Accurate molecular atom selection in VR

E. Molina[1] and P. Vázquez[1]

Abstract

Accurate selection in cluttered scenes is complex because a high amount of precision is required. In Virtual Reality Environments, it is even worse, because it is more difficult for us to point a small object with our arms in the air. Not only our arms move slightly, but the button/trigger press reduces our weak stability. In this paper, we present two alternatives to the classical ray pointing intended to facilitate the selection of atoms in molecular environments. We have implemented and analyzed such techniques through an informal user study and found that they were highly appreciated by the users. This selection method could be interesting in other crowded environments beyond molecular visualization.

(see https://www.acm.org/publications/class-2012)

CCS Concepts

• ***Human-centered computing*** → ***Interaction design process and methods;*** *Activity centered design;*

1. Introduction

The objectives of this work revolve around advancing research in Immersive Analytics [MSD*18] for biological data, more specifically for the visual analysis of molecular dynamics simulations. Molecular visualization virtual reality systems (e.g., UnityMol [DCP*14, LBO*20]) are still not on par with desktop and present some limitations in interaction, collaboration, or data visualization [GBS*18]. We will address some of these problems: the interaction and accurate atom selection. Today they still represent obstacles to achieving a virtual reality system that allows a detailed analysis of molecular simulations.

Currently, there are various systems designed to visualize molecules in VR such as UnityMol, Nanome [KBL*19], ChimeraX [PGH*21] or Molecular Rift [NGEB15]. A characteristic that unites them is the method of selection of atoms, mainly carried out by raycasting [Pie18]. This method allows the selection of the atom that intersects with a ray that is generated from the controller to where the user points. This technique is easy to learn and intuitive, but it has several problems, for instance, the effect of hand vibration or user fatigue that lead to erroneous selections [AA13]. This can be highly frustrating, and worsens when the elements to select are small and cluttered, such as in the case of molecules.

To overcome this problem, we propose and evaluate two different techniques that decouple the selection procedure in two steps: an initial ray-based selection (likely on an atom close to the final goal), and posterior a navigation through the neighbors thanks to visual cues that does not require pointing precision.

For this project, we will use the HTC Vive with its controller and UnityMol, a molecular viewer and prototyping platform, coded in C# with the Unity3D game engine. It is developed at the LBT laboratory (IBPC institute of CNRS in Paris).

2. Advanced atom selection techniques

We propose two new pointing techniques intended to facilitate the precise selection of atoms by allowing movement between neighboring atoms. We call these techniques: *Ray + Arrows* and *Ray + Colors*. Both techniques work with the same two-step process:

1. An initial selection is made using the Raycasting method.
   - The selected atom is marked.
   - The system automatically highlights a set of up to 8 neighbors the user can travel to.
2. The user hops to the neighboring atom of interest by just using a direction of the controller touchpad and the trigger.

The region in which neighbors are searched for is defined by a radius that can be easily configured by the user. Each candidate destinations are in one of the main directions: up, down, left, right and the corresponding diagonals. And these directions map to eight regions of the controller's touchpad. Although the interaction with the neighbors follows the metaphor, each technique provides visual feedback differently (illustrated in Figure 1).

Method 1: Ray + Arrows. The available neighbors are shown by a yellow arrow and a yellow ring around the corresponding atom. Both elements are oriented so that their planes are perpendicular to the user's vision. A guide appears in the upper left peripheral view, showing the user which directions are available. The user can select the desired direction, resulting in the arrow and the ring turning white as feedback. In the same way, the direction indicated in the

DOI: 10.2312/evp.20221121

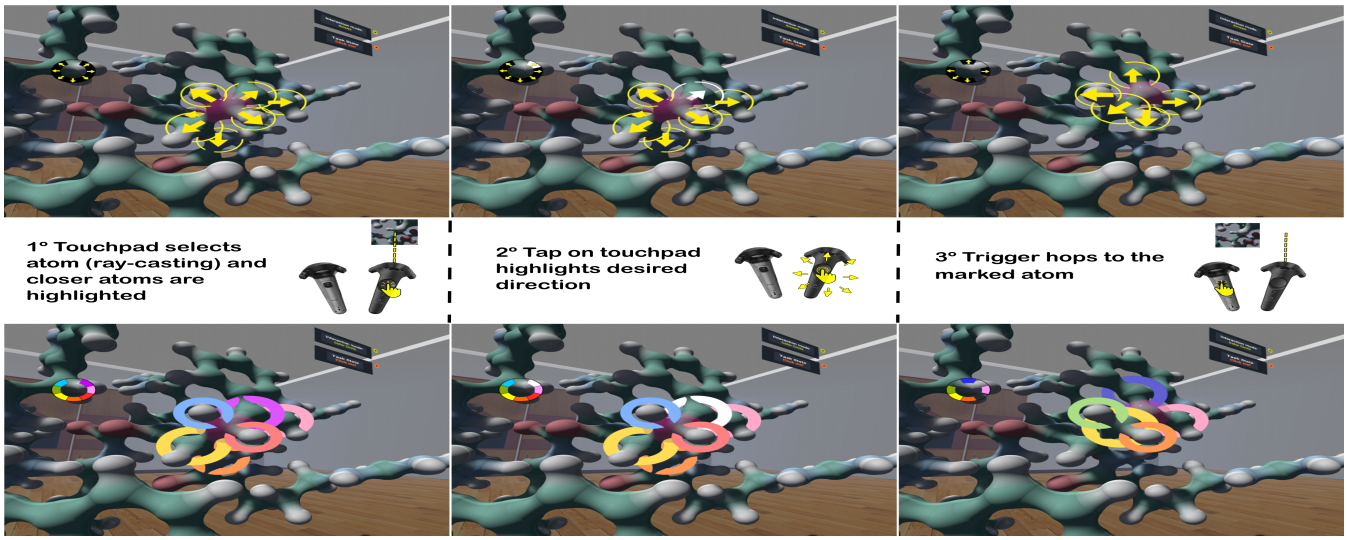

Figure 1: *Process to select an atom and choose and navigate to the available neighbors.* ***Up:*** *Ray + Arrows technique.* ***Down:*** *Ray + Colors technique.*

guide turns white. The rationale behind that is that we believe that showing arrows naturally leads to the user to decide which touchpad direction is the desired one.

Method 2: Ray + Colors. Following the same model as in the previous method, we show the possible neighbors employing a colored ring that surrounds the corresponding atom, oriented perpendicular to the user's vision. These rings are of a different color, identifying the different directions they represent. In the same way, a guide is displayed in the upper left periphery that will show the available directions utilizing the corresponding colors. Likewise, the ring and the color in the guide of the selected direction turn white when their direction is selected. In contrast to the previous method, although here the directions need to be learned, the visual cues (rings around atoms) are seemingly more visible in cluttered scenes.

Neighbors calculation. In both cases, the available neighbors are obtained with the selection sphere centered on the currently selected atom and the directions are calculated by a transformation to a new coordinate system. The new system is made up of:

$$\text{A = current atom position, C = Camera position}$$
$$\text{Origin = A, } \vec{Z} \text{ = A - C, } \vec{Y} \text{ = Camera up, } \vec{X} = \vec{Z} \text{ x } \vec{Y}$$

With these new coordinates we will know the corresponding direction obtaining the angle defined with $\arctan(\frac{y}{x})$.

3. Evaluation and conclusions

After a pilot study with a naive user who suggested some changes to the interface, we carried out a user study to compare the use of Ray + Arrows, Ray + Colors, and Raycasting techniques. 9 participants with ages between 18 and 36 carried out the experiment. Only 3 of them had medium or high experience in VR. Users used each technique to perform six searches with a protein of less than 200 atoms, 2M7D from the PDB database [BKW*13], and another protein of about 17000 atoms, 6EZN [WKE*18]. The experiments were performed using Latin squares to sort participants, to avoid learning and fatigue effects. Before the experiment, the users filled out a consent questionnaire and thereafter, a tutorial on the operation of the tool was done. Then, the tests were carried out. Finally, a questionnaire about the methods was filled out. The questionnaire had 19 questions that had to be answered in a 1-7 Likert scale. Finally, they had to give a global score from 1 to 10 to each technique. The users showed a preference for Raycasting (8.625) over Ray + Arrows (8). Ray + Colors was the least valued technique (7.375). However, the results are not conclusive since, although users prefer raycasting when evaluating from 1 to 10, in other questions such as evaluating the ease of achieving the objective on the Likert scale from 1 to 7, they have very similar results: Raycasting 5,25, Arrows 5.25 and Colors 5.125. In addition, most users stated that the ray was more cumbersome with the large molecule and that the option to navigate to neighboring atoms was very useful in this context. On all usability questions, Arrows and Colors ranked over 5 (in 1-7 Likert scale): ease to achieve the desired goals (5.25 and 5.125), easy to learn (5.375 and 5.25), managed to achieve the tasks (5.875 and 5.25), understandable representation (6 and 6), visual cues for candidate atoms (6.25 and 5.875), comfort (5.75 and 5.25), perceived speed (6 and 5.375).

In this paper, we presented two new pointing techniques for accurate selection of small elements in cluttered scenes. A small semiformal study was carried out, which showed both techniques were understandable and easy to use. Users still seemed to prefer the ray interaction instead of the newly developed techniques, albeit recognizing that it was difficult to use when molecules are huge. In the future, we want to quantitatively measure and compare the actual performance in terms of time, errors, and fatigue, of the new methods regarding ray selection with a broader set of users.

References

[AA13] ARGELAGUET F., ANDUJAR C.: A survey of 3d object selection techniques for virtual environments. *Computers Graphics 37*, 3 (2013), 121–136. URL: https://www.sciencedirect.com/science/article/pii/S0097849312001793, doi:https://doi.org/10.1016/j.cag.2012.12.003. 1

[BKW*13] BYRNE A., KIER B. L., WILLIAMS D. V., SCIAN M., ANDERSEN N. H.: Circular permutation of the trp-cage: fold rescue upon addition of a hydrophobic staple. *RSC Adv. 3* (2013), 19824–19829. URL: http://dx.doi.org/10.1039/C3RA43674H, doi:10.1039/C3RA43674H. 2

[DCP*14] DOUTRELIGNE S., CRAGNOLINI T., PASQUALI S., DERREUMAUX P., BAADEN M.: Unitymol: Interactive scientific visualization for integrative biology. In *2014 IEEE 4th Symposium on Large Data Analysis and Visualization (LDAV)* (2014), pp. 109–110. doi:10.1109/LDAV.2014.7013213. 1

[GBS*18] GODDARD T. D., BRILLIANT A. A., SKILLMAN T. L., VERGENZ S., TYRWHITT-DRAKE J., MENG E. C., FERRIN T. E.: Molecular visualization on the holodeck. *Journal of Molecular Biology 430*, 21 (2018), 3982–3996. URL: https://www.sciencedirect.com/science/article/pii/S002228361830696X, doi:https://doi.org/10.1016/j.jmb.2018.06.040. 1

[KBL*19] KINGSLEY L. J., BRUNET V., LELAIS G., MCCLOSKEY S., MILLIKEN K., LEIJA E., FUHS S. R., WANG K., ZHOU E., SPRAGGON G.: Development of a virtual reality platform for effective communication of structural data in drug discovery. *Journal of Molecular Graphics and Modelling 89* (2019), 234–241. URL: https://www.sciencedirect.com/science/article/pii/S1093326318303929, doi:https://doi.org/10.1016/j.jmgm.2019.03.010. 1

[LBO*20] LAUREANTI J., BRANDI J., OFFOR E., ENGEL D., RALLO R., GINOVSKA B., MARTINEZ X., BAADEN M., BAKER N. A.: Visualizing biomolecular electrostatics in virtual reality with unitymol-apbs. *Protein Science 29*, 1 (2020), 237–246. URL: https://onlinelibrary.wiley.com/doi/abs/10.1002/pro.3773, arXiv:https://onlinelibrary.wiley.com/doi/pdf/10.1002/pro.3773, doi:https://doi.org/10.1002/pro.3773. 1

[MSD*18] MARRIOTT K., SCHREIBER F., DWYER T., KLEIN K., RICHE N. H., ITOH T., STUERZLINGER W., THOMAS B. H.: *Immersive analytics*, vol. 11190. Springer, 2018. 1

[NGEB15] NORRBY M., GREBNER C., ERIKSSON J., BOSTRÖM J.: Molecular rift: Virtual reality for drug designers. *Journal of Chemical Information and Modeling 55*, 11 (2015), 2475–2484. PMID: 26558887. URL: https://doi.org/10.1021/acs.jcim.5b00544, arXiv:https://doi.org/10.1021/acs.jcim.5b00544, doi:10.1021/acs.jcim.5b00544. 1

[PGH*21] PETTERSEN E. F., GODDARD T. D., HUANG C. C., MENG E. C., COUCH G. S., CROLL T. I., MORRIS J. H., FERRIN T. E.: Ucsf chimerax: Structure visualization for researchers, educators, and developers. *Protein Science 30*, 1 (2021), 70–82. URL: https://onlinelibrary.wiley.com/doi/abs/10.1002/pro.3943, arXiv:https://onlinelibrary.wiley.com/doi/pdf/10.1002/pro.3943, doi:https://doi.org/10.1002/pro.3943. 1

[Pie18] PIETROSZEK K.: *Raycasting in Virtual Reality*. Springer International Publishing, Cham, 2018, pp. 1–3. URL: https://doi.org/10.1007/978-3-319-08234-9_180-1, doi:10.1007/978-3-319-08234-9_180-1. 1

[WKE*18] WILD R., KOWAL J., EYRING J., NGWA E. M., AEBI M., LOCHER K. P.: Structure of the yeast oligosaccharyltransferase complex gives insight into eukaryotic n-glycosylation. *Science 359*, 6375 (2018), 545–550. URL: https://www.science.org/doi/abs/10.1126/science.aar5140, arXiv:https://www.science.org/doi/pdf/10.1126/science.aar5140, doi:10.1126/science.aar5140. 2