REASONING WITH ATOMIC-SCALE MOLECULAR DYNAMIC MODELS[1]

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Abstract

The studies reported in this paper are an initial effort to explore the applicability of computational models in introductory science learning. Two instructional interventions are described that use a molecular dynamics model embedded in a set of online learning activities with middle and high school students in ten classrooms. The studies indicate that middle and high schools students can acquire robust mental models of the states of matter through guided explorations of computational models of matter based on molecular dynamics. Using this approach, students accurately recall arrangements of the different states of matter, and can reason about atomic interactions. These results are independent of gender and they hold for a number of different classroom contexts. Follow-up interviews indicate that students are able to transfer their understanding of phases of matter to new contexts.

Introduction

Computational models represent a class of models that appear to have great promise in education. Computational models are based on mathematical algorithms that approximate fundamental laws and exhibit behavior that reproduces some important observed phenomena. In many situations, the educational challenge is to help students understand the relationship between the underlying mathematics and the resulting behavior of the system.

Although computational models often rely on sophisticated mathematics, they can be designed to allow learners to acquire important concepts without needing to master formal mathematical proof. Because the prerequisite mathematics has heretofore been the primary medium of explanation, curriculum designers have found it difficult to convey fundamental understandings of many technical subjects. Computational models offer an attractive alternative that could support major changes in the science curriculum.

One way to utilize computational models in education is to have students develop models using general-purpose environments like Stella[2], Model-It (Metcalf, 1999), multi-agent Logo (Colella, Klopfer, & Resnick, 2001; Wilensky & Resnick, 1999), and AgentSheets (Repenning, 1993). While this is a most promising area of development, student learning through model construction has proven to be difficult to implement in typical schools, challenging to many teachers, and inefficient because it can divert scarce class

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[2] See http://www.hps-inc.com/index.htm

time from the intended content to the details of building models in the construction environment.

This paper addresses the educational impact of computational models that are created by curriculum developers rather than students. Our models are based on a few fundamental rules of atomic interactions that exhibit emergent behavior that reproduces important aspects of the properties of materials, including the states of matter. Computational models of this sort that are sufficiently interactive and thoughtfully integrate student exploration and reflection of the model into instruction can support deep learning. As with all discovery-based learning, a balance must be struck between free exploration that can be time-consuming and procedural instruction that can be more efficient but leave students with only a superficial understanding. Many rich educational computational modeling environments have been developed, and their potential has been convincingly demonstrated for increased learning of various topics (Roberts, Feurzeig, & Hunter, 1999).

Molecular dynamics models represent a promising class of computational models that could have broad application in science education. A molecular dynamics model uses classical mechanics and approximations of atomic forces to compute the motions of collections of atoms and molecules in either two or three dimensions. Many of the core ideas of thermodynamics can be seen in molecular dynamics models, such as temperature, conservation of energy, entropy increase (the idea that the most disordered state is most likely), the equipartition principle (the average kinetic energy of all objects in thermal equilibrium is the same), and the ergodic hypothesis (time average of some parameter like kinetic energy is the same as the average at one time over all particles in a system.) Many of the behaviors of complex systems that could previously be predicted only from complex statistical calculations can be seen in dynamic models consisting of fewer than a hundred atoms. Examples include the ideal gas law, thermal equilibrium, phase changes, latent heats, crystal structure, diffusion, thermal expansion, osmosis, compressibility, gas absorption on solids, and solubility. In the language of complexity theory, these large-scale phenomena “emerge” from the simple rules governing the agents (atoms and molecules) that make up the system.

Molecular dynamics models are widely used in research for the same reasons that they could be useful in education: to explore emergent behavior of systems too complex for closed solutions and to follow the evolution of these systems. The ability to visualize what happens to collections of interacting atoms and molecules under many different conditions and rules gives the researcher a deep, intuitive understanding of the system under study. In effect, the interactions of atoms could become as familiar and predictable as our macroscopic world. If this familiarity and predictability could be passed on to beginning students, large parts of physics, chemistry, and biology would be more comprehensible and easier to learn at an earlier age.

An understanding of the interactions of atoms and molecules could be a valuable unifying theme in introductory science. An instructional strategy that took advantage of molecular models could have a major impact on science education by increasing student understanding of atomic-scale phenomena. Well-designed learning opportunities that use molecular dynamics models could help students develop this understanding starting in the earliest grades. Learning experiences based on molecular dynamics tools should help students develop more scientifically accurate mental models of atomic-scale phenomena which should in turn help them to reason more effectively at different

levels like experts (Chi, Glaser, & Farr, 1988; Glaser, 1989). Such learning could be based on fewer, more fundamental principles and will have a far broader predictive capacity. This should reduce the amount of memorization required by increasing the logical connections between ideas.

Previous Research

Learner Conceptions of Matter

Much of the research on student conceptions of matter points to difficulties students have in understanding the relationships between matter, states of matter, and the particulate theory (Nussbaum, 1985). For example, research has shown that many students in middle school are familiar with the terms "atoms" and "molecules," yet they maintain inconsistent alternative ideas about the underlying nature of matter. While they know that atoms and molecules exist and that matter is made of tiny particles, many believe gas is not material, as it cannot be touched or seen (Smith, Maclin, Grosslight, & Davis, 1997). Students not only have great difficulty understanding the basic properties of invisible molecules, they also have difficulty explaining changes in state in terms of molecules (Novick & Nussbaum, 1978; Nussbaum & Novick, 1981). They assume that there is a direct relationship between the macroscopic properties of a substance and the atomic properties of its molecules. For example, many learners believe that ice is made of cold, hard molecules that do not move (Berkheimer, Anderson, Lee, & Blakeslee, 1988).

Using carefully designed instructional strategies, researchers have shown that it is possible to teach middle school students about the arrangement of atoms in the three phases of matter as evidenced by their ability to reproduce pictures representing the three phases (Driver, 1985; Griffiths & Preston, 1992; Millar, 1990; Nussbaum, 1997). Most of the reported successful instruction in this area tests only whether students can produce the correct atomic-scale description of a macroscopic situation. This tests for memory, not reasoning. For instance, students in Johnston & Driver's study (Johnston & Driver, 1989) learned to draw reasonably accurate atomic-level pictures of solids, liquids, and gases, but there was no evidence that they could use these pictures to explain or predict other phenomena. These atomic-scale visualizations must appear to students as extra mental baggage that has little predictive value and might even seem counter-intuitive. From a student's perspective, this is simply more useless information that must be memorized.

It is questionable whether the effort to teach students to reproduce these pictures is worthwhile, because, as taught, pictures that represent how atoms are arranged have little explanatory power and fail to help students reason about related effects such as thermal conduction, change of state, or the compression of gases (Linn & Songer, 1991; Nussbaum, 1985; Stavy, 1990). For instance, Linn and Songer found that atomic-scale arguments do not help middle school students understand thermal conductivity and that a continuous model of heat flow was more effective.

Because of these difficulties, educators recommend delaying the introduction of atomic-scale models until high school (The National Research Council, 1995). Only then, they posit, do "high-school students develop the ability to relate the macroscopic properties

of substances that they study in grades K-8 to the microscopic[3] structure of substances." Yet high school biology, usually first in a series of science courses, and chemistry, depend on understanding the kinetic molecular theory and the relationship of the atomic scale world to the macroscopic phenomena students encounter (Bodner & Domin, 1996; Krajcik, 1991; Nakhleh, 1992). If atomic-scale models are not taught in middle school, it makes learning high school science considerably more difficult. We hypothesize that typical middle school students can learn atomic scale phenomenon through guided exploration of molecular dynamics models (Tinker, 2001b).

Atomic Scale Models

Animations of atomic scale systems can look very much like the output of one of our computational models. In both cases the user sees a lot of atoms or molecules moving on the screen. The difference between animations and computational models involves flexibility and interactivity. An animation might simply run like a video clip or it might have several video clips that are selected according to some input. For instance a popular atomic scale animation shows several different clips of atoms moving at speeds that depend on the temperature setting. In contrast, a molecular model of atomic motion is computed from the details of the motions and interactions of the atoms. As a result, students can experiment with the system and generate an infinite number of accurate models. Nevertheless, there is much to learn from research with animated atomic scale models (Birk, 1997; Burke, Greenbowe, & Windschitl, 1998; Copolo & Hounshell, 1995; Trunfio, 1990; Wu, Krajcik, & Soloway, 2001).

Kozma and colleagues experimented with animations of atomic motion in diffusion and chemical equilibrium that are embedded within a full teaching environment of lecture and experimentation. College student learning of significant concepts about diffusion increased significantly (Kozma & Russell, 1997). In addition, they showed significant decrease in the number of misconceptions. Using a four-fold divided screen displaying video, animation, graph, and symbolic representation, students were able to control the display modes, select experiments, and run and pause displays. In some cases, the screen was too complex and students failed to understand the connections between the various representations. To focus student attention on the molecular motions, this research team developed an animation tool that students use to generate illustrations of their understanding of atomic-scale interactions (Schank & Kozma, 2002). This is a promising way to reveal student mental models and to help them consolidate ideas and experiences they have had into more consistent mental model, but may not be as useful in generating those mental models in the first place.

Research Design and Methods

This paper describes the results of middle and high school students' use of a powerful molecular dynamic model in curricula that address the phases of matter. This investigation represents an initial test of the *Molecular Workbench* molecular dynamic system as well as *Pedagogica*, a control environment that is used to guide student investigations

[3] We prefer to use the terms "atomic-scale" or "nano-scale" rather than "microscopic." The latter term implies visibility using a microscope or micrometer-scale, both of which are inaccurate descriptions of atoms.

and assess student performance (Horwitz & Christie, 1999). We simply were looking at the ways in which learning environments based on dynamic models increase cognitive competencies: In what ways can they enhance students' understanding of the content? Can students reason more accurately about the nanometer-scale world of interacting atoms and molecules? At what age can students begin to reason about molecular dynamic behavior? In particular, we studied how guided student exploration of interactive dynamic molecular models might impact student understanding of atomic-scale phenomena and the relationships between these phenomena and observable, macroscale phenomena. To explore these questions, we created learning activities in *Pedagogica*, administered these activities to ten groups of students, and looked for learning gains and transfer. The research reported here focused on determining whether the use of models based on molecular dynamics helped students learn about the states of matter.

The Technology: Molecular Workbench and Pedagogica

The *Molecular Workbench*

The materials used were based on the *Molecular Workbench*, a two-dimensional molecular dynamics application written in Java and available as open source from the Concord Consortium[4]. This software calculates the motion of atoms subject to the following forces:

- Lennard-Jones forces, based on a potential that has an attractive inverse sixth-power attractive term and an inverse twelfth-power repulsive term. Students can vary the strength and radius of the attractive part.
- Chemical bonds approximated by adjustable harmonic forces in both the radial and angular directions.
- Electrostatic forces based on Coulomb's Law that are used when ions or polarized atoms are present.

The computational engine uses Newton's Second Law to calculate each atom's motion under the applicable forces in short time steps. Every few steps, the screen is redrawn to create the illusion of smooth motions of the atoms. The computations are sufficiently fast on a typical modern personal computer that a model consisting of over 100 atoms appears to be smooth and responsive. A sensitive indication of the accuracy of the model is that for the models reported here, the total energy in the system remains essentially constant for long runs.

The *Molecular Workbench* application has many options as illustrated in Figure 1. Any number of four kinds of atoms can be placed in the container. The mass, charge, diameter, attractive force, color, location, and initial velocity of each can be controlled by the user. Atoms can be linked to make molecules. The container can have reflective or cyclic boundary conditions. Barriers can be added to the container. The simulation can be started, stopped, stepped, and rerun in either direction. Temperature can be controlled or measured. A variety of output objects can be coupled to the model to record parameters such as temperature or potential energy. Two or more models can be placed on the same page for comparison. Many other options are available.

[4] http://concord.org

Pedagogica

The *Molecular Workbench* is too complex to be an effective learning environment for beginning students. Even if they learned all the controls, students could easily become lost and use their time inefficiently. In addition, teachers could fail to grasp how such a very general model best supports specific learning goals and instructional strategies. In order to learn efficiently and effectively from an open-ended model like the *Molecular Workbench (MW)*, students need pedagogical supports that convey appropriate concepts, allow for exploration, and require student reflection about their thinking (White, 1993; Wilensky, 1999).

To convert *MW* into a powerful educational experience, strategies are needed that foster reflection that is sufficiently open-ended so that students learn through inquiry rather than being told the right answer, but it also sufficiently directive so that students do not get lost or miss the point. It is difficult to balance openness with direct instruction and the best balance point is different for different students. Often, educational software includes print student manuals that provide some of these functions. Other modeling tools have attempted to provide the guidance and reflection through "scaffolding" that is built into the software. The software approach can be more responsive to the user, but has proven difficult to develop (Jackson, Krajcik, & Soloway, 1998; Jackson, Stratford, Krajcik, & Soloway, 1996; Metcalf, 1999).

Instead of building specific scaffolding into each model, researchers at the Concord Consortium have developed a general solution based on *Pedagogica* an application that controls a model (Horwitz & Christie, 1999; Horwitz & Tinker, 2001). *Pedagogica* can take over control of one or more applications, allocate screen space to each, pass data to and from them, monitor student choices and actions, and make context-sensitive responses. *Pedagogica* is itself controlled by a script written in JavaScript that can be easily edited and delivered over the Internet. Under the control of these scripts, *Pedagogica* can take over the user interface, disable unneeded options, and structure the learning experience into a series of linked pages. The resulting combination is called a *hypermodel* (Horwitz, 1996; Horwitz & Christie, 1999; Tinker, 2001a)

The research reported here used *Molecular Workbench* controlled by *Pedagogica* scripts to create molecular dynamics hypermodels. Figure 2 illustrates the appearance of one of these hypermodels.

The Instructional Material

Beginning students need to start with simple models that have just a few options. For instance, we start the study of phase change by allowing students to explore one atom in a box, changing just the initial velocity and elasticity of collisions with the container. Next, they explore the total energy of two atoms that can collide to discover that kinetic energy is conserved in all collisions. Without guidance, students will seldom stumble across these ideas and will, therefore, lack understanding of energy conservation in many-atom systems.

Even when students do discover important ideas through guided inquiry, they often fail to articulate their discoveries. As a result, they can lack appreciation for the significance of their discovery and cannot transfer their learning to new contexts. Articulating their findings through discussions, performances, or reflection is a necessary part of the learning process. For instance, students working with Horwitz's earlier GenScope ge-

netics model were able to solve complex genetics problems in the model while failing to recognize the same content in a paper test (Horwitz, Neumann, & Schwartz, 1996). When additional pedagogical and metacognitive prompts were added to GenScope, students significantly outperformed the control group as well as all previous GenScope users (Hickey, Kindfield, & Wolfe, 1999).

The curriculum materials used in this research were delivered in two ways 1) a States of Matter "mini-module" that required five class periods; and 2) States of Matter activities integrated in a semester-long high school unit. Both modalities combine dynamic atomic-scale computer models and activities with similar hands-on laboratory and kinesthetic activities.

The "Mini-module" States of Matter Design

To draw students into a study of the behavior of atoms and the properties of matter, the unit begins with a real world example of a volcanic eruption in Iceland. Students are asked to reason about changes of states of matter using the kinetic molecular theory. We expected them to be able to explain how molecules themselves do not change during physical alterations in substances such as melting, and reflect on the different arrangements and motions of molecules in solids, liquids and gases.

The activities in the unit are organized around the following sequence:

Activity One: What Happened? Students begin, first, by doing a hands-on activity that has them describe matter as particulate and not continuous. They then read about a volcano eruption in Iceland and identify several real-world examples of different states of matter.

Activity two: A Closer look at Matter. Students complete a laboratory activity about phase change, in which ice changes to water and dry ice changes to gas at room temperature. They then compare dynamic computer models of macroscopic and atomic-scale solids, liquids and gases.

Activity Three: Just Add Heat. Students use the dynamic model to experiment with how changes in temperature relate to changes in phases. Students describe the motion of molecules, their relative proximity to each other, and compare different substances as heat is added. Students also use the model to investigate the role of inter-atomic forces as substances make the transition from gas, to liquid, to solid.

Activity Four: A tight squeeze. Students complete a hands-on activity and a model-based activity to relate macroscopic space filling properties of substances to atomic-scale properties.

Activity Five: An Explanation. In this last activity students revisit models and explanations they developed at the beginning of the unit of the changes of state, and revise them.

Longer Unit: Atoms in Motion

In this semester-long unit, students explore the basic characteristics of atoms and how behavior at the atomic scale can explain what is observed at the macro scale. To draw students into this study, they are challenged to explain how and why a hot air balloon floats. To explain this fully requires understanding such fundamental concepts as prop-

erties of matter, motions, forces, and transfer of energy. More specifically, the curriculum addresses the following key 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.

The curriculum is divided into seven sections. The third section on diffusion and the sixth section on phase change incorporate the same molecular dynamics models used in the States of Matter unit. The following describes the context in which the models were embedded:

Section Three: Diffusion

Through computer models and laboratory activities students investigate matter in its various states and how these states reflect different arrangements and motions at the atomic/molecular scale. In addition students explore in a laboratory investigation how multiple random collisions of particles (atoms) will cause an odor (molecules of gas) to diffuse into the surroundings and how molecules of different masses will diffuse at different speeds.

Section Six: Phase Changes

In this section students explore the role of attractive forces between atoms and why this is needed to model phase changes. Students experiment using the computer model with changes in temperature and space filling properties of the different phases of matter.

Key Concepts

In developing the materials, both units attended to the relevant science education standards (The National Research Council, 1995) and the following learning objectives:

Students were expected to be able to:

- Observe a phenomenon that helps students define that matter is particulate.
- Describe what a gas, liquid, and solid looks like at the atomic level.
- Describe the behavior of particles in each phase of matter.
- Compare the macroscopic characteristics with atomic-scale characteristics for the three phases.
- Observe changes in matter when they manipulate temperature.
- Predict what macroscopic phase they will be in as they manipulate the temperature of the atomic-scale model.
- Investigate the role of inter-atomic forces in making the transition between gases, liquids, and solids.
- Predict what happens when a gas, liquid or solid is compressed.

The activities are organized around the development of specific concepts. The primary instructional strategy involves asking student to interact with molecular dynamic models and to draw static models to explain their thinking.

Implementation Studies

Classroom Studies

Eight classroom studies were conducted using the States of Matter mini-module. The materials were tested in two middle schools in Massachusetts. The materials were tested in two middle schools in Massachusetts. These research studies were done in 8th grade heterogeneous physical science classes with an average size of 20. Class periods were 55 minutes in length. The regular science teacher administered the teaching intervention. Six laptop computers with the software loaned to each classroom. Students worked in pairs or groups of three on the computer activities. During Activity Two, Three and Four (described above) the classes were divided such that half of the students were on the computers completing the activities while the other half were completing the associated hands-on activities. After approximately 20 minutes student pairs switched. Debriefings were done the first five minutes and the last five minutes of each class. The teacher spent the majority of time supervising students working on the hands-on activities because the computer activities were largely self-directed. The data were collected by group for the work done on the computer while other worksheets and the pre- and post-tests were collected for individuals.

Additionally, two classes participated in the Atoms in Motion implementation. These classes were drawn from a four-year Massachusetts suburban high school. The Atoms in Motion curriculum was delivered in 11th grade Chemistry 2 classes. Chemistry 2 is designed to teach students the basic chemical principles ordinarily taught in a one-year high school chemistry course, as well as the methods of questioning and reasoning used by scientists. Students taking this course tend to have trouble with mathematics. These classes included 20-50% students on Individualized Education Plans and other non-special education programs. Classes had an average of 22 students. Class periods varied from 45 to 75 minutes in length and met either three or four days a week. The regular science teacher administered the teaching intervention. Eight laptop computers with the software included were used in each classroom; students worked in pairs or groups of three for the computer activities.

Module	Duration of Module	Grade	Class Subject	Number of Classes
States of Matter	1 Week	8th	Physical Science	8
Atoms in Motion	1 Semester	11th	Chemistry 2	2

A Closer Look at Matter

Activity two in States of Matter and activity eight in the Atoms in Motion curriculum are representative learning experiences that use the same molecular dynamics model. In these activities students do a hands-on activity related to matter in different phases and interact with computer models of macroscopic and atomic-scale models of solids, liquids and gases. Students relate macroscopic properties for the three phases of matter to the atomic-scale properties depicted in the molecular model as illustrated in Figure 3. By directly relating observable macro-scale properties to the atomic-scale behavior of atoms students are given the opportunity to develop their own kinetic conception of the particulate model of matter. This activity was designed to promote learning of the following concepts:

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- The atoms or molecules of a solid are generally spaced as closely together as possible and vibrate in place where the distance between two molecules does 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, gases have, comparatively, a great deal of space between their atoms or molecules. Gases fill whatever container they are in. The distance between two molecules change a great deal, sometimes they are close to one another and sometimes they are far apart.

While working with the computer activity, students were asked to reflect on their observations. For example students followed the following prompts:

Prompt: Choose a solid. Highlight a molecule and describe the movement of one particular molecule of that substance.

Typical student responses include:

Student pair A: They're very large and they vibrate to move. They're close together in an organized fashion.

Student pair B: The molecule is closely packed in with the other molecules, and can barely move. It seems to float around, and continuously bounce off the other molecules.

Prompt: Choose a second molecule. Describe how the two molecules move. Pay specific attention to the distance between the two molecules.

Typical student responses include:

Student pair A: They are separated by three molecules and they continue to vibrate without moving very much.

Student pair B: Both molecules move in the same way; moving in a seemingly random pattern, probably resulting from bouncing off the other molecules that are so close to it. The two molecules are staying the same distance apart from each other.

Student pair C: The molecules are very tightly packed together and they're moving. The two highlighted molecules stay in the same place.

Student pair D: The molecules are vibrating, bouncing off the surrounding molecules. The distance between the two is always the same. They never move from their spot

Students observe and describe molecular models for solid substances, liquids, and gases. Then students are asked to compare the different states of matter:

Prompt: Describe the differences between solids and liquids.

Student pair B: The molecules of a liquid have just enough room to move, whereas the molecules of a solid are so closely packed, they cannot really move at all except in a slight circle.

Student pair E: The difference between liquids and solids are the arrangement and movement of the molecules. Liquids are not as neat, and solids are in orderly rows. They move pretty much the same, but liquids are not as tightly packed as solids and molecules flow past each other.

Student pair D: [The difference is] The movement of the molecules and the distance between the two highlighted molecules. In the liquid molecules the distance between the two changed slightly. In the solid substances the distance does not change and atoms just vibrate.

Prompt: Describe the differences between liquids and gases.

Student pair B: The molecules of gases are free flowing, and have plenty of room to move. They also move very fast. The molecules of a liquid can move, but not very much. There are also many more liquid molecules then gas molecules.

Student pair D: The atoms of the gas appear to move more randomly and they are farther apart. The distance between the two highlighted atoms change constantly.

The questions above are examples of near transfer tasks that required students to reflect on their observations of the model while looking at the model. Additionally, the activity included a few embedded assessment questions. Examples follow:

Prompt: Solids don't normally change shape when placed in a container how can you explain this on the basis of what you have seen?

Student pair A: On what I've seen solids don't normally change their shape because the molecules don't move positions.

Student pair B: Because there is not much room for solid molecules to move, they can not change position, and therefore the solids can not change shape.

Student pair E: Solids don't normally change shape because their molecules are very close together and they can't pass each other so they always stay in the same place.

Prompt: Liquids usually take the shape of their container, so how can you explain this on the basis of what you have seen?

Student pair A: I can explain this because as liquids flow, the molecules flow.

Student pair B: Liquid molecules have enough room to move slightly. They push against each other to move, and slide past each other so they can flow.

Student pair D: The molecules are moving, changing positions compared to each other, flowing.

Student pair E: Liquids normally flow because their molecules are free to move past each other.

The answers to these questions required students to apply their understanding of the molecular arrangement of the different states of matter to explain some observable macroscopic phenomenon. In this case they needed to reason about the macroscopic space filling properties of solids, liquids and gases, as it related to the molecular arrangement of the molecules.

Results

Pre-Post Test Comparisons

An examination of the effectiveness of the States of Matter module and the Atoms in Motion module was conducted using pre- and post-tests to assess student content knowledge. Many of the pre- and post-test questions were designed to cover content in which misconceptions had previously been reported in the literature. Additionally, questions focused on determining how students reason from the models to solve problems. Students were asked to apply their understanding to phenomenon not previously encountered in the curriculum. The pre- and post- tests consisted of six questions for which students were asked to give brief answers and draw diagrams. The tests did not count toward students' grades.

Student answers were coded for correct content. The statistics were done using StatView® (1999). The inter-rater reliability, assessed in scoring two classes, was 89.9%. In all classes analyzed, eight middle school classes and two high school classes, students scored higher on the post-test then they did on the pre-test. A paired T-test revealed that, in nine of the ten classes, the post-test scores for content knowledge were significantly greater than their pre-test score. It is important to note that in the one class in which a statistically significant result was not obtained (Class 5), the implementation of the States of Matter module ended abruptly due to school-wide scheduling conflicts. A majority of students missed several class periods and many missed the post-test.

Module pre-post test analyzed	Class	Mean Diff.	DF	t-value	P-value
States of Matter	1	6.056	18	7.369	<.0001
States of Matter	2	7.688	16	12.010	<.0001
States of Matter	3	4.833	11	4.166	.0016
States of Matter	4	4.833	12	4.529	.0007
States of Matter	5	2.222	8	1.871	.0982 not.sig
States of Matter	6	6.750	19	8.876	<.0001
States of Matter	7	4.000	12	5.808	<.0001
States of Matter	8	3.846	12	5.754	<.0001
Atoms in Motion	1	2.909	22	5.534	<.0001
Atoms in Motion	2	8.333	12	7.348	<.0001

An analysis of variance (ANOVA) was computed in order to determine whether there were any statistically significant differences on the total post-test score based on gender, the independent variable was gender of the student, and the pre-test score was used as a covariate. The analysis revealed that there was no statistically significant difference found between the boys and the girls on post-test for any of the classes analyzed.

Additional analysis was done on questions that appeared on both the States of Matter tests (administered in the middle school) and the Atoms in Motion tests (administered in the high school). Comparisons indicate that the high school students overall did better then the middle school students on the same questions, but not significantly.

A subset of randomly chosen student responses were analyzed for the inclusion of incorrect ideas regarding the bulk properties of atoms and molecules. On the pre-test 54% of the students either wrote statements that indicated they thought the properties of the atoms and molecules in a substance could be described by the macroscopic properties of the substance or were unable to answer the question. In the post-test, these same incorrect concepts appeared in only 23% of the students.

Student Reasoning

We conducted a study of the ability of students to transfer their understanding. One measure of transfer can be based on the quality of student reasoning about atomic-level phenomena and their manifestations at the macro level. The following is a presentation of student reasoning and transfer that reflects understanding influenced by the Molecular Workbench models and curriculum.

On the pre- and post-test students were asked the following question:

"Suppose you were the size of a water molecule, and could stand on a water molecule in a glass of water. Someone takes the 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 require students to reason at both the macroscopic and atomic-scale levels, and it would require notions about the motions and forces of the molecules and about the density of the molecules. This question sets up a situation that requires students to take what they understand about the different states of matter and apply it to the phase change in a new abstracted context. The students were encouraged to notice features that previously may have escaped their attention or conflicted with their prior conceptions and to focus on which features were relevant. The assessment sets a new context, in which the learner is expected to engage in a "What if…" problem solving question outside the context of the computational model.

The following are examples of the most common types of change in conceptions:

Student S:

Pre-test: I would probably feel a lot colder, and the water molecules would not be moving around.

Post-test response: The molecules would begin to align and move more slowly. It becomes cold.

Student T:

Pre-test: The water goes from a liquid to a solid. The water expands and inside, you can see ice crystals. The water becomes really cold and you can sometimes see air bubbles.

Post-test: The water changes from liquid to solid. Once the water turns to ice the molecules slow down and clump together in a rigid form.

Student U:

Pre-test: The molecule that I stand on expands to a larger size. There is little space to move and the temperature has decreased to cold.

Post-test: As it gets colder the molecules group into a tight organized pack. The molecules only vibrate slightly.

Student V:

Pre-test: The surface is solid and slippery. The water is condensed and you can not "see through."

Post-test: The molecules in the ice have slowed down from when they were in the liquid form.

Student W:

Pre-test: I would see the water molecules expand.

Post-test: The molecules would get closer together and only move very little.

The above examples focus on students who exhibited fairly well-documented misconceptions. In many cases, students did not use any conceptions about molecules in their descriptions at all. In the post-test responses, students relate the difference in the state of water to the motion of the particles and their arrangement. These initial findings suggest that we have successfully created a learning environment in which students learn to use atomic-molecular reasoning to decipher the macro-scale world. Student explorations of these models appear to lead to a good understanding of connections between atomic-scale events and what they observe at the macroscopic scale. Students use the models to describe properties at both levels.

Student Interviews

Interviews were used as an additional source of data. Twelve semi-structured interviews were conducted following an interview protocol that lasted for an average of 30 minutes. The interviews were conducted to gain insight into interesting or unexpected findings. Students were interviewed in groups of three. The open-ended responses to the questions provide quotes that are the main source of the data. The measure of success was based on the quality of student reasoning about atomic level phenomena and their manifestations at the macro-level.

The following excerpts from interviews are examples of students' ability to transfer their understanding to both new representations and new situations. These examples demonstrate the robust nature of students' mental models of molecular density and of the different movements of the molecules for the different states of matter.

The task involved interpreting graphs of the distance between randomly-selected atoms as a function of time. The question, context, and graphs were unlike anything that the students had encountered in the activities. Although the models had atoms with different distances between them, the activities had no representation of this as a graph of separation against distance. Thus, the task required that students correctly interpret the graphs, and relate their interpretation to their mental models of the distances between atoms in different phases of matter.

An analysis of student interviews revealed that 10 out of 12 students were able to transfer their knowledge of molecular movement in the different states of matter and the density of molecules to interpreting the data in this new context. The remaining two

students only needed to be given some insight into how to interpret the graphs before being able to analyze the representation correctly.

Prior to this interview students had not been challenged to interpret representations of the molecular state of matter in any way other than describing verbally the dynamic model they observed. The following is an excerpt from one of the interviews.

> *Interviewer: Here you have a box of molecules and you have your eye on a molecule, you pick one at random, and then you pick another molecule at random and you are going to watch the distance between the two molecules and see how that varies. So here is a case that we are looking at where here is a graph of the distance between them as it varies in time. What do you think is true about the material? (Interviewer is showing the first graph in Figure 4)*

(insert Figure 4)

> *Student 2: Would it be like a solid? Because they are staying at the same distance, because they are probably just vibrating in the same area.*
>
> *Interviewer: And suppose you watched the two molecules and the distance between them begins to look like this? (Interviewer is showing the second graph in Figure 4)*
>
> *Student 1: A gas.*
>
> *Interviewer: And why do you think it is a gas?*
>
> *Student 1: Because they [the molecules],their distances are far apart and move a lot.*
>
> *Interviewer: So, now suppose you are watching the two molecules and you see this. (Interviewer shows Figure 5)*

(Insert Figure 5)

> *Student 1: It could be like it is a solid at first and that as it melts it turns to a liquid and then a gas or whatever, it is like a phase change.*
>
> *Student 3: See, I know it is going from one phase to another but I can't decide whether I want that beginning one to be a solid or a liquid because it all depends on how much time we are looking at there.*

It is noteworthy that Student 3 had such a sophisticated mental model of the different states of matter that time became a factor in interpreting the initial phase, as he appears to have learned that the density of the molecules in a liquid and a solid are similar and that it is only over time molecules in a liquid slides past another molecule. An excerpt from another interview reveals similar reasoning.

> *Interviewer: …and here is the distance between the two molecules that you are watching in one material and how it changes through time and here is the distance you are watching in the other material and how it changes through time. What can you say about these two materials?*
>
> *Student 4: Maybe this one on the right is a gas and this one on the left is a solid. Or that one (pointing to the one on the left) could be a liquid. Because when something is a solid the molecules are more tightly packed together so the difference between them won't vary that much, it doesn't matter if they are this far apart or this far apart (arm movements) they are not going to get farther apart because mostly in a solid the molecules are just shuffling around but in a gas the molecules are free to move all over the place wherever they want so the graph will be up and down.*

Interviewer: So what do you think happened here?

Student 4: You heated up the liquid or the solid and it became a gas.

In one interview, two of the students had difficulty interpreting the graph. As graphs had never been correlated to the models in the states of matter unit.

Student 5: The difference here is the temperature is staying relatively the same where as here it looks like the molecules are heated up and cooled down and heated up.

Student 6: That is the distance not the temperature.

Interviewer: This is the distance between two molecules….

In this case, it took a little while to help the students interpret the graphic representation. But once they became comfortable with the new context they were able to apply their conceptualizations of the different phases of matter fairly accurately.

Interviewer: So if you saw this when you watched the two molecules what would you think?

Student 6: A phase change, probably liquid to gas.

Interviewer: And you?

Student 5: Yea, they were heated up. I mean if it is a liquid they have a lot of collisions with each other, and then if it gets heated up [the molecules] start moving faster and they get further away.

Another question designed to see if students reasoned from the macroscopic properties or the atomic-scale properties was asked in the interview: "Do you think a liquid is more like a gas or more like a solid? Why?" As was evidence in the post-test responses, students used their experience with the models, their knowledge of the motion of particles and the relative proximity of particles in different states to respond. The following is an excerpt from one of the interviews. What is interesting in this excerpt is the way in which the student reasons from both a macroscopic and atomic-scale view in order to make the decision:

Interviewer: All right one more question, do you think a liquid is more like a solid or more like a gas and why?

Student 1: I can't really make a decision on which ones are more alike because solids, liquids and gases are all relatively the same depending on the temperature or what the object is….

Interviewer: The same stuff, you are absolutely right. If I take a single molecule of water out of ice, and a single molecule of water out of a glass of water, and a single molecule of water out steam they are identical. But the question is not about a single molecule but about a "gillion" molecules.

Student 1: Yeah, I don't know, I guess…liquid and solids are more alike.

Interviewer: Because?

Student 1: Because a liquid can still be somewhat hard like a solid and they [molecules] are not really moving around as much, kind of like a solid, and the molecules are close together like a solid and probably less likely to break apart like a solid. Like jumping on concrete is like jumping out of an airplane and hitting water, ….but you jump in the air you really don't feel nothing.

In the excerpt below, students could not persuaded to change their ideas based on macroscopic space filling properties. They instead focused on the movement and proximity of particles as a way to decide.

Interviewer: All right one more question, do you think a liquid is more like a solid or more like a gas and why?

Student 2: More like a solid.

Interviewer: Because?

Student 2: Because the molecules are a little more spaced out than a solid but they are moving at a relatively similar speed.

Interviewer: What do you think?

Student 3: I agree.

Interviewer: Despite the fact that if I look at it macroscopically a liquid sort of fills the container, a gas sort of fills the container and a solid keeps it shape?

Student 3: A gas has much more space in between their atoms than (unless the pressure was changed significantly) much more space in between than a liquid does and a solid.

Discussion & Conclusions

These data indicate that middle and high schools students can acquire fairly robust mental models of the states of matter through guided explorations of computational models of matter based on molecular dynamics as evidenced by significantly higher post-test scores when compared to pre-test scores. Using our approach, students accurately recall arrangements of the different states of matter, and can reason about atomic interactions. These results are independent of gender and they hold for a number of different classroom contexts. Additionally, a close evaluation of students' responses about the bulk properties of atoms and molecules revealed that many fewer students had misconceptions following the intervention as compared to these responses on the pre-test. Lastly, follow-up interviews indicate that students are able to transfer their understanding of phases of matter to new contexts, suggesting that the knowledge they had acquired was robust. In comparing middle school to high school student performance, there were too many differences in the treatments and populations to draw any conclusions about the impact of grade level on learning with these materials.

In the standard curriculum the three states of matter are most often described by static qualitative characteristics. Students taught in the traditional way fail to understand that atoms in all three phases are in motion. They tend to use macroscopic space-filling properties as the main way to distinguish among the different phases and they often come away with the idea that the particles in solids are close together, liquids are far apart, and gases are very far apart. After using our approach, students' thoughts regarding the different states of matter are based on density of particles, on movement of particles, and on the macroscopic properties.

In the literature reviewed, questions were raised concerning middle school student ability to reason about atomic scale phenomena. National Standards recommend not teaching students about molecular phenomena before high school. Our results suggest that

interactive molecular dynamics representations and guided activities provide an instructional strategy that gainsays this advice.

There were several features of our materials that may have contributed to student learning:

Computational models. In our materials, the same underlying computational model appears in numerous contexts. We suspect that this provides several advantages: 1) students gain familiarity with the representation and the way in which atoms interact, 2) the model parameters can be set by the student, giving a sense of control and interactivity, and 3) a large number of different configurations can be explored, and 4) the macroscopic properties of the model emerge from the details of the atomic-scale interactions in just the way that the corresponding properties emerge in real atoms.

Connections between the macroscopic and atomic scales. Our approach provided many situations such as illustrated in Figure 3, that provided links between the macroscopic world and atomic-scale interactions.

Guided exploration. The activities were designed by teachers who had a deep understanding of the required balance between open-ended exploration and direct instruction.

As mentioned above, there are multiple factors that could have contributed to the positive learning gains yielded. On the basis of these data we cannot empirically tease out the effects of each of these different aspects of the intervention, nor was the study designed for this purpose. A future study in which we experimentally control for each aspect of the intervention could yield important findings about which features of the implementation were most important in supporting students' learning. It is also important to design additional studies to identify other possible instructional features that are important.

States of matter represents only a small fraction of the science content that can be addressed by molecular dynamics. The *Molecular Workbench* can be used to support learning across introductory physics, chemistry, and biology. The emphasis on atomic-scale interactions can provide a unifying theme that can unite these fields and accelerate learning of all three. Understanding atomic-scale interactions provides an essential grounding for students entering biotechnology and nanotechnology, two of the fastest-growing fields of science. If the initial research reported here can be duplicated and expanded to new topics, science educators will have evidence for the effectiveness of curriculum that is enabled by an important new tool: molecular dynamics models.

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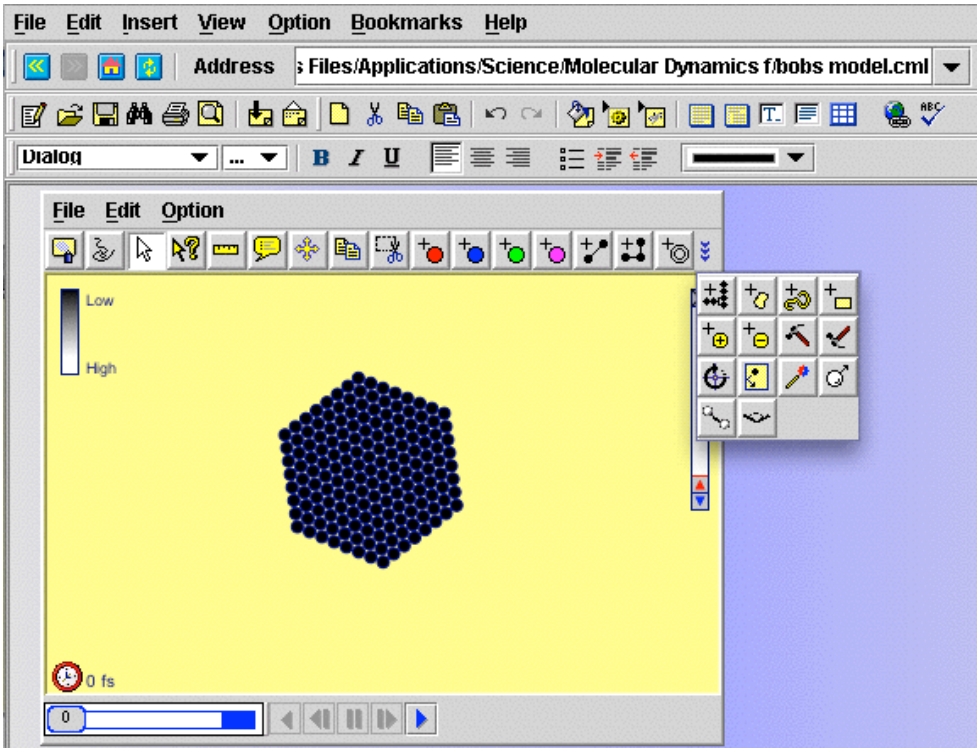

Figure 1. A typical Molecular Dynamics model, illustrating some of the available options.

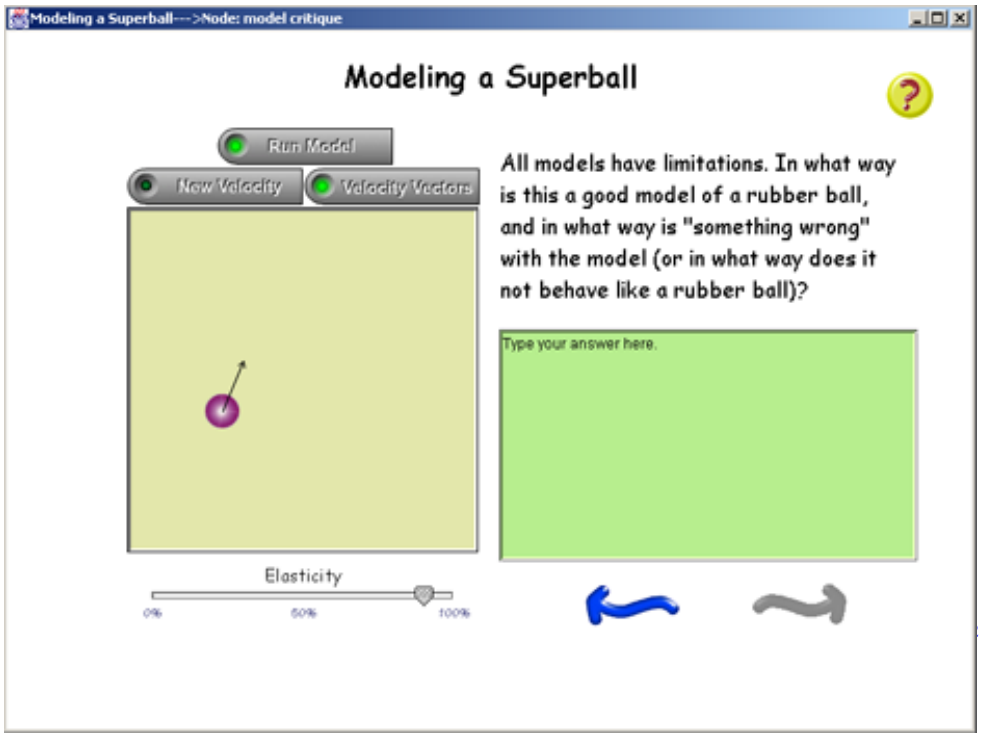

***Figure 2. An example of a molecular dynamics activity generated by* Pedagogica**. *A view of the* Molecular Workbench *engine is shown on the left. All its normal controls are disabled and replaced by controls generated by* Pedagogica*. The right-facing "go on" arrow is inactive until some response is made. A previous screen showed how to obtain help by pressing the question mark.*

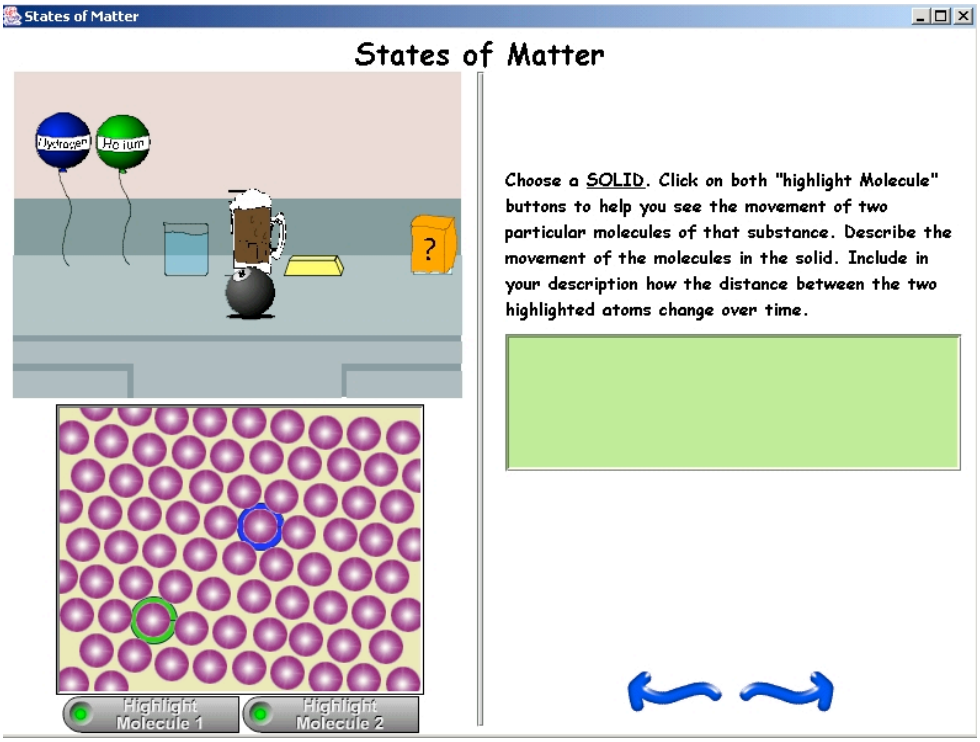

Figure 3. A view of The States of Matter Activity*. Students are prompted to choose the solids, liquids and gases in the window at the top, observe the molecular model of the objects in the window below and describe how the distance between two highlighted molecules change overtime.*

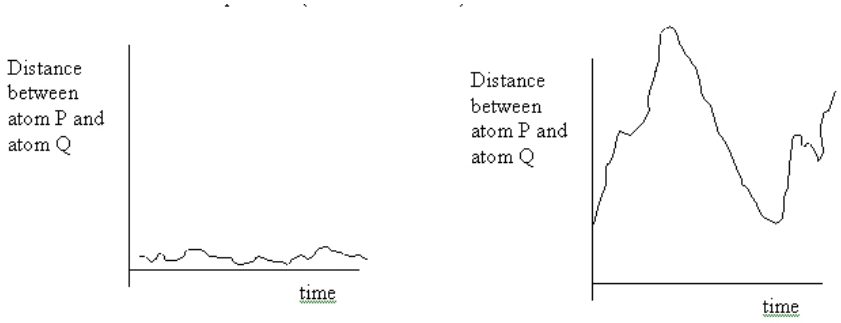

Figure 4: Graphs shown during interviews

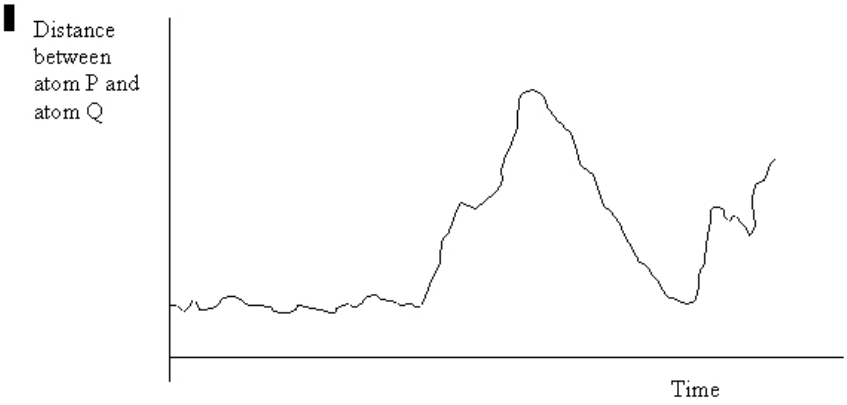

Figure 5: Graph showing change of state used during the interview.