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Computational Experiments for Science Education

Computational experiments based on solving fundamental physics equations bring authentic science to the classroom.

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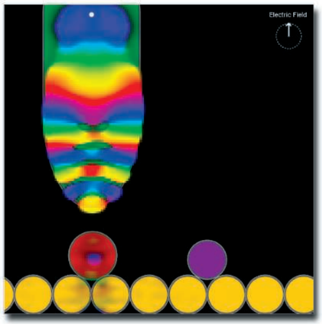
Computational physics, which provides digital representations of natural phenomena by solving their governing equations numerically, has transformed areas as diverse as scientific research, engineering design (*1*), and film production (*2*). It is also changing the way science is taught. The *Molecular Workbench* (MW) software, http://mw.concord.org, developed by the Concord Consortium, illustrates this perspective. MW models atomic-scale phenomena on the basis of molecular dynamics and quantum mechanics calculations, which enables students to carry out computational experiments to investigate and learn a wide range of science concepts.

The atomic world is alien to students: Electrons, atoms, and molecules are too small to be seen, and their interactions resemble nothing in the everyday observations that shape our intuitions. In the world of electromagnetic forces, thermodynamics, and quantum mechanics, there is little that students can assemble or tear apart with their bare hands in order to learn how those rules work. Traditional static ball-and-stick models of molecules fall short of conveying those essentially dynamic rules.

When direct hands-on experiences are not feasible in the classroom, computational experiments provide attractive alternatives. Inquiry through computational experiments is similar to inquiry through real experiments: Students observe visualizations, raise "what-if" questions, formulate hypotheses, design and conduct investigations to test their ideas, and, finally, analyze and interpret results. In some cases, good simulations can be just as effective as their real counterparts (*3*, *4*).

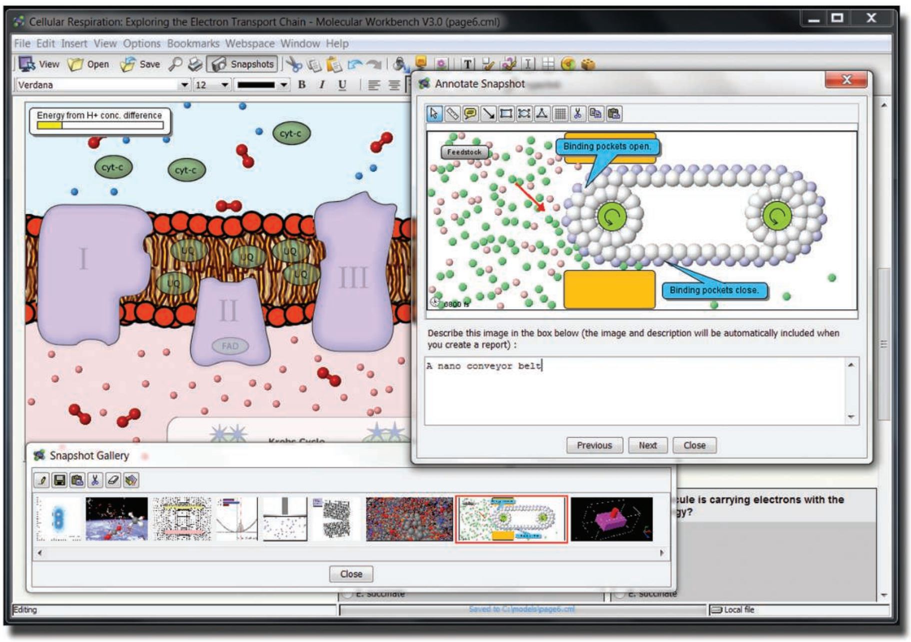


Scanning tunneling microscopy simulation. Using MW's quantum dynamics engine, the tunneling current from the probe tip to an atom sitting at the surface of a substrate is dynamically visualized. The electron wave is colored by the phase.

For a computer simulation to become a versatile experimentation tool, a computational engine capable of accurately simulating many real-world situations is needed. Each instance of such a generic engine models a specific phenomenon. For example, the computer models of a pendulum and a spring are two engines for solving Newton's equation of motion. The two appear to be different, but they are computed using the exact same engine.

MW is a tool for designing and conducting computational experiments with atoms and molecules, based on molecular dynamics and quantum dynamics simulation methods that originate from molecular modeling research (*5*). These computational methods approximate the fundamental laws in the world of atoms and molecules, and so MW's computational engines create dynamic visualizations of atomic motions and electron waves (see the first figure). The molecular dynamics engine uses classical mechanics to predict the motion of atoms according to the forces computed from potential energy functions that model interatomic interactions (*6*). The quantum dynamics engine solves the time-dependent Schrödinger equation to predict the propagation of wave functions in potential fields that model atomic-scale structures (*7*). The engines can be configured to simulate real or thought experiments. Users can intervene in the calculation by changing variables as the engines run. The results are visualized instantaneously, which allow users to observe and interact with the emergent phenomena. Using MW's capacity for embedding computational experiments in curriculum materials, we and other MW users have created hundreds of classroom-ready interactive online lessons that have been widely used.

The computational engines in MW cover a broad scope of science topics, including gas laws, states of matter, chemical bonding, chemical reactions, electrostatics, heat transfer, fluid mechanics, fractures, quantum



Simulation snapshot. An image taken from the simulation of a hypothetical nano conveyor belt designed to selectively transport molecules across a membrane.

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mechanics, diffusion, osmosis, self-assembly, and so on (see the second figure). The fact that many seemingly disparate phenomena emerge from a couple of computational engines that employ only a few general scientific laws demonstrates the unity of science, a profundity noted by physicist Richard Feynman in his famous lecture that opened the field of nanotechnology: "I am inspired by the biological phenomena in which chemical forces are used in repetitious fashion to produce all kinds of weird effects" (*8*). This unity is key to addressing the problem in U.S. science curriculum, famously described as "a mile wide and an inch deep" (*9*). Recognizing this problem, the Conceptual Framework for the New Science Education Standards has put forward a "more coherent vision" to move in the direction of "fewer, higher, clearer" standards (*10*).

An integrative tool such as MW can support novel instructional strategies that focus on the conceptual unity of otherwise fragmented factual knowledge. For example, the microscopic pictures and the macroscopic properties of the three states of matter are typically taught as individual facts. But all of them can be explained and connected using a single computational experiment with a particulate model: Students add particles into a container under a piston, adjust their properties, and run molecular dynamics simulations to see what happens. They discover that gas particles move freely to assume the entire volume of the container, liquid particles flow to occupy the lowest part of the container, and solid particles vibrate and maintain a fixed volume and shape. When pushing the piston, they find that a gas can be significantly compressed, whereas a liquid or a solid can hardly be. Gradually raising the temperature of a solid, they observe how it softens, collapses, melts, evaporates, and expands. They can even fiddle with the interaction potential among particles to study how it is responsible for the formation of each phase. Such a computational experiment unites many different ideas and provides the micro-macro connections needed for developing a deeper, more coherent understanding.

The fundamental physical laws used to build MW's engines ensure the accuracy and depth of many computational experiments they support. For example, the First and Second Laws of thermodynamics, the Boltzmann distribution, Fourier's law of heat conduction, Raoult's law, Pascal's principle, Archimedes's principle of buoyancy, and the ideal gas law can be discovered or tested. This capacity extends learning to the level of quantitative analysis, which is an important part of scientific experiments.

An open-ended tool such as MW allows students to construct their own artifacts to generate and evaluate their own ideas. Learning through creating a computational experiment to answer a challenge complements learning through interacting with an existing one (*11*).This approach sets a higher goal for students and often motivates them to learn more actively. For example, when teaching the ideal gas law ($PV = Nk_BT$), instructors can ask students to design computational experiments to investigate a number of interesting questions, such as, "Why doesn't the law include molecular mass as a factor?" and "Why should *N* be the number of molecules but not the number of atoms?" These questions are hard to answer without a mastery of complex mathematics and statistical mechanics. But with MW's graphical user interface, students can bypass those barriers and come up with computational evidence and explanations. What would have been difficult to accomplish is simplified to visual manipulations.

General and physical chemistry students in a pilot study produced nearly 150 computational experiments to explore principles and applications in chemistry; such as ionic bonding, purification, and fuel cells. When challenged to come up with designs that break the ideal gas law, students created surprising solutions. They studied factors ranging from molecular size and mass, the strength and range of the van der Waals attractions, to covalent bonding. One student even meticulously constructed a setup that showed the correlation between the gas laws and the law of energy equipartition. The creativity of these students was unleashed. Their experiences of learning chemistry were transformed into fruitful science explorations.

MW represents a successful application of computational physics to developing effective learning tools. The generations of computational scientists who contributed to the theory and practice of the subject presumably did not anticipate that one day their techniques would benefit thousands of schools all over the world. In fact, education and research share a common goal: to understand how the world works. It is, therefore, not a surprise that a research technique can be successfully converted into a learning tool. This makes us wonder how many other tools invented by scientists and engineers are still waiting to be "discovered" by educators and translated into educational technology.

About the Authors

Charles Xie is the computational physicist who created the Molecular Workbench. **Robert Tinker** is the founder of the Concord Consortium. **Barbara Tinker** was the project manager. **Amy Pallant** is a senior educational researcher. **Daniel Damelin** is a senior curriculum developer. **Boris Berenfeld** was a senior scientist. Robert and Boris served as the principal investigator (PI) and co-principal investigator of several molecular literacy projects that developed the molecular dynamics engine. Charles served as the PI of a nanotechnology project that developed the quantum dynamics engine." **Group portrait:** A. Pallant, D. Damelin, B. Tinker, B. Berenfeld, C. Xie, and R. Tinker.

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