



HAL
open science

A Multimodal VR Framework for Interactive Molecular Simulations

Alex Tek, Benoist Laurent, Nicolas Férey, Marc Baaden

► **To cite this version:**

Alex Tek, Benoist Laurent, Nicolas Férey, Marc Baaden. A Multimodal VR Framework for Interactive Molecular Simulations. EuroVR-EVE 2010, Nov 2010, Orsay, France. hal-03977463

HAL Id: hal-03977463

<https://hal.science/hal-03977463v1>

Submitted on 27 Feb 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

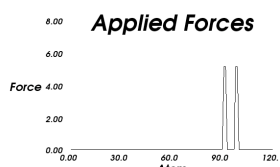
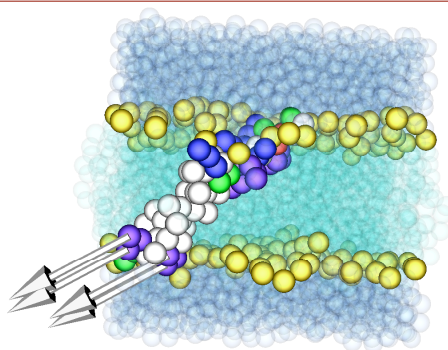
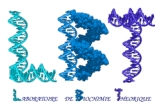
L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

A Multimodal VR Framework for Interactive Molecular Simulations

A. Tek¹, B. Laurent¹, N. Férey², M. Baaden¹

¹ CNRS - IBPC - Laboratoire de Biochimie Théorique – alex.tek@ibpc.fr

² CNRS - LIMSI - Venise group – ferey@limsi.fr



Molecular simulation is nowadays becoming a routine technique in structural biology. Recent progress along with increasingly widespread access to substantial computing power now enables the study of macromolecular systems in interactive time. Visual inspection of MD trajectories is a good way to quickly discover general trends and perform initial analysis.

Interactive Molecular Simulation (IMS) provides visualisation of and interaction with a simulation in progress, as well as possible on-the-fly control over simulation settings. Yet, few simulation and visualisation programs implement these features or often lack functionalities such as dynamic “live” analysis tools or efficient rendering.

Our goal:

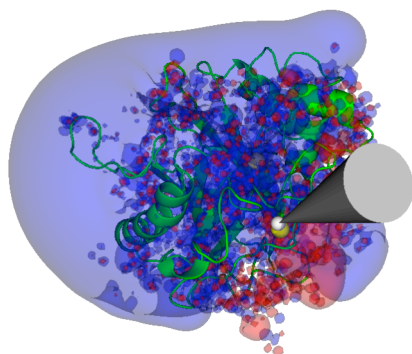
Providing a framework combining IMS with multimodal rendering and facilitating the development of new features and tools. Here we present our **BioSpaghetti** prototype. It uses VTK (Visualization ToolKit) which provides high-level features, such as isosurface rendering of electrostatic potential maps.

With VTK it is possible to visualise up to several hundred thousand particles in interactive time using a GPU shader implementation of spherical representations. VTK was encapsulated into a Cocoa application, allowing us to quickly develop a GUI using the XCode and Interface Builder tools.

Interactive Molecular Simulation and real-time plots

With VTK it is possible to visualise up to several hundred thousand particles in interactive time using a GPU shader implementation of spherical representations. VTK was encapsulated into a Cocoa application, allowing us to quickly develop a GUI using the XCode and Interface Builder tools.

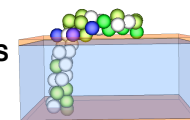
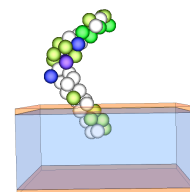
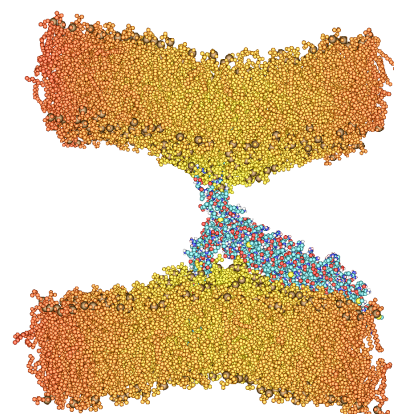
Rendering of potential isosurfaces for the MyPal [2] application



Features:

- Interactive rendering of large macromolecular systems (>300,000 particles)
- Atomistic and Coarse-Grained representations
- Interactive Molecular Dynamics (IMD) using MDDriver [1]
 - Easy picking of particles
 - Force feedback rendering of forcefield for haptic arms
- Visual feedback (e.g. colour mapping) of multiple variables
- Isosurface rendering
- Dynamic “live” plots
- 3D guides placement

Visualisation of membrane thickness



Use of 3D guides for an IMS protein insertion in an implicit membrane

References:

- [1] N. Férey, O. Delalande, G. Grasseau and M. Baaden; J Comput Chem 30, 2009, 2375-2387 <http://mddriver.sourceforge.net/>
 [2] O. Delalande, N. Férey, B. Laurent, M. Guérout, B. Hartmann, M. Baaden; Pacific Symposium on Biocomputing 15, 2010, 205-215

This work is part of the FlowVRNano project funded by ANR (ANR-07-CIS7-003-01), <http://www.baaden.ibpc.fr/projects/fvnano>



EuroVR-EVE 2010

Joint European Meeting « First EuroVR -SIGs workshops & EVE inauguration »

May 6-7, 2010

Université Paris-Sud, Orsay, France - <http://eurovr-eve-2010.limsi.fr/>

