# Pck, a software for pockets detection and analysis

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Pck homepage : http://alnitak.u-strasbg.fr/Pck/

With the growing number of structures in the pdb, a great variety of programs and algorithms have been developed to address the difficult problem of the automatic detection of cavities in a given structure. Unfortunately the vast majority of these efforts are imperfect, uneasy to install, or show cryptic outputs when they are at all freely accessible.

We developed a free software to detect pockets and ease their analysis through a Plugin in VMD (Humphrey *et al.,* 1996), one of the most used visualization software.

## Pocket detection

Usual approaches for the automatic detection of pockets can be broadly divided in three categories considering the approach on which their algorithm relies : *discretization*, where the protein is sliced in a cubic grid; *mostly geometric* where a first step consist in filling holes with probe spheres; and *combinatorial* that uses computational geometry tools to represent a molecule and it's voids.

This latest approach, introduced by Edelsbrunner (Edelsbrunner 1995) decomposes molecules by a partition of tetrahedra whose vertices are the atoms centers. In this model, pockets can be both naturally and formally defined, as well as their mouths. Pockets are represented as polyhedra composed of triangular facets, the vertices being the atoms that contribute to the border of the pocket.

## Pck Description

Our software is accessible via a VMD plugin provided as a Tcl package. This plugin allows one for visualization and interaction with pockets. It interfaces with our Internet server that actually achieves computations. The server is written in C++ using the CGAL library (CGAL 2006) for the computational geometry framework.

Two detection algorithms are actually implemented :

**tight** is an implementation of Edelsbrunner algorithm (Edelsbrunner 1998) for the detection of buried cavities and tightly opened pockets.

**wide** for the detection of clefts, pit and other wide opened pockets. In some aspects it resembles Peters Algorithm (Peters 1996).

The output of the software comprises the pockets facets, distances between pockets, volumetric properties, and a globularity index for each pocket.

Moreover, since pockets facets carry information about their vicinity they are merely classified as "border","mouth","almost mouth", and "thin closure". The latest showing a thin closure between neighbor pockets that might possibly be merged.

## References

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CGAL, Computational Geometry Algorithms Library, http://www.cgal.org