

## **Samuel and Hector's Experiences and Perceptions of nanoHUB Simulations as Learning Tools: a Case Study Approach**

### **Research Design**

The aim of this study is to provide holistic and meaningful descriptions of professors' experiences and perceptions of nanoHUB simulations as learning tools. Therefore, it is required not only to describe how professors perceive the tools, but also how they experience their use of such tools. In this particular study the research question I am trying to answer is:

What are instructors' perceptions and experiences of using nanoHUB simulation tools as part of their instructional practice?

Since the aim of this research study is to describe, analyze, and understand experiences in educational settings (Marton, 1981); phenomenography will be used as the method of inquiry. According to Marton (1994):

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. These differing experiences, understandings, and so forth are characterized in terms of "categories of description," logically related to each other, and forming hierarchies in relation to given criteria. Such an ordered set of categories of description is called the "outcome space" of the phenomenon concept in question. (p. 4424)

The study involved two faculty members who are part of the Network for Computational Nanotechnology (NCN) and who have used nanoHUB simulations as part of their instruction. These faculty members voluntarily participated in a one-hour interview and think-aloud protocol.

Case study was selected as the unit of analysis. The data analysis of this research study began with individual case studies of each participant and then the cross-case pattern analysis was conducted. Data analysis started by reading and transcribing the interviews. Once I transcribed the interviews, the analysis proceeded with open coding. For inter-rater reliability purposes, four coders participated in this phase. From the codes that were generated, I grouped together all of those that were related, and used Wiggins and McTighe's backward design model as a framework for organizing such data in three major themes. Wiggins and McTighe (1997) present a "backward design process" (p.9) 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. In identifying the desired results, Wiggins and McTighe provide a further classification of three levels for establishing curricular priorities one embedded inside another and ranging from knowledge worth being familiar with to enduring understanding.

The next step in the data analysis was to classify the data into these three themes and decide the level of strength or weaknesses of each coded statement. I did so by focusing in a scale from 0 to 10 as well as by looking at frequency of appearance of each statement. Then I proceeded with the writing of the findings.

## **Data Analysis and Interpretation**

In the following sections I will describe ways in which Samuel and Hector described the simulation tools, as well as their approach in designing the content, assessment, and pedagogy for incorporating them into their classrooms.

### **Samuel and Hector's Experiences of their use of the nanoHUB Simulation Tools**

#### Samuel

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

#### *Learning Outcomes*

Samuel has been using several of the nanoHUB simulation tools as part of his graduate course in semiconductor devices. He used the nanoHUB throughout the entire semester and at different points in time. Samuel's instruction focused on helping students “*developing an intuitive understanding*” of the phenomenon under study. He did that by designing learning activities that either would 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...*

Throughout the nine homework assignments, Samuel followed an approach in which each homework assignment was part of a progression in the level of complexity.

The last one though, he targeted to integrate 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 Samuel, this activity not only served as a final project integrating all the knowledge of the semester, but also it 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*

Samuel focused his assessment in students designing devices to 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*” and asked 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 related to 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, Samuel scheduled feedback sessions outside lectures. When I asked him about the process of providing feedback Samuel 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.*

Samuel identified that probably this feedback is 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 are uploaded on the nanoHUB and have an easy access 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 Samuel was to first introduce the concepts during class and then assign the homework. Homework assignments were designed by Samuel 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 those 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.*

Samuel 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 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.*

For the case of the first homework assignment Samuel designed it as an exploratory activity. Samuel gave an opportunity for the students to get familiarized 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 Samuel's pedagogical approach, he usually provided to his students a starting point. Sometimes it consisted on a model to be tested in the simulation tool, some initial parameters that should be met, and/or some others consisted of a model to be implemented (i.e. writing a Matlab script) outside the nanoHUB. Then, the output of such 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...*

### Hector

Hector teaches graduate courses related to materials science engineering at a Midwestern university. Before joining his actual university about three years ago, Hector worked in a nationally recognized research laboratory. Hector also gained about for years of teaching experience while studying his Doctoral Degree. Hector has also been awarded

for his research and teaching efforts.

### *Learning Outcomes*

Hector has developed and used the Materials simulation toolkit as part of his research agenda. Actually, as a faculty member, he uses it in different courses and for different purposes. For the course we are collecting data from, Hector used the simulation toolkit to convey one particular topic at certain point in the semester.

Hector's goal in using this simulation tool was to help his students develop an intuitive understanding of the phenomena under study. In particular, he tried to convey what are the fundamental atomic level mechanisms that govern how materials behave. He explains that once students have this intuitive understanding, they will "have a better chance in developing better materials".

*The main idea is to give students more of a... help them develop a more intuitive understanding of how materials work at atomic scale, so when they see the atoms moving it is easier for them to capture, you know... to imagine what the fundamental mechanisms are that govern hmm... the behavior of materials. That is the research we do.*

As we can see from the last sentence of the above paragraph, Hector is trying to bring his research experiences into the classroom. He further explains:

*... conceptually when you do atomistic simulations those are the steps you have to go through running simulations is very similar you go through the same steps that you do in an experiment.*

### *Evidence of Learning*

Hector focused his assessment in students' ability to predict behavior of materials

according to specific parameters and comparing them with experimental values. During my first conversation with Hector he did not mention any aspect of his feedback and assessment strategies. Therefore I had a look into his homework assignment. I identified that although most of the exercises were related to computation of specific values; he gave as an option to his students to read a journal article and predict parameters of a specific material using the simulation tool and then compare his solution with the solution given by the authors.

In a follow-up interview I asked him what was his assessment strategy. He explained that basically he posted the solution on a website and later on he requested the students to grade themselves. If students have further questions related to the assignment, Hector invited them to either talk to him or talk to the teaching assistant.

#### *Instructional Approach*

Hector used the simulation toolkit to convey one specific concept of the curriculum. Therefore he used it for a short period during the semester. Hector's instructional approach was twofold. He first introduced the concepts during class time and then proceeded to make a demonstration of the simulation tool for his students. Part of that demonstration included helping students get familiar with the tool and understand the type of inputs and outputs it requires. Once introduced these two aspects in class, then he assigned the homework.

Hector explained that the simulation toolkit has some pre built-in models so that students can have a starting point.

*Alright so the first thing you do is to set up your input model, and we have a list of pre-built-in models, and I am going to select from this list, from this example a*

*platinum nanowire... So nanowire is a small cylinder made out of platinum ok. I am going to pick one of those and then with the rest of hmm... hmm the options here you can change the properties, you can make the model bigger or smaller replicate it and do manipulations of the initial model, so that gives you some flexibility as to... from those... from that list of pre-built models you can have much wider variety of initial structures for the simulations.*

A particular aspect of this simulation toolkit is that not only it is a simulation, but also a visualization tool. Therefore, Hector designed homework assignments with the intention of helping his students identify how aspects of the input will not only be reflected on the output plots, but also on the behavior of the atoms shown in the visualization tool.

*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.*

According to Hector, this process of comparison will eventually help his students make predictions on “*how materials behave from first principles*”, giving his students new possibilities to eventually design better materials.

*...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 [scientists to] design [...] 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.*

## **Samuel and Hector's Perceptions of the nanoHUB Simulation Tools**

### **Samuel**

Samuel considered nanoHUB simulation tools as convenient because they allowed his students to solve hard analytical calculations easily through simulation. Another feature of the simulation tools mentioned by Samuel is that his students had the capability to use different models run with different parameters that would run 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...*

Samuel also made a comment on one of the nanoHUB simulation tools' particular characteristics; namely their simple interface. In the same comment, Samuel 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.*

Samuel also mentioned that a specific element of simulation tools which make them unique was that it gave him an additional capability that could not be replicated on 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...*

### Hector

Through my entire conversation with Hector, he described that nanoHUB simulation tools provide his students the ability to see “*what is happening with the atoms,*” almost providing his students with the ability to design materials they have never encounter before.

*...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 designers, design 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.*

Hector also made positive comments related to the user interface. He explained that the interface was designed in such a way that it imitates the same process or steps that should be conducted in a similar experiment.

*... conceptually when you do atomistic simulations, those are the steps you have to go through running simulations. It is very similar you go through the same steps that you do in an experiment. So the way we defined the graphical interface is that it is conceptually or is designed in a way that it mimics those steps that you*

*do and it helps students or users in general understand at what level you know, each approximation is being made.*

Hector also gave me some examples of the flexibility and variety that provides the simulation tool.

*...you can change the properties [of a model], you can make the model bigger or smaller replicate it and do manipulations of the initial model, so that gives you some flexibility as to... from those... from that list of pre-built models you can have much wider variety of initial structures for the simulations*

During our conversation with Hector, he also pointed out as an advantage the complexity behind the simulation tool as well as its research quality.

### **Cross-Case Analysis**

For the case of both instructors, it has been identified that learning experiences accompanied by simulation tools were used to convey concepts having “endurance value beyond the classroom” (Wiggins and McTighe, p.10). While Hector used the simulation tool to convey one specific learning goal of the course curriculum, Samuel made an intensive use of the simulation tools within the entire semester following a progression of complex activities culminating in a design challenge. Samuel and Hector reported that their goal while using the simulation tools was to give their students a sense on how investigations must be conducted in their areas of expertise as well as ways in which professionals work on those disciplines.

Wiggins and McTighe second stage is to identify acceptable evidence on knowing what students have achieved. Both instructors, Samuel and Hector designed assessments of the types of performance tasks featuring real challenges. However, it seems that in

both cases the professors do not devote enough time to provide feedback to their students. They usually post the solution of the homework assignments on a website but do not devote next lecture class time to go over the homework and solve doubts. This feedback instead, is done either by request or by scheduling extra sessions to do so. The main reason for that might be due to the fact that professors have a lot of material to cover during the semester, as well as the fact that running the simulation tool takes some time.

The final stage in the Background Design Process (Wiggins and McTighe, p.9) is the planning of learning experiences and instruction. When instruction is accompanied by a complex simulation tool, both instructors pointed out they not only take the time to explain concepts related to the phenomena in study, but also they had to spend some time explaining how to operate the simulation tool. Both instructors commented that nanoHUB simulation tool includes pre-built-in models, suggesting that these may serve as scaffold for students within their initial interactions with the simulation tools.

The overall approach for Hector and Samuel for instruction was to first introduce the basic concepts in class, describe the models and analytical and practical ways in which those models could be solved, and then solve the same models by simulation. Then they elicited from their students to compare the approximations done in class versus the exact solutions computed by the simulation tools.

Samuel and Hector reported that nanoHUB resources appear to be appropriate tools for academic use because they see the benefit of the flexibility for students to be able to compute the exact solutions in a short period of time, with multiple models, and with multiple representations. Samuel and Hector also emphasized as one asset of nanoHUB simulation tools their capability to allow their students to “see” phenomena

that cannot be “seen” with other means. While Hector emphasized the idea to “*see how atoms behave,*” Samuel emphasized the idea to “*look inside the device*”. Two more advantages of nanoHUB simulation tools mentioned by Hector and Samuel were the friendly graphical user interface and the high quality of these tools to be used for research.

## **Conclusion**

Samuel and Hector seem to incorporate the simulation tools in an efficient way. Efficient in the sense that students are able to apply their knowledge to solve practical situations close related to students’ areas of interest, as well as efficient in the sense that they provide to their students opportunities to reinforce concepts learned in class with homework assignments that allow students multiple opportunities of practice, comparison, and reflection.

Samuel and Hector’s experience with the nanoHUB indicate that there is a potential of integrating the nanoHUB simulation tools into formal learning experiences. Instructors interviewed have leveraged its potential using nanoHUB simulation tools in providing their graduate students with authentic learning experiences in which knowledge was successfully applied to practical applications. But clearly more detailed research studies are required aiming to identify if instructors who teach undergraduate level courses follow similar approaches, and if these undergraduate students perceive the learning experiences favorable. Therefore, next steps include (see Figure 1): a) interview and think aloud protocols with students from undergraduate and graduate level courses; b) interview other professors in order to make a deeper analysis on identifying factors of success and failure; and c) identify and interview professors who teach undergraduate

level courses who are incorporating nanoHUB simulation tools. Informed by these results, interventions will be designed considering factors found to be of success; these interventions will be mainly focused to undergraduate level courses as well as courses in which students' expectations range from moderate to low.

Future research topics that will inform better ways of incorporating simulation tools to learning experiences will include ways in which we can increase nanoHUB potential as a learning resource that is developmentally appropriate as well as ways in which experts use the nanoHUB as an expert tool to think with. It is anticipated that the results from this research, will provide curriculum developers as well as computational simulation tools developers with a stronger foundation from which to design simulations for learning as well as the instructional materials that accompany them.

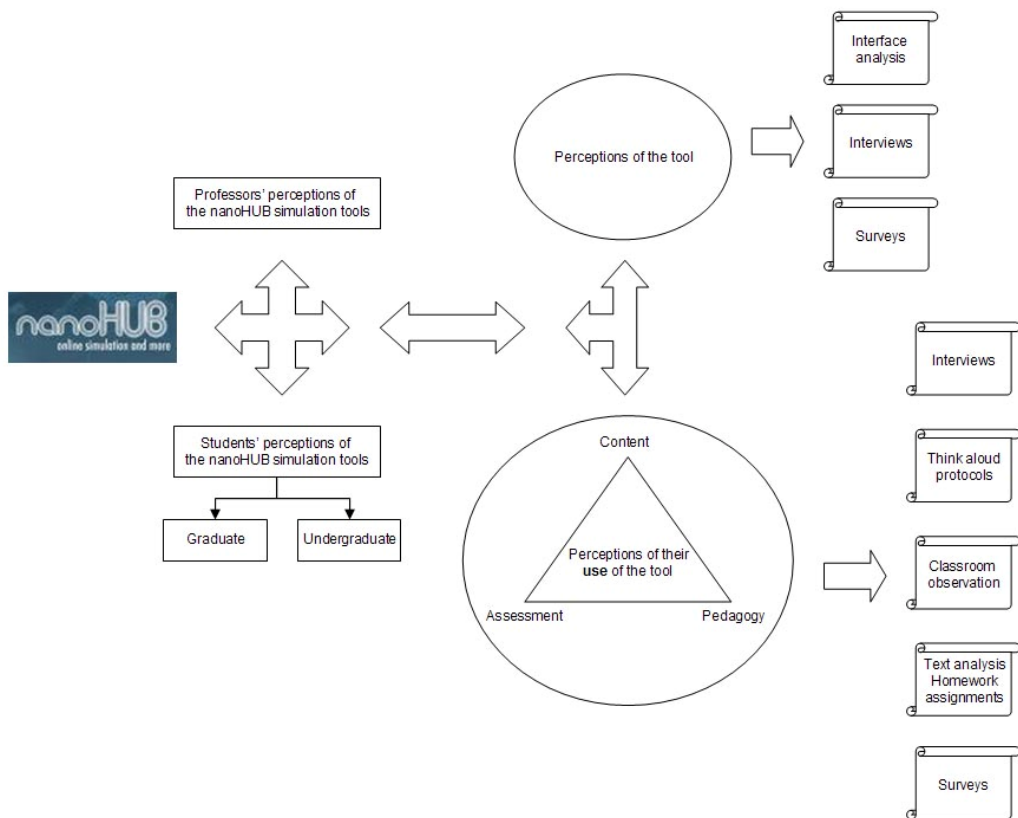


Figure 1: Data collection and data analysis methods

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