M. Zemek: Tunnels in Static and Dynamic Protein Molecules

Biochemists use a computer analysis of existence and proportions of the tunnels (cavities), leading from a biochemically significant place inside a protein to its surface. I will describe a geometric approximation of the tunnels and an application of the regular triangulation for its computation.

The geometry of a protein is not static – the positions of atoms change in time and a long sequence of "molecule snapshots" have to be explored to find a stable tunnel. In the second part of my speech, I will describe our new method, which uses a spatial coherence of a tunnel and a clustering of atoms to accelerate the processing of a sequence of snapshots.

I am sure you all are busy therefore my speech will be short (30 – 45 minutes).