A VR Framework for Interacting with Molecular Simulations

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Introduction

The *NAMD-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.

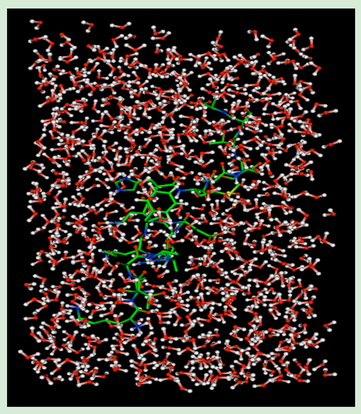
Software Architecture for IMD in a VR context

We use the ***MDDriver* 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.

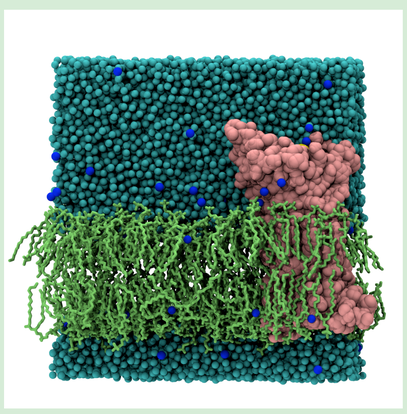
Why using VR techniques for Molecular Simulations

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.

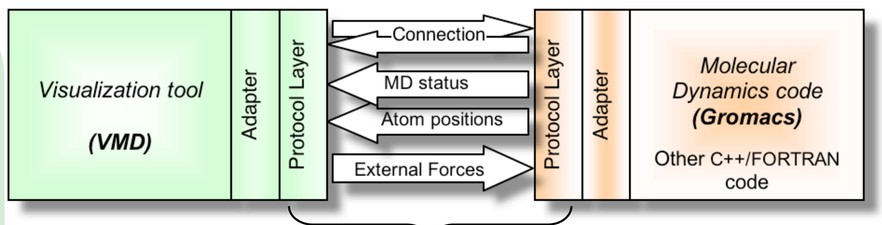
Visualising a simulation in progress with various Molecular User Interfaces

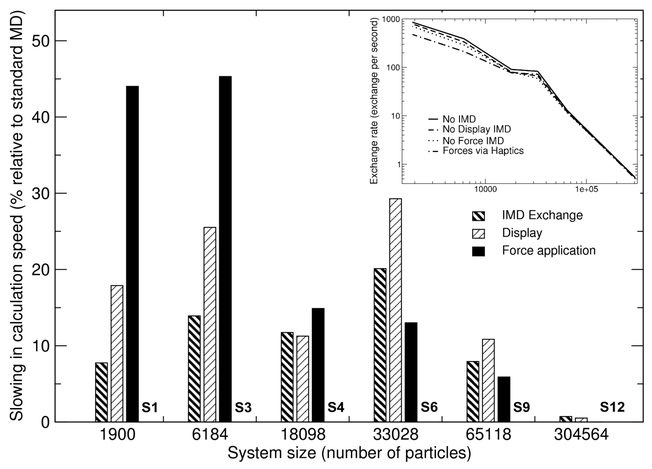


VTK : visualising a polypeptide in solution

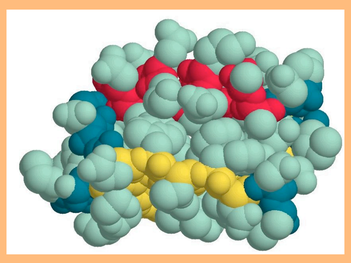


VMD : visualising the OmpT enzyme

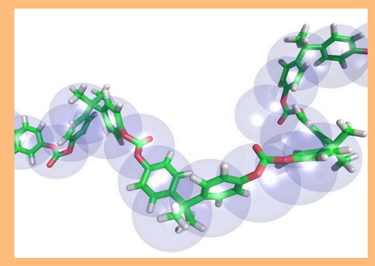




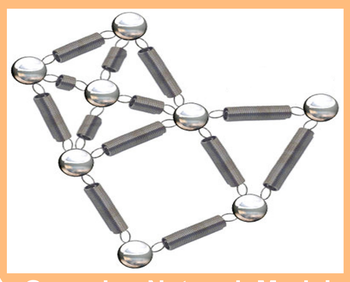
Using various simulation methods and/or models [5]



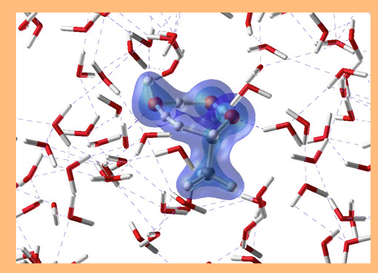
All-Atom Model



Coarse Grained Model



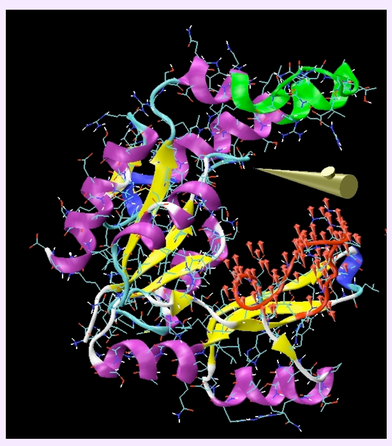
Gaussian Network Model



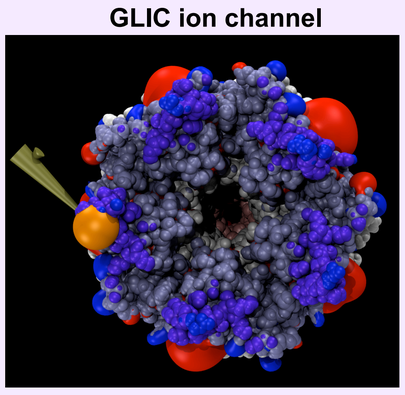
Quantum Mechanical Model

Interacting with dynamic models in real time using innovative devices and paradigms

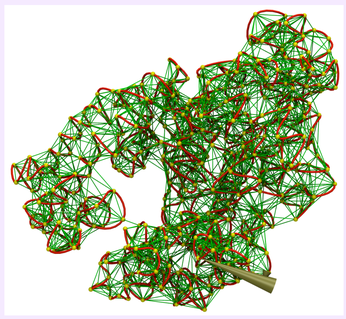
Interactive constraints (user applied forces) on a loop (red) of the GK enzyme



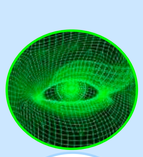
Exploring potential fields and isosurfaces of the GLIC ion channel



Improve mechanical properties of DNA transferase using elastic network (GNM)

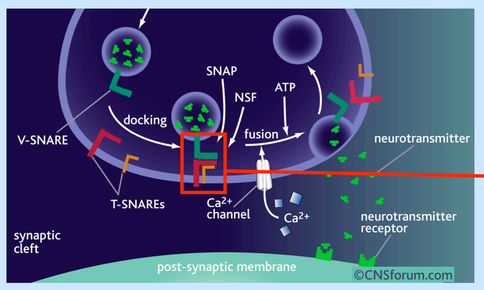


Relevant biological application : membrane fusion induced by the SNARE complex

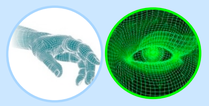


Instant visualization feedback (Low and High VR contexts)

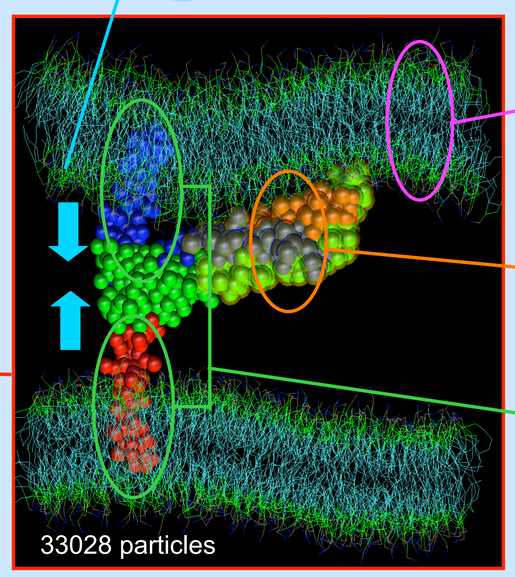
Haptic feedback (High VR context)

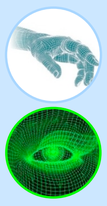


Synaptic membrane fusion

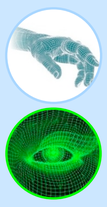


Mechanical process of SNARE action

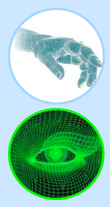




Lipid bilayer behaviour



Inner structural coherence of the SNARE complex



Trans-membrane helices insertion (different in depth, orientation, strength)

Perspectives

Evolution of this VR framework is ongoing as a larger module, FVNano, to be encapsulated into the FlowVR middleware [6], 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:
MDDriver 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

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