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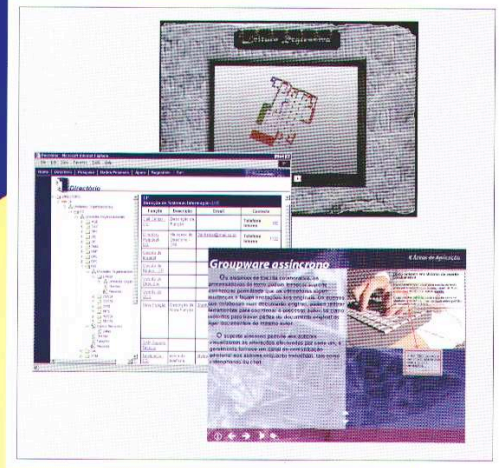

Courseware for Telework Training

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.

German Abstract

Mit den neusten Fortschritten im Rahmen der Virtuellen Realität (VR), ist die Betrachtung komplexer Daten und das Aufbauen angemessener Modelle möglich. Diese Fortschritte brachten neue Möglichkeiten für die Darstellung und Betrachtung von 3D Objekten. Daten erhalten eine progressive Wichtigkeit, im wissenschaftlichen Bereich, und dort besonders in der Atom- und Molekularwissenschaf, den Dynamischen Fluiden, etc. Die Abteilung für Physik der Universität Coimbra, Portugal, das Exploratorium Henry der Seefahrer, das Zentrum für Graphische Datenverarbeitung (beide in Coimbra) und die Hochschule für Technologie und Verwaltung Guarda, entwickeln z.Z. das Projekt »Virtuelles Wasser«, eine virtuelle Umgebung um Chemie und Physik zu erlernen. Dieses Projekt umfasst das Knowhow mehrerer Bereiche (Computer Simulation in Physikalischen Systemen, Graphische Datenverarbeitung und Wissenschaftliche Ausbildung) um eine wissenschaftlich-pedagogische Darstellung und Betrachtung des Wassers zu erreichen. Das hier vorgestellte Projekt ist das erste, das atomare und molekulare Umlaufbahnen, elektronische Dichtigkeit, dynamische Wassermoleküle für flüssige und gasförmige Phasen sowie Phasenübergänge darstellt.

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.

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. 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 Centre (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 scenarios 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[3].

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 behaviour 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.

Our Problem

Innovative practices using computers are being tried for teaching and learning science[4]. VR has been touted as a powerful teaching and training tool because[5], [6]:

- 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[7]:

- 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.

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.

System Configuration and Models Development

»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 (cf. 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.

Concerning the software, we use WorldToolkit (from Sense8), to create 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[8], that performs the water molecule calculations (namely geometry optimization, electron density, etc.) and the freeware Molden[9] 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.

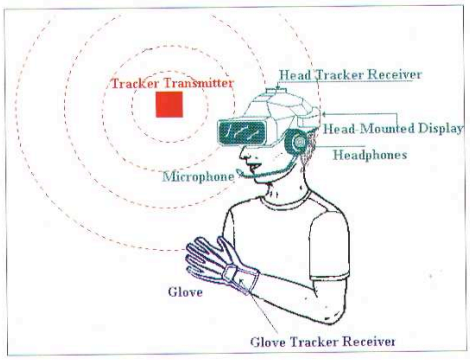

Figure 1: The virtual reality hardware interfaces

The Training Environment
Scenery exploration is preceded by navigation in a training environment. 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.

The Quantum Mechanics Virtual Environment
In this scenery we deal with the geometry of the water molecule (cf. Figure 2-a), its electron density (cf. Figure 2-b), and molecular orbitals (cf. 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 travel through molecular orbitals, ad molecular density and better understand the water molecular structure in order to clarify the chemical bonding.

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,

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

(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

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

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 (cf. Figure 3-a). The solid phase is also examined (cf. 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.

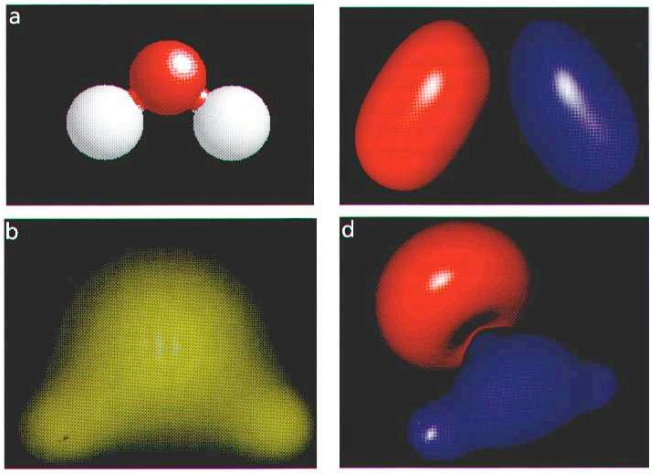

Figure 2: Some 3D models of the quantum mechanics virtual environment: a) ball-and-stick representation of water molecule; b) equidensity surface representation of the same molecule; c) the third and fourth occupied molecular orbital representation of water molecule (the total electron density is obtained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

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

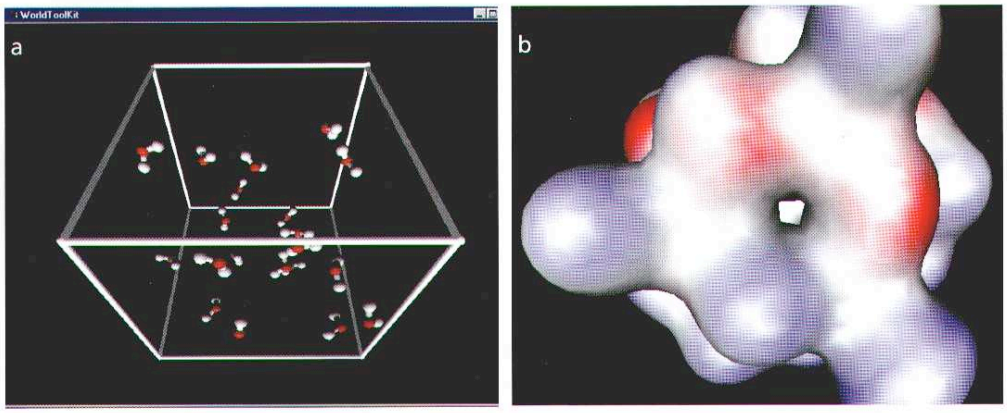

Figure 3. Images from the molecular dynamics environment: a) the gaseous phase, with the ball and stick model, showing twenty molecules in a box; b) The ice phase, with the same number of molecules, but with the electron density representation. These pictures were created using the same software as in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

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 analysed.

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