ABSTRACT

Computer science enrollments have started to rise again, but the percentage of women undergraduates in computer science is still low. Some studies indicate this might be due to a lack of awareness of computer science at the high school level. We present our experiences running a 5-year, high school outreach program that introduces information about computer science within the context of required chemistry courses. We developed interactive worksheets using Molecular Workbench that help the students learn chemistry and computer science concepts related to relevant events such as the gulf oil spill. Our evaluation of the effectiveness of this approach indicates that the students do become more aware of computer science as a discipline, but system support issues in the classroom can make the approach difficult for teachers and discouraging for the students.

Categories and Subject Descriptors
K.3.2 [Computer and Info Science Education]: Computer science education

General Terms
Design, Experimentation, Human Factors

Keywords
high school outreach, interactive worksheets, chemistry

1. INTRODUCTION

We present a high school outreach program that introduces high school students to computer science in the context of interactive worksheets developed in Molecular Workbench. High school outreach is important because the enrollment of underrepresented groups in computer science such as women and minorities is still quite low. Carter [3] surveyed 836 high school students from a variety of backgrounds about their impressions of computer science and whether they were considering computer science as a major. Unfortunately, 80% of the students surveyed had “no idea what Computer Science majors learned.” This is a major issue in Colorado due to the lack of computer science courses being taught in high schools. From 2005-2011, only 1.5% of the 116,281 Advanced Placement STEM (Science Technology Engineering and Math) exams taken in Colorado were the computer science exams [7].

Based on such observations, we introduced some computer science concepts to local high school students in coordination with their current science curriculum. Our team includes two high-school chemistry teachers, three summer research undergraduates (all women), and a computer science assistant/associate professor. Additionally, during the summers of 2008 through 2012, we developed interactive worksheets using Molecular Workbench [15] and then deployed the worksheets in the classroom during the school years. The worksheets include chemistry and computer science concepts about current events such as the gulf oil spill and issues that students find generally interesting such as how mobile devices work and what materials are used to make the mobile devices. During the summer of 2012, we held a 3-day, hands-on workshop for a group of 19 junior high and high school teachers to teach them how to develop interactive worksheets for their classrooms.

In many regions throughout the country, related outreach programs are in place or currently in development. In a three-day summer workshop, Hart et al. [5] presented an outreach program where high school math teachers learned ways to incorporate computer science related examples into their courses. Owens and Matthews [8] have developed and piloted a four-week CyberCivics unit for AP Government in which high school students explore computer science topics and gain hands-on introductory programming experience in the context of computing issues related to electronic voting. To provide support for teachers in surrounding districts, they plan to train civics educators to implement this unit when they return to their classrooms. These examples all share the theme of incorporating computer science concepts into current curricular standards.

To evaluate our approach, we developed four different surveys: three that were given to students over a 5 year period
and one that was administered a month after the summer workshop for the high school teachers. The goal of the surveys for the students was to determine what impact the electronic worksheets with computer science concepts had on their attitude and understanding of computer science. The goal of the survey for the high school teachers was to determine how feasible such an approach is in the long term. Are other junior high and high school teachers willing to use such technology in their classroom and become computer science ambassadors? We also qualitatively evaluate the 5 year experience and indicate what worked and what did not.

2. CREATING THE WORKSHEETS
The goal of the project was to introduce high school students to computer science without the benefit of formal computer science courses offered at the high school. We did this by introducing computer science concepts alongside chemistry concepts within interactive worksheets. Some of the worksheets that have resulted from this work include[1] building atoms[2] (1) (2) evaporation[3] (3) movie/entertainment industry[4] and (4) the gulf oil spill. Some of these concepts were described in the previous section. Additionally, simulations were also used directly to convey chemical concepts, as in the case of building atoms one sub-atomic particle at a time to teach atomic theory.

The primary goal was to introduce students indirectly to computer science as a discipline alongside chemistry concepts using relevant topics. We developed worksheets that described Facebook and internet safety, a worksheet that described computer science concepts that are portrayed correctly and incorrectly in movies and video games, and a worksheet that described materials used in mobile devices alongside computer science concepts such as wireless networking. Perhaps the best example of this was a worksheet that used the gulf oil spill to illustrate how oil and water interact. The worksheet also describes how computer simulations and high performance computing are important for predicting the course of the oil spill and where to deploy cleanup crews.

2.3 Motivating the Teachers
The chemistry teachers involved in the project consider teaching chemistry their highest priority. Since the main goal of this project was to introduce computer science within the context of a chemistry course, it was important to keep the priorities of the teachers in mind while designing the project. The teachers found they were motivated to participate in this project due to a number of factors: (1) the interactive worksheets seemed to help students with abstract chemistry concepts, (2) the Colorado curriculum calls for the use of models in K-12 science, (3) the electronic worksheets helped keep students engaged, and (4) the high school teachers were able to earn a stipend and course credit over the summer.

When field tested in Spring 2009, the success of Molecular Workbench in chemistry was qualitatively evident. Students were not only actively engaged in the learning process, but made enthusiastic comments to each other with phrases like “Oh, I get it now!” and “This is fun. We need to do more of this.” It seemed that a greater number of students gave correct chemical explanations of the relative rates of evaporation in lab reports and appeared to struggle less with these sections than in past years on unit assessments.

One useful aspect of the interactive worksheets was the ability to include hints and/or answers so students have the ability to check their own understanding of specific concepts and receive immediate feedback at critical checkpoints. Teachers experience difficulty with larger classes in navigating throughout the classroom to answer questions and provide individual feedback, so this enables the teacher to monitor for common misconceptions and address these directly during class discussion at the conclusion of the activity.

Besides introducing local high school students to computer science as applied to molecular dynamics simulations, we also wanted to address specific high school curriculum requirements. Standard 5 in the Colorado K-12 science standards requires that “models are used to analyze systems involving change and constancy” for high school students. Using interactive computational models to help meet this requirement also helps students visualize the atomic-level interactions that result in the macroscopic-level observations they make during a laboratory experience. In chemistry,
students have the ability to observe what is happening at the macroscopic level through a laboratory experience but may not make the connection to the abstract, or what is happening at the molecular and atomic level. MW enables the visualization of microscopic interactions along with the ability of students to interact with these simulations.

The interactive aspect of the models helps keep students engaged, which is critical due to programs such as the new Response to Intervention requirement in Poudre School District [9] where students not performing to their academic potential must be identified and may require programs and additional staffing that must be supported by funding not available under current economic conditions. These additional benefits of this approach to high school outreach increases the possibility of involving non-computer science faculty at the high school level.

Finally, everyone’s time is valuable. To maintain a high level of commitment for five years, the two high school teacher participants received a stipend over the summer and university credit for a group study course. The stipend and university credit were planned and paid for through an NSF CAREER grant.

2.4 Example Interactive Worksheets

2.4.1 Worksheet for Evaporation

For AP Chemistry, the application of intermolecular forces to evaporation rates was selected as a curriculum target because prior familiarity with existing simulations led to a belief that this particular topic would lend itself easily to molecular modeling. Previous unit assessments of student understanding of this topic also indicated this to be an area of conceptual weakness. The MW activity, which builds on previously developed worksheets [11], precedes the actual experiment performed by the students to measure the evaporation rates of different substances. Utilizing MW, we believe that students will apply an understanding of intermolecular forces to evaporation rates with greater proficiency and to greater conceptual depth than in years past.

Students’ fundamental difficulty with understanding intermolecular forces seems to stem from the lack of ability to visualize the particles that interact, as well as the confusion of intermolecular forces with the bonds between the atoms themselves. By using MW simulations, students interact with visual representations of the forces in meaningful comparisons, which appear to translate into increased concept acquisition and retention through anecdotal evidence and preliminary student feedback.

2.4.2 Worksheet for Precipitates

Through the MW worksheet “Introduction to Solutions,” students are led through a series of models and questions related to the solution process to help them understand the properties a particular solute and solvent must have in order for a solute to dissolve. Animating the solution process allows the student to have a better grasp of solution properties that differ from that of the solvent alone. It also represents how chemical reactions occur in solution. Figure 1 shows the dissociation in water of the ionic compound silver nitrate, which breaks into $Ag^+$ and $NO_3^-$. Figure 2 demonstrates the formation of the $AgCl$ precipitate, an insoluble product resulting from the mixing of the previous ionic solutions. This worksheet builds off of models previously placed in public domain on the MW website [10][12].

During the development of this activity, some limitations of the software became evident. Because of the small mass of the atoms, gravity has little effect on them. In order to simulate a precipitate that sinks, we must introduce a larger number of atoms. At this point, the software no longer runs smoothly and the particles jump from one position to the next. In order for the molecular simulation engine to achieve the teaching goals of the worksheet, unrealistic parameters needed to be set on both the charges of the ions and the gravitational field strength. This was necessary to enable the proper ions ($Ag^+$ and $Cl^-$) to form the precipitate, the spectator ions ($Na^+$ and $NO_3^-$) to remain in solution, and only the precipitate to fall to the bottom of the container. Introducing parallelism could potentially allow the model to operate efficiently with the necessary number of particles.
and remove the need to set an unrealistic gravitational field.

2.4.3 Worksheet for Parallelization
Motivated by the need for more ions in the precipitate worksheet (see Section 2.4.2) and the goal of introducing computer science concepts to high school students, we used the Java concurrent library to parallelize parts of the molecular dynamics simulation engine in MW. We also added functionality to enable users to initiate the number of threads of parallelism and display its effect on simulation execution time. For the initial presentation of the parallelization worksheet, we borrowed a quad core from CSU.

The parallelization worksheet first illustrates the “non-smooth” updates that medium (e.g. 500 atoms) and larger (e.g. 1000 atoms) models experience in comparison to a “smooth” small model (e.g. 100 atoms). The worksheet then describes how performance problems can be analyzed by profiling the code and analyzing the methods and loops in the computation that require the most execution time. Finally, the worksheet overviews parallelization and steps the students through an experiment where they modify the number of threads and use the capability of graphing over multiple simulations to observe speedup versus number of threads.

It was not possible to build the parallelization worksheet within the existing MW framework, so we modified the Java implementation to expose control over the parallelization level. We also created a new graph type within MW to plot results such as speedup over multiple runs of a simulation. In our modified version it is now possible for a user to specify the number of threads to use when running simulations. The built-in capabilities of the scripting language allow parallelism to be set from various easy-to-use places such as sliders, spinners, etc. The second part of the support for parallelism is the ability to graph the effects parallelism has on simulations. Previously, the Molecular Workbench had a built in graphing capability; however, it only was designed to graph data that changes as a simulation runs (such as potential energy) rather than data that changes between simulations. We added a new form of graph; this one collects data for each simulation at the end of a time limit specified by the user, and displays the data in real-time. It can be graphed as a scatter plot or a mean of all data for each number of threads.

3. SHARING WHAT WE LEARNED
For the culmination of the five-year outreach project, a three-day summer workshop was offered to high school science teachers within Poudre School District. The workshop was held June 18-20, 2012 in the Computer Science building at Colorado State University. A total of 18 teachers participated in addition to the original two high school teachers that ran the workshop.

The original two high school teachers wanted to share their experiences in the classroom using Molecular Workbench especially in light of the school district’s push for more technology in the classroom. With the approval of a 2010 Mill Levy and Bond issue, the Poudre School District has committed to “refresh technology and provide technology support for student learning opportunities” and “purchase and install technology in district schools to provide learning opportuni-

ties for students.” One focus of the district is to provide a laptop computer for every high school student, starting with the incoming freshmen of the 2011-2012 school year. This commitment requires educators to investigate technology-based teaching methodologies. The idea for the three-day workshop was to provide support and time for teachers who will be incorporating these technologies into their curriculum this fall.

On the first day, we told the teachers about the overall outreach project and about computer science. Teachers were encouraged to suggest computer science as a possible discipline for students. Then we introduced teachers to the Molecular Workbench application and the idea of the electronic worksheet. Teachers were encouraged to explore Molecular Workbench simulations and worksheets in addition to other online simulations. Teachers spent the next day modifying existing electronic worksheets or developing paper and pencil worksheets and electronic worksheets to use in conjunction with existing online simulations.

During the final day of the workshop teachers shared the lessons produced, in addition to their concerns about and difficulties associated with technology-based lessons. Teachers were able to utilize the time to produce lessons geared to a variety of skill levels and science content. For example, a physics teacher developed pen and paper worksheets to be used in conjunction with PhET simulations. Two ninth grade Biology teachers modified an existing Molecular Workbench electronic worksheet on cellular transport mechanisms. Another teacher developed an electronic worksheet to be used with photosynthesis and respiration simulations accessed through another website. These lessons were then placed in a Dropbox folder to provide common access to lessons generated through the workshop.

Teacher comments during the workshop included, “Besides learning about some great learning tools, and learning from other great educators, it was just really fun.” and “Best workshop in a long time! Appreciate it!” The teachers as a group requested that this specific workshop be offered each summer. The small stipend, single university course credit, and lunch each day was a nice silver lining and showed that we respected the teachers time and effort. A survey taken a month after the workshop found that all of the survey participants (7 teachers) felt the workshop had the right balance of instruction and worktime. Six people felt the workshop was just the right length, and one person felt it could be longer. Everyone was willing or very willing to attend a similar workshop in the future. There were mixed responses in terms of whether the credit and/or stipends were needed. The university credit seemed to be the most attractive and important incentive. Most importantly, everyone indicated that they would be using the worksheets in their classrooms at least once per year, with 2 people indicating they would be using one each week.

4. EVALUATING THE IMPACT ON COMPUTER SCIENCE ATTITUDES

http://www.psdschools.org/about-us/board-leadership/major-initiatives/2010-mill-levy-bond
The main goal of the project was to introduce high school students to computer science within the context of their required chemistry courses. We evaluated the impact of this approach using three surveys. The first survey was developed by an undergraduate research assistant. The second survey was developed by another undergraduate summer student, but was based on the work of Hoegh and Moskal at the Colorado School of Mines [6], where they developed a survey tool to measure the attitudes of high school students about computer science. The third survey was developed after doing a statistical analysis of the results of the second survey.

In this section, we describe the results of each of the surveys. Unfortunately, the approach we developed did not have as much of an impact on computer science attitudes as we had hoped. Though this approach introduced the students to computer science and cleared up some misconceptions about the field, technical difficulties experienced with the machines and the network used in the high school to deploy the interactive worksheets caused some negative results in terms of how students viewed the usefulness of computer science.

4.1 The 2008-2009 Survey
During the spring semester of 2009, the computer science associate professor and an undergraduate research assistant visited Poudre High School and had students in AP Chemistry and one IB MYP (the Middle Years Program of the International Baccalaureate Program) Chemistry section complete a survey based on what the students knew about computer science and its applications. Two example questions were, “When you think of a computer scientist, what best describes what comes to your mind? [Someone who mostly writes computer programs, Someone who mostly does research, Someone who mostly installs/fixes computers or computer systems, Someone who mostly builds computers, Someone who mostly helps people when their computers aren’t working, I don’t know, Other]” and “Have you ever thought about being a computer scientist for a career? If so, are you planning to pursue this career path?”. Out of the 43 students who took the survey, 18 thought of a computer scientist as someone who mostly writes computer programs and 12 thought of a computer scientist as someone who does research. About 7 of the 43 students indicated that they were interested in becoming a computer scientist.

In the first session, the students worked with the evaporation worksheet, and in the second session, they worked with the precipitates and parallelization worksheets. The students were also asked about what they liked and did not like in the worksheet as well as for suggestions to improve the worksheet. Many of the students liked the graphical/visual interface and the interactivity. The dislikes were more varied and included the desire for more interactivity, for a bug with the thermometer to be fixed, they wanted harder questions, and they did not like that they had to print out the finished worksheet. Their suggestions included making more interactive activities, providing more facts/explanation, figure out technical issues, and present more real-life applications. The second group of students liked the worksheets because they were interesting, included simulations, and had diagrams. They disliked the worksheets because they had to read a lot, they “didn’t like Molecular Workbench,” they “did not finish so didn’t see the point of it,” and “felt that the longer questions were difficult to understand.”

4.2 The 2010-2011 Survey
To more accurately measure the impact of this program on high school students' attitudes toward computer science, we developed a survey based on the work of Hoegh and Moskal at the Colorado School of Mines [6]. Ideally, nineteen questions were to be asked both before and after Molecular Workbench activities to gauge student attitudes toward computer science. During the 2010-2011 school year, only pre-activity data was reliably gathered and analyzed to determine the validity of the survey instrument itself.

This second survey included the following quote: “Computer science is the study of computation – what can be computed and how to compute it.” [16] The quote was included to give the students some idea of what computer science is since most of these students had never taken a computer science course.

Table 1 shows the survey, which was designed to measure three constructs of student attitudes toward computer science: understanding, interest, and usefulness. The understanding construct included four questions (4, 8, 11, and 15), interest comprised six questions (3, 5, 7, 10, 12, and 14), and usefulness included four questions (2, 6, 9, and 13). The remaining questions gathered demographic information or prompted students to begin thinking about computer science applications and thus were not grouped into a particular construct. Items themselves were not actually questions but rather statements whereby students were asked to respond using a four point Likert scale: strongly disagree, disagree, agree, and strongly agree. A neutral category was not included in order to encourage students to make a positive or negative decision. Many of the questions were adapted from the work of Hoegh and Moskal.

The responses to the questions were coded on a scale from one to four, with the highest score reflecting the most positive response. The sample size was 150 students, grades ten through twelve, male and female, taken from General Chemistry, IB MYP Chemistry, and Advanced Placement Chemistry.

As was done in the Hoegh and Moskal [6] paper, we analyzed the Cronbach’s alpha for each set of questions to determine how well that question fit within each construct. The usefulness construct was seen as problematic since the responses to those four questions together do not meet the 0.7 threshold. It is interesting to note that the entire data set taken together had the highest Cronbach’s alpha, suggesting that the entire sample can be viewed as mapping to a single construct.

Upon doing a factor analysis to determine which questions correlate, we found that instead of having three constructs, we appeared to have only two constructs. Therefore we decided to only pull two constructs from this initial survey for a
Table 1: Questions on the 2010-2011 survey.

| #  | Question                                                                 |
|----|--------------------------------------------------------------------------|
| 1  | Question 1 did not use the Likert scale for its answers.                 |
| 2  | Developing computing skills will be important to my career goals.        |
| 3  | I hope I can find a career that provides the opportunity for me to use computer science concepts. |
| 4  | I am comfortable learning computing concepts such as setting up a home network and developing an excel spreadsheet with macros. |
| 5  | Students who are skilled at computer science are just as popular as other students. |
| 6  | I use my computer for solving day-to-day problems at home/school.        |
| 7  | I am interested in learning computer science concepts and skills.        |
| 8  | I find it easy to use computer applications for class assignments.       |
| 9  | Computer science concepts and skills are useful for everyone in every profession today. |
| 10 | I would like to see how computer science concepts are used in the development of video games and movies. |
| 11 | I understand that performing long division and other arithmetic tasks by hand can be described with a procedure, or algorithm, which in turn can be programmed into a computer. |
| 12 | I am likely to take a computer science class in college.                 |
| 13 | Developing computer science skills will help me secure a better job.     |
| 14 | I find that using computers within the context of other courses helps aid understanding of concepts not directly related to computing such as chemistry, history, and english. |
| 15 | I am comfortable learning computer science concepts and skills.           |

more rigorously administered pre and post survey. Table 2 shows the questions that were selected for the 2011-2012 school year survey and the reasons why the questions were selected in parentheses.

We decided to use a 15 question survey encompassing 3 constructs: Interest, Understanding, and Misconceptions. We decided to give the survey one week prior to the delivery of the Molecular Workbench lesson, and the identical post-survey within one week after the lesson.

4.3 The 2011-2012 Survey

Based on the survey analysis from the initial trial, an improved survey was given to students during the 2011-2012 academic year to assess the change in interest in, understanding of, and misconceptions around Computer Science through using computer simulations to learn Chemistry concepts with Molecular Workbench (MW) software. Students were given identical surveys both before and after an hour long interactive series of MW worksheets ranging in content from atomic structure, intermolecular forces, and nuclear chemistry for separate populations. Ideally, the pre-survey was to be given within one week prior to the MW experience and the post-survey within one week after. Problems with the hardware, both access to machines and network reliability, prevented ideal protocol from being followed in two of the three student populations.

The goal with the 2011-2012 survey was to determine if the electronic worksheets had an impact on student attitudes about computer science. To measure this we used a paired t-test, where we looked at the pre and post survey data for each student and tried to determine if the overall results were significant. A low p-value, <0.05, is statistically significant.

Table 2: Questions on the 2011-2012 survey. The factor loadings are from factor analysis and > 0.4 is considered significant.

| #  | Question                                                                                                                                 |
|----|-----------------------------------------------------------------------------------------------------------------------------------------|
| 1  | I am interested in learning computer science concepts and skills. (Question 7 in Table 1)                                              |
| 4  | I hope I can find a career that provides the opportunity for me to use computer science concepts. (Question 3 in Table 1)               |
| 7  | I am likely to take a computer science class in college. (Loaded very well on the Interest Factor in the post-survey data, 0.837)        |
| 10 | Developing computer skills will be important to my career goals. (Question 2 in Table 1 even though it was previously grouped in the usefulness construct) |
| 13 | I like to use computer science to solve problems. (adapted from Heersink and Moskal)                                               |
| 2  | I find it easy to use computer applications for class assignments. (Question 8 in Table 1)                                             |
| 5  | I use a computer for solving day-to-day problems at home/school. (Question 6 in Table 1 even though it was grouped in the usefulness construct) |
| 8  | I am comfortable learning computer science concepts. (Question 4 in Table 1)                                                            |
| 11 | Developing computer science skills will help me secure a better job. (Usefulness question in the post-survey that loaded very well on the Understanding Factor, 0.708) |
| 14 | I use computer science skills in my daily life. (adapted from Heersink and Moskal)                                                   |
| 3  | Computer science is primarily about writing programs.                                                                                  |
| 6  | Computer scientists spend all their time sitting in front of a computer.                                                               |
| 9  | Most computer scientists have poor social skills.                                                                                    |
| 12 | Most computer science jobs are being outsourced to other countries.                                                                  |
| 15 | Computer professionals are not likely to be involved in solving real world problems.                                                 |
The entire data set represented three distinct sections: pre and post survey data from General Chemistry students during an atomic structure unit, pre and post survey data from MYP Chemistry students during a nuclear chemistry unit, and pre and post survey data from AP students during a unit on intermolecular forces. Individual student responses were correlated and the paired T test was performed on the entire data set representing 101 separate students. (Approximately one-third of the data represented only pre-survey information and was removed.) Only questions 1 and 3 showed significant change in response (p-value < 0.05), with mean delta values of -0.238 and -0.178 respectively. This corresponded to a decrease in Computer Science interest as measured by question 1 and a decreased belief that Computer Science is only about writing programs as measured by question 3. The decreased interest was somewhat reinforced by a marginally significant negative result when the entire interest construct (questions 1, 4, 7, and 10) was analyzed with the paired T test: p-value = 0.0525, mean Δ = -0.0644.

When the data was split into its three distinct student populations, additional results could be gleaned. Some data was determined to span outside the time periods represented by these three populations and was thus removed. Using only the MYP Chemistry data (N = 26), the paired T test showed marginally significant results (p-value = 0.0501 in both cases) for questions 1 and 12. Interest again decreased (mean Δ = -0.269) and the misconception response measured in question 12 increased by the same amount (mean Δ = 0.269). No significant result could be gathered when the constructs were analyzed as a whole. It must be noted that a time lag of two months between pre and post survey data most certainly impacted the MYP Chemistry results. The cause of this time lag was the lack of availability of dependable computers on which to perform the surveys.

Significant results (p-value < 0.05) were seen with only the General Chemistry students for questions 1, 8, 14, and the interest construct as a whole (N = 17). Interest in computer science went down as measured by question 1 and the entire construct, mean Δ values = -0.529 and -0.206 respectively. If computer science understanding is indeed measured by question 8 (it did not load on the appropriate factor), it went up by mean Δ = 0.235. This, however, was balanced by a decrease in the average change in understanding responses as measured by question 14, mean Δ = -0.235. This is confirmed by an insignificant change in the understanding construct as a whole (p-value = 0.255). Lack of availability of dependable computers also impacted the General Chemistry results. The small number of machines available meant that the pre and post surveys were performed in teams, with each response representing a combination of two student opinions. The reliability of these results were therefore also questioned.

Finally, when only the AP student data (N = 29) was analyzed, questions 7, 12, 13, 14, and the understanding construct (questions 2, 5, and 14 combined) each showed significant change. Here ideal survey protocol was observed. The interest in Computer Science seemed to increase slightly, though question 13 did not load uniquely on the interest factor. Belief in the misconception described in question 12 decreased, while understanding of Computer Science increased as measured by question 14 and the entire construct.

Within the second-generation 15 question student Computer Science attitude survey at the high school level, 7 questions emerged as viable measures of what we labeled as Interest in Computer Science and Understanding of Computer Science as a field. Cronbach’s alpha measurements >0.7 supported the reliability of questions within each construct. Factor analysis >0.4 confirmed the loading of each question on its appropriate factor.

When the data was separated into its three distinct student populations, the paired T test on each population revealed little if any significant change in student attitudes toward Computer Science when having a Molecular Workbench computer simulation experience in a Chemistry setting. In the most reliable data set, the AP Chemistry students, what we labeled as understanding of the field of Computer Science was shown to have increased slightly, corresponding to a significant decrease in a particular Computer Science misconception. A perceived increase in student interest in Computer Science as measured on questions 7 and 13 among the AP population is balanced by the negative finding on question 1 among the entire data set encompassing all the Chemistry students surveyed. It is important to note that the lack of availability of dependable computers and network access at the high school level not only prevents the collection of reliable data but may be a contributing factor in the interest of students in the field of Computer Science.

5. CONCLUSIONS
Computational models are critical to the way science is currently done in university and industry research labs, but their use in K-12 classrooms has been limited. Molecular Workbench provides an excellent platform for integrating computational models and particle simulations into the high school classroom. Electronic worksheets are designed to teach students scientific concepts through the interactive manipulation of models and simulations, either reinforcing conventional teaching techniques or replacing them altogether. Research shows that concept acquisition is much more effective through active rather than passive student engagement.

The use of computational models at the high school level provides a vector for increasing awareness of the applications of computer science and computer science concepts. Student survey results (in a school where there is no computer science course) show that there is a varied understanding of what computer science entails and interest in computer science. Student surveys indicate that some computer science misconceptions were fixed throughout this process, but the barrier of getting the technology to reliably work is a larger issue than expected.

6. ACKNOWLEDGMENTS
This work is sponsored by NSF CAREER grant CCF 0746693. We would like to thank Shinjini Kar and Kate Ericson for their aid in putting together worksheets and survey questions for this project. We would also like to thank Christopher Wilcox for his work parallelizing MW.
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