



FROM VISION TO DECISION

SEMINAR FRIDAY 26.10.12

PLACE: Dept of Radiology (H112), «Biblioteket»

TIME : 12:00-13:00

TITLE:

Parulek and Reuter: Interactive visual analysis of protein simulations: cavity extraction
Lampe: Enlighten - an Interactive Tool for Visual Analysis of Multi-Dimensional Data

SPEAKERS:

1. Julius Parulek , UiB, Postdoc, Department of Informatics
2. Natalie Reuter, UiB, Researcher, Department of Molecular Biology
3. Ove Daae Lampe, CMR

ABSTRACT

Identification of cavities in proteins is determinant for understanding substrate-receptor recognition, designing drugs or for protein design. Molecular dynamics (MD) simulations are a powerful in silico tool to investigate protein structures and have the potential of revealing surface evolution and cavities. However cavity analysis from MD simulations data is limited because of data size (thousands of time-steps) and complexity (tens of thousands atoms). The positions in space of the atoms define the protein 3D structure and the protein surface. In this talk we will briefly introduce molecular dynamics simulations, its potential and imitations for cavity identification. Then we will present a novel method to extract, analyze and visualize the cavities of proteins and their evolution over simulation time. Finally we will demonstrate the efficiency of this method on a few use cases.

