A VR Framework for Interacting with Molecular Simulations

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Introduction

The NAMO-VMD [1-3] ensemble provides access to Virtual Reality (VR) devices for interacting with a Molecular Dynamics (MD) simulation in real time. In this interactive approach, named Interactive Molecular Dynamics (IMD), the use of VR peripherals yields good results for the analysis and study of complex biological systems. On the given simulation timescale, reversible and non-reversible events can be examined during the simulation. Our goal is to improve this approach by designing a VR framework, for developing tools dedicated to IMD in a VR context. This framework should allow developers and users to add new VR interaction paradigms and additional feedback modalities in order to provide new ways for steering a simulation and analysing its results.

Software Architecture for IMD in a VR context

We use the MD_driver library for interfacing a molecular User Interface (UI) with an MD simulation engine (GROMACS [4]) through a network connection. Thanks to this protocol, the new atom positions computed for each simulation timestep by the simulation, are sent to the molecular UI. The user can apply forces on atoms via this UI, which are then sent to the simulation and are taken into account in the next simulation step. As alternative molecular UI, we chose the visualisation toolkit VTK, allowing to quickly design visualisation and interaction paradigms dedicated to IMD. The VRPN library is used to manage VR devices, such as tracking devices for 3D interactions or haptic devices to provide force feedback to the user.

Why using VR techniques for Molecular Simulations

System exploration is easier using a 3D mouse or a haptic device to interact with molecular objects. Force feedback via haptics is especially well adapted to force-based methods such as molecular dynamics. It provides intuitive tactile feedback and enables the user to apply forces upon the virtual objects in order to guide or steer the simulation. A better perception of the three-dimensional organisation of large and complex biomolecular assemblies can be obtained by stereovision tools. The display surface can be extended on multiple screens in order to provide an immersive feeling to the user and create a collaborative work context.

Perspectives

Evolution of this VR framework is ongoing as a larger module, FVNano, to be encapsulated into the FlowVR middleware [5], a library designed for exchanging and synchronizing VR events and data between computers.

Summary

We propose a virtual laboratory for IMD in a Virtual Reality context, composed of the following libraries and tools:

MD_driver library provides new generic tools to connect calculation and visualization modules necessary for IMD simulations

vtk-based interactive MUI allows rendering of molecular simulations

vtkVRPN library manages Virtual Reality devices, such as trackers and haptic devices

References


See also http://mddriver.sourceforge.net and http://www.baaden.ibpc.fr/projects/fvnano/