# A Multimodal VR Framework for Interactive Molecular Simulations

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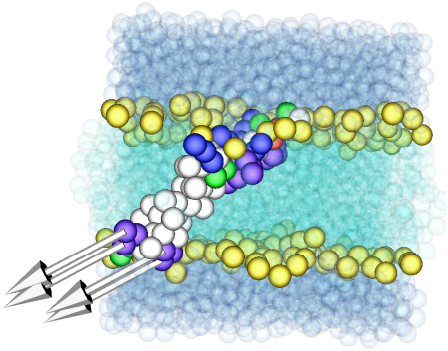
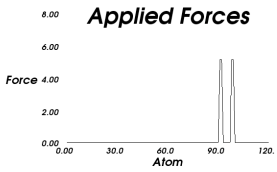





**Interactive Molecular Simulation and real-time plots**

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.

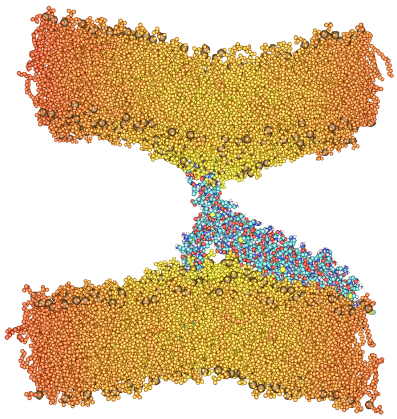
Interactive Molecular Simulation (IMS) provides visualisation of and interaction with a simulation in progress, as well as possible on-the-fly control over simulation settings. Yet, few simulation and visualisation programs implement these features or often lack functionalities such as dynamic "live"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

**Our goal:**

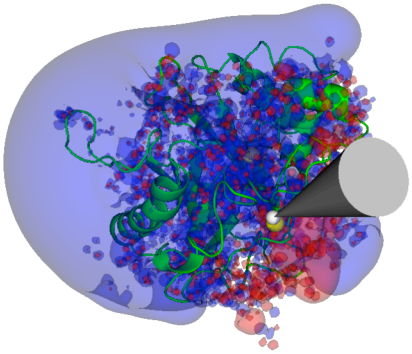
Providing a framework combining IMS with multimodal rendering and facilitating the development of new features and tools. Here we present our **BioSpaghetti** prototype. It uses VTK (Visualization ToolKit) which provides high-level features, such as isosurface rendering of electrostatic potential maps.

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.

**Visualisation of membrane thickness**

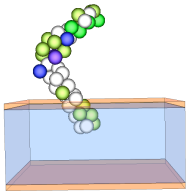


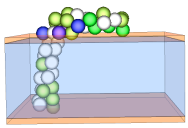
**Rendering of potential isosurfaces for the MyPal [2] application**



**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





**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. Guéroult, 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