Virtual Reality Learning Objects of Molecular Structures

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Abstract
Chemistry students experience a number of problems during the learning process in subjects like molecular biology, biochemistry and others, particularly when they study molecular structure, since it is generally complex and abstract. This paper describes a proposal of learning object development to support understanding of molecular structures, using multimodal virtual reality technology. This paper also comments the development of a test bed for analyzing the possible applications and limitations of the technology and pedagogical contents of learning objects in virtual reality.

Keywords: Metadata, learning objects, multimodality, virtual reality, molecular structures.

https://doi.org/10.23106/dcmi.952108486

1. Introduction

Students experience a number of problems during the learning process of subjects like molecular biology, biochemistry and others, particularly when students study molecular structure, since it is generally complex and abstract. Many students have difficulty to comprehend three-dimensional structures of atoms that build up a molecule (conformation), the way molecules bond to one another, their reorganization, classifications, and biochemical reactions. All this happens at submicroscopic scale, having intangible characteristics (1, 2). Since the fifties, students and teachers have been using plastic and wooden molecular model sets in their courses with fairly good success, although these models present some limitations, since they are insufficient to show certain characteristics of atomic bonds, and other key values about structure (3). Moreover, sometimes they are difficult to manipulate and store. As well as using model sets, students nowadays use computerized graphical models of molecules, with better interactivity and more precise bonding and structure values. These take advantage of scientific visualization techniques for better understanding of molecular structure (4). However, although graphical models are relatively easy to find on the Internet and to show on a computer monitor, few of them contain detailed information about their physicochemical characteristics and other contextual information. That is, they generally only show their graphical molecular structure.

The last developments of virtual reality (VR) technology have supported the analysis and comprehension of molecular information, using scientific an information visualization techniques, and interactivity techniques that have eased the visualization and manipulation of molecular models, making use of more than one human sensory channel at the computer interface, especially in a virtual reality environment (5). This is called multimodality. It is possible to "touch" a graphical representation of a molecular model in a virtual reality environment, as well as to feel with the sense of touch the intermolecular forces of that model (6). It is also possible to represent information of molecules into auditory parameters (7), so the bonding force of two molecules can be represented as auditory pitch variations, along with its visualization.

Since many of the molecular models downloaded from the Internet lack of contextual information (i.e. information on molecular interactions and physicochemical properties), our research proposes a definition of learning objects of molecular structure that include contextual information, as well as educational guidelines about its use, based on virtual reality technology. Our hypothesis in this study is that the application of learning objects with virtual reality will effectively support the didactical use, reuse, and comprehension of molecular information.

1.1 The Concept of Learning Object

The learning object concept has been proposed as an important paradigm within the field of information and communication technologies applied to education, because past

https://doi.org/10.23106/dcmi.952108486

literature has been argued that with them it is possible to carry out a better planning, design and organization of technological resources in education. Currently, there many definitions of learning object. Wiley (8) defines it as “any digital resource that can be used and reused to support learning”. This is related to CUDI’s (9) definition: “A learning object is a digital information entity developed for the generation of knowledge, abilities and attitudes according to the necessities of the learner, and that it corresponds to a concrete reality”. The IEEE concisely defines a learning object as an entity, being digital or not, that can be used, reused or make reference of, during the learning based on technology (10).

1.2 Learning Objects and Virtual Reality

It has been recently proposed the application of learning objects based on virtual reality technology (11). Virtual reality can be defined as a computer-generated space in three dimensions (also called virtual environment or virtual “world”) that is highly interactive and immersive. Immersion is the sensorial feeling of “being there”, inside the virtual environment, which leads to a psycho-physiological sensation called *presence*. VR is multisensorial, that means it is possible to use more than one human sense to interact with the virtual environment. The integration of human sensory channels in virtual reality is called *multimodality* (12, 13), where the participant can use special devices to interact with the virtual environment. Figure 1 shows a fully-immersive virtual reality system.

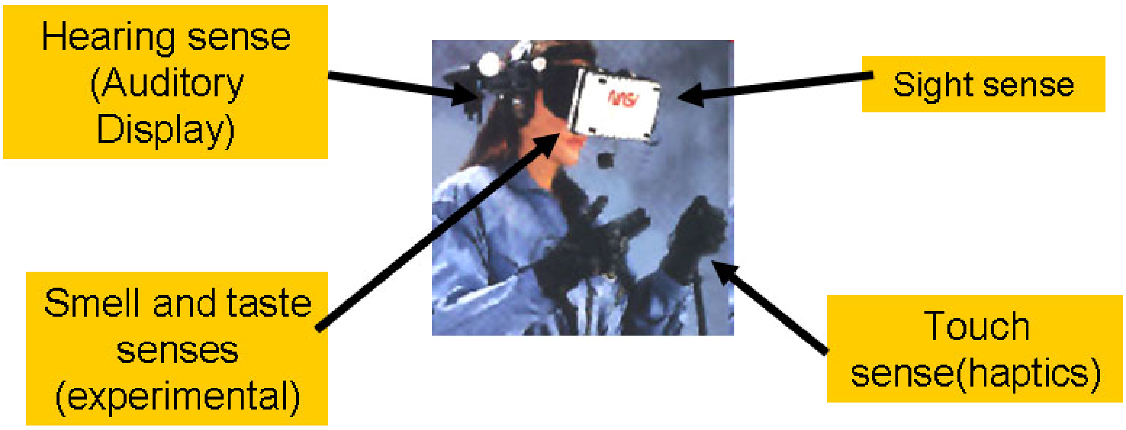

Figura 1. Fully immersive virtual reality system. Image Courtesy of NASA.

Applications of VR can be carried out with more modest equipment like the one shown in Figure 1. There are versions of virtual reality technology that uses conventional desktop computer and monitors (called desktop virtual reality) to display the virtual environment or other types of computer displays.

Virtual reality has been applied in education since more than a decade, where its characteristics of presence, interactivity and multisensoriality have been researched and applied, where students make us of them to watch and control simulations and models of

https://doi.org/10.23106/dcmi.952108486

scientific phenomena (14). For example, VR has been applied to medicine schools, where students learn anatomy and morphology of the human body through virtual organs. These can be converted into learning objects, because they can be reused and transformed to suit any educational goal or need to diversify their didactic applications at the medicine school. The concepts of presence and interactivity can be essential part of the virtual reality learning objects (VRLO) by supporting their form and function. More importantly, highly interactive VRLOs could facilitate the comprehension of abstract or complex concepts in science education (15) and in other areas of knowledge.

2. Related work on learning Objects and Metadata in Virtual Reality

The research about learning objects in virtual reality has been scarce, probable due to the development of actual powerful personal computers (necessary for running virtual reality applications in a relatively smooth way), and the relatively recent application of VR to education. Past literature shows early investigations on development of metadata and learning objects to carry out catalogs of online virtual museums (16), where metadata and the learning objects are shown in an online virtual reality environment. Those objects are described following international museum classification standards and codified in XML.

3. Metadata Definition for VRLOs

It is possible to use many of the principles and guidelines of the IEEE Learning Task Committee (LTSC) for the definition of learning objects in virtual reality, in conjunction with the Dublin Core Metadata Initiative (DCMI) (17). It is important to note that the metadata definition for VRLOs require special characteristics. Their design poses a real challenge, since it is necessary to know technical and pedagogical aspects of virtual reality, especially about multimodality, computer graphics, sound, tactile information, and other types of sensory information.

In order to have a correct definition of metadata and learning objects in virtual reality, it is necessary to develop them based on software engineering methodology and a robust metadata definition, as it is described in the IEEE Learning Objects Metadata.

4. Test bed for learning objects of molecular structure

Our research project has developed hundreds of 3D graphical models of molecular structures, which can be used in molecular biology, biochemistry and related subjects. For instance, we developed a virtual molecule of DNA that has been used in biochemistry courses (Figure 2).

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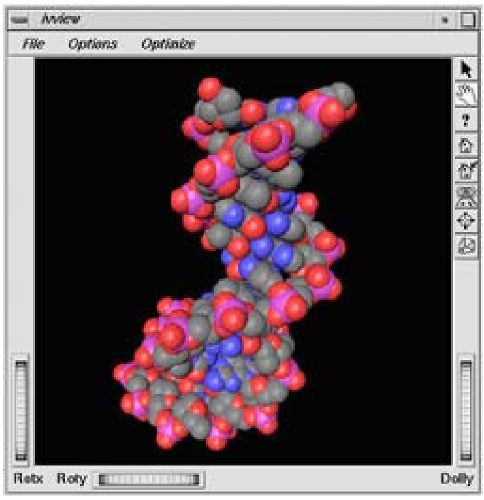

Figure 2. 3D model of a molecule of DNA

The development of 3D models of molecules, even if it is an automated task, is not trivial. It is necessary to find out special text files, generally stored in Protein DataBank (PDB) format on the Internet that defines the creation of the molecular structure model. There are specialized Web sites that handle a digital library of PDB files of biological macromolecular structures, such as the PDB databank (http://www.rcsb.org/). PDB files store metadata about the 3D structure of the molecule (conformation), position of each atom in the structure, its chemical elements, energies, and even data about the researchers and the laboratory that synthesized the molecule and created the PDB file. Once the PDB file is found and downloaded from the Internet, it can be converted into a virtual reality file format, such as Virtual Reality Modeling Language (VRML), a popular markup language for defining virtual environments. Molecular modelers and open source programs for doing the conversion of PDB into VRML have been developed, albeit they need considerable computer power and memory to perform the conversion, especially if the molecular model to be converted has thousands of atoms.

As it is stated in (18), the importance of learning objects resides in their reusability, allowing the use of one learning object for various educational applications. For example, the virtual molecule shown in Figure 2 can be reused for biochemistry, molecular biology, pharmacology, or other medicine courses, depending on the characteristics that can be taken from the original leaning object.

According to past experiences, we consider that it is necessary to ask a number of fundamental questions in early stages of the development of learning objects in virtual reality:

What are the input/output virtual reality devices that will be applied in conjunction with the VRLO?

Which of the sensory channels will be involved to interact with the VRLO, and

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how are they going to be integrated (multimodality)?

How much degree of immersion is going to be needed?

How about the navigation style and the type of interactions the participant will carry out with the virtual environment that houses the learning object(s)?

Will the learning objects have ç representations? For instance, a molecular model can be represented as “ball and stick” or “CPK” types.

How are the characteristics of the virtual environment display? Is it going to be displayed on a computer monitor, a large projection screen, in a virtual reality head-mounted display? Will it be rear projected?

How are the characteristics of the audience? What is their average age? Are most of them passive students? Have they had previous experience with 3d models?

How are the characteristics of the hall or classroom where the VRLOs will be displayed and used? Does it become dark enough so a data projector can be effectively used?

The answers of the above questions will define certain metadata of the virtual learning object, particularly to define technical aspects of their educational use.

Figure 3 depicts our proposal of a hypothetical structure of a VRLO, where the metadata of the 3D model, tactile, visual, auditory, gustatory and olfactory information, as well as extra information on its educational usage, is encapsulated.

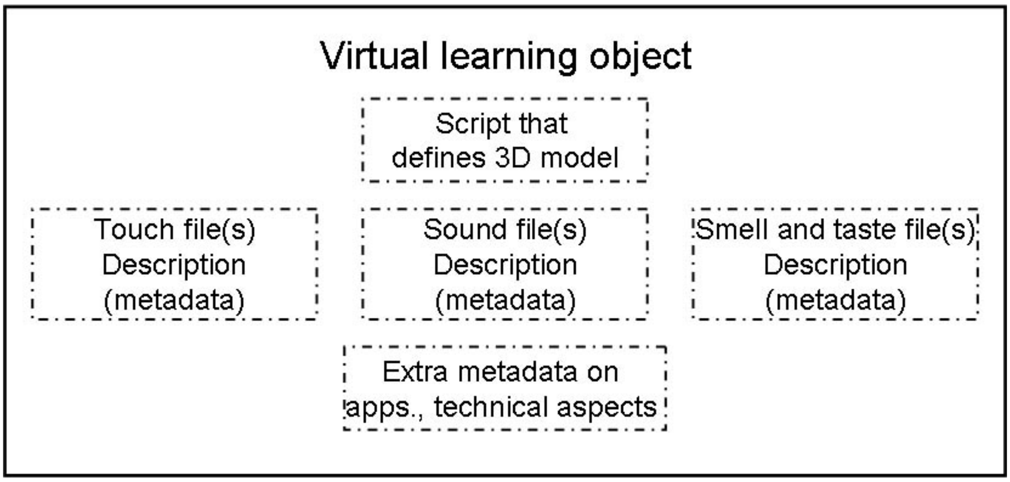

Figure 3. Our proposed structure of a VRLO.

The programming of models can be done using VRML or X3D, and the metadata definition can be defined in XML. It is also possible to use scripting languages like

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Python or Tcl/Tk for metadata and sensory information definition. The virtual learning environments could reside in a digital library that can be locally or remotely accessed, as proposed by (19).

5. Conclusions.

The development and application of virtual learning environments is feasible if it is based on software engineering development methodologies, strong educational theories, and adequate technology application. It also need to be based on standardized learning object initiatives such as the ones from the IEEE and Dublin Core. Nowadays, this research project has produced hundreds of 3D models of molecules that will be integrated in VRLOs as test bed. We consider that they can effectively support sciences learning, based on their adequate design and application. We are currently planning usability and media comparison studies about the application of VRLOs of molecules using a computer monitor, a large projection screen, and a virtual reality head-mounted display.

6. Acknowledgements

This research is being funded by a PROMEP grant from the Mexican Ministry of Education, no. UCOL-EXB18.

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