

# Visualising molecules: on-line simulations and virtual reality

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Science education, in particular physics education, is being changed by the use of new technology. One of the most promising means of teaching and learning science is the Internet. A lot of material has appeared on the Web. Its impact in education has in most cases still to be evaluated.

Relatively small and less developed countries like Portugal offer interesting ground for observing the dissemination of computers in science education. The Portuguese Physical, Chemical and Mathematical Societies set up, in 1991, a common action – “Softsciences - for creating, producing and distributing software for learning Science and Mathematics, especially at the middle and high schools levels. “Softsciences” had the intention of making somewhat “softer” the learning of the so-called “hard” sciences, but without compromising rigour. The Ministry for Education and the Ministry for Science and Technology have supported this project.

In 1997 all software programs were brought together in a CD-ROM, under the suggestive title “Omniscience”. A multimedia program was included (“Multimedia Periodic Table”) as well as copies of Web pages with abundant teaching and

learning resources. A copy of the CD-ROM was given to all (around 1500) Portuguese middle and high schools. “Omniscience” has a home page with the address: <http://nautilus.fis.uc.pt/~softc/omni98>, through which new materials have been offered (in Portuguese).

Our work in the group “Computers in Science Education” at the Centre for Computational Physics of the University of Coimbra, which gained experience with “Omniscience”, is now centred on on-line materials. The Web gives much more accessibility and universality compared with off-line programs (see, for example, Web Multimedia Periodic Table in <http://nautilus.fis.uc.pt/st2.5/>). On-line simulations in “Java” are a convenient format for representing many physical phenomena in a pedagogic way. They may be used interactively, without the need for downloading and installing.

Another method for visualizing and manipulating scientific concepts goes under the name of virtual reality, a technique where virtual scenarios are felt as real by users. This novel technique, which is becoming cheaper, needs further testing and evaluation.

We describe here two recent experiments which are being carried out by us and which use on-line simulations and virtual reality in the teaching and learning of the structure of matter.

## “Molecularium”: On-line simulations in Physics and Chemistry

In the project “Molecularium” we aim to produce a set of computational simulations for the Internet dealing with various physical-chemical processes (<http://nautilus.fis.uc.pt/molecularium>). Based on recent Internet technologies, our aim is the teaching and the learning about the microscopic world. One of the main problems in science education is experienced by students when faced with abstractions. Computer visualization tools are particularly effective to overcome this problem. For example, when learning the atomic and molecular structure of matter, the

progressive familiarization with scientific models benefits from static and dynamic representations of the building blocks of matter.

The simulations that we are building relate to thermodynamical concepts (pressure and temperature), phases (solids, liquids and gases) and phase transitions, energy and entropy, and some assorted chemical phenomena (chemical equilibrium, salt dissolution, etc.). Our target groups are final year high school students and university freshmen.

One simple example of the “Molecularium” aims to help students to understand how food (containing water) is heated in a microwave oven (<http://nautilus.fis.uc.pt/molecularium/mw>). Rotating a button, radiation is transferred to the molecules (Fig. 1) which start to undergo faster rotation. Their vibrational and translational motion is also increased and the thermometer rises, indicating an increase in temperature. Of course, one of the drawbacks of this simulation is the lack of quantal features, such as the quantum nature of molecular rotation.

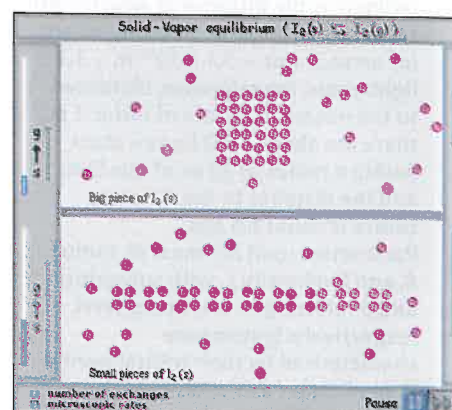
Another example is the solid-vapor transition in iodine (<http://nautilus.fis.uc.pt/molecularium/sv>). It helps students to understand the influence of the division of the solid phase in the microscopic rate of the transition (Fig. 2). They could graph why iodine sublimation gets faster when the substance is pulverized.

## “Virtual Water”: Virtual reality for understanding of water

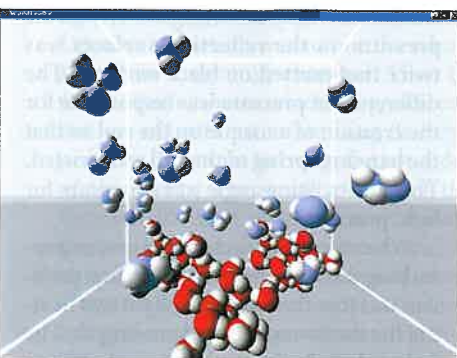
Some of the animations in the “Molecularium” are in 3D (Fig 1). Virtual reality (KALAWSAKY, 1993) extends the traditional 3D graphics world to include stereoscopic, acoustic, haptic (i.e., related to touch) and other feedbacks to create an al-



**Fig. 1:** Water molecules inside a microwave oven. This picture was created in “Java”. Translations, rotations and vibrations take place at the same time.



**Fig. 2:** Solid-vapor equilibrium for different divisions of the solid. For simplicity, the iodine molecules are represented as single spheres which are vibrating in the solid phase.



**Fig. 3:** Snapshot of a virtual reality simulation of water showing the vapour - ice transition. The blue objects make up the gas phase while the red ones are the solid phase (the color is for pedagogical convenience and may be switched off). These pictures were created with "Visual C++" on "WorldToolkit".

most complete sense of immersion. A stereo image gives a stronger sense of depth. The hardware for virtual reality consists of real-time graphics generators, stereo displays or views, tracking sensors, sound machines, and haptic devices. Tracking sensors – which determine the position and orientation of the viewer's head, hands, body parts or other inputs – allow the calculation of stereo images, the manipulation of models and the navigation in virtual environments. Sound "machines" provide a sense of location and orientation of certain objects and activities in the environment. Haptic devices vibrate and touch the user's body enhancing the interaction.

Water is an abundant substance but also one with unusual properties. For example, it has a maximum density at 4°C in the liquid state and, below 50°C, the isothermal compressibility grows with cooling (cold water is more "squeezeable" than warm water). Moreover, the solid floats on the liquid unlike in other substances.

We are using virtual reality as a tool to introduce students to the molecular bonding and structure of water. Using head-mounted colour displays and haptic interfaces, students navigate through an environment created with specialized software ("World Tool Kit"). The environment, under the title "Virtual Water" (<http://nautilus.fis.uc.pt/rv>), is designed to illustrate scientific concepts such as molecular orbitals and densities, molecular geometry, and the phases and phase transitions of water itself (Fig. 3).

Our molecular dynamics simulations use the equations of Newtonian Mechanics integrated with Verlet's algorithm. We

assume classical dynamics because more realistic simulations (incorporating quantum effects) are also much more computationally demanding (SPRIK and PARRINELLO, 2000). We also assume that the force between any pair of molecules depends only on the distance between them, using the Lennard-Jones potential. Some programming tricks were used to obtain a compromise between realistic behaviour and pedagogical utility.

Water molecules in the liquid phase tend to cluster. Computational and laboratory work has focused on the detailed characterization of the water dimer, trimer, tetramer and large clusters. Some of these isomers are transient structures. The cyclic hexamer (Fig. 4), one of the newest morphologies found in simulations of liquid water, is shown in our virtual environment.

Students exposed to our computer environment were very enthusiastic. One of them wearing a glove said: "I never thought of touching molecules!". Although a quantitative evaluation of the educational impact of our materials is still under way, the virtual environment seems to be a valuable tool. All textbooks and almost all available computer simulations that discuss these concepts stick to 2D representations, so that the change to a 3D world is quite a dramatic step. The "touch and feel" dimension is an additional stimulating feature.

Problems we faced in implementing our system were the price of hardware / software and the implementation of good graphics and haptics interfaces. A problem in generalizing the use of programs like ours is the "technophobia" of some teachers, which contrasts to the extraordinary computer abilities of some of their students.

#### Enter the Internet

Internet is a road to the future. Though the bandwidth in communication channels is not yet satisfactory, the Internet is becoming gradually the preferred vehicle for all those materials. Teaching and learning processes in multimedia formats on the Web have the obvious advantage of making educational content freely available. Molecular simulations in the Web, in a simple and modular format ("Java"), such as those we have described, seem particularly well suited to this new pedagogical genre.

On the other hand, virtual reality offers additional features such as stereo viewing and haptic interaction. The very idea of navigation inside the microscopic world preceded modern computers (see "Mr. Tompkins" book by George Gamow, from



**Fig. 4:** The cyclic water hexamer, which may be regarded as the smallest piece of ice.

which a new edition has appeared (GAMOW and STANNARD, 1999). Our "Virtual Water" project turns this idea "real". We are thinking about a Web version, running either Java or VRML (the Internet 3D language).

Both projects point ways to the future of technology in science education. Computational tools may indeed facilitate the understanding of some scientific concepts. But the complexity of the challenges faced by scientific education does not find a panacea in the new technologies. Many changes are needed, computer technologies being only one of the ways to achieve an improvement.

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