

Molecular Modeling and Visualization Tools in Science Educationⁱ

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Summary

The goal of this symposium is to present and discuss how advances in computer hardware, scientific visualization, and computational methods of visualization, has enabled multiple conceptual and visual representations of atomic and molecular concepts. These advances in molecular modeling and visualization enable students to manipulate a variety of visual representations of abstract concepts, explore these concepts, and, therefore, bring the study of science closer to the doing of science. We will present several projects funded by the National Science Foundation (NSF) to create research-oriented, user-friendly, molecular modeling education tools that facilitate multiple visual representations.

Much of science is submicroscopic. It is difficult for students to see the connection between the submicroscopic world of atoms, ions, and molecules, and the macroscopic properties of matter. Computational research in the sciences makes very effective use of available computing resources in simulating the behavior of complex systems. Routine use of these simulations is possible because of the development of interactive (i.e., real-time, individually controlled) visualizations in three dimensions. The coupling of simulations with

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Powerpoint presentations are available online at:
<http://polymer.bu.edu/narst2003/>

visualization presents scientists with a powerful description that matches the three-dimensional dynamic nature of their field. Now more than ever before, computational science tools are being placed in the context of science education tools.

Students have many problems understanding dynamic three-dimensional processes. A glance at any general chemistry textbook shows a multiplicity of representations used in different contexts with no correlation between representations or why one was chosen. Some students can switch contexts easily; but most do not integrate the knowledge or extract from them representations to ideas the experts see in them. While experts use different models and switch easily between them when solving problems, students tend to believe the representation as a complete model of the concept (Reif, 1987).

We need to develop better techniques for sharing multiple mental models with students, and help students develop the ability to choose a proper model. Computer graphic representations are being used to show students different ways of seeing diagrams (Brasell, 1987). But students develop intuition by doing, not by seeing, and this is precisely what the new technologies allow us to consider (Smith and Jones, 1989).

The projects represented in this symposium are consistent with the major goal of the science curriculum standards to understand macroscopic features in terms of microscopic interactions that give rise to them. A key feature of the projects participating is the use of molecular visualization, a science technique perfected in recent years that programs the actual structure and motion of atoms and molecules based on the laws that govern their motion. Thus the student can actually see, in real time, the microscopic behavior and in some cases, using split-screen software programs, can simultaneously see the corresponding macroscopic behavior. By changing the conditions of the system (e.g., temperature), the student can better understand how both sub-microscopic and macroscopic properties depend on these conditions. These materials can be used across a continuum of intellectual depth, from the demonstration of qualitative concepts to a full-fledged tool of exploration and self-discovery, and they can be used to teach a wide range of topics from the national science curriculum standards.

The focus of this symposium will be to describe the various approaches and visualization technologies of each project, discussing the range of visual representations, as well as how these multiple representations are enabling students to learn difficult concepts.

ChemSense: Shared Responsibilities within A Knowledge Building Environment

<http://chemsense.org/>

ChemSense is a research and development project to examine the impact of representations, chemical investigations, and discourse on chemistry learning. The work intersects several theoretical approaches to learning, which include

collaborative project-based investigations (Krajcik et al., 1998), representational competence (Kozma & Russell, 1997), the design of chemistry curriculum (Coppola, 1999), and knowledge building (Scardamalia & Bereiter, 1996; diSessa, 1993). ChemSense includes a set of tools (software and probeware) and curriculum activities that draw on this theory to scaffold students' learning of chemistry. These tools and activities are based on designs by curriculum integration teams of researchers, chemists, teachers, and developers, informed by learning theory and related technologies (e.g., 4M-Chem, CSILE, ESCOT), and grounded in authentic classroom use.

Our current work builds on the hypothesis that providing students with a richer, more diverse means of expressing their chemical understanding, increases the chances that students will be able to demonstrate their level of understanding. In turn, teachers will be able to assess and assist them better. From this working hypothesis develops the "shared responsibility" model embodied in our ChemSense Knowledge Building Environment. Our model challenges the research and curriculum development community to provide teachers with tools and approaches to help students develop their conceptual understanding through representational expression and through collaboration with teacher and peers. It also challenges teachers to integrate this tool in ways that are meaningful and appropriate to their classroom and school environment.

ChemViz: Chemistry Visualization of Atomic and Molecular Structures
<http://chemviz.ncsa.uiuc.edu/>

This NSF funded project, ChemViz: Visualizations in Teaching Chemistry, grew out of the quest to discover ways to render certain basic concepts of chemistry more vivid and visible to young learners. Due to the microscopic nature of chemistry, many of its basic constructs and processes are "invisible" to students. Historically, chemistry educators have tried to render chemical structures and processes more visible through the use of vivid, albeit excessively simple, visual metaphors such as the solar system serving as a model of the structure of an atom. While marginally useful in early stages of learning, such metaphors eventually interfere with a rich understanding of basic chemical concepts. More recent pedagogical work has suggested that computer-generated three-dimensional animations of certain basic processes, molecular bonding for example, are capable of providing students with this type of richer visualization. It has also been suggested that such visualizations help students obtain a better grasp of the abstract aspects of chemistry, such as calculating algorithmically-based solutions to problems.

Building on these more recent findings, the ChemViz project proposed a pedagogical approach that starts with a computational experiment on an abstract concept, and then proceeds to present the model (the visualization) to interpret the experiment. The computational experiment approach allows, in contrast to theory and experimentation, students to explore how the laws of chemistry behave. In a computational experiment students can do simulations that visually and dynamically replicate the behavior of a complex chemical process. An example, prevalent in this project, is the numerical solution to the

Schrödinger equation. In a computational experiment, students learn by doing because they can manipulate their learning environment, testing different computations against models in an iterative fashion.

In order to explore this pedagogy, the investigators proposed to develop tools that would allow both teachers and students to do the simulations and visualizations easily and routinely so that the students develop an intuitive understanding of the chemistry laws behind the models. Besides computation and visualization, a third pivotal piece in this approach is access to a high-performance computing environment (e.g., a supercomputer) to conduct the simulations and create the images in time-frames (a few seconds of computing time) that make the manipulations feasible and at least theoretically useful from a pedagogical perspective.

The Molecular Workbench Project

<http://workbench.concord.org/>

The goal of the Molecular Workbench project is to enhance our understanding of how students can use dynamic models to enhance their reasoning about atoms and their relationship to macroscopic phenomena. Not only physics but also so much of chemistry and modern biology is based on a "molecular view," but this is seldom addressed in beginning courses because it is very difficult to learn from static pictures and narratives, or even simple animations. By supporting guided student explorations of interactive, dynamic models, students can get a deep conceptual understanding of atomic-scale phenomena and their relationship to macroscopic phenomena. Project-generated data show a significant enhancement of atomic/molecular reasoning for students using project materials.

The project is based on the Molecular Workbench, an extensive, professional-grade molecular dynamics model that we have written in Java. The basic model is based on classical mechanics using the force laws that apply to atoms and molecules: Lennard-Jones potentials, electrostatic forces, and elastic bonds. Combinations of these objects can be created, placed in a container, given a temperature, and allowed to propagate in time. Students can use these models to generate phase changes, explore diffusion and thermal conductivity, and even simulate osmosis.

Initial research with a curriculum based on the model, scripts, and off-computer activities has been designed to re-visit some of the research on student understanding of the phases of matter. Since most prior research has been done with static drawings of the atomic arrangements in different phases of matter, it is not surprising that the literature show that middle school students have great difficulty with this domain. Many educators had concluded from these studies that explanations based on the properties of atoms and molecules should be avoided before high school.

Using dynamic representations and the guided interactions that the software supports, the project finds that middle school students' learning is greatly

accelerated. After exposure to these materials over five class periods, students can accurately recall the arrangements of atoms in gasses, liquids, and solids. In addition, they appear to have built a sufficiently robust mental model of the topic to predict new results by reasoning about the interactions of atoms and molecules.

Heretofore, even a conceptual understanding of these topics required advanced mathematics, so at the secondary and beginning college levels these topics were either ignored or taught as unrelated facts that needed to be remembered. Entropy, chemical energy, osmotic pressure, catalysis, reaction rates, chemical equilibrium, solutions, hydration, self-assembly and other phenomena should be easier to learn and more memorable if students understand how the simple rules of atomic interactions give rise to these phenomena.

Virtual Molecular Dynamics Laboratory

<http://polymer.bu.edu/vmdl/>

Since 1989, the Center for Polymer Studies Education Group has been focused on developing materials for high school and undergraduate science education that is based on cutting-edge science research. How can leading-edge research possibly be usable in high schools? Because of the simplicity of the rules embedded in the physical models, the availability of computers to apply these models to large systems, and the ease with which students successfully manipulate the resulting interactive visual displays. Our materials introduce both the process and content of modern science, without a decades-long time delay between a scientific discovery and what the student can investigate the next day.

In science research, computers in general and molecular dynamics in particular, have transformed how science is practiced. Being able to visualize and bridge the gap between the sub-microscopic and macroscopic, we think, helps students learn valuable scientific content. But that's the tip of the iceberg. Much more than learning science content, using computers as complex tools to solve otherwise intractable real-world problems is a powerful 21st century skill. Large-scale computational models are used to design new drugs, to solve the mysteries of Alzheimer's, cancer, and other debilitating diseases, predict weather and other aspects of our environment, and on and on. Only recently has the gap between the computational power of the typical research and the computational power that you can find in many classrooms been reduced to almost zero. This opens up exciting opportunities, we think, for science education and science research to come together.

The Virtual Molecular Dynamics Laboratory consists of hands-on activities and computer-based virtual laboratory experiments (SimuLabs) that engages students to investigate the role of sub-microscopic motion and interactions in the context of traditional chemistry, biology, earth science, and physics curricula. The Virtual Laboratory allows students to experience a scientifically honest world in which molecular motions are computer directly from the elementary molecular interactions and displayed in real time as they are computed. The Virtual Molecular Dynamics Laboratory enables the student to visualize atomic motion,

manipulate atomic interactions, and quantitatively investigate the resulting macroscopic properties of biological, chemical and physical systems

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