

Interface between proteins

Simon Ziza
6 months internship
Student at CPE Lyon

David Ritchie and Bernard Maigret

Introduction : Intersurf ++

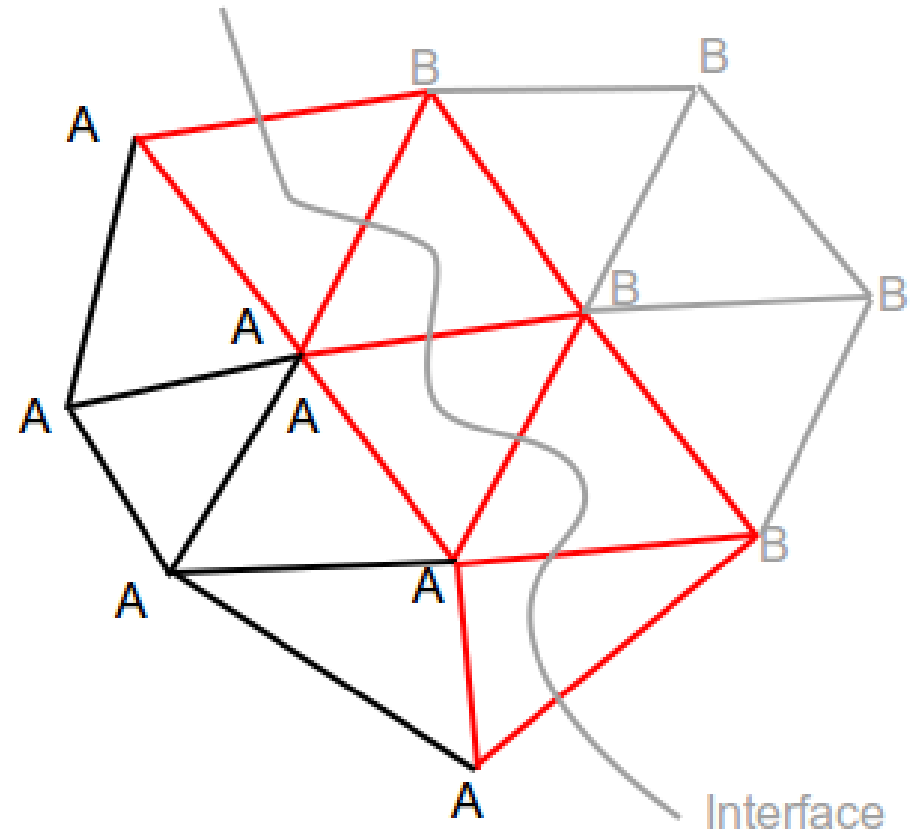
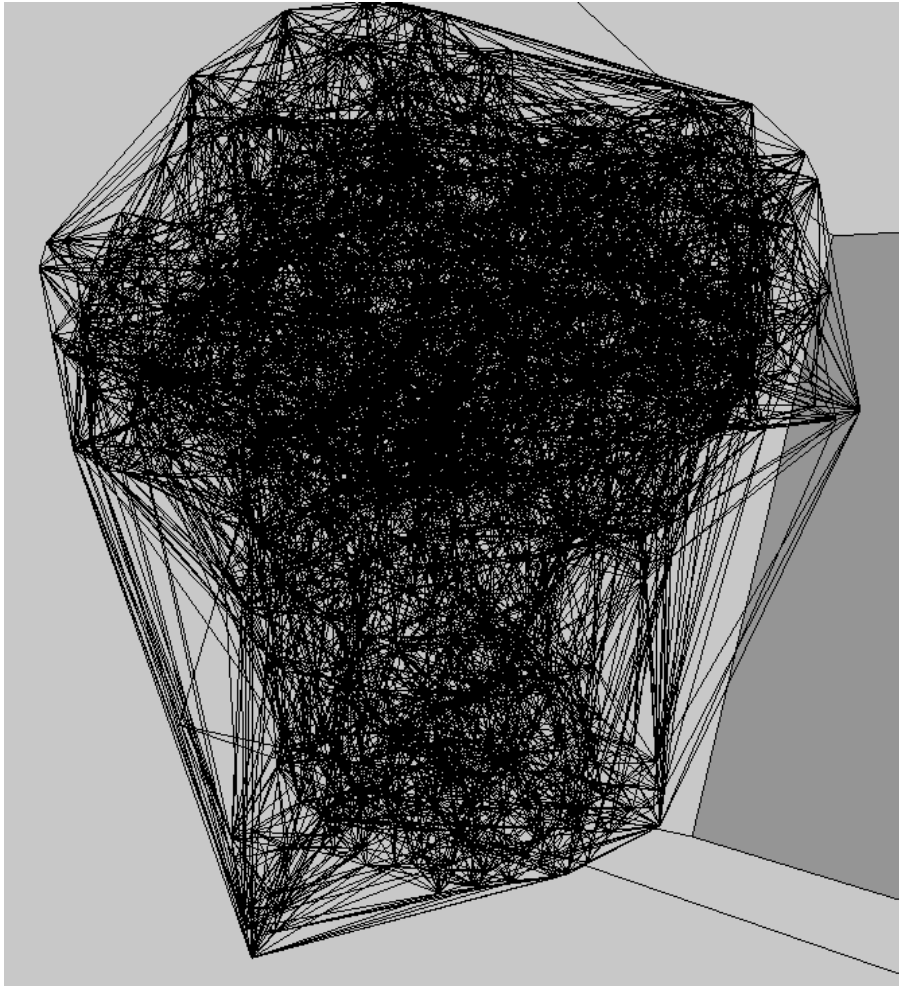
- **Finding dynamically the interface between two proteins**
- **Calculate the new interface when one or several atom(s) has moved**

Existing Software

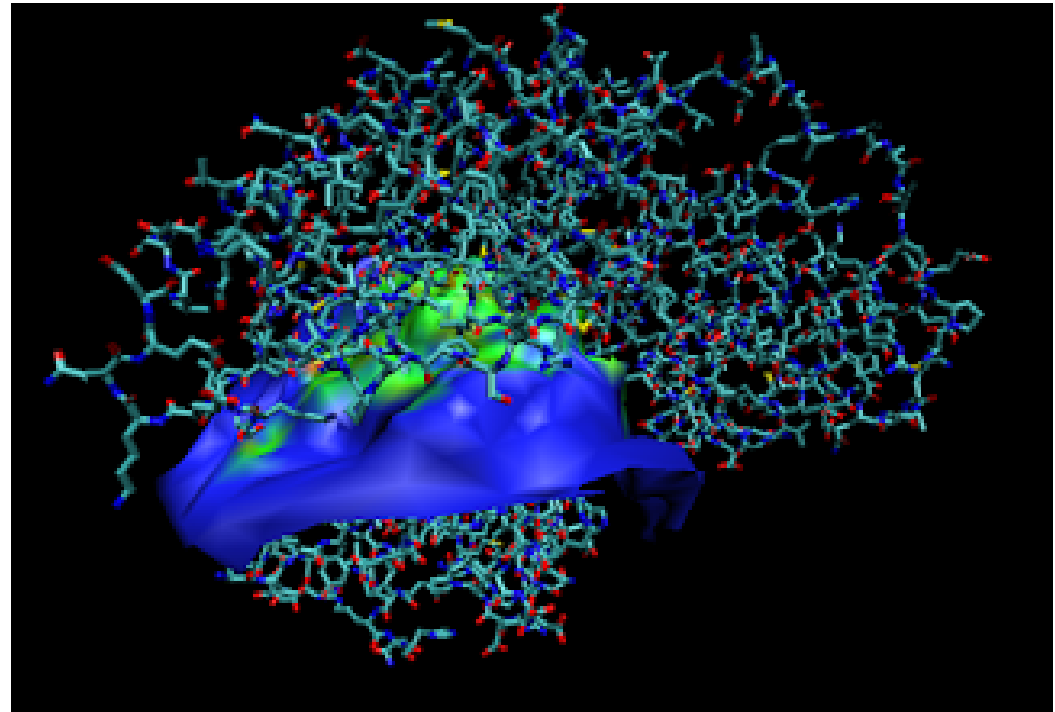
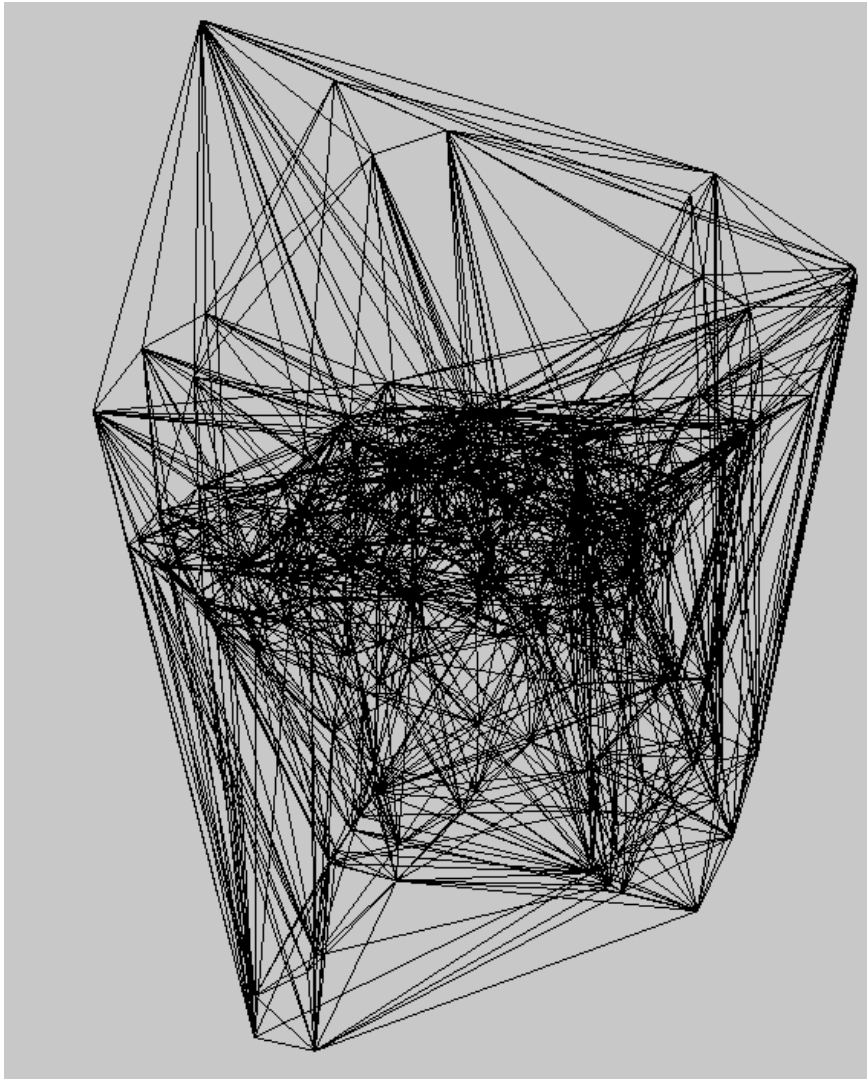
- **Intersurf** : Static calculation of a surface between proteins (works as a module for VMD)
- **VMD** : Protein visualization (*.pdb)



Delaunay Tessellation



Delaunay Tessellation





: Software library to compute geometry algorithms

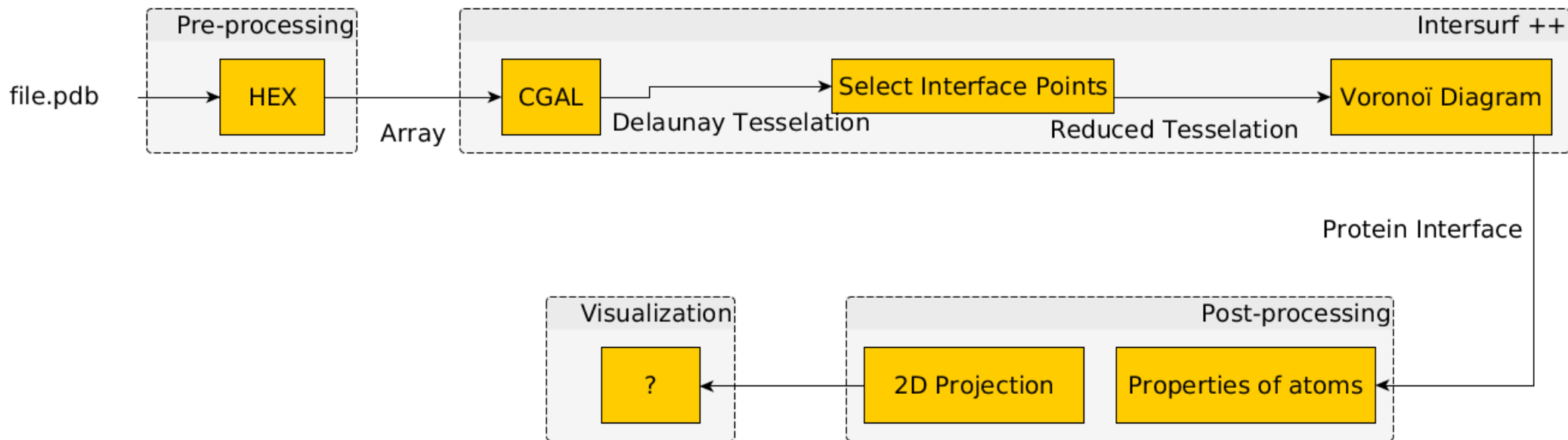
- **Advantages**

- **Great pre-defined structures (Delaunay Triangulation)**
- **Fast calculation**
- **Fast location**

- **Disadvantages**

- **Amount of information and structures**
- **Hidden data**
- **Visualization (Using Qt5)**

Software processing pipeline



Next functionalities

- **Dynamical display**
- **Information regarding the atoms**
- **2D Projection (Comparison of complexes)**

Thank you for your attention.