

**Laboratoire de Biochimie Théorique**  
Institut de **Biologie Physico-Chimique**  
13, rue Pierre et Marie Curie  
75005 PARIS

# **S E M I N A I R E**

**Silke Wieninger**

Laboratoire de Bioinformatique structurale, Institut Pasteur,  
Paris

**« A More Dynamic View on Protein Domains »**

Structural domains are frequently used to analyze functional motions of proteins. Although domains are intuitively thought of as compact structural units, various criteria are employed for their assignment. We developed a method for identifying protein domains using directly dynamic data obtained from an Elastic Network Model. Our program CoMoDo (Covariance of Motion Domains) clusters residues into domains of different hierarchical levels based on covariances of atomic fluctuations. The so-called dynamic domains facilitate the study of conformational changes and the effect of ligand binding on protein dynamics. A comparison to domains assigned manually shows that human assignments are often influenced by evolutionary or functional aspects and that recurrent secondary structure patterns can be deceptive. In contrast to standard domain assignment methods, we do not perform any postprocessing steps imposing restrictions on discontinuous domains, intercalating segments or split secondary structure elements. We even allow for intersubunit domains in multimeric proteins, believing that valuable information about protein dynamics can be gained from those special features of dynamic domains.

**Jeudi 23 juin 2016**  
**14h30**

**SALLE DE CONFERENCES**