Using Virtual Environments for Studying Water Phases and Phase Transitions

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In recent years, many studies have dealt with students' reasoning in science. Those studies suggested that pupils, in different degrees, have difficulties in understanding matter phases and phase transitions. To increase pupils understanding of phases and phase transitions, we are developing the "Virtual Water" project, a virtual environment centered on the learning of the structure and properties of water in its different phases. Within this environment, the molecular dynamics in the solid, liquid and gaseous phases of water and the corresponding phase transitions take place in three-dimensional space, with the possibility of haptic interaction with the molecules.

Keywords: **Virtual reality, virtual environment, water, phases and phase transitions**

1 Introduction

All substances undergo dramatic changes in their qualitative properties when certain parameters pass through particular values. Matter phases and phase transitions have received considerable attention in the framework of research on children's understandings in different ages and development stages [1-4], [10], [15].

Ice melting is an everyday example of a phase transition. When the temperature increases, keeping the pressure constant, the molecular vibrations become gradually more violent and thermal expansion occurs. Since this increase of vibration amplitude is gradual, one might expect that the macroscopic properties of water would also undergo a smooth change. While this is true for most temperatures, there is a well-defined temperature for which something dramatic happens: a sudden change in the properties of the substance and the appearance of a liquid. The liquid, in its turn and at a higher temperature, undergoes another phase transition going into a gas.

Few pupils use the corpuscular theoretical model taught in school to explain these processes. Indeed, their knowledge and understanding of the corpuscular theory of matter is sometimes very fragmentary. They apply it in some situations but not in others. For example, they may apply the corpuscular theory to explain gases but not to explain solids and liquids. There are also cases where pupils say that the shape and size of molecules changes when the state of matter changes: the shape of molecules depends on the shape of the vessel, molecules of solids are the biggest while gas molecules are the smallest for Portuguese children (13-15 years) [9], etc.

Other studies of students' conceptualization of phase transition from liquid or solid to gas have indicated that some children have difficulties conceiving gas as a substance [6] [12]. As students do not develop the general idea of gas prior to formal learning, the perceptual clues for detecting and identifying gases are weaker than for liquids and solids. Although pupils know some properties of air, they do not compare air with other gases, claiming that other gases do not have the same properties as air. A frequent explanation is that air is a big bulk system [11]. Gases are frequently linked by some invisible entity, something immaterial, for example energy in various forms. Kircher [5] also reports that high school pupils understand gases as a continuous substance with no empty space between particles.

Since the use of images is a powerful tool for understanding complex and/or abstract information and since immersion in virtual environments is a recent technique which needs to be explored and evaluated, a virtual environment for studying phases and phases transitions is being developed by the Physics and Mathematics Departments of the University of Coimbra, Portugal, the Exploratory "Henry the Navigator", in Coimbra, and the High School for Technology and Management of the Polytechnic Institute of Guarda. We have named it “Virtual Water”.

2 Overview of the Molecular Dynamics Virtual Environment

"Virtual Water" (VW) is a set of virtual environments designed to help in the instruction of high school students of Physics and Chemistry (it might also be useful for freshman university students). The main goals of this virtual reality application are:

a) To provide an educational environment for students to explore some microscopic concepts which they are taught in class.

b) To develop a practical knowledge concerning the application of virtual reality techniques to education, contributing with data on the usefulness of virtual reality [13-14].

The molecular dynamics component of VW is devoted to understanding some water properties and studying its phases and phase transitions by computer simulation. These simulations are based on the corpuscular theory of matter and use the equations of Newtonian Mechanics. We assume that the dynamics can be treated classically because more realistic simulations (incorporating quantum effects) are cumbersome and more computationally demanding. We also assume that the force between any pair of molecules depends only on the distance between them.

The interactions using *dataglove* allow the user to act and change the environment in order to distinguish the properties of solids, liquids and gases. The *cybertouch* system associated to the dataglove enables the user to experience some molecular behaviors that are impossible to feel in real world. For example, in the solid phase the user may fly through the ice structure and learn about it (Figure 1). Using the *dataglove* the user is able to break the ice and with the *cybertouch* system he can feel the increase of molecular vibrations with the temperature. While breaking ice may be a common macroscopic experience, watching the network of hydrogen bond and feeling molecular vibrations, for example, are quite uncommon experiences. On the other hand, in the liquid and gas phases, it is possible see and try to grab a molecule, understanding by direct experience that its speed is bigger than in the solid phase.

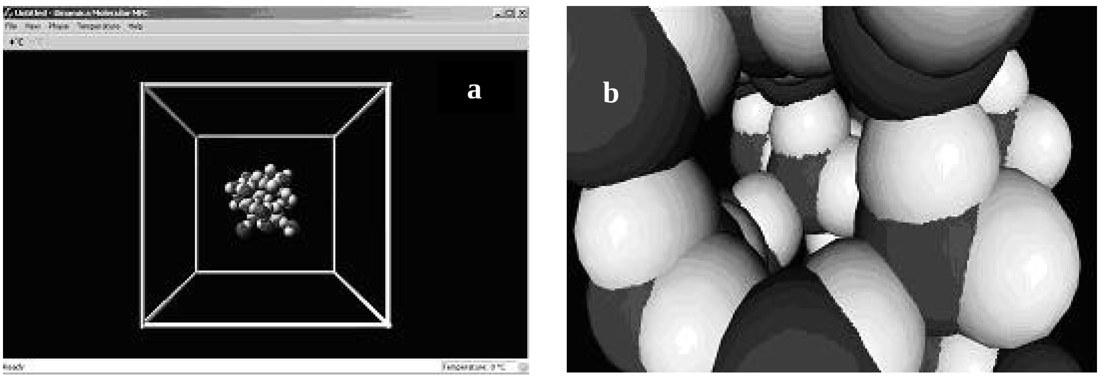

Figure 1: Two frames from the water solid phase (ice) of our molecular dynamics environment: a) balls model of a group of molecules; b) flying through the ice structure.

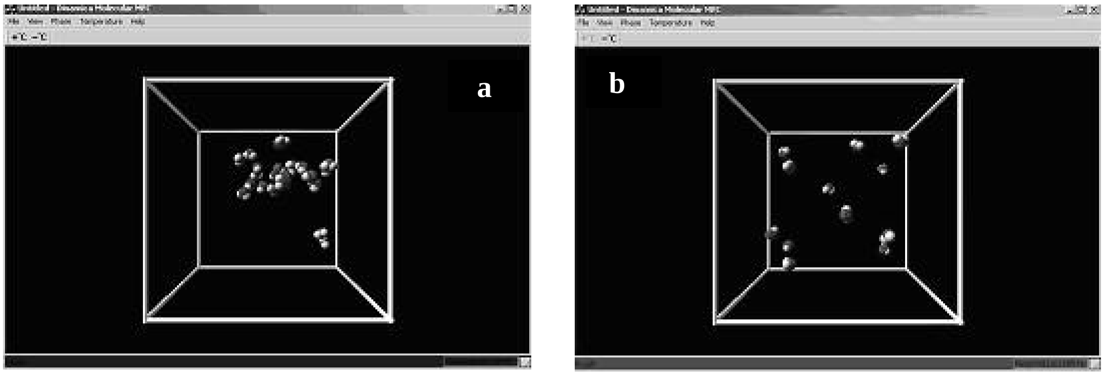

Figure 2: Frames from the water liquid and gas phases: a) the liquid phase, with the balls model of twelve molecules; b) The gas phase, showing the same molecules. These pictures, as well as those of Figure 1, were created with *PC Gamess*, *Molden*, *3D Studio Max*, being the dynamics implemented in *Visual C*$^{++}$ on *WorldToolkit*.

Using balls models of water molecules the user may interiorize the corpuscular theory of matter. Since the molecular dynamics simulation takes place in a box (closed system) it is easy to understand that the molecules are the same in solid, liquid or gas phases. It is clear from our virtual environment that, in any phase of water, empty intermolecular spaces are present, these being smaller in the solid and liquid phases than in the gas phase (Figure 2). The density is different in the three phases.

For designing the VW models we used the free software *PC Gamess* [8], that performs the calculations on the water molecule, and *Molden* [7], for the molecular representations. For model development and optimization we used commercial software packages (*Mathcad* and *3D Studio Max*) and *Visual C*$^{++}$ for implementing the molecular dynamics algorithm. Concerning the definition and creation of the virtual scenarios we used *WorldToolkit* (from Sense8). For navigating in the virtual environment and interacting with our models we use a *dataglove* with *cybertouch* system (for haptic information) from Virtual Technologies.

3 Conclusions

Important strategies in teaching Physics and Chemistry are based on central the idea that matter consists of particles but the fact that these are invisible hinders sometimes the development by students of the right scientific concepts. However, the analysis and comparison of various results in the pedagogic literature show that some incorrect concepts and their relationships are simply transferred from the macroworld to the micro world. In fact, there is a firm link between the concepts on matter structure and empirical knowledge of macroscopic phenomena.

If students accept the corpuscular theory mainly for gases and not for solids and liquids, it is advisable to confront them with this contradiction and to treat specifically the processes of phase changes from gas to liquid, and *vice versa*, in terms of identity of substance, identity of particles and conservation of the number of particles. Similar procedure applies to students who accept better the corpuscular theory for solids.

The use of immersive virtual environments and haptic information, although recent, seems to be a powerful means for visualizing and understanding complex and/or abstract information. Actions like grabbing a molecule, breaking hydrogen bonds networks, feeling molecular vibrations, flying through channels in ice and through the empty spaces of molecules in liquid and gas phases (as in George Gamow's book "Adventures of Mr. Tompkins"), etc. are impossible in real world but possible in computer simulations.

"Virtual Water", our virtual environment for studying phases and phase transitions based on corpuscular theory of matter is promising to make progresses along the indicated directions. We are acquiring new means in learning and teaching the Physics and Chemistry of water and building knowledge on virtual reality techniques and tools, which can later be applied to other problems. In particular, our experiment with virtual reality should point out what are the most effective educational benefits and also to indicate the weaknesses of this new technology in an educational setting.

Feedback from pupils is being collected and analyzed in order to quantify the pedagogical usefulness of our virtual environment. Of course, if these techniques prove to be successful, teacher's strategies should incorporate them. We hope that, with tools like the one we are developing, intangible experiments become more and more concrete and that this fact may facilitate the development of scientific models among science students.

Acknowledgements

The authors thank Prof. Dr. Victor Gil, from the Chemistry Department of the University of Coimbra, for his precious suggestions, and Prof. Dr. José Carlos Teixeira, from the Computer Graphics Center of the same University, for his technical advice. We also wish to acknowledge the assistance of the students Nuno Pereira and Eduardo Coutinho, who have developed the molecular dynamics component of "Virtual Water". This research was supported in part by the Portuguese Foundation for Science and Technology (project PRAXIS/FIS/14188/1998).

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