TAMING SCIENCE MODELS FOR CLASSROOM USE

Boris Berenfeld, Dan Damelin, Amy Pallant, Barbara Tinker, Robert Tinker, and Qian Xie
The Molecular Workbench Team, Concord Consortium
http://workbench.concord.org
boris@concord.org

Model building is a fundamental part of science. Many scientists labor long hours adding small but important details to a model. The excitement of science reaches a peak when new data confirms a proposed model, or forces the modification of fundamental parts of a model. The image of Watson and Crick assembling the skeleton on the outside and pair bases inside the DNA helix comes to mind, with their subsequent delight as parts of the model finally fit together.

Highly maneuverable computer-based models give students the opportunity to participate in exciting discoveries of their own. The kinds of models used in research, however, rarely are found in education. In this article, we will consider the adaptation of research-grade models for the classroom, and the importance of the accompanying instruction that allows students access to and experimentation with models. Finally, we will present some research findings obtained in schools in which the use of our dynamic molecular models was tested.

Why do scientists need models?

The goal of one category of computational modeling in research is to build a comprehensive model of a process or phenomenon that mirrors reality so precisely that it has both explanatory and predictive value. Models of weather, plate tectonics, and the growth of a coral reef or cell are in this category.

In other cases, scientists build models that purposely strip out details so that the remaining, simplified components more clearly reveal the fundamental mechanism. Sometimes simplification is essential just to produce a model that can be computed.

Models range from scale models, such as a model car, or a ball and stick model of a molecule, to the purely mathematical. Most models are incomplete, growing as the scope of experimental data expands, as in the case of modern models of carcinogenesis. Most theory can be represented by a model, which has the power both to explain phenomena and to predict the impact of variations in values and relationships.

Today Crick and Watson might well have created their model on a computer instead of constructing their beautiful DNA model from machined parts. Computer models have greatly improved the ease of trying new molecular configurations, or exploring various forces applied to the structures. Investigators can easily ask "what if" questions such as: What if we change pressure? Increase the temperature? Change elasticity? Change the angle of attachment, polarity, or distance between chemical groups? What if we try this compound instead of that?

Why does science education need computer models?

In our classrooms today, students rarely build and use even physical models. When they do use models at all, they serve largely to illustrate rather than expand upon the content on which students are working. They rarely work as a vehicle for prediction and discovery. This is a waste.

Models make for good education. Models can supplement hands-on experiments, and can do so economically. In addition, their abstract nature furthers student learning of new orders of analysis. Providing students with access to good models will assure that students have opportunities to abstract essential principles, to explore relationships among parts, and to experiment by manipulating variables.

Today an emphasis on model-based reasoning fits in with the current view of science education. It appears that modeling software that is sufficiently flexible and requires students to interact or construct their own models can engage students in authentic scientific inquiry and reasoning. (Tinker, 2001,[1] Gobert and Clement 1994,[2] 1999,[3] Sabelli, 1994,[4] Linn & Muilenberg, 1996[5]). Interactive models can address core ideas in a visually engaging way that makes them more accessible to students with vastly different learning styles. Research is showing that, as students are able not only to run the models but also change key variables, they are more likely to remember and transfer their learning to new situations.

Computer power increases. During the last decade, the power of machines for student computing has increased almost a hundred-fold. Sometimes the question is asked: Why do schools need power machines? While there is no need for extremely powerful and fast machines to browse the

web or edit text, in fact a lot of computer "horsepower" is required to run a good dynamic model. These computer models allow investigators to calculate and display in real time interactions between significant number of components, visualize objects that are too many and small to see, or move too fast, or are too big, and require visualization of interactions with many other objects. These generally require many computational steps.

Seeing the molecular world. The arrival of computer models for the classroom is timely. The need for models of the molecular world is particularly acute, as this world is out-of view and different enough from the macroscopic world to require special attention. Discoveries of atomic-molecular phenomena, furthermore, are driving current research. A good model addressing fundamentals of the molecular world (e.g. thermal motion, conservation of energy, polar and non-polar interactions), furthermore, can be called upon in many science settings.

Computer models can help bridge the gap between professional science and classroom laboratory exploration, but the pathway between the two needs to be walked with care. Research-grade models are notoriously large, computationally heavy, and assume much preexisting knowledge. It is easy to overwhelm students with models that are too unappealing and detailed. It is also easy to give students misconceptions by oversimplifying them. Our challenge is to make models that are both good teaching tools and that are scientifically accurate.

The Molecular Workbench Project

The goal of the *Molecular Workbench Project* http://workbench.concord.org, funded by the U.S. National Science Foundation (NSF), has been to research whether the use of atomic scale models can improve student reasoning about atoms and molecules, and how atomic scale properties relate to macroscopic phenomena. Not only physics, but also much of chemistry and modern biology is based on a "molecular view," but this is seldom addressed in beginning courses, largely because it is very difficult to learn from static pictures and narratives, or even simple animations. It is the thesis of the Molecular Workbench research that, by engaging students in scaffolded model-based experiments with interactive, dynamic models, they can obtain a deep conceptual understanding of atomic-scale phenomena and their relationship to macroscopic phenomena.

How we have developed middle ground models: The *Concord Modeling Workbench* software

The *Molecular Workbench Project* has developed an atomic/molecular engine capable of being used in the classroom as an underpinning to teaching fundamental science. The *Concord Modeling Workbench (v. 1.1)* is freely available at http://workbench.concord.org/modeler/index.html.

The *Concord Modeling Workbench* software is an extremely versatile set of modeling tools based on current research in computational physics, which can be used to compute and visualize the motion of ensembles of atoms and molecules. The motion of each entity is estimated using classical dynamics and applicable forces, from Van der Waals potentials, Coulomb interactions, and harmonic approximations, to bonds, external fields, and boundaries. Meso-scale objects and their interactions are supported. (**e.g. See Fig. 1)**

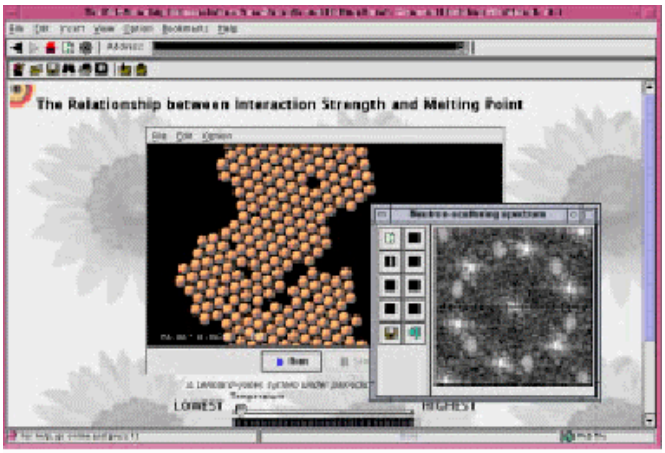

Figure 1: The Concord Modeling Workbench with one of its more professional displays.

Source: Concord Consortium

The resulting ensembles can illustrate energy conservation, gas laws, pressure, phase transitions, chemical bonding, chemical reactions, Maxwell velocity distribution, osmosis, electrolysis, electrophoresis, liquid crystals, polymers, and more. Preexisting models can be used by high school and college students to explore a vast range of content, or students can use the Concord Modeling Workbench tools to develop their own models. Models for students at any specific level can be built using the strategies described below.

We have taken several different approaches to 'taming' this research-grade science model, which can work as is in a college classroom fairly comfortably. The first approach (A) has been to develop ways for teachers and curriculum developers to work directly with the model, selecting and modifying the buttons and sliders, as well as text and pictures associated with the models. The second approach (B) has been to use a language for programmers, *Pedagogica*, developed by Paul Horwitz's group at the Concord Consortium, which supports closer control of a model and the user interface.

A. *The Concord Modeling Workbench* software is more than a single atomic/molecular program, however. It provides you with a modeling engine integrated with a What-You-See-Is-What-You-Get (WYSIWYG) word processor that can be used to write styled text, insert JPEG and GIF images, import models and simulations, create/edit models,

and hyperlink other Web resources. We will amplify this description below:

With the Concord Modeling Workbench's integrating software environment, the user can easily create, visualize, annotate, contextualize, cross-link and distribute dynamical models.

Interact with model at various levels of sophistication. You can set up, interact with, or edit a molecular model using its original user interface, which usually has many hierarchies of menus and dialog windows for setting up a model, changing a model's states and controlling a simulation.

Design interfaces. You can design a simpler interface that can be used to control the model with constrained degrees of freedom. For example, for activities exploring a molecular view of states of matter, changing temperature may be the only thing that a teacher would require students to do. Therefore, a slider that controls the temperature of the molecular model, and the model itself, would be adequate in those particular activities. Teachers can select these tools from an array of sliders, buttons, combo boxes and more.

Annotate and illustrate models. The *Concord Modeling Workbench* enables you to create (or choose) these essential elements, and annotate them with text and images, on a conventional document interface.

Save models and documents. Once you have created such a document, everything on the workspace can be saved (in XML format). When a document is saved, the current states of the embedded models are saved. When a document is opened, those saved states will be the initial states of the models. If you are particularly interested in saving intermediate states and analyzing patterns of particular molecular trajectories, the *Concord Modeling Workbench* allows you to record a simulation.

Share over the Web. Any standard HTTP server can securely distribute documents you have created, which can be viewed/downloaded by any end user all of the World using the *Concord Modeling Workbench*. Students, using only the *Concord Modeling Workbench*, therefore, can develop molecular dynamics models, annotate them and share them over the web with one another for discussion.

B. Pedagogica Our model can also be programmed for use in middle and high school classrooms with the assistance of a script, *Pedagogica*. *Pedagogica* is a scripted control environment developed to overlay models (Horwitz & Christie, 1999[6]). A *Pedagogica* script can define a user interface, set up the initial conditions, define the interactions with the model, coordinate multiple applications, define text and response windows, and record users' responses and use of the model. (**See Fig. 2**) It generates records that can provide feedback to teachers and data for researchers. A branching sequence of pages that include models can be scripted. *Pedagogica* scripts, written in JavaScript, are currently being used to control some activities within the *Molecular Workbench Project*.

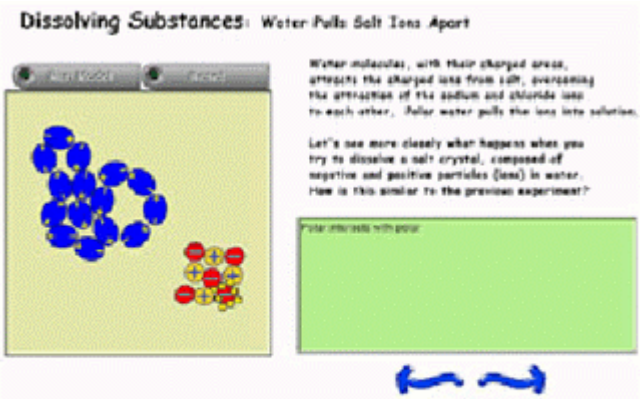

Figure 2: A scripting language that interfaces with models, *Pedagogica* allows the curriculum writer to control deeper aspects of the model.

Source: Concord Consortium

These two approaches provide a rich set of strategies for dealing with models, from the direct configurations of models that most users will be able to do easily and simply with only the *Molecular Modeling Workbench*, to the programming of key variables with the model-oriented scripting language, *Pedagogica*.

Our modeling strategies have had to adjust to different content. While Gas Laws and Phases of Matter required fairly straight-forward manipulation of scientific formula, modeling water has so far required a more "roll up the sleeves" approach, making rules for the model that are close approximations to the behavior of ions in water, and ions as they pass through membranes. Our model for DNA coding of protein, however, has some of the simplicity of Gas Laws. These differences reflect science progress: the actual structuring of water is still a hotly disputed mystery. DNA to protein, while unclear in many individual cases (there are after all, at least 60,000 proteins), is at least clear about the codon-to-amino acid connection.

Case Example: States of Matter

Students completed a molecular dynamic activity in which they observed various macroscopic phenomena typical of the three phases of matter, and then compared these properties to the microscopic properties depicted in the molecular model. (**See Fig. 3**) By directly correlating observable macro scale

properties to the micro scale behavior of atoms in matter, students could develop their own kinetic atomic and molecular perspective of the particulate model of matter. In addition, the activity had students highlight and observe two selected atoms or molecules in each phase and observe the relationship between them.

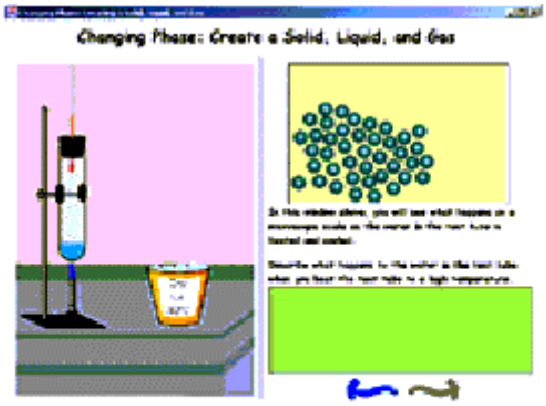

Figure 3: A dynamic model (upper right on screen) is synchronized with an animation using *Pedagogica*.

Source: Concord Consortium

The goal of the activity was to help students develop through interaction with the model and observations of the macro and microscopic behavior the following mental models:

• The atoms or molecules of a solid tend not to move very quickly and are generally spaced as closely together as possible and vibrate in place where the distance between two molecules do not change over time.
• The atoms or molecules of a liquid are also generally spaced closely together. However, the atoms or molecules of a liquid tend not to stay in one place. They slide by each other, allowing the liquid to conform to its container.
• Finally, gasses have, comparatively, a great deal of space between their atoms or molecules. Gases fill whatever container in which they are. The distances between two molecules change a great deal, sometimes they are close to one another and sometimes they are far apart.

Case Example: DNA to Protein

In building a good science model, the curriculum developer and programmer should take into account known facts, prioritized to emphasize critical aspects of the process or phenomena.

When experimenting with our DNA to Protein model, students discover first-hand that:

1. The genetic code is written as a linear sequence;
2. There is co-linearity between genetic code and the protein sequence. The longer the portion of the code you read, the more protein you get as one line codes another line;
3. Code is written in codons without comas; and
4. Codons sit next to each other in line and each dictates the position of one amino acid in the chain;
5. The genetic code is redundant.

We built a model based on these assumptions. The model operates with a chain of amino acids linked to a genetic code table. A codon representing three consecutive nucleotides, A, T, C or G, controls the position of every amino acid. Each nucleotide can be replaced by another three or deleted. Each codon is linked to a specific amino according to the genetic code. Our model also includes the concept of redundancy – several codons can code the same amino acid. Working with the model, students are able to observe changes in the protein folding as a response to any alteration of the genetic code.

This model, though simple, allows students to explore the value of two different types of mutation, substitution and deletion of nucleotides, and the relative role of these mutations in affecting the shape of a protein. (**See Fig. 4**) They also can explore for themselves that some substitutions do not affect the sequence of amino acids because of the redundancy of the genetic code (or the location of the mutation).

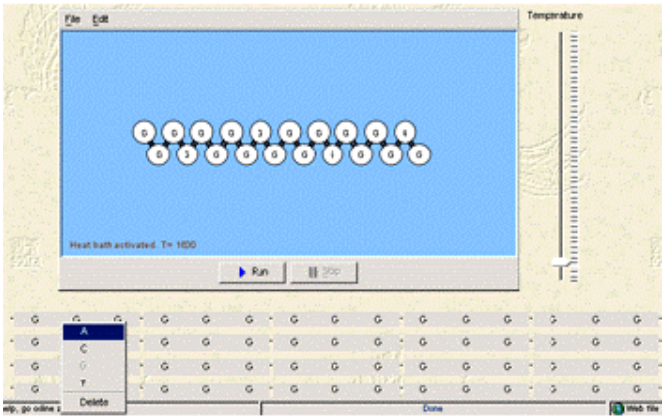

Figure 4: The model DNA to Protein. While simplifying the process of information transmission, students nonetheless see the effect of coding specific amino acids, and experiment with mutations.
Source: Concord Consortium

This means that in principle they can rediscover the role of the redundancy of the genetic code in maintaining the relative stability of proteins.

Educational Research Using Mini-modules

The centerpiece of the *Molecular Workbench* research includes "mini-modules" lasting no longer than one week. Each one includes *Molecular Workbench* signature software that focuses on macro-to-micro connections and atomic-scale models. The software was used to generate model-based activities for the following content: *The States of Matter*, a

module focused on the arrangements and motions of molecules in matter in its various states; *Water in and Around our Cells*, a module that addresses the essential ability of water to dissolve and transport some substances and not others, and the role of membranes in regulation of concentrations of dissolved substances; and *Monomers to Polymers*, a module that explores the ways monomers can be assembled into key polymers: particularly proteins and the relationship between the primary structure (the sequence of amino acids) and the shape of a protein.

While the mini-modules represent a focused effort of the research, student evaluation is also being done in classrooms able to run the *Molecular Workbench* curriculum for a significant part of a semester. The curriculum *Atoms in Motion*, has students explore the science of molecular kinetic theory and characteristics of atomic behavior underlying macroscopic phenomena. To draw students into a study of the abstract concept of invisible atoms, students are challenged to explain how and why a hot air balloon flies. In order to explain this fully, the curriculum addresses the following concepts: all substances are made of atoms and molecules; these particles move randomly; the temperature of atoms and molecules are directly related to their kinetic energy, which is the energy of motion related to mass and velocity; and pressure is due to the repeated impacts of molecules.

Using the above curriculum modules, students can learn about causation and emergent behavior that relate to the content from the National Science Education Standards such as the structure and properties of matter, chemical reactions, motions and forces, interactions of energy and matter, biomolecules, form and function, and cell regulation.

Approximately 500 students to date have participated in our testing. These students were drawn from 8th, 9th, 10th and 11th grade classes in Massachusetts. A pre- and a post-test was given to students in every class to assess their content knowledge. For example, the following question was asked in the pre-test of *States of Matter* to determine students' understanding about the relationship of macroscopic properties of matter to microscopic properties, as well as to learn about students conceptions or misconceptions about matter in its various states.

Suppose you were the size of a water molecule, and could stand on a water molecule in a glass of water. Someone takes that glass of water and puts it in the freezer. After a while the water turns to ice. How does what you see and feel change?

If answered in an expert manner, this question would have students reasoning at both the macroscopic and microscopic levels, and it would employ notions about the motions and forces of the molecules. In the pretest, more than 2/3 of the students either responded to this question with answers that contained misconceptions regarding the bulk properties of atoms and molecules, or were unable to answer the question. This includes some classes that had studied the subject before using the curriculum. In the post-test, the misconceptions appeared in less than 1/5 of the students. In all classes analyzed, students scored significantly higher on the post-test then they did on the pre-test.

In addition, however, the research was looking at the ways that these environments, with interactivity and control over the stimuli, increase cognitive competencies. Can students accurately reason about the microscopic world of interacting atoms and molecules? Overall, our research has shown that, by learning through model-based experimentation, supported with guided interactions, students appear to have developed sufficiently robust mental models of atomic-scale processes. These models have enabled the students to explain macroscopic phenomena and predict new results by employing atomic scale reasoning.

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