Physica A 177 (1991) 281–293
North-Holland

Learning science through guided discovery: liquid water and molecular networks

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Dedicated to Michael E. Fisher on the occasion of his 60th birthday

In every drop of water, down at the scale of atoms and molecules, there is a world that can fascinate anyone. The objective of "Learning science through guided discovery: liquid water and molecular networks" is to use advanced technology to provide a window into the submicroscopic, and thereby allow students to discover *by themselves* an entire new world. We are developing a coordinated two-fold approach to high school science teaching in which a cycle of *hands-on* activities, games, and experimentation is followed by a cycle of computer simulations employing the full power of computer animation to "ZOOM" into the depths of this newly discovered world. Pairing of laboratory experiments with corresponding simulations challenges students to understand multiple representations of concepts. We thereby provide students with the opportunity to work in a fashion analogous to that in which practicing scientists work – e.g., by "building up" to general principles from specific experiences. Moreover, the ability to visualize "real-time" dynamic motions allows for student-controlled graphic simulations on the molecular scale, and interactive guided lessons superior to those afforded by even the most artful of texts. While our general approach could be applied to a variety of topics, we have chosen to focus first on the most familiar of molecular networks, that of liquid water. Later we will test the generality of the approach by exploring macromolecules such as proteins and DNA.

1. Introduction

Michael E. Fisher – Professor of Mathematics, Physics and Chemistry – is known for many things, not the least of which is his commitment to quality education. Indeed, many of the key ideas in mathematics, physics and chemistry of the second half of this century have originated from Professor Fisher and his students. What better proof can there be of his ability to educate? Moreover, Professor Fisher's Ph.D. training as a mathematician has enriched his career at the interface between chemistry and physics. Thanks to scholars like Professor Fisher, there has been a tremendous upsurge of interest in the opportunity to unify a large number of diverse natural phenomena from a variety of fields.

Has the time come for some of the recent discoveries of "the Fisher era" to make the leap from the research laboratory to the introductory science curriculum? The lack of computing power in the high school classroom has unfortunately been a barrier to

0378-4371/91/$03.50

this transfer in the past, but within a decade this situation will change. Very recent advances in computer technology provide the power of mainframe systems in relatively compact and inexpensive personal computers. Soon the computing power of even a supercomputer will be available on a desktop at a price comparable to today's personal computers. Over the next decade this tremendous computing power can and probably will become available in schools throughout the world. Here we discuss the possibility of harnessing this new technological resource as a teaching tool for specific topics in math and science, focusing on molecular networks and the most familiar substance of all, liquid water.

The members of our community are in a unique position to construct an innovative approach to this problem that serves to draw together mathematics (especially elementary probability) and various disciplines of science, capitalizing on a student's natural curiosity about nature to drive the desire to learn basic mathematics. Our approach, which we call "Learning science through guided discovery", is based on our experience that science is a field of endeavour as exciting and aesthetically rich as literature and art. A new teaching and learning paradigm is necessary to convince students that science is more than a collection of laws and equations in a textbook. We want to give students the opportunity to explore, to try, even to play and enjoy "on their own" in much the same fashion that we scientists do research in our labs.

One objective of "Learning science through guided discovery" is to use technology to provide a link between submicroscopic particles and the macroscopic world, and thereby allow students to discover and explore a new world with a minimum of supervision. We are developing a coordinated two-fold approach:

(i) A cycle of *hands-on* activities, games, and experimentation – involving tactile participation of all students and leading to a limited range of "tentative results", followed by

(ii) A cycle of desktop computer simulations employing the full power of computer graphics visualization to "ZOOM" into this newly-discovered world, a "virtual reality" that can approach an *interactive* version of an OMNIMAX theater.

One tangible outcome will be an answer to the question *Can desktop computer simulations really be used as a tool for learning about real science*? Is it possible that *far greater educational value results when students themselves have complete control of the simulations – as much control as we scientists have over our own laboratory experiments*? Answers to student questions, resolution of student misconceptions, and eventual personalized student discoveries are all "guided" by a clear set of cues which we build into the desktop computer display. Such an arrangement allows students to choose the parameters of the simulation system, and observe the results – thereby reducing the tendency of non-verbal students to "turn-off" to abstract concepts.

We emphasize that our approach is not only to impart scientific information but also to introduce students to modeling – one essence of "*doing science*". Our protocol

capitalizes on the natural *scientific* curiosity of high school students to discover how things "stick together" and their fascination with the "magic" of real-time dances of molecules. The student learns

- How to ask scientifically valid questions, as well as how to use both experiment and computer simulation to answer the questions.
- How to formulate a strategy for obtaining realistic answers to his or her questions via the same combination of experimentation and computer modeling that real scientists use when approaching questions.
- How to test the validity of the models proposed, by directly comparing the predictions of the model with direct observations on the real world.

It is unfair and unrealistic to expect students new to a subject to "discover" *on their own* results that professionals in the field are only now learning to appreciate. That is why our activities and software provide a structured exploration space in which the student directs the construction of randomly generated models that are individually unique (never before seen, not even by the teacher) but, in collective profusion, are predictable (and in this sense, "orderly"). These predictable results – often the subject of recent research – arise naturally out of the transparent simplicity of the governing physical models for these systems, their embodiment in games and activities, and the wealth and variety of cues available on modern desktop computer displays.

How does the novice acquire discovery skills? Just as cues can be added and made mutually reinforcing, so can they be gradually withdrawn. As students become more and more accustomed to the display, the program can leave them more and more to their own devices – for example by retiring commands from obvious buttons to pull-down menus. At the same time new resources can be introduced with a wealth of buttons and other cues that can be, in turn, gradually relegated to menus. Eventually the program becomes a "professional tool", with cues and motivation provided primarily by the student's developed ability to explore and discover.

At each stage in this process the desktop computer proves itself to be a more and more accomplished *slave* as the student grows to become a more and more powerful *master*. Growing student mastery does not depend on reading comprehension or mathematical background. Mastery consists of directing the desktop computer qualitatively: more statistics (larger samples), higher temperature, lower pressure, different graphs, a larger network.

Each deeper level of exploration by the students results in gradual *removal* of cues from previous levels and *activation* of cues for subsequent levels. Of course, parameters and alternatives must be set by close personal observation of individual students as they use the programs. A wider spectrum of feedback results from recording every keystroke and mouse-button press and replaying them in the presence of the student as he or she offers running commentary.

Does such a strategy of guided discovery succeed? We have recent experience with some steps in this sequence: brief hands-on games and activities followed by desktop

simulations and extensions. These are popular and engaging to high school students from both urban and suburban settings, for females and males, for minority and majority students. A central goal of our work is to explore *other* stages in this sequence: the tailoring of cues on the screen to tempt the student onward to both guided and unguided explorations. The results of our study provide both data and guidelines for others attempting to use advanced desktop computers in teaching.

In the remainder of this article, we offer some specific examples of the innovations we are attempting, and of the advanced technologies that we bring to bear. The key fact is that very recent advances in technology, which can essentially put the power of a mainframe computer in a high school environment, have the potential to revolutionize the teaching of certain topics in science and mathematics to students of all ages.

2. Water – the "liquid of life"

We now present an extended scenario for our unit on the hydrogen bond network of liquid water. Liquid water is centrally important in itself, but it is also an example of the kind of topic that is simply impossible to present in our style without greater computing power.

One of the objectives of "Learning science through guided discovery" is to provide a link between the submicroscopic and the macroscopic views of the world. Currently, students are asked to learn about and believe in this submicroscopic world without ever seeing it – yet it forms the basic structure of our bodies and of everything around us. Molecular dynamics simulations are the only way in which students can view this submicroscopic world. Molecular dynamics is a very simple application of the most widely taught of all scientific laws, Newton's laws – familar to every high school student. One produces a time sequence of "frames" which display a close-up view of several hundred water molecules and the bond network linking them together. The molecules push and pull one another via a *pair potential*, which closely approximates the interactions of water molecules brought about by the formation of chemical bonds. Molecular dynamics simulations have also been carried out for a variety of other liquids. Each liquid has its own characteristic pair potential. The student appreciates that a single physical law, Newton's law, is sufficient to describe the hydrogen bonded network of liquid water.

Chemical bonds are the atomic glue that hold matter together. Atoms are linked by bonds to form molecules as small as molecular hydrogen (with only two atoms) and as large as DNA (which can have millions of atoms). In high school chemistry, students learn about the nature of bonds at atomic and molecular scales, with emphasis on ionic and covalent bonds.

Chemical bonds also play an extremely important role at much larger length scales.

In a *crystalline solid*, atoms or molecules are arranged in a regular array – repeated over and over – and are held in place by rows and columns of chemical bonds. In a *molecular gas*, the molecules are not joined to one another; they fly along straight-line trajectories and occasionally collide.

Liquids, by contrast, have more complicated structure and much more complex dynamics than either solids or gases. Accordingly, they are far more difficult to model. This is one reason why high school courses seldom address the subject of liquids in detail. However, a great deal is now known about both the structure and the dynamics of liquids. Much of this recently acquired knowledge is not so complex as to be beyond the level of a high school student. In fact, the results of much of the research are as elegant and simple as they are exciting – and we seek a way whereby this new knowledge can be taught. Unfortunately, standard teaching approaches are inadequate – particularly for learning about the dynamic, time-dependent motions of liquid particles.

Water is known as an "associated liquid" because in addition to the *intramolecular* chemical bonds that hold together each individual water molecule, there are also many *intermolecular* bonds linking different water molecules together. In an ice crystal the intermolecular bonds form a regular pattern; in contrast, the network of bonds in liquid water is disordered, with no easily discernible pattern.

Furthermore, in a liquid, the bond network is not static, but changes rapidly over time. Bonds flicker on and off as water molecules travel throughout the liquid. The network structure rearranges itself as often as a million times per microsecond. Thus it is impossible to characterize the submicroscopic properties of the bond network by displaying a picture in a textbook. Ideally, students should be able to view a moving picture – which is now possible using the newest generation of "desktop supercomputers".

During the 1980s, excellent pair potentials have been developed to describe the submicroscopic interactions in water. There is a consensus among physicists and chemists that what is affectionately called "computer water" is in fact a remarkably accurate approximation to real water. With the powerful tool of molecular dynamics simulation, we can now probe the nature of liquids at the submicroscopic level – without leaving the high school classroom.

Molecular dynamics simulations are conceptually so simple that they are not limited to the study of liquid water. In fact, molecular dynamics techniques have been used to describe a vast range of physical systems. Students can alter the form of interactions in water to simulate other liquids and to study their corresponding properties. For example, students can be guided to design liquids which have unique properties (i.e., strange phase diagrams, etc.). In particular, we feel that *interactive* computer animation provides a unique opportunity to integrate the current subject matter of high school physics and chemistry (and even biology) with guided discovery.

We are developing an integrated software package as well as a set of personalized

hands-on games, experiments, and instruction manuals. Here are descriptions of some displays on which we are working. With the help of powerful desktop computer technology, students take an "animated walk" through the world of the submicroscopic. Using the ability of computer graphics to simulate a three-dimensional world on a two-dimensional screen, students are immersed in a awe-inspiring bath of molecules swimming about their heads. This effect becomes even more pronounced if we use the supercomputer graphics to create 3D movies viewed with 3D glasses! The desktop computer allows students to experience this world as if they were living among the atoms. Moreover, in the computer-generated world the student has complete control of all the parameters of the molecular bath and therefore can observe directly and immediately the consequences of changing these parameters.

Thus one goal of "Learning science through guided discovery" is to design a set of desktop computer software and optical disc packages which introduce students to the *dynamic* (i.e., time-dependent) side of natural phenomena. Such simulations allow students to realize that this submicroscopic world is as beautiful and as exciting as the large-scale world we live in. A longer term goal is to allow the students to *interact* with these simulations thereby permitting them to change the simulated world as well as stimulating classroom discoveries through the simulations of physical processes.

We also test the utility of the newest generation of emerging desktop computers for on-screen simulations of the actual motion and bonding patterns of molecules. These user-friendly high-speed desktop computers offer a substantial fraction of the power of a CRAY XMP to a student – so that he or she can escape many current restrictions on the scope of questions that can be asked and answered. Such "desktop supercomputers" will almost certainly be within the budgets of many high schools by the year 2000, if not before. Even now a IBM RS6000 with ten terminals costs less than ten personal computers.

The figures present examples of screen output from the software we have developed for students to explore the properties of water using computer simulations. In all cases, a primary goal is to allow for a choice among many representations of the same physical system, so that the particular path taken by a student in achieving understanding is under his or her control. The figures are based on configurations of a system of 216 molecules that result from a molecular dynamics simulation of water. However, instead of showing the molecules themselves, the student can choose to visualize the system in terms of its energy content and organization. In fig. 1 are shown the pair interactions of seven particular molecules with the other molecules in the system. Here, the strength of the interactions between distinct pairs of molecules is shown by lines between molecular centers; the boldness of each line is proportional to the strength of the corresponding pair interaction. It is immediately evident that there exist an entire family of interactions between a given molecule and the rest of the system, an observation which suggests the importance of collective behavior in determining the overall properties of the system. The student can then focus on particular kinds of

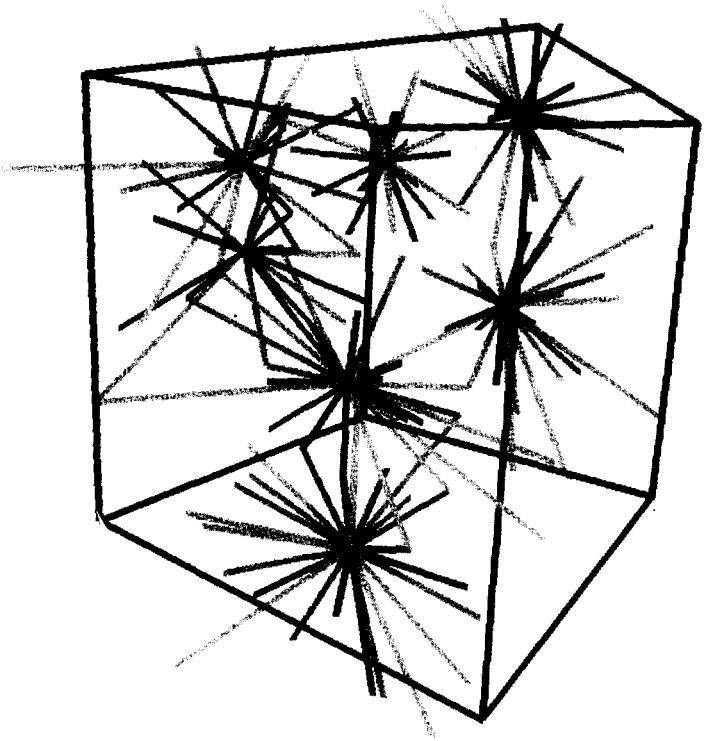

Fig. 1. A frame from a molecular dynamics simulation of water molecules. Here, only seven of the 216 molecules present on the simulation box (blue) are shown. Instead of showing the molecules themselves, the bonds between each of these seven molecules and all other molecules in the box are shown as lines. The boldness of the line indicates the strength of the attractive interaction between molecules.

interactions. For example, how dispersion (Lennard-Jones) forces are significant only at short range, whereas electrostatic forces are felt over much longer ranges. Alternatively, by combining this bond-strength representation with information on atomic positions, it can be seen how the electrostatic forces are dependent on molecular orientation, indicating the microscopic origin of water's tetrahedral bonding geometry.

A way of showing the distribution of energy while also allowing the actual molecules to be rendered is presented in fig. 2a. Here, each molecule is given a color representing the strength of its total interaction with all other molecules combined. Fig. 2b shows the color scale used. The purple molecules are most strongly bonded to the rest of the system, indicating that they are favorably positioned in their environment, while the red ones are least strongly bonded, and thus poorly related to their neighbors. The distribution of different colors throughout the system points out two features of the liquid. First, that all molecules are not energetically the same, even when the energy considered is the energy of interaction with all other molecules in the system. This demonstrates the occurrence of fluctuations within a macroscopically homogeneous liquid. Secondly, we see that, consistent with this spatial variation of molecular prop-

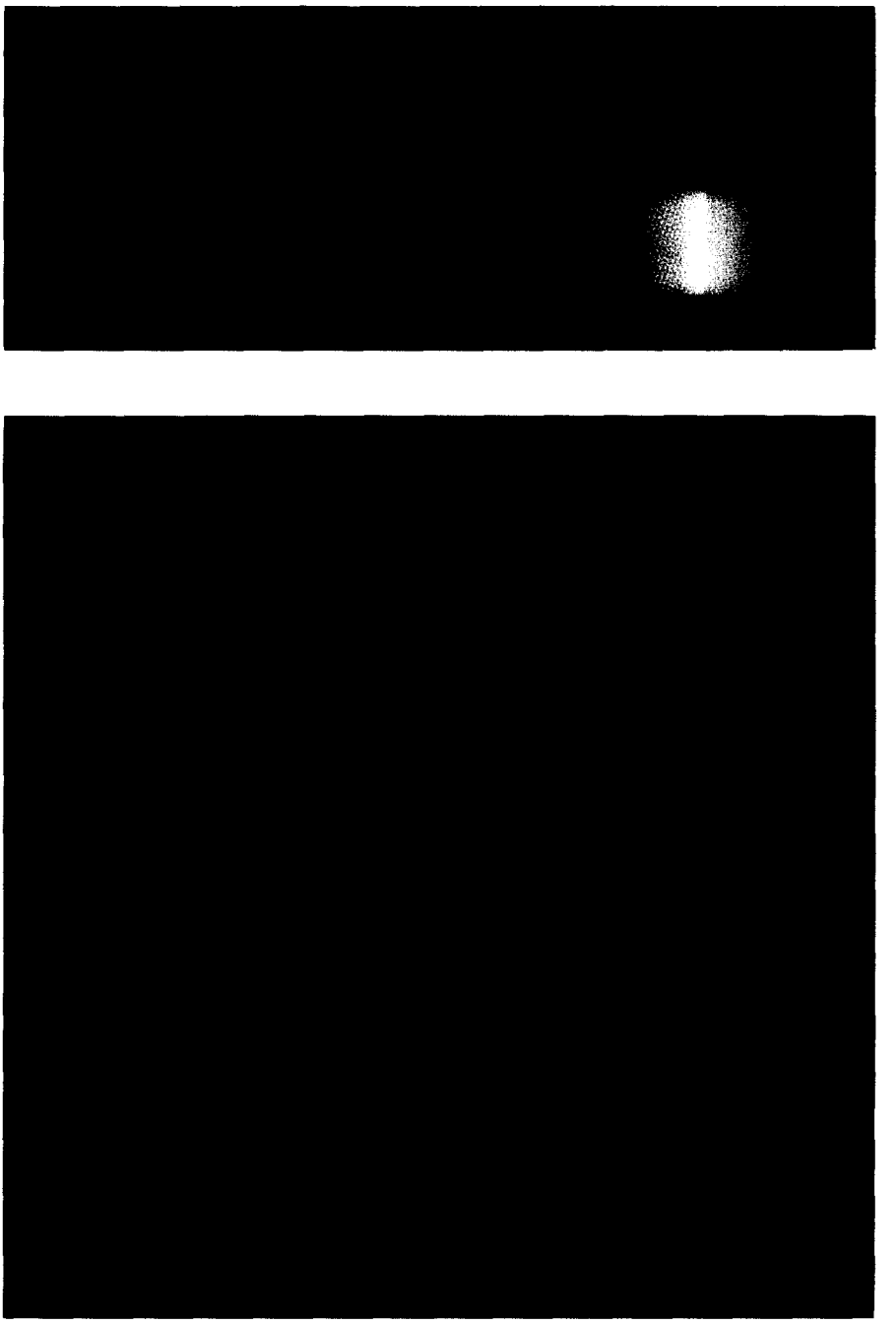

Fig. 2. (a) The same frame of the simulation as seen in fig. 1 is shown here with all molecules displayed. The color of each molecule indicates the strength of

erties, there are correlations among molecules in that there exists a tendency for molecules of a particular color to be surrounded by similarly colored molecules. Students can try to estimate the length in space (and in time) of these correlations, guess how this length is affected by changing temperature or pressure, and then test their guesses by running the simulation further at the new state point. Furthermore, specific molecules can be isolated and their immediate environment studied, to look for correlations between local structure and a molecule's energy. If students see a resemblance between the surroundings of "purple" molecules and the local molecular environments seen in a microscopic view of an ice crystal, then they can link the concept of a fluctuation to that of a locally ordered region which can be a "seed" for the crystalline state, and thus gain insight into how first order phase changes occur.

The network of hydrogen bonds in liquid water is revealed by showing only the strongest pair interactions, as shown in fig. 3. As a static picture, it is clear from this rendering that liquid water is a fully connected structure – in fact, it looks like a gel. This high degree of connectivity, which places the system of water molecules far above

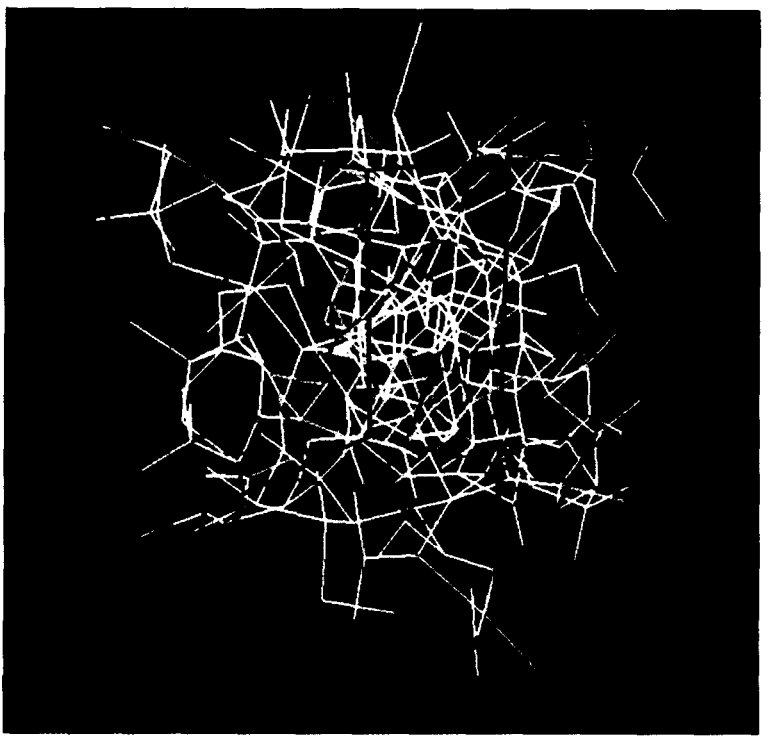

Fig. 3. The same frame of the water simulation shown in figs. 1 and 2, is here displayed with only the strongest of the pair interactions drawn. The results is a view of the spanning network of hydrogen bonds found in liquid water.

its percolation threshold, is an important clue to understanding the anomalies of water as a liquid. This type of extensive connectivity (i.e., high energy hydrogen bonds) is vital to understanding the origin of water's high specific heat. The fact that the network is generally four-coordinated shows that the molecules are not close packed (in which case we would predict 12 nearest neighbors), and so generate a configuration that sacrifices compactness to gain internal energy. This is a simple way to reveal the special relationship in water between energy and entropy, which is ultimately responsible for water's anomalous thermodynamic properties, such as its density maximum.

The microscopic view of bonding in water is completed by allowing the students to study the real-time evolution of the system. Fig. 4 is a frame from a simulation of a system of ten water molecules which runs in real time, and is rendered for viewing with "3D" glasses, so that both the spatial and temporal bonding associations may be monitored in the most realistic way. This presentation provides striking insights into how important dynamics are to the concept of a bond. Pairs of molecules which in snapshots look strongly bonded still exhibit significant librations and vibrations with respect to each other. Students can appreciate how bonds break and new bonds form, in part because of, and in part in spite of, the degree of motion shown by bonded molecules. In this way, the role of temperature, defined as the amount of molecular

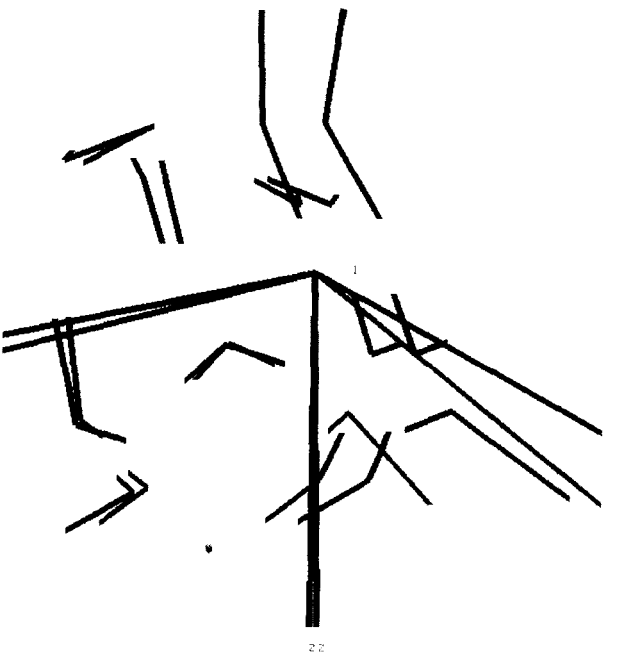

Fig. 4. A frame from a "3D" simulation of ten water molecules that runs in real time on the computer display. (The viewer must wear appropriate glasses to see the "3D" effect.)

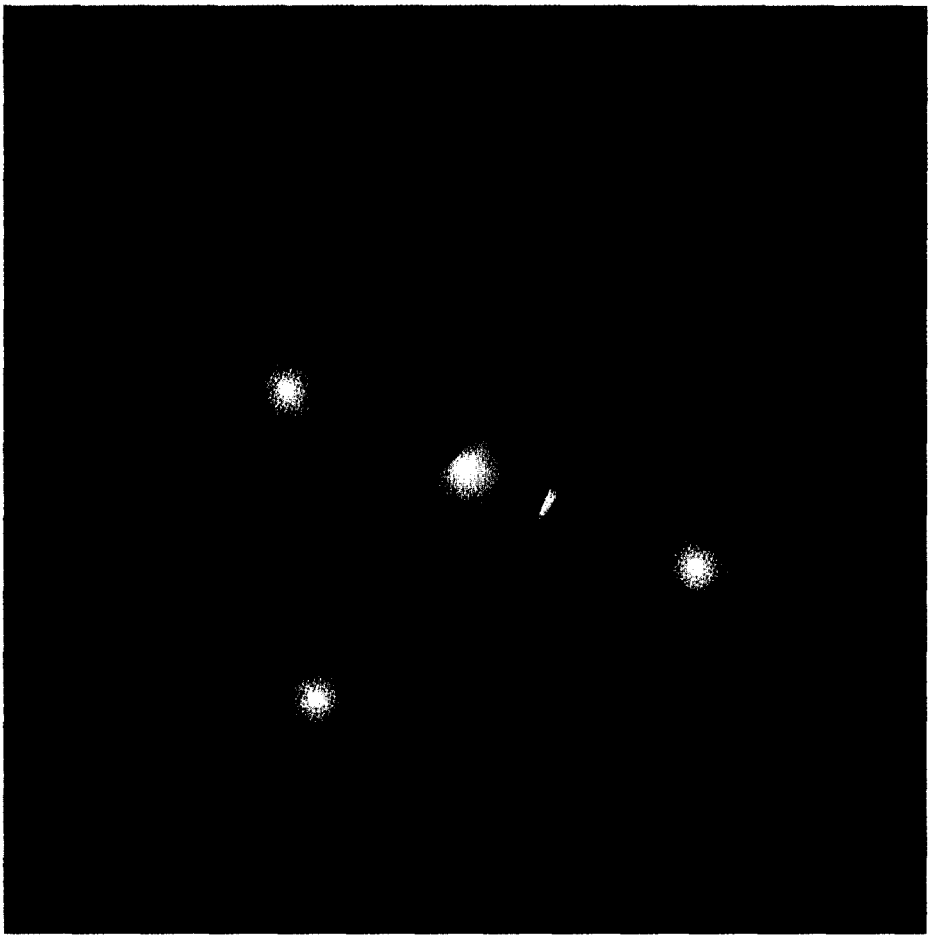

Fig. 5. A detailed view of a specific local environment of a water molecule from the simulation also shown in figs. 1–3. The central molecule is orange; its nearest neighbors are shown in blue.

motion, in determining the state of a condensed matter system can be visualized.

Fig. 5 shows an example of how students can "dissect" the system of molecules in order to study specific features more carefully. Shown is one particular molecule (orange) surrounded by only its immediate neighbors (blue). By working with specific molecular arrangements, and selectively displaying different groups of molecules, such as nearest neighbors only, or second nearest neighbors only, students can be introduced to the important concept of a radial correlation function. "Frame-by-frame" analysis of local bonding arrangements can also show how bonding arrangements change, as a bond to one receding neighbor is exchanged for a bond to a new approaching neighbor.

3. Discussion and summary

We have begun to study the extent to which students make meaningful connections between what they see simulated on a computer screen and what happens in real life. The role of the hands-on experiment or activity which serves as the counterpart to the computer-based simulation we study through careful observation of the students themselves, and compared with other ways the sciences are traditionally taught. Of special interest are interdisciplinary ventures joining science teachers from two or more disciplines to teach important concepts.

We are also trying to discover cognitive outcomes. Professionals from diverse backgrounds fuse their respective talents – professors in the scientific disciplines, professors in education and cognitive science, research associates, graduate students, undergraduates, high school science teachers, and high school students – all interact in the work of the project in ways that cast aside the traditional "pecking order" or disciplines. In particular, it is interesting to see the impact our bright and energetic graduate students have on the choice of courses and major as well as the career plans of younger students as they work together in developing and trying the new materials.

Perhaps most interesting and novel is the influence this work in educational development is having on *our* science graduate students – who normally have no opportunity to work on educational issues. Already there is impressive evidence to suggest that the process itself has important benefits for the participants. In particular, we have found that involving women graduate an undergraduate students as mentors in our interactions with high school students attracts female high school students and gives them role models in scientific research. This direct influence is amplified when the graduate students involved in the education project are concurrently carrying out research on the same subject. Indeed, we may be in the process of discovering and documenting a new paradigm for engaging graduate students on a regular basis in high school education – a part-time *Education Corps* (which could become for the 1990s what the *Peace Corps* was for the 1960s).

In sum, we arouse the innate curiosity of students – so that the next time the child confronts a familiar substance, he or she asks questions such as *"Why is this substance the way it is?"* and *"How does nature make this substance work the way that it does?"* By replacing the *"videogames of the arcade"* with the *"videogames of the desktop supercomputer"*, can we encourage even the most ardent science-phobe to discover for himself or herself the interactive aspects of science? By exploiting the breathtaking speed of a CRAY X/MP supercomputer housed in a package the size of a bread box, can we offer a money-back guarantee *that no student will ever again complain of boredom?*

Acknowledgements

This article is based on an extensive collaboration with many individuals. In addition to those joining as co-authors, the collaboration includes C.A. Angell, R. Blumberg Selinger, A. Geiger, M.H. Shann, S. Sastry, S. Schwarzer, D. Stauffer and E.F. Taylor. The support of the Education and Human Resources Division of the National Science Foundation, Apple Computer, and the IBM Corporation is gratefully acknowledged.