Development of a Virtual Reality (VR) Platform for Visualization of Molecular Data for Biomedical Research and Classroom Learning

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Due to its complexity and robustness, the study of molecular structure can become an unpassable challenge to many learners. Better methods must be designed to improve the learning curve by focusing on increasing the interactivity of studies/research related to molecular structure. The application of Virtual Reality (VR) is therefore crucial to reducing the difficulty curve and increasing the interest in studies and research related to molecular structures such as chemistry and biology. Therefore, the application of VR technology would greatly help increase interest and foster a more interactive learning environment for students to study molecular structure. By combining various VR applications, hardware, and a large safe space, students can freely interact with molecules and their intricate structure within the VR space.

While Nanome can be used to create an extremely informative and interactive group learning environment allowing students to interact with molecular structures within the VR environment, the process of converting existing macromolecule data into the Nanome presentation format is not beginner-friendly and require technical and specialized knowledge. The goal of this project is to derive an easy to implement a workflow that can create an interactive VR classroom environment by utilizing the Nanome.

To provide a user-friendly and faster way to rapidly create and organize Nanome presentation slides from a set of molecular structure data and their respective presentation slides, the Nanome Macro Maker (NaMaMe) web service has been created based on the following steps: First, a website for NaMaMe is created to allow users to access the web service. The site has two main text input, one for the desktop folder name, and the other for the NaMaMe Input. Then a PHP server is created to accept the user's text submission on the website and forward the two text inputs above to the Python program. After that, a Python program has been written incorporating the PyMol library for parsing molecular structure data format. Python is one of the most efficient programming languages as it gives greater flexibility in storing different types of data and faster processing in the python environment. The main task of the Python program is to take in the names of the PyMol session file (.pse format) and the slide title to generate the result LUA macro script. Technically, the python program first converts the input data from the website in CSV format to Python-specific Data Structures (List). By using Python List, user input is separated into three columns to help to build the Lua Scripts. The size of each column represents the number of slides or molecules that the user wants to show in Nanome. This macro script allows for the creation of Nanome slides combined with molecular structure data (from PyMol session files) in a very short time and is very easy to set up. The Lua macro script provided by the NaMaMe service can greatly reduce the time and technical knowledge required for the making of detailed Nanome presentation slides, allowing anyone to produce educational Nanome presentation slides. The NaMaMe service has proven to be an essential tool in raising interest in the study of molecular structure.

The use of virtual learning tools is a great way to enrich core science education for students, Nanome achieves this by integrating a 3D virtual reality viewing experience with molecular interaction and manipulation in a team environment. It is important that Nanome is utilized more often by teachers to encourage more students to be interested in the study of molecular structure. Hence the NaMaMe web service has been created to reduce the time and effort required to produce Nanome presentation slides through the use of Lua macro scripts generated from user input to the website. In addition, the usage of Lua macro script provided by the NaMaMe service can be mastered in a matter of minutes, reducing the time and technical knowledge required to create comprehensive Nanome presentations. Nanome's intuitive interaction features, combined with a robust 3D VR environment can become a great catalyst in accelerating the drug discovery process, helping researchers and scientists from various disciplines and backgrounds, and allowing structure-based design collaboration in real-time. Innovative workflow designs such as NaMaMe and Nanome are needed to enhance the student-teacher interactions within the classroom, helping to provide a much more immersive learning environment.