Virtual Water: An Application of Virtual Environments as an Educational Tool in Physics and Chemistry

Jorge F. Trindade

Physics Department and
High Education School for
Technology and Management,
Polytechnic Institute of Guarda
Phone: +351-71-222634
P-6300 Guarda, PORTUGAL
jtrindade@ipg.pt

Carlos Fiolhais

Physics Department and
Center for Computational
Physics, University of Coimbra
Phone: +351-39-410624
P-3000 Coimbra, PORTUGAL
tcarlos@hydra.ci.uc.pt

Vitor Gil

Chemistry Department of the
University of Coimbra and
Exploratory Henry the Navigator
Casa Municipal da Cultura
Phone: +351-39-703897
P-3000 Coimbra, PORTUGAL
vgil@cygnus.ci.uc.pt

Abstract

"Virtual Water" is a project which aims at constructing a virtual environment of water molecules as an education tool. The main goal is to enable the user to visit attractive and enjoyable virtual scenarios that make the structure and properties of water more amenable to master. The virtual environment is comprehensive, enabling explorations at both the atomic and macroscopic levels. In particular, molecular geometry, molecular orbitals, molecular electron density, normal vibrational modes will be addressed, as well as a simulation of the molecular dynamics for the liquid and gaseous phases and the phase transitions.

Background

For the learning of some topics of Physics and Chemistry (atomic and molecular science, reaction kinetics, fluid dynamics, etc.) the visualisation of objects and data in 3D space is becoming increasingly important. Misconceptions can arise when students try to match what they know about the physical world from their own experience and what they are being taught in class ([Cle82], [Min82], [Mcd84], [Sty96]). For example, students often associate ice melting with an increase of speed of the water molecules during the process. However, students are normally not able to use their observation to understand this microscopic concept.

Computational means are very common today in education as a tool for solving this and other kinds of problems. Some interactive and immersive computer environments have been found to help the student [Ded95]. A way to correct a wrong mental model consists in allowing the student to explore it using a simulation and contrast the results with the correct model and reality.

Up to now, the use of computational means in science education has been restricted mainly to 2D representations that the students could use to build more refined mental models ([Dis87], [Den96], [Tao97]). However, the most recent computational advances have created new possibilities. Virtual reality (VR) is a modern technology, allowing the visualization of complex data and building better conceptual models [FT98]. It is designed to make the user believe that he is actually inside the artificial environment, as opposed to being an external observer looking in. Virtual environments can represent various aspects of a natural environment or even a totally artificial world. The inclusion of haptic information and direct manipulation increases the impression of being immersed in a real situation.

Although the concept of VR has been around for almost thirty years, until recently its use has been limited to specialised research labs. High-quality solutions are not yet affordable, but we are now able to develop VR based educational applications, which can be improved in the future. VR has a definite role to play in education. However, it should not be forced into a subject when another method is available that teaches better or as well in a more economic way.

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 applied to the learning of Physics and Chemistry.

Among various reasons that justify the choice of water, two should be singled out: (a) it is an ordinary theme common to a large spectrum of domains of Physics [LSP93], Chemistry [Lai87] and Biology [GK97], and (b) its scientific study has motivated a large number of investigators, due to its unique characteristics [Sta97] and led to the revelation of unknown properties [LFK98]. With the increased power and availability of computing resources, it is becoming more and more common to model aqueous systems atom by atom, moving each molecule in response to the forces acting on it. A better understanding of water, in its different functions and aggregation states, is only possible if the structure of the water molecule itself and the behavior of molecules are grasped.

This work combines the know-how of different fields (quantum theory, computational simulation of physical systems, computer graphics and science education) in order to arrive at a visualization of water which is useful from the pedagogic-scientific viewpoint.

Overview of "Virtual Water"

"Virtual Water" (VW) is an application of VR designed to aid in the instruction of high-school and undergraduate Chemistry and Physics students. Own main goals in producing VW are:

a) To provide an educational environment for students to explore some microscopic concepts which they study in class.
b) To develop a practical knowledge concerning the application of VR techniques to education.
c) To contribute with data on the usefulness of VR. People in the field have an intuition that VR can have a good impact on the way people learn. But believing that VR is useful is not enough. That usefulness has to be proved.

The topics approached in our project cover aspects of quantum mechanics and molecular dynamics. First, we deal with the geometry of the water molecule, its electron density in connection with chemical bonding, and molecular orbitals (Figure 1). Second, we aim at understanding some water properties by simulation. In different conditions of pressure, volume and temperature and using simplified equations as those of Newtonian mechanics, with the Lennard-Jones potential, the user is able to interact and change the environment in order to study the liquid and gaseous phases and phases transitions (Figure 2). The solid phase is also examined. We assume that the dynamics can be treated classically because realistic simulations (with quantum effects) use complicated forces [LSP93] and are much more computational demanding. We also assume that the force between any pair of molecules depends only on the distance between them. The repulsion at small distances is a consequence of the Pauli exclusion principle. The dominant weak attraction at larger distance is due to the mutual polarization of each molecule.

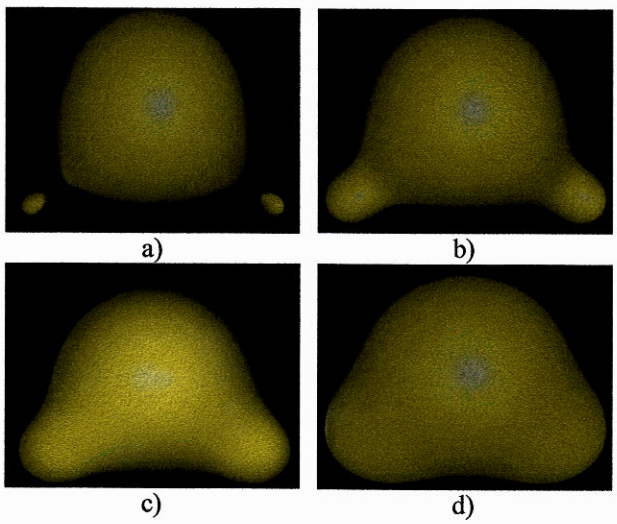
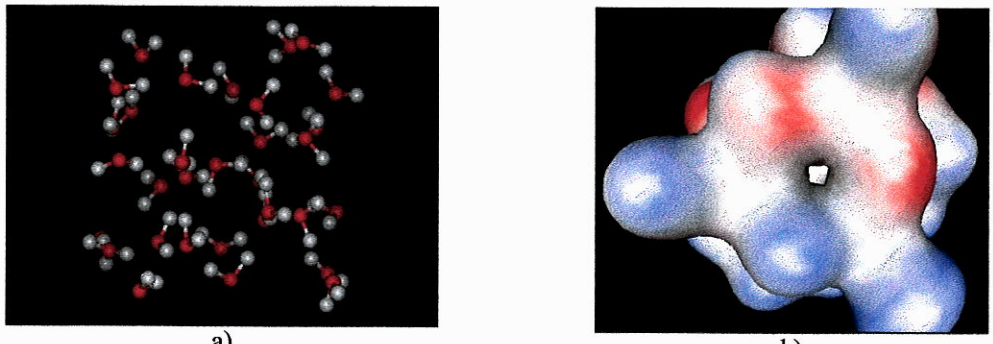


Figure 1: Some 3D representations for the water molecule electron density. The situations a), b), c) and d) represent equidensity surfaces, corresponding to decreasing values. The pictures were produced using *Molden* and *PC Gamess*.

The scenery exploration is preceded by navigation in a training environment. The goal is to help the user to achieve good adaptation to the hardware interfaces and provide some training in interacting with virtual worlds.



a) b)

Figure 2: Two frames from the molecular dynamics environment: a) the gaseous phase, with the ball and stick water model, showing twenty molecules in a box; b) The ice phase, with the same number of molecules, but now with the electron density representation. These pictures were created using the same software as in Figure 1, being the dynamics implemented in *Visual C*$^{++}$.

We use the following hardware: one PC with Pentium II at 233 MHz, with 128 Mb of RAM using an ultra-high-speed video board and a 3-D sound audio card. 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 (Figure 3). This class of hardware will not be common in classes for several years, but it allows us to deliver a product with minimal quality.

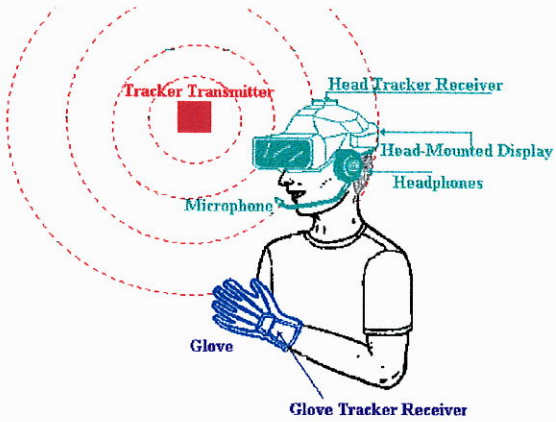


Figure 3: The virtual reality hardware interfaces.

Concerning the software we use the *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 models of the VW, we use mainly the freeware *PC Gamess* [Gam], that performs the calculations related with the water molecule (namely geometry optimization, electron density, etc.) and the freeware *Molden* [Mol] package for molecular representation. For the second part we use commercial software packages (*Mathcad, 3D Studio Max* and *Autocad*) for models development and optimization and *Visual C*$^{++}$ for the implementing of the molecular dynamics algorithm.

In order to understand how can molecular dynamics is implemented, we present the method used for that simulation.

The molecular dynamics simulation

For simplicity, we assume that the dynamics can be treated classically. Newton's equations are solved for each molecule starting from initial positions and velocities and using the force acting on each molecule. We calculate the positions and velocities of each molecule at successive times. Let us present in detail the dynamics algorithm. We assume that the molecules are spherical and chemically inert (the representation is nevertheless given by a stick and ball model) and that the force between any pair of molecules depends only on the distance between them. In this case the total potential energy U is a sum of two-particle interactions:

$$U = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} u(r_{ij}), \tag{1}$$

where $u(r_{ij})$ depends only on the distance r_{ij} between particles i and j. The most important features of $u(r)$ are a strong repulsion for small r and a weak attraction at large r-value.

One of the most common forms of $u(r)$ is the Lennard-Jones potential:

$$u(r) = 4\varepsilon\left((\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6} \right). \tag{2}$$

The length σ and the energy ε parameterize this potential.

The forces on each pair of molecules are:

$$\vec{F}(r) = -\vec{\nabla}u(r) = \frac{24}{r}\varepsilon\left[2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]\hat{r}, \tag{3}$$

where $\hat{r}$ is a unit vector.

The system configurations at successive times Δt are calculated from Newton's equations for each molecule with mass m:

$$m\frac{d^2\vec{r}_i}{dt^2} = -\vec{\nabla}_i \sum_j u(r_{ij}) \tag{4}$$

To solve this equation we adopt the Verlet algorithm [GT96]:

$$x_i(t+\Delta t) = 2x_i(t) - x_i(t-\Delta t) + \frac{F_{x,i}(t)}{m}\Delta t^2 + 0(\Delta t^4) \tag{5}$$

$$v_{x,i}(t) = \frac{x_i(t+\Delta t) - x_i(t-\Delta t)}{2\Delta t} + 0(\Delta t^3). \tag{6}$$

The $x_i(t-\Delta t)$ is calculated by:

$$x_i(t-\Delta t) = x_i(t) - v_{x,i}(t)t + 0(\Delta t^2). \tag{7}$$

In Figure 4 we see the final result for the gaseous phase simulation. One of the new aspects of this work is the 3D representation for molecules instead of the usual 2D. The same algorithm has been applied to the liquid phase and gas-liquid phase transitions. 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 twenty 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 such 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 must be made.

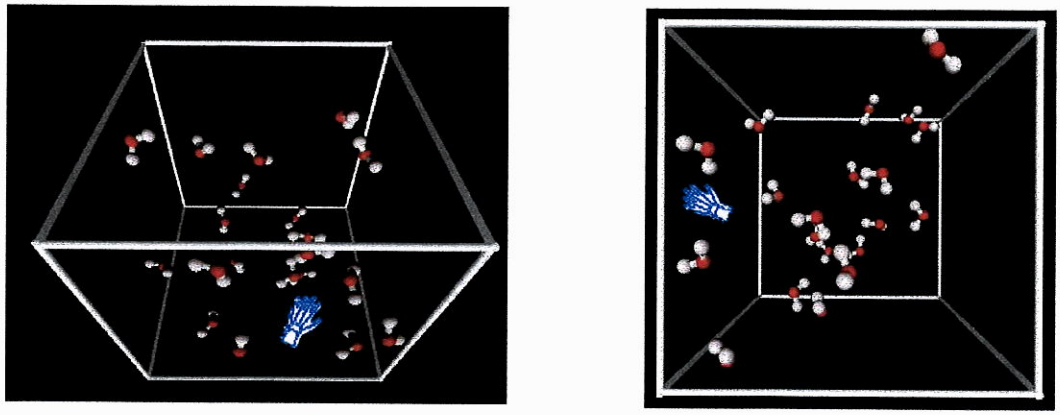


Figure 4: Two perspectives of the gaseous phase molecular dynamics. Using the head-mounted display, the head-tracking device allows the user to look where he likes. With the glove he can manipulates objects (*e. g.*, catch a molecule). These virtual scenarios were obtained using *WorldToolkit*.

Conclusion

The use of graphics is, indeed, a powerful tool for visualizing and understanding complex and/or abstract information. Immersion is a recent aspect to be explored and evaluated. A virtual environment for the teaching of Physics and Chemistry is being developed to study the possibilities of virtual reality in teaching and learning. The main objectives are:

a) Get new means in learning and teaching the Physics and Chemistry of water.
b) To build knowledge of VR techniques and tools which can later be applied to other problems.
c) 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 new technology in an educational setting.

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