International Journal of Engineering Education Vol. 28, No. 5, pp. 1033–1045, 2012
Printed in Great Britain

0949-149X/91 $3.00+0.00

Student Views of Engineering Professors Technological Pedagogical Content Knowledge for Integrating Computational Simulation Tools in Nanoscale Science and Engineering*

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The ability to explore the physical world at the nanoscale has opened up an affluence of technological advances with the potential to improve human life. Further, it has been complemented with significant advances in simulation-based engineering and science (SBE&S). Having become a crucial part of the present infrastructure, SBE&S is central to the application of advances in the conductance of scientific research and engineering practices. These facts clearly signify the need to integrate the use of computational simulation tools in 21st century engineering education curricula as one way to bridge the gap between school engineering and work engineering. The guiding research questions for this study are: (a) What technological pedagogical content knowledge do professors have for incorporating computational simulation tools to convey nanoscale science and engineering-related concepts and practices? and (b) How do students react to an instructor's technological pedagogical content knowledge with computational simulation tools? This study coupled the methodological framework of a case study with the theoretical framework of TPCK. Open-ended interviews, classroom observations, and document analyses were conducted with six engineering professors teaching undergraduate and graduate courses related to nanoscale science and engineering. Thirty-three students of these courses were also interviewed. Analyses present detailed descriptions of how instructors integrated computational simulation tools to support the learning of nanoscale-related concepts. Findings revealed that computational simulations were perceived by students as effective learning tools. Also revealed was that students continued to confront difficulties when interacting with these tools. Implications for education and educational research in engineering relate to the development, the research and implementation scaffolds, and the transparency at the physical/conceptual, mathematical, and computational levels to understand and then overcome student difficulties in learning with computational simulation tools.

Keywords: computer simulations; computational simulations; engineering education; technological pedagogical content knowledge; nanoscale science and engineering; qualitative research methods

1. Introduction

The ability to explore the physical world at the nanoscale has opened up an affluence of technological advances with the potential to improve human life. Further, it has been complemented with significant advances in simulation-based engineering and science (SBE&S) [1], which allows researchers to test hypothetical devices and materials that have not (or could not have) yet been manufactured. Therefore SBE&S offers unique insight into the study at the nanoscale by allowing the observation of internal phenomena that cannot be physically measured.

SBE&S has been proposed as a new discipline in engineering science in which modern computational methods, computational thinking, devices, and collateral technologies are combined to address problems far outside the scope of traditional numerical methods [2]. It applies the power of computing to extend analytic, statistical, and probabilistic methods, enabling the understanding and investigation of richer and more dynamic worlds and, at the same time, revealing new and sometimes counterintuitive patterns and relationships. Therefore it has become a crucial part of the present infrastructure and is central to applying advances to the conduction of scientific research and engineering practices [1].

These facts clearly signify the need for integrating computational simulation tools in 21st century engineering education curricula as one way to bridge the gap between school engineering and

* Accepted 1 June 2012.

work engineering; this disjuncture has been described as one requiring a significant effort to be correctly addressed [3]. As a step toward accomplishing this need, the Network for Computational Nanotechnology (NCN) created a cyberinfrastructure called nanoHUB.org with the goal to transform nanoscience to nanotechnology through online simulation-based engineering and science [4]. NanoHUB.org is a web-based science gateway that provides scientific-computing-based simulations that experts in nanoscience commonly use to build knowledge in their field. However, the resources nanoHUB provides began to be used for instructional purposes because of the following key characteristics: (1) they were produced by researchers for domain-specific NCN areas; (2) they are seamlessly accessed online from a web browser powered by a highly sophisticated architecture that taps into national grid resources; (3) they provide a consistent interactive user-friendly graphical user interface known as Rappture, designed to make computational models accessible to non-experts [5]; and (4) they can be used to engage students in authentic research and engineering activities similar to the work done by their instructors, who are also scientists and engineers [6].

To approach the complex nature of this work, we required a methodological approach that would allow us (a) to study issues in depth and to approach the phenomenon without being constrained by predetermined categories of analyses or standardized measures; and our participants (b) to define factors and influences they found significant and crucial to describe their experiences. Therefore this study required qualitative research methods of inquiry coupled with a conceptual framework that would allow capturing the interplay among content, pedagogy, and technology. We therefore used TPCK [7–9] to identify how instructors transformed content knowledge into a more conceptually understandable version for their students by blending content knowledge with technological and pedagogical methods. Specifically, our purpose was to identify how instructors intended learning outcomes can inform the design of specific pedagogical methods for integration with computational simulation tools and how students react to instructors' pedagogical methods to incorporate the use of computational simulation tools in meeting their intended goals and objectives. Specific research questions for this study:

(a) What technological pedagogical content knowledge do professors have for incorporating computational simulation tools to convey nanoscale science and engineering-related concepts and practices?
(b) How do students react to an instructor's technological pedagogical content knowledge with computational simulation tools?

This study concentrates on six case studies of engineering professors who integrated computational simulations and learning tools with an emphasis into how students perceived the effectiveness of these efforts in their learning. For this purpose, we use Technological Pedagogical Content Knowledge [8] as a framework to provide rich descriptions of instructors approaches for integrating computational simulation tools and more importantly to identify how students reacted to these approaches in terms of their perceived learning experience. We believe that describing instructor approaches 'calibrated' by students' views of these same approaches in their learning can result in effective pedagogical methods for integrating computational simulations as learning tools for nanoscale science and engineering.

2. Methods

2.1 Theoretical framework

Technological pedagogical content knowledge (TPCK) informed the data analysis and the interpretation of this investigation. TPCK is an extension of Shulman's notion [10] of pedagogical content knowledge (PCK) with technology. TPCK is a conceptual framework for capturing the interplay among content, pedagogy, and technology [8]. Research has identified that the acquisition of PCK is essential for instructors to provide proper instruction and to help improve students' conceptual learning [11]. TPCK has been used as a framework for (a) pedagogy for teacher education, (b) for learning technology by design, and (c) for research [8]. In this study we used TPCK as a descriptive framework to document how instructors integrated computational tools at a certain point in time and not as pedagogy for teacher education or as a way to learn technology by design. In Fig. 1 depicts Mishra and Koehler [15] definition of TPCK. In this figure, stressed in dark, are the elements that are the focus of this study. Table 1 describes the conceptual differences between selected TPCK's elements for this study such as technological pedagogical content knowledge (TPCK), pedagogical content knowledge (PCK), technological content knowledge (TCK), and technological pedagogical knowledge (TPK).

We propose that the acquisition of TPCK is especially needed for engineering educators to integrate technological and digital tools such as cyberinfrastructure to facilitate proper instruction and to support the improvement of students' conceptual

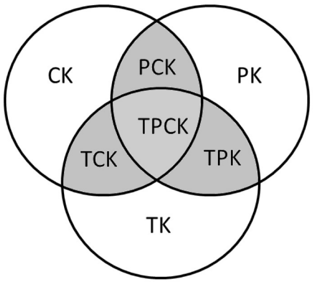

Fig. 1. Mishra and Koehler's definition of technological pedagogical content knowledge (TPCK) and focus of the study. CK: content knowledge, PK: pedagogical knowledge, TK: technological knowledge, PCK: pedagogical content knowledge, TCK: technological content knowledge, and TPK: technological pedagogical knowledge.

learning of complex phenomena. TPCK was used in this study to connect instructors' understanding of SBE&S and its integration with their subject domain. In particular, TPCK provided us with an analytical frame for organizing data on instructors' cognition [12] and their current educational practices and beliefs for integrating SBE&S. It also allowed us to identify how instructors transformed their content knowledge into a more conceptually understandable version for their students by blending content knowledge with technological and pedagogical methods.

PCK assumptions that guided this investigation: (a) instructors become experts in a specific subject area through the construction of specific knowledge that informs them of superior teaching methods for that subject; (b) instruments can be devised to identify and measure PCK; (c) PCK can be shared with other educators for use in their classrooms; and (d) articulations by instructors about attitudes, beliefs, and knowledge mirror teacher practice in the classroom [13]. Because TPCK is a class of knowledge that would not typically be held by technologically proficient subject-matter experts, by technologists who know little of the subject or pedagogy, or by teachers who know little about that subject or about technology [8], we have adapted our definitions of TPCK for engineering faculty in this study as depicted in Table 1 as related to the focus of the study.

These adaptations were required because most members of the engineering faculty are expert researchers in an engineering domain and most likely have had no formal training in pedagogical methods, learning theories, or instructional design. For this study, TPCK was used as a way to identify how instructors conceptualized their content knowledge, technological knowledge, and pedagogical methods to integrate SBE&S in nanoscale science and engineering-related courses.

2.2 Methodological framework

Case study design was considered to be appropriate for this study because it provides methodological tools to approach in-depth investigations of complex interactions between content knowledge, pedagogical knowledge, and technological knowledge within a naturalistic setting. Yin [14] defined case study as 'an empirical inquiry that investigates a contemporary issue in depth within its real-life context, especially when the boundaries between phenomenon and context are not clearly evident.' A case study of a situation, she said, should include data about individuals' behaviors, perceptions, and

Table 1. Focus of the study and adapted elements and relationships of TPCK for our study

Element	Definition based on Mishra and Koehler 2006	Adaptation for this study
Pedagogical Content Knowledge (PCK)	Knowledge of pedagogy that is applicable to the teaching of specific content. This includes knowing what teaching approaches fit the content, and also knowing how elements of the content can be arranged for better teaching.	Current practices for teaching engineering subject domains
Technological Content Knowledge (TCK)	TCK is knowledge about the manner in which technology and content are reciprocally related. Although technology constrains the kinds of representations possible, newer technologies often afford newer and more varied representations and greater flexibility in navigating across these representations.	Knowledge about the use of cyber-infrastructure and nanoHUB in particular
Technological Pedagogical Knowledge (TPK)	TPK is knowledge of the existence, components, and capabilities of various instructional technologies as they are used in teaching and learning settings, and conversely knowing how teaching might change as the result of using technologies.	Knowledge of cyber-infrastructure and SBE&S affordances for learning
Technological Pedagogical Content Knowledge (TPCK)	TPCK is the basis of good teaching with technology and requires an understanding of the representation of concepts using technologies and of pedagogical techniques that apply technologies in constructive ways to teach content. It also requires knowledge of what makes concepts difficult to learn and how technology can help to redress some of the problems students face; knowledge of students' prior learning and knowledge of how technologies can be used to build on existing knowledge and to develop new epistemologies or strengthen old ones.	Knowledge and practices related to cyberinfrastructure for learning, i.e., cyber-learning

attitudes and should be collected from multiple sources. We coupled the use of a case study with grounded theory approaches to analyze the data. Grounded theory is a theoretical framework in which themes and findings emerge directly from the data. Strauss and Corbin [15] described it as a systematic approach of data collection and analysis where theory is inductively derived from the study of the phenomenon it represents. The process of inductive analysis consists of a process of identification of differences and similarities in the data, resulting in a set of categories and themes and their properties and interrelations [16]. Our research study started with individual case studies of participants' experiences followed by a cross-case pattern analysis. Specifically, the unit of analysis included individual instructors and their students within individual classrooms and comparative cases across all of them.

2.3 Participants

The participants in this study were selected from a population of faculty members involved in the Network for Computational Nanotechnology (NCN) who used simulation tools available on the nanoHUB as part of their instruction. Participants were identified by evaluating the statistical usage metrics registered on nanoHUB.org. That is, when a peak in the statistical usage data for users from the same institution was identified, we contacted instructors at that institution to determine whether nanoHUB-based tools were being used in instruction and to invite the instructors to participate in the study. Five faculty participants (nanoHUB users) were invited to participate in this study, as well as a professor who used a commercial numerical computing environment and programming language. Interview data were also collected from 33 students enrolled in courses taught by faculty members participating in this study. Students were selected to voluntarily participate if they were enrolled in an engineering course whose instructor incorporated simulation tools as part of the learning activities. The recruitment of student participants was done at the end of each class in which the instructor had agreed to participate. Random selection was done if several student participants from the same class volunteered to participate. Pseudonyms were used to protect instructor and student identities.

2.4 Data collection methods

Semi-structured interviews, classroom observations, and document analyses were selected as the data collection methods. The interviews were video-recorded and transcribed by a third party. They started with structured guiding questions asked in a fashion as open as possible to let the participants choose the dimension of the question they would like to answer; consequently revealing the participants' relevance structure [17]. From the six instructors who participated, the lead author requested permission of five of them (Sanders, Hass, Richardson, Denner, and Bowen) to allow her to observe their lectures for an entire semester. These observations were useful because they allowed the researcher to establish rapport with students and to gain a general understanding of the subject matter and of the instructors' pedagogical methods. We also conducted document analysis of the faculty syllabi.

The interviews with instructors started by asking general information about the students and the course and continued with specific questions about their intentions and methods for incorporating simulation tools into their courses. We asked, for example, what are the outstanding objectives of the course? To what extent do the simulation tools help accomplish these objectives? In terms of educational benefits, what are the advantages of the simulation tool(s) used in the course(s)? What was considered to have helped the students most during their learning process? How activities are best structured to achieve learning goals?

Interviews with the students focused on their learning experience in a particular homework assignment in which they used simulation tools. Sample questions asked of students, for example: What was your experience of using the simulation tool as part of your homework assignment? What do you think was the purpose of the homework activity using the simulation tool? What was it the professor wanted you to learn? Which portion of the assignment did you find the most challenging? How did you overcome those challenges? When you were solving the homework assignment, how confident were you with the required knowledge to solve it? After completing the activity, what was new for you that you did not know before? Why are you taking this course?

2.5 Data analysis methods

For the data analyses, we employed the case study approach [18] coupled with grounded theory analysis of qualitative data [19, 20]. Specifically, once all interviews were transcribed, we employed two techniques called open coding and axial coding for each. During open coding we conducted the first level of abstraction in conceptualizing major ideas. During axial coding, we reassembled the data to identify their explanations and relationships. Our theoretical framework, TPCK, guided the identification of themes during the process of axial coding. That is, once the data were coded openly the first time to identify general categories, these categories were grouped into themes identifying (a) pedagogical content knowledge, (b) technological pedagogical knowledge, (c) technological content knowledge, and (d) technological pedagogical content knowledge. This process of individual transcript analysis was first conducted for the six instructors and then for each of their students who participated in the study.

2.6 Trustworthiness of the study

The trustworthiness of this study was addressed through Guba's four criteria [21] of a trustworthy study guided by provisions proposed by Shenton [22]. We addressed the credibility of the study in all stages since its conception until the data analysis was finalized. For instance, during the design, we utilized well established methods for data analysis, combining case study designs with grounded theory approaches for analyzing the data. Before collecting the data, classroom observation allowed the researchers to develop an early familiarity with the context of the research and also allowed the researchers to establish rapport with students who later volunteered to participate. During the data collection process credibility was addressed by random selection of participants if several students from the same class volunteered to participate (which was the case for all these instructors). During data collection process we utilized tactics to ensure honesty of participants giving them opportunities to refuse to answer or participate. Similarly, during interviews with the participants, we utilized probes to elicit detailed data leading to iterative questioning. During the initial data analysis process the research team conducted thick descriptions of the findings, then ongoing debriefing sessions were conducted where findings were questioned and verified against data. Additionally, a content expert in nanoelectronics sporadically joined the discussions of the team to verify for technical accuracy. Finally, we conducted member checks with four of the six instructors to verify the accuracy of the findings.

Transferability was addressed by selecting test beds in two different disciplines that deal with phenomena at the nanoscale such as electronics and materials engineering. Dependability was addressed by using multiple overlapping data collection methods, such as interviews, document analysis, and classroom observation approaches with an initial survey (reported in a different article) and detailed reporting of the process of data collection method and the use of proper research practices appropriate to answer the research questions. Finally, confirmability was considered by the overlapping of data collection methods, providing rich descriptions of the data analysis, and providing enough evidence through quotes to demonstrate that findings derived from the data and not from researcher bias.

3. Results

Results from this study will focus on the core four elements of our theoretical framework as shown in Fig. 1. The three elements PCK, TCK and TPK will be described briefly while TPCK (at the center) will be described in-depth. In addition, we will also provide detailed descriptions of students' views of their professors TPCK.

3.1 Pedagogical content knowledge

During classroom observations it was identified that engineering professors extensively used two main instructional and learning strategies to convey nanoscale phenomena. The first was to use diagrams, abstractions, and other representations as the main vehicle to convey the content knowledge of the course. The second most commonly used strategy was to first introduce the simplest case of a specific phenomenon, and then build on that understanding to convey more-difficult phenomena. These explanations also included posing examples of what happens 'at the bulk' looking at phenomena from a top-down view and then compared that example with phenomena at the nanoscale looking at phenomena from a bottom-up approach. These two strategies were supported by the use of computational tools to (a) bridge qualitative understandings with mathematical relationships, and (b) to demonstrate the interaction of multiple elements (e.g., materials with thousands of atoms) in a given system.

Through graphical representations, professors usually conveyed a qualitative understanding of the phenomenon under study; second, they used these representations to make a connection between the behavior and structure of a certain system and mapping some features to specific aspects to a mathematical model. A second common learning strategy used by professors was to explain the concept by means of the simplest case and to use that case as an introduction to more-complicated cases.

3.2 Technological content knowledge

The technological content knowledge of the professors focused on how they envisioned their use of nanoHUB computational tools as a way to convey or facilitate specific knowledge or skills related to the subject domain. At a course level, the professors had four overlapping goals for incorporating computational simulations in their courses: (1) To develop an intuitive/qualitative understanding of the physics governing the behavior of a phenomenon under study; (2) To become intelligent users of the tools demonstrated by student abilities to conduct inquiry activities with the tool and to critically evaluate the validity of the results; (3) To apply modeling and computational techniques as well as related science and engineering concepts and ideas; (4) To transfer this knowledge and these skills to engage in engineering design and other problem-solving activities.

3.3 Technological pedagogical knowledge

Professors had students run or build computational simulation tools as instructional activities designed to accomplish their intended learning outcomes. Their most common pedagogical approach began with direct instruction of theory and models defining the behavior of a physical phenomenon and demonstration of their problem-solving process (or analysis process of exemplar problems), followed by homework assignments posing both well-defined and ill-defined problems. Class demonstrations also included how to use the computational tool. The homework assignments typically required students to solve engineering problems by means of running experiments to collect and analyze data, design devices, and/or build models. Professors who taught undergraduate courses limited their use of the nanoHUB simulations to two or three occasions during the academic term, whereas instructors who taught graduate courses were more likely to use the tools more frequently and more intensively throughout the term (i.e., from five to eight simulation tools). These professors used homework assignments and/or projects as evidence of students' learning. Through these instruments, they could monitor students' learning progression toward course objectives and provide feedback to support progress toward these goals.

Ways in which professors integrated computational tools by running them included the design of homework that integrated concepts for the characterization and design of devices. Ways in which professors integrated computational tools by building them included a variety of learning experiences to stress the application of computational techniques, discrimination of different computational methods to describe phenomena at different scales, understanding of degrees of approximation of specific models, and solution of convergence issues.

3.4 Technological pedagogical content knowledge

The professors' technological pedagogical content knowledge was primarily implemented in two different ways. Drs. Sanders, Denner, and Bowen integrated simulation tools as pedagogical aids with the overall goal to help students better understand the phenomenon under study. Drs. Hass, Richardson, and Brown incorporated the tools as the center of their pedagogy because these courses focused on modeling and simulation tasks.

Through classroom observations and conversations with instructors, we identified that the most common goal was for professors to provide 'hands-on experience' with the simulation tools and have students practice concepts and techniques that were introduced in class. The homework assignments were mostly focused on exercises that allowed comparisons of concepts learned in class with results from the simulations. For example, Dr. Sanders explained that in one homework assignment, 'the students took the analytical calculation they had done in class and did that first. Then they ran a simulation tool and compared results, explaining what was similar and what was different. . . comparing theory versus simulation.'

He further explained that although the exercises done in class are approximations to the exact solution, with the simulation tool students can solve the exact ones. Therefore they had the opportunity to compare those solutions and draw some conclusions to identify 'how it really works.' The first homework assignment was designed as an exploratory activity in which the students became familiar with the simulation tool and with the output and what that output means, thus giving them 'some feel for how these devices work, what voltages you apply to them, and what currents flow.' The pedagogical approach Dr. Sanders used provided students with a starting point that consisted of a model to be tested on 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. The output of such a model was input for the nanoHUB simulation tools.

Dr. Denner designed homework assignments to leverage students' reasoning abilities and their capacity to connect the 'math and the real reality.' As part of those assignments, Dr. Denner sometimes asked his students to use MATLAB, a numerical computing environment and programming language: '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. Play around with it and develop an understanding.' Moreover, Dr. Denner explained that by using MATLAB, students did not need to spend a lot of time solving the mathematical portion of the assignment. He said that sometimes this portion may be overwhelming. Dr. Denner also provided scaffolds to approach homework solutions in the form of simple MATLAB codes. '. . . People can download these codes from the nanoHUB. And my purpose in giving these codes was so that students could use them as templates. It's more like you can see how to write a code. Write one for yourself now.'

Dr. Bowen designed the homework assignments related to nanoHUB as a series of steps from the simple to the more complex. Students first had to solve the analytical solution. Next they created a computational solution with MATLAB and then ran the nanoHUB tool to compare the solutions. He explained that he wanted the students to be more critical of their solutions, and if they were doing it wrongly, actually return to their approach and attempt to develop the right solution.

On the other hand, Dr. Hass described this course as a 'hands-on class' in which students explored a variety of models ranging from simple to complex, starting by describing these models at the levels of atoms and electrons and moving on to describe them with continuum equations. He explained that an important component of the course involved using the nanoHUB as a tool to understand and implement modeling techniques, and also as a tool to run simulations. He described the different tools and different ways in which they used nanoHUB. In particular, they used the workspace where students programmed simplified versions of a specific simulation tool. Students, he explained, 'will gain just enough confidence to know what's inside the box. They may not know every single detail about what's there, but they will have a flavor of it.' He compared and contrasted his approach, using the workspace to program parts of the tools and using the readily available simulations, 'so part of the objective will be 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 of a simulation run.'

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 where students 'have to be able to distinguish between the physical part from the numerical part.' Because his course was not a programming course, he wanted his students to focus more on the modeling part than on the computational part. Therefore he gave them a starting point, in this case a script, in which they could start modifying or building on top of it. As he said, 'I'm going to give them something they can actually just tweak to do that. And the tweak is very simple, but understanding where to do it is what's going to take them two weeks.'

Dr. Brown described her main pedagogical approach for the course as 'project-based learning.' She designed projects so students could go through a progression and combination of experiences to attain the course's learning goals. Dr. Brown employed a pedagogical approach similar to Dr. Hass's in which she assigned students to model a simple version of a simulation tool: 'They learn how a commercial simulator works because they have built their own, so now the commercial simulator is no longer a black box to them.'

3.5 Student views of professors' technological pedagogical content knowledge

Thirty-three students expressed their opinions about one of the six professors' technological pedagogical content knowledge for incorporating computational simulation tools in their engineering courses. These students reported two main reasons for taking one of the six specific courses described here. For 21 of these students, the reasons for enrolling in a course were that the course content was closely related to their research interests. Nine commented that even though their research was not on that particular topic, they considered this knowledge important. Three mentioned they had taken the course because it was one of the core courses required for their engineering degrees. These 33 students reported having perceived four general learning goals: nine perceived to have an insight of current technologies and practices. Examples of their experiences relate to better comprehension of the state-of-the-art of transistor technology or having experiences they might expect to have in industry. Sixteen students perceived the learning goal as being able to identify some kind of cause-effect relationship of physical phenomena. It might be, for example, understanding how current flows in very small devices, or how carriers behave in a semiconductor when disturbed by light, or how the varied dimensions of a nano wire affect strength. Fourteen students perceived the goal of the course and/or homework assignment as being capable of representing physical phenomena by means of simulation tools. They include being able to understand the physics behind the simulation tools and to use a computational tool to graphically represent these concepts and ideas.

When the 33 students were asked how confident they felt in approaching the solution to the homework assignments related to the use of computational tools, two general responses were found. Fourteen felt very confident with the prior knowledge enabling them to be able to approach the solution of the homework. They claimed they gained such knowledge either from their past courses or from the lectures related to the homework assignment. For example, one student pseudonamed Payton explained how he was able to relate portions of the homework assignment to descriptions provided by the professor during class:

> Payton: 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 when I see that code and the program, then I immediately understand what to do to modify or to change.

However, students still confronted some difficulties when approaching the solution to their homework assignments. Eight mentioned that they had no deep understanding of the physical phenomena, four had difficulties solving a particular hand calculation, and five more lacked a programming background. Payton described an instance where he couldn't deal with the syntax and had difficulties understanding the concept of stability:

> Payton: I think in this homework there are two parts, one is theoretical, and one is implementation. I would say I had problems in the implementation part because of the syntax thing. Also the theoretical part. I think that I have something I need to understand a bit more, such as stability. Just today I was reading some papers. So I still need to know the theoretical part of stability and the criteria there — criteria for convergence and whether it is stable.

Other aspects related to student limitations on their learning were related to what students called the 'transparency' of the simulation tool. For example, 13 students, including 2 undergraduates, wanted to know which equations were being solved and to see the calculations as well as the underlying assumptions of the model. Others wanted to have access to the code. Here an undergraduate student named Harper described how he wanted access to the computational model on the nanoHUB:

> Harper: I would like to see explanations of how to use it, and then maybe not as much the concepts, but the explanations of how nanoHUB is getting these solutions. That's because I remember a homework assignment where we were supposed to calculate values, and then we were supposed to look at the values that nanoHUB was getting, and they were always slightly different. As I now I think about it, that was because they do a different type of computation than what we do. I want to say that what we do is like a straight line and then a drop-off, whereas they have something like a continuous line. But that was never really made clear when I was using the tool. I didn't know why the values were always slightly off. So I believe that the two big things I would like to see from them are this: more of an explanation about their math and how they're performing the computations, and then more information on how to actually go about using the tool.

As a means to overcome the limitations described above, students identified three general types of supports embedded in the nanoHUB that were very useful when they approached solutions to the homework assignments. Nine students identified online lectures as being very useful when approaching the solutions. Six identified the templates and blueprints of codes, i.e., short scripts or codes, as helpful in implementing their own solutions. Also, two students commented that the predefined (default) values of the parameters are helpful because when they did not know what to enter as those values, the default values gave them a reasonable response. One student, Harley, described how she used the online lecture to approach a solution to the homework assignment. When doubts still remained, she was later able to further clarify them with the professor.

> Harley: If I have to talk about the last homework in the molecular dynamics— it was pretty intriguing, actually. The questions made us think about how to apply knowledge that we had learned through the classes. In the class, the professor actually made us go through the nanoHUB simulation, for example, what data were to be input, at what point, and what they meant. So it made a lot of sense when I was actually using the tool myself. And the simulations actually made me think a lot about the physics involved. Professor Hass's presentation was really good. I had a few doubts when I was going through it, but I cleared them up with the professor at a later class.

Another way to overcome student learning limitations with computational tools was through multiple feedback mechanisms. Eleven students mentioned that their instructor provided them with the solutions to their homework assignments. For them the solutions were sufficient to identify their problems and to self-correct their understanding of the concepts and skills targeted by the assignment. Six students mentioned that when the sample solution to the homework assignment was insufficient, the teaching assistant and the instructor were very helpful in relieving their doubts.

Even though students experienced some difficulties, all but one agreed that they had learned something new. Some described their learning experiences at a course level, and others in the specifics of the homework assignment. Sixteen students mentioned having learned how the physics relate to the real world, e.g., understanding the behavior of a transistor in a very small scale, or behavior of atoms in a certain material. Six other students have learned how to conduct specific measurements. Four mentioned having learned to be critical of the output of simulations, and three of them also learned how to find a way to verify if the simulation tool is performing correctly. Lastly, three students reported learning new computational techniques, and four others mentioned that besides learning computational techniques, they also gained deeper understanding of the physics of the studied phenomenon.

When students were asked how they had benefited from learning by the use of computational simulation tools, they focused on four main areas. Six mentioned convenience because the tools solved difficult and complex calculations for them and helped them simplify complex models. Another useful factor was related to the output of these tools. Twenty students mentioned especially that output of the simulation helped them to realize how each parameter affects the output; that is, the simulation gave them some sense of how physical phenomena behaves. Another benefit, perceived by seven students, was the opportunity to experiment and to 'play around' with ideas through hands-on experiences with the simulation tools. Seven others saw the tools as an aid to verify the correctness of their hand calculations and/or of their own programmed simulation tool.

4. Discussion

This section discusses the identified themes that emerged from the combination of the two major research questions related to the technological pedagogical content knowledge of engineering professors for incorporating computational simulation tools to convey nanoscale science and engineering-related concepts and practices and their students' reactions to the use of such tools for teaching. Due to the different focus and scope of the interviews conducted with instructors (at the course level) and students (at the homework assignment level), the results are presented describing general trends as opposed to specific links between students' viewpoints based on individual learning experiences in a particular homework assignment in which computational simulation tools were used and instructors' TPCK.

4.1 Theme 1: Integrating computational simulation tools can result in meaningful learning experiences for learning nanoscale science and engineering concepts and principles

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 this study, and contributed to their current interests and academic goals. Some instructors focused on conceptual understanding and engineering skills, and others emphasized computational techniques. Three general methods for incorporating simulation tools into engineering courses were identified: simulations to predict system performance relative to a design task, simulations built as part of a modeling task to predict model performance relative to observed phenomena, and a combination of both. These two trends are analogous and can be aligned with using versus building simulation tools [23] and learning from models versus learning by modeling [24]. Of special interest is that these instructors have used expert computational simulation tools for leveraging different types of learning goals to convey concepts and skills with enduring value beyond the classroom [25].

A learning goal shared by most of the instructors was to develop their students' abilities and intuitive understanding of the phenomenon under study, and further, to enable these students to become critical users of simulation tools. A second learning goal was for the students to become familiar with literature in the area of study. Although some instructors focused on conceptual understanding and engineering skills, others emphasized computational techniques. For example, Drs. Sanders, Denner, and Bowen dedicated a large part of their courses to convey the governing fundamental physical principles of devices (e.g., circuits and semiconductors). Dr. Sanders went further into these fundamentals by describing the behavior of nano devices, and he also focused on their design and evaluation. On the other hand, Drs. Hass, Richardson, and Brown focused their courses on teaching modeling and computational techniques. They emphasized the application of these techniques to approach engineering tasks.

Students reported two main reasons for having taken the courses in this study: because the study is closely related to their research and because they considered this knowledge important for future educational and professional activities. The perceived general learning goal was to have an insight of current technologies and practices. Most students agreed that they had learned something new using and/or building with computational simulation tools. Some mentioned learning how (a) the physics models relate to the real world, (b) to conduct specific measurements, (c) not to blindly trust simulations, (d) to find a way to judge if the simulation tool is doing what it is supposed to do, and (e) to implement computational techniques. Therefore students and instructors described consistent expectations of the learning outcomes for the specific courses.

The main instructional approach the instructors followed was to first introduce the physical principles defining the behavior of a device, material, or phenomenon in class, and then to have the students apply these principles with the homework assignments, using the simulation tools. This approach has been referred to as 'direct guidance' [26]. According to Kirschner and his colleagues, direct instructional guidance refers to information provided to students that fully explains the concepts, procedures, ideas, and skills required to learn. Kirschner et al. argued that direct guidance is more effective and more efficient than minimally guided instruction. Similarly, Bodemer et al. [27] reported that not having the appropriate prerequisite knowledge is one of the reasons why even supporting learners in processes of discovery learning does not lead to better learning outcomes. For this group of students, direct guidance provided them with the required knowledge to approach the solution to their homework assignments.

?twb=.2w>By using the simulation tools as part of the homework assignments, the students were expected to notice, 'by playing around with these tools and developing understanding,' that there were differences between 'theory versus simulation' or 'math and reality.' For example, Dr. Bowen first asked his students to solve the analytical solution, then the same equation by employing MATLAB, and finally through nanoHUB to check out the solutions of the two previous steps. On the other hand, instructors who focused their courses on the computational and modeling techniques emphasized that they have followed what they called 'hands-on' or 'project-based' approaches in which students had an opportunity to interact and/or implement simulation tools to know 'what's inside the box.' They followed a series of learning strategies to provide opportunities for their students to be able to compare and contrast aspects of (a) programming their own simulation (a simple version or a portion of it), and just run a simulation tool; (b) using different user interfaces (e.g., graphical and non-graphical); and (c) using different models embedded in different simulation tools.

Students perceived that they benefited from using simulation tools because they found them both convenient and helpful. They were convenient because simulation tools solved difficult and complex calculations and because the simulations helped to simplify complex models. The output of the simulation enabled them to realize how each parameter affects the output, giving them some sense of the physical phenomena. Lastly, the simulation tools gave students hands-on experience that at the same time allowed them to experiment.

4.2 Theme 2: Students need transparency and soft and hard scaffolding for using computational simulations as learning tools

Students also experienced some limitations in their learning. They wanted more simulation tool transparency. On page one of Transparent Interfaces: Model and Methods [28], Tanimoto defined transparency as 'a property of systems where the inner workings and the design of the system are visible to users.' Students wanted to know which equations were being solved and to see the calculations and the underlying assumptions of the model, and some wanted access to the code. However, we identified a polarity where students who ran only the simulation tools wanted to program their own tools, while 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 the supports provided to students. Part of this need has already been fulfilled by scaffolds that have been incorporated. However, transparency of the underlying models of the physics needs also to be addressed. The two most common approaches for simulation transparency are the black box and glass box simulations [29]. The glass box simulations differ from black box simulations by providing learners with visibility [30]; i.e., the ability to inspect and modify the equations [31].

Students were also asked how confident they felt with their prior knowledge at the moment they approached the solution to their homework assignments. Two general responses were found: either they felt very confident, or they lacked some knowledge or skill (e.g., lacked understanding in the physics, the mathematics to represent the physics, or programming skills). Students who felt confident with their prior knowledge mentioned that instructors provided them with that knowledge as part of the lecture. Students who were lacking certain knowledge or skills felt they lacked them from prior courses and/or because instructors assumed they had them. For example, instructors assumed that students knew how to approach the solution to a particular differential equation.

Students commented on various strategies their instructors employed to help them overcome their prior knowledge limitations: soft and hard scaffolds. The distinction made by Brush and Saye [32] between soft and hard scaffolds for supporting (individual) student learning is that soft scaffolds are feedback, questions or information provided by the instructor, and perhaps also by peers, but hard scaffolds are embedded (or hard-wired) into the computer learning environment. According to Tabak [33], the best approach for implementation is by targeting a synergy between both. In this specific case, students received soft and hard scaffolds during the solving of their assignments. They identified three types of hard scaffolds that were useful to them while solving their homework assignments. One was the online lectures on the nanoHUB that functioned as an embedded expert guidance [34], which helped them to activate their prior knowledge. The second was the use of programming scripts that served as templates and/or blueprints for implementing their own scripts. The third was the predefined or default values embedded in the simulation user interface. Soft scaffolds provided by the instructors were opportunities provided to students to have additional clarification through interactions with the teaching assistant, instructor, and/or peers. The scaffolding strategies employed by the instructors are consistent with previous findings, which argued that a successful use of simulation tools needs adequate but not intrusive scaffolding [24, 35–39].

Three models have been identified that describe ways to integrate hard and soft scaffolds with computer simulation tools. Quintana et al. [34] described a set of scaffolding guidelines that include (a) the use of representation and language that bridge learners' prior conceptions, (b) organization of tools and artifacts that make disciplinary strategies explicit to learners, and (c) use of multiple representations that make explicit underlying properties of data. Similarly, de Jong and van Joolingen [40], as well as Veermans, van Joolingen, and de Jong [41], identified a set of strategies, heuristics, and tools intended to (a) activate students' prior knowledge (e.g., providing extra information to the simulation learning environment in the form of a hypertext/hypermedia system, incorporating intelligent tutoring systems), (b) help students in their process of hypothesis generation (e.g., providing a hypothesis menu and offering hypothesis scratchpads), (c) scaffold students in their design of experiments (e.g., advising students to change only one variable at a time, to try extreme values), and (d) aid students in their data interpretation process (e.g., providing tools for making predictions and receiving feedback). Kali and Linn [42] also 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. Guidelines from these three models can be adapted and integrated as scaffolds for computational simulation tools.

5. Implications

The results of this study have implications for education and educational research in the fields of engineering education and learning design and technology. Especially, these results can directly inform the design of learning objectives and instructional interventions to encompass some of ABET's Criterion 3 outcomes (particularly A–K) [43], together with the use of computational simulation tools in the fields of nanoscale science and engineering. These results also identified initial components to be used toward the development of an instructional design theory for computational simulation tools in engineering education. This theory can integrate some principles and guidelines that are consistent with previous research and with findings from this study. For example, from the three models described above that integrate scaffolds with computer tools, common elements include (a) the use of multiple representations and language that can help learners integrate prior knowledge; (b) make disciplinary strategies accessible and explicit to learners; and (c) integrate multiple levels of representations to make thinking visible. Similar common elements have also been identified through the investigation of engineering professors' technological pedagogical content knowledge and students' reaction to the use of computational tools in the classroom (i.e., soft scaffolds, hard scaffolds, and transparency). Therefore specific scaffolds and strategies that have been suggested for overcoming students' difficulties while using or building computer simulations can be adopted or adapted to be integrated with computational simulation tools, as depicted in Table 2.

On Table 2 we propose a transparency and scaffolding framework [44] that integrates these two elements at three different levels of representation: (a) at the physical/conceptual level, (b) at the mathematical level, and (c) at the computational level. By integrating transparency and scaffolds at these three different levels, learners can (a) compare and contrast multiple levels of representation, (b) bridge from a qualitative understanding to a quantitative understanding of phenomena, and (c) gain access to disciplinary strategies for creating and representing knowledge.

Implications for educational research in engineering derive from the proposed framework and relate to the implementation of design-based research approaches [3, 45]. Through the use of design-based research approaches, scaffolds and transparency can be developed, researched, and then integrated with the computational tools. This iterative cycle between development, research, and implementation can also be integrated at the three identified different levels of representation (i.e., physical/conceptual, mathematical, and computational). These three levels can be integrated by researching and improving engineering professors'

Table 2. Framework for researching and developing scaffolds and transparency with computational simulation tools.

<table>
<tr><th>Transparency and scaffolding level</th><th>Physical/Conceptual level</th><th>Mathematical level</th><th>Computational level</th></tr>
<tr><td rowspan="2">Researching and integrating instructor knowledge into soft and hard scaffolds</td><td colspan="2">Pedagogical Content Knowledge</td><td></td></tr>
<tr><td></td><td colspan="2">Technological Pedagogical Content Knowledge</td></tr>
</table>

pedagogical content knowledge and technological pedagogical content knowledge, as depicted in Table 2.

6. Conclusion

Engineering education researchers have pointed out that the role of technological and digital tools in engineering education has been extremely undertheorized [3]. This study provides new insights into the definition of engineering-related learning outcomes and the associated pedagogical approaches for achieving such outcomes when incorporating computational simulations for learning. Also, by employing qualitative research methods of inquiry, we have accounted for the interactions of professors' technological pedagogical content knowledge and their students' reactions for integrating computational simulation tools in naturalistic engineering learning contexts. The outcomes of this study therefore provide general guidelines toward the development of learning materials for using computational simulations as learning tools. These outcomes also indicate the potential of integrating the computational simulation tools into formal learning experiences in terms of learning outcomes and pedagogical approaches.

Computational simulations in learning contexts are a means to an end. That is, simulations are teaching tools used by instructors to promote an understanding of procedural and declarative knowledge in their students. Instructors strive to have students develop abilities to regulate their own learning-designing activities that range from simple to complex. As such, the development of learning activities and instructional materials and their use together with the computational simulation tools should be informed and improved through continued research.

Acknowledgments—This work was supported by the U.S. National Science Foundation via NSF Grant # 0817486 and EEC-0634750. Support from the Department of Computer and Information Technology, School of Engineering Education, and from the Network for Computational Nanotechnology at Purdue is also gratefully acknowledged.

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