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Exploring Active Stereoscopic Molecular Visualization in the Classroom

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Abstract: Scientific visualization of molecular models in the classroom using high-quality computer graphics can be a powerful means to support students' learning of molecular structure. The objective of this paper is to analyze the feasibility of using PyMOL (an easy-to-use molecular model visualization program) in a classroom for learning and teaching molecular structure, with the support of active stereoscopic visualization. This paper describes a technical study on the testing of shutter glasses and a data projector used to display molecular models in a classroom. The paper also lists recommendations on their application in class.

Introduction

One of the ultimate goals of applying scientific visualization in the classroom is to support students' understanding of visual aspects of physio-chemical phenomena, where students link already-learned scientific knowledge with new knowledge being taught visually

(Ricketts et al., 2018). Scientific visualization can be enhanced using techniques such as stereoscopic and high-quality computer graphics. These techniques have been successfully researched for supporting teaching and learning of molecular model structure (e.g. Berry & Baker, 2010). Stereoscopic projection (a technique that enhances the depth illusion in computer graphics using stereopsis) of molecular models greatly support students' understanding of molecular structure, making some of its visual aspects more salient and exploiting 3D perception capabilities (Waddington, 2001).

The objective of this paper is to analyze the feasibility of using PyMOL in a classroom for learning and teaching molecular structure, with the support of active stereoscopic visualization. PyMOL is an open-source molecular modelling visualization program used in both research and education (Schrodinger LLC, 2021). This paper describes the importance and feasibility of scientific visualization in class done on PyMOL with low-cost stereoscopic projection, providing a list of recommendations related to molecular model visualization in classroom.

PyMOL is widely used in chemistry and similar courses, and it is capable of displaying 3d molecular models as high-quality anaglyphs (a visualization technique that uses green-red or blue-red glasses). It also allows active stereoscopic projection where users wear shutter glasses. These glasses have transparent LCD lenses that work by shutting (darkening) the left and right LCD lenses in a rapid sequence, typically at 60 frames per second (FPS) each, hence the name active stereoscopy. This shutting sequence is synchronized with a data projector signal. Many recent data projectors have the DLP-Link (TM) standard that provides active stereoscopic projection. DLP-Link works by displaying a flash of white light very briefly on the screen projection between each video frame. A sensor from the shutter glasses captures that white frame that synchronizes the left and right lenses shutting. Active stereoscopic visualization is very effective for showing molecular structure and has been applied in structural biology research and in other areas of science (Sommers et al., 2017).

The Technical Study

We conducted a short technical study to analyze whether PyMOL can be an effective software tool for conducting interactive molecular visualization in class using stereoscopic projection. Three people (a student, a biology professor and a computer science specialist) tested a molecular model visualization running on PyMOL using stereoscopic projection with a data projector and using active shutter glasses.

We used active shutter glasses made by Boblov, part number JX-30 (see Figure 1). These glasses cost about $20USD each, and have a battery that is rechargeable using a micro-USB cable. They are compatible with DLP-Link data projectors.

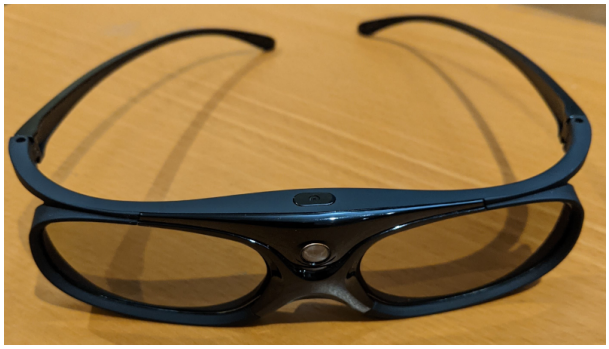

Figure 1: The active shutter glasses used in the technical study.

As Figure 1 shows, the glasses have a sensor in between the lenses. This sensor picks up the visual signal emitted by the DLP-Link data projector in between the video frames projected on the screen.

A BenQ W1080ST 1080p DLP-Link data projector was also used, costing about $800 USD. This projector was used to display molecular models in PyMOL using stereoscopic projection. This projector provides 2000 ANSI lumens (a standard measure of the quantity of visible light emitted by any source), which works well in a semi-dark classroom.

The DLP-Link data projectors such as the one used in our study synchronizes with the shutter glasses by doing stereoscopic visualization with DLP-Link technology. It is not necessary to use extra hardware such as infrared (IR) emitters with this configuration. This facilitates the set up of stereoscopic projection in class. Fortunately, PyMOL can be used to activate stereoscopic display used for DLP-Link projections with a graphics card that supports active stereoscopic projection.

In this technical study, we used a desktop computer with the following description: iBUYPOWER Elite Gaming PC Computer Desktop, model ARCW 105A. System: AMD Ryzen 7 3700x 8-Core 3. 6GHz, 16GB DDR4-2666 RAM, running Windows 10 64-bit operating system. The computer has an NVIDIA GeForce GTX 1660 graphics card.

In our technical study, we used Windows 10 operating system with the respective graphics card driver installed on it. It seems that some recent NVIDIA cards from the GeForce series (such as the GeForce GTX 1660 card) support active stereoscopic visualization with PyMOL. NVIDIA's Quadro series of graphics cards are also recommended.

Figure 2 shows a person donning shutter glasses and visualizing a molecular model on PyMOL in a classroom.

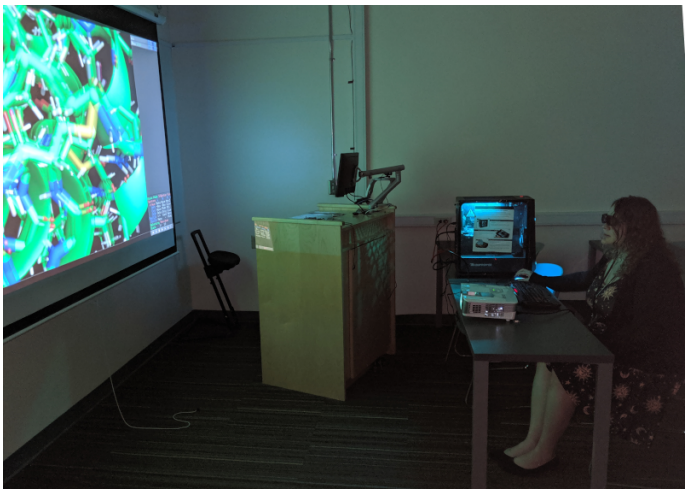

Figure 2: A molecular model visualized in PyMOL.

As it can bee seen in Figure 2, the user interacted with the visualized molecular model using a regular mouse. The user is seated right in front of the projection. The projection's field of view is quite wide in case many students would like to visualize it at the same time. The data projector that we used in our study has a short throw, allowing it to install it conveniently close of the projection screen or hanging it from the ceiling. In addition to testing the shutter glasses close to the screen, we tested the shutter glasses at a distance of approximately 10 meters from the projection. The glasses at that distance were still performing stereoscopic visualization effectively. To test the stereoscopic visualization system, we opened a number of molecular models on PyMOL, including the molecule of human insulin. Its Protein DataBank (PDB) file can be downloaded from: http://www.rcsb.org/

3d-view/jsmol/2hiu. PDB is a standard text format that defines important molecular data, such as the molecular atoms' 3D position. Once we downloaded the PDB file, we opened it in PyMOL by selecting File / Open from the main menu. From PyMOL, we could also open the molecule by typing the following command at PyMOL's command line (PyMOL>): fetch 2hiu.
To activate the stereoscopic visualization in PyMOL, we selected from the menu bar: Start > PyMOL > PyMOL > PyMOL 3D Launch > PyMOL Stereo. Once we selected that option, the data projector then automatically switched to active stereoscopic projection (3D).

Recommendations

Based on the above technical study and from previous studies that we have conducted on molecular visualization in the classroom (e.g. Garcia-Ruiz, Valdez-Velazquez, Gomez-Sandoval, 2008; Garcia-Ruiz, Santana & Molina, 2014), we have organized these recommendations to carry out before, during and after molecular visualization sessions in class:

Before

- Make sure to use an appropriate silver or white projection screen. It should be as rigid as possible, otherwise it will distort the molecular model projections.

- Make sure that all the shutter glasses are clean (e.g. they do not have finger streaks on their lenses, using a microfiber cloth for cleaning them) and sanitized. In addition, be sure that the shutter glasses' batteries are fully charged.

- Before the class starts, it is advisable to check the number of students who will take the class to see if there are enough shutter glasses available.

- Before wearing the shutter glasses, ensure that students do not have any medical or physical condition that may arise with the shutter glasses' use, because, as in other visualization systems, it may trigger seizures in susceptible students due to the shutter glasses' rapid shutting sequence.

- We have found that PyMOL is easy to use overall, and is suitable for supporting in-class scientific visualizations. However, it can take some time to download and install it for the first time. PyMOL is free for classroom use, but instructors will need to register on PyMOL's website first. PyMOL's website is: https://pymol.org/2/

- Run a dry test with the equipment by trying out the stereoscopic visualization to see if you need to adjust the operating system's or the data projector's options. It is recommended, before starting the class, to try out the shutter glasses' synchronization with the DLP projector and ensure that the projector brightness is optimal and the classroom is dark enough. The shutter glasses use a chip that synchronizes the frequency of the images emitted by the projector with the image that the glasses receive, thus ensure that all students (even the students seated at the back of the classroom) will perceive the stereoscopic visualization correctly.

During

- A teaching assistant can manipulate the computer mouse and PyMOL while the instructor explains a the molecular model on one side of the projection.

- A way to save model interaction time and to make molecule visualization more efficient, the instructor or teaching assistant can type scripts in PyMOL during class. This is a useful scripting tutorial: https://pymol.org/tutorials/scripting/index.html
  For example, this simple script line colors non-carbon atoms by element:
  color atomic, not elem C
  Remember that scripts are typed at PyMOL's command element.

- It is advisable to review what has been displayed with PyMOL at the end of the classroom and compare the reviewed molecular model against similar ones (for example, the difference between human and pig insulin molecular models), but this will depend on the learning objectives that belong to the classroom session.

- In case students experience any discomfort symptoms, such as dizziness, disorientation, heaviness in the eyes, headache, or itchy eyes, it is best that they remove the shutter glasses immediately and rest. This discomfort is generally a transitory effect (Zhang et al., 2013). It is recommended to limit the use of shutter glasses to a single short time. People with visual conditions, e.g. people with only one functioning eye, lazy eye, or strabismus, may not be able to efficiently perceive the stereoscopic display effect in the classroom. In this case, it is best not to rely on stereoscopic visualization alone for conveying crucial or highly relevant molecular structure information.

After

- Remember to set the data projector in stand-by mode to save energy and to cool down the projector lamp, and then turn the projector off. If you disconnect the data projector right after using it, you can damage the lamp.

- It is necessary to disinfect the shutter glasses after class, especially in times of the COVID-19 pandemic. We do not recommend using rubbing alcohol to disinfect the glasses, because it may affect the glasses' coating. We do recommend using pre-moistened disinfecting cleaning wipes. Hygiene is very important when using shutter glasses multiple times by different students. Ideally, each student should have his/her own shutter glasses to avoid spreading of infections, since sharing contaminated shutter glasses with several students could transmit eye or skin diseases, such as conjunctivitis, or fungi, not to mention the SARS-CoV-2 virus. The cost of shutter glasses such as the ones described in this paper have decreased considerably and may be affordable to many students.

Conclusions

This paper described a technical study about testing active shutter glasses and a data projector used to display molecular models in a classroom. The paper also listed recommendations on what to do before, during and after the use of stereoscopic projection of molecular models in the classroom.

We are currently testing stereoscopic projections of molecular models through a ViewSonic PX700HD data projector that handles 3500 lumens. This projector may be beneficial for classrooms that are not completely dark. We will also test whether many pairs of active shutter glasses can be used at the same time, and whether the students wearing

them can be seated with at least 2 meters of separation (maintaining the so-called social distance) following COVID-19 health recommendations. Future work will include running a pilot study with five students, and running an extended study to gather significant feedback of the efficacy of the molecular visualization approach from a broader group of participants. We are planning to apply pretests and post-tests on molecular model knowledge to see any learning gains when using the stereoscopic molecular visualization. We will also apply usability and user experience (UX) questionnaires to analyze the participants' stimulation, overall impression, motivation, efficiency and efficacy of use, among other human-computer interaction and interaction design aspects.

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