Πρόγραμμα Μεταπτυχιακών Σπουδών

ΤΕΧΝΟΛΟΓΙΕΣ ΠΛΗΡΟΦΟΡΙΚΗΣ
ΣΤΗΝ ΙΑΤΡΙΚΗ ΚΑΙ ΤΗ ΒΙΟΛΟΓΙΑ

Short Course:

MODELING MACRO-MOLECULAR COMPLEXES AND ASSEMBLIES

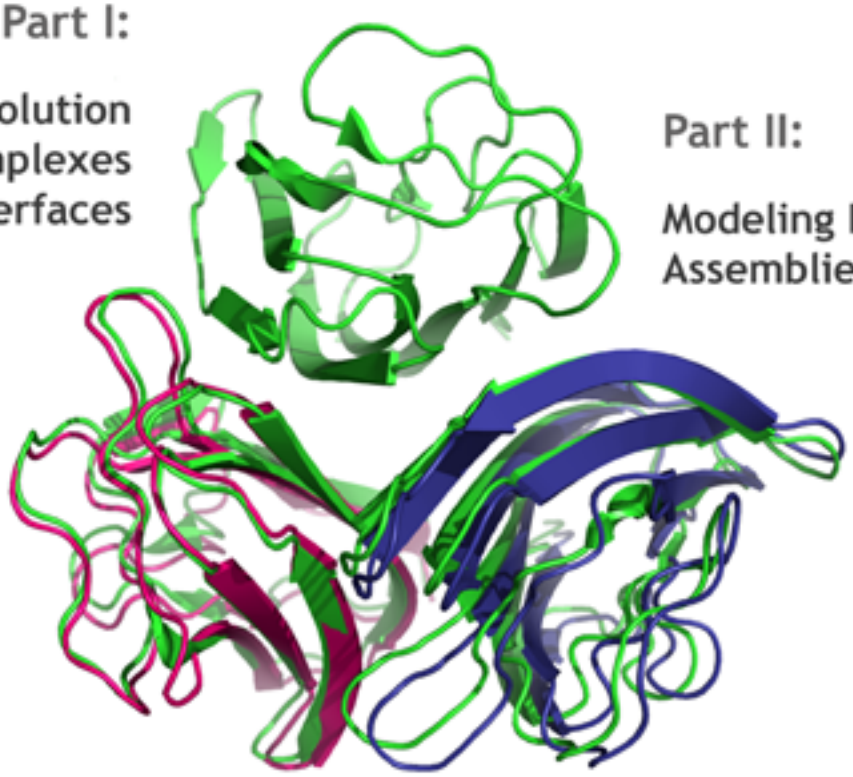
Tuesday 14 May 2013: 14:00-17:00, Room A1
Wednesday 15 May 2013: 10:00-13:00, Room D

-- Frédéric Cazals --

Algorithms-Biology-Structure,
INRIA Sophia-Antipolis, France

Part I:

Modeling High Resolution Protein Complexes and their Interfaces



Part II:

Modeling Large Protein Assemblies

> Geometry is not everything, but it is the most fundamental thing
>
> (Michael Connolly)

Syllabus:

This course will discuss recent algorithmic developments revolving on the investigation of the structure-function relationship in structural biology. The first part will focus on atomic resolution models of small complexes, typically involving two partners, and will show that finer geometric and topological models yield more accurate biophysical and biological descriptors. The second one will focalize on the emerging trend of reconstruction by data integration, which targets molecular machines involving up to hundreds of macro-molecules, and will show that advanced constructions allow one to make a stride towards atomic resolution models of such assemblies.

From a methodological standpoint, this class will touch upon computational geometry and topology (affine and curved Voronoi diagrams, alpha-shapes), programming techniques (dynamic programming, greedy algorithms), and also statistics (statistical tests, p-value calculations).

Part I: Modeling High Resolution Protein Complexes and their Interfaces

-- Protein complexes: key questions
-- Geometric intermezzo: Voronoi diagrams and relatives
-- Describing protein interfaces
-- Mining biophysical properties at protein interfaces
-- From protein interfaces to protein binding patches
-- Connexions with docking, scoring, and binding affinity predictions

Part II: Modeling Large Protein Assemblies

-- Large protein assemblies
-- Reconstruction by data integration
-- Toleranced models and curved Voronoi diagrams
-- Assessing the reconstruction of large protein assemblies
-- Designing toleranced and coarse-grain models
-- Studies in mass spectrometry: stoichiometry determination and connectivity inference

Short CV:

Frédéric Cazals is research director at INRIA Sophia-Antipolis Mediterranee, France, where he leads the group Algorithms - Biology - Structure (ABS, *http://team.inria.fr/abs*). He holds an engineering degree in Biological Sciences from the Institut National Agronomique Paris-Grignon (Paris, France), a master degree in theoretical computer science from Ecole Normale Superieure and Ecole Polytechnique (Paris, France), and a PhD in theoretical computer science from the University of Paris VII (Paris, France).

His research interests encompass computational structural biology (modeling protein complexes and assemblies, modeling the flexibility of proteins), as well as geometric and topological modeling (applied differential geometry, computational geometry, computational topology, shape learning).

He recently co-edited the book entitled Modeling in Computational Biology and Biomedicine (Springer), which pitches success stories at the interface biology/medicine - computer science - applied mathematics.