or conditions; b) implications involve making deterministic predictions of conditions and states based upon plausible cause-effect relationships; c) making inferences implicate reasoning backward from effect to cause; and d) explanations entail the comprehension of structural and functional interrelationships among the system components and the causal relationships between them.

Covariation, the relationship existing between two events, has been identified as a potential cue that two events are causally related (Zimmerman, 2000). Koslowski (1996) noted that in real scientific practice more than covariation is needed when making causal attributions such as causal mechanism, which is the process by which a cause can bring about an effect. Koslowski alleged that these causal mechanisms allow scientists to determine which correlations between perceptually salient events should or should not be considered. Furthermore, Koslowski recognized bootstrapping, the interdependent use of covariation and mechanism information, as a requirement of scientific reasoning. That is, to reason scientifically includes sound decisions such as “to treat a covarying factor as causal when there was a possible mechanism that could account for how the factor might have brought about the effect and were less likely to do so when mechanism information was absent” (Zimmerman, 2000, p. 123). Generally causal reasoning allows scientists to predict and control the environment by structuring chaotic flux of events into meaningful episodes (Buehner & Cheng, 2005). In terms of experimental design, Langley and his colleagues (1987) explained causality as the change occurring in a dependent variable when the value of an independent variable is altered. Similarly, they explained bootstrapping as the use of evidence in conjunction with theory to test hypotheses. In addition, Dunbar and Fugelsang (2005) identified that causal reasoning is extensively used when scientists encounter unexpected findings.

Inductive and Deductive reasoning

Inductive and deductive reasoning are two of the most frequently used types of reasoning in the scientific process that may lead scientific discoveries. Sloman and Lagnado (2005) defined inductive reasoning as a mental activity that takes us from the observed to the unobserved. They alleged that the essence of inductive reasoning relies in "its ability to take us beyond the confines of our current evidence or knowledge to novel conclusions about the unknown" (p.95). Dunbar and Fugelsang (2005) explained that inductive reasoning is used by scientists when they try to recognize the rule that governs them by observing a series of events. Or as stated by Popper (2002), inductive reasoning involves making inferences passing from singular statements to universal statements. That is, passing from accounts of the results of observations or experiments to hypotheses or theories.

On the other hand, deductive reasoning refers to the process of identifying conditions and/or assumptions in which an hypothesis may lead to, or is deducted to, a conclusion (Dunbar & Fugelsang, 2005). That is, testing hypotheses or theories by means of empirical applications of the conclusions that might be derived from it (Popper, 2002). Deductive reasoning has the main strength that if an argument is judged to be logically valid and if the premises are true, then they will lead to true conclusions as well (Evans, 2005). However, Dunbar and Fugelsang alleged that inductive and deductive reasoning may sometimes lead to errors. Such is the case for content and context errors that are commonly found in deductive reasoning. A context error, for example, may assume a conditional relationship that is actually bi-conditional. A content error may modify the interpretation of a conclusion based on its degree of plausibility.

Distributed reasoning

Distributed reasoning has been defined as a reasoning process used when scientific discovery processes are applied and is done by groups of scientists, not individual scientists (Dunbar, 1999). Distributed reasoning has also been described as particularly important at critical moments like hypothesis formation, experimental design, data interpretation, and discovery (Dunbar, 1999; Thagard, 1997). Dunbar alleged that the most common event occurring during social interactions is an attempt to consider multiple representations and explanations for the data, model, or theory in question. The result may take multiple forms, sometimes the result is a generalization, some times multiple hypotheses can be generated. Dunbar argued that as varied the group knowledge base is, the better the result. For example, if a group has a varied background, multiple and different analogies may be generated to solve or explain the problem under study.

Scientific Discovery Processes

The scientific discovery process is a special case of problem solving that involves a cognitive information processing perspective (Langley et al., 1987). Under the cognitive information processing perspective the main source of knowledge is reason (Driscoll, 1994). Therefore, under this perspective reasoning processes take an important role. When applying scientific discovery processes, related scientific ways of thinking or reasoning include causal, analogical, inductive, deductive, and distributed reasoning among others. Langley and his colleagues postulated problem solving as “an information-processing system that creates problem representations and searches selectively through trees of intermediate situations, seeking the goal situation and using heuristics to guide this search (p.8).” Langley et al. argued that ways in which the scientific discovery process is similar to problem solving in that it involves decomposing the problem into simpler ones and attacking those sub problems. However, they also pointed out some differences, such as scientific discovery is often a social process, extending over long periods of time, with goals that are not perfectly defined. Concentrating on the similarities with problem solving, the heuristic-search paradigm has been widely accepted as the general way of solving problems. Langley et al. also argued that which heuristic to select depends on the information concerned to the structure of the task. They also argued that there are different kinds of heuristics, some more general than others. Heuristics derived from very specific knowledge are called strong methods, while more general heuristics are denoted weak methods. These two types of heuristics form a continuum of the abstract to the more domain specific where one end includes very general algorithms requiring little specifics of the domain knowledge, and go toward requiring more information about the specific task, then more domain specific skills are required (Langley et al.).

General activities that take place during the scientific process and that are similar and/or part to the weak methods are: gathering data, finding descriptions of the data, formulating explanatory models, and testing them. The order in which these activities occur is usually cyclical and non-linear. When there is not a set of previously known laws, the discovery process is data-driven or inductive. When the goal is to confirm or extend a theory or model it is theory-driven or deductive. According to Langley et al. (1987), the relationship of these two types of scientific activities is related with the strong and weak methods as follows: when theory or model is being tested, the use of strong methods is more extensive and the discovery procedures involve more domain-specific knowledge. In contrast, when a data set is the starting point and the search is for a generalization, model, or theory to explain them, the use of more general methods—i.e. weak methods are more extensive. These methods can also be called domain-general strategies. In the same way, Klahr and Simon (1999) identified the two main components of expertise as strong methods described as domain-specific methods, and weak methods described as general control structures for search (i.e. hill climbing, means-ends analysis, analogy, etc.). A model that was influenced by the work of Simon and his colleagues is the Scientific Discovery as a process of Dual Search (SDDS) model. This model, proposed by Klahr and Dunbar (1988), is an integrated model of scientific discovery that combines domain-general strategies as well as domain-specific knowledge. The SDDS model is described as a process of search in two spaces: the hypothesis space and the experiment space. The search in the hypothesis space is informed by prior knowledge and the intention is to identify hypotheses that can account for some or all of the phenomena in question in a more concise or universal form. The search in the experiment space has the intention to conduct multiple experiments as a way to induce new hypotheses from scientific discovery. The first approach is usually followed by what Klahr and Simon (1999) called theorists, while the second approach is followed by experimenters. In addition to these two processes, Klahr (2002) identified the evaluation of evidence as the process that provides the primary coordination between search in the two spaces.

Key components of contemporary scientific experimentation are the design of experiments and the structuring of research in order to take advantage of unexpected findings (Dunbar, 1999). Dunbar described experimental design as a number of basic processes or steps (a strong heuristic used by experimentalists to produce measurable results). According to Dunbar, the first step consists of choosing an overall method for investigating the hypothesis. He explained that during this step the relation between theory and experiment is the strongest. The second step involves unpacking the design by asking questions about components and values assigned to them. Sub-steps involved in unpacking the design include the verification of the robust internal structure to the experiment, optimizing the likelihood that the experiment will work, performing cost/benefit analyses on possible design components, and ensuring that the results of the experiment will be accepted by the scientific community. One of the important parts of designing experiments is the consideration of experimental and control conditions. According to Dunbar, these conditions have two functions: to guard against error and to generate potentially important unexpected findings. Dunbar explained that an unexpected finding occurs when the result of an experiment is different from what was expected. Dunbar described that after conducting an experiment the next step involves comparing experimental conditions and numerous other conditions. When findings are unexpected the next step is to identify whether the findings are due to methodological error, faulty assumptions, or new mechanisms. In order to identify possible explanations of why the finding was unexpected, replication or change of a protocol is usually done. When the case is that multiple unexpected findings were obtained after discarding methodological error or faulty assumptions, usually new models emerge. Additional procedural activities to scientific processes usually performed during experimentation include: using apparatus, observing, measuring, recording and interpreting data, performing statistical calculations, and so on (Zimmerman, 2000).

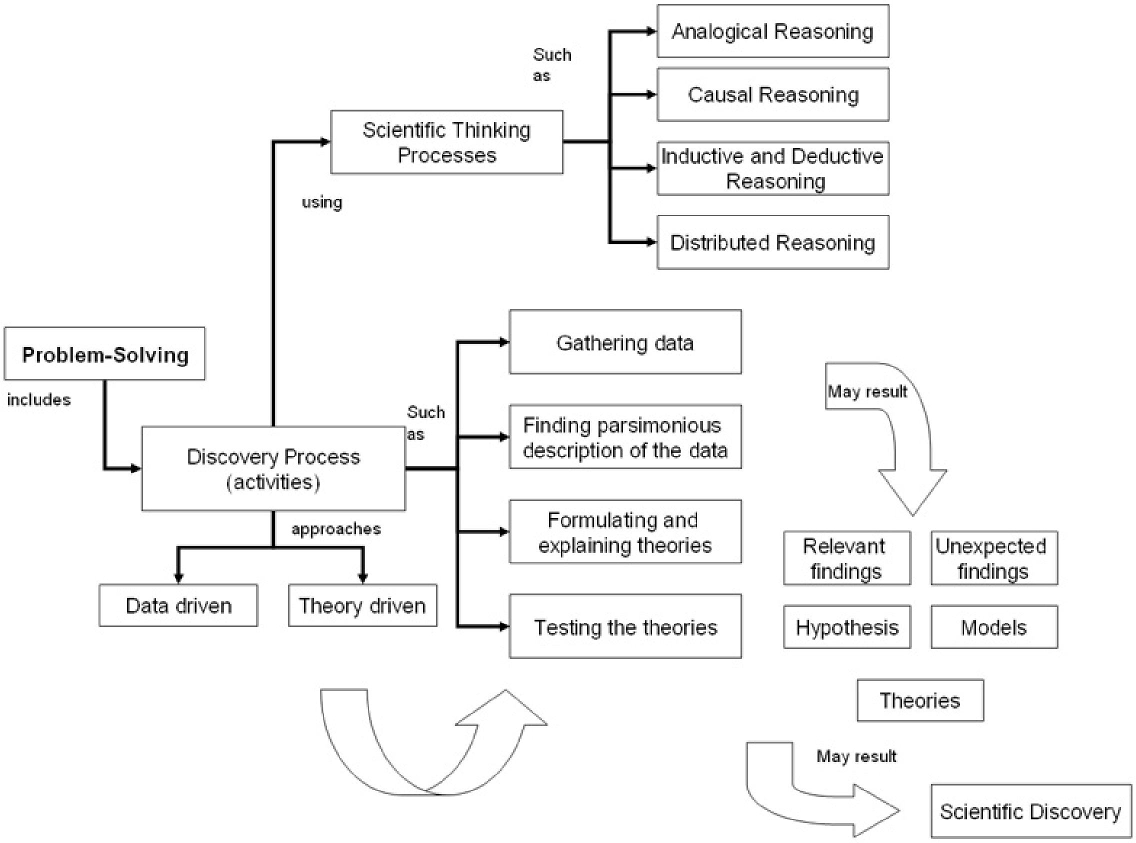


Figure 2.1. Relationship between scientific discovery, scientific thinking and scientific discovery processes.

Figure 2.1 depicts my understanding of the relationship between discovery processes, scientific thinking, and scientific discovery. Discovery processes are considered as a type of problem solving activity consisting of a series of activities or steps that can follow two general approaches—i.e. theory driven or data driven. Scientific thinking is the cognitive part that regulates the discovery processes. Some of these ways of thinking include analogical, causal, inductive, deductive, and distributed reasoning. The result of the combination of these two processes and activities may result in findings such as models, hypotheses that may lead to a scientific discovery.

Mental Models and Modeling

Mental models have been defined as a representation of entities, persons, events, processes, and the operations of complex systems (Johnson-Laird, 2005). Specifically, Johnson-Laird defined a mental model as a structural analog of a real-world or imaginary situation, event, or process constructed by the mind while reasoning. Nersessian (1999) added that a structural analog is "a representation of the spatial and temporal relations among, and the causal structures connecting the events and entities depicted and whatever other information that is relevant to the problem solving task" (p.11). According to Johnson-Laird, thinking involves relying on mental models as a way to enable the thinker to anticipate the world and to choose the course of action. He alleged that this form of reasoning is based on internal manipulations of these models. Similarly, Nersessian (1999) argued that reasoning entails the execution of thought experiments on internal models. Nersessian described modeling practices as the processes of constructing analogical models and reasoning through manipulating them. She argued that the ability to reason with models develops as people learn domain-specific content and techniques. Therefore, reasoning with models entails the formation of a conception of the mental model first, followed by further abstraction to create a formal expression in the form of mathematical model, law, axiom, or theory (Nersessian). Or as stated by Hestenes (1987), in order to understand a mathematical model, a corresponding mental model is required. The processes involved in creating these formal expressions include: a) the representation of one system by another, b) the self-conscious separation of a model and its referent, c) the explicit consideration of measurement error, and d) the understanding of alternative models (Lehrer & Schauble, 2000). Herein, I refer to the process of the creation of formal expressions as modeling.

Scientific Inquiry Learning

Lehrer and Schauble (2006), identified several characteristics of what it means to think scientifically. They argued that scientific thinking is a matter of acquiring strategies for coordinating theory and evidence, distinguishing patterns of evidence, and understanding the logic of experimental design.

Theories of scientific inquiry learning are usually based on theories of scientific discovery (de Jong & van Joolingen, 1998, p. 180). Schauble et al. (1991) identified two main elements of scientific inquiry learning: a) reasoning processes, also called cognitive processes and b) content and structural characteristics of domain knowledge. While the first element refers to processes such as hypothesis testing, measuring, estimating, etc., the second one refers to concepts and misconceptions that people hold, relationships between concepts, comparison between novice and expert knowledge in a specific domain, etc. de Jong and his colleagues (2005) further subdivided the latter process into generic and domain knowledge. They also subdivided reasoning processes into metacognitive and discovery skills. According to de Jong et al., generic knowledge is the knowledge required to understand qualitative or quantitative relations and to appreciate structures of models in a general sense; and domain knowledge is the amount of prior knowledge that a learner has about a specific domain. de Jong et al. defined metacognitive skills as the ability to regulate and control one's learning behavior, while discovery skills were defined as scientific behaviors that can be learned and transferred from one research area to another. de Jong and his colleagues identified these processes as the determinants of discovery learning.

Quintana et al. (2004) and Zimmerman (2000) identified two requirements for solving meaningful problems in inquiry learning: the metacognitive knowledge mapped to the Schauble et al. (1991) reasoning processes, and the concepts and in general disciplinary knowledge mapped to Schauble et al. content and structural characteristics of domain knowledge. There is positive feedback between how theories and knowledge guide experimentation, and how experimentation is the basis for changing students' conceptions (D. Klahr, Fay, & Dunbar, 1993; Schauble et al.). For a summary of the elements and processes involved in scientific discovery see Figure 2.2.

Figure 2.2 depicts my understanding of scientific discovery learning as composed of strong methods and weak methods. Strong methods composed of generic and prior domain knowledge and weak methods composed of transformative and metacognitive skills, may lead to learners' ability to solve meaningful problems.

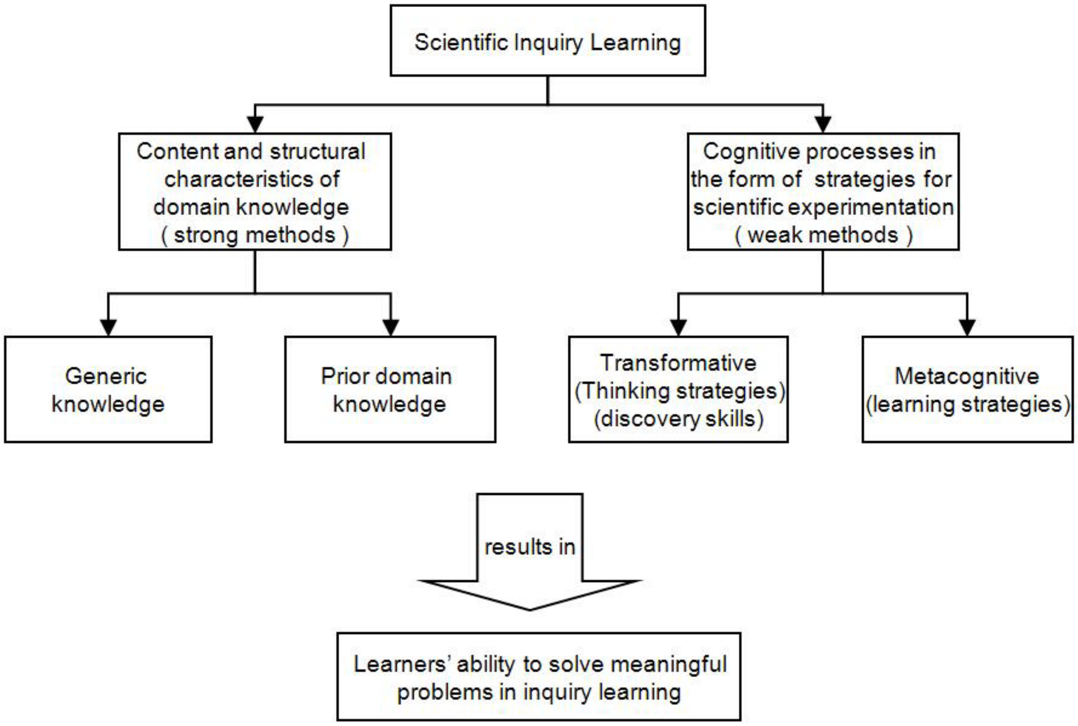


Figure 2.2: Elements and processes involved in scientific inquiry learning

Njoo and de Jong (1993), in an attempt to gain a deeper understanding of the processes that constitute exploratory learning through simulation, conducted observations and think-aloud protocols of university students working in pairs. The students worked on an assignment together with a simulation tool. The outcome of this study was an inventory of 22 exploratory learning processes classified in four main categories: a) transformative processes, b) regulative processes, c) operating the simulation, and d) general processes. Similar classifications were later proposed by Quintana et al. (2004) who identified the constituent process of science inquiry reasoning as: a) sense making, b) process management, and c) articulation and reflection. Since both approaches overlap and complement each other, I propose the following as the constituent processes of scientific inquiry learning with simulation: a) transformative processes, b) metacognitive processes, and c) interaction processes. While the two first cognitive processes are related to scientific discovery and therefore are desired outcomes of scientific inquiry learning; the third one is introduced when collaboration and communication processes take place. This collaboration takes place among team members and communication and interaction with the simulation tools.

Transformative Processes

Transformative processes involve the basic inductive and deductive process operations of analysis, hypothesis generation, testing the hypothesis and evaluation (Njoo & de Jong, 1993; Quintana et al., 2004). Analysis, also called orientation, involves making a broad analysis of the domain such as looking and finding information, exploring models, identifying the variables and the qualitative relations in the model, and identifying the quantitative relations in the model (de Jong, 2006b; Njoo & de Jong, 1993). Hypothesis generation involves choosing for consideration a specific statement about the domain followed by the formulation of a relation between one or more variables and the identification of parameters in the simulation model (Njoo & de Jong, 1993). Hypothesis testing or experimentation involves the design of the experiment, making qualitative and quantitative predictions, manipulation of internal and external variables, data and local output interpretation, and conceptual output interpretation (Njoo & de Jong, 1993). Then a conclusion about the validity of the hypothesis is made (de Jong, 2006b). Finally, the evaluation consists of the process of judging and generalizing based on the findings (Njoo & de Jong, 1993). Although these processes are presented in an ordered manner, this does not mean that learners follow this particular sequence. For example, some learners may use what Klahr and Simon (1999) called an experimentalist approach, while others may follow a theorists approach (de Jong, 2006b; van Joolingen & de Jong, 1991).

de Jong and van Joolingen (1998) and later on de Jong (2006a) identified several difficulties that students may encounter in relation to these transformative processes. They argued that students tend to have difficulties in choosing the correct variables to work with in the process of analysis. Learners in the process of hypothesis generation have difficulties in identifying testable hypotheses and do not drop an original (non-working) goal rather than stating a new one. They also found that students tend to avoid stating hypotheses that could have a high chance of being rejected. The potential source of these problems, as identified by de Jong and van Joolingen as well as Quintana et al. (2004), include the possibility of insufficient prior knowledge.

The problems found during hypothesis testing were the students' inability to design effective experiments and to translate theoretical variables into manipulable and observable ones. de Jong and van Joolingen (1998) argued that part of the problem is due to the fact that students haave a tendency to confirm a hypothesis rather than to disconfirm it, sometimes not trying to understand the model and instead looking for a particular outcome; or do not test the hypothesis at all. The researchers also identified as a problem that students change too many variables at the same time resulting in their inability to draw conclusions. Finally, for the case of the hypothesis evaluation process the problems described were the students' inability to: a) draw the correct conclusions from the experiments, b) link experimental data to their hypothesis, and c) make predictions and interpret the data correctly. The sources of these problems include the fact that students do not use all the information they were provided, but only a limited set of it.

To address these problems Quintana et al. (2004) presented a set of scaffolding guidelines that include the use of representation and language that bridge learners' prior conceptions, organization of tools, and artifacts that make disciplinary strategies explicit to learners, and use of multiple representations that make explicit underlying properties of data.

Examples of successful scaffolding strategies identified by de Jong and van Joolingen (1998) to activate students prior knowledge include: a) providing extra information into the simulation learning environment in the form of an hypertext/hypermedia system, b) incorporating intelligent tutoring systems, and c) providing instruction before using the simulations or prompting students with just in time information embedded in the simulation environment. Other examples intended to help students in their process of hypothesis generation are the use of: a) a hypothesis menu that presents parts of hypothesis, variables and connectors, b) hypothesis scratchpads that allow learners to assemble their own hypothesis, c) predefined spreadsheets that require/force students to make qualitative predictions, d) a list of predefined hypotheses and e) forcing students to state their hypothesis before allowing them to conduct experiments.

de Jong and van Joolingen (1998) as well as Veermans, van Joolingen and de Jong (2006) identified a set of heuristics intended to scaffold students in their designs of experiments, such as advising students to vary only one variable at a time, try extreme values, generate several additional cases in an attempt to confirm or disconfirm hypothesis, and provide examples of adaptive advice and/or intelligent advice based on student's experimentation behavior. Strategies for helping students in their data interpretation process include tools for making predictions and receiving feedback. An example is the inclusion of graphic tools that allow students to draw curves depicting their predictions and providing feedback showing them the correct curve together with explanations.

Modeling is a complementary approach to transformative processes that involves causal and analogical reasoning. Scientific modeling has been identified as a scientific inquiry learning approach including key components such as creating models embodying aspects of theory and data, evaluating them using criteria such as accuracy and consistency, revising them to accommodate new theoretical ideas or empirical findings, using them, and engaging in discussions about models and the process of modeling (Schwarz & White, 2005). On the other hand, simulation tools for modeling may provide new ways of creating models, testing ideas, and analyzing data. According to Schwarz and White (2005), by using this approach students can: a) represent and externalize their thinking, b) visualize and test components of their conceptual ideas, c) advance in their thinking and develop subject matter expertise, d) develop accurate and productive epistemologies of science, and e) better reason about scientific evidence and better integrate their conceptual knowledge. Similarly, van Borkulo, van Joolingen, Savelsbergh, and de Jong (2008) described the modeling process as a way to: a) create the models to represent ideas, b) run the model to compute the values of the variables as they develop over time, c) identify the course of events predicted by the model, d) evaluate the calculated values by comparison with predictions or data collected in an experiment, and e) accept the model or decide to revise it. By applying Klahr and Dunbar

SDDS framework, van Borkulo and her colleagues argued that in this approach the model would be an element of the hypothesis space and the data evaluating the model would derive from the experiment space. Moving within the hypothesis space may represent changes in the model while moving within the experiment space may represent the search for empirical evidence in the model.

A more detailed approach in the area of physics instruction is the modeling process presented by Hestenes (1987). According to Hestenes, an initial stage before the formulation of the model would be the description of the model. In this stage the output is a set of names and descriptive variables of the model together with physical interpretations for all the variables. A second stage would be the formulation stage of the model in which physical laws are applied to determine the equations (e.g. equations for the model and subsidiary equations of constraint). The third step described by Hestenes is the ramification stage. In this stage the properties and implications of the model are described. The final stage is the validation stage that involves the evaluation of the ramified model.

Difficulties identified by Schwarz and White when adopting model-creation instruction are: a) instructors may lack modeling knowledge, b) instructors may face curricular and time constraints, and c) students may not always understand the purpose of engaging in the process of modeling (Smith as cited in Schwarz and White, 2005). The approach proposed by Schwarz and White to overcome some of these difficulties involve providing students with opportunities for carrying out experiments to test competing hypotheses and by providing opportunities for debating the merits of alternative models. This approach proved to be successful with young learners, who were able to identify abstract representations as models and to show how models can be used to predict and explain. However, these students still demonstrated some difficulties in evaluating and revising the models. On the other hand, for the case of older learners, Hestenes (1987) proposed a dialectical teaching strategy with the following elements: a) explicit formulation of systems that are part of common sense beliefs, b) check for external validity for consistency with empirical evidence, c) check for internal consistency among beliefs, and d) comparison with alternative and/or conflicting beliefs.

A different approach to modeling is what Penner (2000) called synthetic modeling. Synthetic modeling is different from other forms of scientific inquiry such as testing theories. It involves reproducing the functionality of the phenomena of interest typically by means of computer-based tools. According to Penner, in educational settings this type of modeling is valuable because it allows the: a) capturing of student's conceptions of natural phenomena, b) improving students understanding of the natural world, and c) reflecting on students own thinking and doing. With this approach Penner alleged that the focus is not on the correctness of the model, but on the degree to which the model behavior can account for the real phenomenon to be modeled. These types of models based on differential or partial differential equations are powerful tools for exploring dynamic phenomena. Penner also addressed three main drawbacks of this modeling approach: a) the level of interaction with real-world systems makes these mathematical models inflexible or fragile, b) models based on calculus may be beyond the mathematical capabilities of learners, and c) highly abstract mathematical models are far from the student's everyday knowledge of the world. Penner did not suggest strategies for overcoming these drawbacks; however, he emphasized the use of programmable media as a way for learners to engage in deep and precise mathematical and scientific modeling. Three educational approaches of modeling described by Lohner, van Joolingen, Savelsbergh and van Hout-Wolters (2005) are: explorative modeling, expressive modeling, and what is called inquiry modeling. In explorative modeling learners explore a given model and possibly extend it. In expressive modeling learners construct their own computer model. In inquiry modeling learners combine these two approaches by integrating a modeling environment into an inquiry-learning environment. The process suggested by Lohner et al. to incorporate inquiry modeling involves merging the modeling cycle proposed by White and Shimoda (1999, as cited in Lohner et al.) and a generic modeling process. They argued that both approaches are similar since both resemble the way scientists work. This process consists of the following transformative processes: a) the orientation stage that can be merged with the model sketching process, b) the hypothesizing stage that could be combined with model specification and prediction of the output, c) the experimentation stage where the model is implemented and run multiple times, and d) the conclusion stage in which the model is evaluated.

Metacognitive Processes

Metacognitive processes involve learners' awareness of their own cognitive processes, as well as their ability to control them (Weinstein & Mayer, 1986). In the context of scientific discovery learning, Quintana (2004) referred to these as articulation and reflection processes that include constructing, evaluating, and articulating what has been learned as a result of conducting experiments. Metacognition also refers to the students' ability to control their cognitive processes by selecting among cognitive strategies such as monitoring, evaluation, and revision of their strategies they used. Njoo and de Jong (1993) referred to these processes as regulative processes. Regulative processes include the strategic decision in controlling the inquiry process (Quintana et al., 2004), through planning, verifying, and monitoring (Njoo & de Jong).

de Jong and van Joolingen (1998), Quintana et al. (2004) as well as de Jong (2006a) concluded that, in general, learners face difficulties in planning and monitoring their progress. Quintana et al. also argued that these processes not only refer to the results found in an experiment but also the reflection on the learning process and the acquired knowledge (de Jong, 2006a). Researchers argued that part of the problem is difficulties students with low prior knowledge have setting their own goals (de Jong & van Joolingen, 1998), learners lack strategic knowledge (Quintana et al., 2004), and learners are easily distracted with unimportant managerial tasks (Quintana et al., 2004).

To address these problems Quintana et al. (2004) suggested organizing the task in steps or providing useful boundaries to learners such as embedding expert guidance together with the simulated learning environment and reducing cognitive demands by automating non-salient tasks. Quintana et al. also recommended providing reminders and guidance to learners to help them facilitate planning, monitoring, and articulation in order to conduct reflection through their inquiry process.

de Jong and van Joolingen (1998) reported the following examples as successful implementations of scaffolds addressing difficulties with regulative processes: a) sequencing the instruction and the experimentation process, b) using gradual progression in the level of complexity, c) providing support for planning tasks, d) providing prompt questions as a way of guidance, e) offering tools to store and manage numerical and nominal data from experiments, f) providing structure and systematic environments requesting students to write down variables, parameters, hypothesis, predictions, etc., g) using a system that allows students to select previous experiments in order to provide a comparison point, h) designing different types of assignments with different cognitive purposes such as assignments for investigation, assignments for specification and prediction, and assignments for explication, and i) incorporating reflection prompts in the form of short questions asking about learners' progress and actions.

Interaction Processes

Interaction processes refer to processes involved in operating the simulation (Njoo & de Jong, 1993), and any other technology that is involved as part of a learning task (e.g. chat tools, text editors, etc). I would also consider other interaction processes such as those described by Swan (2003), who identified four different types of interaction: a) interaction with content, b) interaction with peers, c) interaction with instructors, and d) interaction with interfaces. According to Swan, interaction with content refers to learners' interactions with the course materials and the concepts and ideas they present; interaction with instructors refers to ways in which instructors teach, guide, correct, and support learners; interaction among peers refers to ways of interacting among learners such as debate, collaboration, discussion, peer review, etc.; and interaction with interfaces refers to interaction that takes place between the learner and the technology.

Interaction with the interface requires cognitive effort that if not appropriately designed, will distract the learner from the main task. For example, Clariana and Strobel (2007) argued that increasing the amount and complexity of the simulation output, will result in an increase in the learners' cognitive load. According to Woods (1991) designing for availability and accessibility are the elemental factors of data display in the area of human interface design. He suggested however, that interfaces designed only for data availability are not able to address the problem of data overload. He further explained that interfaces designed for availability do not provide cues for the users to help them decide what the right data is at the right time. An example of a technique that addresses this problem is signaling (Mayer, 2006), which refers to a technique in which certain cues are added to the system to help the learner identify how to process the material.

Although a whole set of literature exists in the area of human-computer interaction as well as in the area of human factors that addresses these problems specifically, this is not the main focus of this dissertation work so I will briefly discuss the general principles of interface design for multimedia learning. Mayer (2006), presented seven techniques for coping with complexity in multimedia learning: a) offloading the presentation of information in spoken rather than in printed form, b) segmenting to provide control to the learner for self-paced instruction, c) pre-training to provide previous instruction in the names, characteristics of system components as well as basic operation, d) weeding of extraneous materials that are non-relevant to the topic, e) signaling system capabilities to provide cues on how to process the material, f) aligning the presentation of printed words near corresponding parts of graphics, and g) synchronizing the presentation of narration and animation simultaneously.

Two more aspects that can be considered as part of the interaction processes that are also highly related with the transformative processes are the level of fidelity and level of transparency of the simulation. According to Alessi (2002), fidelity refers to the level of realism, also described by Cannon-Bowers and Bowers (2007) as authenticity. In this sense, Alessi argued that for the case of educational simulations fidelity not only should be high, but it must also be simplified. Alessi as well as Reigeluth and Schwartz (1989) also discussed the relationship between the level of fidelity and learners expertise; they argued that when learners are novices, lower fidelity may be better. A second way in which data overload may be addressed (Woods, 1991) is by implementing dynamic fidelity (Alessi, 2002; Reigeluth & Schwartz, 1989) that occurs when the realism and complexity of various simulation elements begins at a low level and increases gradually (2002).

Tanimoto (2004) defined transparency as “a property of some systems where the inner workings and the design of the system are visible to users” (p.1). The two most common approaches for simulation transparency are black box and glass box simulations

(Resnick et al., 2000). Glass box simulations differ from black box simulations by providing learners with visibility (Du Boulay et al., 1999); i.e., the ability to inspect and modify the equations that constitute the simulation's model (Murray, Winship, Bellin, & Cornell, 2001). Murray and his colleagues argued that while using a black box approach in a simulation is done purposefully, there might be situations in which students need to be able to inspect the form and function of the equations or rules that drive the simulations. Alessi (2002) provided the following scenario as an example: The black box approach may be used if the learning goal is concrete or situational and deals with particular observable variables of situations, or when the main purpose of inquiry is to identify a relationship between variables. In the glass box approach, students can benefit more if the activity is more explanatory. In this case students have to hypothesize about the underlying principles or mechanisms and the same is true when the learning goal is to criticize an existing model. In addition, authenticity as well as transparency have been related to the students' level of engagement (Cannon-Bowers & Bowers, 2007; Resnick et al., 2000) in which the learning environment causes learners to engage in cognitive processes in similar ways as experts do.

Two research needs identified by van Joolingen, de Jong and Dimitrakopoulout (2007) related to the interaction between peers and instructors are the need to identify ways in which collaborative inquiry can be incorporated into computer simulations for inquiry learning and the need to identify what the role of the instructor should be, as well as what is the right combination between scaffolds from the instructor and scaffolds from the software. For the case of incorporating collaborative learning with discovery learning, Okada and Simon (1997) conducted an experiment in which they compared students working alone with students working in pairs in a computer micro-world. They found students who worked in pairs were more successful in their discoveries and were more active in the explanatory activities. They also concluded that explanatory activity is not predictive of discovery unless it is combined with appropriate experimentation. However, research has not provided the answer to how to implement collaboration in computer simulations with inquiry learning, although successful principles of collaborative learning in the engineering education domain might be applied. Such is the case in the pedagogies of engagement proposed by Smith et al. (2005). They suggested the following guidelines for successful implementation of formal cooperative learning groups: a) positive interdependence that can be established by the instructor using strategies such as setting goal interdependence, setting role interdependence, etc. b) face-to-face interaction that can also take the form of online interaction using technologies such as chat rooms or discussion forums, c) individual accountability/personal responsibility that involves assessing each students' individual performance, d) teamwork skills built by directly teaching them skills such as decision-making, trust-building, communication, etc., and e) group processing, which can be implemented together with metacognitive processes such as articulation and reflection.

CHAPTER III

METHODS AND RESEARCH DESIGN

Rationale and Significance

The media versus method debate was initiated by Clark (1983) after conducting a meta-analysis of quasi-experimental controlled studies focused on media comparison. He argued that the choice of a specific media for delivering instruction does not directly influence the students' learning benefits. Clark also concluded that what produced differences was the method and not the media. I agree with Clark that the method of instruction is critically important, but from my perspective he made three wrong assumptions. First, after reviewing the studies that Clark selected, I noted that he did not use a variety of media. He focused on face-to-face teaching as the comparative control group versus teaching with media such as television or computer-based learning. Second, by considering only quasi-experimental designs, he did not take into account the interaction among different variables that usually take place in complex learning settings. Third, he argued there is independence between the instructional method and the media. Today, however, technological advances allow not only the merging of method and media (Linn, Davis, & Bell, 2004), but also provide affordances that support instructional strategies that without technology would not be possible (Winn, 2002). 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 (Kozma, 1991).

Computer simulation tools can provide students with the ability to do things that they could not do in the real world (Winn, 2002). Therefore, by means of under experimental or quasi-experimental designs, extensive research has been conducted that is focused on how to support inquiry learning with computer simulations (de Jong, 2006a;

Linn et al., 2004; Quintana et al., 2004). However there are still a number of research issues that need to be addressed. One type of research issues that needs further investigation is related to gaps in this area, and the second is related to the method of inquiry. For the case of gaps in the field that need further investigation, de Jong (2006a) pointed out the following research issues need to be further investigated: a) the impact of the complexity of the cognitive tools in the students' memory capacity, b) ways in which the learning environment may adapt to the differences and levels of expertise among students, c) ways to combine collaborative and inquiry learning, and d) achieving the right balance between inquiry learning and direct instruction. In relation to the last point, Hennessy and her colleagues (2007) noted the need for studies that will contribute to identifying the role of the instructor when incorporating simulation tools. In particular, identifying how instructors in different settings think about the pedagogical affordances of inquiry learning environments (van Joolingen et al., 2007). Furthermore, there is a need to identify effective ways to provide instructors with appropriate supports to facilitate appropriate scaffolds (Brush & Saye, 2002).

The majority of the methodologies used to study the second research issue, the method of inquiry, have the drawback that have not taken into account the interaction between different variables that usually effect in complex learning environments. Such may be the case with the influence of students' expectations of the task or the effect of direct instruction. Consequently from a research design point of view these studies lack ecological validity; from a practical point of view, there is a lack of practical application of previous findings (Winn, 2002).

In summary, for this study I had adopted a cognitive information processing perspective in which the most important source of knowledge is reason. I therefore identified the scientific thinking processes that inform and support scientific discovery processes. These ways of thinking may include causal, analogical, inductive, deductive, and distributed reasoning among others. The scientific discovery process is a special case of problem solving that involves the application of processes and procedures such as analyzing the problem or experiment, gather the data, generate, test, and evaluate hypotheses and so on. By identifying these ways of thinking and experimenting I have tried to understand how these same experiences have been adopted in learning environments through scientific inquiry. In particular, I have focused on the use of computational simulations for understanding and building models, and have tried to identify the problems and the gaps that exist in this area.

Table 3.1: Overview of research studies

	Study One	**Study Two**	**Study Three**		
Method	Survey	Phenomenography	Case Study		
Chapter	I	IV	V	VI	VII
Participants	Graduate students (G) Undergraduate students (UG) Freshmen undergraduate students (FUS)	Instructors (I)	Instructors (I) Students (S)		
	G=189 UG=24 FUS=338	I = 6	I=6	S=25	I=4 S=25
Focus of Inquiry	What are engineering students' perceptions and experiences of computational simulations as learning tools?	What are qualitative different ways in which engineering instructors perceive and experience computational simulations as learning tools in terms of their learning outcomes?	What are engineering instructors' perceptions and experiences of computational simulations as learning tools in terms of their learning outcomes, evidence of the learning and pedagogical approaches?	What are engineering students' perceptions and experiences of computational simulations as learning tools?	How do engineering students' perceptions and experiences of computational simulations as learning tools compare to their instructors' perceptions and experiences of the same tools?

In order to capture the complexity of learning environments that adopt this type of tools, this study therefore builds upon the body of knowledge of scientific discovery processes with computer simulation tools for learning. In this study I attempted to identify different qualitative ways in which students and instructors perceive and use simulation tools in a naturalistic learning environment. Therefore, appropriate guiding research questions for this study were:

1. What are instructors' perceptions and experiences of using simulation tools as part of their instructional practice?
2. What are students' perceptions and experiences of using simulation tools?
3. What are students' reactions to professors' goals and instructional approaches of using simulation tools?

In Table 3.1 I present an overview of the different studies that were developed as part of this dissertation work. Even though these studies focused on similar aspects of the world such as perceptions and experiences, they differed and complemented each other in multiple ways. Study One differed from Study Two and Study Three in the research methodology. While Study One employed quantitative research methods, Study Two and Three employed qualitative research methods. Whereas, the quantitative portion was more objective focusing on counts and measures of aspects of the world, the qualitative portion was more subjective identifying descriptions and meanings of aspects of the world.

Study Two and Study Three had a fundamental distinction in their perspectives. Marton (1981) differentiated between what he called the first-order perspective and the second-order perspective. While the first-order perspective aims at describing various aspects of the world; the second-order perspective aims at describing people's ideas and/or experiences of various aspects of reality. The emphasis of Study Two was on the second-order perspective while the emphasis on Study Three was on the first-order perspective. Marton (1981) argued that first-order and second-order perspectives are complementary in the sense that "we would deal with both the conceptual and the experiential, as well with what is thought of as that which is lived. We would also deal with what is culturally learned and with what are individually developed ways of relating ourselves to the world around us (p.181)." On the other hand they are autonomous in the sense that the second-order perspectives cannot be deduced from descriptions arrived at from the first-order ones.

Finally, the three Phases of Study Three focused on two different populations. Phase 1 focused on instructors' perceptions and experiences with simulation tools, Phase 2 focused on students' perceptions and experiences with simulation tools, and Phase 3 compared and contrasted both experiences. Specifics of the methods of inquiry employed are described below.

Method of Inquiry

The goal of this study was twofold. The first goal was to describe different ways in which instructors and students perceive and experience computational tools. The second goal was developing a model for the use of computational simulations as learning tools. An appropriate two-phase research design that allowed the identification of different ways to experience simulation tools, and then identify and make comparisons among them required a multiple-case research study design. The data analysis for this research study therefore began with a phenomenographical study to identify different ways simulation tools were perceived and experienced. The study continued with individual case studies of participants' experiences followed by a cross-case pattern analysis.

Study Two

Since one of the goals of this study was to describe and explain experiences in educational settings; methods of phenomenography were borrowed to conduct the initial inquiry process (Marton, 1981). Characterizing how something is thought about, experienced, perceived, and/or described in terms of their content is by definition a qualitative question (Marton, 1988). By using methods of phenomenography, I sought to describe and explain instructors and graduate engineering students' perceptions, experiences, and conceptualizations of simulation tools in a learning task.

Phenomenography is a research method specialization that developed from empirical bases rather than philosophical or theoretical ones (Aakerlind, 2005; Marton, 1994). Phenomenography originated in Sweden in the late 1970's and was first reported in 1981 (Marton, 1981). According to Marton, "phenomenography is the empirical study of the limited number of qualitatively different ways in which various phenomena in, and aspects of, the world around us are experienced, conceptualized, understood, perceived, and apprehended (p. 4424)."

Marton (1981) made a fundamental distinction between what he called the first-order perspective and the second-order perspective. While the first-order perspective aims at describing various aspects of the world; the second-order perspective aims at describing people's ideas and/or experiences of various aspects of reality. The emphasis of phenomenography is on the second-order perspective. In other words, phenomenography is not uniquely concerned with the phenomena being experienced and thought about, the human beings who are experiencing or thinking about the phenomena, or the perception and thought as abstract phenomena separated from the subject matter of thought and perception. Phenomenography is concerned with the relations and conceptions of human beings and the world around them; whether these conceptions are right or wrong (Marton, 1988).

The main outcomes of a phenomenographic study are "categories of description" and the distribution of subjects among them (Marton, 1994, p. 4424); while the first result is qualitative in nature, the second is a quantitative one (Marton, 1981). The categories of description are different experiences, understandings, and so forth reasonably related to each other and forming hierarchies in respect to a given criteria. These logical hierarchies of categories are denominated the "outcome space." Marton emphasized that the appearance of the same categories of descriptions in different situations is stable and generalized between them; even though it might be the case that individuals experience different categories at different times.

Study Three

During Study Three a cross-case analysis was conducted. According to Eisenhardt (1989), the case study is a research strategy focused on understanding the dynamics within single settings. In this case, the setting focused on each individual engineering course employing multiple levels of analysis within a single study. Starting from the categories of description identified in the first phase, common themes and patterns among the instructor and his/her students were described. This in turn, contributed to a grounded theory of use of computational simulations as learning tools by focusing on perceptions and experiences.

Participants

The participants for this study were selected purposefully from a population of faculty members involved in the Network for Computational Nanotechnology (NCN) who used simulation tools as part of their instruction. Six faculty participants who used the nanoHUB.org as part of the instruction were invited to participate in this study. One more professor who used a commercial numerical computing environment and programming language was also invited to participate. The study also included 25 students enrolled in courses taught by the faculty in this study. Several criteria were used to select participants. First, students were selected to participate if they were enrolled in an engineering course whose instructor incorporated simulation tools as part of the learning activities in the course. Also, the simulation tool was incorporated at a curricular level rather than a lesson level, and the students volunteered to participate in the study. Since the NCN is a multi-institutional center lead by Purdue University, other universities also participated. Instructors involved with this study were using the nanoHUB.org resources as part of their own ongoing course improvement.

Procedure

For the case of participant professors in the study, the directors of the Network for Computational Nanotechnology together with Dr. Brophy and I invited six faculty members who used computational simulations as instructional tools to participate in this study. Faculty willing to participate in the study were interviewed to identify their perceptions, goals, and instructional approaches for using computational simulations as learning tools. We also requested that the professors provide a copy of the assignment description accompanying the simulation tool. Of the faculty members participating, those at Purdue University were invited to participate in a second level of analysis in which they were asked for permission for me to conduct classroom observations.

Students were invited to participate in this study at two different levels. I used the anonymous survey that has been used in the past by instructors as a formative feedback for their course. All students were invited to complete this anonymous survey that focused on their attitudes towards the simulations and their experiences while interacting with them. The second level of student participation consisted of interviews and reflection/think-aloud protocols of students interacting with the tools. The recruitment of participants was done after class, when the instructors and TAs had left the classroom, so that students did not feel pressured to participate. For each student in the class, I provided an individual index card containing a schedule of days and times at which I could conduct their interviews. Interested students put their names and email addresses in the corresponding slot of days and times in which they are available to meet with me, and returned the card to me. Random selection was done if several participants have signed up in the same time slot; although preference was given to female students. Students selected for participation in the interviews were contacted by email for the meeting location. The compensation for students participating in the study was a $25.00 gift certificate.

Data Collection Methods

Booth (1997) suggested open-ended deep interviews as the most common and dominant method of discovery. Interviewing permits an in-depth exploration of a particular topic or experience and, thus, is a useful method for interpretive inquiry (Charmaz, 2006). Some other methods could be applied, such as group interviews, observations, drawings, written responses, historical documents etc. For this study I collected the data using a variety of methods: semi-structured interviews, reflection protocols, surveys and classroom observation. Recorded semi-structured interviews were the main data collection method. Interviews started with structured guiding questions asked in as open fashion as possible to let the participants choose the dimension of the question they would like to answer; consequently revealing the participants' relevance structure (Marton, 1988). These interviews gathered data about participants' reflection on their experience of the phenomena dealt with (Marton, 1994). The interviews explored different ways in which the interviewees were aware of their experience with the simulation tools (Marton, 1997). The conversation focused on interviewees' experiences, goals, beliefs, approaches; and I helped them reflect on how they have experienced simulation tools in the context of a particular engineering course. The main focus of the interview questions were aimed at identifying instructors' perceptions and experiences within three main areas. These areas were based on Wiggins and McTighe's backward design process (1997) composed of three main stages including: a) identifying the desired learning outcomes, b) determining the acceptable evidence of learning, and c) planning the experiences and instruction. The interviews were recorded with a digital video camera. The interview protocol used for all of the instructors is displayed below.

Opening Statement:

We would like to thank you for the time you had taken to participate in this study. The purpose of this study for us is to try to learn more about how professors use nanoHUB resources as part of their instruction. Therefore we would like to ask you a few questions about your goals and process for the use of the simulation tool. And, as a manner of procedure though before we get started, we'd like to record our conversations mainly to help us remember what we talked about.

We would also like you to please take a time to read and if you agree sign the consent form. (note: give a moment for the participant to read the consent form and explain all items).

Do you have any questions for me before we get started?

Interview:

1. Who are the students? What is the level of the students?

2. What type of course is this? (e.g. graduate, undergraduate)

3. How many students are usually in your class?

4. What is the course about? What are big objectives of the course?

5. How often do you use the nanoHUB?

6. To what extent does the nanoHUB help you accomplish these objectives?
   —OR—
   How do you use the nanoHUB to accomplish these objectives? (e.g. in the classroom, in the homework assignments, etc)

   [PROBE—probing for more in-depth detail of the uses and goals of the use of simulation tools.]

7. Please describe what you consider as acceptable evidence that students have achieved these objectives.

8. In terms of educational benefits, what are the advantages of the simulation tool(s) you used in your course(s)?
   —OR—
   What do you consider most helped your students during their learning process?

   [PROBE —how do you think the simulation tool(s) lead to students' conceptual understanding (e.g. explain or predict behavior).]

   [PROBE —What is it about the simulation and/or the learning activities that help students develop a practical understanding and/or the fundamental relationships of the (mathematical) model?]

9. How do you structure your activities to achieve your learning goals?

10. What do you think are the most important features of these activities around nanoHUB simulations that promote learning with understanding? (I.e. students' ability to reason about these models to be able to explain and predict their behavior).

    [PROBE —what is it about the way you set up the activities, or the way your students use it that promote this learning with understanding?]

    [PROBE — do you ask your students to make some kind of interpretation of the output?]

    [PROBE — How do you see students guiding their own inquiry with these simulations?]

    [PROBE —when do you think they make the insights they need to be able to use these concepts in their own investigation of questions they may generate?]

11. What aspects of the simulation tool(s) do you consider inhibited your students' learning processes?

12. Not considering computational performance, what do you consider can be done to make nanoHUB more useful for students' learning?

13. Is there anything else you would like to tell us about nanoHUB simulations?

The interview protocol used for all of the students is displayed below.
Opening Statement:

Thank you again for agreeing to participate in our study. Before we start I need inform you about our process and request your consent to participate in the interview.

<Explain IRB form and protocol>

PART 1 - We are interested in learning more your experience with the recent homework involving the nanoHUB simulations. Could you please tell me…

1. What was your experience of using the nanoHUB for the first homework assignment?

2. What do you think was the purpose of the homework activity using the nanoHUB simulation?

    - What do you think was the professor learning goal?

3. Which portion of the assignment did you find the most challenging?
    - What was difficult about that part?
    - Using your homework and the simulation. Could explain for me how you approached the problem and the specific areas you had difficulty? Please feel free to provide description of your thinking used to get past your difficulties with the problem.

4. When you were solving the homework assignment, how confident were you with the required knowledge to solve it? Was your prior knowledge sufficient to complete the activities? What was missing? What questions would you like answered in order to be better prepared to work on an activity like the one in the assignment?

5. After completing the activity, what was new for you that you did not know before?

   – OR--
6. What have you learned from this activity?

7. How did the simulation tool help you the most during this home work activity?

8. How did the simulation tool inhibit your learning process?

   – OR--
9. Did you have difficulty interpreting the output?

10. How confident are you of your level of performance for this homework activity?

11. What kind of feedback are you expecting to have?

12. What kind of feedback would you like to have?

13. How long did you use this particular simulation tool? (In hours and or number of times).
    - Do you think this was time well-spent?

14. What more could have been done to improve your success toward learning the material with the nanoHUB resource?

15. How do you think you can apply what your have learned in homework 1 to solve a real problem or situation? Explain. (Examples can be used).

16. Have you used and/or will you use the simulation for your own interest? If so, why and how?

17. Do you have any suggestions for how to make this learning activity more effective for your learning?

PART 2 - I have several additional questions about the course in general

1. Why are you taking this course?
2. How this course compares to others you have taken as a graduate student? (e.g. level of difficulty, etc)
3. How is this course related to your areas of interest? Is the material or topic exciting for you?

I also used the anonymous survey used in Study One that is based on the survey that has been used in the past as a formative feedback of instructors for their course. Surveys were collected using an online server. Once I conducted the interviews and collected the surveys, each interview was transcribed by a third party and I conducted the initial coding. I also conducted the initial analysis of the surveys at the level of descriptive statistics. Classroom observation was conducted for four engineering instructors at the graduate level. The classroom observations were done during an entire semester with the purpose of identifying how simulation tools were incorporated into the learning classrooms. These observations helped me identify the context in which computational simulation tools were used in engineering courses and certain points in the semester to collect data from students in the form of interviews.

Data Analysis Methods

For Study Two, I chose the phenomenographical guidelines of Marton (1997) to conduct an inductive data analysis:

1. Since the analytical procedures of phenomenography are very similar to those of grounded theory (Richardson, 1999); the researcher starts the analysis by transcribing verbatim the interviews, and proceeds by applying the systematic procedures suggested by Strauss and Corbin (as cited in Patton, 2002) to code the data; i.e. open coding followed by axial coding. While in open coding I conducted the first level of abstraction in conceptualizing major ideas, in axial coding I reassembled the data so explanations and relationships of the data may be done.
2. The researcher identifies initial categories describing different ways of experiencing the phenomena. In this particular study I identified students and instructors perceptions and experiences of computational simulation tools and organized and analyzed the data according to that.
3. The researcher conducts this process for each topic or phenomenon one at a time and identifying the similarities but most importantly differences.
4. Since the same participant may express more than one way of experiencing the simulation tools, the researcher abandons the borders between the participants and focus on the experience itself. In this study this was done because the goal was not to identify the ways in which an instructor and student experience the simulation tools, but to identify different ways instructors and students experience the simulation tools in an inquiry learning task.
5. The researcher looks for the structurally significant differences with the intention of clarification. In my case, I looked for how instructors and students defined a specific portion of the experience with the simulation tools.

6. The researcher reduces the analysis outcomes to identify and group expressed ways of experiencing the phenomenon and develops a set of "categories of description".
7. The researcher does several runs of the analysis to determine if the categories are descriptive enough and indicative of the data; this may result in an "outcome space."
8. Then, the researcher orders and identifies logical relations among the categories of description. I did so by identifying relationships between categories of description and comparisons between student's conceptions across different topics.
9. Finally, whenever possible, the researcher conducts member checking.

In short, in Study Two data analysis consisted of an iterative and comparative process involving the continual sorting and restoring of data, ongoing comparisons between the data, and the development of descriptions and comparisons between the categories themselves. Or in practical terms, transcripts and/or selected quotes were grouped and regrouped according to perceived similarities and differences along varying criteria (Aakerlind, 2005).

The principal results of the phenomenographic study are the "categories of description" and the "outcome space". These mean "a description for each of the ways of experiencing a phenomenon and how those ways of experiencing are related to each other" (Orgill 2007, 136). The results are then re-applied to the data so frequencies of the statistical distribution of the categories may be visualized.

For Study Three I chose a case study approach (Eisenhardt, 1989) together with a grounded theory approach (Charmaz, 2006) as guidelines to analyze data for building theory from case studies. In this study the specific cases were four engineering graduate courses whose instructors incorporated simulation tools as part of their pedagogy. According to Eisenhardt, case studies can involve single or multiple cases and multiple levels of analysis.

1. The researcher conducts within-case analysis involving detailed case study write-ups (i.e. descriptions) of each site. This is done in order for the

researcher to become intimately familiar with each case as a stand-alone entity.

2. By developing within-case analysis the researcher identifies patterns emerging of each case before generalizing patterns across cases.
3. The researcher then conducts a cross-case analysis searching for patterns looking at the data in many divergent ways.
4. The researcher selects categories and then looks for within-group similarities coupled with intergroup differences. In this study, the dimensions were the components of Wiggins and McTighe (1997) “backward design process” (p.9) to discuss the participants’ experiences. This process is composed of three main stages. These stages are: a) identifying the desired learning outcomes, b) determining the acceptable evidence of that learning, and c) planning the experiences and instruction.
5. Graphing techniques may be used by the researcher such as 2 x 2 or other cell design to compare several categories at once.
6. Then the researcher proceeds with theorizing, looking for patterns and connections rather than linear reasoning by employing constructivist and objectivist grounded theory approaches as recommended by Charmaz (2006). Constructivist grounded theory originates from interpretive thinking and “sees both data and analysis as created from shared experiences and relationships with participants” (p.130). Likewise, objectivist grounded theory flows from positivism with the belief that data is real and does not focus on the process of production. Charmaz explained that in order to theorize as a grounded theorist, blending both of them together is the best approach.
7. The researcher corroborates the evidence from one data collection method with another one to make the findings stronger and better grounded. In cases when evidence conflicts, the researcher reconciles the evidence by probing deeper on the meaning of the differences. This becomes an iterative process of theory and data comparison that results in the accumulation of evidence from diverse sources on a single well defined construct.

8. Finally, the researcher constructs a compelling argument by discussing how and where his/her work fits or extends relevant literature. This includes an explicit claim why the grounded theory makes a significant contribution to the field.

Researcher Bias and Perceptivity

As the researcher for this qualitative study, there were several potential biases that might have had influenced the results of this research study. However, being aware of my personal biases in the initial stages of the study helped me identify the ways to keep those biases in check.

As an engineer and instructional designer my first instinct was to try to improve practice in my field. Therefore, I was potentially biased toward suggesting ways to improve the educational experiences. Regular discussions with my advisors, as well as keeping a research journal helped me keep this bias in check. As the interviewer, I sought to be open and allowed the data to emerge flexibly, built trust and rapport with my participants, and was reflective and reflexive (Patton, 2002). During the interviews, I concentrated on my participants' awareness and reflection and not on mine (Marton, 1997). As data analyst, I separated description from interpretation from judgment and bracketed my preconceived ideas focusing on similarities and differences between ways in which simulation tools are experienced by the participants (Marton, 1997). I targeted a deep understanding of what participants said and what the experience meant to them.

Another important bias I had is the fact that I do not possess knowledge of the subject matter. Although I cannot change this fact, I conducted recorded classroom observations that gave me a better understanding of how the instructors incorporated the simulation tools into their classrooms, and a way to better interact with my participants during the interviews.

Quality and Credibility of the Study

To make my study credible, I used generic techniques proposed by Patton (2002). In the data collection stage the classroom observations allowed me to gain understanding on how instructors incorporate the simulations, have a general understanding of the knowledge of the subject matter, and establish rapport with my students-participants.

During the interviews I built trustworthiness and credibility through pleasant, purposeful interactions with participants. Also, I was open and reflective and allowed the data to emerge flexibly (Patton, 2002). Finally, I concentrated on my participants' awareness and reflection and not on mine (Marton 1997).

During the analysis of Study Two I made sure to meet the three primary criteria proposed by Marton and Booth and as explained by Akerlind (2005, p. 323) for judging the quality of an outcome space in the phase one of this study:

1. that each category in the outcome space reveals something distinctive about a way of understanding the phenomenon;
2. that the categories are logically related, typically as a hierarchy of structurally inclusive relationships; and
3. that the outcomes are parsimonious—i.e. that the critical variation in experience observed in the data could be represented by a set of as few categories as possible.

During the analysis of Study Three I followed the internal validity for case study analysis proposed by Eisenhardt (1989):

1. discover the underlying theoretical reasons for why a relationship exists. This is done in order to provide a good understanding of the dynamics of such relationship;
2. measuring constructs and verifying relationships by judging the strength and consistency of the relationship within and across cases; and
3. display in detail the evidence and procedures when reporting the findings so that readers may apply their own judgment.

In addition, during the analysis and interpretation stages I systematically searched for alternative themes, divergent patterns, rival explanations and negative cases; an important aspect for identifying the categories of description. I separated description from interpretation from judgment and bracket my preconceived ideas, focusing on similarities and differences between ways in which simulation tools are experienced by the participants (Marton 1997). Also, I targeted a deep understanding of what participants said and what the experience meant to them. In the data analysis process, I sought for multiple ways to verify the data collection and analysis by means of coder and dialogic reliability checks with my advisors, participants, and research group members (Aakerlind, 2005). I also reported any personal data and professional information that might have affected data collection, analysis, and interpretation. Additionally, I spent sufficient time in the field and took repeated measurements to increase the reliability of the study.

In particular, 30% of the interviews with instructors were coded by three other researchers. For the case of the students' interviews, 20% of them were coded by three other researchers as well. For both cases, once coded the interviews independently, the group got together and discussed the coding schemes until we got into a consensus. Also, when the analysis phase ended, I conducted a member checking process with 50% of the instructors interviewed.

Ethical Conduct of the Research

Ethical approval for this study was obtained from the Institutional Review Board. The two main ethical aspects considered were getting students' consent and maintaining participants' confidentiality. A signed IRB approved consent form (see Appendices A and B) was obtained from each participant. This consent forms discussed specific aspects of the study such as the purpose, specific procedures that were used, duration of the participation, risk to the individual, benefits to the individual, the level of compensation for the participant, extra costs to participate, confidentiality aspects, and the voluntary nature of participation in the study. When the participant signed this letter I obtained his/her consent to participate in the study.

In written and in verbal form I emphasized to the participant the voluntary nature of their participation and their right to stop participating at any time. I also described the procedure to withdraw their data if they do not want to take part in the study any longer. And I emphasized that their participation, or their non-participation, has no bearing on their grade.

Steps were taken to maintain participants' confidentiality as well as steps for their identity not to be disclosed. For example, pseudonyms were used to identify the data, instructors were not notified about the students who participated in the study, and all documents and electronic files were kept appropriately in order to avoid an information breach.

Contribution to the Field

Findings from this study provide engineering and science instructors, curriculum developers, as well as simulation tools developers with useful insights and a stronger foundation from which to incorporate simulations into engineering courses, design simulations for learning, as well as the instructional materials that accompany them.

CHAPTER IV

STUDY TWO: INSTRUCTORS' GOALS FOR INCORPORATING COMPUTATIONAL SIMULATIONS AS LEARNING TOOLS

Computational simulations have been used by both scientists and instructors as tools to support their scientific inquiries. In learning contexts, studies related to simulations and visualizations have shown that these type of technological tools can lead to significant improvements in students' understandings of the concept in question (Williamson & Abraham, 1995). However, these studies did not consider the complexity of learning environments, or detailed how instructors' specific learning goals inform their pedagogical approaches when incorporating simulation tools into their learning environments. According to Hennessy and her colleagues (2007), research studies focused on instructors' support of students' construction of links between scientific theory and empirical evidence have valuable educational implications. Implications from these studies include design consequences for curriculum-related activities and emerging computer-based learning technologies. For example, one implication is to identify how instructors in different settings think about the pedagogical affordances of inquiry learning environments (van Joolingen, de Jong, & Dimitrakopoulout, 2007) and the right combination between inquiry learning and direct instruction (de Jong, 2006; Rieber, 1992; Swaak, de Jong, & van Joolingen, 2004; Swaak, van Joolingen, & de Jong, 1998). Identifying instructors' learning goals and appropriate pedagogies may inform effective ways to use simulation tools as strategic components for guided instruction. The guided instruction would use these tools to support speculative activity, address prior conceptions and enhance understanding of the limitations of the target scientific theories (Hennessy et al., 2007). However, few studies in the literature focused on instructors' use of simulations in their pedagogical methods. From those few studies, none have focused on college-level engineering instructors.

Therefore, in this second study I examined the different qualitative ways in which instructors use computational simulations as learning tools in terms of their learning goals and pedagogical approaches.

Methods

For this first stage, I employed methods of phenomenography described in the previous chapter to document instructors' perceptions, experiences, and conceptualizations of simulation tools in their engineering courses. Therefore, the result of this Study Two was to identify the limited number of qualitatively different ways in which computational simulations were experienced and perceived by engineering instructors as part of their courses. In order to accomplish this result, I conducted the following data analysis.

Once I had conducted interviews with each of the six instructors, the interviews were transcribed, half by me and half by a third party. Once I received the transcripts from the third party, I then reviewed them by watching the recorded interview and making notes and corrections on the transcripts. Next, I proceeded to analyze them, starting with reading through all of the data for each of the instructors interviewed. I reviewed each interview transcript holistically to understand what the participants were saying about ways and reasons of incorporating computational simulations as learning tools. By individually analyzing such statements, I was able to identify two big themes in which instructors talked about the way they experienced simulation tools. One was about their purposes and reasons why they incorporated simulation tools and the other big theme was related to ways in which they incorporated simulation tools. I identified the first one as the instructors' learning goals (see Table 4.1), and the second one as the instructors' pedagogical approaches (see Table 4.2). To maintain instructors' confidentiality and have their identities concealed, pseudonyms were used. After reviewing each interview and identifying these themes, I began with open coding for one instructor at a time. I then proceeded by conducting axial coding for each of the interviews.

Table 4.1 Initial categories of description of learning goals

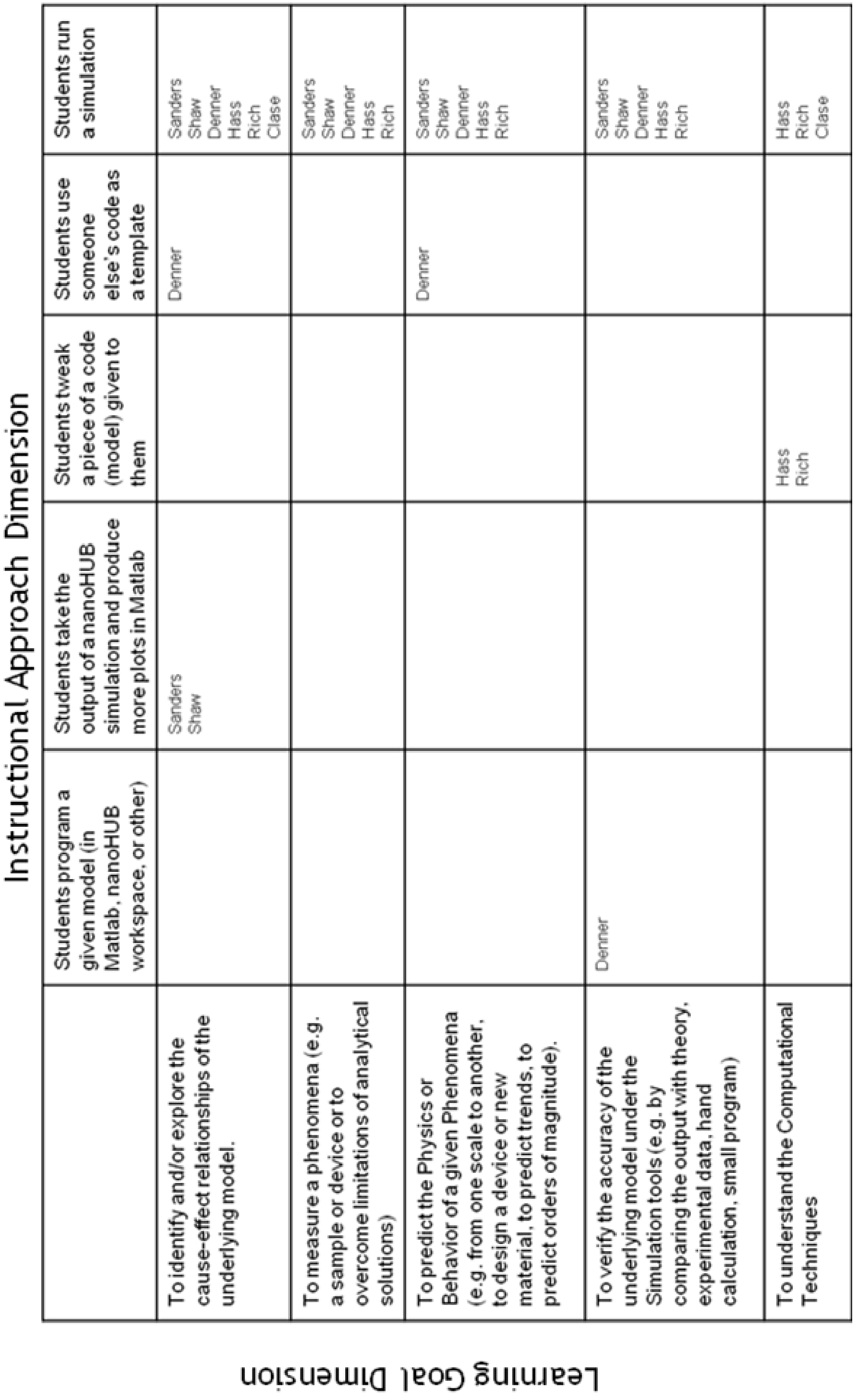
Learning goal	**The way of experiencing simulation tools involves…**
To solve realistic engineering problems • Hass • Richardson • Clase • Sanders	…realistic engineering problems concerned with the application of scientific concepts to solve engineering problems. For example, transforming theory into a useful calculation (or computational model) that can be used to analyze a problem.
To identify the underlying Physics • Hass • Richardson • Clase • Sanders • Shaw • Denner	…running simulations to understand and/or explore the cause-effect relationship of the underlying model. This way of experiencing the tools is concerned when simulations are used when analytical solutions are limited and instead computational/numerical solutions are used. This way of experiencing simulation tools includes using them as a laboratory experience, such as when a sample or device is being measured.
To predict the Physics or behavior • Hass • Richardson • Sanders • Shaw • Denner	…using the tools to predict behavior of a certain phenomena (e.g. from one scale to another, solubility of a chemical solution, stability of phases, etc). For example, to design devices (or prototypes of these devices) by simulation until physical structures are suitable.
To test the accuracy of the output • Hass • Richardson • Sanders • Shaw • Denner	…the identification of experimental and/or theoretical tests to verify the correctness and accuracy of simulation tools.
To identify the computational techniques • Hass • Richardson • Clase	… using and understanding of approximations and numerical techniques to solve computational problems.

Table 4.2 Initial categories describing instructional activities

Instructional Approach	**Description**
Students program a given model	Students use a computational programming environment such as MATLAB or nanoHUB workspace to implement a particular model. This approach also includes the creation of a simple model and building upon that model, adding more physics content as the course progresses.
Students take the output of a simulation tool and visualize the data in a different tool	Students take the output of a simulation tool and program more plots in a different tool. For example, students take the output of nanoHUB which becomes the input for creating more plots either in MATLAB or Excel.
Students are given a piece of code to change	Instructors provide students a framework in the form of a piece of code and students have to implement or change parts of it.
Students run a simulation	Students run a particular simulation and interpret the output
Students use someone else's code as a template	Students start with a template that serves as an example or starting point for creating their own programs.

As suggested by Marton and Booth (1997), in this stage I conducted my analysis focusing on one aspect of the object at a time while holding other aspects frozen. In other words, in the first pass I focused only on those statements in which participants described their purposes for incorporating computational simulations as part of the participants' instruction, and on the second pass I focused on ways for incorporating computational simulation tools into their learning environments. I continued my analysis by creating individual summaries of instructors' purposes and different ways in which instructors experienced the simulation tools. These summaries included excerpts of the interviews and a brief description of my interpretation. Since some of my participants described how they incorporated simulation tools in different courses and at different levels (i.e. graduate and undergraduate courses), I started to analyze all my interview transcripts in a collective way. I went through the entire transcripts several more times and coded them all focusing on the two aspects mentioned above: the purpose and the ways for incorporating simulation tools into instruction. For each distinct statement found I identified the instructors who have experienced it and excerpts of the interview were included to support that statement. Having identified and coded statements related to purposes and ways in which instructors incorporated simulation tools; the next step was an attempt to identify my initial set of categories of description.

Table 4.3 Instructor's learning goals versus pedagogical approaches



Instructional Approach Dimension

Learning Goal Dimension

	Students program a given model (in Matlab, nanoHUB workspace, or other)	Students take the output of a nanoHUB simulation and produce more plots in Matlab	Students tweak a piece of a code (model) given to them	Students use someone else's code as a template	Students run a simulation
To identify and/or explore the cause-effect relationships of the underlying model.		Sanders Shaw		Denner	Sanders Shaw Denner Hass Rich Clase
To measure a phenomena (e.g. a sample or device or to overcome limitations of analytical solutions)					Sanders Shaw Denner Hass Rich
To predict the Physics or Behavior of a given Phenomena (e.g. from one scale to another, to design a device or new material, to predict trends, to predict orders of magnitude).				Denner	Sanders Shaw Denner Hass Rich
To verify the accuracy of the underlying model under the Simulation tools (e.g. by comparing the output with theory, experimental data, hand calculation, small program)	Denner				Sanders Shaw Denner Hass Rich
To understand the Computational Techniques			Hass Rich		Hass Rich Clase

After completing this first iteration I discussed the results with another experienced researcher in qualitative methods who also conducted research related to the use of simulations for conceptual change. Per his suggestion, I constructed a matrix showing the learning goal and the pedagogical approach (see Table 4.3). Part of the discussion of that meeting focused on deciding whether the first category—to solve an engineering problem, was not a category but an implicit goal of the rest of the categories. The researcher and I decided that we could not make a decision at that point and that further analysis was required. After the discussion with the researcher I proceeded to describe in more detail each of my categories of description resulting in my second iteration of categories of description (see Table 4.4).

While conducting this second level of analysis I concluded that my category--to solve engineering problems was not a category related to the learning goals, but more a category related to an instructional approach that could take the form of a structured or ill-structured problem. A second distinction identified was that using simulation tools as a laboratory experience to measure a sample or device did not belong to the category –to understand the underlying physics. The reason for this distinction is that when instructors use simulations for measuring purposes, students may not be required to know the underlying model. On the other hand, when simulations are used to understand the physics, knowing the underlying model is part of the learning goal. At this point I started to look for the internal structure of my categories of description. To accomplish this, I searched for extracts from the data that were pertinent to each category and compared them against the context of individual interviews and against other interviews that talked about related themes. The result was two separate hierarchies depicted in Figure 4.1. One associated with simulations that are used (left) and the second in relation to when simulations are built (right).

Table 4.4 Second iteration of categories of description of learning goals

Learning goal	**The way of experiencing simulation tools involves…**
To identify the underlying Physics • Hass • Richardson • Clase • Sanders • Shaw • Denner	… running simulations to understand and/or explore the cause-effect relationship of the underlying model. This way of experiencing the tools is also concerned when simulations are used when analytical solutions are limited and instead computational/numerical solutions are used.
To measure a phenomena • Hass • Richardson • Sanders • Shaw • Denner	… using such tools as a laboratory experience such as when a sample or device is being measured.
To predict the Physics or behavior • Hass • Richardson • Sanders • Shaw • Denner	… using the tools to predict behavior of a certain phenomena (e.g. from one scale to another, solubility of a chemical solution, stability of phases, etc). This way of experiencing simulation tools also includes the design of devices until physical structures are suitable.
To test the accuracy of the underlying model • Hass • Richardson • Sanders • Shaw • Denner	…identifying experimental and/or theoretical tests to verify the correctness and accuracy of simulation tools.
To identify the computational techniques • Hass • Richardson • Clase	…using and understanding of approximations and numerical techniques to solve computational problems.

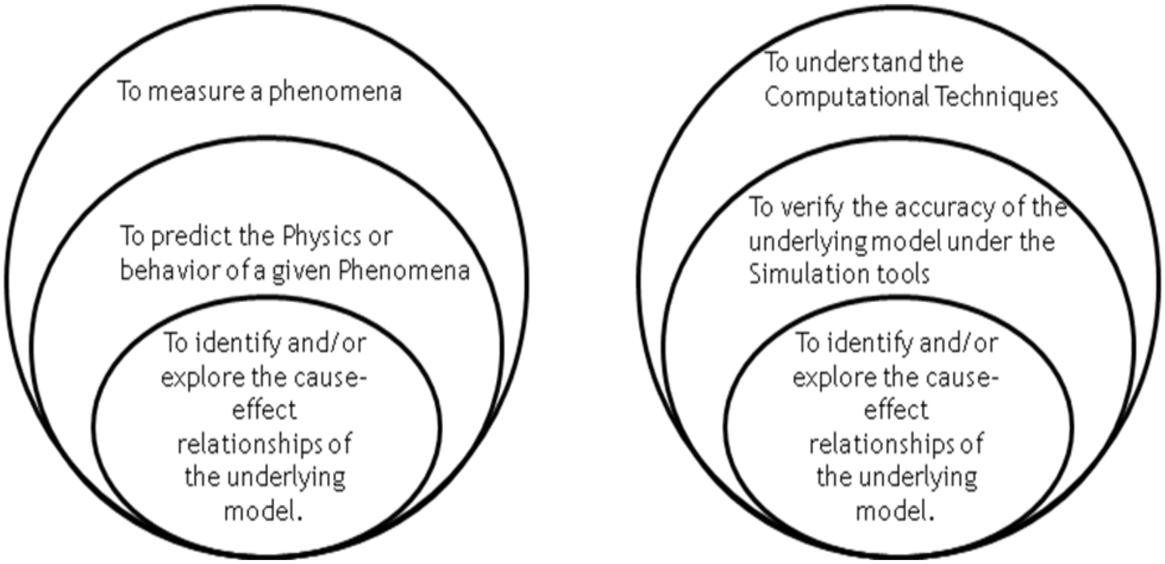


Figure 4.1 First iteration of the outcome space

At this point I reviewed the transcripts again and I identified that this internal structure was incomplete. One instructor, Dr. Denner, expressed a particular way of using simulation tools that none of the others mentioned before. He explained that when he faced a situation in which he used a simulation tool not built by him, before starting any design of a particular device, he verified the accuracy of the underlying model under the simulation. He did this by creating a very simple code representing the simplest case and compared his result with the one generated by the simulation tool. Dr. Denner explained that if the responses were similar, and if he was really convinced, then he proceeded with the design activity. Dr. Denner's argument pointed out a different way in which he experienced the simulation tool that suggested the internal structure presented in Figure 4.2. However, when I compared this new representation against the context of the extracts drawn from all of the interviews, this structure was not holding its hierarchical structure.

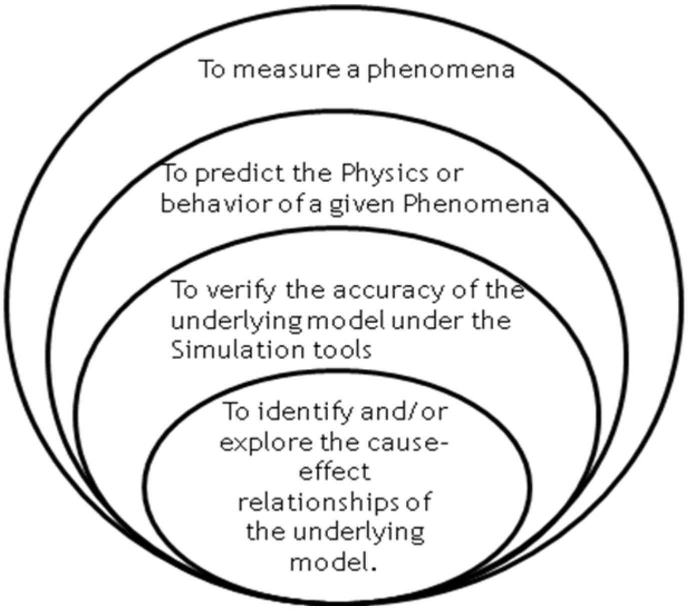
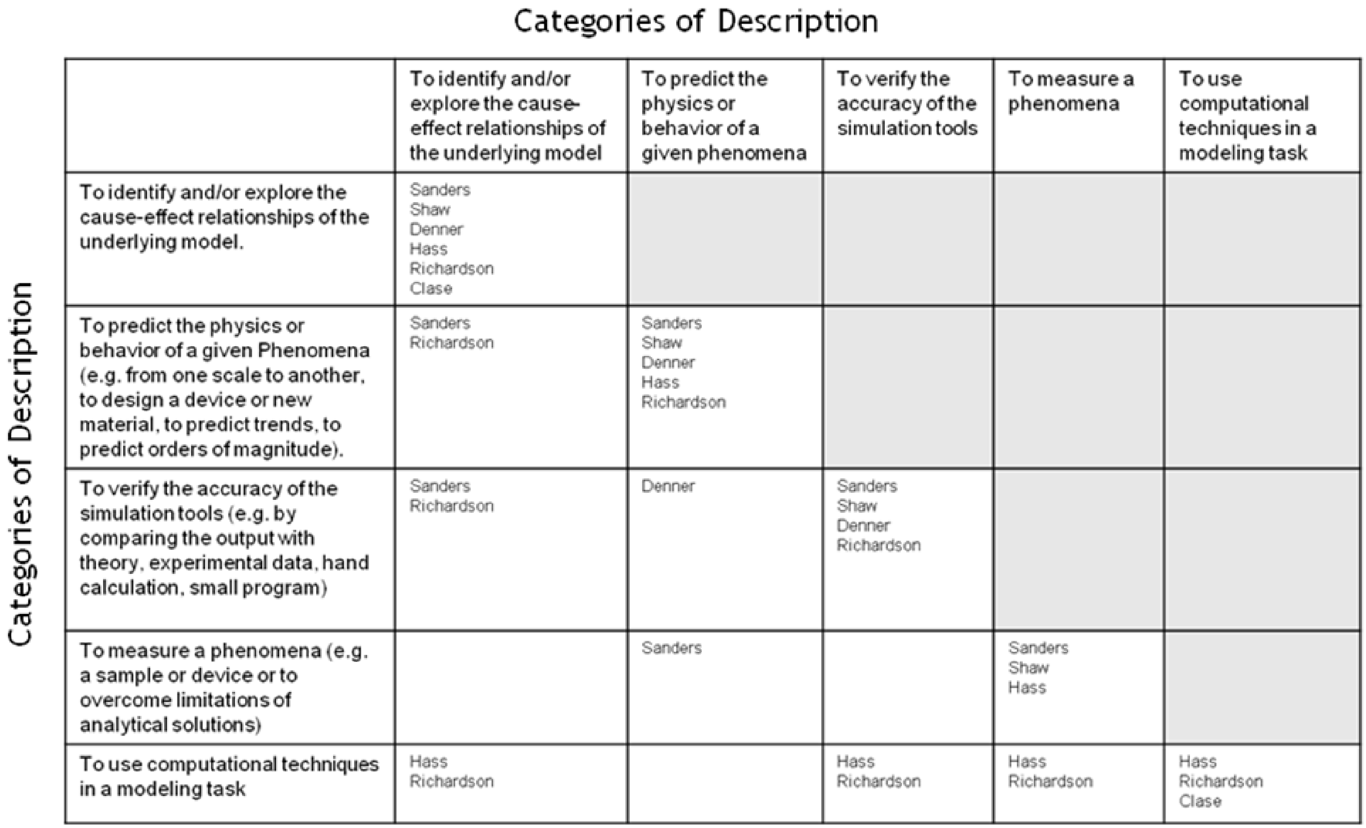


Figure 4.2 Second iteration of the outcome space

After conducting this second iteration I talked again with the senior researcher. We reviewed all the categories of description, but this time we were more careful in looking at specific excerpts of the participants' interviews to corroborate the categories. We were more comfortable with the internal structure of the categories of description presented in Figure 4.1 but we needed a further analysis to corroborate the internal structure depicted in Figure 4.2. We agreed to conduct a third iteration for inspecting the data comparing extracts upon the same and related themes. To gain a better perspective of which participants were experiencing each of the categories of description, I created a matrix having the same elements in the two dimensions—i.e. the categories of description (see Table 4.5). This matrix allowed me to select each aspect of the phenomenon one at a time and inspect it across all of the subjects. Then, from those participants experiencing the phenomenon I concentrated on the way instructors experienced the simulation tools and the way they expressed those experiences in order to identify the variations. I repeated this process over and over for each category of description until clarity was found. The result was the outcome space depicted in Figure 4.3.

Table 4.5 Distribution of participants among categories of description



Categories of Description

Categories of Description

	To identify and/or explore the cause-effect relationships of the underlying model	To predict the physics or behavior of a given phenomena	To verify the accuracy of the simulation tools	To measure a phenomena	To use computational techniques in a modeling task
To identify and/or explore the cause-effect relationships of the underlying model.	Sanders Shaw Denner Hass Richardson Clase				
To predict the physics or behavior of a given Phenomena (e.g. from one scale to another, to design a device or new material, to predict trends, to predict orders of magnitude).	Sanders Richardson	Sanders Shaw Denner Hass Richardson			
To verify the accuracy of the simulation tools (e.g. by comparing the output with theory, experimental data, hand calculation, small program)	Sanders Richardson	Denner	Sanders Shaw Denner Richardson		
To measure a phenomena (e.g. a sample or device or to overcome limitations of analytical solutions)		Sanders		Sanders Shaw Hass	
To use computational techniques in a modeling task	Hass Richardson		Hass Richardson	Hass Richardson	Hass Richardson Clase

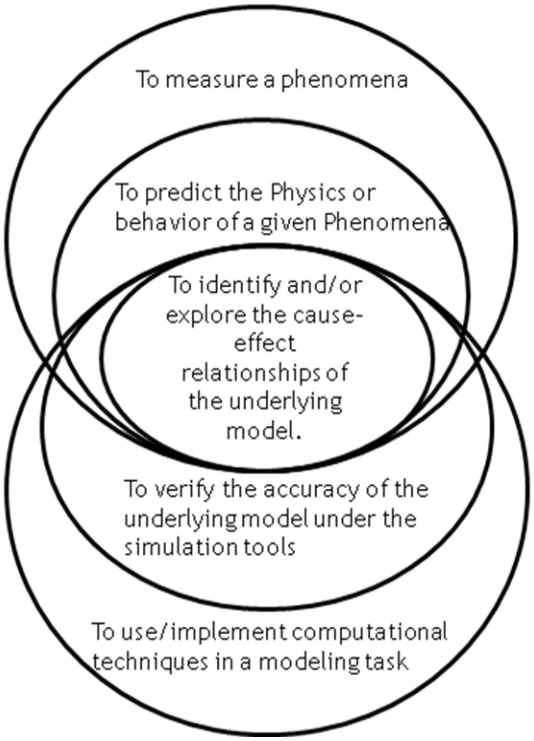


Figure 4.3 Third iteration of the outcome space

Once I identified the categories of description and the outcome space, I created new instruments for data collection. These instruments consisted of a table with each identified learning goal and a brief description. The second instrument was different combinations of the diagrams depicting possible progressions and relationships between the learning goals (see Figure 4.4).

These instruments were used by the researcher to conduct a member checking process with three of my participants. When I met with my participants I first asked them to read the learning goals and the descriptions provided in the table. I asked them if they agreed with the learning goals and with the corresponding descriptions. Then, if required, I made the appropriate changes in the descriptions. Afterwards, I showed them the diagrams one by one. Per each diagram I asked my participant if he/she agreed with the levels of the learning goals. I took notes and observations as required. Finally, I asked if they could think of other ways in which they might have experienced the simulation tools in terms of their learning goals that were not represented in the descriptions.

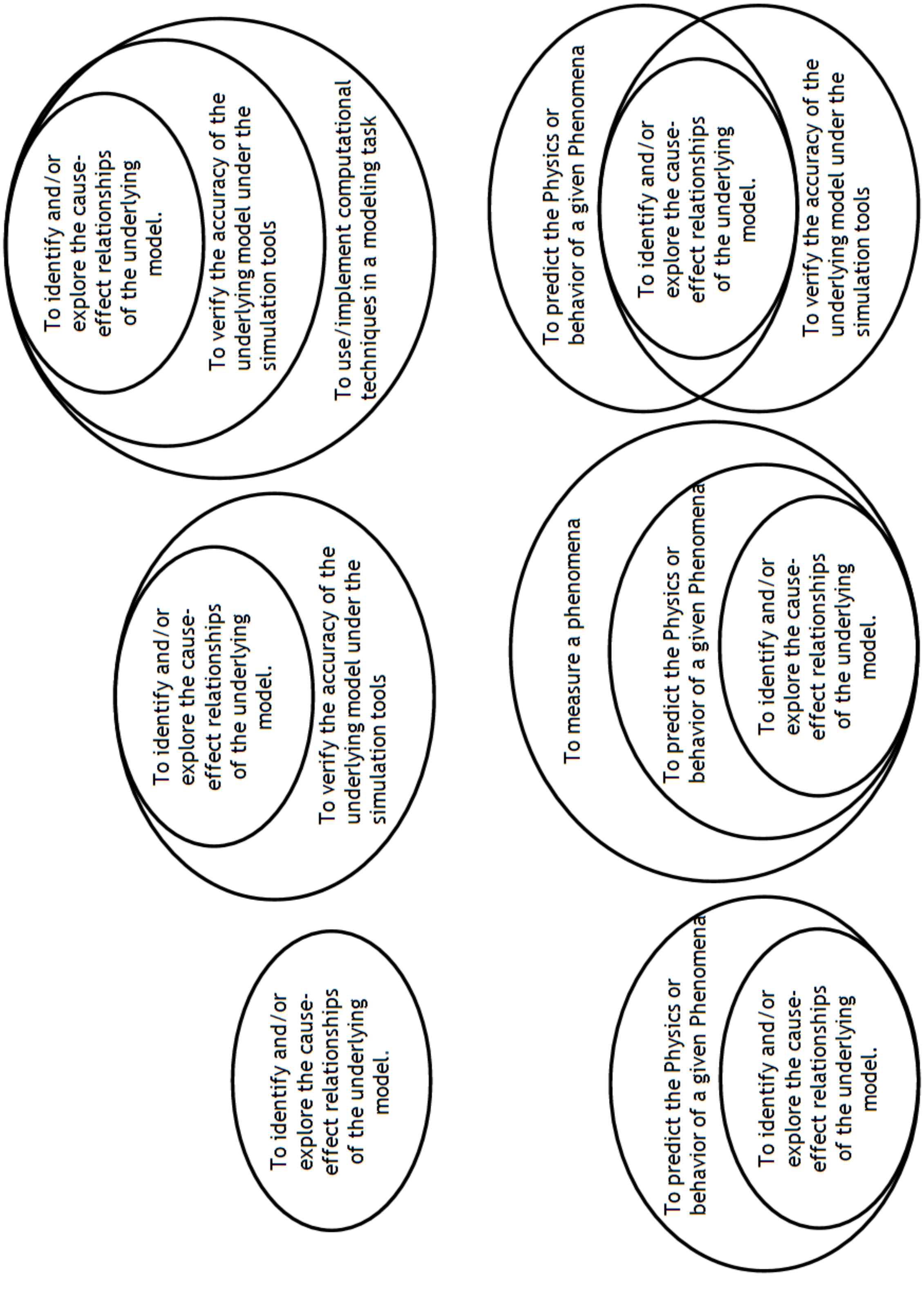


Figure 4.4 Diagrams of learning goals forming a hierarchy

Table 4.6 categories of description

Learning goal	**The way of experiencing simulation tools encompasses…**
To understand the cause-effect relationship of the underlying model	…understanding and/or exploring the cause and effect relationships defining a particular computational simulation by running the simulation. It is also concerned with the comparison of analytical solutions with computational/numerical solutions.
To collect data as in a laboratory experiment	…conducting virtual collection of data (i.e. measurements) to characterize a phenomenon versus running physical devices in a laboratory.
To validate the results or performance of an experiment	…validating empirical results of a performed experiment (or design) with a target specification or performance. Can also lead to changes in the inputs of the experiment so improvements may be achieved.
To predict the results and/or performance of an experiment	…using the tools to predict behavior of a certain phenomena. Also includes design tasks.
To test the accuracy of the simulation's underlying model and its implementation	…verifying the accuracy and precision of the simulation model by comparing and contrasting empirical and/or theoretical experiments with computational experiments.
To use and implement computational techniques in a modeling task	…using and understanding approximations and numerical techniques to solve computational problems by building computational algorithms used in simulations.

After conducting the member checking process a sixth category was identified. The category –to measure phenomena was broken down into two different categories. Dr. Sanders explained that he sometimes asked his students to measure phenomena to validate a design, and sometimes he asked his students to just collect data like in a laboratory experiment. More specifically, validating the output of an experiment was performed together with a design task. Also, students needed to be familiar with the cause-effect relationship of the simulation's underlying model. When used as a tool for collecting data, the simulation tool was usually used as a black-box model (see Table 4.6). The output of this iteration became my final categories of description and outcome space.

The categories of description identified in the analysis, as well as the internal structure of these categories, resulted in the outcome space for this initial phase of the study. Each of the elements of this outcome space and its internal relationship are explained in the following section.

Results

This section presents the findings of the ways engineering instructors experienced computational simulations as learning tools. The six different categories of description and their internal relationship resulted from the experiences of the six engineering instructors who participated in this initial phase of the study. The findings include the explanation of each category of description and the evidence of their internal relationship.

The Outcome Space

The six categories of description resulting from this study identify how instructors experienced simulation tools as part of their instructional experiences. The categories and the distribution of participants among those categories are summarized in Table 4.7.

Marton and Booth (1997) explained that the criteria for quality set of descriptive categories must include: a) each category must tell something distinct about each particular way of experiencing the phenomenon, b) each category has to stand in a logical relationship with one another, and c) the system should be parsimonious for capturing the critical variation in the data. A set of categories of description containing this criteria form the outcome space. The outcome space comprises the distinct ways of experiencing the phenomenon and the relationships between them. That is, the complex of categories of description encompassing the different ways of experiencing the phenomenon is the outcome space (Marton & Booth, 1997). According to Marton and Booth (1997), the relationships between the categories of description form a hierarchy that can be defined in terms of a structure of increasing complexity. Marton and Booth explained that this complexity can be defined in terms of subsets of the component parts and relationships within more inclusive or complex ways of experiencing the phenomenon. Therefore, two additional components of the outcome space include the differences between categories of description (see Table 4.8) and the structure of increasing complexity (see Figure 4.5).

Table 4.7 Categories of description and distribution of participants

Learning goal	Participants	The way of experiencing simulation tools encompasses…
To understand the cause-effect relationship of the underlying model	Hass, Richardson, Clase, Sanders, Shaw, Denner	…understanding and/or exploring the cause and effect relationships defining a particular computational simulation by running the simulation. It is also concerned with the comparison of analytical solutions with computational/numerical solutions.
To collect data as in a laboratory experiment	Sanders	…conducting virtual collection of data (i.e. measurements) to characterize a phenomenon versus running physical devices in a laboratory.
To validate the results or performance of an experiment	Hass, Richardson, Clase, Sanders, Shaw, Denner	…validating empirical results of a performed experiment (or design) with a target specification or performance. Can also lead to changes in the inputs of the experiment so improvements may be achieved.
To predict the results and/or performance of an experiment	Hass, Richardson, Clase, Sanders, Shaw, Denner	…using the tools to predict behavior of a certain phenomena. Also includes design tasks.
To test the accuracy of the simulation's underlying model and its implementation	Hass, Richardson, Clase, Sanders, Shaw, Denner	…verifying the accuracy and precision of the simulation model by comparing and contrasting empirical and/or theoretical experiments with computational experiments.
To use computational techniques in a modeling task	Hass, Richardson, Denner	…using and understanding approximations and numerical techniques to solve computational problems by building computational algorithms used in simulations.

Table 4.8 Differences in categories of description

To collect data as in a laboratory experiment	⇨	To understand the cause-effect relationship of the underlying model	The approach of using the simulation tools is experienced as a black-box model for collecting experimental data as opposed to understanding first principles.
To understand the cause-effect relationship of the underlying model	⇨	To predict the results and/or performance of an experiment	This approach of using the simulation tools assumes students know the underlying model and will use that knowledge to perform a prediction task.
To predict the results and/or performance of an experiment	⇨	To validate as in a laboratory experiment with verification purposes	The result of an experiment is validated against some performance measures or target standards.
To understand the cause-effect relationship of the underlying model	⇨	To test the accuracy of the simulation's underlying model and its implementation	This approach of using the simulation tools is experienced by testing the output of the simulation with the simple case of the analytical solution.
To test the accuracy of the simulation's underlying model and its implementation	⇨	To use computational techniques in a modeling task	This approach of using simulation tools is experienced in a modeling task where students implement a physical model or parts of a physical model by applying computational techniques. Students perform tests to validate the correctness of the model and the implementation.

The categories of description, the differences between such categories of description, and the structure of increasing complexity of the categories are discussed in detail in the following sections.

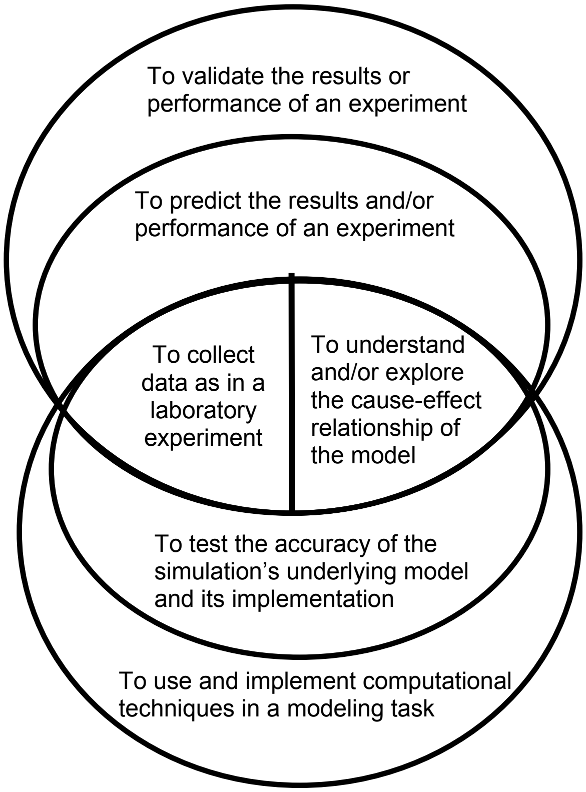


Figure 4.5 Structure of increasing complexity of the categories of description: the outcome space

Categories of Description

Learning goal: To understand the cause-effect relationship of the underlying model (Hass, Richardson, Clase, Sanders, Shaw, and Denner)

This way of experiencing simulation tools entails running simulations to understand and/or explore the cause-effect relationship of the underlying model. This way of experiencing the tools is also concerned when simulations are used when analytical solutions are limited and instead computational/numerical solutions are used. This is done with the intention to have students compare and contrasts the approximation with the exact solution. For example, Dr. Richardson emphasized that the purpose of using the tools is for students to be able to focus on the physical aspect. Likewise, Dr. Hass explained how he used simulation tools to explore the physics:

> Dr. Richardson: In a traditional course using simulation, and simulation tools, is more like a novel thing. The students may not be expecting that. And it allows – it's a tool, it allows them to explore physics that they cannot explore on the back of the envelope.

Dr. Hass provided an example of how he used simulation tools to convey the cause and effect relationship of the underlying models:

> Dr. Hass: So when we did this in class we tell students we explain the tool a little bit we talk about the input files, you know the input windows, what they mean, what type of method is being used.
> But and even though students are not experts in the actual methodology to do the simulations, they understand what the approximations are and what is the accuracy that they would expect, how realistic description we do. And then, once the simulation is done, and they look at the results, they can look at—for example the load versus deformation curve stress strain and then they can look at what the atoms, the location of all the atoms are at different stages.
> So what I've asked, you know, what they do is they try to correlate a feature that they observe in the behavior of the material in the deformation—load deformation curve with what the atoms are doing.
> Or in another example they study melting they heat up a sample I don't necessary tell them they need to see melting but they heat it up at one point the sample actually melts and they see what happens and they can plot for example volume as a function of temperature.
> So what you see when a thing—material, a solid melts, so if it is a crystal in solid and goes to the melt, the volume will jump, so the volume is increasing because of thermal expansion he heated up, but when the phase transition occurs, there is a discontinuous jump in the volume, there is a discontinuous jump in the potential energy, so they can see that and then they look at the—were the atoms are and they can say aha! So it looks very different.

Dr. Denner explained that his goal was for the students to not only physically understand the phenomenon but also why this phenomenon happens. He also emphasized that his intention was for students to get familiar with the real phenomenon by using simulation tools and understand the cause and effect relationship of the model:

> Dr. Denner: So that where I see it more like is that in all of this physics and engineering, there's this mathematical part of the problem that you have an equation which supposedly describes some real life situation. So let's say I have a set of equations that are supposed to give me the current versus voltage characteristic of some transistor. Now, the important thing

> is how to get students to see the connection between the equation and the real world.
> … Just coming out with particular plots and seeing what happens if we change certain parameters. And again, those equations will give you automatically if you run it with MATLAB; the point is then to physically understand why that would happen. And, in an exam I would give them a density of states; tell them, okay this side is hot, this side is cold; now tell me which way the current should flow. MATLAB would have given them that directly. But, when they're doing it in an exam, they don't have MATLAB but hopefully have understood enough that they can say which way the current will flow for example.

Dr. Hass also explained how the simulation tools helped his students overcome the limitations of analytical solutions:

> Dr. Hass: …So, we have equations that we cannot solve analytically, so we use computers to solve those equations; plug them and solve them many times, whatever. But the driver is the application.

Dr. Sanders also emphasized how by using simulation tools, students were able to look at the physical phenomena without any simplification. That in turn allowed them to understand the physical phenomena:

> Dr. Sanders: …Most of the assignments then were trying to reinforce concepts that we discussed in the lecture. Where we'll take the simplest approach that we did in the lecture and now we'll do an actual simulation without any of the simplifying assumptions and we'll see how it really works.

In the same way, Dr. Shaw discussed how using simulation tools students could get rid of any simplification and actually let students compare approaches, the classical approach and the quantum approach. While the first one could be solved analytically, the second one cannot:

> Dr. Shaw: …But, the important thing is give nanoHUB tools, you know, they are more advanced; they are some of the tools are fully quantum mechanicals, so students can readily see, you know, readily verify what is the – you know what is the difference between classical or analytical calculation and the quantum mechanical uh, calculation, right? So now, I have them work, okay, compare the real, you know, in the textbook you know that is found in the textbook, you know. And similar, you know similar results you know that you get from nanoHUB simulator.

> Now, it's not only they just compare, but I ask them why do you see the difference between these two results; the textbook course and the nanoHUB course? They have to explain. So right there, this would be because the nanoHUB tools, you know, they basically you know, do solve between uh, say shorting an equation, or differential equation, which is – which the textbooks are not doing. So, things like that. They, you know.

Dr. Hass also emphasized the importance of the engineering application of those models:

> Dr. Hass: …And obviously, the input and the outputs are important because we don't want to—to have you know, this not enough applied mathematics course, so we don't want them just to learn the model, we want them to learn how you use the model to solve engineering problems…And get them some, you know, get them to become more or less familiar, while having an intuition for how the models work.

The instructors therefore incorporated simulation tools into their instructional experiences when their main learning goal was for students to understand the physics. That is, they used them to help their students understand and/or explore the cause and effect relationship of the underlying model. This learning goal also included having students learn to recognize the difference between the analytical solution and the numerical solution of that model.

Learning goal: To collect data as in a laboratory experiment
(Hass, Richardson, Sanders)

This way of experiencing simulation tools includes running multiple experiments to collect data. This way of experiencing the tools describes situations in which the simulation tool is used instead of using any device or tool in a laboratory. Dr. Sanders explained that the way he experienced simulation tools regarding this learning goal was when he asked his students to measure a transistor. He explained that in this particular case he was more interested on how the transistor is functioning than on the theory behind that behavior. Students did this by extracting experimental data from the simulation tool:

> Dr. Sanders: They log onto the nanoHUB, they ran the simulation, hum— and then just answered some questions – so this was sort of as you

> went to a lab and did a measurement of a transistor and see how these things function.
> Interviewer: so loosely a kind of a virtual lab, where you use the simulations as a way to generate the data
> Dr. Sanders: Right, and basically explain that the point of the course now is to explain why these characteristics are the way they are, what controls – so the whole point is that they will get some feeling for what the electrical characteristics of these devices look like without any of the theory as to why does this, just see what a typical one looks like and get calibrated.

Dr. Sanders also explained that this data were analyzed and come up with some conclusions:

> Dr. Sanders: So there where a whole series of those that there were couple at the end that there were more ambitious, so this one hum — this homework 8 that I have here, so this was like a virtual lab, that these are the kind of measurements that that device engineers frequently go in a lab and do, and it gave them a chance to do it by simulation. so those, you know going in the lab, they have this data, how do you analyze this data to extract some important parameters from the technology so you can see is there some particular aspect that's limiting the performance, so it's the kind of routine measurements that they should know how to do, but since it's not a lab course they don't have an opportunity to do it in a lab, they do it by simulation.

Dr. Hass has also incorporated simulation tools as a way for his students to collect data. In his case, the goal for his students in collecting data was for them to be able to compare experimental data taken from a macroscopic sample with the data generated by the simulation tool:

> Dr. Hass: …We actually use this same tool in an early class; in the lab class. We had the last week we spent doing a competition lab if you want and they had to carry out stress strain curves themselves on much bigger samples, and their task was to carry this competition exercise and then compare the results they get in the computer with the results they got in the lab with a macroscopic sample and there are many differences and the fact that the wires are so small actually makes it big difference, so if you look at the load hum – the load displacement curve that we've got here, it's a – it looks, you know, the shape is the same but looks different, has some, hum – so some of the features that you see in very small scales you don't see in macroscopic scales…

The experiences of instructors included in this category explained how they use the computational simulations as a way to collect experimental data. In this particular case, instructors were not concerned with their students knowing what is behind the simulation. Their primary interest was focused on the phenomena being measured; its performance and/or its behavior.

Learning goal: To predict the results and/or performance of an experiment (Hass, Richardson, Sanders, and Shaw)

This way of experiencing a simulation encompasses using the tools to predict behavior of a certain phenomena (e.g. from one scale to another, solubility of a chemical solution, stability of phases, etc). This way of experiencing simulation tools also includes the design of devices until physical structures are suitable. The focus of this category is in the prediction, which most of the time involves a design task. Dr. Sanders discussed how he incorporated this learning goal by having students design transistors to meet industry targets:

> Dr. Sanders: Now I have scaling, so this is more of a design challenge. So more as lower by making transistors smaller over technology generation. So I – so let's see, we took the next generation, this is one that Intel just announced about three weeks ago they put in manufacturing, but a year ago it was next generation, so we gave them a previous generation, we gave them some simulation input parameters for a previous generation and we said your job is to design a next generation so that it functions properly. This is what the ways engineers do. And they would do it all by simulation.

Dr. Hass explained that it is important for his students to be able to predict how a material will behave. He explicated that by understanding how the material behaves at the atomistic level, from first principles, his students would be able to predict how a material will perform:

> Dr. Hass: We work on different areas, with different classes of materials, but the common theme is that we try to understand what is happening with, form a molecular point of view, what is happening with the atoms so we want to be able to predict how materials behave from first principles, you know as supposed of using experiments.
> So that is why we take a look at a very fine scales instead of quantum mechanics and computing all the way up and the reason for doing that is

> that hum—then our simulations can predict in principles once we validated a particular approach with materials with experiments you can— because everything is from first principles you don't use experimental data to tune your models then you can predict the behavior of new materials that you have never met and so that allows for computer materials design, so doing—designing new materials on the computers before you actually make them in the lab.
> So that is something that is not very doable today I mean it is still kind of almost a dream. You know, we are getting closer.

Dr. Richardson provided the same explanation in terms of chemical solutions. He explicated how it is important for students to be able to predict and figure out trends.

> Dr. Richardson: So what I did was to – for my class of thermal class, thermodynamics, right, developed, and you can see it here, let me pull it up – develop – this is the same window three times, right? And this is all the students see, right?
> There's something called "chemical activity" where for example, you know the temperature, what happens is that the chemical activity of the material changes— being able to figure out trends, and actually, this is using actual real numbers, right, you can predict if this – if this in this case chemical solution is going to mix or demix, right, in this case.
> And this is a full class just talking about the – the thermodynamics of this one.
> And then I send them to the computer lab in this case, completely off the – off the hours of the class and ask them to—to—to tell me their – their order of magnitude and trends of what they should expect will happen, right? That's one of them.
> But this one I think it's – I think this is one of the best tools that we have, you can see this one has a lot of parameters, right? And—and what happens in this class is that I just release one module a week. And when it's released once it only has one – one uh, – one slider, right? And you can see that, you can predict that the material is going to mix, or demix, or what phase is going to be more stable than which one, right?
> And at that point, they—they leave the class, or they graduate from the class knowing what will happen if they made something very tiny, for example.

Instructors who experienced simulation tools in this way emphasized their intention of having their students be able to make predictions by observing performance and behaviors of the phenomena being simulated.

Learning goal: To validate the results or performance of an experiment

(Hass, Richardson, Sanders, Shaw, and Denner)

This way of experiencing simulation tools includes using simulation tools as in a laboratory experience, such as when a sample or device is being measured and then compared to a desired specification or performance. This task is performed after an experiment has been conducted. Therefore, and as different from collecting data as in a laboratory, and this way of experiencing simulation tools usually follows a prediction task, such as an experiment or design. Students then, have to evaluate if the experiment was conducted appropriately and if the results are as expected. For instance, Dr. Sanders asked his students to design a device, and together with that task, he asked the students to meet specific industry standards. That transistor not only had to meet the standards but be a well behaved device. This involved an iterative process between designing and testing:

> Dr. Sanders: …So that's the way it's structured in here, and the transistor design has evolved for so long that its, there are relative small number of basic measurements, you do these measurements and pretty much know everything about the transistors – so – so that's what they're doing in this design problem, they take the bigger device that behaves properly, they shrink it and they should understand now that I need to do these half key dozen measurements and look at these half dozen key parameters and they're going to tell me everything I need to know about what's happening with this device— and then you look at, ok which one is the biggest problem and that's how I'm going to work on the first.

Dr. Shaw also made clear his intention when assigning a task related to design a device and validate it.

> Dr. Shaw: …From a pre – from a predefined – from a predefined device, preselected – a selected device they—they understand what's – what's in, what are the novel phenomena.
> Number two is, they have to design the device. Like they have to optimize the configuration. They have to, you know, vary; they have to vary the device, things like that. So that they have to optimize characteristics. So one thing they have to – they have to simulate you know, lot of simulations.
> So, the first part, where you have to see where one of these features, where one of these novel phenomena from the device, you just do a single simulation, you know.

> You pick a device, you pick a predefined device and then you see what—what is happening.
> But, the second question is on designing the device. Like, okay, now that you – now that you know what – what happens in a device; now you design the device. You change the dimension of the device; you change the environment of the device; and you change the modeling of the device so that you get best out of it. You get – you get the best characteristics; optimized characteristics.

Participants who experienced simulation tools for having students validate the results or performance of an experiment, used them to corroborate the outcome of an experiment to a desired specification or performance target.

Learning goal: To test the accuracy of the simulation underlying model and its implementation

(Hass, Richardson, Sanders, Shaw, and Denner)

This way of experiencing simulation tools includes the identification of experimental and/or theoretical tests to verify the correctness and accuracy of simulation tools. Validating the accuracy may involve identifying if the model is correct as well as the computational technique used to implement it.

Dr. Richardson described this experience for his students as a way for them to become critical users of the simulation tools. He also emphasized that students should not trust what they have created until they have conducted enough tests and have enough evidence that what they have programmed is correct.

> Dr. Richardson: And—and they – one of the things we have discussed recently is uh, let's see how do I put it, they—I want them to realize that they should always be suspicious of what they program. And that they should not trust it, and they should – they should test – find as many tests experimental, and theoretical, until they're satisfied enough, right, not completely though, satisfied enough to—to say something about the physical problem, right?

Dr. Richardson explained that students should be checking the physical aspects as well as the implementation. He also explained different ways of approaching the problem.

> Dr. Richardson: Um, so in – in class you know, you build a model. In this case in FYPY let's say you try to solve an infusion equation, right? So the first thing that you do is, if you have them properly trained is, "How do I know that this is working?"
> And then the first – and then the next question that comes to mind is, "What do I know about the problem?" What – what should I expect the diffusion of something to go. So, I – I pull out a book on diffusion and compare it point by point, which is I am hoping they will do. Or uh, uh, they also can, I don't know, they can run another simulation which is another way to do it.
> And—and just developing these built in, uh, how do I say this, not arguments, but this built in checks, that's something – that is – that is very important, right?

Likewise, Dr. Sanders emphasized the importance of being critical and intelligent users of the tools. That is, to verify if the program is correct and is giving accurate results.

> Dr. Sanders: Now some of the other problems they've used to tool to – to amplify in some concepts in the class; or they've used the tool instead of going into the lab and doing a measurement; they sort of treat the results of the simulation as though they were in the lab actually doing a measurement and then they—they analyze it.
> Now, this—this one is a little – a little different and the explanation is – really comes from this—this paragraph here in the homework assignment that, it's to sensitize them to the fact that when you're using the simulation tool you have to be a very critical, intelligent user. You have to know how to decide for yourself whether you have the program set up right, and it's producing results that you believe.
> So, you know, in this case I had an interesting thing happen. We're using a new tool, and uh, obviously there are a few rough edges in it. There is one particular thought that as we used in the previous assignment, I looked at it and I think, "I don't think that's probably where it says it is."
> And uh, the purpose of the assignment there are really two parts:
> First of all, determine whether – what's being plotted here really is what the labels say is being plotted.
> And the second part, which is more challenging and I don't expect many students to get, is to figure out what actually is being plotted if it's – if it's really not what it says it is.
> So, it's the kind of thing that I think people that use simulations programs are—are used to doing.

These instructors experienced simulation tools as a way to verify the accuracy of the simulation's underlying model as well as how it is implemented. This verification process is conducted when the student is the creator of the simulation as well as when he/she is a critical user of it.

Learning goal: To know and implement computational techniques
(Hass, Richardson, and Clase)

This way of experiencing simulation tools encompasses the use and understanding of approximations and numerical techniques to solve computational problems.

For Dr. Clase, when he used simulation tools to have his students learn computational techniques, he wanted his students to understand what it means to do computational calculations to an extent that they are able to read a theoretical paper and be familiar with the content.

> Dr. Clase: Um, and so one thing I wanted was for them to understand um, what it means to do calculations in this field; in the field of nanoscience. And, I think that's – it's clear that everyone got that out of this class.
> Uh, what I hoped for in addition to that, going beyond that, but didn't – certainly didn't expect everyone to was that some people might say, that it's useful enough that they would start to incorporate calculations in their own research.
> Uh, but at the very least I wanted to be sure that even if it's just to the extent that these experimental researchers when they read a theory paper they now have much more of a sense of what went into that paper.
> Right?
> So, what I wanted to teach was what levels of theory do what in nanoscience? And, how do you – how do you take a level of theory and turn it into a useful calculations? And then how do you turn that useful calculation into something that's useful in a real problem, um, and that's meaningful?

Dr. Hass, as well as Dr. Richardson, explained that the learning goal of their course was that students understand the simulation techniques and some of its applications.

> Dr. Hass: …In this particular course that we will teaching this semester, the—the goal is for the students to understand the concepts and the ideas behind the simulations, the physics behind the simulations, approximations and numerical issues behind the simulations.
> So the driver are the simulation techniques. That's what we want them to learn. And, we use applications to do that.

> We do computation to solve engineering or scientific problems. And so, we—we are always concerned about the application. We want to use what we learn to—to look at nice examples of calculations that might be of interest.
> But the main – but the focus of the course is not an application, but a series of techniques that allows us to solve many applications.
> Dr. Richardson: …But the tricky part is who can actually model? Right? And actually be able to simulate and actually do engineering using a computer.
> And that—that's actually the goal, right? And—and with that in mind, and what—what I have done is – is to first establish a link in that respect, right? Telling them, well there's a connection; it's called multi-scale modeling, right? What you can – you can either take results from—from ab-initio or atomic simulations and then input it into these models, right? Or, you can just go through the experiment on the lab right?

The instructors whose experiences comprised this category discussed how they used simulation tools in modeling tasks. The main goal of these participants was to convey to students how to understand and implement computational techniques to solve engineering problems.

Category Differences and its Structure of Increasing Complexity

The differences in the ways simulation tools have been experienced by the six different instructors have resulted in the structure of increasing complexity shown in Figure 4.5. This section discusses the differences on the categories of description experienced by the engineering instructors who participated in this study as well as the resulting structure of increasing complexity.

"To understand the cause-effect relationship of the underlying model" as different from "To collect data as in a laboratory experiment."

The approach of using the simulation tools is experienced as a black-box model for collecting experimental data as opposed to understanding first principles.

Dr. Hass emphasized this difference when he explained that his point was to have students understand the cause-effect relationship of the model by first principles than from collecting data.

> Dr. Hass: We work on different areas, with different classes of materials, but the common theme is that we try to understand what is happening with, form a molecular point of view. What is happening with the atoms so we want to be able to predict how materials behave from first principles, you know as supposed of using experiments, so that is why we take a look at very fine scales instead of quantum mechanics and computing all the way up. And the reason for doing that is that hum— then our simulations can predict in principles once we validated a particular approach with materials with experiments you can—because everything is from first principles you don't use experimental data to tune your models then you can predict the behavior of new materials that you have never met and so that allows for computer materials design, so doing—designing new materials on the computers before you actually make them in the lab. So that is something that is not very doable today I mean it is still kind of almost a dream. You know, we are getting closer.

Equally, Dr. Sanders made the same distinction by explaining how he used the simulation tools in the first homework assignment. Dr. Sanders explained he wanted his students to become familiar with the device without really going into the physical aspects.

> Dr. Sanders: Yeah—so— yeah I can see, like the very first example I am assuming that they know nothing about it, they just run it and they look at the results and it's like they're doing a lab measurement.
> I am asking them some questions about that. That maybe would be useful to see some quick run through on how you run the program and how you do the results, something like that.
> But most of the other ones, the all of the concepts should have been covered in class so the actual mechanics of implementing and inputting into the tool, maybe is something they need some help with, what all of those things mean should be things that we hope at that point they know...

In the following excerpt, Dr. Shaw clearly explained the distinction between just collecting data to characterize a predefined device and the difference between having students design a device:

> Dr. Shaw: Number one is they can – they can basically they can, uh, you know, they can start with a, with a device, with a predefined device that I ask them well I mean use this – this dimension, this configuration, and see the characteristics.
> So they'll work the phenomena. From that you know they – they understand what is happening in the device. That's the first thing.

> From a pre – from a predefined – from a predefined device, preselected – a selected device they—they understand what's – what's in, what are the novel phenomena.
> Number two is, they have to design the device. Like they have to optimize the configuration. They have to, you know, vary, they have to vary the device so that they have to optimize characteristics. So one thing they have to – they have to simulate you know, lot of simulations. So, the first part, where you have to see where one of these features, where one of these novel phenomena from the device, you just do a single simulation, you know.
> You pick a device, you pick a predefined device and then you see what—what is happening.
> But, the second question is on designing the device. Like, okay, now that you – now that you know what – what happens in a device; now you design the device. You change the dimension of the device; you change the environment of the device; and you change the modeling of the device so that you get best out of it. You get – you get the best characteristics; optimized characteristics. You know?
> Get at the true essential parts.

Using the simulation as a black-box model represents the most important distinction between these two ways of experiencing the simulation tools. While in one category understanding the cause-effect relationship of the underlying model is the most important aspect, in the second one this aspect is hindered to have students focused on the phenomena being measured.

"To understand the cause-effect relationship of the underlying model" as different from "To predict the results and/or performance of an experiment."

This approach of using the simulation tools assumes students will know the underlying model, the cause-effect relationship, and will use that knowledge to perform a prediction task.

Dr. Sanders explained how he experienced simulation tools in this way. He described how he first had his students understand the cause-effect relationship of the model. He then assumed students already had that knowledge in order to proceed with the design task.

> Dr. Sanders: …Yes, so by that point, you know, they should understand why— why we have these goals, you know, there's power supply voltage that needs to operate that, there's some amount of current that needs to

> deliver, there's amount of leakage current that it can't exceed when it is supposed to be off, and they should understand by that point why those are important for circuit designers. Hum— and then when they design the device, you know, they are just – they are trying to achieve those.

Dr. Richardson also explained a similar approach. He explained how he first taught his students the thermodynamics principles during class, and then in the lab students conducted experiments in which they had to predict the behavior of specific samples:

> Dr. Richardson: So what I did was to – for my class of thermo class, thermodynamics, right, developed, and you can see it here, let me pull it up – develop – this is the same window three times, right? And this is all the students see, right?
> There's something called "chemical activity", where for example, you know the temperature, what happens is that the chemical activity of the material changes, right?
> Being able to figure out trends, and actually, this is using actual real numbers, right, you can predict if this – if this in this case chemical solution is going to mix or demix, right, in this case? Right?
> And this is a full class just talking about the – the thermodynamics of this one.
> And then I send them to the computer lab in this case, completely off the – off the hours of the class and ask them to—to—to tell me their – their order of magnitude and trends of what they should expect will happen, right?
> That's one of them.

This way of experiencing simulation tools places emphasis on students conducting prediction tasks where they use the physical principles to guide the design or modeling process.

"To predict the results and/or performance of an experiment" as different from "To validate the results of an experiment with verification/confirmation purposes."

This approach of using simulation tools is experienced when the result of an experiment is validated against some performance measures or target standards.

Dr. Sanders used simulation tools in this way. He discussed that in the first homework assignment, students had to collect data in order to characterize a device.

However, he later on explained how students used this same knowledge and techniques to validate their own designs.

> Dr. Sanders: In this part is reasonably well structured and that is actually the first homework problem we do the kind of measurements that you typically do to characterize a transistor and, you know, there are four or five different measurements and there are five or six different device parameters that you pull off of that, so that's the way I think about the problem.
> I look at—at the major characteristics of this device, what is the sub threshold slope what' s the off current, what's the DIBL, what is the on current, I look at that, and, you know, I can look at the characteristics and I can immediately tell, ok is this a bad device?
> And I can look at it and I can see ok, this will have a high serious resistance, this one has very bad short channel effects— that I can just look at this half dozen key measurements that people do and I can interpret those and I can say, ok is there's a problem, I think I pretty well know where the problem is.
> So that's the way it's structured in here, and the transistor design has evolved for so long that its, there are relative small number of basic measurements—you do these measurements and pretty much know everything about the transistors— so— so that's what they're doing in this design problem.
> They take the bigger device that behaves properly, they shrink it and they should understand now that I need to do these half key dozen measurements and look at these half dozen key parameters and they're going to tell me everything I need to know about what's happening with this device. And then you look at, ok which one is the biggest problem and that's how I'm going to work on the first.

Dr. Sanders also explained how in homework assignment nine, he pulled together all the knowledge students obtained from the course and designed a smaller device. As part of the task, students had to meet simulation performance standards and follow an iterative process of validation and design until those standards were met.

> Dr. Sanders: Now you know, then maybe the most challenging one was this scaling exercise, that's homework nine, where they tried to use all of the knowledge they had in class about what controls the performance, what are the issues when you make the device smaller, what are you trying to achieve in terms of the electrical performance and we give them a simulation tool and we ask them—I think we— we give them— parameters that are targets.
> Because the semiconductor industry is kind of mapped out where it wants to go. So they have some targets where this is how much current we

> want, this is the lights of the channel, this is the thickness of the insulating layer.
> Hum—but we give them these targets and then we say use the simulation tool to design a transistor that meets these targets.
> So—so, you know there is some—what they need to do is to do a simulation, interpret the results, so using their knowledge of the course, look at the results and say ok this transistor suffers from too much DIBL ok. How do I— how do I fix that? And then they should realize while in class we learned the DIBL is controlled by two dimensional electrostatics and has something to do with the depth of the junction, and the thickness of the oxide, using that, they adjust the parameter and try to— try to improve it so that all of the key performance targets are met.
> So that, you know, that exercise was really designed to try of pull together everything they've used in the course and— you know, this is what engineers at Intel do every time they do the next technology generation you know what performance targets you want to meet and you try to design the transistor in order to meet those. And they can do all of that by the simulations.

Validation of an experiment is done after conducting a prediction task. A prediction task, as explained earlier, is usually informed by physical principles. Therefore instructors who experience simulation tools in this way want their students to first be informed from physical principles and then conduct a prediction task of a specific phenomenon. Additionally, the output of the prediction needs to be verified or corroborated with some target parameters or predetermined standards.

“To understand the cause-effect relationship of the underlying model” as different from “To test the accuracy of the simulation’s underlying model and its implementation.”

This approach of using the simulation tools is experienced by testing the output of the simulation by applying physical principles. For example, to test the validity of the simulation’s underlying model by comparing the output with the simple case of the analytical solution.

Dr. Richardson explained the way he introduced the simulation tool to his students. He explained that first students learn about the physics, the cause-effect relationship of the model, and then, by using that knowledge he expected his students to become critical users of simulation tools and to evaluate them:

> Dr. Richardson: No, I put animation on that, yes. But I didn't tell them anything about the tool, right? Because yes I want them to – to learn first about the physics than to just start pushing buttons, because in my previous experience with this other class, right, with—with the thermo class that you see down here, right, my previous experience here is that I could expose them to this first, they will not think about the problem, right? They will just like what they see, right? And, I want them to think of – in physical terms, right?
> So, I don't want them to be users of the code; I want them to critically use it, right? To use it as a guideline, and if there's something that's not right, they can see it right away, right? In general, right; regardless if it's a modeling class or not, right?
> So, anyway what I do when I actually ask them to use a commercial software is well okay, it's fine, you're gonna' use the commercial software, right? So, homework number one is I want you to tell me all the thermodynamic error – at least 10 thermodynamic errors in this code. You know, and they and—and they – it's if you do know thermodynamics, if you actually know thermodynamics it doesn't take more than 10 minutes to find 10 errors, right?

Dr. Sanders also made this distinction when he described how a particular homework assignment was different than the rest. He also explained what approach he expected his students to follow. That is, by means of physical principles, simple calculations, students would be able to identify the errors in a particular simulation tool and possibly the causes of it.

> Dr. Sanders: Now some of the other problems they've used to tool to – to amplify in some concepts in the class; or they've used the tool instead of going into the lab and doing a measurement; they sort of treat the results of the simulation as though they were in the lab actually doing a measurement and then they—they analyze it.
> Now this—this one is a little – a little different and the explanation is – really comes from this—this paragraph here in the homework assignment that, it's to sensitize them to the fact that when you're using the simulation tool you have to be a very critical, intelligent user. You have to know how to decide for yourself whether you have the program set up right, and it's producing results that you believe.
> So, you know, in this case I had an interesting thing happen. We're using a new tool, and uh, obviously there are a few rough edges in it. There is one particular thought that as we used in the previous assignment, I looked at it and I think, "I don't think that's probably where it says it is." And uh, the purpose of the assignment there are really two parts:
> First of all, determine whether – what's being plotted here really is what the labels say is being plotted.

> And the second part, which is more challenging and I don't expect many students to get, is to figure out what actually is being plotted if it's – if it's really not what it says it is.
> So, it's the kind of thing that I think people that use simulations programs are—are used to doing.

Becoming critical users of simulation tools is a key characteristic that differentiates these two categories. By applying their knowledge of the physical principles, students verify the accuracy of the simulation tools. This is done in terms of implementing the right model as well as the model being implemented accurately with the appropriate computational technique.

"To test the accuracy of the simulation's underlying model and its implementation" as different from "To use and implement computational techniques in a modeling task."

This approach of using simulation tools is experienced in a modeling task where students implement a physical model or parts of a physical model by applying computational techniques. Students perform tests to validate the correctness of the model as well as the implementation.

Dr. Denner explained his approach of using computational simulation tools in his course. For example, when discussing about how his students used MATLAB to implement the Schrödinger equation he explained as follows.

> Dr. Denner: I have always felt that using a – because I am really trying to teach people how to let – that you can take these equations and connect it to the real world without relying on anybody else's tools or anything.
> So to me this is almost like a replacement for analytical methods.
> We all learn that okay, here's a differential equation, solutions look like Cosines and Sines, that kind of thing.
> And to me this is like the 21st century version of that almost. You don't have to go to cosines and Sines, you can just program it in, and do it for yourself. Nothing difficult. It's not one of those very difficult things that someone superior has to write a code for you, and then all you can do is run it.
> They have this confidence about the equation itself that we are really just trying to extract the meaning from this equation.

From the above quote, it is clear that Dr. Denner wanted to emphasize the physical aspect of the problem and how, by using MATLAB, solve differential equations in an easier way. Dr. Denner also emphasized in his course the importance of constant checking model implementations against the physical phenomena:

> Dr. Denner: …But that's it. The other thing I've often stressed, and I feel that in all areas is important is that in physics, and all that, I always say that it's really an experimental science. So, it's very important always to compare with the other.
> So, and this is where I've felt again that somehow a lot of this teaching tends to get very mathematical, like a Schrödinger equation, where does it come from? Well, there's all these postulates, etcetera, etcetera.
> Whereas the way I would say it, how do you know – is anything right about the Schrödinger equation? Well, because when you calculate the energy levels, it exactly matches what people have measured from the hydrogen atom very carefully. And this is how the Schrödinger equation was discovered in the sense that people had all these answers, and they were looking for an equation that would fit it. That's really exactly how this works. If you are constantly checking against nature, you have a way of measuring something. And, how do you have any confidence in solving your equation, is only because those energy levels fit the experiment so well.

Dr. Richardson also used simulation tools in a similar manner. He explained this experience by describing three levels of importance. Dr. Richardson talked about first knowing the physical aspect of the phenomena, second the mathematical aspect, and third the computational aspect. He also mentioned how is it important to identify when the model or the numerical part would not work:

> Dr. Richardson: Like, what I want them to see is that they can attack, they can be able to model materials that are geometrically complicated, by using tools that already exist, right?
> And—and be aware, think of three levels.
> Think of the physics level, which is the most important one because, and I insist on that all that time that there's really nothing, never gonna' be more powerful than their, than their intuition, and their knowledge of the problem, right, that the computer is just a tool, right?
> They also have to understand it from the point of view of the mathematics of the problem.
> And, the third one is in the computational aspect of it. Right?
> And the computational part, right, you show them well, I will show them right, what – what part of a model can break, and what numerical part of it will not work, right?

Dr. Richardson also explained how, once his students implemented their own simulations, the verification process is part of this implementation process. In this particular case, Dr. Richardson wanted his students to compare the performance of their simulations against results in published literature.

> Dr. Richardson: They're going to have to write their own simulation. And—and it's an – there's a lot of literature out there, and as a reference I'm gonna' give them a paper right, which they can compare against so they know when something is physical or unphysical, right? Because again the goal is that they – that they can – they can actually make this relationship, right?
> If they run a model, they should be able to see this is physical, this is not working, and be able to make the distinction.
> Why? Because in real life, when they're actually out there trying to solve a real problem, if they cannot tell this difference between what is physical and what isn't physical, they won't be able to fix the problem, right?
> And—and they – one of the things we have discussed recently is uh, let's see how do I put it, they—I want them to realize that they should always be suspicious of what they program. Right?
> And that they should not trust it, and they should – they should test – find as many tests experimental, and theoretical, until they're satisfied enough, right, not completely though, satisfied enough to—to say something about the physical problem, right?

The way of experiencing simulation tools by these instructors informed a structure of increased complexity. With the instructors' explanations I identified that understanding the physical aspect is key for being able to test the accuracy of a simulation tool and to be able to implement a model by means of computational simulation tools.

Summary of Results

The primary goal of this phase of the study was to identify qualitative different ways in which engineering instructors experience simulation tools. As a result, an outcome space was generated composed by six categories of description. These six categories represent the learning goals instructors had when incorporated simulation tools as part of their courses. The six categories of description are:

- To understand the cause-effect relationship of the underlying model
- To collect data as in a laboratory experiment

- To validate the results or performance of an experiment
- To predict the results and/or performance of an experiment
- To test the accuracy of the simulation's underlying model and its implementation
- To use and implement computational techniques in a modeling task

The way instructors experienced simulation tools in their research contexts confirm general ways in which simulation tools were used in an educational contexts. However, this study also reveals new ways of incorporating these tools that have not been documented in learning contexts. Additionally, these categories also reveal similarities in the way experts conduct their research. These similarities and differences are discussed separately in the final chapter.

CHAPTER V

STUDY THREE - PHASE 1: INSTRUCTORS' PERCEPTIONS AND EXPERIENCES OF COMPUTATIONAL SIMULATIONS AS LEARNING TOOLS

Little research has been done to identify reasons why and the way in which computational simulations are adopted by instructors to support their teaching and the learning by students. Furthermore, none of the examples that do exist involve college-level engineering instructors. From the more than one hundred references consulted for this study, only Hennessy et al. (2007) reported the results of interviews done with secondary-level instructors who have incorporated simulation tools as part of their learning activities. Hennessy and her colleagues conducted two studies to investigate how teachers incorporate computer-based technologies such as simulations in the science domains, particularly concentrated in identifying the adaptation process of pedagogical approaches to the classroom setting. The research questions investigated were: a) How can teachers support students in using interactive technologies to access the theory-world of science? and b) How is the pedagogy associated with this goal shaped by the cognitive resources that learners bring to bear and by the structuring resources available in the specific educational setting?

The participants of the first study were four science teachers from different schools who created new lesson designs for using computer-based technologies—i.e. multimedia simulations in their teaching. The data collection methods were video recordings of teachers implementing the lessons and a semi-structured post-project interview with the teachers. The researchers reported the pedagogical approaches teachers found more appropriate to implement when incorporating simulation software into teaching and learning. Teachers concluded on three pedagogies they believed exploited the intrinsic properties of the simulation software resulting in effective teaching and learning. These pedagogies were: a) allowing students to engage in hands-on experiences offering them a degree of control over their inquiry approach to investigating posed questions, b) pointing out the imperfections of the simulation's underlying model coupled with additional research conducted by students to clarify their own understanding, and c) employing multiple teaching strategies according to student's level such as more emphasis on the visual representations and addressing the assumptions on which the underlying model is based. In a consecutive study the researchers also focused their discussion on the roles of the teachers as facilitators, and the relationship between the students' abilities and the way the simulations supported their learning. Hennessy and her colleagues' (2007) second study was conducted with the purpose of documenting the strategies that evolved from the integration and use of technology into classroom practices in secondary-school mathematics and science. The participants were ten focus groups composed of three or four participating teachers. The results of this study were eleven case studies varying from professional practice, school, student group, and topic. The researchers focused their discussion around the pedagogical strategies practitioners devised and the role they took. The researchers also pointed out internal and external constraints practitioners encountered and ways in which practitioners had overcome them. They pointed out the importance of instructors' pedagogical approaches. Their conclusion included benefits in students learning as a result of exploiting the intrinsic properties of these technologies by applying them with the adequate pedagogical approaches. These approaches were appropriate individual and team student experimentation, direct instruction to facilitate conceptual change, and posing "What If" questions that engage and challenge learners.

The two studies offered by Henessy et al. present effective guidelines to implement pedagogical approaches teachers found to be effective for students' learning. However, these studies do not present how these pedagogical approaches are aligned with learning outcomes and the corresponding evidence of the learning. Furthermore, these studies were conducted at a secondary level with mathematics and science teachers leaving the gap of identifying how these same approaches are incorporated at an engineering college and graduate level. In the following section I focus my analysis in engineering instructors' perceptions and experiences of computational simulations as learning tools. This portion of the study is an extension of the phenomenographic study presented in Chapter IV. For Chapter IV the purpose of the study was to identify as much variation as possible of ways in which instructors incorporate the tools into their instruction in terms of learning outcomes at an activity level. This chapter presents a more holistic view focusing on how instructors integrate their learning outcomes at a course level together with evidence of the learning and pedagogical approaches.

Methods

Inductive and qualitative methods were used to construct individual case studies on how instructors perceive and experience the use of computational simulations as learning tools. I employed the case study approach (Eisenhardt, 1989) together with a grounded theory approach (Charmaz, 2006) as guidelines to analyze data for building theory from case studies. For a detailed description of the method of inquiry, participant selection, data collection method, and analysis, refer to Chapter III.

In this analytical stage of the study I individually studied six engineering instructors to develop in-depth descriptions of each of them (Merriam, 1988). Narrative descriptions were framed around Wiggins and McTighe's backward design process (1997). Wiggins and McTighe present a "backward design process" (p.9) composed of three main stages: a) identifying the desired learning outcomes, b) determining the acceptable evidence of that learning, and c) planning the experiences and instruction. These results were compiled in individual case study reports. The individual cases were also compared to identify common themes and patterns (Merriam, 1998) and the result of this comparison process is presented in the summary section. I interviewed instructors who incorporated computational simulations into their pedagogical approaches. The instructors were identified through the initial survey taken as part of Study One. These survey data helped to identify instructors who were using simulation tools through an entire semester or teaching graduate courses, and had positive responses to the use of these tools from their students. These instructors were given the pseudonyms of Dr.

Sanders, Dr. Hass, Dr. Richardson, Dr. Shaw, Dr. Clase and Dr. Denner. These instructors were part of the Network for Computational Nanotechnology (NCN) and they were initially contacted through this organization. From the six instructors who participated in this study I requested permission of four of them (Sanders, Hass, Richardson and Denner) to allow me to observe their lectures for an entire semester. These observations were useful because they allowed me to establish rapport with students and gain a general understanding of the subject matter. The first two interviews were conducted at the end of the Fall 2007 with Dr. Sanders and Dr. Hass. Dr. Sanders and Dr. Hass were interviewed again at the end of the Fall of 2008 together with Dr. Richardson and Dr. Shaw. Dr. Clase was interviewed in the Summer of 2008 and Dr. Denner was interviewed at the beginning of the Spring 2009. Each interview was conducted by a senior researcher while I was in charge of note taking and audio recording the interviews. The individual interviews were semi-structured, conversational, and lasted approximately one hour. A detailed version of the interview protocol is presented in Chapter III. The interviews were transcribed by a third party and me. I then continued my analysis by reading through the interview transcripts several times and conducting open coding (Patton, 2002). Once finished with open coding I developed categories seeking for internal homogeneity and external heterogeneity (Patton, 2002) In this iteration, I categorized my themes around Wiggins and McTighe's backward design process (1997). I also identified what instructors considered major advantages and disadvantages of simulation tools. The next step was to write individual case studies for each of the instructors. In doing so, I grouped the quotes that belonged to the same category (i.e. learning goal, assessment method, pedagogical approach, advantages and disadvantages). I reread each of the quotes and, if necessary, regrouped them where I thought they belong. If two quotes described two of my categories I put them in both. Once my quotes matched my categories I proceeded to identify the most representative quotes for each category and followed by documenting each individual case. Finally, I examined all the cases together to inspect similarities and differences in order to establish consistent patterns across multiple cases.

Results

Dr. Sanders Perceptions and Experiences of Simulation Tools

Dr. Sanders is a faculty member in an electrical engineering program at a Midwestern university, and has more than 30 years of experience in engineering teaching and research. Before joining academia, he gained corporate experience working in the integrated circuit industry. Dr. Sanders' teaching and research have been recognized with several awards.

Learning Outcomes

Dr. Sanders has been using several of the nanoHUB simulation tools as part of a graduate course in semiconductor devices. He used the nanoHUB throughout the semester, at various times. Dr. Sanders' instruction focused on helping students develop "an intuitive understanding" of the phenomenon under study. He did this by designing learning activities that would either imitate a lab experience or activities researchers would conduct for industry development:

> … this homework eight that I have here, so this was like a virtual lab. These are the kind of measurements that device engineers frequently go in a lab and do, and it gave them a chance to do it by simulation…

One way in which Dr. Sanders used the tool was to have his students experience a situation in which they "have to be a very critical, intelligent user." This means that students had to evaluate and, by means of applying physical principles, identify if the output of the simulation tool is correct:

> Now this—this one is a little – a little different and the explanation is – really comes from this—this paragraph here in the homework assignment that, it's to sensitize them to the fact that when you're using the simulation tool you have to be a very critical, intelligent user. You have to know how to decide for yourself whether you have the program set up right, and it's producing results that you believe.
> But you know, then you have to be able just to step back from it, and ask, "Okay, do the results make sense?"

Throughout the nine homework assignments, Dr. Sanders followed an approach in which each homework assignment was part of a progression in the level of complexity. However in the last homework, he targeted integration of all the knowledge gained through the semester, which he defined as a "design challenge":

> Now, you know, then maybe the most challenging one was this scaling exercise, that's homework nine, where they tried to use all of the knowledge they had in class about what controls the performance. Those are the issues when you make the device smaller…

According to Dr. Sanders, this activity served not only as a final project integrating the semester's knowledge, but it also tried to imitate an in-industry experience:

> … so this particular one, sort of integrates all of the knowledge in the course, and kind of explains, this is... if you are going to be a device-development engineer in Intel or something, this is basically what you are going to be doing, trying to do work like this, if you are a circuit designer or someone who is just using that technology to understand how the devices operate, you know, this is in what Intel spends two or three years on every time they move to the next technology generation...

Evidence of Learning

Dr. Sanders focused his assessment on students designing devices meeting industry target parameters. While in one assignment he asked his students to "look at a paper that presents some measured data from a current generation" asking them to "tweak the parameters in the model so they can get a best fit"; in the final assessment he went beyond making it a "design challenge," asking his students to meet parameters of a next generation device.

Since most of the activities that involved the nanoHUB simulation tools were related to homework assignments, solutions were posted on the website. After students saw their responses and had a chance to corroborate them with the solution, Dr. Sanders scheduled feedback sessions outside of lectures. When I asked him about the process of providing feedback Dr. Sanders said:

> Yeah, that's the problem, in the course I didn't have enough time to do that. We had a couple of help sessions that we scheduled in the evening and we went through a couple of homework assignments explaining... this is what you should have learned from the homework assignment... probably we didn't do as many of those as we should have... hmm so my challenge the next time.. I think, there wasn't enough of that... we posted the solutions, but I think that really needs some discussion.

Dr. Sanders recognized that this feedback was not enough, but he mentioned his willingness to try different arrangements taking advantage of the fact that he recorded all his lectures the last time he taught the class. These lectures were uploaded on the nanoHUB and are easily accessible for students:

> We had maybe two or three, possibly four but it was not enough. I was even thinking that I can use some of the recorded lectures and instead of using the class. Because with all the material I had to cover, it was very difficult to devote class period to discuss the homework, so I may try next time to assign, ok listen to the lecture on your own time and now I'm going to use class time to discuss homework assignment this time. I don't know how that's going to work.

Instructional Approach

At the macro level, and with the exception of homework one, the most common instructional approach followed by Dr. Sanders was to first introduce the concepts during class and then assign homework. Homework assignments were designed by Dr. Sanders with the intention to provide practice for students. At the micro level, most of the times, the homework assignments were focused on exercises that allowed the students to compare concepts learned in class with results from the simulations. For example, for the case of homework two:

> They took the analytical calculation they have done in class and they did that first, and then they ran a simulation tool and they compared results and explain what was similar and what was different…compared theory versus simulation. They do some of the quantities that we were talking about in class and compared them to with what the theory says is should be.

Dr. Sanders explained that while the exercises done in class are approximation to the exact solution, with the simulation tool students can solve the exact ones. Therefore students had the opportunity to compare those solutions and draw some conclusions and identify "how it really works":

> …we have to make lot of simplified approximations so it work out, you know equations for this, hum... that you really go about it in practice, now we are going to run a simulation that solve the equations properly without these approximations, and we are going to see how it really works and which of these approximations are good and which of them aren't so good and things like that.

In the case of the first homework assignment, Dr. Sanders designed it as an exploratory activity. He gave an opportunity for the students to become familiar with the simulation tool as well as with the output and what that output means:

> So if I look at this first one it's just that, this one most students don't have any hands on experience with transistors, they don't know what the current/voltage characteristics look like, so we just want them basically get them some experience this device has three terminals, you hook it up and apply voltages, these are the currents that you measure, this is how a typical device behaves, this is how much voltage you typically apply, you know 1 or 1 point 2 volts, this is how much current typically get. So it was just to give them before they start the course to get them some feel for how these devices work, what voltages you apply to them and what currents, flow...

As part of Dr. Sanders's pedagogical approach, he usually provided his students with a starting point that consisted of a model to be tested in the simulation tool, initial parameters that should be met, and/or a model to be implemented (i.e. writing a MATLAB script) outside the nanoHUB. Then, the output of such a model became the input for the nanoHUB simulation tools:

> Well so I guess, you know, what we give the students as a starting point is a current generation device that behaves well, and we tell them ok we want you to shrink the size of this device and has to perform in this way, so the first step would be just to go and properly reduce the dimensions…

Perceptions of Simulation Tools

Dr. Sanders considered nanoHUB simulation tools convenient because they allowed his students to solve hard analytical calculations easily through simulation. Another feature of the simulation tools mentioned by Dr. Sanders is that his students had the capability to use different models ran with different parameters that would give different outputs:

> …so I can choose where I want the plot... let's turn that off just to save time, but normally they would want to plot that too, so this tells them what kind of output plots they would get through the terminal characteristics of the device that like you are measuring if you want to do it on a lab...

Dr. Sanders also commented on one particular characteristic of the nanoHUB simulation tools: their simple interface. In the same comment, Dr. Sanders made clear that nanoHUB simulation tools have a high level of complexity that is transparent to the students:

> Yeah, now this one is actually... it has a simple interface underneath it, is an industrial strength tool underneath, it's one that was developed at Bell Labs a few years ago, so the simulation that's doing is nontrivial, it might take a few minutes here... Now what we've tried to do is to simplify the interface because it would typically take a graduate student maybe a few weeks to learn the full interface to run in this tool. This is the kind of tool that you would run in industry hum... it can do a lot but there's a complicated input format that you specify in the file and we really don't want to use class time for all of that, you can easily spend a week just explaining how you run the tool, how you set up an input file and we are trying to eliminate all of that.

Dr. Sanders also mentioned that a specific element of simulation tools that make them unique is that it gave him capability that could not be replicated in the lab.

> So now, if I want to go in, I can look inside the device, so that's the kind of data I would just give them in the lab and measure the device, but what the simulation allows you to do is to look inside the device and if I want, I can take a look and see a electric field inside the device... let's see if we can...

Dr. Hass' Perceptions and Experiences of Simulation Tools

Dr. Hass teaches a 500 level course for graduate students and advanced undergraduate students related to modeling and simulation of materials.

Learning Outcomes

Dr. Hass explained that the main goal of the course was to teach simulation techniques as well as the related concepts and ideas:

> In this particular course that we will teaching this semester, the—the goal is for the students to understand the concepts and the ideas behind the simulations, the physics behind the simulations, approximations and numerical issues behind the simulations.

Although knowing the simulation techniques are the main focus of the course, it was also important to: a) identify how these techniques can be applied to solve scientific or engineering problems, b) identify what is the level of accuracy, c) be able to interpret the results, and in short d) "understand enough that they can be critical users":

> We do computation to solve engineering or scientific problems. And so, we—we are always concerned about the application. We want to use what we learn to—to look at nice examples of calculations that might be of interest. But the main – but the focus of the course is not an application, but a series of techniques that allows us to solve many applications. We'll pick applications as we see fit to exercise what we learned about the techniques.

Dr. Hass provided an overview of the topics taught in this course. He explained that he focused on the physical phenomena, computational aspects of different models and its degrees of approximation. This included everything from an atomistic point of view:

> And uh, so we talk about the physics and the approximations in the physics that we do. We'll talk a little bit about the computational aspects uh, of those models. And we'll talk about a variety of different models that describe materials with different degrees of approximation and course some materials. Describe in very, in a lot of details, describing atoms and electrons.

Evidence of Learning

Dr. Hass explained that his evaluation method is through a mid-term project and a final exam. Additionally, Dr. Hass said he gave students homework assignments as a means for students to practice and as a means for himself to know what students understood. Although those assignments were not graded in detail, Dr. Hass made sure students completed them. Alternatively, when students were not able to finish the assignments, he gave opportunities to complete them:

> So, we don't actually give them you know they're – it's a advanced course, so we're not going to give them uh a lot of feedback, or you know a grade on the homework except that whether you know they've accomplished, or we wanted to do something complete, or whether they need to redo something. If they're clear they didn't understand what was asked about that…we'll give feedback based on the – on the homeworks…[if] lots of them frequent the same thing, we're going to address it. If it's – or we'll do it more on an individual basis if someone doesn't complete homework. We're not going to grade it in detail, but we will – I will make sure that they're following it.
> And so ((I: Um-hum.)) the homework will be such that it allows me to more or less know whether students are understanding or Falling behind, and to make sure that the students can actually do what's expected from—from that.

Instructional Approach

Dr. Hass described this course as a "hands-on class" in which students explored a variety of models ranging from simpler to more complex, describing those models starting at the level of atoms and electrons to describing them with continuum equations:

> And we'll talk about a variety of different models that describe materials with different degrees of approximation and course some materials. Described in very, in a lot of details, describing atoms and electrons. From then we take a step out and we average out the electrons and we keep that atoms. And then we take another step and we'll group a bunch of atoms into single parts, and then we go all the way to the continuum, and rules, simulations where don't have atoms solve continuum equations.
>
> So we work the – the stuff through this hierarchy of models starting with as much detail as we need to describe the material and go all the way to very coarse descriptions that you can use to describe a whole airplane or something where you really don't worry about every single atom.

Dr. Hass explained that an important component of the course involved using the nanoHUB.org as a tool to understand and implement modeling techniques. Dr. Hass described the different tools and different ways in which they used nanoHUB.org. In particular, they used the workspace and simulation tools:

> So—so one way we will use the nanoHUB work stations – so the nanoHUB has one of the tools, actually an essential tool, it's the ability to open what's called a workspace which is in UNIX uh, desktop. So, like I have here, and it appears inside of your browser, bump it up. And so the students, they have access to a computer. They type in commands, and they can compile and do stuff like that.
>
> With the workspaces, what we want to do is that the tools that run this like the geeks run, you know, or the experts run these things, they login their computer they can see the source code, they can see the input decks, you know, you need to know more about this stuff, and it's not, you know you have to make your own graphics, but it allows you to really tweak this, tweak this, and plug this the way you want to.
>
> So, at the beginning there'll be – in this class we want them to learn that what's inside the codes. So, we'll start with simple codes that solve simple problems but so that the students can actually look at the code and know what's inside and know that there's no magic or whatever.
>
> Um, this – as I said these are very sophisticated models for they take many, many years to develop um, so—so they will be working on little pieces of this, or simplified versions of this; but they will just to gain enough confidence that they know what's inside the box. They may not

> know every single detail about what's inside the box, but they have a flavor of what's inside the box.
> So the workspaces allow them to look at – inside the code, and the online simulation tools allow them to really uh, or to just run simulations. And so – so part of it will be in looking at what's in the guts of the problem, maybe modifying little things. And part of it is just running and analyzing the results.

Dr. Hass also implemented some cooperative pedagogies:

> They will be doing, yeah, so, we have to discern that—that last year they worked in common projects, and they collaborated. But then, in doing the simulations, but then each of them have to perform their own analysis and turn in their own work. So they collaborate and they can discuss, but then at the end of the day it's uh, individual analysis.

Perceptions of Simulation Tools

Dr. Hass pointed out that one of the biggest advantages of nanoHUB is easy access, which gives his students freedom to work from any place at any time and saving costs:

> So, that's very beneficial uh, in teaching because then the students are not limited to using the computer the labs, you know, the times that they are available. But they can log off, go home, re login and look at you know everything should be like they left it.
> So, it gives them extra flexibility.

In addition, Dr. Hass pointed out other capabilities of nanoHUB.org, such as the flexibility to share sessions that allow distance collaboration:

> If something's not running for a student, we – they can share the workspace with us, and we can look at what they're doing, and say, "Well, you're doing this wrong." …you can share this work space, or something's not running, they can use it to collaborate and we'll explore that. So, you know, they can say, "Well I can share my workspace with Alejandra; she can take a look at what I'm doing and say, 'well, you're running that wrong, or I'm getting a different results." Assisting, and collaborating from their home, but like sitting on the same computer.

Dr. Shaw's Perceptions and Experiences of Simulation Tools

Dr. Shaw is an assistant professor in the Department of Electrical and Computer Engineering at a Midwestern University. He has been an active contributor to the nanoHUB.org since 2005. He has participated in the development and/or update of approximately ten simulation tools. In addition to his experience in computational science, Dr. Shaw has more than ten years of teaching experience. Dr. Shaw teaches a course in nanoelectronic devices to M.S. and Ph.D. students that is not a required course.

Learning Outcomes

Dr. Shaw explained that during the course students explore and discuss many types of nanoelectronic devices, such as nanotransistors, nanomemory devices, energy conduction devices, solid lighting devices, and nano-bio devices. His focus was on the practical aspects rather than on fundamental theory. However, he provided a general theoretical introduction to all the types of devices, "the underlying physical principle from quantum mechanics":

> …this course basically, you know this nanoelectronic device course that I've been teaching for the last two semesters, basically this course will go from the device issues, what are the problems in nano devices; what are the phenomenon in the nano devices, how do you know fix those things. And, things like that. Not – not big, very fundamental theory, but just the essential theory of nanoelectronic devices…

Dr Shaw also explained that another component of the course was to understand the characteristics of these nanodevices and the problems related to achieve those characteristics from a technological point of view, a fabrication point of view, a design point of view, and a modeling point of view. For example, from a modeling point of view, Dr. Shaw explained the kinds of theoretical and practical considerations students must do:

> …like if you want to model these devices, what approach do you needed like, is it fully quantum mechanical, or semi-classical, or classical approach will be enough? Or, these things…so, not only understanding the quantum mechanical phenomena, but also to you know, to have some idea, to deliver up some idea how to use these uh, novel phenomena to, you know, to optimize the device design or to innovate new device concepts.

Dr. Shaw also explained that during the course he attempted to build upon students' knowledge of circuit design:

> Uh, basically you know, the objective is to – so, I mean here in my school we have a good – good uh, curriculum in circuit design, so many students are really you know circuit designers so now that I – now that I'm

> teaching the device course, so they're basically they're learning also the device perspective, and what the device issues are… they really need the device background for circuit design, designing.

Dr. Shaw introduced the nanoHUB simulations for specific purposes. One of which was to have students become familiar with the software environment to "how to simulate a device; how to design a device; and, how to see the essential physics." Dr. Shaw also explained that he used several tools, about eight to twelve, extensively during the semester. A second purpose was to do advance calculations and compare and contrast different ways to get the mathematical solutions to a problem:

> …the important thing is give nanoHUB tools, you know, they are more advanced; they are some of the tools are fully quantum mechanicals, so students can readily see, readily verify what is the – you know what is the difference between classical or analytical calculation and the quantum mechanical uh, calculation, right? They have to also understand the underlying you know equations, and why the – where the difference is coming from; things like that.

Evidence of Learning

Dr. Shaw's mechanism for identifying students' learning was through homework assignments. During the semester he designed a variety of activities targeting different learning goals. In one assignment, for example, students had to compare by simulation the performance of nano devices with the performance of conventional bulk MOSFETS. In these types of assignments, Dr. Shaw explained that the advantage of solving this problem by simulation is that now students do not have to do extensive calculations. However, they can identify some values by looking at the curves:

> They don't have to do extensive you know calculation here. You know, they just, you know, they are familiar with –they have they become familiar with advanced issues; conceptual understanding. So I basically emphasize some on conceptual learning.

Dr. Shaw usually structured his assignments in the following way: He first asked his students to view a lecture on the nanoHUB.org and then asked two or three questions from that presentation. The next questions were usually related to theory and the last questions must be answered by means of the simulation tools. What is similar in all of the questions is that students must explain and justify what they have learned. Through these explanations Dr. Shaw evaluated the students' levels of understanding:

> The first question begins, you know, with the seminar; watching the seminar and asking some questions, two or three questions on that seminar. The second question is a series of questions, so they have to say, they have to derive a formula, they have to do some calculations. So they have to derive one equation, a hand calculation, and apply it in a MOSFET. And two questions, you know, I ask on nanoHUB, but there are like several parts in each question. So I have to say, I have this source to use SHRED and then I ask them to verify to testify some statement. So, they justify; they verify what they learned in the class…so that the students really uh, you know learn something beyond the tools. It's not just of the phenomena, but just making some comments you know, that's the thing actually. So, every question will – you know, will have a part where they have to explain what they have they learned.

Instructional Approach

Dr. Shaw's strategy in introducing new concepts and ideas was to build on students' prior knowledge of devices at larger scales:

> So basically –you're gonna' build on what they know about MOSFET, and then they'll probably understand, "Oh, I see why you can't go any smaller." And so then you're introduce new ideas. But at the very – I guess I'm thinking as more of a global sort of level, right, this kind of major ideas…

As explained earlier, Dr. Shaw also designed homework assignments that involved: a) watching seminars or lectures on the nanoHUB.org, b) doing some calculations, and c) running the simulation tools. His goal in asking the students to watch the seminars was to identify the current research in this area. His goal in asking students to do some calculations was to convey an underlying theory. Finally, his goal in asking students to run the simulations was to have students understand, simulate, and design the devices. Also, he used the simulation tools as a means to compare and contrast different ways to do the calculations:

> So, basically by watching the seminars you know students are learning you know the most advanced, you know, ongoing research you know, on this particular topic or field.
> Now, the second question, the pure, you know that, the where they have to derive some formulas, some equation, or you know, some material calculation, you basically are learning some you know underlying theory.

> Um, calculations, math, you know math and models, you know, things like that.

Dr. Shaw also emphasized that by using the simulation tools, his goal was to have students understand and identify different ways to compute solutions. In order to do this, Dr. Shaw designed activities that make students compare and contrast different ways to compute calculations and the results of those calculations:

> I can add one thing. You see expert equations are simplified, very approximate. Like when you see a textbook you know, you – the equations in the textbook are very approximate. Now these calculations are not valid for quantum or small nanoelectronic devices. But, the important thing is give nanoHUB tools, that are more advanced; there are some of the tools are fully quantum mechanicals, so students can readily see, you know, readily verify what is the – you know what is the difference between classical or analytical calculation and the quantum mechanical uh, calculation, right? So now, I have them work, okay, compare the solution in the textbook and similar, similar results you know that you get from nanoHUB simulator.
>
> Now, it's not only they just compare, but I ask them why do you see the difference between these two results; the textbook and the nanoHUB? They have to explain. So right there, this would be because the nanoHUB tools, you know, they basically do solve between uh, say shorting an equation, or differential equation, which is – which the textbooks are not doing. So, things like that.

Dr. Shaw explained that he used two approaches to designing activities that used the simulation tools. One was by means of evaluating and discussing a predefined device, and the second was by asking the students to design the device:

> So, the way they learn, they have to first of all, you know, they can do two things. Number one is they can – they can basically they can, uh, you know, they can start with a, with a device, with a predefined device that I ask them well I mean use this – this dimension, this configuration, and see the characteristics. So they'll work the phenomena. From that you know they – they understand what is happening in the device. That's the first thing.
>
> Number two is, they have to design the device. Like they have to optimize the configuration. They have to, you know, vary, they have to vary the device, things like that. So that they have to optimize characteristics. So one thing they have to – they have to simulate you know, lot of simulations.
>
> So, the first part, where you have to see where one of these features, where one of these novel phenomena from the device, you just do a

> single simulation, you know. You pick a device, you pick a predefined device and then you see what—what is happening. But, the second question is on designing the device. Like, okay, now that you – now that you know what – what happens in a device; now you design the device. You change the dimension of the device; you change the environment of the device; and you change the modeling of the device so that you get best out of it. You get – you get the best characteristics; optimized characteristics. You know? Get at the true essential parts. How they learn things.

Most of the times, Dr. Shaw asked his students to conduct additional analysis of the data to get curves or characteristics that the simulation tools do not provide. Dr. Shaw considered this is a way to get students more involved with the tools:

> So, now this is really important because if I had asked only them to, only you know, just draw some – you know just do the download – the nanoHUB and submit it as homework, I'm sure that they will – they're not taking it as seriously basically. So, by asking them that well, uh, you know, uh, you know, extract some – extract something else from the variable uh, extract something you know from those and plot that. I think that—that—that's how I'm getting them involved – more involved with the tools.
>
> So, I mean, I—I ask them to extract something beyond what is available you know from nanoHUB. And then, that way, you know I can raise my – whether they are learning things or not. Yeah.

Dr. Shaw also used cooperative pedagogies in which he asked his students to build a virtual community on the nanoHUB.org as a way to have students discuss and disseminate their learning about nanoelectronic devices:

> So, they basically have a – you know, they create a group on nanoHUB…so there's a group of students – the students created a group actually to discuss things that – to communicate, you know, themselves basically, they create a group, study group…

Perceptions of Simulation Tools

Dr. Shaw commented on the advantages that nanoHUB.org provided to his students and himself. First, he found it extremely valuable that students, by just looking at curves, could identify phenomena without doing hand calculations.

He also thought that by having students interact with the nanoHUB.org simulation tools they would be more familiar with any other type of simulation tools they might encounter in the future. Dr. Shaw commented about the accessibility of the nanoHUB.org simulation tools. In particular, he mentioned the other advantages that they are free, of easy access, and the tools are concentrated in a single place. Also, he mentioned the advantage of simulations running on different computers than the students' and the fact that it is secure:

> Now, we can, you know we can cover you know lots of devices really quick because we have the simulators here. It doesn't take much time you know to draw the curves, and you know to say you don't have to look through many, many textbooks and everything is we get just from a single um, repository, a single hub right? We don't have to go through you know, just have to find these things in different places, we have everything in a – in a same place, right?
> And I can get, you know, the students really can get connected to the community you know. I mean that's the sense – this feeling is really great. And that's really the – that's another point actually I want to add, you know I mean. I have a heard from the students that they're connected to the community; nano community.

Dr. Shaw also commented on the limitations of the nanoHUB.org simulation tools. During our conversation, he mentioned that some simulation tools have a limited number of outputs, but that he overcame these by asking students to extract the data and analyze it using other programming computational tools such as MATLAB. Other limitations he mentioned were that when tools are updated sometimes the documentation is not updated. He suggested that there must be a way to let users know about such updates since this causes confusion and long waiting times for them.

Dr. Clase's Perceptions and Experiences of Simulation Tools

Dr. Clase is a scientist and group leader of two research centers at a large Southern University. Dr. Clase has also taught a course of computational nanoscience designed for graduate students and senior undergraduate students. The approximate number of participants in this course was from fifteen to twenty students.

Learning Outcomes

Dr. Clase explained that the main goal of the course was to provide students with the fundamentals of different computational techniques that are used when exploring and solving nanoscience problems:

> Okay. So, the way I wanted to make this class unique was that I um, I wanted to provide a fairly broad survey of tools that could be used in uh, in, in the compute – I mean, you know, in computational tools that could – could be used in nanoscience problems, for nanoscience problems…
> So, what I wanted to teach was what levels of theory do what in nanoscience? And, how do you – how do you take a level of theory and turn it into a useful calculations? And then how do you turn that useful calculation into something that's useful in a real problem, um, and that's meaningful?

Two other learning outcomes Dr. Clase expected from his students were to appreciate the usefulness of these techniques and eventually adopt them in their research practice, as well as to become familiar with the literature in this area:

> Uh, what I hoped for in addition to that, going beyond that, but didn't – certainly didn't expect everyone to was that some people might say, that it's useful enough that they would start to incorporate calculations in their own research.
> Uh, but at the very least I wanted to be sure that even if it's just to the extent that these experimental researchers when they read a theory paper they now have much more of a sense of what went into that paper. Right?

Evidence of Learning

Dr. Clase designed homework assignments for having students practice concepts learned in class and projects as indicators to identify students' learning:

> I could see it clearly in the final project – I gave final projects instead of a final exam, and it was clear in these projects what these—these kids picked up. And, it was a lot so.

Another indicator of students attaining class goals was that some students adopted computational approaches to their research:

> Um, and I would say you know, for – for at least five or six student that—that's the case, and they're doing calculations still now well after the class is over. Um, maybe even for more that I'm not talking to.
> So that was, I felt like that was a huge success. That—that almost half the class found from this class that simulations could be helpful for their own research. So that was – that was another goal and one of these sort of indicators that – that this course was a success.

Instructional Approach

An important component of Dr. Clase's approach was using simulations as a hands-on method to predict properties that occur at real nanoscale systems:

> And, uh, instead of just showing the basic equations behind each tool, behind each concept, like classical molecular dynamics F=MA; quantum mechanics ordinary equation, you know, uh, and so on and so forth. Beside – you know, instead of teaching all of that and all of the things that goes into that, I really wanted them to get their hands dirty and get hands on experience in – um, right away.
>
> So they learn an equation, and that day there's a homework assignment on solving that equation with a tool.
>
> And so what – what I really tried to emphasize was that – um, that look here is what – I'm showing you a broad set of ways of simulating systems uh, with many different levels of approximations. And um, but I'm not just showing it. I'm letting you do the simulations and that's where the nanoHUB came in, and it enabled me to do that so I could – I could have the students um, you know going back to classical – classical molecular dynamics, F=MA, okay we talk about all the things that go into solving that equation, and that very day we solve it on the nanoHUB for a nanotube.
>
> So not just for some really unrealistic system that you usually do like uh, you know, like everybody really does a simple thing; harmonic potential kind of thing – but for a real system that they have in their TM images, in their lab, in their research.
>
> And um, that was the point. I wanted to make it uh very hands on, very interactive, and realistic for them.

Dr. Clase developed a simulation tool specifically for this purpose. However, he made an important distinction between the tool he created and the majority of the tools that are in the nanoHUB.org. What makes his tool different is that Dr. Clase developed it for educational purposes rather than for research purposes. In doing so, he decided to limit input and output parameters to the tool and to provide default parameters:

> And, you know, what was different was that the tool I put quite a bit of time into designing for the course had major blinders on it right? So, here's a tool, an electronics structure tool that is hundreds of, no millions of lines of code that has enormous numbers of options. Right? It probably has you know 500 different input options if you really sort of look at it all together. And, I gave them eight. Okay. And, everything else I – I set for them under the hood.
>
> But, I gave them eight, and I gave them all kinds of example problems, and I made everything else automatic, and what it did was it—it took

> away these things that can distract from learning – let's say what I wanted to teach.
> And so, you know, I had to make choices for them, and set some defaults and so forth. But, it's good enough to teach, you know, to teach the concept I wanted to teach…
> By putting blinders on the input and putting blinders on the output. You know? You just don't want them to see all of that output, you want them to see the right output.

By using simulation tools in this way, Dr. Clase had the specific goal that students focus on the physical phenomena rather than on the computational part:

> And that's the thing, you know, that is how experimentalists view a lot of calculations, and I wanted to use this class to say, "Look, these calculations can be very valuable and let's not think about the – the CS part, let's not think about the complexity of these codes, let's think about the science we're trying to get to, and the understanding, and how could these simulations maybe help in that?" You know?

However, Dr. Clase also mentioned that students wanted more functionality with his simulation. Dr. Clase was able to provide that functionality due to the fact that he was incorporating new changes to the tool as students were providing feedback:

> Um, you know, and then, and then, the dramatic simplification of the inputs is another big part of it. And—and how to do that intelligently so that you, you know, I—I—I tried to stick to, and this changed 'cause people kept asking me for more functionality so I added it, but I tried to stick to a rule of about seven choices in any code. And then they all kind of got bumped up to 10 or something.

Perceptions of Simulation Tools

Dr. Clase explained that one of the biggest advantages in his students' learning when using simulations was in the outputs. When we asked him what aspect of the simulation helped his students the most he answered:

> Um, but, uh, so it depends a little bit on the tool, but I would say that it's more in the output. You know, and the "Aha!" moment is um, "Oh, I see how band structure relates to structure now – to the, you know, or I see how the density of states can be affected by something I'd do on the input." But, if they didn't have this way of—of looking at the outputs very, very easily and not going into the, you know, the actual text output files and all that um, it would be much less useful to them.

Dr. Clase also mentioned that this approach of using the simulations allowed him to focus on specific aspects of the course he wanted students to pay attention to the most without getting distracted with secondary technical aspects:

> But, two years ago when I taught it I made, um, like before I had to make little interfaces for them to do calculations and so forth. And it's just, it's much, much better. Um, much – they can do much more um, with the – this toolkit that we were able to develop on the nanoHUB. And so it's really allowed me to go much further with – with taking out the kind of computational science aspects which I didn't want to do, like LINUX and parallel computing, and you know, compiling, or whatever, you know, and just focusing on equations, the levels of theory that we need, the kinds of problems you can solve; really going after the real ideas of the problems.

Another advantage Dr. Clase perceived as very useful was that by using the tools, he was able to incorporate real and complex examples in his lectures:

> So not just for some really unrealistic system that you usually do like uh, you know, like everybody really does a simple thing; harmonic potential kind of thing – but for a real system that they have in their TM images, in their lab, in their research.
> And um, that was the point. I wanted to make it uh very hands on, very interactive, and realistic for them.

Also, Dr. Clase mentioned that this same simulation tool has the flexibility of being adapted to other different courses.

> So, in a way um, it was being able to have that flexibility of putting those blinders on, but – but really using the tool on what I wanted to teach, you know, and trying to keep it flexible enough so that it was still actually pretty useful to a more general public.
> That was – that was really advantageous… the same code can have a totally different set of blinders on… it can even take the same code or any of the codes I took, and put them into a totally different course with different in – completely kinds of inputs and outputs, you know, not completely different but very different, and that you could teach something different.

However, Dr. Clase pointed out that these "blinders", when students attempt to use the simulations for their own research, may become a challenge:

> Now, and could that tool actually be used for research the way it was developed with all those blinders? Not sure. Maybe in the context that I

> convey today where you have a kind of way of probing ideas. But that you then needed to bring those ideas to a theory group.

Dr. Clase pointed out some limitations his students encountered related to usability aspects and performance. Among others, Dr. Clase mentioned that students had limited number of jobs per user to execute and that slowness in the execution was a problem students faced.

Dr. Richardson's Perceptions and Experiences of Simulation Tools

Dr. Richardson is a faculty member in a materials science engineering program at a Midwestern university. Before joining this university about three years ago, Dr. Richardson worked in a national institute conducting research on the development of codes and theoretical tools for the analysis of microstructurally complex materials.

Learning Outcomes

Dr. Richardson has been using several of the nanoHUB simulations as modeling tools for his graduate course in modeling and simulation of materials. Dr. Richardson taught the second half of this course after Dr. Hass. His focus for this second half was on the continuum.

> And basically we are going from—from the atomistics to describe the time evolution of materials which is related to how one would process a material, and we will ultimately end in a – in a position where one would model materials that are not evolving in time, right? But they are very – you show them that at some point materials can become very complicated.

Dr. Richardson's main goal was to help his students "be thinking in the conceptual terms and not be just a programmer," and by that he meant ability to "model, simulate, and do engineering with the computer." Dr. Richardson believes that for this class, students must think at three different levels: the physics, the math, and the computational part:

> Think of the physics level, which is the most important one because, and I insist on that all that time that there's really nothing, never gonna' be more powerful than their, than their intuition, and their knowledge of the problem, right, that the computer is just a tool, right?

> They also have to understand it from the point of view of the mathematics of the problem.
> And, the third one is in the computational aspect of it. The computational part, right, you show them well, I will show them right, what – what part of a model can break, and what numerical part of it will not work, right?

Dr. Richardson used two main types of simulations as modeling tools, one in which students were actually modifying the code, and another in which the code was hidden behind a user interface. Dr. Richardson pointed out that he used the second type of modeling tool to help students develop an intuition of the phenomena under study:

> And I want them to develop that intuition, which they will not develop using FyPy because there they will actually see the code. So, I want them to see two aspects of modeling, right? One where they actually have to write it; and another one where you have this other big piece of software and they have to believe in the results, right?

Dr. Richardson had a third goal for his students to accomplish at the end of the course. He wanted his students to be critical and knowledgeable about the literature in this area:

> … students should distinguish, what should, what is – what is a good paper, and what is a bad paper. That's a talent that they have to develop, and the only way to do it is by exposing it, right?... And at the same time be able to integrate different concepts, right, which, I think in this case is important.

Finally, Dr. Richardson also wanted his students to realize that "they should always be suspicious of what they program" and do some calculations to verify whether their model is correct:

> And then of course, we go over the analytics, right, just to show that when you actually do the – the numerical model, your model should at least reproduce the—the analytics.
> If it doesn't do the analytical part of it then it's not gonna' fly. It's just not gonna' work at all.

Evidence of Learning

Dr. Richardson explained that the solutions to the homework assignments were the evidence of students' learning. He said the homework tests each and every aspect to be covered, and if students know what they are doing, they will be able to bring a model that works. However, there were some times in which students were not able to get the correct solution, and in those cases, Dr. Richardson's approach was the following:

> Well, in some cases they can not tell me – they cannot bring a model that works. And something I do tell them is, well if you cannot tell me why it works, I want you to tell me some ways of working right? And I think that's then enough. Sometimes it's a good enough answer.

For example, specific activities students did as part of their homework assignment were to write their own simulations, compare their results with those in the literature and identify the type of phenomena. If some discrepancies appeared in their results, he then expected his students to engage in a problem solving approach and be able to identify the source of the problem and attempt to fix it.

> They're going to have to write their own simulation on uh, on micro structure evolutions of material. And—and it's an – there's a lot of literature out there, and as a reference I'm gonna' give them a paper right, which they can compare against so they know when something is physical or unphysical. Because again the goal is that they – that they can – they can actually make this relationship.
> If they run a model, they should be able to see this is physical, this is not working, and be able to make the distinction. Why? Because in real life, when they're actually out there trying to solve a real problem, if they cannot tell this difference between what is physical and what isn't physical, they won't be able to fix the problem.

In order to be able to accomplish the assignment successfully, Dr. Richardson expected that students should follow a decision making process similar to this one:

> …I will not tell them how to differentiate that – a specific model from another one, but I will give them the means so that if they are out there in the world, they can, they will be – "Oh, this model is—is not good because it's violating the principle. All of the limitations of this model has such and such. But, oh if I could take this one and extend it, right?" Which basically takes – takes the theory of thermodynamics and extends it so that you can see how materials evolve in time. And—and it's concept – it has a lot of uh, it gives – it has the beauty that you can use concepts that they're supposed to know, right, like uh, uh, for example they have a temperature field, or a concentration, right, concentration field, or – or they can see that sometimes something it grows at expense of the other one, right? And—and you want – I connect that to thermodynamics.
> And then based on that, the sphere of the mathematics, because this is not a – this is not a – a math class, right, I'm sure that from here you can

> build a model that looks like this, right? And they all have the structure, right? And, based on that you can – you can build a model, too, too.
> And then of course, we go over the analytics, right, just to show that when you actually do the – the numerical model, your model should at least reproduce the—the analytics. If it doesn't do the analytical part of it then it's not gonna' fly, right? It's just not gonna' work at all.
> So the basic process of what you anticipate them having to go through is they basically have to make a decision where they have to change the model—and then they have to basically evaluate the results and come up with some rationale—where—where the model breaks. When you can blame the numerics; when – when you can blame the analytics; when you can blame yourself. And so as part of the rationale, that's where the content should come out—as far as understanding the physics.

Instructional Approach

Because Dr. Richardson's portion of the course started in the middle of the semester, his initial approach for introducing new topics was to build on what Dr. Hass had already taught the students. In particular his strategy was:

> …to show that there's a link between what happens on the atomic level and the continuing level and show that there's not only a theory but that there's a direct – direct relationship of what happens at those learning skills to higher, or courser learning skills. And—and with that in mind, and what—what I have done is – is to first establish a link in that respect, right? Telling them, well there's a connection; it's called multi-skill modeling, right? What you can – you can either take results from—from ab-initio or atomic simulations and then input it into these models, right? Or, you can just go through the experiment on the lab…And they will find that as compared to what happens at the atomic level where you really have a very well defined theory, which is called quantum mechanics, at the continuing level you have a slew of theories, right?

His second approach for introducing new topics was by means of simulations as modeling tools. In particular, he used two different modeling tools for attaining two different goals:

> Oh, yes, and so we are using – we are going to use, I am going to use in order to be able to describe again the equilibrium and the kinetics of materials two main tools, right? One is called FyPy is not a piece of software that has GUI, it's not a piece of software that you can just simply click buttons and learn. It's actually a set of libraries that allows you to cast partial differential equations, right? …That's—that's the beauty of that program, right? That you can write with that set of libraries, that you can write a program in a matter of minutes, and of

> course there's a disclaimer here which is, if you know what you're doing, right?
> And the other one is called OOF Which is uh, it's also public domain code. That one is actually – does have a GUI. And – and there's a reason for that. This one has a GUI because it's not a – a – you wouldn't want to see the back end of that program, so that a user can focus on the physical aspects of it, right? …And I want to use that tool just to teach the technique of finding elements. Which is uh – uh – at its very core it's a mathematic – it's a very simple technique, but the details on how to use it, right, and how to distinguish a good simulation from a bad simulation does require you to have a much more friendly interface than simply a script, right, when you see the actual code. And I want them to develop that intuition, which they will not develop using FyPy because there they will actually see the code. So, I want them to see two aspects of modeling, right? One where they actually have to write it; and another one where you have this other big piece of software and they have to believe in the results.

In order to expose students to learning experiences that will help them identify the physics from the numerical components of a modeling situation, Dr. Richardson designed homework assignments related to the specific topics covered in class. For example:

> They will have to have – there will be a set of homeworks addressing different aspects including the numerical stability; convergence; measure refinement; and all these aspects, right, that you want to distinguish from the physical problem that you're solving, right? And in between of course, they will probably have to learn some physics, right, because they have – they have to be able to distinguish between the physical part from the numerical part, right? Yeah.

However, since Dr. Richardson's course was not a programming course, he wanted his students to focus more on the modeling part than in the computational part. Therefore he gave his students a starting point, in this case a script, in which they could start modifying or building on top of it.

> And they actually – I – in—in the lab I'm gonna' give them something they can actually just tweak to do that. And the tweak is very simple, right? But understanding where to do the tweak is what's – what—what – that's what's gonna' take them two weeks.
> And, it's gonna' be really, really simple from that point of view. Right? They're not gonna' have to actually write the program, right? Because I think if I had done that, we would have raised the expectation of what a student should do before they – what the prerequisites for this class, right?

> And this – if they just have the script, they just say, “Oh, this is the physical part of the problem that I need to modify, so this is the one that I have to change in the code.”
> And of course they have to compare, right, the analytical part with the – with the numerical part.
> And—and of course I’m hoping to do this at least twice, right? Where we walk them through the motion for two physical problems, right, that I – that I have already covered in class. And—and yeah, that’s pretty much it.

Dr. Richardson also used techniques of cooperative learning in which students needed to work together to get to the solution…

> I—I am a big fan of group work, right? I do want them to work together, because as much as probably the first and the second problem they will – they will be able to do it on their own, by the time they get to the last problem, they will realize that only if they work together they can do it, right?

Perceptions of Simulation Tools

An advantage that Dr. Richardson mentioned in using nanoHUB simulations as modeling tools is the times when analytical solutions can no longer be solved without computational methods:

> At some point I show them well, yeah if you can solve this equation, it’s an important equation, but there’s a point in which a piece of paper won’t do, right? And at that point you have to go to a computer.

Other advantages Dr. Richardson pointed out are easy access, flexibility, and the research nature of the tool.

> One of – both – they’re both very flexible in the sense that uh, they—they both can be extended to simulate any type of material. They are research rated tools, but they’re gonna’ be used for education. And, one of them – and they’re both public domain.

Dr. Richardson explained some other practical reasons of why nanoHUB simulations are very helpful. He identified that from the point of view of the student they do not need to pay or install anything. From the point of view of the instructor, he does not need to administer and install any kind of software:

> And then at that point I start introducing computational methods. And— and let’s see, and it’s at that point where the nanoHUB becomes very

> helpful. Why because, well there are two reasons: one, in one of the issues that we had in previous years, and previous modeling classes, and this is just a, how do I say this, a—a logistic and strategic aspects to using a computer. Maybe computer has a literal operating system, right? Every computer has its own issues installing the software, and if you're going to teach modeling, you don't want the installation of the packages to be the limiting rate, right. To basically defeat them before they actually start using them.
>
> And for that, the nanoHUB is perfect because you don't have to install anything, and it doesn't matter if I'm running it on a Mac, if I'm running it on a PC, if I'm running it on a Linux box, right, it doesn't matter. But they basically just go there and just it, right? And that's—that's a very, very convenient. Um, and that's one point of view from the student.
>
> From the point of the view of the professor, and I don't have to administer the cluster, or administer individual machines. I basically just go and say just—just do it. I don't have to – have to worry about that at all. Which I think is extremely convenient, and it can save me a ton of time doing that.
>
> And actually there are administrators that you can talk to if you really want to—to interact more closely to with the framework of the nanoHUB, and but they're extremely helpful. And um – and that's from that—that point of view.
>
> From the point of view of doing what we want to do, is that we show that all these link skills, couple, also the nanoHUB is very convenient, because then they can – they are in the position of taking all of these different tools and putting them together to make a much more complicated simulation.

Dr. Denner's Perceptions and Experiences of Simulation Tools

Dr. Denner is a faculty member in an electrical engineering program at a Midwestern university. Dr. Denner has about 30 years of engineering teaching and research experience and has received prestigious awards because of his contributions to teaching and research.

Learning Outcomes

Dr. Denner teaches a course related to fundamentals of nanolectronic devices to senior undergraduate and graduate students. Dr. Denner described his course as somewhat different than others in the sense that the content is relatively new and unique. He explained that his focus in developing this course is more like helping incorporate the latest physical principles behind nanoelectronic devices but in an understandable, undergraduate level. Dr. Denner also explicated that the main topic addressed in this course is for students to identify how current flows in very small devices.

> And what it has to do with about how current flows in very small things. And that's just nanoelectronics there. And for an engineering point of view, I guess that the reason that's very important is each one of our laptops has about a billion transistors in it. What makes it so powerful is that you've got a billion of them working together. And the reason they can fit a billion in something that small is because each one is extremely small…So, an important engineering problem is how to design those transistors in terms of current flow through something that is hundreds of atoms long. And so this whole course is about how to understand that.

In the process of conveying the overall learning goal, Dr. Denner also wanted to help his students understand the relationship between the models and the real world:

> Real world meaning saying a current versus voltage that an experimentalist would actually measure. How to make the connection between that math and the real reality.
> And there they actually have to reason that well since what – since my equation says this is what will happen, so as I do this, this is what should happen etcetera... And so that is the only thing I'd say I try to stress a lot, because I feel otherwise that people have this feeling gradually in all kind of area, that I have seen too many students who think that physics can't really be understood; all you can do is kind of listen to what people say and then repeat it.
> And, what I try to tell people is, no it really can be understood, and it's a very human form of knowledge where you know, you are constantly checking and things evolve, etcetera, etcetera. And, everything you believe in, there's a very good reason why you believe it; because it fits certain class of experiments.

Evidence of Learning

Dr. Denner's ways to identify students' learning were exams and homework assignments. Furthermore, Dr. Denner explained that he expected that having students do the homework assignments will result in better understanding of the phenomena and consequently better performance on exams. He explained this relationship as follows:

> …So, they calculate it but then in the exam what I ask them more is – at that time they don't have the MATLAB code on a computer or anything but them I'm saying, "Okay, now if I did this, what do you think the shape of the current versus voltage should look like? Is it like this? Or,

> like that?" And there they actually have to reason that well since what – since my equation says this is what will happen, so as I do this, this is what should happen etcetera…
> And, in an exam I would give them a density of states; tell them, okay this side is hot, this side is cold; now tell me which way the current should flow. MATLAB would have given them that directly. But, when they're doing it in an exam, they don't have MATLAB but hopefully have understood enough that they can say which way the current will flow…

Dr. Denner gave feedback to his students by posting solutions to the assignments on the course website.

Instructional Approach

Dr. Denner's instructional design approach for the course was to focus on a few important concepts and concentrating his teaching efforts on those concepts:

> … apart from my general philosophy of I try so a lot of courses I've seen, often they stress on learning lots of things. But, I usually stress saying that choose a few, but then know it really well so that you – so I kind of stress more like okay these are the things, but you should be absolutely clear why it is, and I'm not going to try to give you lots of information. But, whatever I give you will be solid and for exams and everything I will expect you to understand this well.

A particular characteristic of Dr. Denner's pedagogical approach was that instead of using phenomena at the microscale as a bridge to understand phenomena at smaller scale, he started from an atomistic approach, arguing that this is easier to understand.

> … And, what I've always tried to convince that if instead you start from small things, they look a whole lot simpler, than if you try to take your jumbled understanding of big things and then try to project it down smaller.
> …So, I'm starting from this hydrogen molecule, but what I'm explaining, I feel like I can explain to a high school student. I mean a good high school student who knows about energy levels and hydrogen atoms and all that…
> …Now I can explain that under what conditions the hydrogen molecule would conduct very well; when it wouldn't. While – why copper conducts very well, and say glass doesn't. That's much harder to explain. That's a more complicated thing.
> On the other hand, when you think from this point of view, you can kind of see why gradually.

In addition to lectures, Dr. Denner designed homework assignments with the intention to leverage students' reasoning abilities and be able to connect the "math and the real reality." Sometimes, as part of those assignments, Dr. Denner asked his students to use MATLAB. MATLAB is a numerical computing environment and programming language that Dr. Denner thought corresponds to this century's technique to approaching analytical methods:

> And there they actually have to reason that well since what – since my equation says this is what will happen, so as I do this, this is what should happen etcetera.
> But that reasoning ability I'm hoping is coming from doing all those MATLAB examples ((I: Um-hum, um-hum.)) you see. Again, those equations will give you automatically if you run it with MATLAB, the point is then to physically understand why that would happen. And what I want to stress there again is that this course is not about how to write MATLAB. It's really about trying to understand it. And, play around with it, and develop an understanding.

Moreover, Dr. Denner explained that by using MATLAB, students did not have to spend a lot of time solving the mathematical portion of the assignment. He said that sometimes this portion may be overwhelming for his students.

> The other thing I've seen with these analytical methods is that if your mathematics is a little weak for various reasons, I mean, then often that process of getting analytical solutions becomes so overwhelming that you never get to appreciate the physics of it. Or whatever, because just keeping sines and cosines straight and keeping the pies in the right place, that more or less overwhelms you completely. But this way, even if you are mathematic – analytically not that good, you can still appreciate a lot of this. Because you could write that code relatively easily.

Dr. Denner also provided his students with scaffolds to approach the homework solutions in the form of simple MATLAB codes.

> …people can download these codes from the nanoHUB actually. And my purpose in giving this was just that, okay you can use this as your template. Not that these are CAD tools; sophisticated computer aided design tools that you should be using. It's more like you can see how to write a code. Write one for yourself now. It's more as an example.

Perceptions of Computational Tools

Dr. Denner pointed out that in his class, MATLAB is a very useful resource. He also explained that when the computational task is small, he usually prefers to write his own code to make sure the initial conditions and assumptions are appropriate to the problem he is trying to solve:

> So, most of my period I have done without MATLAB…And I know that learning MATLAB kind of expanded my horizons enormously. So that lots of things I can now easily do, that I couldn't do before. So to me it was a big challenge there.
>
> And, if I just used a code that somebody else wrote, I never would have acquired that confidence. I'm not quite sure what he did, what he assumed, how much I can trust it, etcetera. So I never, I personally wouldn't use a code by someone else but once in a while I've done it this way.

However, Dr. Denner has faced a situation in which he needs to use a complex simulation tool developed by someone else. In those cases, he always tests the results of the simulation to an extent.

> There is a well-known simulation tool or something that has been developed by 30 years of work, and I want – and of course I can't redo that in any set way. But even then I've sometimes done it this way: write my own little code; and compare some simple answers; and make sure I'm getting exactly what they're getting, so that I know exactly what they're doing. But the difference is that my code of course is not optimized. So, it does in one hour what that does in one minute.

Summary of Results

The six engineering instructors who participated in this study incorporated simulation tools by creating meaningful learning experiences for their students. In particular, these instructors used expert and educational simulation tools for achieving different learning outcomes to convey concepts and skills with enduring value beyond the classroom. One learning goal shared by most of instructors was the ability to develop students' intuitive understanding of the phenomenon under study and, at the same time, become critical users of simulation tools. A second learning outcome was for students to become familiar with the literature in the area of study. While some instructors focused more on conceptual understanding and engineering skills, others emphasized computational techniques. For example, Dr. Sanders as well as Dr. Denner focused a large part of their courses on the fundamental governing physical principles of nano devices. Dr. Sanders went further these fundamentals describing the behavior of nanodevices and also focused on the design and evaluation of devices. Similarly, Dr. Shaw focused on the practical aspects such as the applications of nanoelectronics devices. On the other hand, Dr. Hass, Dr. Richardson and Dr. Clase focused their courses in teaching modeling and computational techniques, and emphasized the application of those techniques to approach engineering tasks.

Most instructors in this study used simulation tools as a part of homework assignments and projects. For these instructors the most common way to provide formative feedback was by posting the solution of the assignments on the course website. Some of the instructors incorporated the simulations with mid-terms and final exams.

The main instructional approach instructors followed was to first introduce in class the physical principles defining the behavior of a device, material, or phenomenon and then have students apply these principles with the homework assignments using the simulation tools. However, the instructors who focused their courses on the computational and modeling techniques followed what they called a hands-on approach in which students had an opportunity to interact and/or implement simulation tools in the computer lab. Another feature incorporated in their pedagogical approaches was the use of recorded lectures uploaded on the nanoHUB.org. Dr. Sanders, Dr. Shaw and Dr. Hass asked their students to look at the online lectures as part of homework assignments. Dr. Denner, on the other hand, recorded all his lectures while he taught and then uploaded these recordings onto nanoHUB.org. A different pedagogical strategy Dr. Clase incorporated was limiting the number of input parameters of the simulation tools so students can focus on specific aspects of the phenomena under study.

Instructors such as Dr. Hass, Dr. Richardson and Dr. Shaw incorporated cooperative pedagogies. Dr. Hass and Dr. Richardson encouraged students to interact face-to-face and online, and Dr. Shaw asked his students to build a virtual community in the nanoHUB.org.

Overall, these instructors believe nanoHUB.org simulation tools and computational simulation tools in general are convenient for them to teach with and for their students to learn with. They are convenient for instructors because they do not have to install any software or manage students' accounts; convenient for students because they have conceptual and technical benefits for their learning. Conceptual benefits may include students' ability to solve hard analytical calculations easily through simulation. Furthermore, students can overcome the limitations of analytical solutions. As a result, students can focus on the values depicted on the curves rather than doing extensive calculations. Also, simulation tools provide additional capabilities they cannot replicate in a laboratory. Instructors also mentioned that simulations are useful for their students because they are flexible; they can run different models and different simulations with different parameters and will get different outputs. Additionally, instructors can incorporate real and complex examples. Technical benefits include the ability of using online simulations that are easy to access at no cost for students. The user interface is friendly and students have a lot of computational power under the hood.

Limitations identified by few instructors included the limited number of outputs of the simulation, outdated documentation, and performance issues.

CHAPTER VI

STUDY THREE - PHASE 2: STUDENTS' PERCEPTIONS AND EXPERIENCES WITH COMPUTATIONAL SIMULATIONS AS LEARNING TOOLS

Although many studies have investigated the affects of prior domain knowledge on students' inquiry processes, few have looked into how values, perceptions, attitudes, and beliefs affect learning with simulations as learning tools. One example borrowed from the area of conceptual change was conducted by Pintrich, Marx, and Boyle (1993). Pintrich and his colleagues showed the need to study how goals, values, self-efficacy, and control beliefs mediated students' processes of conceptual change. A study related to the use of computational simulations and students' beliefs was conducted by Windschitl and Andre (1998). Windschitl and Andre investigated the interaction between either an exploratory or a confirmatory condition and students' epistemological beliefs. They found that students with more sophisticated epistemological beliefs—i.e. one's beliefs toward knowledge and the process of building knowledge, performed better when allowed to explore. However, students with less sophisticated beliefs performed well when given explicit directions on how to use the simulation.

More studies are needed to explain the relationship between learners' characteristics such as motivation, self-efficacy, beliefs, expectations, perceptions, attitudes, and how these influence their strategies for scientific inquiry learning through simulation, and domain specific strategies for guiding inquiry (Cannon-Bowers & Bowers, 2007). Also more research based on instructional methods need to be identified to respond to differences between learners and their developing knowledge and skills (Alessi, 2002; de Jong, 2006).

Overall, the existing literature does not provide much insight into how engineering students perceive the use of computational simulations as part of their courses. Therefore, by adopting a first-order perspective, I attempted to identify how computational simulations for learning were perceived and experienced by engineering graduate students who took part in three engineering courses.

Methods

The goal for this phase of the study targeted identifying engineering graduate students' perceptions and experiences using computational simulations as a learning tool. Data were collected for this phase of the study through interviews with students whose instructors allowed classroom observations to document how instruction was implemented. Students' participation consisted of a one hour interview. Interviews were conducted with different students at various points during the semester.

In total, 42 students volunteered to participate in the study. From those, I interviewed 27 students during the Fall of 2008 semester, but I was unable to use two interviews because of technical problems with the video recordings. Eleven of the students interviewed attended Dr. Sanders' course, nine attended a course that Dr. Hass' and Dr. Richardson's co-taught and five attended Dr. Denner's course. The pseudonyms of the participants and their instructors are detailed in Table 6.1.

Table 6.1 Summary of participating students per instructor

Instructors	Dr. Sanders	Dr. Hass	Dr. Richardson	Dr. Denner
Students	Libo John Isison Arash Valerie Joe Howard Jack Jonathan Allison Maria	Jake Drew Jim Uday Kyle	Lawrence Rajiv Melanie Robert	Dimitris Tom Connor Maurice Steve

The total number of student participants reported in this study is 25. Each data collection period focused on a particular homework assignment. Dr. Sander's student interviews were collected at two points in the semester. Six interviews were conducted at the beginning of the semester and the remaining five towards the end of the semester. Dr. Hass' student interviews were conducted in the middle of the semester and Dr. Richardson's and Dr. Denner's towards the end of semester. The individual interviews were semi-structured, conversational, and lasted approximately one hour. I began by asking the students about their general experiences of using computational simulations as learning tools. My next questions focused on aspects related to the perceived goals of the class, particular assignments, the instructor's method of assessment and pedagogical approaches. Finally, we ended the interview discussing their academic and research interest related to the course and the usability aspects of the nanoHUB tools. Chapter III contains the specific protocol questions.

Since the interviews were transcribed by a third party, I reviewed the videos with the written transcripts to verifying its accuracy. Once verified, I continued my analysis by reading through the interviews several times and proceeded by conducting open coding, followed by conducting axial coding. In this iteration, I again grouped my themes around Wiggins and McTighe's backward design process (1997) as in Phase 1. I also identified what students considered to be the major advantages and disadvantages of simulation tools as learning tools. After conducting this coding process, I wrote descriptions and summaries of the interviews by grouping together themes related to the learning goals of the classes, assessment methods, pedagogical approaches, and advantages and disadvantages of simulation tools. These write-ups provided me with insight and helped me become familiar with each case as a singular entity (Merriam, 1988). The next step conducted was to compare individual cases in order to push to generalization of patterns across cases. As an organizational aid in this process, I decided to display the identified themes arranged in a matrix. In the first column, I wrote a general way in which students perceived or experienced a particular simulation tool as part of a course. On the following columns I marked the participants who were experiencing the tool in the same way. If I identified a different way of experiencing or perceiving simulation tools during this process, I added a new row with a brief description of the experience or perception. I did this process in an incremental way. For example, I created my initial descriptions based on a single interview. When I analyzed the second interview, I compared and contrasted it with the first one, marking similar ways of experiencing the simulation tools and adding different ways. For the third interview, I compared and contrasted it in the same way first with the initial interview followed by the second one, leading me to more sophisticated understandings of how students experienced and perceived the computational simulation tools. I conducted this comparison process first among students for each individual engineering instructor and then across all of them. I did so by selecting categories or dimensions, looking first for within-group similarities and then coupled them with intergroup differences. When a pattern from one data source was corroborated by the evidence from another, the finding became stronger and better grounded in the data (Merriam, 1988).

Results

Students Perceptions and Experiences of Dr. Sanders' Course and Approach of Incorporating Simulation Tools

In general, Dr. Sanders' students perceived the course as a well-designed course that was difficult at the same time. Some students agreed that the main goal of the course was to give a thorough understanding of the physics of semiconductor devices. Here are some excerpts of Libo and Maria who described their understandings of the goal of the course:

> Libo: I think it is um, this course is not like the physics or mathematics course that teaches some fundamental things that everyone needs to know. It is not that everyone needs to know kind of course, but it is good for some experimentalists, it is good for some theorists who just study the physics like quantum mechanic. This course can give them the feeling of how the physics phenomena show up in some model devices in real cases. So this course can be crucial for device person because like 80 percent of device we are using, so this course will describe in every aspect what um, what is good for it and bad for it and what it can not reach, kind of what it needs to do to be better and why people are using it. So I think um, this is a good course. But not for people who study like cosmetic area or some people who study some other aspect but people who do device, transistor things.
>
> Maria: In this course actually I used three or four tools which are hum— there on the nanoHUB and basically it gives us some insight into the physics of the device and um plots that it gives that help us to

> understand the principles of the device, which is part of the class and it helped a lot in capturing the basic concepts which were talked about in this course. So it became more clear using it.

Most of the students interviewed were taking the course for either of two main reasons. One of them is because Dr. Sanders is a very good instructor and the second one is because the topic is interesting and useful for them. For example, Libo, John, Isison, Arash, and Howard all had similar opinions:

> John: I am taking it as an elective. Well, I guess a couple of reasons. First of all um, I guess the general feeling in the department among students and I think professors too is that um, Professor Sanders is a very good instructor and his courses are good. I am also interested in the material, um, in the devices and things that are part of the course.
>
> Howard: Oh yeah, um it is very interesting because hum— for my— my goal to take this class is that I want to know what really happens in the nano scale transistors. So, you know a lot of things happen when you shrink the size to a small. So that kind of software give you a very direct and simple insight of what happens, like if you have these kind of conditions you will see what. It is kind of very intuitive I think…
> …Hum— since hum— basically, my major area is ME, so generally I am a device people but not this specific device. But I also always want to know, like transistors are the most popular things in the world, so I just want to learn more. It is not related to my research but I want to know more.

Interestingly, other students such as Valerie, Joe, and Allison, who were not doing their research in this area, were interested as well. They believed that the topic was not only interesting, but also important:

> Valerie: Uh, ok, when I came to do my masters here, first I did my undergrad in India, I came here to get my masters and hum— when I started with my masters, I took courses in different areas, like my first semester I took one in like computer architecture, I took one in design, one in solid state, I took three courses and I liked the solid state area better.
> So I started taking courses in solid state and I was funding myself and finally when I got funding I was basically supposed to do research in the area of microwaves because that's where I got my funding, so but, I really liked solid state, and its unfortunate I couldn't find someone who could ever fund me in that area, and when I did my masters research for microwaves, I really never thought that I would have my PhD in

> microwaves too, so that's how I got into the area of microwaves, not that I don't like the area, but studying wise, I like more solid state, I am not very comfortable studying electro-magnetics and all that stuff, uh— though hum— I am very good at doing the microwaves, but hum— my heart lies with solid state, I like solid state more.
>
> Allison: Um, I think so— I think it's interesting and like I said a lot of these, the stuff we learn is more relevant now because it's about the short channel transistors and the transistors getting smaller now, so hum— I think it's more important to know this now than any other time in history, so I am glad I took this class. And hum— even though it's not exactly my area, it definitely helps me to know this, because then I have a wider, larger understanding of circuits and stuff.

Eleven interviews were conducted with Dr. Sanders' students. Six of them were interviewed at the beginning of the semester with Libo, John, Isison, Arash, Valerie, and Joe; and five towards the end of the semester with Howard, Jack, Jonathan, Allison, and Maria. While the first homework assignment was well-structured, the second one was more ill-structured or open ended. Dr. Sanders' students' perceptions and experiences of learning outcomes, evidence of the learning, and instructional approach are discussed below.

Learning Outcomes

Dr. Sanders' students, Libo, John, Isison, Valerie, and Jonathan, identified the goal of homework assignments as a self-exploration of current technology to get a feel about what transistors look like. In particular, these students described the goal of the course as wanting them to get an insight into the state of the art of the transistor technology.

> Isison: Um, for homework one, I think well it was a simulation to simulate CMOS technology and it is 45 nanometers, and Intel is using 45 nanometer processor right now. So it is more or less like, a little example, or a little self exploration into this current technology. It's just nice example. Um, it is fairly simple so I think the purpose of this homework overall, it just lets the student have a feeling of where the current technology is standing um, how you can extract key device performance parameters out of the results. We only have two exams; the first is drain current against voltage. The second one is string current versus the drain voltage. So we only have those two curves as the parameters for the results. So we can't get too much out of it, but we can extract key parameters of those two curves.

> Libo: This homework one? Um, the purpose is for, what the homework design is to let the students get insight into this state of art, the transistor technology we are using right now in 2008. And um, um, so to discover what um, cause in the homework you can adjust different parameters and values to get different output so in that aspect you can see what the parameters control what aspects the most. Basically that is the aim of the homework.

For example, in the first homework assignment, Arash and Joe identified the goal as an overview of the MOSFET fundamentals to see by simulation what it looks like, and how input parameters affect transistors. Students also mentioned a goal of being able to see what the changes on the MOSFETs are when the dimensions got smaller.

> Arash: The purpose of this homework was the refreshment on the MOSFET fundamentals, to see really we know what is things of the MOSFET, like what is the on current, what is the turn off rate, what is it like. And I think mostly it is to know what is the ID characteristic and what the output is of the MOSFET when the dimensions go lower, like the scale because it is not just really normal MOSFET and we have, we see some changes. And I think the purpose mostly was to us go and look how it is and get an idea of what we are looking, how much the current, how much the resistance, how much those stuff like that.
>
> Joe: Um, well I think it was to understand how those input parameters affected the transistors and to kind of see, and to simulate it and to see how it actually affected them.

For the case of the ninth homework assignment, Howard identified the learning goal as to expose them to real world industry experiences.

> Howard: The homework is just tell you the real world. Like if you go into a company, sometimes definitely we have used a lot of commercial software so we know even if it is tens or hundreds of thousands of dollars, there is a lot of— lot of problems inside. So if you just trust the simulation software, like I mean, in school maybe you can say the simulation software gave me the wrong results, so but in the real world in a company it is not forgivable. So it is very important you know what it software are doing, and how to fix it.

Howard, Jack, Allison and Maria also explained that in homework assignment nine, Dr. Sanders wanted them to identify what the software was doing, how to fix it, and in general to become critical users of simulations:

> Maria: Ok he actually wanted to hum— wanted us to play around with the various options of the tool and hum— and look at it in a particular point, and particularly analyze the plot that it gives, not just like believing the plot which its giving and how we can make use of the plots and our knowledge in physics of the device to convince us that the results the tool is giving is relatively wrong.
> So it's like, even if some particular, even if a plot shows that it is plotting one particular quantity, we just need to verify that it is indeed that kind of thing, by using some other plots or using some physics of the device or by using some hand or self calculations, just to verify that its giving the proper results. So he wanted us to hum— become more critical users of the tool rather than blindly following, or blindly accept what the tool is giving.

> Jack: Well on several occasions in class he discusses how um, when you run a simulation you need to make sure that you understand what is going on in the simulation and you understand or are able to test the results.
> So I know that some of the tools on the nanoHUB we found out have been giving results that weren't exactly what they should be. Whether it was just that the plot was mislabeled in a certain way, or um say like, there's a certain thing in the math behind it that is a little bit off. Visually it looks fine, but if you actually get down and pay attention to what certain things are doing at certain times, you will find that there's something wrong.
> And I think that was the point of this homework to point out to all of us that some of these simulation tools are up there and based off of things used in industry and have been used in industry for years, and um, it's only years after that we have been using it that someone comes along and looks at a certain plot and needs that certain plot to look a certain way and it doesn't and then they start asking why and come to find out that it is wrong in some way.

When discussing prior knowledge, in general, most of the students were comfortable with their prior knowledge and thought that if they didn't have it, Dr. Sanders would have provided them with that knowledge. For example, Libo, Isison, Valerie, Joe, and Maria said that they possessed the knowledge to approach the solutions of the assignments. However, for the case of homework assignment one, most of the students used the online lecture as a review for approaching the solutions to the homework.

> Valerie: Um, I have taken a basic uh, course, like a 606 course in my masters, I didn't take it here at Purdue, it took it at another State

> University, and um, it was not, like the first part, especially this part was not new to me, like as in the device itself, like the, the device itself is familiar to me, like I have studied it in detail to an extent, but I have never studied anything specifically for small scale devices, I have just in general like what would be the most device characteristics and that kind of stuff.
>
> Isison: Well, I think before I have taken undergraduate level course, so I do believe I have sufficient knowledge to answer the questions. Of course that requires me to refresh my memory a little bit, but on nanoHUB there is one lecture taught by Professor Sanders, again on the MOSFET device review, so that helped me a lot as well. So by using the previous knowledge and the lecture notes, I can answer every question and be pretty confident of what the answers are.

However, it seems homework assignment nine was challenging for a few students. For example, Howard, Jack and Jonathan had difficulties with the assignment and were not confident with their performances on the assignment.

> Howard: Um, actually before I think everything you— everything you need to use has already been taught in the class and hum— and in the textbook.
> The thing is that I have to hum— like some of them— those kind of rules is really hum— like you know you have to understand the physics very well.
> So hum— since this class covers a lot of things, for me I am not a— I am not a transistor people, so hum— I need some— for me— I needed some time to really get a, get those kind of things in my mind. That is the difference like I think for those kinds of things; those kind of homework will be not so hard for those guys, like those students in Professor Sanders' team and physics.

Evidence of Learning

Two main components are discussed in this section. One relates to what students perceive as new knowledge they have gained throughout the course, and the second one relates to Dr. Sanders' feedback mechanisms.

Although most of the students interviewed had exposure to similar courses, John, Arash, Valerie, Joe, Isison, and Allison pointed out that there were many things that were new for them. For example, they have not been exposed to different metrics, and they learned those by doing homework assignment one.

> Arash: This homework assignment actually it was pretty good. Like how we compute the on channel I didn't know that much. And then how exactly can we like, what the threshold linear and what the threshold saturation, you know I didn't know the difference and from this homework I know. And actually the good thing is that this course is pretty good in explaining everything, the review of the MOSFET fundamentals, it was a big difference. I mean it explained everything.
>
> Valerie: Um, like I have um, everything was, like I know I have studied MOSFET, but I don't remember was exactly is on current, what exactly is DIBL, I think now I know kind of, what is on current and what is off current, I didn't know there would be two separate like threshold voltages like Vdsat and VDLen, which um, Professor explained in the lecture. Yeah, the online presentation which was part of the homework too, first go through the lecture and then do the homework. So um, like I didn't know there would be two threshold voltages and which one was what. Hum— I didn't have clear understanding of MOSFET, I was familiar with the MOSFET, but hum— I didn't have like a clear understanding of MOSFET. Hum— and uh— and its different when you study something in detail like this and its different when you are browsing through, learning MOSFET as a new device, you wouldn't be concentrating observing so much where is on current where is off current, you maybe learn how the device operates and you know that kind of stuff, I have never learned MOSFET quite in detail.
> …So first we just plotted these curves and then we plotted a log ID versus VDS curve and most of the parameters can be got from log ID versus VDS curve, you can get VDSAT, threshold swing, what is on current, off current, so that is entirely, like finding out the parameters from one curve that was very different for me, like I have never learned that. Now I know...

Other students, like Libo, Jack, and Maria commented that what they learned was relating the physics of the world with the outcomes in the behavior of the device.

> Libo: Um what I learned is kind of like the approach, like in homework one they have basically four projects, four problems, and problems can ask you change the different parameters to see what effects this outcomes.
> So I take a deeper step into it and hum— think about what the physics course that is actually what I learned. So what I mean is that first I run the tool and it gives me the output so I know this two parameters control the output the most.
> So I take a deep thinking into why in the physics world this is available, this is realistic so I realize some physics phenomena and I say, yes that is why, that is reasonable why these tools and even the real world these two

> parameters will affect this outcome the most, because the physics is like that.

> Jack: Um, since I am primarily working with nano wire transistors and this is a highly transistor based course, it is very similar. So a lot of what I have learned in this course has actually helped me in my research because um, a lot of times in my research would say well use this equation and it wouldn't exactly say why or how or where it came from or what that equation represents. So this course has given me a lot better insight into that and it's done a lot better job than other courses I've had that should have done the same thing. I don't recall you know why but it might just be the amount of time I pay attention in this class.

Arash, John and Isison commented that they learned a sense of what current transistors look like.

> Isison: Hum— I think the most important thing I learned from this activity is um, the techniques to use to extract those key parameters. Question number one was about extracting those key parameters off of those graphs. I know those things before but as I said previously, I need to refresh my memory, so by doing it again, I refreshed my memory and have review the key things that I will need later on in this course.
> And the second thing I learned with this simulation tool, which I had actually never used this one before, I had never seen this one before, it gives me a good knowledge of where the current technology is standing with the 45 millimeter technology, of what the transistors characteristics look like. This is actually the first time I have ever seen that, so in general it basically reviews my knowledge, refresh my mind and gives me a good look at where we are standing today.

Howard, Jonathan, Allison, and Maria commented that they learned to not blindly trust simulations; that they have to find a way to judge if the tool is doing the right calculation:

> Maria: Hum— hum— I don't think I had learned anything new conceptually. But of course it gave me an experience of how to look at a tool more critically rather than believing it blindly, and it hum— it taught me that spending some time to convince myself that it is putting out the right results it worthy, it is worthy because later on if I proceed with believing the tool that it is giving the right results, I might land into some problem that is going to be more difficult, so figuring it out in the hum— in the first, initially will save a lot of work later on, so that was one thing which I had learned from this, spending a little time initially to convince myself that the tool is working properly is worthy and this gave me a

> chance to have a hands on experience of that kind of critical analysis of the device.
>
> Howard: Hum— the one thing that hum— there are basically two things that I have learned. One thing is that you can not, there is a way that when you have simulation software, you can not blindly trust it, you have to check it. That is very important, since in the industry you have to use a lot of tools, sometimes you will have to use a well known commercial kit, things will be relatively ok because there is a lot of source, but sometimes for a very specific application, you will use some homemade software kits.
> Generally, you are unlucky; generally those guys will not give you any documents or any support to test it by yourself. Another thing is that like you got to find some way to, another important thing is that you have to find a way to judge if it is right or not. That means you have to be able to simplify the model and get some quick results and compare to the results of the simulation software that means you have to have some deeper understanding of some physics and you have been able to get some quick numbers in your mind to compare with the results.

When discussing the feedback mechanisms, most of the students, including Libo, Arash, Valerie, Joe, Howard, Jack, Jonathan, and Allison, mentioned that they were comfortable with the way Dr. Sanders provided feedback. They said the posted solutions to the assignments had enough details for them to identify their solutions to the problems:

> Howard: Hum— generally the solution is quite clear, very clear…Actually I would say that the homework is all graded by the TA, and hum— he is a senior graduate student, he is not getting his funding from this course. So I would say the grading is not hum— generally I don't look at the grades, because he didn't grade it very carefully, but they have a very detailed solutions, so I just directly go to the solutions and I know what I am doing, where I am a little bit wrong.
>
> Jonathan: Well I am quite happy with the feedback because the course itself is very well designed course, and the homework even if it is quite difficult and tough it still gives us the nice feedback because the professor has some engineering sense, he is a professor but also an engineer so he provides us very thorough understanding of what he had been working on with us very efficiently, like his lectures are nice and the homework well designed, it is not just repetition of previous courses like Fall 2006, like he always modifies and develops new homework. So yeah, it really helps me a lot.

However, two students, Valerie and Jack, pointed out that sometimes Dr. Sanders didn’t give enough details during lectures and homework assignments, especially on the math, and sometimes he expected students to show that knowledge on the exams.

> Jack: I think one of the problems in this class right now is the way the professor has us doing a lot of conceptually based things with the homework assignments, and lectures he goes through a lot of concepts and doesn't really do into any detail in a lot of the math, and then on the exams he suddenly expects us to know all the math, which I thought was kind of an issue for me personally because I'm not really good on the math side of things, but when it comes to concepts I can get them pretty well. So I think the homework assignments are really good in understanding the concepts but when it comes to knowledge of final equations, manipulating equations to fit certain criteria, I don't think it helps much at all.

Instructional Approach

Howard, Jack, Valerie and Allison commented about Dr. Sanders' instructional approach. Howard explained that Dr. Sanders taught the knowledge and the methodology needed to approach problems that happen in the real world. Jack mentioned the approach was appropriate in order to get a good feel of what the current technology devices are. Jonathan explained that Dr. Sanders provided thorough explanations, that lectures are approachable, and that the homework was well designed.

> Howard: Well this course covers a lot of things. Like, it covers I will say the content of this course is very broad, and also um, Professor Sanders is really great professor. He not only tells you the knowledge but also how to solve, the methodology, to solve the problems, what is in the real world and what happens in the future. Those kind of view things, it makes this course different. He is a leading researcher in this kind of area, so his words give you kind of a lot of different things. He won't tell you just what it is but what it used to be and what it will be, what the limitations are.
>
> It is very helpful for you if you really want to, like for me, I am doing a kind of different device and I am thinking about if they have such limitations there is one that our device can compete with the nano transistor, in some specific applications, is what I am thinking. It is very interesting.

Students identified benefits in their learning when approaching the homework assignments with simulation tools. Libo, Isison and Howard said that, in general, simulation tools helped their learning. John mentioned he enjoyed using the simulation tools. Other students made specific comments on how simulation tools help them. Joe, for example, said that simulations helped him because they solve complex equations for him. Libo pointed out the convenience of not having to do the real experiment in the lab. Howard focused on how the simulation tool helped him by simplifying a complex model.

> Joe: How did it help me the most? Hum— well it's definitely a lot faster than trying to solve equations especially when they are nonlinear and very difficult to solve analytically, so I mean it made it possible to solve some of these problems I think.
>
> Libo: What I think the tool is important is hum— its like hum— its a simulation tool so you don't need to do the experiment. Now you can easily play around with the channel length, the oxide thickness, the geometry structure of the device and temperature and hum— hum— sub-threshold voltage, you can play around simply by just changing the numbers and simulate and see the results. So I think the whole process will give you a very comfortable feeling of the device. You will not get frustrated like in a real world experiment in lab, you go there and do the experiment and you fail a lot of times and now you don't have to worry about that. Just click it and it will give you output, you can measure all the important. In the output you have some curves, so you can measure the different points of the curves and some properties of the curves, to see the important things.
>
> Howard: Yeah there is hum— two things. Uh, one is that hum— the simulation tool hum— sometimes if you are thinking a problem with the functions, you will be not so, so clear or some obvious, like if I change one parameter how the curve will change. If you just want to see the functions, that would be not very direct, maybe a change where you can set this parameter by different values and look at the curve, you explicitly know what is happening there and how it has changed. I think that is one thing that helps you to know. If I want to this performance to be higher or lower, I have to increase or decrease one of the parameters; that is very helpful to see it. It is very useful to see if from the simulation software. Another thing is that um, in simulation software you can eliminate a lot of options and make simplifications. A lot of functions they have they say we have lots of options, before the nano simulation software they can not use very complicated algorithms and it considers everything.

The possibility to look at and interact with the output of the simulation tools—i.e. the curves and graphs, was identified by Libo, John, Isison, Jack, Maria, and Jonathan as one of the most important benefits of simulation tools. Some of these students described this experience as a hands-on learning experience:

> John: Um well I think probably the biggest thing is that it gives the student an opportunity to put their hands on it themselves instead of just listening to a lecture and get a feel for it. Its great that you can change parameters and see how things change based on those things without having to do a rigorous process by hand which I think is very helpful. Um, and just in general it gives the student I think a good feel of how things are supposed to be and what to kind of expect.
>
> Jonathan: Oh it is very simple, we can solve it by hand but we can see how the wave functions are formed in like, in like a graphical way so it is very simple, I mean it's very nice to verify what the results are in real, and we can simulate various shapes, for example I mean we just use boxes, we can just solve box type structure but in that case we can simulate the pyramid structure and dome shaped structure and we can use it to verify that techniques.
>
> Maria: …It gives the plots of, gives the various things, like density, electric fields and things inside the device, so a lot of the things in which we just hum— understand by analytical things, we get to see those things inside the simulation and hum— again also play around by changing things used in the device, and see the effect of using different models and how exactly a device performs, the quantum mechanics and the things we learn in the class, the concepts we learn in class we can see how it actually works in the device since it gives the internal values.

Perceptions of the Tools

Students identified several advantages of nanoHUB.org simulation tools. Libo mentioned the advantage that it is online and he has easy access. Arash, Valerie and Libo mentioned that it is convenient because they also have access to many different tools in a single place. John and Isison pointed out aspects such as the tools are research-based, and therefore they can, in some way, trust the results. Students also commented on usability aspects. For example, John, Isison, Arash, Valerie, Joe, Jack, and Howard talked about the ease of use and ease in learning how to utilize the user interface. They mentioned the interface is very intuitive and that they can easily interact with it:

> Joe: Well, I think it is fairly easy to use. It is definitely very user friendly in the fact that all the parameters are listed conveniently and it does the plots and all you have to do is switch between the plots you want to use. After I figured this out, um, that became useful on the last one because I had to run like simulations, and I reran them three times, I ended up running like twelve simulations or fourteen or something like

> that, anyway I ran a bunch so this was nice to switch back and forth um because when you did that, it wasn't changing the axes. So you could, and it didn't work more than four at a time, but I would run like four, I changed the parameters plus or minus ten percent and then run this, and then switch back and forth between these for two individual parameters and that way I didn't have to resize the axes.
>
> Isison: The most significant thing I felt was first of all it is very convenient. It has very clear layouts, and I am a student and this program has the parameters that I can understand. You know I go into to the interface and I see, ok those are the key parameters I can change and they are very easy to change as well. For example, if I try to put the number that is too large or too small, it will tell me that I made a mistake and each of the input parameters also have little explanations to go with it. If I do not know what that parameter stands for or what that means, I can actually learn a little bit from the description.
>
> Valerie: Hum— I think hum— the most important thing is that its easy, like you can log into at any technology device, like 30 nanometer or 40 nanometer, like they have a bunch of stuff and you can always compare results, so I can choose NMOS 45 nanometers and I can choose NMOS 100 nanometers and then put them on the same plot and see how they differ and everything.
> Getting the curves, it uh, it was very simple, all you had to do was like click and then just get the technology that we need and then give all the parameters that were right there and then it was simple and very easy.

However, students mentioned several limitations of the simulation tools. Some of them are technical, related to usability and performance, and some of them conceptual. Valerie, for instance, explained she wanted more capabilities from the tools. For example, she wanted to have additional plots and the ability to do differentiation.

> Valerie: …I wanted to see GM versus VGS as ID curves, but there is no option to do that. The only two plots that it would let us plot um, one is the ID curves, the ID versus VDS curves and then the other one was the ID versus VGS curve and that would, yeah it would plot it in both block scale and non-block scale, it was the option to choose that, but it wouldn't let us plot GM versus ID curves, which I believe is also a very important curve which um, which lets us see where the device is struggling, where the device is weakening, where the device is in threshold and all that stuff.

Further, students such as Arash and Jack pointed out the need to be able to mark on the graph; and students such as Valerie and Joe would like to see more tick marks on the graphs.

> Valerie: Yeah, the thing is you can have different simulations and then show them all in the same plot, uh, but you know, there was nothing like uh, I couldn't calculate, lets say I wanted to fix my cursor at one microgram and I wanted to see the difference in each case but there was no line, there was nothing like a cursor which I could do, you know, uh, the best way for me to do it is you know, take these points, take it into Excel or something, put the cursor or put a line there and then check for each individual case because um, because otherwise in each of the cases I had to actually see, it was quite challenging actually and I don't know if I had approached the problem correctly,
>
> Joe: Well the painful part was the fact that, just um, there wasn't enough tick marks on the bottom scale, so I had to make my own and you couldn't click on the line except for a specific simulated points, so I don't know, it wouldn't be nice like my calculator where you can trace the line and then interpret points in between or even if you could just click on the two lines and give it a value and it would automatically measure it or something, I don't know, just because of the limitations in there it made it really difficult to do the measurements I guess. I spent hours with the stupid paper ruler trying to measure how far along the lines were apart, literally hours.

Other students, like Jonathan, expressed a desire for better documentation and organization of the tools; documentation not only on the technical aspects, but also on the conceptual ones. For example, Jonathan mentioned that simulations sometimes have many options and he sometimes doesn't know the physical meaning of such variables.

> Jonathan: Hum— well I mean the online lecture is very good, I use it very frequently, but the tool side, there are too many tools out there that works, that works similar. I can't choose what tools to use, so for tool side, we need some organization or something like that, and documentation. There are like, how many tools are there, like over 100 right? Yeah I mean, that is a good thing to have all those tools in one website but it's again for us, it is kind of difficult to figure out what tools to use in various research topics so that is one problem I think.

One striking finding is that students (i.e. Isison, Arash, Valerie, Joe, Howard, Jack, Allison, and Maria) would like to have more information about what is "under the hood." Some of them are more interested in seeing the physics, the underlying model.

What are the assumptions and equations they are solving and how, and what, are the implementation algorithms?:

> Maria: Um...maybe um, in this particular case maybe making a little bit of the source code known to us so that might help to figure out what exactly it is doing, but that may or may not help because it could be a very long code and you won't be able to make out all that is happening, but seeing it for those who are interested can go through and really understand what is happening, maybe that option would help. Otherwise, I guess the tools are fine. They give us most of the required, values of most of the required things needed for the student to really understand the concepts, how exactly things change with the parameters and the length and stuff. And all of the parameters can be changed for the graphical interface. In that sense the tools are fine.
>
> Isison: Will be a disadvantage— hum— well from my experience I know what is running under those simulation tools, a very complicated physics code. Hum— the manner of the things that are in that code is not aware by me. I am not aware of those difficult physics involved, so when I use analytical solutions to come to results and then I compare my results with the simulation, it is usually they don't consist. So I have a question that why is this happening and that could be something interesting for me to investigate. Hum— but by using the tool alone, it is fast and saves time, but it really doesn't tell me what uh— how it came with that solution. So I think that is the main disadvantage of simulation tools. It doesn't actually tell you what are the physics. It only takes input and gives you output, that's it.
>
> Joe: Yeah, well, um, I guess, its more of understanding what the parameters were because where it was, where the simulation was done for us you know I wouldn't be able to recreate the plots, I could measure the plots and I could derive the parameters from it, but I didn't actually make the plots so I guess that is one drawback. Hum— and maybe that would be helpful to show the equations that its solving obviously. Maybe not all the code but maybe the equation and how it's solving for all the parameters.

Students Perceptions and Experiences of Dr. Hass' Course and Approach of Incorporating Simulation Tools

Five students were interviewed for the portion of the course Dr. Hass taught. As opposed from other courses, these students had different backgrounds. Jake is an aeronautical engineer, Drew and Uday are mechanical engineers, Jim is an industrial engineer, and Kyle is a physicist. According to Dr. Hass' students, the overall goal of the course was for students to be able to identify what happens at the nanoscale as compared to micro and macroscopic scales. In particular, Dr. Hass' portion of the course focused on an overview of molecular dynamics simulations and the physics and initial conditions governing the nanoscale phenomena. Another goal of the course was to have students get familiar with the literature in this area. Jake compared and contrasted his personal interests with the goals of the course and Drew discussed in detail Dr. Hass' goals of his portion of the course:

> Jake: So, hum— my current research is hum— does a lot of finite element modeling of materials, specifically composites, and hum— there's a lot of movement in the industry to be able to be able to do the top down and bottom top sort of modeling, the entire materials system from constituent properties all the way up to the homogenous properties, So, and to be able to predict failure in these composite materials by matching what happens globally to what's going to happen on the smaller scales, and back and forth. So, that's basically is what this entire course does. It starts at the bottom and it works it way to the top with different ways to model materials and the different tools that you need. So it felt like it would be a good introduction to what's happening in the industry that I plan on going into.
>
> Drew: So I think professor, I think hum— the main motive of hum— doing molecular dynamics is to reveal something that happens at the nano scale which doesn't happen at the usual millimeter centimeter macroscopic scales as we call it. Hum— through molecular dynamics he designed I think projects to reveal the exact size effect of material properties. So what does the stiffness of a material, how stiff it is you know, how stiff is a big steel bar which is maybe a centimeter big versus a steel bar that of maybe ten nanometers long. We particularly did it for platinum nano wires so we did a platinum nano wire which was about five nanometers or three nanometers in diameter, which is really just like hum— you know, ten or five atoms in the diameter direction, hum— and we were looking at terms of that it was stiffer than hum— bulk material that we usually see. So, uh, I think one of the very important aims of Professor Hass was to get across the message of interpreting how to run simulations, how to run molecular dynamics simulations very well, what are the things you need to keep in mind, what are the conversions, or what are the time step or all the other simulation parameters, but the more important part of it was to reveal the new nano scale physics that comes out of the molecular dynamics and the exact, so supposing I am stretching the nano wire in one direction, hum— everything that happens to atoms

> inside the solid can be seen in molecular dynamics, and hum— that was one of the aims to understand why a smaller wire which is three nanometers in diameter is different than a bigger wire, and you know all that can be understood by seeing how atoms move when they are deformed. So in the bulk wire atoms have, hum— no where to move sort of, they run into each other, but when a wire has a free boundaries what happens is dislocation of hum— of different starts to form, it can escape out of the boundary. So things like that, those are things that you can see hum— from the tool, how atoms move, so in there too there is also provision of getting a snapshot of atoms, that is how atoms arranged at every time step, so if you keep seeing sort of a movie of the atoms you can understand what it happening to every atom and that was more important to realize what are the physics or what are the microscopic uh, details of anything like this in the simulation and things like that, so I think that was thing to get the physics across for me because the microscopic details of hum— the formation and all kind of materials together.

The general perception of the course is that it was a broad overview of multiple topics ranging from the nanoscopic scale to the macroscopic scale. Jake described the course as broader and faster than others, while Drew described it as an overview of topics with hands-on application, and Kyle wished the course could have gone in greater depth.

> Drew: Hum— [the course] is more applied, hands on, but its also because more topics are in depth, it is sort of an overview of topics more than extreme details of topics, so most courses that I have taken have focused literally on just one very particular aspect, so they are much more detailed than this course, but on the other hand they were more theoretical and less applied, less of the simulations like this, hum— also I think this is a broader course, I usually take courses in electric engineering and computer science so this hum— coming into material science for the first time it was a different experience, sort of what was more interesting to material science people.
>
> Jim: Yes, yes. I hum— I like the course very much. I mean, when I say this is a typical graduate course it is, hum— I mean that it is different from undergraduate courses, I mean in this course hum— the professor teaches us some basic theories and basic fundamental theories during the lectures and then hum— gives us some homework assignment or do some work on nanoHUB and but hum— if you want to finish homework or projects, only the knowledge from the lecture is not enough and hum— this hum— so this project just hum— force us to dig some more information and go to read more papers or related hum— theories to finish the homework or the projects and in this process we just get

> more familiar, get a good appreciation of the course material and finally hum— we get a better understanding of this topic. I think this is very good in terms of a graduate course.

Drew, Jim, Uday and Kyle mentioned that the course was relevant for them because it was related to their research. Jake, on the other hand, mentioned that, for him, this course was a good introduction to what is happening in industry. For Uday, this course was a preparation to be able to read a book that is relevant for her research area:

> Uday: Yeah, its not, I don't know even if it is truly relevant to my research but my professor says it is, and so basically I'm listening to him and uh— there is a book that I want to read which says hum— the relationship between thermodynamics and mechanics, so hum— all of this course has something to do with my research. So, it clears up my basics plus it ties up to an overview of other huge research things in my work, so yeah, and it probably will make me read that book in a better way, its very, he said don't try to read it all you wont understand, that's what he says, you need a lot of basics for that, so I think I am actually building up my basics to read that book.

Learning Outcomes

Focusing on the final project of Dr. Hass's portion of the course, students broadly described the learning goal as to have students experience doing molecular dynamics simulations.

> Jim: Hum— I think that the purpose for this project should be some, uh some initial and a general exposure to real molecular dynamic simulations. But uh, like I said, this simulation is pretty simple and pretty straightforward, but it can still give us some, hum— some knowledge of how molecular dynamic simulation is run.
>
> Uday: Ok, So if, if I have to talk about the last homework in the molecular dynamics, hum— it was pretty intriguing actually, I mean there is hum— the questions made us think as to how to apply our knowledge that was actually, I mean knowledge that we have got through the classes. So hum— in the class Professor actually made us go through, all through the nanoHUB simulation, like what data to be inputted at what point, and what it means, so it made a lot of sense when I was actually using the tool myself.

When discussed if students possessed the prior knowledge to approach the solution to the project, most of the students agreed they have been exposed to the important concepts during lecture. However, Jake and Jim felt that they still needed more explanation or to dig more into literature to grasp a particular concept. On the other hand, Drew and Kyle mentioned they had all the required background to approach the solution to the project.

> Jim: Ok um so, for this question I think that I have part of the knowledge, I mean, I have part of the knowledge that I need to solve this problem. I would include that hum—with the, with the larger x and y was larger in the x and y directions, the stress will go down. I mean, uh— I know this from my previous knowledge, but hum— in the, in the field of nanoscale simulation and scale of molecular dynamic simulation, uh— still need some more research in the literature to get some meaning with this problem and hum— I did go to the literature review to get some papers to discuss the hum— mechanical response of the nano wires and uh— I got information that linked to carry out this simulation. But, but, to be honest, frankly hum— this simulation itself is not hard at all. I mean it is easy, to frankly, the result I mean, uh, how to explain it hum— the result that we got from the simulation, um, we need to go to the literature to...
>
> Interviewer: I see, to interpret the graphs.
>
> Jim: Yes, to explain the results in a logical way.
>
> Interviewer: That's the difficult part.?
>
> Jim: Yes, that's the difficult. I mean, hum— the simulation itself is uh, very easy, since we are using the molecular dynamics toolkit in our hub and they have uh, they have set our everything for us, we just use our mouse to click which parameters to use, which material to use and uh, step times and total time and the temperature or anything else and then we click similar and it was relatively easy and hum— but, yeah, its easy to run a simulation but uh, to explain the result we need some more knowledge about the mechanical response of some nano wires.
>
> Jake: Hum— I felt like I had heard of all the steps before, like when I was looking through the um menus and stuff, I had heard of the things, but I didn't really understand what each of the options were until I had communicated with Dr. Hass more. Like, in the homework assignment, we just used something that was already made, I forget what the homework assignment was, but I know we had a homework assignment where we used the tool but we didn't have to build something from the unit cells and we could just use the default potential, so like, I knew he had talked about what the different potentials were but I still like

> off the top of my head I couldn't tell what the difference between them would be, like how the results would change with the different potentials.

Evidence of Learning

When students were asked what was new for them that they did not know before, most of them reported having learned something new, except Kyle. However, most of them learned different things. For example, Jake learned about quantum physics and about the behavior of materials. Drew learned how to interpret the late formations of materials. Jim learned more about molecular dynamics simulations and in particular this helped him realize how molecular dynamics work. Uday realized the differences between nanoscale and macroscale wires.

> Drew: Hum— ok, so uh I first had this time, you know, how uh nano wire, what are the properties on the nano wire. Hum— is it, it is really interesting because the nano wire was stronger than the bulk materials so um, that was something that was very important useful knowledge which I think because I also worked in my research in the are of nano scale systems it was important to understand this. I would say this is the most important knowledge that came out of it. Second was the microscopic detail of why a nano wire is stronger than the bulk material that was probably also very important too. So through following the atomic properties we understand how atoms deform if they are in a big system versus if they are in a small system. So I mean that was something that I learned.
>
> Uday: The fact that hum— when you are doing a nano scale the Young's modulus could be so different when compared to a macro scale wire, was actually, I, it took me a lot of time to take that first of all, the wires could get so stiff when they go to nano scale and getting to know that was very exciting.

Students reported having received initial feedback for their projects in the final presentation. After that final presentation, students were also required to deliver a final report. The interviews were conducted after the final presentation but before receiving the feedback from the final report. Therefore, students just commented about the kind of feedback they would like to receive.

> Jim: Ok, hum— feedback from Professor, I think hum— uh— the most important feedback that I would like to hear is why uh, we got hum— I mean why the result of our result stress is even lower than bulk material. I don't know, so if hum— Professor can um, uh give us more

> guidance or tell us, um, which is wrong so that we got a wrong result, I think, um, I think that will be great.

Jake commented about the feedback he received versus the feedback he would like to receive for the other homework assignments. He mentioned he would have appreciated it a more detail feedback. He discussed his problem as follows:

> Jake: Alright, so based on the homeworks, what he has done is just looked to see if you did it, but I think he weighs these projects more heavily, so in the homeworks, it was just check off if you did it, so I think what I would expect is maybe hum— yes you made the right conclusions, no you made the wrong conclusions. But hum— maybe he might say, well why did you use this or why did you use that if I didn't explain something too well, but um, I'm not totally sure what to expect I guess because we haven't had anything that had, so since the homework isn't graded, he hasn't put that much feedback into it, so we haven't had anything with feedback yet, so I've never had him before, so I don't know.
>
> Interviewer: I see, would you like to have more feedback? Do you think that would be really useful for you?
>
> Jake: Yeah, because, hum— like on the first homework, I did almost everything almost completely wrong and I didn't realize it until I got to the second homework where we needed to use some of the answers from the first homework, that hum— it was just simple things that I was rusty on integration or something, and had he said, Oh you're doing this all wrong you need to try this or something, so that on the second homework I went to talk to him and I figured out all the problems I had on the first homework, fixed all those, and then was ready to do the second homework. So it would have been nice to have, well, this is a little screwy or this isn't the right answer instead of yeah you did it. Because I know if I do it or not.

Instructional Approach

The instructor's approach to the course was described by Jim as one in which the lecture was followed by an assignment related to simulations and culminating with a final project.

> Jim: Hum— first, first we um, we got some uh theoretical background from professor's lectures and this is theoretical part and then we got the nanoHUB and the presentation by professor and we uh, it is about how to run the molecular dynamics simulation toolkit on nanoHUB and uh, by viewing that presentation we know how to use the toolkit and

> finally when we are doing the project, we uh, we got more detail information how the simulation was run exactly and um, by the completion of this project, I think we, uh we have much better knowledge how the simulation was run in the molecular dynamic simulation toolkit and I think this is what I have learned, the learning process sort of.

Dr. Hass also included an online presentation on how to use the simulation with the final project. Jim, as well as Jake and Uday, commented that this presentation helped them in approaching the solution to the final project.

> Uday: Ok, So if, if I have to talk about the last homework in the molecular dynamics, hum— it was pretty intriguing actually, I mean there is hum— the questions made us think as to how to apply our knowledge that was actually, I mean knowledge that we have got through the classes. So hum— in the class Professor actually made us go through, all through the nanoHUB simulation, like what data to be inputted at what point, and what it means, so it made a lot of sense when I was actually using the tool myself. So hum— the simulations actually made me think a lot as to, I mean the physics behind it was quite apparent and the nanoHUB it has got hum—, especially the molecular dynamics simulation tool kit that we used, it had this presentation which Professor Hass has showed, so that hum— presentation was a very good view of that the size does matter in the presentation, that was really good, uh— there were a few doubts that I had when I was going through the presentation as well, which I could clear up with the professor.

Even though students had access to the online presentation in the nanoHUB.org, some students had difficulties setting up the model in the simulation tool. For example, Jake had difficulties getting the simulation cell to match with the super cell size. Drew had difficulties setting up the dimensions, the geometry to do this particular experiment. Jim mentioned that the most challenging part for him was to set up the periodical boundary conditions. He mentioned that he was still confused with these issues at the moment he was interviewed.

> Jake: Yeah, the um, getting the simulation cell matched to the super cell size because, um, we didn't know that if you put your mouse over where you select what kind of unit cell you have, we didn't know that it came up with the lattice parameter there. So, at first we were trying to guess what he put the lattice parameter until we could talk to him [Dr. Hass] and those simulations gave us crazy answers, because we were slightly off. So like the simulation cell has to be perfectly matched

> to the super cell or else you loose the periodicity and the z direction and you induce stresses that aren't there.
>
> Drew: Ok, hum— the midterm project probably the most uh— challenging was to go ahead and run uh— to go ahead and set up the geometry and understand how to, how you are going to do a particular numerical experiment, so that in terms of suppose I have to generate a nano wire and I am pulling it and these ends are the, the most, uh— one of the challenging tasks was to understand what are the correct ways of doing this, so you have to make this uh— dimensions sort of infinite and this dimension has to be finite, so it took me a while to understand how to do that on the tool…

The benefits some students perceived from the molecular dynamics simulation was by means of the graphs. Jake, for example, mentioned the graphs gave him more insight into the physical phenomena. Uday said the simulation gave her another perspective and made her think in different ways. Here, Drew explained in detail how simulation tools helped him in his learning:

> Drew: In my learning of the topic oh— Actually, so I would say that simulation is the only way to learn hum— so if we had not done these simulations, hum— although we would know the concepts from talking, sort of surface knowledge of what everything is and what is molecular dynamics how it is simulated, but when you are doing simulations you understand what the more scientific aspect and more quantitatively what is molecular dynamics. So what is the effect of time steps, what are fluctuations, uh— what are they why are they important, how do you simulate a problem of temperature flow or heat flow versus how do you simulate a strain or bending of wires and all these simulation aspects are different from one another. So although all that was taught in concept in slides it is only through simulation that we finally understand what is the meaning of each of these things. Hum— and uh— and also hum— you know when we do the simulations we play around with the simulation tool kit, with the nano scale with lots of options, so you play around and you see uh— when is molecular dynamics simulations stable, when it gives useful results, how does it compare experimentally obtained data you know in labs and things like that...
>
> Interviewer: So you did that? Or you are just giving me examples?
>
> Drew: No I mean we compared it from the experimental data that is available in literature only and we uh— although I did not do experiments myself someone else has done experiments so we compared, we always try to compare things against that and we tried to see that you

> know if you have the tool kit available to you, you can change everything and run it more and more, so we sort of found out you know what is the most important determinant of hum— of say this problem....

Students also commented about their team interaction. Jake and Kyle described it as difficult mainly because of bad communication among the members. In contrast, Jim and Uday mentioned some benefits of interacting in teams, such as being able to check the results with each other and to clear doubts. Drew commented he would have preferred smaller teams for better interaction.

> Kyle: Hum— having to, or rather the collaboration with your group mates. Because it, because you're doing different simulations hum— and everyone comes from a different, all the people in my group were, had different backgrounds. None of them were from the same major and hum— I know at least two of the people I was working with are hum— are graduate students but I'm not sure about the third one. So we are all coming from different backgrounds, and we're not sure, everyone has their own, has developed their own language when talking with each other, so you have a barrier from that. And then you also have, hum— having to have, one of our group members didn't have, didn't understand the simulation techniques, so we were, we had to explain to them how to actually perform the simulation, or what was actually, what actually the simulation was doing.
>
> Uday: Yeah. So that way, it, and even the group we had a few discussions like I was in a group of four so, um, we actually went around twice for the project and that actually cleared up lots of other doubts I had.
>
> Jim: Hum— some in the first few days, some result were not same, and then we, hum— we wrote some comments on the wiki and we finally got why we got different uh, result. And we hum— and we figure out who is right and who is wrong and then we use the same correct parameters and the same correct uh methodologies to interpret the result, and hum— I'm pretty sure what we have done, I mean based on our knowledge, its right.

On the other hand, Uday also commented that the wiki was very useful for the team interaction.

> Uday: …we had the wiki and we had discussions, um, I was kind of out of those discussions initially because I mean this time was very tough for me, but it actually helped me a lot for the project, we had like pages and pages of discussion, lots of discussions going on for the project

> and such, so its kind of immediate, you approach something, there is a change, if you want, or if the other person wants to make a change he just downloads it and then he can post it too, and then the new person downloads it and its kind of fast, at least you're not putting so much bulk into your mailbox, so that way its um, and actually you can ask Professor you can peep into others projects and see what they are doing and you can learn a lot with the questions you have and stuff, in fact there is another person in another project, we were made into two groups, one project into two groups, the other group guy actually sent me an email asking ok I am not understanding you have to explain to me, since we had the other discussions I could explain to him what Professor Hass was saying and how to apply things that was the key, so that really helped.

When students were asked how they think their learning process could be improved, they suggested the following: Jake and Jim said it would help them to read more theoretical papers to better understand the underlying concepts. Uday and Drew agreed they would like to see more structures, more materials, and more physics problems. They also agreed it would be helpful for them if more help files or videos accompanied the simulation toolkit. Kyle suggested it would be very helpful if he creates his own simulation.

> Uday: Hum— probably its not the simulation I should say if you are looking at generally the molecular dynamics, you can go to higher scales so you wouldn't know what would happen at larger time scales, I think it's a general problem of the molecular dynamic simulation, you can't understand what's happening at larger time scales basically, so that I think it requires, as professor said, it requires a lot of uh— computer capability to get that— as I am saying it could be slightly flexible as to the potentials, hum— or some user defined elements like there were aluminum, platinum, nickel, so mainly there were all cubic.
> If there were some other uh— structures as well we could, I thought actually of working on different structures so ok what would happen if this structure were different, I definitely would get things to be different, so if the slip planes were different my Young's modulus would be— so that is another aspect where I had an idea which is actually there in project report, I mean the initial plan that I had in mind so that was another one which the tool kit could improve on, if it is able to uh— look at other structures for us to interpret.

Perceptions of the Tools

General comments students made about the tool and about the nanoHUB.org are positive. Jim perceived the materials simulation toolkit as a very convenient tool. Drew mentioned that the interface is very good. Jake mentioned that the nanoHUB.org in general is very easy to navigate, but he had some problems with the visualizations (or "visualizer" as he described them). Uday described it as very systematic and easy to use.

> Jake: So, overall, the nanoHUB is pretty easy to navigate. And it easy to, uh— find the tools that you want to use, hum— some, I noticed that some of the tools don't have as much, uh— background material ready. There's like the, you can select about this tool and just gives you a general description but it doesn't always give you like, how to use the tool necessarily, and hum— that would be nice. And also, a lot of times, you'll run something, so at least in the, the project we would run three or four simulations in a row and then on the fourth one get halfway through and it would fail, and then we couldn't get back to the same visualizer, at least I didn't see an easy way to get back to the same visualizer to bring back the old data. I know that its saved, like all our data gets saved, but how to access that easily with the nanoHUB— you know what I mean?
>
> Uday: It was very systematic basically, the tool kit was simple and systematic, so uh, when I am actually putting my cursor on each of them, it actually tells you what it is, so I, ok, for starting off a problem you have the materials part there in the first step and then the second part is ok what kind of potential do you want to use, the specifications, and then it goes to ok now what are your lower conditions or your forced conditions, that was in the next part, so it was basically very simple and systematic and that was a very key uh— thing for any new person who wants to learn what's happening, uh— say, it is very user friendly basically, uh, there are certain parts which uh kind of missing, or I should say if there was a way in which you could put your user defined potential instead of what were there, I don't know what complications it would have for us to think of a potential which is so involved that they define default values, if we are thinking of a new potential then I don't know how many mistakes we would make, but if there as something of that it would be more flexible, uh— and, yeah—basically systematic and easily approachable, you wouldn't expect really, looking at the… I mean you wouldn't get scared looking at the tool kit, it's very user friendly.

Regarding performance, Kyle described his experience as bad. He said that the simulation was crashing most of the time. He said that even though the simulations are running in the cloud, users have partial access to it. Jake also pointed out the same comment saying that the computational power they have access to is very limited.

> Kyle: …it's easier for me to just run things locally on a, on a computer I've managed because it's easier to actually get the data, that's

> the problem I see with doing the cloud computing, is that you don't always have access to one hundred percent of the resources, which is a problem I see. For example hum— I'm currently working with uh— Dr. Richardson and one of the simulations I will probably be running this semester I will just have to generate files large enough that if it were done by cloud computing it would run out of space.

Drew and Kyle commented about the transparency of the materials simulation toolkit. Drew said that not being able to see what is happening inside the simulation is a limitation. Kyle said he couldn't learn anything because of this lack of transparency.

> Kyle: I have an idea of what's happening behind but I'm not exactly sure. I'm not 100 percent sure of what's going on because I've run similar simulations using similar techniques but I, I didn't learn anything about making a simulation, all I learned was about running one. The problem I had was that it wasn't transparent. I couldn't see what was going on, so I didn't know, and that also made, for me it made uh— understanding whether something was actually physical or not, made it a little, a little less, or made it a little more difficult more me to understand it. Because actually whenever we ran into the problem of not being able to visualize the, the cells, because you couldn't tell if your initial set up was correct or incorrect, or was poorly conditioned.

Students' Perceptions and Experiences of Dr. Richardson's Course and Approach of Incorporating Simulation Tools

Lawrence, Rajiv, Melanie and Robert were the students who participated in the interviews related to Dr. Richardson's portion of the course. These students also had a diverse background. Lawrence had a materials engineering background as well as Melanie. Rajiv had a mechanical engineering background and Robert an electrical engineering background. These four students perceived the course in different ways. Rajiv described it as not a very difficult course. Melanie described it as a typical graduate course. Lawrence described the course as different in the way the homework assignments were considered and also because of the diverse background of the students.

> Lawrence: I think this course is unique in the sense that the homework isn't really a part of your grade, like it's not a weight percent of your grade but you have to complete all the assignments in order to pass the class, so it's an interesting take. Some classes will say the homework is optional, some will say you have to do the homework and at the end it's ten percent of your total grade, but in this class, they aren't

> giving that option, you can't pass the class unless you do all the homework.
> Another thing that is different I would say it that there is more disciplines in this class than the other graduate materials class, this one has people from mechanical, electrical, from all. Because computational is the hot thing right now so people are trying to predict new materials or devices without having to actually process it in the lab.

On the other hand, Robert mentioned it was a bit difficult of a course since it covers a lot of things, leaving out details. Lawrence had the same perception that the course is very broad. Actually, he was somewhat disappointed because of that.

> Robert: Hum— actually for me since hum— I think hum— it hum— it covers a lot of things I guess so since it covers a lot of things maybe it hum— it skips some details of some things, so the difficulty level I think is a little bit more than average.
>
> Lawrence: I was actually disappointed in the start too because a lot of people in the class don't have a quantum mechanics background, and I do, so I thought it was going very slow and somewhat lacking depth, and I'm sure it was helpful to people who have never done it but I have been doing this for a while so I was a little bit disappointed in that part. And the molecular dynamics part I didn't have a lot of experience with so I found that very interesting. The phase fields and stuff, it's good to know and it's interesting, but if I would have known exactly everything laid out in the class I probably would have considered taking a different class, but it's been useful I would say, not so much thirsting for interest, but definitely I can see the usefulness.

The four students interviewed commented they are taking this course because they are interested in learning how to do computation. Lawrence thought it is convenient to have these skills. Rajiv got interested in the molecular dynamics when he had once seen Dr. Hass' seminar series. Melanie, on the other hand, would like to continue in graduate school and focus her research in this area. Robert is focused on doing simulations of electrical nano devices, and wanted to have the experience from the materials engineering point of view.

> Melanie: Yeah, this is one idea of I have in doing my graduate here I want to do this because I like going into the lab, and at the same time because I have been doing this for like almost a year, and I really believe that there are more description that can really describe what happened in the small scale, so what I want to do in the future is that I would build a

> model that is small, and expand it to a big model that would explain what I did in the experiment. So this really gives me a touch of what I am going to do in the future, and I love it.
>
> Robert: This class...actually I hum— am working in electrical, like some problems with nano technology, so basically in our research we also do simulations of electrical nano devices, but I just wanted to know, I wanted to see this thing from a different perspective. How material engineers do these things. So I thought that it will broaden my understanding of these things.

Learning Outcomes

These students had different perceptions of the homework assignment's learning goal. Melanie had the broadest perception of the learning goal saying that the goal was to have an experience in doing research in this area. Rajiv and Robert had a similar perception describing the purpose of the assignment - as a practical experience on how to implement the equations taught in class. Lawrence described the learning goal as to have a conceptual understanding of the phase field starting from the first principle of thermodynamics and how to implement a simulation that will solve the required computations.

> Robert: Oh ok so in this particular course a large portion is based on some numerical theories, so hum— he [Dr. Richardson] is teaching a theory that in order to implement this, we need to use some way to implement that material, in particular homework, I think the goal is to implement that portion of the theory and to see how hum— how this theory works and what is the result, how the like some numerical things like stability and just to check these things and to really apply the theory, and to really hum— get some results and to see how things are happening.
>
> Lawrence: Hum— I think he really wanted us to see where phase fields really come from, the first principle of thermodynamics, and tie that all the way into how to implement it and run a software program and use computations to solve it. It was hum— a very difficult assignment and it actually encompassed quite a lot, it was almost like telling a story. It started you off at the beginning and you had to know the first principle of thermodynamics, you go through analytically derived results, and then you get to a point where you can't solve it by hand anymore and then you have to go write code, and the process of learning about actually writing code, troubleshooting to code, and then interpreting the results and then going back and seeing if the results fit with what you started with. So it

> was, I think his purpose was to give you a taste of everything from the start, how it ties into the computation, how to interpret your computational results, and then how to see if they actually make sense, do they match with what you started with?

Students encountered some difficulties in approaching the solution to this assignment because of lack of prior knowledge. While Lawrence and Robert struggled with the implementation because of lack of programming experience, Rajiv and Melanie had some problems with understanding the physical concepts.

> Lawrence: Hum— well from the physics standpoint I was very confident and the mathematics too, but my background is in physics and math, but it isn't in computation which is the reason I am taking this course is to try and learn how to implement the physics and math but I wasn't confident at all really in the computational stuff. If he wouldn't have given us the blueprint to start with, I wouldn't have had a clue where to begin doing the problem. We got the blueprint and I was able to do enough research and collaboration with my peers to hopefully have gotten the right result.

> Melanie: It is way beyond me I think, like I feel like that, mainly because I don't have any classes before this that taught me all these physical kind of, like this is my first class in this so I am really, really overwhelmed cause my physics background was like two or three years ago, and physics of classical mechanics have nothing to do with this. And all these equations that appear in the class, those are the first times that I saw those equations.
> …So every time when he shows the slides, that will be the first time that I have seen the equation. A lot of people in the class they really know what's going on because they have seen it before, so it is related to their research and they know what's going on but to me, it was like always my first time, and I have no quantum mechanics background.

Evidence of Learning

Lawrence provided a general description of the structure of the course focusing on the assessment components:

> Lawrence: There is a final exam. There are two big group projects, we already did one, so you get a grade on that. You get a grade based on your cumulative group project based on your first half with Dr. Hass' material and then a grade on the big project for Dr. Richardson's material and then a grade on the final exam, and those are the three components plus you have to do all the homework.

Focusing on the specific homework assignment where students had to use FyPy, students described the new knowledge they received. Lawrence, Rajiv and Robert commented that they have learned how to set up and solve partial differential equations using FyPy. In addition, Lawrence commented he learned how to do phase field modeling, Rajiv have gained a general idea of the concepts taught in class, and Robert also got confidence in implementing simulation tools. In contrast, Melanie learned how to work like a real researcher.

> Rajiv: Hum— I mean, just hum— basically like applying the equations and stuff. What I have learned new is that hum— I learned how to program at least, maybe not in all entirety, but in parts of Python which I have a little bit, although I had a little bit of background in Python because I use another modeling simulation software, so I learned that and then I learned how to assemble equations for the phase field method. So, how to solve the Allen-Cahn equation, or if I really wanted I could solve the Cahn-Hillard equation. So then I learned about, I knew in advance the stability issues with implicit method as well as explicit, so then I ran simulations using both methods to see how it actually does make a difference, so these things I learned about it.
>
> Lawrence: Hum— well in general, I didn't know about phase field modeling, I mean it was something that was out there but I didn't know, you don’t have to use polarization you can use electro mechanical quantities, you can use mechanical quantities, etc. and so I have learned about being able to model different phase fields, which I did not know coming into the course.

When these interviews were conducted, students had not yet experienced any formal feedback from Dr. Richardson. However, students thought Dr. Richardson may post the solution or a suggested solution in the course wiki. Rajiv, Melanie and Robert pointed out that he may probably discuss some overall mistakes during class time. Melanie commented that she can just go and talk about specific doubts with the instructor.

> Melanie: Hum— I started by going through all the notes, going through the notes and the slides, understanding the question, and see whatever I can, and if I couldn't I would just ask my friend and um because we have two programs that Professor Richardson wanted us to download, just go through that and see and know what we are expected to have and if I can't understand I will just go see him and ask for help.

Instructional Approach

Melanie described Dr. Richardson’s pedagogical approach for conducting lectures. Melanie compared and contrasted her experiences in Dr. Richardson’s course as compared to other undergraduate courses:

> Melanie: Hum—I, also because I understand that this is a graduate course, waiting for the professor to guide us one step to another—because like, doing undergrad study the professor will kind of guide you like, bring you one step to another. Here we have this big gap that you know, we need to jump ourselves. I can’t like, I can’t really expect the professor to teach step by step because this is a graduate course...

When students were asked about the challenges they encountered when approaching the solution to the homework assignment, students responded in the same lines as they responded about their confidence in their prior knowledge. Lawrence, Melanie, and Robert mentioned they did not have the computer background. Melanie added she was not able to understand the concept at a higher level of abstraction. Rajiv said he had some problems with one value that did not come out the way he expected, and he did not know whether he had done something wrong in the implementation. Robert also mentioned not having grasped the concept of stability.

> Melanie: Yeah I know a little piece here and there everywhere, but I can not put it in the big picture and see what's happening as a whole. Like maybe I know phase field the derivation over here, I know the derivation of Allen-Cahn, but I just can't put them together and see what's happening in the big picture, how are they interrelated to each other, and yeah that's my problem.
>
> Robert: I think in this homework there are two parts, one is the theoretical part and one is the implementation part, so in the theoretical part as well. The one I say I had problems in the implementation part is the syntax thing. Also the theoretical part I think that I have hum—something I need to understand a bit more, like the stability like just today I was reading some paper, so still some I need to know in the theoretical part of stability and the criteria there hum— criteria for convergence and whether it is stable or not. I found that in the class lecture for me it was not enough I guess. So particularly I have to even see in other literature about stability, the numerical simulation, so I, that part I think I have to work on.

As we can see from Robert's explanations, the students employed some strategies to overcome those challenges. Rajiv, as well as Robert, looked into the literature that the instructors recommended. Melanie opted to talk with her classmates and with Dr. Richardson. Additionally, Lawrence and Robert commented that Dr. Richardson, during class time, gave a blueprint to students as a starting point for the solution to the homework. Both students agreed that this starting point had been a very good help.

> Robert: Uh— initially I, since I did not know the language, so even um, before starting this, I thought that it could be a little bit challenging, but when I see a particular example code that the professor showed us in class and he ran it, then we I see that code and the program, then I immediately understand what to do to modify or to change.
> Lawrence: For me, I have a lack of computer science background, so actually writing the code. In class, Professor Richardson went through and started it for you, so you had a good base, which I would have been lost without completely, but he left out key things that were difficult for me to figure out.
> I had to do a lot of reading on Python on my own, and collaborate with other students to eventually figure out these things that I didn't know how to do before.
> So writing the actual code for the electric field, so the phase field that we were modeling is how the polarization changes with applied electric fields. So he set up for us a model that didn't include an electric field, so you just model, so had a phase field equation that looked at whatever the polarization was given some initial conditions, the extension was having to take the electric field, add it, and then see how the phase field changes. And to do this, you have to import mathematical tools that aren't already there and you have to know how to make things evolve in time, so all the functions that we had before you can just define the function to solve it, but in this case, you want to value the electric field at every step in the equation, so you have to know how to put it into loops and stuff. All that stuff I did not know and I learned that, and it was the hardest part.

Students discussed the characteristics of doing a modeling task that helped the most in their learning processes. For Lawrence, the output on the viewer helped him realize whether he had done the coding correctly. For Rajiv, it represented a way to verify the correctness of his analytical solutions. It also represented a way to understand the physics and its implementation. For Melanie, using simulations in a modeling task represented many advantages in her learning. It helped her see phenomena that are really small and apply what she has learned in a laboratory setting. Also, it helped her to prove whether her knowledge is correct by means of the output. Finally, it also helped her to understand the physics.

> Rajiv: Hum— just basically the output I get of whatever I have inputted so trying to understand how M and K vary or where, how many number of elements do I need for the simulation to be stable, what is the time step I am required to be stable to that way it helped because analytically got a particular time step but what I found out when I implemented it is that that wasn't the right value, I had overestimated analytically what my time step should be. So some things like that, it helped later on.
> …But if hum— in a sense I like this one because I could implement it on my own, so it helped me understand the physics as well as implementation of it, but just understanding how physics work in itself is a different issue in a sense.
>
> Melanie: Like, generally it is something very interesting to me, because in the lab we can't really see something that is that small, just like in materials we can do like fractures and stuff, but it doesn't go to like nanometer, we can't see it or whatever, but when we are using nanoHUB we have a lot of, a lot of time we can really see, like where they start to fracture and stuff like that. It is really nice because we can't really do it in the lab, and we are able to use it.
> Also, I think sometimes when using the simulation it helps me to understand the physics as well, instead of using the output to explain the physics I will use the output to understand the physics behind it, because it is easier for me to visualize something using a graph than using nothing, like at this point they give your maximum or whatever I can tell, and as I look at the graph I can see this happens at this point, why is it happening, something like that.

Perceptions of the Tools

Students made general comments about the simulation tool as well as about the nanoHUB.org. Lawrence commented that it is convenient and useful to have all the software installed in a single place. Robert, on the other hand, compared and contrasted FyPy with MATLAB for solving partial differential equations. He said that it is easier using FyPy.

> Lawrence: Um, I hadn't used nanoHUB until I took this class. So that was my first time registering and the class used it for the first part, both the quantum mechanics and then the molecular dynamics, and now we are using it for Phi Pi. It's useful because a lot of the stuff is already there and installed, if you go to the store and you buy a computer and you

> install Linux on it, you don't already have Phi Pi, and it takes a lot of time, it's a pain in the neck to compile everything but in the nanoHUB it's already all there for you at your fingertips.
>
> Robert: Yeah, in fact I think hum— I did not know about this FyPy tools, like this is basically running on Phyton so this is a particular library or model, so I think, in fact I am amazed, so I have been for partial differentiation equation I have been using some other tools like MATLAB something like that, but this is so much handy.

Rajiv commented that not being able to have access to the code hinders his learning experience:

> Rajiv: I had mentioned that since it is extremely closed you can just use the graphical interface, it just does a little bit hinder, say if I want to hum— because when you have a graphical interface there are only a certain amount of things that you can do with the simulation tool. Hum— you can't change certain things like for example, hum— in Professor Hass' part of the course for the molecular dynamics tool, uh— in their simulation software which says something is coming soon. So in the sense those are the things which I want to implemented because it is so closed in a sense. It's not open a lot. I mean it is good but still sometimes, that would benefit if it were a little bit more open in a sense.

Students' Perceptions and Experiences of Dr. Denner's Course and Approach of Incorporating Simulation Tools

Five students, Dimitris, Tom, Connor, Maurice, and Steve who attended Dr. Denner's course for the semester of Fall 2008 were interviewed. Some students, such as Steve and Tom, described this course as a hard course for an undergraduate level but at the same time, simpler than a graduate level course.

> Steve: This is definitely a higher level than any class I took there. As far as undergraduate level it's definitely the hardest undergraduate level I've – I've seen… However, I think it's much simpler than the other graduate courses. Um, at least it's a lot simpler than I'm taking a class on semiconductor devices called Solid State Devices and that's very much involved in the quantum mechanics view – do a lot of that at the beginning as compared to a day or two in this class.
> And uh, and we've also done density of states and other stuff. And, it's a lot more in depth than this.

Dimitris commented that for him, this course is unique because of the instructor's approach. He also mentioned he enjoyed it.

> Dimitris: I think it's uh – no, no, no, I have to emphasize I think, uh, I think this is the – I mean, uh, okay, to be honest, I think this is the best class I ever had in my educational history.
> I have to, since the professor won't see it, okay. I just to let you know. Okay? This I think this is – I think yes, by far I would say, yes. I'm very, very excited to be here to have this class.
> And, the homework is – is – it has the same.
> I take two other courses. I feel that in comparison with them this is uh, the most conceptual one.
> It is the most enjoyable one.
> You never think of the—of the, okay you say you're compensated by the richness of the ideas, you don't really feel, "Oh, I have to spend time on this," because you – you get compensated by the – the ideas.

Learning Outcomes

In general, Dr. Denner's students identified two main learning objectives related to homework assignment one. One was related to the physical concept of conveying how current flows in very small devices, as described by Maurice and Steve. The other one, as identified by Tom, Connor, Maurice, and Steve, was related to introducing MATLAB as a computational technique to represent phenomena. In addition, Dimitris mentioned that Dr. Denner's intention was to give them tools to try new ideas and validate equations.

> Maurice: Um, so, let's see the purpose of homework one. To familiarize people with MATLAB.
> And then um, so, um, one of the basic um, devices in your computer is a transistor. And, um, so the purpose of homework one was to get people up to speed at what happens in that transistor as certain conditions change.
> So, like, here you change voltages you know, over your transistor; and then, you know, what happens with the current basically.
> So, you have different – different parts of your transistors, like three different parts: source, channel, and drain.
> So, you can change your voltage on those parts and see what happens with your current. So, that was like the whole basis of that homework.
>
> Interviewer: And, talking on a more general level, do you think his goal was for you to find something new? Or, just to practice? Or—

Maurice: Just to verify what he had done in class.
So, I mean he gave us the equation in the class, you know. but how to actually turn those equations into something meaningful on the computer; or how to, you know, ‘cause there’s certain things you can do by hand that the computer’s not going to be able to do, you know.
But, there are certain things you know, it’s like the difference between an analytical solution, an analytical solution you can do by hand, you know.
But, on a computer they’re not going to give you – you’re not gonna’ put like some text in your computer and it can give you the text back.
So, you have to do things numerically. But I think that’s the – one of the big things with homework one is you have to break things up into small pieces and then do things numerically, like one at a time, and then put things back together at the end in the plots.
So, I think that’s one of the things with homework one. How to do things numerically instead of just doing it by hand.

Dimitris: I think Professor Denner wants us to – I think has two— two aims.
The one is to give us a graphical representation of the ideas.
When you have a single mathematical equation it’s not easy for the student to – to see the dependence as clearly.
But when you have a graph you can see the dependences. You can see the limited cases. You can see the circulation phenomena; this cannot be seen by the equation itself.
But when you have a graphical presentation, you can see all this info.
The second that I think aim of the professor is to make – make us more independent. So that when we can arrive – when we write um, an alternative equation that we thought of that we can – we can write it in MATLAB to see whether it is valid.
So, he wants to make us independent to try new things so now wrong.
So, um, I think that it’s a good reason to become independent people that think and try new ideas to see whether they are valid or not.
So, I think this too.

These students took the course because they interested in nanotechnology and/or because the course is related to their areas of specialization. For example, Dimitris and Steve commented that the course was related to their research. Tom and Connor mentioned it is going to be useful in their careers, and Maurice mentioned a general interest in nanotechnology. Here, Steve and Maurice share their interests for the course:

Interviewer: And then how does this course is relate to your areas of interest?

> Steve: Pretty directly related um because it's very helpful in understanding how – how electronics work at that small of a level, so ((I: Um-hum.)) definitely.
>
> Interviewer: And, is the material or topic exciting for you?
>
> Steve: Um-hum. I'd say it's – it's definitely exciting to uh learn uh, - it's a – yeah, I guess it's uh, what would I say, um, it's not like well I learned how this works today kind of class, but it is uh really exciting to learn all the different stuff that we've learned about how current works in these different situations. And uh, and I get sense for where we're going and what stuff is – what people are doing to enable us to learn all this stuff, so, it's yeah.
>
> Interviewer: I think you have already answered this last one, but I will ask it anyway. How does this course related to your areas of interest?
>
> Maurice: I'm interested in modeling of nanoscale devices.
> Yes, so, this combines theory and modeling of nanoscale devices. So, it's exactly at the heart of my interest. Yes.
>
> Interviewer: Is the material exciting for you?
>
> Maurice: Yes, as I told you, yes from my educational experience I want to insist on it.
> I—I knew about this course before I came to Greece, uh, to the U.S.
> When I was in Greece I used to discuss this with – I – I had the book before I came here.
> I didn't find the time to study it thoroughly, but I had the self – I had another – so it's uh, it's one of the motivations to be here so I – I can only praise this.

Evidence of Learning

All students reported having learned new concepts and skills by attending the lecture and by solving homework assignment one. Dimitris, Connor, and Tom mentioned having learned more about small scale devices and, in particular, how current can flow on such devices. Other skills students obtained were how to manipulate arrays in MATLAB, as explained by Tom, and how to integrate using MATLAB, as described by Steve. Also, Steve commented that he learned how to manipulate different units, and Tom mentioned he learned to first understand the problem before starting coding and to develop an expectation of his results.

Maurice: I'm really glad I made this decision because this course has helped me understand what's going on.
'Cause like I said, my undergrad I didn't really go over the MOSFET you know, the source channel all that stuff.
We just did the bipolar transistor. Which I think is customary for undergraduate degrees. But now it's – I think things are a lot more clear for me. So.
And plus, you know, at the nano level there's a lot of physics involved in fact most of it's governed by the Schrödinger equation.
So, that's a big – big plus to learn how to implement Schrödinger equation in MATLAB. So, yeah, I've enjoyed it.

Tom: But, I think the one thing that I learned was just that you need to – before writing like I kind of attacked writing my code by just using the equations that were given to me, and kind of taking a plug-and-chug route. Doing a little bit of thinking.
But um, with this problem, and the other problems, you really need to think about what exactly is going on.
And yeah, develop an expectation of your results first before just kinda' going and writing your code.
And so I think that's what I learned is that you really need to like sit and think about what is going on in the problem, and what is trying to be taught before just kind of going in and attacking it and just plugging, you know, just going through the motions.

Regarding the feedback mechanism implemented by Dr. Denner, the most common approach was to post the solutions to the homework assignments on the website. Dr. Denner, as well as his teaching assistant (TA), offered office hours for students to have an opportunity to ask questions and solve doubts while approaching the solution to their homework assignments. All of the students commented that the instructor and the TA helped them a lot to approach this solution during office hours. Also, by posting the solutions, students, such as Steve, benefited from it.

Interviewer: And, did you have any problems approaching the solution to—

Connor: Oh, first of all yeah. I mean, I wasn't an expert of the, you know, the MATLAB, so I mean the first one or two, you know, the homework assignments, I had kind of, okay I wrote it, but somehow it didn't work out.
So, I went to the TA and asked, you know, him what was wrong with it.

> And, he checked the cause and then he showed, okay, you need to change this one. I would just maybe add this one to just one graph, and then I see why I used that. So, that was really helpful.
>
> Steve: Um, I didn't know how to integrate in MATLAB before.
> Um, and actually, um, so I learned that.
> And the – when I – afterwards when I got the assign – or got the homework solutions back, the professor – or TA, or whoever comes up with those had a different way even.
> And I was using it both in method that allows you to do uh, basically not necessarily a numerical integration but like a symbolic integration. Uh, but it still used numerical techniques. And uh, they used it differently, so I learned how to do the integration.
> Um, definitely learned some of the uh, uh potential issues with uh, this particular set, uh— this particular framework is uh— you're dealing a lot with uh, values that could be given in joules or in electron volts and you have to be able to manipulate between the two rounds of – it's a difference of basically a charge of electron. But, you just have to make sure that everything is in place.

Instructional Approach

Dimitris, Connor, Maurice, and Steve commented on Dr. Denner's instructional approach. In general, all of them pointed out how it was easy for them to understand the concepts when he explained them. In particular, Connor pointed out the uniqueness of Dr. Denner's approach and Maurice appreciated how Dr. Denner explained how the concepts relate to real life:

> Connor: But he used a different – a different approach to solve the same thing when we then scaled down the size of the devices.
> So that was – that was – that was pretty new to me.
> The calculations, and everything was different. Everything and was different.
> Okay, he realized the thing to how you know the traditional way, but he—he's wants to somehow to link between that. But his approach completely different.
> It's just caused, you know, like you go top down and bottom up approach, and he just explains how it's, you know, the bottom up approach; if you just go from the molecule size to the big sizes what would happen.
> Because it must be different – I understand that, when you go to, you know the mini scale you know sizes, you cannot use the same approach as you used for being – you know the solids. That's real appealing.

> Maurice: You know but he does refer to things like you know measuring different values hum— you know, physically.
> Which I think is important. I think it's a good point that he's bringing up.
> 'Cause you always have to match – try to match your um, simulations with your data in the real world, you know.
> And, for the most part you know based on what he's said I think the simulations that we've done – or I've done anyway, have matched pretty closely so.
> So, seeing that he's starting to go through grapheme now in class – I think it's highly relevant. 'Cause you gotta' understand you know what governs hum— current; you know, these current versus voltage characteristics. It's the – the density of states.
> And that's what he spent the whole month going over was how to find the density of states in material.
> You know, it's another thing to go out and measure it. Which is one thing that I'd like to learn.

All students, experienced and not so experienced with MATLAB, reported they found the implementation in MATLAB challenging. Dimitris reported having difficulties on how to represent vectors with MATLAB, as well as problems with syntax and how to implement integration. Tom, as well as Connor, reported that in general they had difficulties implementing the concepts in MATLAB. Steve and Tom reported finding it challenging to get the equation to work correctly, as well as having problems manipulating units. Steve and Dimitris had problems doing integration. However, all of them overcame those challenges by asking either the instructor or the TA, and also by reviewing the MATLAB scripts that appeared at the back of the book.

> Tom: I felt uh, it was bad. I mean, it was like my first time kinda' working on MATLAB, and I was excited about this class.
> I felt like I knew what everything meant, but I couldn't get it.
> So, yeah, I was a little disappointed. I was kinda' frustrated, but, I was alright.
> 'Cause I'm not very um, I think we had to use arrays and our arrays were different sizes.
> And, and I kept messing that up, so that was the most difficult part for me, I think, was just trying to keep track of um—
> and also keeping track of units; things of that nature were also very hard in terms of trying to make sure all the units were making sense so that we got you know numbers that were reasonable to each other instead of getting like straight line because one number would be so big compared to the other things.

> …So – I kinda' used the code that was written for the problems in the book too, to kinda' see how the code was written.
> And uh, I found that that was useful, so that was – came in handy.
>
> Dimitris: Yes. Since my experience with MATLAB was a – largely limited, uh, starting from scratch with MATLAB would be a relatively tough problem. But uh, at the end of the book there were several MATLAB scripts uh, that helped me a lot. I just needed to adapt them with uh, the new problems that the professor came up with. So, it was easier.
> …If it weren't for this I would have spent much more without getting a really deep insight in the course. It would be a waste of time. So, I think these scripts helped me.

Summary of Results

Twenty five engineering students were exposed to computational simulations as part of their courses. Students reported two main reasons for taking the specific courses. In general, Libo, John, Isison, Arash, Howard, Dimitris, Connor, Steve, Drew, Jim, Uday, Kyle, Lawrence, Melanie, and Robert (n=15) agreed they took the course because is closely related to their research interests. On the other hand, Valerie, Joe, Jack, Jonathan, Allison, Mom, Maurice, Jake, and Rajiv (n=9) commented that even though their research is not on that particular topic, they considered this knowledge as important to know. They thought that at some point, having this knowledge may become "handy".

These students reported having perceived four general learning goals. Libo, John, Isison, Valerie, Howard, Jonathan, Maria and Jake (n=9) reported that the learning goal perceived was to have an insight of current technologies and practices. Examples of these perceived experiences are better comprehend the state of art of the transistor technology or, in general, to experiences they might have industry. Arash, Joe, Maurice, Steve, Jake, Drew, Jim, Uday, Kyle, Lawrence, and Rajiv (n=11) perceived the learning goal as being able to identify some sort of cause-effect relationship of physical phenomena. For example, understanding how current flows in very small devices, or how the varied dimensions of a nano wire affect strength. Students such as Dimitris, Tom, Connor, Maurice, Steve, Jake, Drew, Jim, Uday, Lawrence, and Rajiv (n=11) perceived the goal of the course and/or homework assignment as to be capable of representing physical phenomena by means of simulation tools. These include being able to understand the physics behind the simulation tools and to use a computational tool to graphically represent those concepts and ideas. Howard, Jack, Allison and Maria (n=4) also identified being critical users of the simulation tools as one of the learning goals for the course. These learning goals included being able to understand what the software is doing, assessing if the calculations are correct, and knowing how to fix it.

When students were asked how confident they felt with their prior knowledge, two general responses were found. Libo, Ision, Valerie, Joe, Maria, Steve, Drew and Kyle (n=8) felt very confident with the prior knowledge to be able to approach the solution of the homework. Howard, Jack, Jonathan, Jake, Jim, Rajiv, and Melanie (n=7) mentioned they didn't have a very deep understanding of the physical phenomena. And Dimitris, Tom, Lawrence and Robert commented they didn't have the appropriate programming background. Students identified two general types of supports that were very useful when they approached the solution to the homework assignments. Libo, John, Isison, Valerie, Joe, Maria, Jake, Jim and Uday (n=9) identified the online lectures posted by instructors on the nanoHUB.org as being very useful when approaching the solutions to their homework assignments. These lectures functioned as an embedded expert guidance (Quintana et al., 2004) that helped students in activating their prior knowledge. Also, Dimitris, Tom, Connor, Lawrence, and Robert (n=5) identified the templates and blueprints of codes—i.e. short scripts or codes as helpful in implementing their own solutions.

Even though students reported experiencing some difficulties, all students but one (Kyle) agreed they learned something new. Some students described their learning experiences at a course level, and some others in the specifics of the homework assignment. Libo, Arash, Jack, Maria, Dimitris, Tom, Connor, Maurice, Steve, Jake and Drew (n=11) mentioned having learned how the physics are related to the real world. For example, understanding the behavior of a transistor in a very small scale, how atoms behave, etc. Other students, such as John, Isison, Arash, Valerie, Joe, and Allison (n=6) mentioned they have learned how to conduct specific measurements. Howard, Jonathan, Allison, and Maria (n=4) mentioned having learned to be critical of the output of simulations and Howard, Allison, and Maria (n=3) also mentioned they learned how to find a way to verify if the simulation tool is performing correctly. Finally, Jim, Lawrence, Rajiv and Robert (n=4) learned new computational techniques.

In general, students perceived the feedback mechanisms for learning as appropriate for advanced undergraduate and graduate courses. Students described the feedback as not very detailed, but for Libo, Arash, Valerie, Joe, Howard, Jack, Jonathan, Allison, Steve, Rajiv, and Melanie (n=11) mentioned the posting of the homework solution was sufficient feedback for helping them self correct their understanding of the concepts and skills targeted by the assignment. The students enrolled in the advanced undergraduate level course also mentioned the teaching assistant and the instructor were very helpful in relieving their doubts.

When I asked students how they benefited in their learning from using the simulation tools, students focused on three main areas. The first benefit was convenience mentioned by John, Isison, Joe, Howard, Jack, and Connor (n=6). They found simulation tools as convenient because the tools solve difficult and complex calculations for them, and because the simulations helped them simplify the complex models. Another important factor students identified as useful for their learning was related to the output of the simulation tools. In particular, students (n=16) mentioned the output of the simulation helped them realize how each parameter affects the output; that is, the simulation gave them some sense of how physical phenomena behaves. The final benefit perceived by Libo, John, Arash, Joe, Maria, Maurice and Melanie (n=7) was the opportunity to experiment and ”play around” with ideas through hands-on experiences with the simulation tools.

However, students also experienced some limitations in their learning. For example, Ision, Arash, Valerie, Joe, Howard, Jack, Allison, Maria, Drew and Kyle (n=10) wanted more transparency in the simulation tools. They wanted to be able to know which equations are being solved, to see the calculations as well as the underlying assumptions of the model. Some others wanted to have access to the code. However, a type of paradox was identified. While students who only ran the simulation tools such as Arash, Howard, Jack and Kyle (n=4) wanted to program their own simulation tools; the students exposed to a modeling task such as Dimitris, Tom, Connor, Maurice, Steve, Lawrence, Melanie, and Robert (n=8) commented about their difficulties in implementing the computational part. Further, as found in Phase 1 of this study, the goals of the instructors did not always include a focus on learning the underlying model because other learning objectives were targeted for the time allowed. This contrast of learning goals is explored as part of Phase 3 of this study.

Students also made suggestions of other features they wanted to have as part of the simulation tools. Valerie, Drew, Jim, and Uday (n=4) suggested it would be desirable to include more options of graphical representations of the data as well as more models. And Jake, Drew, and Uday suggested having more presentations and help files focused on the conceptual (physical) aspect of the simulation tools.

Finally, several students had remarks regarding usability aspects, John, Isison, Arash, Valerie, Joe, Howard, Jack, Jake, and Drew (n=9) described the nanoHUB.org as very user friendly and intuitive. Arash, Valerie, Joe and Jack (n=4) experienced some problems with the interface such as navigation problems, difficulties to read some values from the graphs, how to switch from one simulation output to another, change dimensions of the graph, etc. Libo, Joe, Jake, Kyle and Melanie (n=5) experienced performance issues such as long waiting time, system crashing, and difficulties downloading data.

CHAPTER VII

STUDY THREE - PHASE 3: INSTRUCTORS' AND STUDENTS' PERCEPTIONS AND EXPERIENCES USING COMPUTATIONAL SIMULATIONS AS LEARNING TOOLS

None of the studies reviewed for this research compared perceptions and experiences of computational simulations as learning tools between instructors and his/her students. Also, no studies were found that documented ways in which students perceive instructor's reasons and methods for incorporating computational simulations as learning tools into their learning activities. Furthermore, none of the studies reviewed reported the use of computational simulations placed at a curricular level; a research need also identified by van Joolingen, de Jong and Dimitrakopulout (2007). For example, most of the studies found were conducted at lesson level from approximately three to five weekly sessions. This short period between treatment and posttest may lead to ineffective knowledge building (van Joolingen et al., 2007). Therefore, through a deeper level of analysis I compared and contrasted findings of Chapter V of how instructors perceive and experience simulation tools as a learning tool with findings of Chapter VI about students' perceptions and experiences of simulation tools used for their learning and instruction. Additionally, I included survey data of the three engineering courses collected in the Fall 2008 using the same survey as Study One presented in Chapter I.

Methods

In this third level of analysis I documented students' reactions to instructor's reasons and instructional methods for incorporating computational simulations as learning tools into their learning activities. The data sources for this analysis included four interviews discussed in Chapter V from instructors who were observed for a semester. The instructors who participated were Dr. Sanders, Dr. Hass, Dr. Richardson and Dr. Denner. A second data source was from 25 student interviews discussed in Chapter VI who attended at least one of the three courses taught by the instructors mentioned above. Finally, the third data source was a student survey conducted at the end of the Fall 2008 semester. As explained in detail in Chapter I, The student survey consisted of a Likert scale aiming to identify students' perceptions of their course and the simulation tools used as part of it. The student survey was responded by 40% of Dr. Sanders' students, 41% of Dr. Hass' and Dr. Richardson's students and 20% of Dr. Denner's students.

I started my analysis from the write-ups of descriptions and summaries of the interviews of all of the instructor and student participants. These write-ups contained data categorized among specific themes related to the learning goal of the class, assessment method, pedagogical approaches and advantages and disadvantages of simulation tools. The next step conducted was an iterative process of comparison to generalize patterns across cases. In addition to the write-ups, I also used a matrix to display students' ways of experiencing simulation tools versus their perceptions and experiences. The matrix made an easier comparison process between these factors. Once again I started a process of constant comparison to corroborate the findings by the evidence. I conducted this process of comparison by identifying similarities and differences between each engineering instructor and his/her respective students.

Results

Dr. Sanders and Students' Perceptions and Experiences of Simulation Tools in Engineering Learning Contexts

Dr. Sanders' overall goal for using simulation tools was to show his students how investigations must be conducted in their areas of expertise and ways professionals work on those disciplines. Dr. Sanders' students identified the course goal as gaining insight into the state of the art of the transistor technology. Analysis of the survey data suggested students perceived this course content and learning activities as highly relevant to their areas of interest. The analysis also indicated that the simulation tools supported students' goals and expectations of the course and reported using nanoHUB.org as a very positive experience (see Figure 7.1).

The common assessment method applied by Dr. Sanders was to first have students submit the homework, grade it, and then post the solutions on the website. Most of the students agreed this feedback was sufficient for meeting the course objectives, because the solutions to the homework assignments were very detailed. In general all students commented they learned something new by comparing their homework solution with the posted solution. The survey data showed that students experienced the simulation tools as useful for their learning in comprehending the concepts better than using lectures and readings only. However, they reported inconclusive experiences related to not having trouble in interpreting the output of the simulation tools. Students also reported high confidence in their ability to use the concepts embedded in the simulation tools to approach new problems as well as an increase in their awareness of practical applications of the concepts.

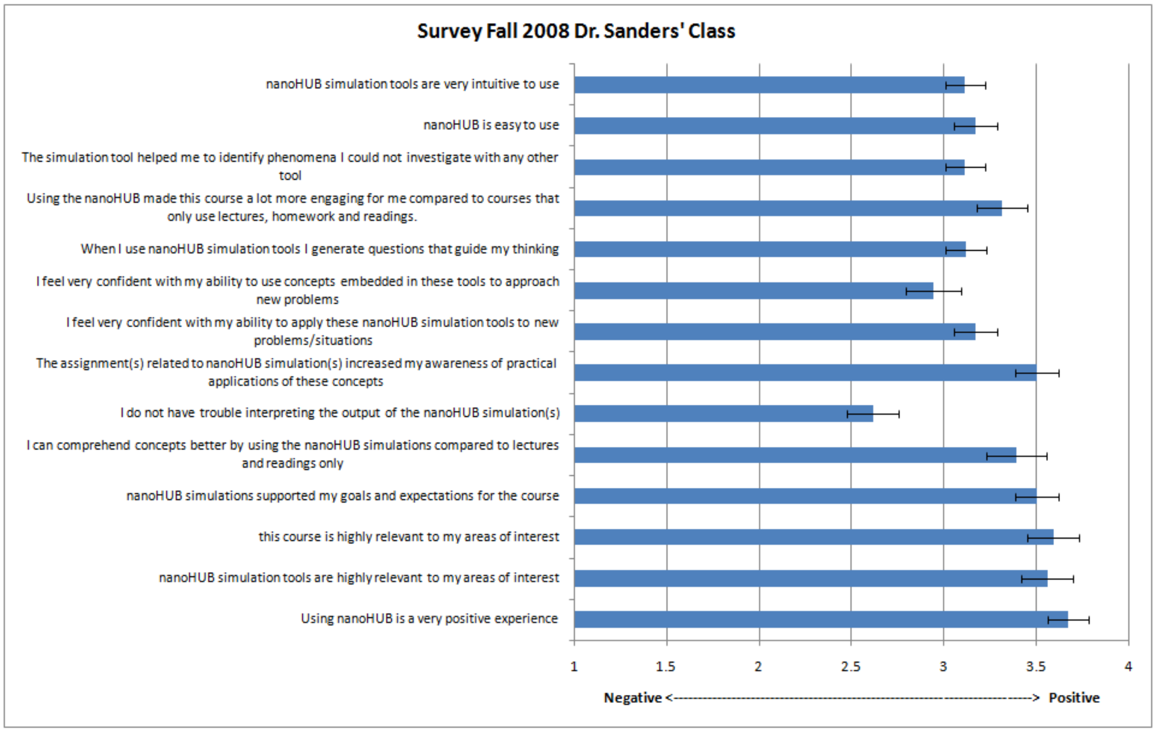


Figure 7.1 Dr. Sanders' students responses to the survey

Dr. Sanders incorporated simulation tools in almost every part of his pedagogical approach, from the classroom to homework activities. He pointed out that he did not only take the time to explain concepts related to the phenomena under investigation, but also spent some class time to explain how to operate the online simulation tools. Dr. Sanders also mentioned he posted online lectures on nanoHUB.org to assist students in doing their assignments. In general students perceived Dr. Sanders instructional approach as appropriate for the course. Students considered Dr. Sanders provided them the knowledge and problem solving methods that are authentic to real world applications. Students also perceived Dr. Sanders' approach as useful; since he provided them with the required knowledge to complete the assignments. Additionally, students reported the online lectures as valuable and useful resources for completing their assignments. The survey data showed students considered the simulation tools as engaging for their learning as well as a means to identify phenomena they could not investigate with any other tool. They also reported the simulations as helpful in generating questions they used to guide their thinking during the assignments.

While Dr. Sanders pointed out three advantages of nanoHUB.org simulation tools 1) easy computation of complex calculations, 2) simple interface, and 3) additional capabilities students cannot get in a laboratory. Students reported the most salient advantages were the simplicity of use, plus easy access and flexibility of the tool to represent the same data in different ways. This is consistent with students' responses to the survey that the simulation tools are easy and intuitive to use. However, students also pointed out the need for additional features to assist in distinguishing different curves when the simulation tool was run multiple times and additional (different) outputs of the data. Students also mentioned the need for better documentation and organization of the tools so they can easily find them and decide which one fits their needs. Finally, most students mentioned they wanted access to the simulations' underlying model. They wanted to know the physics behind the simulations such as models, what are the assumptions, what equations they are solving, and how and what are the implementation algorithms. I further expanded my interpretation of this issue at the end of this Chapter. In the survey students reported the simulations as intuitive and easy to use.

Dr. Hass and Students' Perceptions and Experiences of Simulation Tools in Engineering Learning Contexts

Dr. Hass co-taught a course with Dr. Richardson and reported three main goals for his portion of the course. One goal was to introduce students to simulation techniques as well as related physics such as theories and models associated with a specific phenomenon. Second, he wanted students to be critical users of the tools. A third goal was to have students familiarize with the literature on the area. The students identified a more holistic goal for the course that considered both Dr. Hass' and Richardson's goals. Students mentioned the overall goal of the course was to distinguish between what happens at the nanoscale compared to what happens at the micro and macroscopic scales. In particular, regarding Dr. Hass' portion of the course, students mentioned the introduction to molecular dynamic simulations as a goal for the course. The survey data indicated students perceived this course content as relevant to their areas of interest. Also, they identified the simulation tools as supportive of their goals and expectations of the course. On the other hand, students were mixed in their perceptions of nanoHUB as a positive experience and its level of engagement as a learning resource. The variance was high on these items which could be a factor of any number of events associated with the learning experiences (see Figure 7.2).

Dr. Hass' assessment method consisted of homework assignments and a project involving a modeling task. He provided feedback only in the final project. Students' perceptions of his feedback mechanism were diverse. Only one student reported not having any preference on how Dr. Hass provided his feedback. Another one mentioned he would like to have seen more detailed feedback in the homework assignments. Two more commented they were expecting a detailed feedback on the final project. In general all students commented they learned something new by completing the homework assignments and the project. The survey data showed inconclusive results on how students experienced the simulation tools as useful for their learning, in comprehending the concepts better, and inconclusive in their ability to use the concepts embedded in the simulation tools to approach new problems. Students also reported an increase in their awareness of practical applications of the concepts embedded in the tools. Also, students reported not having problems interpreting the output of the simulation tools.

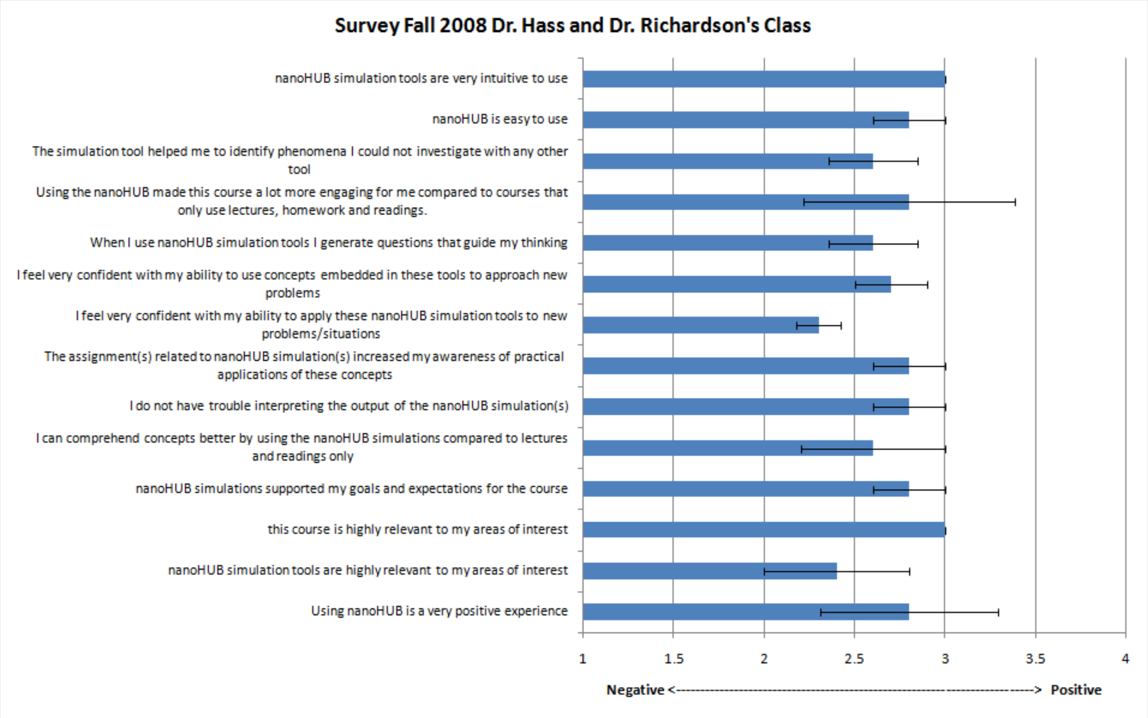


Figure 7.2 Dr. Hass and Dr. Richardson's students responses to the survey

Regarding the instructional approach, Dr. Hass described his course as a hands-on class where he gave students opportunities to explore a variety of models of physical phenomenon and modeling techniques involving numerical methods. He also incorporated cooperative pedagogies. In general students perceived Dr. Hass' instructional approach as appropriate for the course. Students pointed out the online lectures as very helpful in solving portions of the project and most students reported benefits to their learning by using the simulation tools. The survey data indicated students considered simulation tools as engaging for their learning. At the same time, these students reported ambiguous perceptions of nanoHUB tools helping them guide their thinking. They also reported inconclusive experiences from using simulations as a means to identify phenomena they could not investigate with any other tool.

Dr. Hass pointed out easy access at no cost as advantages of nanoHUB.org simulation tools. He also pointed out that nanoHUB.org has capabilities to support collaboration. Students also pointed out the convenience and easy access as evidenced from the interviews and the survey. In addition they also pointed out the ease of use. This was consistent with students' responses to the survey that the simulation tools are easy and intuitive to use. However, as reported in Chapter VI, students also pointed out the need for additional features they believe will help their learning experience. Students believed they need greater control of manipulating various outputs to support their inquiry and wanted visualization to be more user friendly. Students also mentioned it would be helpful if more help files and/or presentations accompany the simulation toolkit. Dr. Hass' students also mentioned they wanted more transparency of the tool, that is, a more explicit indication of what were the governing characteristics of the model.

Dr. Richardson and Students' Perceptions and Experiences of Simulation Tools in Engineering Learning Contexts

Dr. Richardson focused his portion of the course on modeling and simulating properties of materials. In particular he wanted his students to be thinking in conceptual terms about how a model represented the behavior of a material and not merely as programmers transforming equations into computational algorithms. That is, Dr. Richardson mainly wanted his students to develop an intuition of the phenomena under study and become critical and knowledgeable users of the simulations as well as of the literature in this particular area. Similarly his students perceived the goal of the class as to have a conceptual understanding of modeling and simulation of materials (e.g. mathematical phase field models) and how to implement and run those in a simulation. Also, one student mentioned as the learning goal to know how research is done in this area. The survey data indicated students perceived this course content as relevant to their areas of interest. Also, they identified simulation tools as supporting their goals and expectations for the course. On the other hand, some students reported inconclusive experiences using the nanoHUB.org while others reported using nanoHUB was a very positive experience (see Figure 7.2).

Dr. Richardson's assessment mechanisms focused on the projects and the final exam. From Chapter VI, I identified students perceived this assessment mechanism as appropriate for the course. In general, students expected Dr. Richardson to point out what their errors were and some indications on how to fix those. Students also mentioned that if they had further doubts, they could always approach Dr. Richardson to solve those doubts. In general all students commented learning something new by completing the homework assignment. Students grasped a general idea of the concepts as well as general skills to solve partial differential equations using the modeling tool. The survey data showed inconclusive responses in students' experiences with the simulation tools as useful for their learning in comprehending the concepts better and in their ability to use the concepts embedded in the simulation tools to approach new problems. Students also reported an increase in their awareness of practical applications of the concepts embedded in the tools. Also, students reported not having problems interpreting the output of the simulation tools.

Dr. Richardson's instructional approach built on the content (knowledge and modeling techniques) Dr. Hass taught. Dr. Richardson's gave his students a blueprint of the code as an aid to learning because his focus was more on the computational part rather than on the specifics of the programming. . Students reported this blueprint as very helpful because the most challenging part for them related to their programming skills. The suggested readings were also helpful in overcoming this challenge. Other challenges students faced were related to the theoretical portion of the course. One student discussed having problems in understanding the concept of stability while another one was unable to relate all the concepts together because of her lack of prior knowledge. From the survey data it was identified that overall students considered the simulation tools as engaging for their learning. At the same time, these students reported inconclusive perceptions of nanoHUB tools helping them guide their thinking. They also reported inconclusive experiences from using simulations as a means to identify phenomena they could not investigate with any other tool.

Dr. Richardson pointed out as general advantages of simulations the possibility to overcome the limitations of analytical solutions. In particular, he pointed several advantages of nanoHUB simulation tools include ease of access, flexibility of use and the research potential of the simulation tools. He also commented it is convenient for him and his students because these tools eliminate the burden of installing software and managing accounts. One student also identified this advantage of easy use associated with not needing to install the software. Also, most students described the simulation tools as useful. Only one student mentioned he wanted more transparency of the tool. In the survey students reported the simulations as intuitive and easy to use.

Dr. Denner and Students' Perceptions and Experiences of Simulation Tools in Engineering Learning Contexts

Dr. Denner reported his overall course goal as teaching the fundamentals of nano-electronic devices; and in particular, for the first homework assignment, targeted to identify explaining how current flows in very small devices. Similarly, Dr. Denner's students identified that the goal of the first homework assignment was a conceptual understanding on how current flows in very small devices. Dr. Denner's students also identified as a learning goal the introduction of MATLAB as a computational tool to represent this particular phenomenon. The survey data indicated students perceived this course and the assignments related to MATLAB as highly relevant to their areas of interest. They also reported that the assignments related to MATLAB supported their goals and expectations of the course. Students reported using MATLAB as a very positive experience (see Figure 7.3).

The evaluation mechanisms Dr. Denner applied were homework assignments and exams. He also incorporated formative assessment mechanisms, such as posting the solution to the homework assignments and office hours. Dr. Denner's students found these forms of providing feedback to students were very helpful for them and were a key element for completing their assignments successfully. Another element students found very useful for implementing their assignments in MATLAB were the scripts at the instructor provided at the end of the book and that also were uploaded into the nanoHUB.org. In general all students commented they learned something new by approaching the homework assignments together with the solutions. These assignments helped them to reinforce concepts learned in class and new ways and techniques to implement them in MATLAB. The survey data showed that the models students implemented in MATLAB helped them to comprehend the concepts better than by using lectures and readings only. The assignments related to MATLAB also helped students to increase their awareness of practical applications of these concepts and to approach new problems. However, survey data also showed that students still had difficulties in interpreting the outputs of the plots they generated in MATLAB. A possible explanation for this could be that students spent too much time in the implementation so they could not focus that much on the output. Another explanation could be that since this was an advanced undergraduate level class, students were still lacking some expertise.

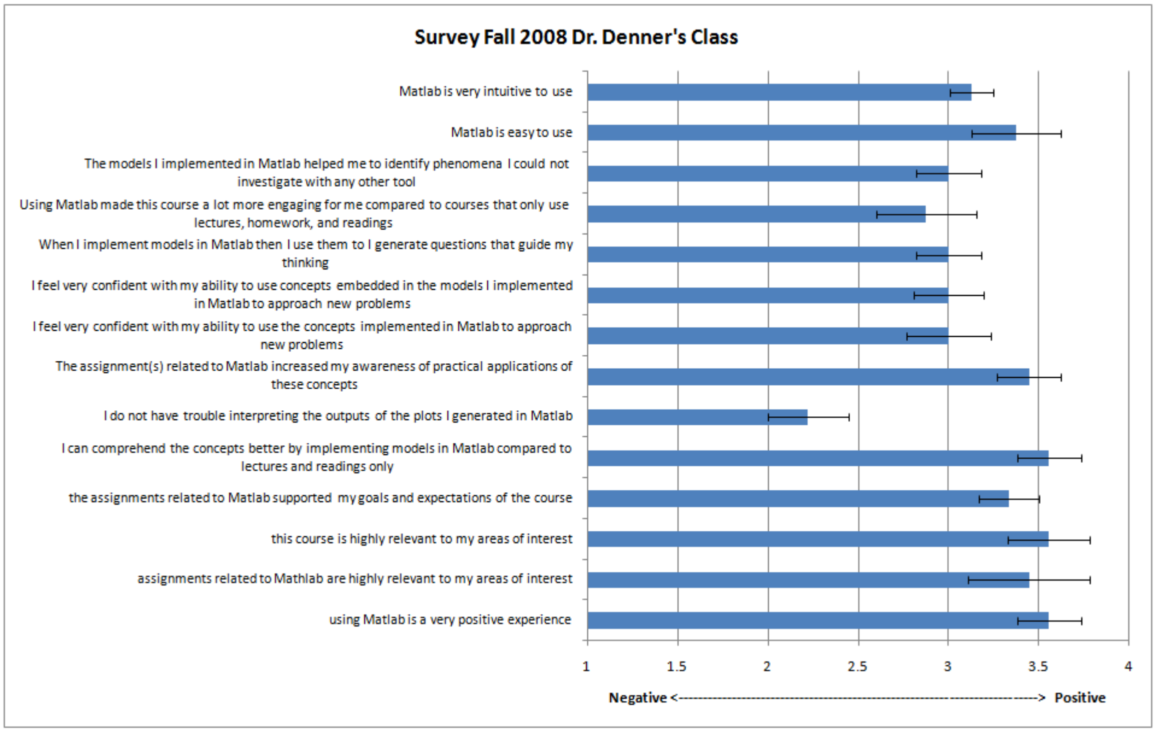


Figure 7.3 Dr. Denner's students responses to the survey

The pedagogical approach Dr. Denner incorporated during lecture focused on an atomistic approach on how current flows in small devices. Additionally, Dr. Denner emphasized what the relationship between the models and the real world is. In contrast, students interviewed pointed out that the concepts taught in class were easy for them to understand. Some students also identified this approach as different and unique and how Dr. Denner made the connection between the concepts and the real life.

In addition to lectures Dr. Denner also incorporated exams and homework assignments. Sometimes, as part of those assignments, Dr. Denner asked his students to use MATLAB to implement models. Students find this task sometimes challenging, but all of them reported having learned from the assignment. All interviewed students overcame those challenges both by asking the instructor or the TA, and also by reviewing the MATLAB scripts that appeared at the back of the book. From the survey data it was identified that students considered the simulation tools as engaging for their learning. These students also reported a positive perception on the homework assignments related to MATLAB in helping them guide their thinking. They also reported a positive experience from using the models they implemented in MATLAB as a means to identify phenomena they could not investigate with any other tool. Students also reported that MATLAB is very easy and intuitive to use.

Summary of Results

The results from the three phases of this study describe how instructors used expert simulation tools as an inquiry device toward achieving learning goals to conveying cause-effect relationships, predict performance of an engineered nanoscale device, and to implement models of nanoscale physical phenomenon. Their students reported having a positive experience learning with simulation tools as part of their homework assignments. Since Chapters V and VI provided a detailed analysis of professors and students' perceptions and experiences with instruction and learning using computational tools, I will focus the summary of this chapter on the possible differences between instructors and students' perceptions and experiences.

Before presenting the differences, In Figure 7.4 I present a summary of the survey designed for Study One showing results from Dr. Sanders', Dr. Hass', Dr. Richardson's and Dr. Denner's courses.

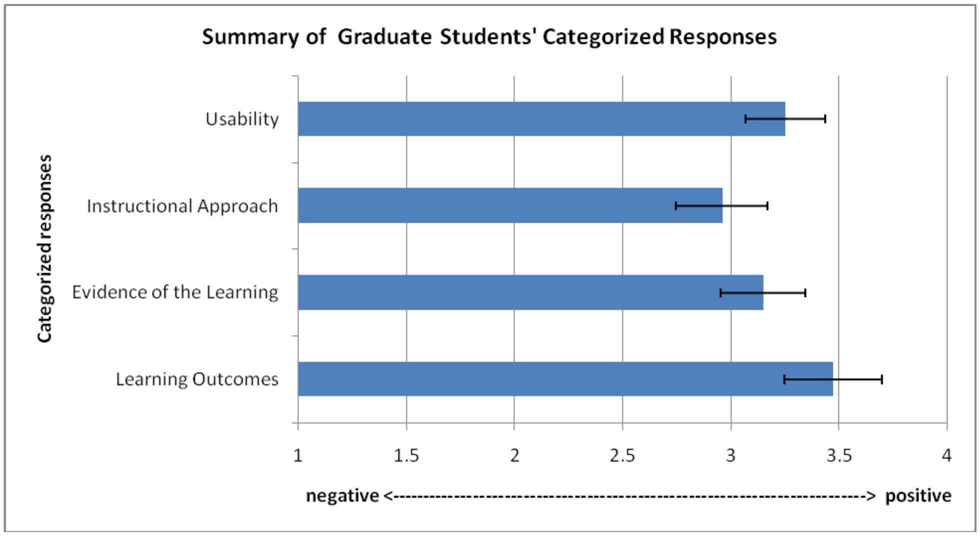


Figure 7.4 Summary of survey responses categorized into usability, instructional approach, evidence of the learning, and learning outcomes

The students' surveys showed mostly favorable results in how instructors incorporate computational simulation tools to learning experiences as confirmed by the low variance shown in the standard error bars. Therefore, I conclude these learning experiences involving computational simulation tools were perceived as positive experiences by the graduate students participating in these courses.

The positive outcome of effective pedagogical uses is encouraging, and to improve the instructional approach a more thorough analysis of meeting intended goals is critical. Therefore, I now explore the general trends where instructors and students differed in their perceptions for using computational simulation tools for instruction and learning. One of these trends relates to the level of transparency of the computational simulation. Many students mentioned they wanted more access to the simulations' underlying model. They wanted to know the physics behind the simulations such as models, what the assumptions are, what equations they are solving, and how and what the implementation algorithms governing the performance of the model. Through interviews with instructors I was able to identify three different levels of transparency that may be implicit in their pedagogical intent. From the interview data I infer instructors view models as having three levels, 1) how a physical phenomenon is represented as mathematical models (e.g. equations defining the physics theory), 2) how these mathematical models can be evaluated “by hand” to estimate the performance of a system, and 3) how these mathematical models can be turned into numerical solutions implemented through computational techniques. Professors provided the first level of transparency through lectures such as explaining what the physics models in terms of equations. Sometimes they also provided the second level following lectures with example problems to estimate the relationship between various factors. Instructors sometimes hid the complexity of third level from students when they want to focus students’ attention on comprehending the physics concepts. They asked students to run the simulation as a “black box” because they were not concerned with how to implement a computational model, only use the tool to perform an engineering activity like designing a nanoscale device. However, based on students’ responses they perceive they need all three levels of transparency. In contrast, instructors with whose learning outcome was to implement computational techniques must achieve all three levels of transparency. These students might have faced a higher level of complexity because of this increase in transparency and encounter difficulties due to their lack of programming skills. Therefore, instruction and/or supports (scaffolds) that appropriately balance both aspects is required as part of the learning experience. This balanced instruction may be attained through scaffolding techniques such as online lectures, manuals and programming scripts that serve as templates or blueprints.

CHAPTER VIII

DISCUSSION AND CONCLUSION

Roadmap of Studies Findings

This final chapter discusses the results of the three different studies conducted as part of this dissertation work (see Table 8.1 for an overview). Table 8.1 describes the roadmap of studies that were developed. These studies are alike because all of them focused on similar aspects of the world: professors' and students' perceptions of computational simulations as learning tools. They are also different in multiple ways. However all of these studies complement each other.

Study One differed from Study Two and Study Three in the research methodology. While Study One employed quantitative research methods, Study Two and Three employed qualitative research methods. Whereas, the quantitative portion was more objective focusing on counts and measures of aspects of the world, the qualitative portion was more subjective identifying descriptions and meanings of aspects of the world. Study Two and Study Three had the fundamental distinction in their perspectives. Marton (1981) differentiated between what he called the first-order perspective and the second-order perspective. While the first-order perspective aims at describing various aspects of the world; the second-order perspective aims at describing people's ideas and/or experiences of various aspects of reality. The emphasis of Study Two was on the second-order perspective while the emphasis on Study Three was on the first-order perspective. Marton (1981) argued that first-order and second-order perspectives are complementary in the sense that "we would deal with both the conceptual and the experiential, as well with what is thought of as that which is lived. Finally, the three Phases of Study Three focused on two different populations. Phase 1 focused on instructors' perceptions and experiences with simulation tools, Phase 2 focused on students' perceptions and experiences with simulation tools, and Phase 3 compared and contrasted both experiences. Specifics of the methods of inquiry employed are described below.

In Study One a survey method was employed to identify students' perceptions and experiences of computational simulations as learning tools. Through this initial study I was able to identify differences in the way students perceived nanoHUB simulation tools; differences such as graduate students reported more positive experiences with nanoHUB simulations than undergraduate students did. This study helped me select the population for studies Two and Three that involved instructors whose students report having a positive experience using computational simulations in their learning experiences. Study Two builds on Study One by identifying qualitatively different ways instructors define learning objectives (learning outcomes) related to the use of computational simulations as learning tools. In Study Two I utilized phenomenographic methods to identify the variance in the ways instructors incorporate these tools as part of their instruction. The outcome of Study Two is a set of categories of description and its internal structure represented in the outcome space. In practical terms, this outcome space represents a model of learning outcomes.

In Study Three I adopted a more holistic approach focusing on learning outcomes, plus I analyzed the data identifying evidence of the learning and pedagogical approaches. By utilizing cross-case analyses in three different phases I was able to identify instructors' perceptions and experiences of computational simulations as learning tools, students perceptions and experiences with computational simulations as learning tools, and a comparison of the perceptions and experiences of these two groups. The outcome of Study Three is an instructional framework for using computational simulations as learning tools. This framework and the model of learning outcomes are presented at the end of the discussion section.

Table 8.1: Overview of research studies

	Study One	**Study Two**	**Study Three**		
Method	Survey	Phenomenography	Case Study		
Chapter	I	IV	V	VI	VII
Participants	Graduate students (G) Undergraduate students (UG) Freshmen undergraduate students (FUS)	Instructors (I)	Instructors (I) Students (S)		
	G=189 UG=24 FUS=338	I = 6	I=6	S=25	I=4 S=25
Focus of Inquiry	What are engineering students' perceptions and experiences of computational simulations as learning tools?	What are qualitative different ways in which engineering instructors perceive and experience computational simulations as learning tools in terms of their learning outcomes?	What are engineering instructors' perceptions and experiences of computational simulations as learning tools in terms of their learning outcomes, evidence of the learning and pedagogical approaches?	What are engineering students' perceptions and experiences of computational simulations as learning tools?	How do engineering students' perceptions and experiences of computational simulations as learning tools compare to their instructors' perceptions and experiences of the same tools?

Discussion

This section discusses the results and analyses of the three major research questions related to instructors' learning outcomes, evidence of learning, and pedagogical approaches for using computational simulations in their courses. This chapter also discusses students' experiences using computational simulations in these courses and their perceptions of instructors' learning outcomes, evidence of the learning and pedagogical approaches for achieving these outcomes.

Learning Outcomes

The results of Study Two generated an outcome space consisting of six categories of description. These six qualitatively different ways in which engineering instructors incorporate simulation tools into their learning activities include the categories of description presented in Table 8.2 and the outcome space presented in Figure 8.1.

Table 8.2 Categories of Description

Learning goal	**The way of experiencing simulation tools encompasses…**
To understand the cause-effect relationship of the underlying model	…understanding and/or exploring the cause and effect relationships defining a particular computational simulation by running the simulation. It is also concerned with the comparison of analytical solutions with computational/numerical solutions.
To collect data as in a laboratory experiment	…conducting virtual collection of data (i.e. measurements) to characterize a phenomenon versus running physical devices in a laboratory.
To validate the results or performance of an experiment	…validating empirical results of a performed experiment (or design) with a target specification or performance. Can also lead to changes in the inputs of the experiment so improvements may be achieved.
To predict the results and/or performance of an experiment	…using the tools to predict behavior of a certain phenomena. Also includes design tasks.
To test the accuracy of the simulation's underlying model and its implementation	…verifying the accuracy and precision of the simulation model by comparing and contrasting empirical and/or theoretical experiments with computational experiments.
To use and implement computational techniques in a modeling task	…using and understanding approximations and numerical techniques to solve computational problems by building computational algorithms used in simulations.

The way instructors experienced simulation tools reveal new ways of incorporating these tools into learning contexts that are not yet documented in the literature. The observations for this research are consistent with results and recommendations found in the literature in the way experts conduct their research. Prior literature described the main instructional objective for incorporating simulation tools into learning contexts as a method to achieve students' understanding of an underlying model describing the behavior of a phenomenon (or system), through pedagogical approaches involving discovery, experimentation (systematic inquiry of comparing and contrasting results), demonstration, or other methods (Alessi, 2000).

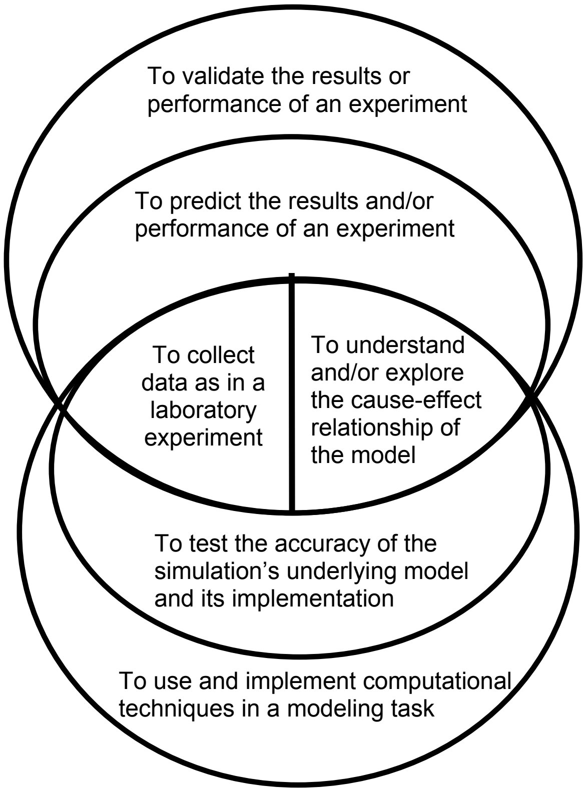


Figure 8.1 The outcome space: a model of learning outcomes

Alessi (2000) described two main ways of incorporating simulation tools into a learning experience: using versus building simulations. According to Alessi, these ways of experiencing simulations affect two types of knowledge; declarative knowledge and procedural knowledge. According to Smith and Ragan (2005), declarative knowledge requires a learner to recall and apply facts, lists, names, or organized information. Procedural knowledge involves the application of defined steps or procedures including algorithms, rules of thumb and/or heuristics. Alessi described the relationship between "building" versus "using" simulations and declarative versus procedural learning as "(1) when learning goals are primarily procedural (e.g. flying an airplane, doing a titration) the learners use simulations built by other people; (2) When learners are building simulations the goals are primarily declarative" (p.182). Alessi's (2000) view of knowledge and learning emphasized the importance of directionality. When the learning objectives are procedural, the learners generally *use* simulations but the converse is not the case. That is, when the learning objectives are procedural the learners use simulations, but when the learning objectives are to gain declarative knowledge, then learners may *use* or *build* simulations. Alessi also warned that although he discussed learning which is either procedural or declarative, he explained that what is more important and quite common situation is when the goals include both—i.e. the procedural and declarative knowledge. The case of the learning goals reported in this study is a combination of declarative and procedural knowledge.

Similarly, de Jong and van Joolingen (2007b), have combined these two approaches in their discussion of model-based inquiry learning. They believed the main objective of learning *from* models (using) and learning *by* modeling (constructing) is for students to build mental models that provide a rich description that explains the behavior of a physical phenomena. Mental models have been defined as a representation of entities, persons, events, processes, and the operations of complex systems (Johnson-Laird, 2005). Specifically, Johnson-Laird defined a mental model as a structural analog of a real-world or imaginary situation, event, or process constructed by the mind while reasoning. I believe this is an implicit goal in the instructors' descriptions of their learning objectives. This assumption emerges from the holistic view of the learning objectives organized in the model shown in Figure 8.1.

In this study, two general methods for incorporating simulation tools into higher education courses were identified; simulations used to predict system performance relative to a design task and simulations built as part of a modeling task to predict model performance relative to observed phenomena. These two general trends are analogous and can be aligned with using versus building simulation tools (Alessi, 2000) and learning *from* models and learning *by* modeling (de Jong & van Joolingen, 2007b). In addition, the evidence provided in this chapter points out other learning objectives that are closely related to what the American Association for the Advancement of Science [AAAS] (AAAS, 1989) described as inquiry learning. The AAAS described inquiry learning as a process involved in exploration and observation of natural and man-made systems, testing of theories to explain or validating design decisions, rework of problem solving task, build a device based on desired specifications, calibrate instruments, collecting experimental data, constructing mathematical models, etc.

On the other hand, the ways in which these instructors have experienced simulation tools reveals a strong similarity in the way scientific activities or processes have been described in literature. For example, according to Langley and his colleagues (1987), general activities that take place during the scientific process are: gathering data, finding descriptions of the data, formulating explanatory models, and testing them. The order in which these activities occur is usually cyclical and non-linear. When no laws exist, the discovery process is called data driven or induction. When the goal of the discovery process is to confirm or extend a theory or model, it is called theory driven or deduction. While most of the instructors followed a similar approach as theory driven, a few of them experienced a data driven approach. Meaning while most of the instructors incorporated simulation tools by first introducing the governing physics theory describing the behavior, a few instructors incorporated simulation tools as an experimentation tool to gather data and find descriptions of such data which illustrate the behavior of a system (device). Other activities similar to scientific processes incorporated by these instructors are: the exploration of models, prediction of results of experiments, testing the results of experiments, the implementation of models, and validation of such models.

Overall, the instructors in this study have incorporated computational simulations following approaches similar to scientific processes. These ways of experiencing simulation tools expand the ways in which simulation tools have been documented in literature. These ways include not only learning goals related to students' understanding the cause-effect relationship of the models, but also learning goals related to collecting and finding descriptions of the data, predicting the results or performance of an experiment, validating the results or performance of an experiment, testing the accuracy of the simulation's underlying model and its implementation, and implementing computational techniques in a modeling task. These ways of experiencing simulation tools may inform better ways of incorporating simulation tools in inquiry learning processes into learning environments.

Engineering instructors have incorporated simulation tools by creating meaningful learning experiences for their students. These experiences have been described as meaningful because they were well perceived by students as reported in Chapter VII and contributed to their current interests and academic goals. Some instructors focused more on conceptual understanding and engineering skills while others emphasized the computational techniques. In particular, these instructors have used expert and educational simulation tools for leveraging different types of learning goals to convey concepts and skills with enduring value beyond the classroom (Wiggins & McTighe, 1997). In general, students reported two main reasons for having taken the courses in this study: because it closely related to their research and because they considered this knowledge as important for them to know for future educational and professional activities.

One learning goal most instructors wanted to convey to their students was to develop an intuitive understanding of the phenomenon under study and, at the same time, become critical users of simulation tools. Being familiar with the literature of the area was also a common learning outcome. The general learning goal perceived by students was to have an insight of current technologies and practices. All students but one agreed they learned something new using and/or building with computational simulation tools. Some students mentioned learning a) how the physics models relate to the real world, b) how to conduct specific measurements, c) how not to blindly trust simulations, d) how to find a way to judge if the simulation tool is doing what it is supposed to do, and e) how to implement computational techniques. Therefore, students and instructors describe consistent expectations for the learning outcomes for the specific courses.

Evidence of the Learning

Most of the instructors incorporated the simulation tools as a part of homework assignments and projects. Once students completed the assignments and turned those in, then the instructor or teaching assistant (TA) proceeded to grade them for correctness, but with limited feedback on solution processes. The most common strategy used by instructors was to first correct individual assignments and then post a detailed solution on the course website. Later on, students had opportunities to have additional clarification through interactions with the TA, instructor and/or peers. This strategy or assessment mechanism is identified as one type of formative feedback. According to Black and Wiliam (2004), the purpose of formative assessment is to promote students' learning through reflection on actions they have taken through their own thought process. They argued that an assessment activity promotes learning if it provides information that can be used by students for assessing themselves and they can refine and re-apply their thinking in activities they are engaged in. Shute (2008) defined it as "information communicated to the learner that is intended to modify his or her thinking or behavior for the purpose of improving learning (p.154)." Another type of assessment mechanism is summative assessment. The purpose of summative assessment is to determine accountability, ranking or competence (Black & Wiliam, 2004). In this study many instructors incorporated summative assessments as mid-terms and final exams. I will focus my discussion on the formative assessment.

Instructors in this study incorporated formative feedback by providing two types of information to the students: verification and elaboration (Shute, 2008). Verification is defined as a simple indication of whether the answer is correct or incorrect. This type of information was provided in students' individual assignments. Elaboration guides the learner toward a correct answer. Elaboration feedback may have two functions: directive and facilitative (Black & Wiliam, 1998). Directive feedback specifically tells the student what needs to be addressed. Facilitative feedback, on the other hand, provides general comments and suggestions as guidance for students in their own revision. The type of feedback employed by the participant instructors was the facilitative type.

Shute (2008) described three cognitive mechanisms of formative feedback that can impact students' learning. One relates to reduction of uncertainty in students' performance, another relates to students' reduction of cognitive load, and the last one relates to the supply of information that may be useful for correcting inappropriate tasks, errors and/or misconceptions. Although not enough evidence was collected in this study to ascertain if students have benefited from the formative assessment through these three cognitive mechanisms, their perceptions of it were identified. In general, participating students perceived the feedback mechanisms as appropriate for advanced undergraduate and graduate courses. The feedback was described as not very detailed in their individual assignments, but for most of the students having the solution to the homework assignments posted was enough.

Pedagogical Approach

Instructors' main instructional approach began in class by introducing the required prior knowledge describing the physical principles governing the behavior of a device or system, and then students practiced applying these concepts during homework assignments using computational simulation tools based on the physical principles. The instructors who focused their courses on the computational and modeling techniques also followed what they called a "hands-on approach" in which students had an opportunity to interact and/or implement computational simulation tools in the computer lab under the guidance of the instructor. Another feature incorporated in their pedagogical approaches was the use of recorded lectures uploaded on the nanoHUB.org. Contrasting from students perceptions outlined in Study Three-Phase 3, students were asked how confident they felt with their prior knowledge. Two general responses were found, either they felt very confident with the prior knowledge to be able to approach the solution of the homework or they didn't have a very deep understanding of the physical phenomena. Not having the appropriate pre-requisite knowledge has been documented as one of the reasons why even supporting learners in processes of discovery learning does not lead to better learning outcomes (Bodemer, Ploetzner, Bruchmuller, & Hacker, 2005). However, researchers have emphasized that successful inquiry learning needs adequate but not intrusive scaffolding (de Jong & van Joolingen, 2007a; Mayer, 2004; Njoo & de Jong, 1993; Reid, J, & Chen, 2003; van Joolingen, de Jong, & Dimitrakopoulout, 2007; Winn, 2002). Brush and Saye (2002) made a distinction between two types of scaffolds to support (individual) student learning. Soft scaffolds are feedback, questions or information provided by the instructor, and perhaps peers, while hard scaffolds are embedded (or hard-wired) into the computer learning environment. According to Tabak (2004) the best approach for implementation is by targeting a synergy between both. In this particular case, students received soft and hard scaffolds during their processes of solving the assignment. Students identified two general types of scaffolds that were very useful at the moment they approached the solution to the homework assignments. One hard scaffold was the online lectures instructors posted on the nanoHUB.org. These lectures functioned as an embedded expert guidance (Quintana et al., 2004) that helped students in activating their prior knowledge. The second hard scaffold was the use of programming scripts that served as templates and/or blueprints that students identified as helpful in implementing their own scripts.

From instructors' perspective, nanoHUB.org computational simulation tools are convenient for instructors as an instructional device and for their students as a learning tool. They are convenient for instructors because they do not have to install any software or manage students' accounts; convenient for students because they have benefits of using simulation tools. Instructors perceive computational simulation tools as convenient because students are able to solve hard analytical calculations easily through simulations. Furthermore, students can overcome the limitations of analytical solutions. As a result, students can focus on the values depicted on the curves rather than doing extensive calculations. Also, simulation tools provide additional capabilities they cannot replicate in a laboratory. Instructors also mentioned they believe simulations are useful for their students learning because the simulations are flexible. Flexible meaning they can run different models and different simulations with different parameters and will get different outputs. Additionally, instructors can incorporate real and complex examples.

From a students' perspective, they benefited from using simulation tools because they found them convenient and helpful at the same time. They found it convenient because simulation tools solved difficult and complex calculations for them and because the simulations helped them simplify the complex models. The output of the simulation helped them to realize how each parameter affects the output giving them some sense of the physical phenomena. Finally, the simulation tools gave students a hands-on experience that at the same time allowed them to experiment.

Students also experienced some limitations for their learning. Students wanted more transparency of the simulation tools. They wanted to be able to know which equations are being solved, to see the calculations as well as the underlying assumptions of the model. Some others wanted to have access to the code. However, a type of paradox was identified. While the students who only ran the simulation tools wanted to program their own simulation tools; the students exposed to a modeling task commented on their difficulties implementing the computational part of the assignments. Therefore, a balance is needed between the complexity of the task and supports provided to students. Part of this need has already been fulfilled for the students by incorporating hard and soft scaffolds mentioned earlier. However other aspects such as fidelity and transparency of the underlying models of the physics need to be addressed too. According to Alessi (2002), fidelity refers to the level of realism, also described by Cannon-Bowers and Bowers (2007) as authenticity. Alessi (2002), argued that in some cases fidelity must be simplified. Alessi (2002), as well as Reigeluth and Schwartz (1989), discussed the relationship between the level of fidelity and learners' expertise. They argued that when learners are novice, lower fidelity may be better. This strategy may result in diminishing students' cognitive load. The other aspect to be considered is transparency. The two most common approaches for simulation transparency are the black box and the glass box simulations (Resnick, Berg, & Eisenberg, 2000). The glass box simulations differ from the black box simulations by providing learners with visibility (Du Boulay, O'Shea, & Monk, 1999); i.e., the ability to inspect and modify the equations that constitute the simulation's model (Murray, Winship, Bellin, & Cornell, 2001). Murray and his colleagues argued that purposefully using a black box approach to learning with simulation might cause students to inspect the form and function of the equations or rules that drive the simulations which ultimately leads to their learning of both, the physical phenomena being modeled and an example of how to model a physical system. As an example, Alessi (2002) provided us the following scenario: The black box approach might be used if the learning goal is concrete or situational and deals with particular observable variables of situations, or when the main purpose of inquiry is to identify a relationship between variables. For the case of the glass box approach, students can benefit more if the objective and learning activity is more explanatory. In this case, students have to hypothesize about the underlying principles or mechanisms, and the same is the case when the learning goal is to criticize an existing model. In addition, authenticity as well as transparency has been related to students' levels of engagement (Cannon-Bowers & Bowers, 2007; Resnick et al., 2000) in which the learning environment causes learners to engage in cognitive processes in similar ways as experts.

On the other hand, a different pedagogical strategy Dr. Clase incorporated was limiting the number of input parameters of the simulation tools. Clariana and Strobel (2007) argued that by increasing the amount and complexity of the simulation output will result in increasing learners' cognitive load. According to Woods (1991) design for availability and accessibility of data are the elemental factors of data display in the area of human interface design. He suggested interfaces designed only for data availability does not address the problem of data overload. He further explained that interfaces designed for availability of data do not provide cues for the users to help them decide what the right data is at the right time. Dr. Clase diminished his students' cognitive load by limiting the input parameters so students can focus on specific aspects of the phenomena under study.

Performance, Access, and Usability of nanoHUB.org Resources

Instructors mentioned the technical advantages of using online simulations as easy to access to research grade computational power at no cost for students. Also, the user interface is easy to interpret and manipulate and students have a lot of computational power under the hood.

Technical limitations identified by few instructors included the limited number of outputs of the simulation, outdated documentation, and performance issues. Similarly, students made suggestions of other features they wanted to have as part of the simulation tools. They wanted more options of graphical representations of output parameters as well as more models of the physical phenomena and more presentations and help files (i.e. hard scaffolds) focused on the conceptual (physical) aspect of the simulation tools.

Like the instructors, students highlighted similar usability aspects of nanoHUB.org as very user friendly and intuitive. However, some students experienced problems with the interface as well as with system performance.

The results of this study indicate the potential of integrating the computational simulation tools into formal learning experiences in terms of learning outcomes, evidence of the learning and pedagogical approaches. Instructors have leveraged its potential using computational simulation tools in providing students with authentic learning experiences in which knowledge was successfully applied to practical applications. In particular, instructors have used expert simulation tools as an inquiry device toward goals ranging from conveying cause-effect relationships and conducting prediction as well as modeling tasks. These experiences, as well as the computational simulation tools in turn, seemed to be well perceived and experienced by the graduate and advanced undergraduate students.

A Model for Using Computational Simulations as Learning Tools

The culmination of these three studies provides new insights into the definition of engineering related learning outcomes and the associated pedagogical approaches for achieving these goals. In this section I summarize a new framework for designing instruction using computational simulations.

Computational simulations can be convenient and flexible learning tools for engineering instructors and students because they quickly perform complex computations while students can a) focus on interpreting outputs of the simulations to answer important scientific/engineering questions, b) explore multiple real and complex models with different initial conditions producing different output conditions. Students' interactions with computational simulations could lead to developing an intuition of the governing physics describing the behavior of a phenomenon and how each input parameter affects (or relates to) the output parameters. Ultimately, this leads to gaining capabilities they cannot achieve in a conventional laboratory. One reason these gains occur from their access to control all the parameters, and access to the expressive visualizations illustrating relationships between multiple parameters. Achieving these learning benefits requires an appropriate balance of teaching and learning aspects of an effective learning environment. A framework or model identifying and illustrating these important aspects for using computational simulations as tools for learning is proposed as a way to illustrate relationships between important engineering learning objectives.

Teaching with Computational Simulations

At a course level, engineering instructors have four overarching goals for incorporating computational simulations into their courses. First, engineering instructors want their students to develop an intuitive/qualitative understanding of the physics governing the behavior of a phenomenon under study. Second, engineering instructors want their students to become intelligent users of the tools demonstrated by their ability to conduct inquiry activities with the tool and critically evaluate the validity of the results. Third, engineering instructors want their students to be familiar with modeling and computational techniques as well as related science and engineering concepts and ideas. Finally, engineering instructors want their students to eventually transfer these knowledge and skills to engage in engineering design and other problem solving activities.

Engineering instructors either have students run or build computational simulation tools as an instructional activity. Running simulations can support students understanding of cause-effect relationship of factors underlying the model, collecting data as in a laboratory experiment, validating the results or performance of experiment, predicting the results and/or performance from an experiment, and testing the accuracy of a simulation’s underlying model and its implementation, and modeling phenomena utilizing computational techniques. Building simulations as an instructional method can support testing the accuracy of the simulation’s underlying model and modeling phenomena by applying computational techniques.

Engineering instructors use homework assignments and/or projects as evidence of students’ learning. Through these instruments engineering instructors can monitor students’ learning progression toward the course objectives and provide feedback to support their progress toward these goals. One instructionally efficient method of formative assessment is to provide an assigned individual grade indicating current performance relative to the instructors expectation accompanied by a generic detailed solution of the assignment or project. This method requires students to compare and contrast their solution to one standard solution process and result. For graduate engineering students this form of formative assessment is convenient and productive toward meeting their learning objectives.

Engineering instructors' most common pedagogical approach begins with direct instruction of theory and models defining the behavior of a physical phenomena, and demonstration of their problem solving process (or analysis process of exemplar problems), followed by a guided inquiry into well-defined and ill-defined problems. The classroom activities are typically followed by homework assignments requiring students to solve an engineering problem by means of running experiments to collect and analyze data, design devices and/or build models. For example, engineering instructors develop students' inquiry skills by running simulation tools to generate data and identify relationships between factors governing the performance of a system. Alternatively, instructors can make the model transparent to the students and ask them to test and explain the limits of a model's performance. Success of this approach requires graduate engineering students having the necessary prior knowledge to self-guide their approach to solving the homework assignments and projects, and the ability to critically evaluate their approach when given an alternative solution.

Learning with Computational Simulations

Engineering graduate students need scaffolds and transparency of the simulation tool so they can benefit in their learning with simulations. Three different levels of transparency were identified. One level relates to how the phenomenon is represented through physical models. The second level relates to how those physical models are solved mathematically. The third level relates to how those mathematical models can be turned into numerical solutions implemented through computational techniques.

Engineering graduate students would learn more if they are able to “see” behind the simulation tools at these three different levels of transparency. That is, to be able to “see” the underlying model, the assumptions, the equations solved, and the algorithms.

Engineering graduate students would learn more if appropriate scaffolds that implement a guided inquiry approach are leveraged. One scaffolding method is to run simulations coupled with online lectures about the theory and/or tutorials explaining how to use the tools and well written examples illustrating how it is used in practice. These self-paced lessons focus on the conceptual aspect of the theories and models and the operational aspect of the computational tool. Scaffolds for assignments involving building simulations are templates containing some initial code or a given code that students need to modify. As mentioned before, these starting points give students a stimulus to react to and requires them to critically evaluate what the initial code can do, interpret the goals of what it is required to do and design a solution that achieve these goals. Several methods can be used to facilitate this process lead by the student including online lectures or tutorials focused on the conceptual and operational aspect of the simulation tool. For graduate engineering students scaffolds such as online lectures and programming scripts serve as a very useful just-in-time support as they approach the solution to the homework assignments.

Implications

The results of this study have implications for engineering and science education, simulation-based learning environments development, and instructional design. In the following sections I describe how professionals (e.g. educators, instructional designers, learning environments developers) in these areas can benefit from this study.

Engineering and Science Education

Implications in engineering and science education are focused on the way instructors identify evidence of the learning and incorporate pedagogical approaches to attain specific learning goals. In particular, this study organizes a variety of learning goals into a model that helps to suggest instructional strategies on how simulation tools can be incorporated to attain such goals. It also provides guidelines on how soft and hard scaffolds can be incorporated effectively and discusses strategies of formative assessment.

Engineering and science instructors may not have awareness on how specific learning goals can be accomplished by certain instructional strategies that incorporate computational simulations as learning tools. By providing instructors with specific learning goals accompanied by effective instructional strategies and formative assessments mechanisms, the design of homework assignments for the use of computational simulations can be more effective. This study provides effective guidelines to incorporate computational simulations as learning tools. These guidelines have been identified as effective as perceived by the students who were exposed to them. However, some limitations were also identified. By identifying students' perceptions of the use of computational simulations as learning tools instructors may realize what are common student difficulties and potential ways to overcome them as they engage in specific activities. For example, when students are engaged in a modeling task that requires the implementation of the model by programming a script, scaffolds such as templates may be incorporated. Understanding of students' difficulties when engaged in learning tasks using computational simulations may help instructors develop appropriate scaffolds to overcome such difficulties.

This study also suggests to instructors new ways of incorporating computational simulations that are more expert-like. For example, an instructor can go beyond the learning goal of identifying cause and effect relationships of a model to a design task and even to the implementation of that model. A similar approach is identified by de Jong and van Joolingen (2007b) as model-based inquiry learning. In this approach de Jong and van Joolingen suggested to first have students explore the cause and effect relationship of a model and then attempt to reconstruct that model so both models will behave similarly. However, as discussed in this study, students sometimes find challenging the implementation of models and scaffolds may be required. In this respect, de Jong and van Joolingen (2007b) alleged that learning from models can only be successful if the student is sufficiently supported at their current development level and considering prior knowledge. This final assertion leads me to the second implication; the development of simulation-based learning environments.

Simulation-Based Learning Environment Development

Implications in simulation-based learning environments development are grounded on students' experiences with the simulation tools. These implications focus on two main aspects, one of them relates to the incorporation of hard scaffolds and the other one to the level of transparency of the simulation tools.

Through this study it has been identified that students perceive scaffolds as helpful in their learning. The identified scaffolds, the ones instructors implemented as well as the ones students pointed out to be useful to have, may be classified in three main areas: a) interface interaction aspects such as how to run simulation tools, how to change the scale etc., b) implementation aspects such as model's assumptions, boundary conditions etc., and c) conceptual aspects such as models, theories, etc. The result of this study suggests possible ways to incorporate scaffolds to support these three aspects. For example, by including online lectures instructors can support the conceptual aspect and developers can support the interface interaction aspect. A second example is by means of documentation such as manuals. By incorporating manuals together with the simulation tools developers can provide scaffolds for interaction aspects (i.e. how to use the tools) as well as implementation aspects (i.e. how those tools are built). Implementation aspects have been identified in this study as one of the least scaffolded. By providing documentation and perhaps an online presentation the level of transparency of the simulation tools can be increased.

Instructional Design

Implications in instructional design derive from the above discussed implications. Instructional designers may serve as the translators between the engineering and science instructors and the simulation-based learning environment developers. Furthermore, implications in instructional design are focused on the orchestration of learning outcomes, evidence of the learning, and instructional approaches. There is a need for an instructional theory for the design and incorporation of computational simulations as learning tools. Reigeluth and Schwartz (1989) developed a general instructional theory for the design of computer-based simulations. They provided a general theory for procedural simulations, process simulations, and causal simulations. According to their descriptions, the closest one to computational simulations is causal simulations. However, as suggested by the name, they just focused on the identification of cause and effect relationships of models. This study has identified five other different learning goals that can be accomplished with computational simulations. Therefore, through these different learning goals, this study provides guidelines toward the development of an instructional theory for the design and incorporation of computational simulations as learning tools.

A second implication relates to the design of frameworks for technology-enhanced support for inquiry learning. Researchers have identified general frameworks for support inquiry learning that may be adapted to support simulation-based learning environments. For example, Quintana et al. (2004) presented a set of guidelines that can be implemented either with soft or hard scaffolds. These scaffolding guidelines include: a) the use of representation and language that bridge learners prior conceptions, b) organization of tools and artifacts around the semantics of the discipline, c) use of multiple representations that make explicit properties of underlying data, d) provide structure for complex task and functionality, e) embed expert guidance about scientific practices, f) automatically handle non-salient routine tasks, and g) facilitate ongoing articulation and reflection during the investigation. Similarly Kali and Linn (2007) suggested a set of design principles: a) make science accessible, b) make thinking visible, c) help students learn from others, and d) promote autonomy and lifelong learning.

In this study I have focused my analyses on experiences related to graduate students. These graduate students perceived the pedagogical approaches instructors implemented as adequate for their learning. However, the guidelines presented by Quintana et al. as well as the ones described by Kali and Linn may be more appropriate when incorporating computational simulations as learning tools at an undergraduate level. nanoHUB.org provides the technical infrastructure to incorporate most of these guidelines and/or strategies but lacks the instructional overlay that can be implemented following the above mentioned guidelines. For example, it provides collaboration tools where students and instructors can share sessions and be able to interact with the same simulation tool at the same time. It also provides collaborative spaces such as wikis that can be used by instructors in their courses. nanoHUB.org also provides instructors with capabilities to upload their presentations and simulation developers with capabilities to upload documentation together with the created simulation tools.

Limitations

This study had several limitations that might have affected the analyses, results, and consequently the outcomes of the study. First, the sample size of the phenomenographic study is smaller than the size recommended by literature. According to Trigwell (2000), the sample size of a phenomenographic study is in the range of fifteen to twenty participants. A second limitation of the study is that most of the instructors were using nanoHUB.org simulation tools that are characterized by their particular user interface. A third limitation of this study might be the potential assumption that the results of this study may apply to undergraduate students. Although I don't have enough evidence than my personal perceptions, these students are highly motivated as well as very familiar with conducting research in their own areas of expertise and might have highly developed metacognitive skills. Based on these limitations future work is suggested in these areas.

Future Work

This study lays a foundation for future research about how computational simulations are used by engineering instructors and students. Several directions for future work suggested by the present study are:

- How instructors incorporate computational simulations as learning tools as part of their lectures? What are the most appropriate ways to incorporate computational simulation tools in a lecture setting?

- How instructors incorporate computational simulation tools at the undergraduate level? How these ways are different from the ones incorporated by instructors at a graduate level? If a gap exists, what can be done to close it?
- What are the qualitatively different ways in which instructors from different engineering disciplines approach the use of computational simulations as learning tools?
- What are students' inquiry learning processes as related to the different categories of descriptions identified in the outcome space?
- What are students' challenges when reasoning with computational simulations? What problem-solving strategies do they use to overcome them?
- How do differences in students' prior knowledge affect their perceptions of computational simulations as learning tools? How do differences in students' prior knowledge affect their inquiry and problem-solving strategies?
- How students' graphing skills affect or influence their understanding and reasoning with computational simulations as learning tools?
- How students' motivations affect their inquiry and problem-solving strategies?
- What appropriate and effective instructional methods may overcome the paradox of transparency and access vs. modeling complexity discussed in Chapter VI?
- Can general guidelines or an instructional design theory of the use of computational simulations as learning tools be helpful for instructors to develop effective learning materials?

Computational simulations in learning contexts are means to an end. That is, simulations are teaching tools used by instructors to promote understanding of procedural and declarative knowledge in their students. Instructors strive to have students develop abilities to regulate their own learning. That is, to only need minimal, unstructured resources for learning. Students, on the other hand, have perceived them as useful for their learning. As such, the development of learning activities by instructors and the use of those activities together with the computational simulation tools by instructors and students should be informed and improved through continued research.

Conclusion

Computational simulations have been used in educational contexts for inquiry learning by allowing learners to develop their understanding of phenomena. However little or no studies have been conducted in naturalistic learning environments and consequently have not taken into account the interaction between different variables that usually affect complex learning environments.

Several outcomes were achieved by this dissertation work. The first outcome is a set of categories of description and the outcome space focused on learning outcomes instructors experience when incorporating computational simulations into their instruction. A second outcome is a general model of using computational simulations as learning tools from the teaching and learning perspectives. These outcomes indicate the potential of integrating the computational simulation tools into formal learning experiences in terms of learning outcomes, evidence of the learning and pedagogical approaches.

Instructors have leveraged the potential of using computational simulation tools in providing students with authentic learning experiences as perceived from their students, in which knowledge was successfully applied to practical applications. In particular, instructors have used expert simulation tools as an inquiry device toward goals ranging from conveying cause-effect relationships and conducting predictions as well as modeling tasks. Graduate students in general show positive perceptions toward how instructors incorporate computational simulation tools into learning experiences.

This study contributes to the body of literature of scientific inquiry learning and the use of computational simulation tools for learning. This study also identifies how instructors in different settings think about the pedagogical affordances of inquiry learning environments such as the nanoHUB.org (van Joolingen et al., 2007); a research need identified by Hennessy and her colleagues (2007). This study also contributes to the identification of effective ways to provide instructors with suitable supports to facilitate appropriate scaffolds to learners in the form of soft and hard scaffolds (Brush & Saye, 2002).

Future research focus will be towards the development of an instructional design theory for using computational simulations as learning tools by identifying students' learning by the construction of mental models with such tools, with a particular emphasis on how undergraduate students learn and the scaffolds they need to use computational simulations as part of instruction.

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APPENDICES

Appendix A. Consent Form Instructor

For IRB Office
Use Only

RESEARCH PARTICIPANT CONSENT FORM
nanoHUB simulations as learning tools
Instructor participation form
Sean Brophy
Purdue University
Department of Engineering Education

Purpose of Research

The purpose of this study is to determine the effectiveness of resources at the nanoHUB website (nanohub.org) as learning tools and to identify opportunities for redesigning the website to increase its potential as a learning environment. In particular, our intent is to describe how experts use the nanoHUB tools for research activities and document their expectations of the nanoHUB resources as part of their course instruction. Results from this research will inform our design of the nanoHUB to increase its potential for supporting both scientific research and instruction.

Specific Procedures to be Used

Your participation will consist of a recorded interview focused on how and why you use the nanoHUB simulation tools in your course and what are the benefits for your students. The interview will also focus on identifying your perspectives on how the tools could be used for solving practical problems. We will also request that you demonstrate how to complete course assignment(s) using the simulation tool on nanoHUB.org website. At the same time, we will request your participation in a recorded talk/think aloud procedure describing the steps to be followed and your rationale for making those decisions.

For the case of some professors at Purdue University, we may also request for you to allow us to conduct classroom observations that will be audio and/or video recorded.

Duration of Participation

The time in which you will be actively engaged in this research process will consist on 30 minute interview and 30 minutes exploring how to solve the assignment with the tool.

If you are one of the professors at Purdue University to whom we have requested to allow us to conduct classroom observations that will be audio and/or video recorded; the duration of the observations will be during the entire semester of Fall 2008.

Risks to the Individual

Your participation in this study will not involve any potential risks to you over and above those risks that would be encountered in everyday life.

Benefits to the Individual

There are no direct benefits to you for participating in this study. However, the indirect benefits of participating in the study may include the opportunity to receive a formative evaluation from the learning activities that accompany the nanoHUB simulation tools. In addition, the perspectives you will provide invaluable feedback to the developers of the nanoHUB who can improve the system to better support your instructional goals and other instructors who use the system.

<u>Extra Costs to Participate</u>
There are no costs for you to participate in this study beyond your time.

Confidentiality

Your confidentiality will be maintained and your identity will not be disclosed to anyone. All steps will be taken to maintain your confidentiality by labeling all data with a pseudonym involving your data. All documents such as transcriptions from recorded interviews, recorded classroom observations (if applied), and electronic files including videos, will be kept by Dr. Sean Brophy in a secure and locked location at Purdue University West Lafayette campus. The documents and electronic files will be kept indefinitely. The only persons who will have access to this data will be Dr. Sean Brophy and Alejandra Magana.
In addition, the project's research records may be inspected by the Purdue University Institutional Review Board or its designees and by the Network for Computational Nanotechnology to ensure that your rights are being protected.

Voluntary Nature of Participation

Your participation in this research project is completely voluntary. Your participation has no bearing on you involvement in the NCN or future use of nanoHUB resources. If you agree to participate you can withdraw at any time without penalty. In order to withdraw your data, you just have to contact Sean Brophy at sbrophy@purdue.edu and request your file to be destroyed.

☐ I am willing to provide a copy of the assignment that accompanies the simulation tool and
Initials participate in the interview and think aloud protocol.

☐ I am willing to share the results of the anonymous survey with the researchers for publication
Initials purposes.

☐ I am willing to allow the researchers to conduct recorded classroom observations. (applied
Initials to professors at Purdue University only).

<u>Contact Information</u>:
If you have any questions about this research project, you can contact Sean Brophy by email at sbrophy@purdue.edu or by phone at (765)496-3316 or Alejandra Magana at admagana@purdue.edu. If you have concerns about the treatment of research participants, you can contact the Institutional Review Board (IRB) at Purdue University, 610 Purdue Mall, Hovde Hall Room 300, West Lafayette, IN 47907-2040. The IRB's phone number is (765) 494-5942. The email address is irb@purdue.edu.

I HAVE HAD THE OPPORTUNITY TO READ THIS CONSENT FORM, ASK QUESTIONS ABOUT THE RESEARCH PROJECT AND AM PREPARED TO PARTICIPATE IN THIS PROJECT.

____________________________________ ____________________
Participant's Signature Date

____
Participant's Name

____________________________________ ____________________
Researcher's Signature Date

Appendix B. Consent Form Student

For IRB Office
Use Only

RESEARCH PARTICIPANT CONSENT FORM
nanoHUB simulations as learning tools
Student participation form
Sean Brophy
Purdue University
Department of Engineering Education

Purpose of Research

The purpose of this study is to identify the potential of resources at the nanoHUB website as learning tools. In particular, we are trying to analyze how students and experts use the nanoHUB tools to guide their gathering of information to answer questions proposed by others and themselves.

Specific Procedures to be Used

Your participation will consist of a recorded interview focusing on your experience using the nanoHUB simulation tools. The interview will also focus on identifying your perspectives on how the tools could be used for solving practical problems. We will also request that you participate in a recorded talk/think aloud procedure as you solve a class assignment that uses the nanoHUB resources. As part of this think aloud interview we will be interested in your rationale for making various decisions.

Duration of Participation

Your participation in this study will take less than 20 minutes for the interview and less than 40 minutes working with the simulation tool. After this time you will be free to complete the assignment at your own pace.

Risks to the Individual

Your participation in this study will not involve any potential risks to you over and above those risks that would be encountered in everyday life.

Benefits to the Individual

There are no direct benefits to you for participating in this study. However, this study may allow you to offer your opinion and perspective for using nanoHUB as a learning resource in a confidential way. These perspectives are invaluable, since they point to existing strengths, weaknesses (as well as perceptions of both), and provide us with guidelines for how to best implement such learning resources in the future.

Compensation
To compensate you for your time and effort to participate in this study you will receive one gift certificate from amazon.com worth $25.00 dollars. The procedure for payment will consist of requesting from you your email address. Once we have purchased the gift certificate for you, it will be sent to your email account. You will be able to redeem it at the Amazon.com website.

Extra Costs to Participate
There are no costs for you for participating in this study other than the additional time you might take to meet with the interviewers before complete a course assignment

Confidentiality

Your confidentiality will be maintained and your identity will not be disclosed. All steps will be taken to maintain your confidentiality by using a pseudonym to identify your data. Your instructor will not be notified about who is participating in this study. At the end of the semester, when all the grades have been calculated and officially posted, the instructor will be made aware of a summary of the results that contain no identification of the participants. All documents such as transcriptions from recorded interviews, and electronic files including videos, will be kept by Dr. Sean Brophy in a secure and locked location at Purdue University West Lafayette campus. The documents and electronic files will be kept indefinitely. The only persons who will have access to this data will be Dr. Sean Brophy and Alejandra Magana.
In addition, the project's research records may be inspected by the Purdue University Institutional Review Board or its designees and by the Network for Computational Nanotechnology to ensure that your rights are being protected.

Voluntary Nature of Participation

You do not have to participate in this research project. Your participation, or non participation, has no bearing on your grade. If you agree to participate you can withdraw your participation at any time without penalty. In order to withdraw your data, you just have to contact Sean Brophy at sbrophy@purdue.edu and request your file to be destroyed.

Contact Information:
If you have any questions about this research project, you can contact Sean Brophy by email at sbrophy@purdue.edu or by phone at (765)496-3316 or Alejandra Magana at admagana@purdue.edu. If you have concerns about the treatment of research participants, you can contact the Institutional Review Board (IRB) at Purdue University, 610 Purdue Mall, Hovde Hall Room 300, West Lafayette, IN 47907-2040. The IRB’s phone number is (765) 494-5942. The email address is irb@purdue.edu.

I HAVE HAD THE OPPORTUNITY TO READ THIS CONSENT FORM, ASK QUESTIONS ABOUT THE RESEARCH PROJECT AND AM PREPARED TO PARTICIPATE IN THIS PROJECT.

______________________________________ ____________________
Participant’s Signature Date

____
Participant’s Name

______________________________________ ____________________
Researcher’s Signature Date

VITA

VITA

ALEJANDRA MAGANA DE LEON

Personal Information	
Name: e-mail: www:	Alejandra Magana admagana@purdue.edu http://web.ics.purdue.edu/~admagana/
Education Background	
Graduate:	Purdue University Engineering Education Ph.D. 2007-August 2009 GPA: 3.91
	Purdue University Educational Technology Master's degree 2006 – 2007 GPA: 4.00
	Instituto Tecnológico y de Estudios Superiores de Monterrey Electronic Commerce Master's degree 2000-November 2002 Average: 93.8/100
Undergraduate:	Instituto Tecnológico y de Estudios Superiores de Monterrey B.S. Information Systems Engineering 1995-2000 Average: 89.8/100 **Honorary mention for the highest average**
Academic Appointments	
Post-doctoral Researcher	Network for Computational Nanotechnology at Purdue University Joint appointment with the School of Engineering Education 2009-Present Under the supervision of Sean P. Brophy and Ruth A. Streveler.

Research Assistant:	Network for Computational Nanotechnology at Purdue University 2007-2009 Under the supervision of Sean P. Brophy and George M. Bodner.
Instructional Designer:	Network for Computational Nanotechnology at Purdue University for the outreach program generation-nano.org 2007-2008
Apprentice Faculty:	Purdue University Spring 2009 ENE 69500 005 Pedagogy Content and Assessment ENE 69500 006 Cognitive Devices in STEM Education
Faculty:	Instituto Tecnologico y de Estudios Superiores de Monterrey-CCM 2002-2005 Spring 2005 CB00812-Introduction to Internet Applications Development group 1 (enrollment: 27 students) CB00858-Application Development with Multimedia group 1 (enrollment 23 students) CB00899-Community Project group 1 (enrollment 10 students) Fall 2004 CB00812-Introduction to Internet Applications Development group 1 (enrollment: 23 students) group 2 (enrollment: 26 students) Spring 2004 CB00812-Introduction to Internet Applications Development group 1 (enrollment: 33 students) Spring 2003 CB00812-Introduction to Internet Applications Development group 1 (enrollment: 29 students) group 2 (enrollment: 28 students)

	Fall 2002 CB00801-Introduction to Computing group 1 (enrollment: 26 students) group 2 (enrollment: 27 students) Additionally I taught The module of Internet Programming three times as part of training courses for industry professionals.
Industrial Experience	
Internet Consultant:	SINERGIA SRL de CV 2000-2004
Analyst, Designer, and Programmer:	Corporativo PRAXIS 1998-2000
Other courses and certifications:	
Computer Science-Educator Workshop	Purdue University Computer Science K-12 Outreach Program October 2006 Computer Science Unplugged One-day Educator Workshop
iCarnegie certification	Curriculum powered by Carnegie Mellon in partnership with Instituto Tecnologico y de Estudios Superiores de Monterrey August 2003 SSD2 - Introduction to Computer Systems
BC401 ABAP Objects:	SAP México August 2003
BC400 ABAP Principles:	SAP México August 2003
SAPTEC:	SAP México November 2002
Publications/presentations	
Referred Conferences:	Magana, A.J., Brophy, S. and Bodner G. (2009) Are Simulation Tools Developed and Used by Experts Appropriate Experimentation Tools for Educational Contexts? *Proceedings of the 116th Annual ASEE Conference and Exposition. June 14-17. Austin TX.*

	Magana, A.J., Brophy, S. and Newby T. (2009) Pre-service teachers perceptions of web-based instructional media: Three different tools one learning goal. *Proceedings of the 20th Annual SITE International Conference. March 2 - 6, 2009. Charleston, South Carolina.* **Outstanding Paper Award Winner**
	Magana, A.J., Brophy, S. and Bodner, G.M. (2008). Professors' instructional approaches and students' perceptions of nanoHUB simulations as learning tools. *Proceedings of the 115th Annual ASEE Conference and Exposition. June 22-25. Pittsburgh, PA*
	Magana, A.J., Brophy, S. and Newby T. (2008), Scaffolding student's conceptions of proportional size and scale cognition with analogies and metaphors. *Proceedings of the 115th Annual ASEE Conference and Exposition. June 22-25. Pittsburgh, PA*
Invited Talks:	Magana A. and Klimeck G. (2007). nano-based education through generation-nano.org Tutorial presented at Supercomputing 2007. Education Program. Reno, Nv.
Poster Presentations:	Magana, A.J., Brophy, S. and Bodner, G.M. (2008), Professors' instructional approaches and students' perceptions of nanoHUB simulations as learning tools. *Graduate Student Educational Research Symposium 2008* and *2nd Latino Scholar Forum*
	Magana, A.J., Brophy, S. and Schaffer, S. (2008), Taxonomy for conceptions of Size and scale. *Graduate Student Educational Research Symposium 2008.* **Best-Poster Award Winner**
	Magana, A.J., and Brophy S. and Bodner G.M., (2007). Analogies and metaphors for scaffolding middle school students' scale cognition. *Poster presented for the Engineering Education Advisory Council April 27 and NSF Review and Site Visit at Purdue University June 18-20*
	Magana, A.J. and Madhavan, K. (2006). Pedagogical foundation for nanoHUB for Kids. *Poster presentation at NSF Review and Site Visit at Purdue University June 20-22.*