

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.

