Virtual Environment of Water Molecules
for
Learning and Teaching Science

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Abstract

Virtual reality is an emerging computer visualization technology which allows educators to place their students into instructional environments heretofore difficult or impossible to achieve. In order to take full advantage of this technology, a virtual environment, "Virtual Water", is being developed. Virtual reality has been recently employed in a few educational applications, but the project presented here is the first application we know of combining aspects as atomic and molecular orbits, electron densities, water molecular dynamics for the liquid and gaseous phases and phase transitions.
Keywords: *virtual reality, water, molecular dynamics, quantum mechanics.*

Introduction

In the past fifteen years, research on physics education has brought a lot of information about the difficulties students have in learning physics. At the same time, the ongoing revolution in information technology has led to new tools for creating innovative educational environments. In response to these developments, a wide variety of new models of physics instruction are available.

People's understanding of what computers can do has shifted dramatically as the size and cost of these devices has decreased while their power has increased. At the beginning, computers were seen as number-crunching machines, but now we have tools to manipulate information, namely in the graphic form. Up to now, the use of computational means in Physics education stood mainly on the creation of 2D representations that the students could use to build more refined mental models. However, recent advances have created new possibilities and the visualization of 3D objects and data becomes increasingly important in learning several scientific subjects (in particular, atomic and molecular science, fluid dynamics, etc.). With virtual reality (VR), the visualization of complex data and the building of more adequate conceptual models is possible [1, 2].

VR is one of the most significative steps towards a natural human-computer communication, allowing an easy presentation and an intuitive grasp of complex data. Virtual environments can represent various aspects of a natural environment or even a totally artificial world. The inclusion of haptic information and direct manipulation contributes to the impression of being immersed in a real situation [3]. Perception, as learning, is an individual act. Since each person evolves a unique psychomotor approach to interacting with a physical environment, individuals have more varied responses to 3D interfaces than to the standard 2D graphical interfaces with menus, windows, and mouse.

The Physics Department of the University of Coimbra, Portugal, the Exploratory Henry the Navigator, the Computer Graphics Center (both also in Coimbra) and the High Education School for Technology and Management of Guarda, are developing the "Virtual Water" project, a virtual environment devoted to the learning of Physics and Chemistry. This work involves the know-how of different fields (computational simulation of physical systems, computer graphics and science education) in order to arrive at a useful scientific-pedagogic visualization of water.

The main goal is to enable the user to visit virtual attractive and enjoyable sceneries where he can learn the constitution and properties of water. The user will be able to interact and "change" the environment to better understand the structure of water. The virtual environment is realistic and comprehensive, allowing for exploring the atomic constituents of water as well

as macroscopic structures. With this environment, the study of the atomic units, the molecule geometry, the molecular orbitals, the electron density, and molecular normal modes is facilitated. Using simplified equations, as those of Newtonian mechanics with the Lennard-Jones potential, simulation of the molecular dynamics of the solid, liquid and gaseous phases and phase transitions, is also available. Realistic simulations use more complicated forces [4].

Description of the Project

The study of water is motivated by the fact that a better understanding of it, in its different functions and aggregation states, is only possible if the water molecule itself and the behavior of a set of molecules in given conditions are understood. With the speed of modern computing resources, it is becoming common in research to model aqueous systems atom by atom, moving each molecule in response to the forces acting on it. These advances should be followed by education applications.

2.1. Our Problem

Innovative practices using computers are being tried for teaching and learning science [5]. VR has been touted as a powerful teaching and training tool because ([6], [7], [8]):
- Supports direct experience of phenomena.
- Is 3D.
- Allow for multiple frames of reference.
- Offers multisensory communication.
- Is physical immersive.

However, current immersive VR technology has several limitations that may impede usability and learning ([9]):
- Head-mounted displays and gesture devices interfere with interaction.
- Input devices have restricted fidelity and versatility.
- The display capabilities are somewhat limited.
- Multisensory inputs can interact to cause unintended sensations and perceptions.

Through the design of "Virtual Water" we have started to determine how the characteristics of VR influence usability and learning. At present, achieving VR's potential to enhance learning requires transcending the interface barriers through paying careful attention to usability issues.

2.2. Our Approach

To design a educational virtual world, we have adopted an iterative learner-centered design approach that focuses on usability and learning. The main goals in producing our application are:
- To provide an educational environment for students to explore some microscopic and abstract concepts, which they are teached in class but are far away from daily experience.
- To develop a practical knowledge concerning the application of VR techniques in education.
- To contribute with data on the pedagogical usefulness of VR. People in the field have an intuition that VR can have a strong impact on learning. But believing in VR is not enough: its usefulness has to be proved.

2.3. System Configuration and Models Development

The interface of our immersive, multisensory environment is typical of current high-end VR. "Virtual Water's" hardware architecture includes a Pentium II processor with 3D graphics accelerator. For the navigation and immersion in the virtual environment, we use the Head Mounted Display V6 from Virtual Research, as well as one Cyberglove with cybertouch (for haptic information), from Virtual Technologies, and a Polhemus Isotrack II magnetic orientation position sensor for two receptors (see Figure 1). This class of hardware will not be common in classes in the next years, but it allows us to deliver a product with minimal quality.
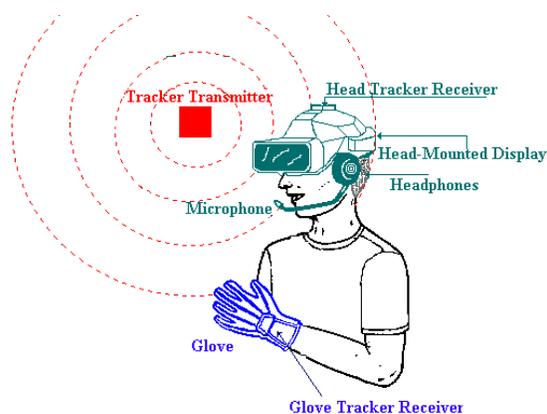

Figure 1. The virtual reality hardware interfaces.

Concerning the software, we use *WorldToolkit* (from Sense8), that serves the definition and creation of the virtual scenarios, and other packages for model development. For the design of the first part (quantum mechanics) of "Virtual Water", we use mainly the freeware *PC Gamess* [10], that performs the water molecule calculations (namely geometry optimization,

electron density, etc.) and the freeware *Molden* [11] package for molecular representation. For the second part (molecular dynamics), we use commercial software packages (*Mathcad*, *3D Studio Max* and *Autocad*) for development of models and optimization and *Visual C++* for implementing the molecular dynamics algorithm.

2.4. The Training Environment

Scenery exploration is preceded by navigation in a training environment. The first "room" which users encounter is the training environment, which contains known objects. The goal is to overcome the disorientation problems which some users experience when first using VR. This virtual scenery is designed to be a simple, familiar environment in which users can become comfortable with the VR hardware before moving on to more complex an abstract environments.
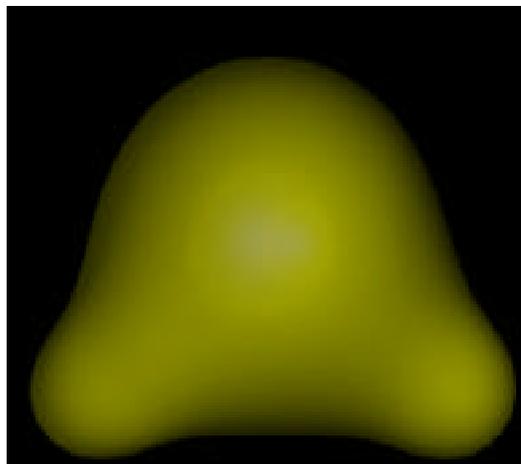
2.5. The Quantum Mechanics Virtual Environment

In this scenery we deal with the geometry of the water molecule (see Figure 2-a), its electron density (see Figure 2-b), and molecular orbitals (see Figure 2-c and d). The 3D models were produced with *PC Gamess* (a program that performs *ab initio* calculations to obtain the molecule geometry), and *Molden* (a program that enables the visualization).
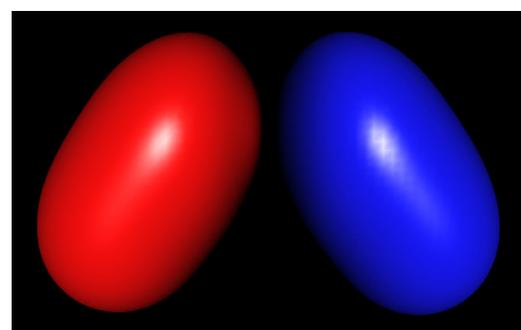
In this virtual environment students can build and travel through molecular orbitals, ad molecular density and better understand the water molecular structure in order to clarify the chemical bonding.
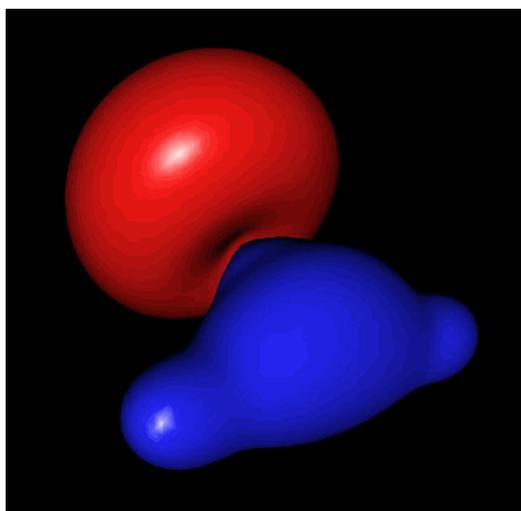
b)

c)

a)
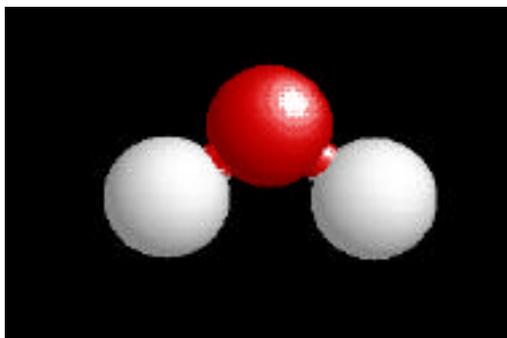
d)

Figure 2. Some 3D models of the quantum mechanics virtual environment: a) ball-and-stick representation of water molecule; b) equidensity surface representation of the same molecule; c) the third and fourth occupied molecular orbital representation of water molecule (the total electron density is obtained adding up the occupied molecular orbits).

2.6. The Molecular Dynamics Virtual Environment

We aim at understanding some water properties by direct simulation. We assume that the molecular dynamics can be treated classically because realistic simulations (with quantum effects) use complicated forces [4] and are much more computational demanding. We use Newton's equations of motion

$$m\frac{d^2\vec{r}_i}{dt^2} = -\vec{\nabla}_i \sum_j u(r_{ij})$$

with the Lennard-Jones potential,

$$u(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right]$$

(the ε and σ are constants).

The repulsion at small distances is a consequence of the Pauli exclusion principle. The weak attraction at larger distances is due to the mutual polarization of each molecule.

Newton's equations are solved for each molecule starting from initial positions and velocities and using the force acting on each molecule

$$-\vec{\nabla}u(r) = \frac{24\varepsilon}{r}\left[2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right]\hat{r}.$$

Then, we calculate the positions

$$x_i(t+\Delta t) = 2x_i(t) - x_i(t-\Delta t) + \frac{F_{x,i}(t)}{m}\Delta t^2$$

and velocities

$$v_{x,i}(t) = \frac{x_i(t+\Delta t) - x_i(t-\Delta t)}{2\Delta t}$$

of each molecule at successive times.

The user is able to interact and change the environment in order to study the liquid and gaseous phases and phases transitions (see Figure 3-a). The solid phase is also examined (see Figure 3-b).

One of the new aspects of this pedagogical work is the 3D representation of the ensemble of molecules instead of the usual 2D. The same algorithm has been applied to the liquid and gas phases, emphasizing their similarity.

In order to assure a real-time rendering (the level of detail which is attainable at a practical speed), the number of molecules in each phase or phase transition simulation has been carefully tested. For example, for the gaseous phase simulations we have used 20 molecules. This restriction is the compromise between the computer graphics capability, molecular models and real-time calculations. Contrary to most computer applications, VR must recalculate the user's view for each frame update, taking account considerations as light sources, shadings, distance from the user, etc. To be effective, all this must be performed several times per second in addition to any calculations that have to be made.
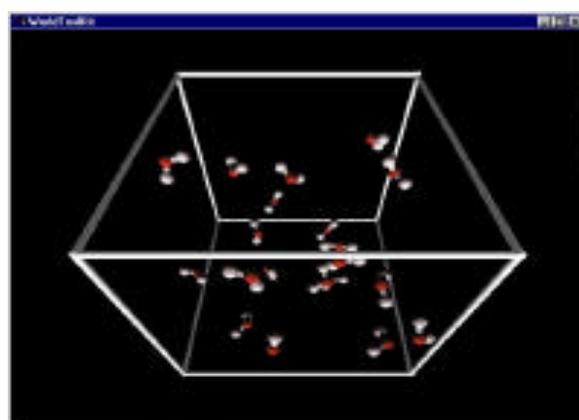
a)
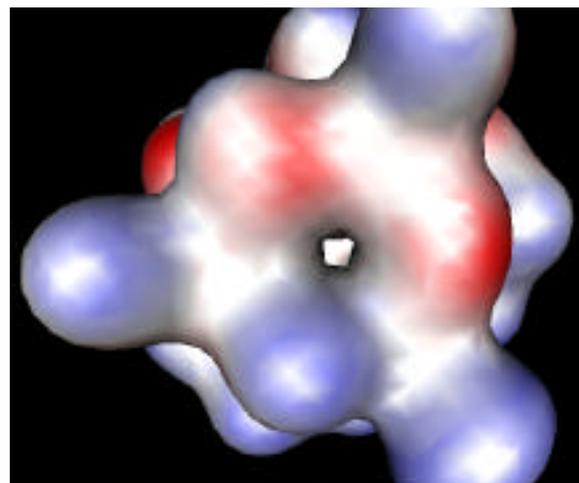
b)

Figure 3. Images from the molecular dynamics environment: a) the gaseous phase, with the ball and stick model, showing twenty molecules in a box; b) The ice phase, with the same number of molecules, but with the electron density representation. These pictures were created using the same software as in Figure 1, being the dynamics implemented in *Visual C++*.

Conclusion

The use of 3D graphics seems to be a powerful tool for visualizing and understanding complex and/or abstract information. Immersion is a recent aspect which has to be better explored and evaluated. A virtual environment for teaching and learning Physics and Chemistry is being developed to study the possibilities of VR in education. The main objectives are:

· Get new means for teaching and learning the physics and chemistry of water.
· To apply VR as an educational tool, in order to determine which aspects of VR provide the most effective educational benefits, and to learn the strengths and weaknesses of this technology in an educational setting.
· To build knowledge of VR techniques and tools which can later be applied to other problems.

Feedback from students still needs to be collected and analyzed.

Acknowledgements

References

[1]   J. Trindade and C. Fiolhais. A realidade virtual no ensino e na aprendizagem da Física e da Química. *Gazeta da Física* **19**, pages 11-15, 1996.

[2]   C. Fiolhais and J. Trindade. Use of Computers in Physics education. *Proceedings of the "Euroconference'98 – New Technologies for Higher Education".* Univ. Aveiro: ed. A. Ferrari, Aveiro, 1999.

[3]   J. C. Teixeira, A. Côrte-Real, P. Bernardes and F. Macedo. Santa Clara-a-Velha: virtual environments and cultural heritage. *Proceedings of CAD & Graphics'97, Fifth International Conference on CAD & CG*, pages 81-88, Shenzhen, China, December, 1997.

[4]   M. Laasonen, M. Sprik and M. Parrinelo. "Ab initio" liquid water. *J. Chem. Phys.* **99** (11), pages 9080-9089, 1993.

[5]   J. C. Teixeira. Environments for teaching computer graphics: an experience. *Comput. & Graphics* **20** (6), pages 927-935, 1996.

[6]   M. Bricken and C. Byrne. Summer students in virtual reality. In Wexelblat, A. (Ed.), *Virtual Reality: Applications and Exploration*, pages 199-218, New York: Academic Press, 1993.

[7]   T. Erickson. Artificial realities as data visualization environments. In Wexelblat, A. (Ed.), *Virtual Reality: Applications and Exploration*, pages 1-22, New York: Academic Press, 1993.

[8]   R. Kalawsky. *The Science of Virtual Reality and Virtual Environments. A Technical, Scientific and Engineering Reference on Virtual Environments*. Addison-Wesley Publishing Company, 1993.

[9]   C. Wickens. Virtual Reality and Education. *Proceedings of the IEEE International Conference on Systems, Man, and Cybernetics, 1,* pages 842-847, New York: IEEE Press, 1992.

[10]   PC Gamess, a program for ab initio quantum chemistry, written by Alex. A. Granovski, Moscow State University.

[11]   Molden, a package for displaying MOLecular DENsity, written by G. Schaftenaar, CAOS/CAM Center Nijmegen, Toernooiveld, Nijmegen, The Netherlands.