15. VIRTUAL REALITY IN SCIENCE EDUCATION: THE *VIRTUAL WATER* PROJECT

TRINDADE, Jorge Fonseca
Physics Department
Institute Polytechnic of Guarda
6300 Guarda
alberto@hydra.ci.uc.pt
&
FIOLHAIS, Carlos
Physics Department
University of Coimbra
3000 Coimbra
tcarlos@hydra.ci.uc.pt

Abstract **- Virtual reality adds a new dimension - immersion - to graphics display. Moreover, the characteristics of this new technology allow for a greater interactivity with the user.**

The *Virtual Water* project is the first work in virtual reality applied to the learning and teaching of Physics and Chemistry done at the Physics Department of the University of Coimbra. The project involves aspects as atomic and molecular orbits, electronic densities, bonds, molecular dynamics, phase transitions, etc.

It is a multidisciplinary work involving areas as computational simulation of physical and chemical systems, computer graphics and science education.

15.1. INTRODUCTION

The recourse to graphics, in particular to three-dimensional ones, for visualizing and interpreting information has been increasing in the research and teaching of sciences. In particular, that recourse is needed in domains where the interpretation of complex information is more demanding, as it happens in molecular modelation. Indeed, there are a lot of chemistry software packages, the most recent including the use of VRML [1,2]. The reasons for such interest are clear: in scientific research it is easier to obtain understanding from a three-dimensional model than from the simple reading of numbers or formulas; in the apprenticeship domain the utility of graphical methods, in particular the immersive ones, is being proved, for instance for forming correct conceptual models [3].

The *Virtual Water* project aims at the conception of an educational environment, joining molecular modelation with immersive three-dimensional graphic representation. The choice of water is justified by the fact that this is a common and relatively simple substance. Its study has interested many investigators who do realistic simulations of water in Physics, Chemistry and Biology [4,5]. However, less attention has been given to the pedagogical exploration of water simulations.

The subjects approached in the project go from the study of the molecule geometry to the structures of the solid, liquid and gaseous phases, through the study of the electronic density and the chemical bonding by hydrogen bridges. Since some studies of water start with atomic orbits, in particular with the hydrogen s, p and d, this subject is also included in the project.

15.2. General Features of the Project

The exploration of the contents is done in two ways (Figure 1):

- Macro → Micro - from the water phases to the atoms (full line in the Figure);
- Micro → Macro – from the atomic orbits to the water phases (dashed line).

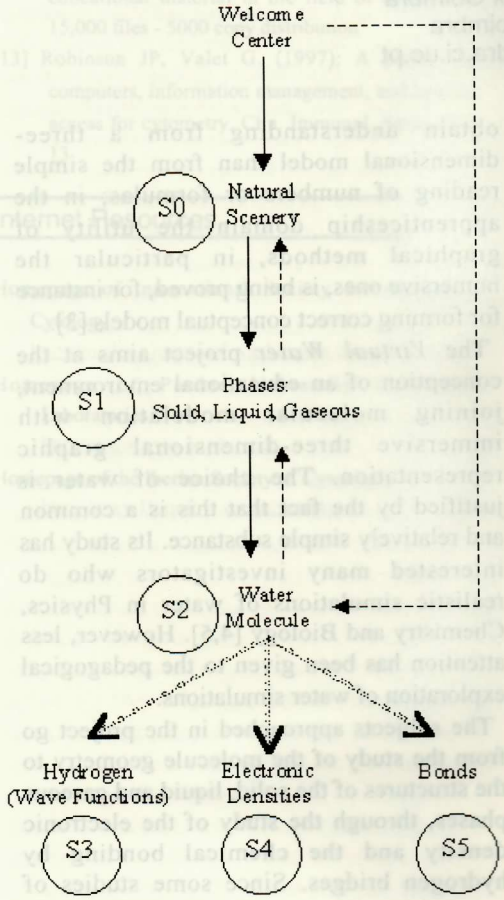

Figure 1- Scheme of the environment *Virtual Water*. The dashed line denotes the content exploration going from the macroscopic to the microscopic side while the full line denotes the exploration going from the microscopic to the macroscopic side.

In any case, the scenery exploration is preceded by navigation in a training environment. The goal is to help the user to achieve good adaptation to the interfaces (glove and Head Mounted Display), navigation and interaction in virtual worlds.

Our project comprises two phases: in the first (which is under way) the visualization of the water molecule geometry (S2), the hydrogen bonds (S5), the water electronic density (S4) and hydrogen wave functions (S3) are done. In a second phase, other aspects will be introduced allowing for the study of phase transitions (S1).

For implementing the virtual environment we use two software packages running in parallel in two PC's. One of the packages, *WorldToolkit*, serves the definition and creation of the virtual scenarios while the other, *Gaussian 94*, does the calculations related with the water molecule namely, geometry optimization (S2) and the electronic density (S4).

We use the following hardware: two PC's with Pentium Pro at 233 MHz, with 64 Mb of RAM, in network, with one of them (that which does the virtual environment rendering) using an accelerator graphic board *Matrox Millennium II AGP* with 8 Mb of RAM. For the navigation and immersion in the virtual environment, we use the Head Mounted Display V6 from *Virtual Research*, as well as one *Cyberglove* from *Virtual Technologies* and a position sensor to two receptors, *Isotrack II*, from *Polhemus*.

The final product of this work will be disposed to the school community through the Competence Center "Nónio-Softciências".

15.3. Conclusion

The use of graphics is, indeed, a powerful tool for visualizating and understanding of

complex and/or abstract information. The immersion capacity is a recent aspect to be explored and evaluated. A virtual environment for the teaching of Physics and Chemistry is being developed to test the possibility of applying virtual reality in teaching and learning. The work is in a preliminary phase of execution, so that its evaluation cannot yet be done.

15.4. ACKNOWLEDGEMENTS

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