FiPy and OOF: Computational Simulations for Modeling and Simulation of Computational Materials

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Abstract

Modeling and simulation of materials has been identified as one relevant skill for undergraduate and graduate students in materials science engineering. To address this need, the course MSE 597I *Introduction to Computational Materials*, aimed to junior/senior undergraduate and graduate students, has been designed to convey concepts and ideas that address the numerical description of the equilibrium and kinetics of materials. To attain the goals of the course, two computational tools, OOF and FiPy, have been incorporated to the class. OOF was used to calculate the spatial distribution of physical fields and the macroscopic properties from images of real or simulated microstructures and FiPy was used as a tool to solve partial differential equations. To investigate students' perceptions of OOF and FiPy as learning tools, two surveys were conducted focusing on learning outcomes, evidence of the learning, and pedagogical approach. By identifying, comparing and contrasting students' perceptions of these two tools we discuss potential changes in classroom implementation as well as changes in the simulations' interface design.

Introduction

Because of the increased application of modeling and simulation tools in the design and optimization of materials in research institutions, academia, and industry, computational modeling and simulation of materials has been identified as one relevant skill for undergraduate and graduate students in materials science engineering (Thornton and Asta, 2005)[1]. Furthermore, the Accreditation Board for Engineering and Technology (ABET, 2009)[2] has also included as part of its criteria for engineering programs including materials, materials processing, ceramics, glass, polymer, metallurgical, and similar the appropriate application of experimental, statistical and computational methods to solve materials selection and design problems. To address this need, the course MSE 597I *Introduction to Computational Materials*, aimed to junior/senior undergraduate and graduate students, has been designed to convey concepts and ideas that address the numerical description of the equilibrium and kinetics of materials. The class adopts a hands-on approach alternating between a classroom and a computer lab lectures. The course focuses on systems that are conceived at the nanoscale and whose resultant properties and performance have an impact on the associated mesoscopic and macroscopic length scales. Topics addressed in class are practical aspects associated to modeling of materials, such as model validation, data fitting, links and incorporation of atomistic aspects to continuum and mesocontinuum models, optimal meshing criteria, and model convergence and stability. In particular, the course focuses on real-life example applications to expose students to advantages and disadvantages of a) phase field, sharp, and level set microstructural evolution methods and b) numerical techniques such as finite differences, finite elements, and finite volumes.

To attain the goals of the course, two computational tools, OOF and FiPy, have been incorporated into the class. OOF (Reid et al., 2009) [3] is a tool designed to calculate the spatial distribution of physical fields and the macroscopic properties from images of real or simulated microstructures (see Figure 1). The code provides an intuitive Graphical User Interface to enable the user to perform Finite Element calculations on materials that are topologically complex, but do not require a Computer Science degree or a deep computational materials background. Homework assignments were designed increasing degree of difficulty, from very simple (running the program and getting acquainted with it) to deploying a full simulation and reproduce and even improve results found in the recent literature (Chawla et al., 2003) [4] .

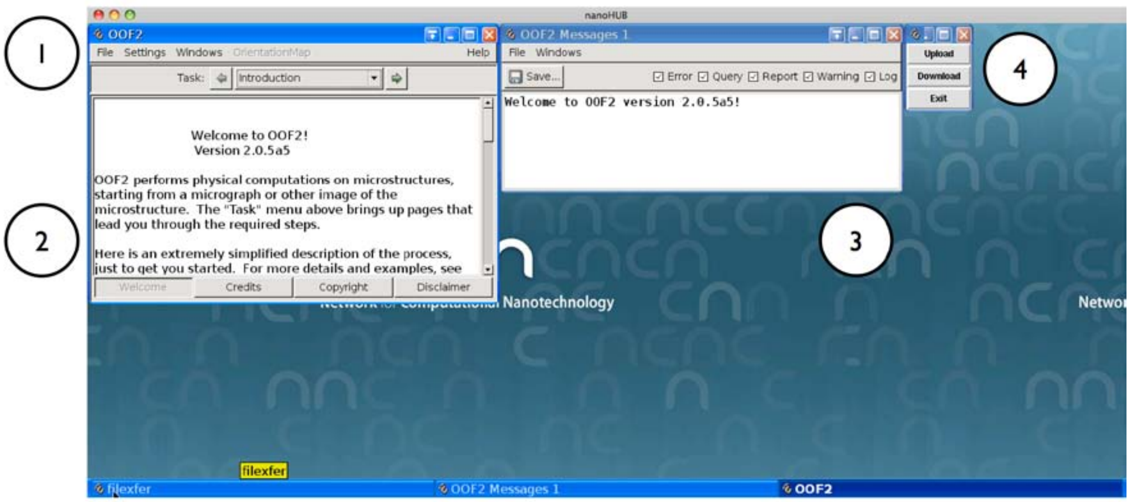

Figure 1. OOF2 web-based interface. At 1, finite element meshes and material properties are uploaded, while at 2, the user selects among an array of menu items operations to perform on the material microstructures. At 3, executed commands, errors and the status of the system are reported. Through the Filexfer, files are uploaded and downloaded: microstructures are added to the system, while macroscopic material properties are reported.

To complement the class, FiPy (Guyer et al., 2009) [5] was used as a tool to solve partial differential equations (see Figure 2). Based on the finite volume method, FiPy provides a set of python-based libraries to analyze the effect of meshing and time-step size on the convergence and stability of parabolic partial differential equations. FiPy provides a web interface called VKML-Live that allows the user to edit, debug, and run their specific applications online is critical to developing new scientific models and share results and databases. VKML-Live completely removes the barrier of installing the libraries and thus the user can focus on developing microstructural evolution models by using FiPy. Homework assignments related to FiPy started by solving the classic diffusion equation (through explicit, semi-implicit, and implicit schemes) and ended solving the microstructural evolution of materials.

Both simulation tools are deployed through the nanoHUB.org (Bartol et al., 2009 [6], Garcia, 2007 [7]). The nanoHUB.org is a web infrastructure developed by the Network for Computational Nanotechnology (NCN) with the main goal to provide research-quality simulations that experts in nanoscience related research commonly use to build knowledge in their field. nanoHUB.org leverages advanced cyber-infrastructure and middleware tools to provide seamless access to these simulations.

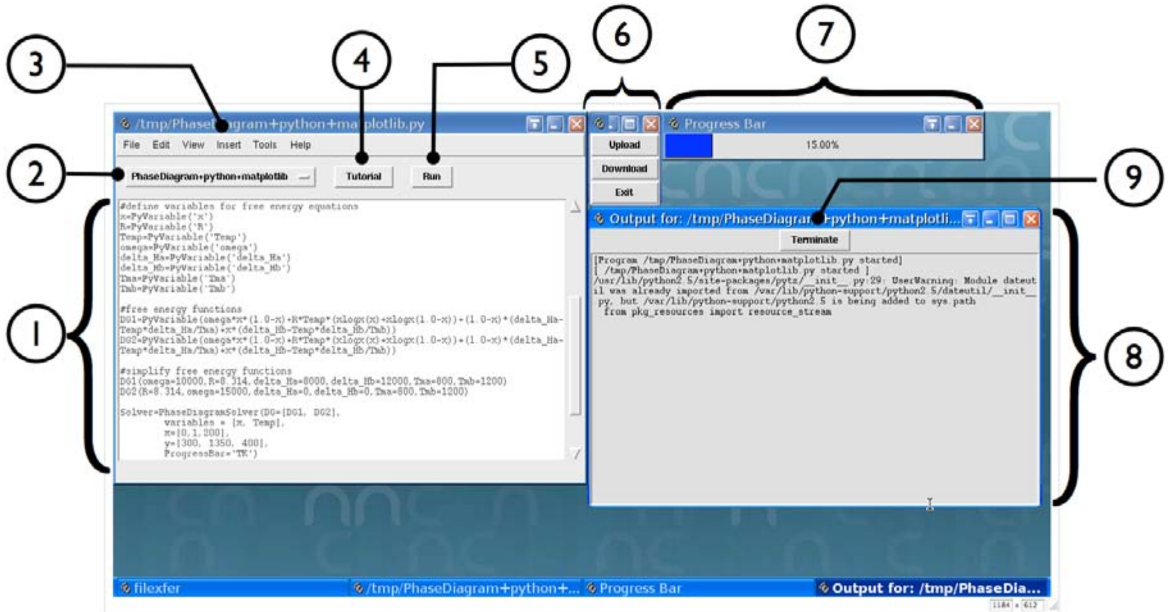

Figure 2. VKML-Live web-based interface. Python scripts are edited online at 1, while the user can select from a variety of examples at 2. The toolbar is shown at 3, where the user can perform standard editing operations, such as copy and paste. For a selected script, a link to any available tutorial can be deployed by clicking at 4. Edited or default scripts can be run at 5. Data, modified programs, images, and databases can be exchanged through the interface provided at 6. Regardless of the deployed application instantiating or not a GUI such as the one shown at **7,** a process control window will be deployed, 8, which can be terminated by clicking at 9.

The purpose of this research study is to investigate how materials science engineering students, perceive FiPy and OOF simulations as learning tools in terms of learning outcomes, evidence of the learning, and pedagogical approach. Therefore, the guiding questions for this study are: a) what are students' perceptions of the utility of these resources for learning?, b) what differences exist in students' perceptions between these two tools? And c) what factors may influence students' ability to engage in inquiry learning experiences? By identifying, comparing and contrasting students' perceptions of these two tools we discuss potential changes in classroom implementation as well as changes in the simulations' interface design.

Methods

Participants of this study consisted of 18 graduate students in materials science engineering (3 female 15 male), who were surveyed twice during the semester. From the entire population, seven were Materials Science students (four graduate students, two seniors, and one junior), and the rest of the class was composed of Electrical and Computer Engineering (3), Mechanical Engineering (6), and Aeronautics and Astronautics Engineering (2). All of them were graduate students. The first data collection was done in the middle of the semester and the second one towards the end. The surveys focused on students' perceptions on OOF and FiPy.

The surveys were administered in the fall semester of 2009 to 18 students 16 of who completed the survey for OOF and 13 of who responded the one for FiPy. The students were asked to participate in a voluntary Likert-scale survey focused on their perceptions of the simulation tools as useful for their learning, relevance to their areas of interest, and ease of use. Students responses were rated in a scale from one to four: strongly agree, agree, disagree, and strongly disagree to each question. Descriptive statistics were used to analyze and report the surveys results.

Results

Wiggins and McTighe's backward design (1997) [8] was used as a framework for grouping answers to the survey questions. 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. We decided to use this backward design as a framework because it encompasses all elements that should be involved in any instructional intervention.

Students reported that they used OOF to generate plots and read values (47%), to generate data (41%), and to implement models provided by the instructor (41%).

Learning Outcomes (content) - This section focuses on the general experience students had, relevance of the content to whether students thought the simulation tools were relevant to their areas of interest as well as their level of satisfaction. Students were positive in their responses of considering using OOF as a positive experience (M=3.35, SE=0.12). Students reported considering the assignments related to OOF as highly relevant to their areas of interest (M=3.19, SE=0.16) and that such assignments supported their goals and expectations for the course(M=3.18, SE=0.18). Students also found the course as highly relevant to their areas of interest (M=3.31, SE=0.15). We also asked students to describe their areas of interests as related to the homework assignments with OOF. Students responded this question by describing the relationship of the assignment to their areas of research:

> "Simulate the deformation of metal foil based on crystal plasticity model. The metal foil is deformed by the laser dynamic forming."

> "My major area of interest in failure prediction over a range of length scales. Finite element models are a core aspect of the analysis methods used to pursue this goal. By gaining an understanding of the mechanics and implementation of the finite element method I am better able to critique and refine results."

> "Want to do diffusion related modeling rather than stress-strain composite materials modeling."

Evidence of Learning (assessment) - In this section we focused on how students perceived OOF as useful for their learning and their transfer of it to practical situations. Students reported to be able comprehend the concepts better by using OOF as compared to lectures and readings only (M=3.0, SE=0.16). Students stated their ability to apply concepts learned in class to the lab practice related to OOF (M=2.8, SE=0.16) and reported an increased awareness of the practical application of the concepts related to OOF (M=3.07, SE=0.18). However, students were somewhat uncertain with their ability to use the concepts learned with OOF to approach new problems (M=2.5, SE=0.16) and some of them had some trouble interpreting the data they generated with OOF (M=2.5, SE=0.16). In the middle of the semester students reported their expectations on their performance of the class as between good and very good (M=3.33, SE=0.13). When we asked students if they will continue to use OOF after they are done with the course, 65% reported they will keep using it to conduct research, 35% reported they will use it for personal learning purposes, 24% reported they will only used if it is required as part of a course and 6% reported that they will probably not use it again.

Instructional Approach (pedagogy) -In this section our focus was on identifying whether OOF was a useful and engaging cognitive device for students' learning. Students reported positive responses of using OOF to generate questions that guided their thinking (M=2.73, SE=0.18), and also positively reported that using OOF made the course a lot more engaging for them compared to courses that only use lectures, homework, and readings (M=3.13, SE=0.18). We asked students how OOF helped them the most during their learning process and some responses were:

> "help me to know how to optimize the mesh from the given photos obtained from the true experimental images. (ex: EBSD....)"

> "The Visualizations"

> "It is a quick way to demonstrate the workflow of a finite element code."

> "Fairly intuitive. Pop-up explanation boxes are helpful."

In contrast, we also asked students how OOF inhibited their learning process. Some responses were related to performance issues, difficulties in learning, and transparency of the simulation tool:

> "No Windows edition. It is not easy for me to use OOF2. I need to install Cygwin and many other needed software. The most part for me is to connect Cygwin and all other softwares needed."

> "I am interested in element development which is not visible to the end user of OOF."

> "Not sure how to refine certain points in a mesh."

Finally, we also asked students what could be done to make OOF more useful for their learning in the course:

> "I found using this tool little complicated. A video demo with very elementary application will be good for the beginners like me."

> "More user friendly and more clarity in what is happening to the program when running."

> "OOF isn't a very user friendly and easy to learn application."

> "User defined elements, element development tutorials."

> "I need a better understanding of the tools and options."

Usability –Students found OOF very intuitive (M=2.94, SE=0.14) as well as easy to use (M=2.88, SE=0.18).

FiPy

Students reported that they used FiPy to implement models provided by the instructor (56%), used to generate data (50%) and to generate plots and then do some reading of values (56%).

Learning Outcomes (content) – In this section we report the general experience students had and their level of satisfaction. We also report relevance of the content to whether students thought FiPy was relevant to their areas of interest. Students were positive in their responses of considering using FiPy as a positive experience (M=3.5, SE=0.17). Students stated they considered the assignments related to FiPy as highly relevant to their areas of interest (M=2.93, SE=0.28) and that such assignments supported their goals and expectations for the course (M=3.27, SE=0.33). Students also reporting considering the course as highly relevant to their areas of interest (M=3.54, SE=0.14). We also asked students to describe their areas of interests as associated to the homework assignments related to FiPy. Students' responses were related to their research:

> "My research area is polymer based solar cell, where I work on process modeling. Fipy based HW like spinodal decomposition is very helpful for my research."

> "Very closely related. My research is in modeling microstructural evolution."

> "My areas of interest are generally related to elastic properties of multi-phased materials. FiPy was used to model various phenomena that occur in materials processing and can determine the micro-structure to be

analyzed with other tools."

"I was only interested in the phase field method. But I really learned a lot from FiPy, especially the phase field examples in the FiPy manual."

Evidence of Learning (assessment) - In this section describes how students perceived FiPy as useful for their learning and their transfer of it to practical situations. Students stated they were able comprehend the concepts better by using FiPy as compared to lectures and readings only (M=3.0, SE=0.16). Students also stated positive responses in their ability to apply concepts learned in class to the lab practice related to FiPy (M=3.18, SE=0.25) and reported an increased awareness of the practical application of the concepts related to FiPy (M=3.15, SE=0.19). Students reported inconclusive positive responses with their ability to use the concepts learned with FiPy to approach new problems (M=2.8, SE=0.17) and some of them had some trouble interpreting the data they generated with FiPy (M=2.5, SE=0.25). Towards the end of the semester students maintained their expectations on their performance of the class as between good and very good (M=3.38, SE=0.14). Students were asked whether they will continue to use FiPy after they are done with the course, 71% reported they will keep using it to conduct research, 43% reported they will use it for personal learning purposes, 14% reported they will only used if it is required as part of a course and 14% reported that they will probably not use it again.

Instructional Approach (pedagogy) –Here we report how students identified FiPy as a useful and engaging cognitive device for their learning. Students reported positive responses of using FiPy to generate questions that guided their thinking (M=2.92, SE=0.14), and also positively reported that using FiPy made the course a lot more engaging for them compared to courses that only use lectures, homework, and readings (M=3.15, SE=0.15). We also asked students how FiPy helped them the most during their learning process and some responses were:

"I can now solve many complicated but important PDE very quickly."

"fipy gives easy way to deal with PDE. we can therefore focus on the physics behind the PDE whiteout being distracted by the numerical problems."

"The examples taught me about the phase field method."

We also asked students how FiPy inhibited their learning process. All responses pointed out that FiPy did not inhibit their learning process. In the last question, we asked students what could be done to make FiPy more useful for their learning in the course:

"some video demo"

"it's perfect. It should have integration routines."

"more user friendly sometimes you get lost in the code"

> "python is quite new for me, so it would be much better if some fundamental about python can be provided before fipy is taught."

Usability –Students reported finding FiPy very intuitive (M=3.0, SE=0.17) and easy to use (M=3.0, SE=0.20).

Discussion and Conclusion

The results of this study indicate students' positive perceptions of OOF and FiPy as useful learning resources to understand concepts and ideas of modeling and simulation of computational materials such as microstructure modeling and design, microstructural evolution, and model development, implementation, and validation. Potential factors that may have influenced students' ability to engage in inquiry learning experiences are first their level of interest of the class as the topics were related to their areas of research. The most beneficial aspects identified by students as related to the tools are in the visualizations that allowed them to better understand aspects related to computational materials. Another beneficial aspect identified was students' ability to focus on the physical phenomena while the simulation tool (i.e., FiPy) took care of the computation of partial differential equations.

Minor differences were identified on students' perceptions between OOF and FiPy as learning tools. These minor differences can be found in aspects that may inhibit students' learning processes. Some of these aspects can be related to performance and usability. These differences may also be related to transparency aspects of the simulation tool; for example, mathematical and/or computational aspects that are not available for the end user. Another aspect that may influence students' learning experience is their prior programming knowledge, as not all students were comfortable programming in Python. A third aspect found in both simulation tools that may have influenced students' learning experience relates to usability aspects. Few students pointed out as a factor to improve the complexity of the interface, as students pointed out that the simulation tools are somewhat complicated to use.

The results of this study point out to several implications for enhancing students' experience using these tools. It has been identified that the inclusion of a tutorial or online demonstration may be beneficial, for not only explaining technical aspects such as description of all options of the tools, but also for explaining theoretical aspects such as how to refine certain points in a mesh. Finally, by these same means (e.g. tutorials, demos, etc.) the transparency of the simulation can be increased by explaining students "what is happening to the program when running".

In conclusion, literature has emphasized the need of integrating computational materials courses into the curriculum. We believe that in this process it is also important to focus not only on the what but on the how these courses are implemented. In this study we have focused on students' perceptions of the use of computational simulation tools as useful for their learning. The inclusion of OOF and FiPy as part of the course Introduction to Computational Materials have offered students an opportunity to apply the main concepts to a topic of their interest focusing on modeling and simulation of computational materials. By focusing on students' perceptions of these tools, we hope that these results may provide useful information and insights into the goals of computational materials science education that can be considered when designing pedagogical aspects.

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