Eurographics Workshop on Visual Computing for Biology and Medicine (2020)
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UnityMol tuning for better Virtual Reality experiences

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Abstract

Molecular representations are taking an important role in communicating ideas, in generating new hypotheses on biological mechanisms and in analysing molecular simulations. However, the current devices used to observe and manipulate these molecular systems are typically limited to the two dimensions of the computer screen combined with a keyboard and a mouse offering limited interaction capabilities. Nowadays, virtual reality headsets offer a more performant and accessible solution. However, adaptations are necessary to fully benefit from the advantages of using virtual reality for scientific visualisation. This poster presents a few examples implemented with the UnityMol software. In addition to immediate applications in teaching, the paradigm shift in interaction and the increased depth perception and shape comprehension of biological molecules are already easing the grasp of these complex systems and will certainly lead to the discovery of new scientific knowledge.

CCS Concepts

• ***Applied computing*** → ***Molecular structural biology;*** • ***Human-centered computing*** → ***Scientific visualization; Virtual reality;***

1. Introduction

Depth-perception is playing an important role in structural biology since the 80's, when a stereoscopic slide viewer made of cardboard [FB80] could be used to visualize molecules in 3D in the classroom. Nowadays, stereoscopic devices such as head-mounted displays (HMDs) provide high-quality rendering with high resolution and framerate. Molecular visualization can benefit from these devices combined with state-of-the-art performant rendering pipelines provided by game-engines such as Unreal Engine or Unity. UnityMol (http://unitymol.sourceforge.net) is a molecular visualization framework that provides classical representations but also offers the possibility to easily extend its features with custom representations while benefiting from up-to-date support for recent HMDs and other mixed reality devices.

2. Desktop to VR

Necessary adaptations were made to provide a smooth experience and a closely related code base between desktop and VR versions of UnityMol. There are two approaches to perform classical transformations on molecular visualizations, mainly translations and rotations:

- Change the camera point-of-view by rotating around a point, usually the center of the molecular system.
- Move the molecular system without changing the camera position.

When no context surrounding the molecular system (skybox, external 3D objects...) is provided, both approaches are completely identical. However, when there is a 3D scene around the molecular system or in a VR context where the user is in a determined geometrical position with respect to the molecule, moving the camera can be troublesome. For example, if a skybox gives a sense of up and down, rotating the camera can lead to situations where the user is upside-down which is not acceptable in a VR context.
For this reason we made UnityMol use the second approach both for desktop and VR contexts.

3. Context

UnityMol VR immerses users in a simple room that provides a familiar context to move in (Figure 1). Indeed, one of the main factors involved in cybersickness is a difference between what the vestibular system perceives (eg when physically walking around the room in VR) and what the visual system receives [LJ00] (eg do any visual cues move confirming the user's displacement). Immersed in an unicolored space, the users do not perceive visual changes in the surrounding, even when they move physically or rotate their head.

Building a room into the 3D scene provides a sense of up and down, as a skybox could do, but also gives visual landmarks and a sense of scale.

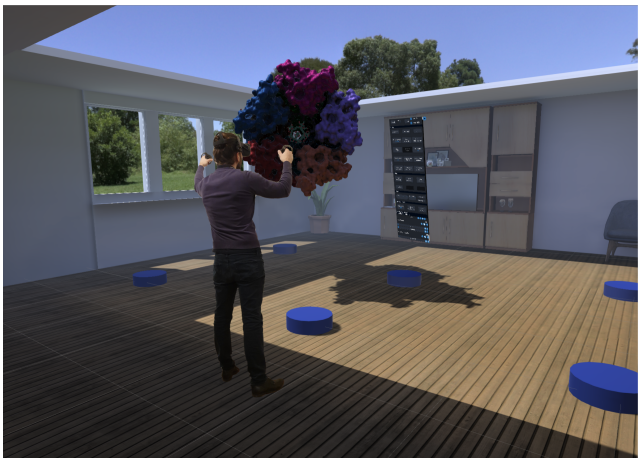

Figure 1: *User immersed in the current VR room provided by UnityMol. VR controllers are used to move and scale molecules (PDB id: 3EAM in this case). Depending on the HMD, users can physically move around the molecular system. Blue pods on the ground are teleporting spots.*

4. Interaction

On top of stereoscopic view, HMDs provide 6 degree of freedom (DOF) interaction devices that greatly ease common molecular transformations such as rotations and translations. Teleporting spots (blue in Figure 1) are given to users to quickly change position and to avoid large physical travels.

Thanks to the VIVE Input Utility plugin (VIU), UnityMol supports the vast majority of common VR controllers and will surely support the next HMD/controller generations.
Several tests have been carried out using hand tracking thanks to the Leap Motion. We plan to provide better hand tracking support as the technology matures, but occlusion and errors in the tracking do not currently allow for a satisfactory experience for extended periods.

5. Annotations

In UnityMol, these enhanced interaction devices also provide a way to do **selections** on several levels (atom/residue/chain) by clicking on atoms to add or remove parts of the molecule to the current selection. Depth-perception and 6 DOF interaction also help with **measuring** atom distances or angles because users can move controllers close to the target atoms.

Another VR-eased feature is **3D drawing** using controllers which is useful to highlight parts of the system or convey graphical information.

6. User interface

The user interface (UI) in VR is an important part of the user experience. For now, UnityMol offers a single panel menu with options similar to the desktop version that are activated by a laser-pointer metaphor of the controllers. For technical reasons, the scale of the UI has to be enlarged and requires a lot of space to be readable and easily usable. Ergonomic studies may be desirable to fine-tune the size and shape of the UI. We are currently simplifying and separating items of the current UI for a better VR experience. This may imply developing an advanced windowing system allowing to organize, group and move windows.

7. Example 1: Molecular exploration

Molecular exploration and visual analysis of complex molecular systems is one of the first tasks structural biologists are interested in. Visual inspection of a molecular dynamics trajectory in VR, for example, can provide helpful insights that could be difficult to observe using standard 2D screens and classical interaction devices. Besides the improved 3D perception, users can choose and adjust a favorable point of view by physically moving "inside" the molecular system. This is particularly useful when molecular scenes are dense, for example when loading electrostatic density maps from APBS [LBO*20].

8. Example 2: Interactive Molecular Dynamics

Interactive molecular dynamics (IMD) is a scenario in which VR and 6 DOF interaction shines because translations combined with rotations are essential for adding localized and precise forces to the ongoing simulation. Two-hand interaction is straightforward in VR and valuable during an IMD session. Controllers also provide haptic feedback by vibrating based on the forces applied to the simulation.

9. Conclusion

Moving from a desktop oriented software to a VR experience requires to take several points into account:

- To increase use time and improve user experience, **cybersickness** has to be avoided. Besides hardware considerations, this implies to avoid forced camera movements but also to provide visual landmarks and performant representations for a constant and high framerate experience.
- Translations and rotations are greatly facilitated by VR **6 DOF** controllers. The way to interact with molecular objects can be transposed to the desktop version for consistency.
- **User interface** has to be adapted to the VR format, in particular scaling UI widgets for readability.

References

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