6.3 Computational Experiments for Science and Engineering Education

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Abstract. How to integrate simulation-based engineering and science (SBES) into the science curriculum smoothly is a challenging question. For the importance of SBES to be appreciated, the core value of simulations—that they help people understand natural phenomena and solve engineering problems—must be taught. A strategy to achieve this goal is to introduce computational experiments to the science curriculum to replace or supplement textbook illustrations and exercises and to complement or frame hands-on or wet lab experiments. In this way, students will have an opportunity to learn about SBES without compromising other learning goals required by the standards and teachers will welcome these tools as they strengthen what they are already teaching. This paper demonstrates this idea using a number of examples in physics, chemistry, and engineering. These exemplary computational experiments show that it is possible to create a curriculum that is both deeper and wider.

1.0 INTRODUCTION

Before starting this paper, I feel obliged to explain how I use the terms "modeling" and "simulation." When studying the function or behavior of a system that involves time-varying properties, I prefer to use "simulations." If only the structure or configuration of a system is concerned, I prefer using "models." For example, a protein model describes a protein structure in a stable state, whereas a protein dynamics simulation describes a protein folding or binding process. But this distinction is just personal. For most of the part, the words "modeling" and "simulation" or "model" and "simulation" can be used quite interchangeably.

Simulation-based engineering and science (SBES) is defined as the discipline that provides the scientific and mathematical basis for simulating natural and engineered systems [1]. SBES is increasingly important in accelerating research and development because of the analytical power and cost effectiveness of computer simulation. Advanced simulation tools based on solving fundamental equations in physics are routinely used to understand natural phenomena and solve engineering problems. SBES is an interdisciplinary subject indispensable to the nation's continued leadership in science and technology [2].

SBES, however, has virtually no place in the current science and engineering curriculum frameworks at the secondary level. Despite the fact that modern simulation tools can run on an average computer and be used just like an ordinary application, it is still commonly thought that SBES mandates advanced mathematics and science, uses abstruse jargon, requires monster supercomputers, works only through the esoteric command line, and cannot be possibly taught or used at the secondary level. As a result, most students are not informed of the modern concepts of SBES and are deprived of an opportunity to develop an interest in it earlier in their education. The consequence of this deficiency may have contributed to the erosion of the nation's leadership in SBES and engineering and science in general [1].

One of the purposes of this multi-disciplinary conference is to create a dialogue that will lead to the development of a national plan for integrating SBES into K-20 education, a literacy framework for SBES, and a research agenda.

How to integrate SBES into the secondary curriculum is a tricky, open question. The U.S. science curriculum is often criticized to be "a mile wide and an inch deep." [3] Incorporating SBES into the existing curriculum must reconcile with the growing national consensus around the need for "fewer, higher, clearer" education standards [4]. The majority of science educators will need to be convinced that the integration of SBES into their curricula will be realistic, constructive, and helpful.

This paper suggests an implementable integration strategy that uses the products of SBES to help teachers achieve their goals in deepening students' conceptual understanding, as set by the new National Science Education Standards [4], and in doing so, conveys the core values of SBES to both students and teachers. To be practical, I will demonstrate how this strategy may work using a few concrete examples in physical science and engineering. Each of these examples shows how students can use a visual, interactive, and constructive simulation tool to conduct and design a sequence of computational experiments to explore a broad set of concepts in great depth. These examples are based on my work on creating simulation tools for science education using research-grade computational methods for solving fundamental physical laws. Resorting to first principles in physics to build educational tools may be considered as overkill by some educational developers, but it is essential to bringing learning experience with authentic science to the classroom. Of more importance, it opens up new, profound opportunities for deeper learning that will not exist otherwise, as the examples will show. Having a strong root in SBES, the examples may be used as stimulating introductions of the theory and practice of the corresponding computational methods behind the scene. By employing well-established pedagogical principles such as design-based learning [5] or constructionism [6] in the curriculum to encourage students to create simulations to answer questions, solve problems, or design systems, learning secondary science and learning SBES can have a significant overlap and a mutual enhancement can consequently occur.

2.0 WHAT IS A COMPUTATIONAL EXPERIMENT?

A computational experiment is a computer simulation of a real experiment or a computer implementation of a thought experiment. Computational experiments complement analytical theories and real experiments by providing a tool for explaining
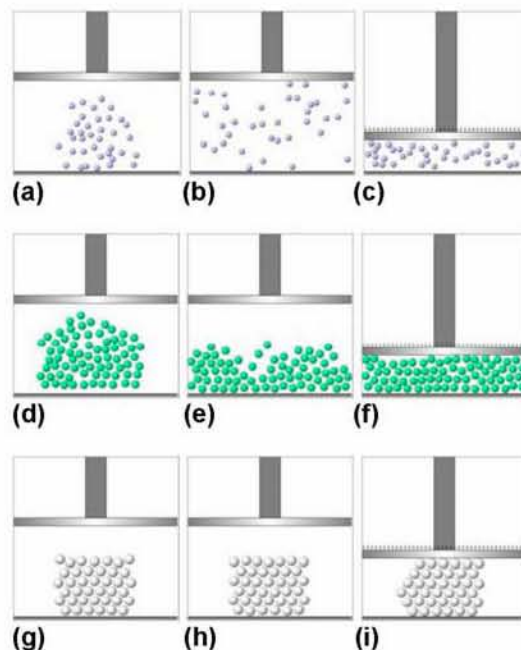
Figure 1: A computational experiment for studying states of matter. The images show if and how molecules of a gas, liquid, and solid students place into a container will fill the space and if they can be compressed. Gas: a, b, c; liquid: d, e, f; solid: g, h, i.

what was observed and predicting what will happen. With all these explanatory and predictive power, computational models, the machinery of computational experiments, have become a key element of science [7]. They are now also considered a pillar of science education—in parallel to mental and physical models—if appropriate user interfaces are provided to make them accessible to *every* student.

Figure 1 shows a computational experiment for investigating the molecular mechanisms underlying some key macroscopic properties of a gas, liquid, and solid. Students can add different types of molecules into a container maintained at a given temperature (Fig. 1a, d, g). If the molecules form a gas, they will quickly fill up the entire container and move rapidly and chaotically (Fig. 1b). If they form a liquid, they will fill up the lower part of the container and move randomly around each other (Fig. 1e). If they form a

solid, they will stay together to form an or-
dered structure (Fig. 1h) and vibrate around
some fixed positions. Now if we apply some
pressure through a piston, the gas will be
significantly compressed (Fig. 1c), whereas
the liquid and solid can hardly be (Fig. 1f, i).

As you can see from Fig. 1, the most impor-
tant properties of the three states of matter
are *all* explained on the molecular basis in a
single computational experiment using just
the mouse. All the related concepts such as
the Kinetic Molecular Theory, diffusion, lat-
tice vibration, and pressure, however dispa-
rate they may be in a textbook, are linked
and unified in the very same computational
model and can be manifested or inquired
through the computational experiment. With
a variety of visualization and analysis tools,
many more details can be discovered. For
instance, students can select a molecule
and visualize its trajectory to examine how it
moves in different states. The force vector,
velocity vector, or kinetic energy shading on
each atom can be shown to provide further
information about molecular collisions.

3.0 GOING DEEPER, REACHING WIDER

The example shown in Fig.1 demonstrates
how a computational experiment can trans-
form the way we teach states of matter. The
new way is simple enough to be applicable
even to lower grades. But the computational
model has a lot more to offer. The example
shows only the tip of the iceberg. What lies
beneath is a great number of opportunities
to go deeper and reach wider.

The computational experiment shows how
matter in different states behaves without
further explaining what makes them behave
so. Figure 2 shows the equilibrium confor-
mations of a molecular system correspond-
ing to three different strengths of interatomic
interactions, which students can adjust
through a graphical user interface shown in
Fig. 2d. This step takes students down to
the level of studying the states of matter in
terms of interaction and energy. It offers an
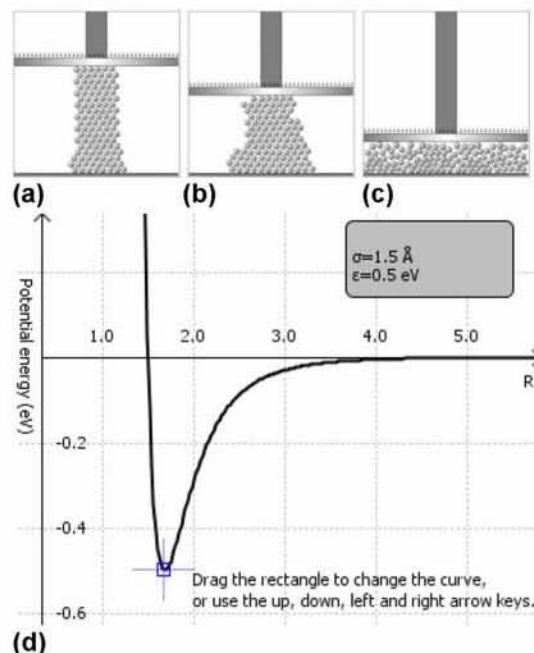
**Figure 2: The effect of interatomic interac-
tions. The potential well depths are: (a) 1
eV, (b) 0.5 eV, and (c) 0.01 eV, respective-
ly. A shape of the interatomic potential
function is shown in (d).**

intuitive explanation of the idea that stronger
attractions result in stronger materials.

With a few more mouse clicks, many other
concepts can be studied. The material
strength can be tested by increasing the
pressure on the piston and observe how the
solid is deformed, which explains plasticity.
By increasing the temperature, the solid will
become more ductile, which then explains
the business of a blacksmith. When the
temperature continues to rise, the solid will
melt down into a liquid to fill the container,
showing a phase change. If the temperature
keeps rising, the liquid will turn into a gas
and start to push the piston up, causing a
dramatic volume expansion. This explains
how heat can do work. Gas laws can also
be studied. Students can discover that un-
der the same pressure, higher temperature
will result in greater volume, and under the
same temperature, higher pressure will re-
sult in smaller volume. Students can even
ask questions not covered in most curricula
about gas laws. For example, the mass of

the molecules can be changed to see if it affects the equilibrium volume of the gas under the same pressure and temperature. Visually, it seems that the mass of molecules should affect the volume, as more massive molecules appear to move more slowly. The frequency at which they bump into the piston is, therefore, lower. But a computational experiment simply shows that molecular mass has no effect, just as suggested by the Ideal Gas Law: $PV=nRT$. This is not easy to figure out just by thinking. Even if one can reason correctly that a more massive molecule will deliver a greater impact when it collides with the piston, some mathematical work is still needed to prove that the two effects cancel out exactly. Where the mathematical skill prevents the majority of students from investigating further, the computational experiment helps them move forward. Beyond investigating the effect of mass, students can even adjust the atomic radius and the van der Waal attraction to explore how the equation of state deviates from the Ideal Gas Las. A comparison of two gases that differ only in atomic radius or van der Waals potential energy shows the effect of excluded volume or intermolecular attraction.

It is probably not an exaggeration to assert that the possibility of inquiry is only limited by the imagination of the experimenter. The breadth and depth of the science embodied in this computational experiment, along with the ease of inquiry afforded by a graphical user interface, suggest the feasibility of creating a curriculum that is both wide and deep using this type of simulations.

This prospect would not have been possible without using authentic science to build the educational tool. The scientific power demonstrated above originates from the application of the molecular dynamics method [8], which is an important tool in SBES for studying nanoscale science and engineering [9]. The computational experiment described above was designed and conducted using the *Molecular Workbench* software, which has a classical molecular dynamics tool tailor-made for science education [10].

I hope you are reasonably inspired by this introductory example. In the following section, I will discuss more about the need to use true science to build educational tools and the implication of this to SBES education. Then I will show more examples in other disciplines in later sections.

4.0 WHY USE ROCKET SCIENCE TO BUILD EDUCATIONAL TOOLS?

The educational software market is largely dominated by cartoon movies, animations, and games. Most of these media were usually produced with multimedia effects as the paramount design goal in the developers' minds. Although many claim to offer computer models, most are insufficiently intelligent to have the desired predictive power. For example, an animation that the user cannot change has only illustrative power but no predictive power at all. An interactive model or game designed to have a limited number of outcomes scripted by the developer can explain the preset causality but nothing beyond. In making the rules for determining the outcomes, many developers seldom perceive a need to exploit the "rocket science"—advanced mathematics and computation based on first principles in science. In the following, I will explain why there is such a need.

A first principle is a foundational scientific law from which many phenomena can be explained and many propositions can be derived. For example, Newton's equation of motion is the first principle in classic mechanics—everything in the domain of classic mechanics can be explained by solving it analytically or numerically. The classical molecular dynamics method that powers the computational experiment shown in the previous sections is based on solving Newton's equation of motion for a system of interacting particles that model atoms and molecules. It is responsible for all the simulations in the computational experiment that explain the myriad of concepts. There is no need for

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students to program all those—everything just emerges from the number crunching done by the computational engine according to the ruling equations.

The molecular dynamics method was, however, not originally intended for education. It was developed to help scientists and engineers explore nanoscience and engineer nanosystems [11]. The generations of computational scientists who contributed to the theory and practice of the method presumably did not anticipate that one day the method would find its place in thousands of schools all over the world. But this should not be surprising at all. In fact, science education and scientific research share a common goal: to understand how the world works. It is, therefore, no wonder that a research tool can be successfully converted into a learning tool.

Perhaps the single most important reason for using first principles to build educational tools is that all the power of explanation, prediction, and creation embodied in them will then be given to *every* student. What else is more important in education than passing students the greatest power and deepest wisdom brought to us by the most brilliant figures in the history of science and engineering? Now that the information technology has empowered us to deliver them through computing, an unprecedented opportunity to revitalize science and engineering education using this enabling technology is right upon us.

Unfortunately, this opportunity is often underappreciated in the educational world. Using first principles to build interactive media is not part of the design guidelines for the mainstream. There are many more domains of science and engineering where the curriculum needs to be transformed in a way similar to what was described in the previous sections. Enormous volumes of literature have existed for how to simulate real world problems by numerically solving fundamental equations such as the Navier-Stokes equation for fluid dynamics and the

Maxwell equations for electrodynamics and photonics. Sadly, there has been little investment and interest in making those powerful methods usable by students and the public at large.

5.0 NEW STANDARDS, NEW OPPORTUNTIES

There is now a chance for SBES to prove its value in education at a large scale. The new National Science Education Standards has put forward a "more coherent vision" of science education [4]. The framework calls for educators to focus on a limited number of core ideas and give time for students to engage in scientific investigations and achieve depth of understanding. It emphasizes that learning about science and engineering involves the integration of both content knowledge and the practices needed to engage in scientific inquiry and engineering design. It recognizes learning as an ongoing developmental progression. Exactly how this vision will turn into actions is a critical question. Given the fact that the results from the 1996 Standards have been disappointing [12], the development of creative ideas to implement the new framework in the curriculum will be more important than ever.

The recommendation of learning from core ideas is not an overstatement. Richard Feynman once noted: "I am inspired by the biological phenomena in which chemical forces are used in repetitious fashion to produce all kinds of weird effects (one of which is the author)." Indeed, the unity of science—that everything can be derived from some basic rules however their appearances and representations may differ— is probably the most profound nature of science. For students to achieve deeper learning, the curriculum must be structured to reflect this nature. Learning should focus on the basic rules as suggested by the principle of Occam's razor and science should be taught as a way of thinking based on them rather than a large collection of facts.

The idea that complexity arises from unity is the holy grail of SBES, too. A simulation

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program uses the same code in repetitious fashion to produce all kinds of results to explain the weird effects observed in the real world. The parallelism between the inner workings of a simulation and the conceptual structure of knowledge it simulates makes it an ideal cognitive tool. Being the scientific discipline about simulations, SBES can be a
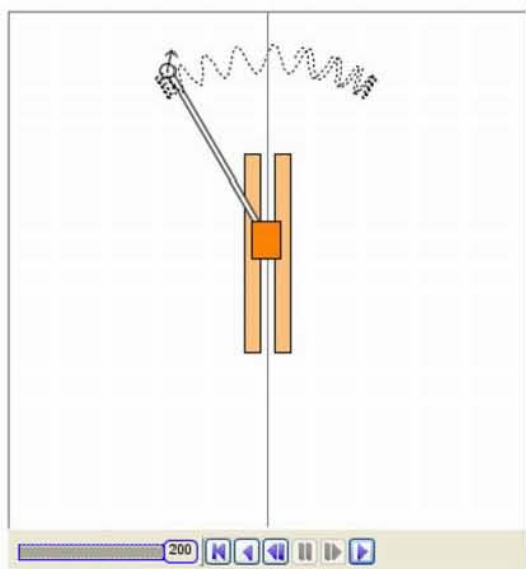
(a)
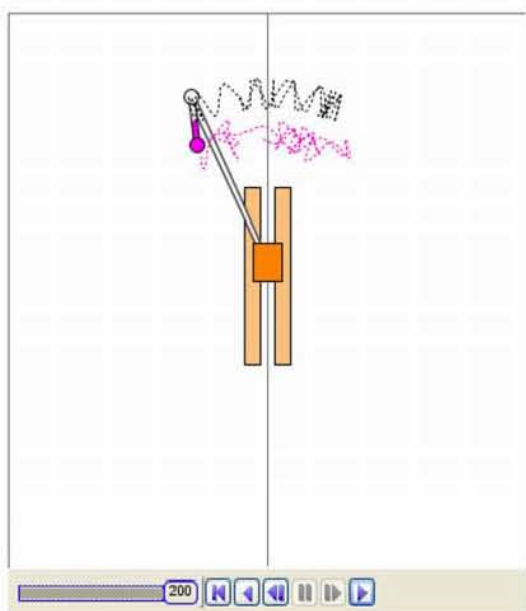
(b)

Figure 3: A computational experiment for studying the inverted single (a) and double (b) pendulums on an oscillatory

cornerstone for building the technological foundation of the new science framework.

Although the framework literally stresses the importance of simulations as a creative engine that drives the scientific and engineering enterprise, simulations are considered more as individual expressions of concepts than as possible systematic solutions to realize the vision. In fact, a simulation tool can be used not only as an inquiry tool to teach known facts as shown by the example of the states of matter, but also as a research tool to explore the unknowns. The latter provides opportunities to teach students to think and practice like scientists and engineers, a wish reiterated in the new standards. A simulation tool constitutes a computational laboratory in which students will ask questions, identifies problems, find solutions, and analyze results. The following computational experiment about the inverted pendulum, a classic problem in dynamics and control theory, shows an example of how this may work for students.

A pendulum is what every student learns in physics. An inverted pendulum is what we get when we turn it upside down after it has stopped swinging. We know this upright position will not be stable. Any blow will knock the mass off from that position. But there are ways to stabilize it. One way is to fix the pivot on a base and rapidly oscillate the base up and down. If the oscillation is simple harmonic motion, the pendulum's motion is described by the Mathieu equation, which has very complex solutions that tell how high the frequency and how large the amplitude should be in order to maintain stability.

An interesting question that immediately follows is: what will happen if we invert the double pendulum? This is a question that would almost instantaneously excite any mathematician or physicist who knows the importance of a double pendulum in nonlinear dynamics and chaos theory. The study of an inverted double pendulum may well worth a Ph.D. thesis. But never mind about the intimidation of the mathematical com-

plexity, a simulation tool can easily bring students to where the mathematicians or physicists stand. Fig. 3a shows a computational experiment designed to test the stability of the inverted pendulum. The amplitude and frequency of the oscillation of the base and the perturbation on the mass can be adjusted to study the dynamic stability. If students want to test an inverted double pendulum, they can just append another mass to the mass as shown in Fig. 3b. Can this chaotic system be stable in the face of the butterfly effect? In other words, does unpredictability necessarily imply instability?

I will leave this interesting question for you to ponder. The central point of this example is that it demonstrates the enormous educational value of a simulation tool in supporting *all* levels of scientific investigations, which in this case range from a well-known problem (a single pendulum) to a less-known problem (an inverted pendulum) and then to an unknown problem (an inverted double pendulum).

6.0 ENGINEERING DESIGN
Engineering is considered an integral part of the new standards. Engineering design is a creative and iterative process for identifying and solving problems under various constraints. It is a core element to engineering like inquiry to science.

Modern engineering methodologies heavily involve SBES. Computer simulations are often used to screen solutions to a particular problem or optimize a design before building the real system. One of the most successful applications of SBES to solve engineering problems is computational fluid dynamics (CFD).

Deeply at the core, CFD involves sophisticated numeric methods for solving the Navier-Stokes equation such as the finite difference method or the finite element method. While it may be inappropriate to teach the nuts and bolts of these numerical methods at the secondary level, it is desirable to teach how engineers use these tools to

solve problems. This is similar to teaching how to use CAD tools to design structures without teaching the computational geometry under the hood. In fact, simulated fluid flows, when visualized, are intuitive enough for students to understand. For example, the Kármán vortex street is mathematically complicated but probably not incomprehensible as similar patterns are not uncom-
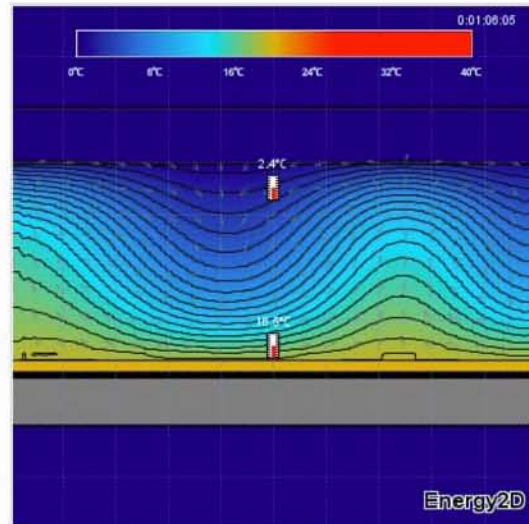
(a)
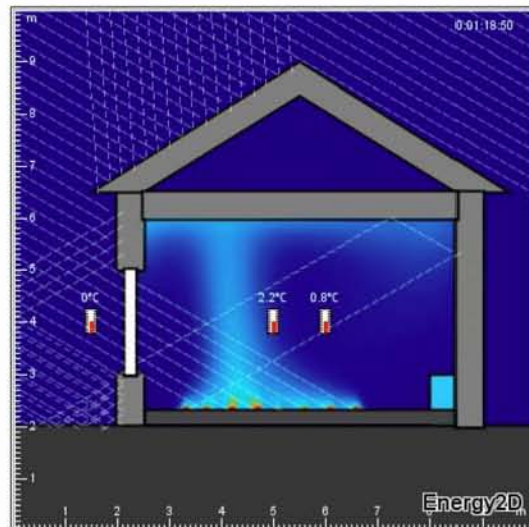
(b)

Figure 4: (a) A computational experiment for studying the Rayleigh-Benard convection pattern of a fluid between a cold plate and a hot plate. (b) A computational experiment for studying solar heating of a house through a window.

mon in everyday life. The key is to develop the user interfaces that will make these tools visually and manually accessible to students and, importantly to engineering, make it possible for students to design with them.

Ironically, while there are numerous CFD tools developed for professionals to tackle engineering problems, little has been done to make a CFD tool for average secondary students to learn with the powerful method. With all the dramatic, artistic effects of flow that worth the volume of a book [13], CFD has enormous potential to bring fun and enjoyable learning experience to the classroom. This potential should not be left untapped any longer.

Figure 4 shows two computational experiments designed using an educational CFD tool called *Energy2D* I created to move towards the goal of providing a versatile CFD laboratory for students. The tool allows the user to set up a 2D thermal system such as a house and run CFD simulations to assess the energy flow within it. Ultimately, this tool will be integrated into a 3D environment for students to evaluate and optimize their designs for real world applications such as a green building, an internal combustion engine, or a cooling system for a CPU. But even the 2D simulations show the richness of science and engineering concepts students can explore. For example, the temperature difference between the hot plate and the cold plate in Fig. 4a can be adjusted to test when the convective pattern becomes turbulent. The angle of sunlight can be changed to investigate solar heating of a house at different times of the day, as shown in Fig. 4b. Virtual thermometers can be placed in the model house to monitor temperature changes at any locations to check if a passive solar design meets the requirements of thermal comfort. When the house is heated internally, a virtual thermostat can be added to maintain the indoor temperature. Students can evaluate energy costs under various conditions and constraints. For example, if the environmental temperature is one degree colder, how much more energy will be needed to keep the house as warm? If the sun is shining into the house through a window, how much energy can be saved? With a learning environment like this, many engineering problems and design challenges can be posed to students.

7.0 DISCUSSIONS
In this section, I would like to make a few further suggestions on how to foster SBES's role in the upcoming reform of science and engineering education.

7.1 Blurring the line between research and education
Modern personal computers have become fast enough to run serious simulations that involve intense computation. The ubiquity of multicore processors in the near future will only make computers even more powerful. What can science education benefit from personal computers that rival supercomputers only one or two decades ago?

Scientific simulation software programs, the direct products of SBES, can capitalize from ubiquitous multicore computing [14]. Powerful simulation tools running on powerful multicore computers have the potential of becoming one of the most powerful scientific investigation tools for education, just like their supercomputing counterparts to scientists and engineers but only much more accessible. Recent studies revealed that children are born investigators, capable of reasoning in a surprisingly sophisticated way about the natural world based on direct experiences with the physical environment [15]. If easy-to-use graphical user interfaces, or even the more modern touch interfaces, are provided, there is fundamentally nothing that can prevent them from becoming amateur scientists and engineers. With powerful simulation tools at students' fingertips, the line between research and education will be blurred and science can then be taught as the way it is. When the difference between learning and investigation diminishes, the curriculum can become a fantas-

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tic journey to discover the jewels of science and engineering.

7.2 Learning from games but not counting on them

Outside education, game developers have adopted first principles far more quickly and aptly. Games need to have realistic look-and-feels in order to be competitive in the market that always demands better realism. Major graphics libraries already provide excellent lighting functions. Realistic motions and flows powered by physics engines such as *Lagoa Multiphysics* and *Maya Fluid Effects* are now available for animators. Real-time physics games such as *Algodoo* and *Crayon Physics* are making inroads into classrooms at the lightning speed. There is a lot to learn from the success of games.

But game developers are only interested in technologies that can entertain the player and are not necessarily willing to invest on things like quantum mechanics, genome dynamics, or climate modeling. The future of science and engineering education cannot rely on the good will of the game industry. It lies in the hands of a strong alliance between scientists, engineers, and educators. The SBES community is among the foremost groups that can lead the charge and bridge the gap.

7.3 Learning by creating simulations

One of the most important affordances of open-ended simulation tools such as the *Molecular Workbench* software is the ability for students to create their own simulations. Only through the creation process can learning be maximally deepened and personalized. This kind of simulation tools offers an important method to implement the theory of constructionism [6] or learning by design [5] for the scientific fields they grow out from. A good user interface will allow students to design any computational experiments to test their own hypotheses. In our field tests with the *Molecular Workbench* software, we found students became very creative once they were given creative tools. We were initially concerned that stu-

dents would just copy each other's design or duplicate a demo, thus invalidating the pedagogy. But this did not happen. On the contrary, it turned out that a surprisingly high percentage of students came up with creative solutions that even professional scientists had never thought of.

Learning science by designing new simulations has a substantial overlap with learning the practice of SBES. Both aim at using simulations to prove a concept or test a design. The only difference is that the mission of the SBES professionals is to explore the unknowns on behalf of the society whereas students are only exploring on their own behalves what is probably only new to themselves. But this difference is not really fundamental, except for a cutting-edge research task requires a higher skill level and a broader scope of knowledge. If an educational tool employs true SBES, some of the modeling skills and knowledge students learn from creating their own simulations in classrooms may end up transferring into SBES literacy and skills. For instance, students may learn some basic data analysis skills that are commonly needed to understand a simulation in both a research setting and an educational setting.

Creating simulations for learning science provides the necessary contextualization for SBES to be adopted in the science curriculum, as well as the driving force for engaging students and teachers to pursue SBES. Nothing is more rewarding than seeing one's own simulations at work. And nothing is more satisfying than seeing one's own students succeeding in doing impressive work. As such, students are more likely to be motivated to learn more deeply and dig under the hood of SBES in order to improve their own simulations. And teachers are more likely to adopt the tools if they see their potential.

8.0 CONCLUSIONS

This paper suggests a strategy for integrating SBES into the science curriculum using computational experiments as the facilita-

tors. How to implement the strategy under the conceptual framework of the new National Science Education Standards was discussed and substantiated by a number of concrete examples in physical science and engineering. It was elucidated that powerful scientific simulations can serve as cognitive tools for learning science and engineering more profoundly. An important outcome of adopting computational experiments in the science curriculum will be that they will also provide pathways to teach the principles and practices of SBES.

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