Sujet 1
Intersurf++

Proposé par : Dave Ritchie

Informations générales

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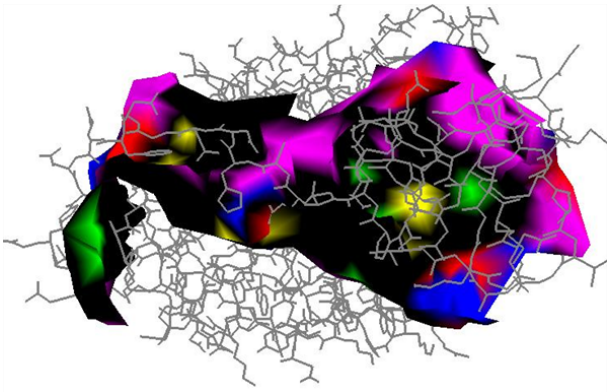

Motivations

Studying protein-protein complexes in 3D can help to understand many fundamental biological processes.

Topic

Intersurf++ : Calculating 3D interfaces between protein molecules

Context

This project is proposed through a collaboration between the Capsid and Vegas research teams. The main objective is to develop a new program to calculate and visualise 3D protein interfaces using the CGAL [1] computational geometry library and OpenGL 3D graphics. An early prototype [2] was developed in C but cannot be interfaced with modern computational geometry library nor with recent protein modelisation software [3]. Ultimately, we want to use the developed program to be able to compare the similarities and differences in protein complex interfaces across related families of proteins, and to measure how interfaces change during molecular dynamics simulations of protein flexibility.

Advisors

The project will be supervised by Bernard Maigret and Dave Ritchie (Capsid) in collaboration with Monique Teillaud and Olivier Devillers (Vegas).

Working program

First, the student will use the CGAL library to compute the 3D Voronoi diagram of two proteins, identify the part of the diagram at the interface between the two proteins. A quality of the relative position of two proteins will be computed according to the distances and chemical properties of the involved parts of the proteins.

Then, several directions will be explored :

— Optimizing the computation of the Voronoi diagram by restricting the computation to the interface area.

— Updating the diagram when the shapes of the proteins are modified without recomputing everything from scratch.

— Extracting 2D signature from a relative position of two proteins to facilitate the management of the database.

Références

[1] The Computational Geometry Algorithms Library, *http ://|http ://|www.cgal.org|*.

[2] N. Ray, X. Cavin, J.-C. Paul, and B. Maigret *Intersurf : dynamic interface between proteins*, Journal of Molecular Graphics and Modelling, 23 (2005) 347–354.

[3] VMD. Visual Molecular Dynamics. *http ://|www.ks.uiuc.edu|Research|vmd|*.