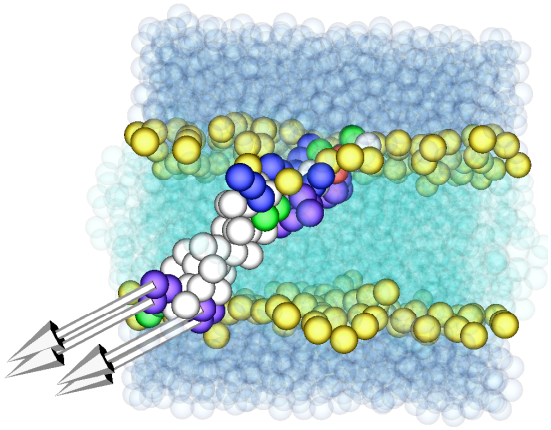

Interactive Molecuar Dynamics and real-time plot

Augmented Dynamics

Enhanced Visualization of Molecular Dynamics Trajectories

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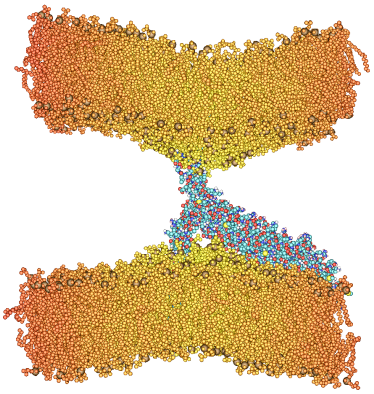
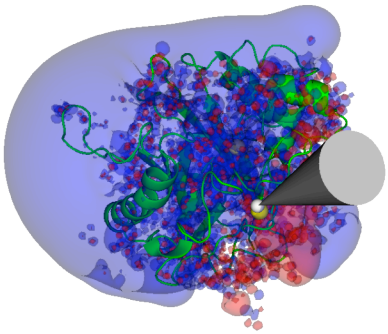
Molecular dynamics (MD) is nowadays becoming a routine technique in structural biology. Recent progress along with increasingly widespread access to substantial computing power now enables the study of macromolecular systems in interactive time. Visual inspection of MD trajectories is a good way to quickly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

Our goal:

Providing a tool capable of "Augmented Dynamics", i.e. visually enhanced representations of MD trajectories. We present here a prototype called **BioSpaghetti.** It uses VTK (Visualization ToolKit) which provides high-level features, such as isosurface rendering of electrostatic potential maps. It allows us to visualize 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.

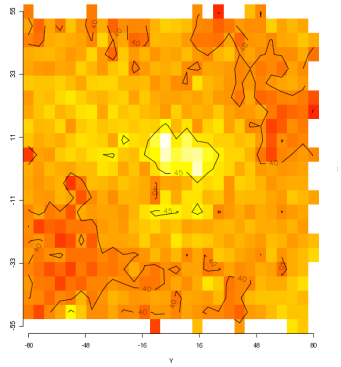




Rendering of potential isodurfaces for the MyPal application

Features:

- Supports of large macromolecular systems (>300,000 particles)
- Atomistic and Coarse-Grained representations
- Interactive Molecular Dynamics using MDDriver [1]
  - Easy picking of particles
  - Force feedback rendering of forcefield for haptic arms
- Colour rendering of multiple variables
- Isosurface rendering
- Dynamics plots
- 3D guides placement



Visualization of membrane thickness : 2D and 3D rendering

Use cases:

MyPal [2]: Molecular scrutin**Y** of **P**otenti**AL**s where ionic probes are immerged into an electrostatic potential map. The potential force feedback and the visualization of the isosurface help to find the binding sites.

Implicit membrane insertion: We implemented a forcefield allowing dynamic insertion and orientation of a protein into an implicit membrane. Here we use 3D guides to visualize the membrane and dynamics plots to see the evolution of the orientation.

Membrane thickness: For the study of membrane fusion induced by a SNARE complex, we coloured the lipids according to the thickness of the membrane.

Perspectives:

- 3D slicing
- Voronoi volumes visualization
- Enhanced shaders for rendering of molecular structure and surface.
- Sound feedback
- Stereoscopic view
- Portable interface (QT)

References:

[1] N. Férey, O. Delalande, G. Grasseau and M. Baaden, *in Proceedings of the 15th ACM Symposium on Virtual Reality Software and Technology*, 91 (2008).

[2] O. Delalande, N. Ferey, B. Laurent, M. Gueroult, B. Hartmann, M. Baaden; Pacific Symposium on Biocomputing 15:205-215(2010)

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