Virtual Reality in the Interactive Computer Classroom

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2 Kurzbeschreibung des Projektes

The detailed visualization of biomolecules, chemical structures and reactions is key to incorporate chemical concepts and for the computer-aided engineering of chemical and biological systems. Although the benefits of the immersive visualization of structures are clear, the most powerful tools with manipulation and visualization capabilities require expensive VR (virtual reality) headsets that are not easily accessible to our targeted audience of groups of students. Our goal is to advance BCI's teaching capabilities by developing our own version of VR-based visualization software using cost- effective solutions. We will first use Nanome, an established application, as a reference and to introduce the VR experience to a test group of students, this application, however, must be restricted to demonstrative purposes given the high costs of the compatible headsets (Oculus, at least 350 EUR per unit). Therefore, we will develop an application to make VR accessible to large groups of students on a regular basis and to be combined with tools already developed in our group for protein engineering, such as PPI-Affinity.

3 Details zum Projekt

3.1 Istzustand vor Beantragung

This project will benefit from the knowledge of the CBE group of 3D engines such as Unity3D and Blender, of Web-based applications development and our state-of-the-art knowledge of chemical and biomolecular simulations and their applications. In addition, our VR tool will be used in combination with the protein engineering module of PPI-Affinity. PPI-Affinity is a machine learning tool implemented by us for the prediction of protein-protein (peptide) binding affinities and for protein engineering applications (J. Proteome Res. 2022, 21, 8, 1829–1841).

3.2 Projektziel/Projektbeschreibung

Goal: to develop a cost-effective virtual reality-based visualization software for teaching activities.

Projektbeschreibung: Analyzing the structures of complex organic compounds, materials and proteins is at the core of chemical and biomolecular simulations aiming to the engineering of chemical and biological processes. While this analysis may be relatively straightforward for the everyday user, it is frequently challenging for the neophyte, especially since "hidden" structural details may be missed. We will create a computational tool for the virtual reality-based visualization of molecules in the context of teaching activities.

There are several well-stablished visualization software solutions available,[1-9] most of them rely largely on a 2D representation of the structures. However, accurately understanding the 3D structure of biomolecular systems is key for biomolecular simulations and the detailed visualization of chemical structures and reactions helps to incorporate chemical concepts. Therefore, the benefits of the immersive visualization of structures are clear. Many tools are already developed or are under development in this direction. They can be divided into three main groups,[2] PC desktop applications, Web-based applications, and smartphone applications. Unfortunately, the most powerful tools with manipulation and visualization capabilities[3, 5, 6] require expensive VR headsets that are not easily accessible to our targeted audience of groups of students.[2] Others alternatives such as Web-based[1, 7] or

smartphones applications[8, 9], although with fewer capabilities, provide simpler solutions using inexpensive headsets such as Google cardboards (8-20 EUR per unit).

Our goal is to advance the Department's teaching capabilities by developing our own version of VRbased visualization software. We aim for cost-effective solutions (ideally using Google cardboards) that can be used in classrooms where a considerable number of headsets is necessary in order to give individual and still affordable access to each student. This project will benefit from the team's knowledge of 3D engines such as Unity3D[10] and Blender[11], of Web-based applications development and our state-of-the-art knowledge of chemical and biomolecular simulations and their applications. We thus aim to improve the teaching experience (with potential applications to bachelor and master research projects) towards a more immersive, real-like visualization of complex molecules. This software could be also combined with our own bioengineering tools such as CL-FEP, PPI-Detect and PPI-Affinity.

References: **1.** Xu, K.; Liu, N.; Xu, J.; Guo, C.; Zhao, L.; Wang, H.-W.; Zhang, Q. C., VRmol: an Integrative Web-Based Virtual Reality System to Explore Macromolecular Structure. Bioinformatics 2020. **2.** Calvelo, M.; Piñeiro, Á.; Garcia-Fandino, R., An immersive journey to the molecular structure of SARS-CoV-2: Virtual reality in COVID-19. Computational and Structural Biotechnology Journal 2020, 18, 2621-2628. **3.** 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 2019, 89, 234-241. **4.** Li, H.; Leung, K.-S.; Nakane, T.; Wong, M.-H., iview: an interactive WebGL visualizer for protein-ligand complex. BMC Bioinformatics 2014, 15 (1), 56. **5.** https://www.samson-connect.net/element/64225415-0c58-6ef2-4b29-f6e78a01e460.html. **6.** Norrby, M.; Grebner, C.; Eriksson, J.; Boström, J., Molecular Rift: Virtual Reality for Drug Designers. Journal of Chemical Information and Modeling 2015, 55 (11), 2475-2484. **7.** K.C. Cassidy, J. Šefčík, Y. Raghav, A. Chang, J.D. Durrant, ProteinVR: Web-based molecular visualization in virtual reality, PLOS Comput Biol, 16 (2020). **8.** https://www.appmindedapps.com/proteinvr.html. **9.** Calvelo M, Porto C, Piñeiro Á, Garcia-Fandino R. Corona VRus coaster: the virtual reality roller coaster of the proteins of SARS-CoV-2. Santiago de Compostela, Spain: 2020. **10.** https://unity.com/. **11.** Kent, B. R., 3D Scientific Visualization with Blender®. Morgan & Claypool Publishers: 2015. http://dx.doi.org/10.1088/978 -1-6270-5612-0.

3.3 Einzelmaßnahmen, Schritte etc.

- Introduction of a state of the art VR tool (Nanome) for demonstrative purposes in the practical sessions of "Computational Protein Engineering and Enzyme Design" (WS) in combination with the protein engineering module of PPI-Affinity. This will require the preparation of tutorials and exercises in this context.

- Generation of the code (with Unity), graphic interface and hand tracking interface compatible with cost-effective hardware (headsets, hand tracking device). This step will require extensive programing efforts as well as trial and error steps, until final optimization.

3.4 Geplante Laufzeit

First version of the code: 8 months
Final version of the code: 20 months (12 + 8 months)

3.5 Indikatoren zur Evaluation des Projektes

Implementation of VR practical sessions for visualization and manipulation of structures in courses taught at BCI such as "Computational Protein Engineering and Enzyme Design" and "Computer-Aided Drug Design".

3.6 Nachhaltigkeit/Verstetigung

The hardware and software of this project can be used by next generations of students.