



Activity Report 2014

Project-Team INRIAALL

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RESEARCH CENTER
Sophia Antipolis - Méditerranée

THEME

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Project-Team INRIAALL

Keywords: Computational Structural Biology, Protein-protein Interactions, Protein Assemblies, Computational Geometry, Computational Topology

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2. Overall Objectives

2.1. Overall Objectives

Computational Biology and Computational Structural Biology. Understanding the lineage between species and the genetic drift of genes and genomes, apprehending the control and feed-back loops governing the behavior of a cell, a tissue, an organ or a body, and inferring the relationship between the structure of biological (macro)-molecules and their functions are amongst the major challenges of modern biology. The investigation of these challenges is supported by three types of data: genomic data, transcription and expression data, and structural data.

Genetic data feature sequences of nucleotides on DNA and RNA molecules, and are symbolic data whose processing falls in the realm of Theoretical Computer Science: dynamic programming, algorithms on texts and strings, graph theory dedicated to phylogenetic problems. Transcription and expression data feature evolving concentrations of molecules (RNAs, proteins, metabolites) over time, and fit in the formalism of discrete and continuous dynamical systems, and of graph theory. The exploration and the modeling of these data are covered by a rapidly expanding research field termed *systems biology*. Structural data encode informations about the 3D structures of molecules (nucleic acids (DNA, RNA), proteins, small molecules) and their interactions, and come from three main sources: X ray crystallography, NMR spectroscopy, cryo Electron Microscopy. Ultimately, structural data should expand our understanding of how the structure accounts for the function of macro-molecules —one of the central questions in structural biology. This goal actually subsumes two equally difficult challenges, which are *folding* —the process through which a protein adopts its 3D structure, and *docking* —the process through which two or several molecules assemble. Folding and docking

are driven by non covalent interactions, and for complex systems, are actually inter-twined [4348]. Apart from the bio-physical interests raised by these processes, two different application domains are concerned: in fundamental biology, one is primarily interested in understanding the machinery of the cell; in medicine, applications to drug design are developed.

Modeling in Computational Structural Biology. Acquiring structural data is not always possible: NMR is restricted to relatively small molecules; membrane proteins do not crystallize, etc. As a matter of fact, the order of magnitude of the number of genomes sequenced is of the order of one thousand, which results in circa one million of genes recorded in the manually curated Swiss-Prot database. On the other hand, the Protein Data Bank contains circa 90,000 structures. Thus, the paucity of structures with respect to the known number of genes calls for modeling in structural biology, so as to foster our understanding of the structure-to-function relationship.

Ideally, bio-physical models of macro-molecules should resort to quantum mechanics. While this is possible for small systems, say up to 50 atoms, large systems are investigated within the framework of the Born-Oppenheimer approximation which stipulates the nuclei and the electron cloud can be decoupled. Example force fields developed in this realm are AMBER, CHARMM, OPLS. Of particular importance are Van der Waals models, where each atom is modeled by a sphere whose radius depends on the atom chemical type. From an historical perspective, Richards [4346], [4335] and later Connolly [4331], while defining molecular surfaces and developing algorithms to compute them, established the connexions between molecular modeling and geometric constructions. Remarkably, a number of difficult problems (e.g. additively weighted Voronoi diagrams) were touched upon in these early days.

The models developed in this vein are instrumental in investigating the interactions of molecules for which no structural data is available. But such models often fall short from providing complete answers, which we illustrate with the folding problem. On one hand, as the conformations of side-chains belong to discrete sets (the so-called rotamers or rotational isomers) [4337], the number of distinct conformations of a poly-peptidic chain is exponential in the number of amino-acids. On the other hand, Nature folds proteins within time scales ranging from milliseconds to hours, while time-steps used in molecular dynamics simulations are of the order of the femto-second, so that biologically relevant time-scales are out reach for simulations. The fact that Nature avoids the exponential trap is known as Levinthal's paradox. The intrinsic difficulty of problems calls for models exploiting several classes of informations. For small systems, *ab initio* models can be built from first principles. But for more complex systems, *homology* or template-based models integrating a variable amount of knowledge acquired on similar systems are resorted to.

The variety of approaches developed are illustrated by the two community wide experiments CASP (*Critical Assessment of Techniques for Protein Structure Prediction*; <http://predictioncenter.org>) and CAPRI (*Critical Assessment of Prediction of Interactions*; <http://capri.ebi.ac.uk>), which allow models and prediction algorithms to be compared to experimentally resolved structures.

As illustrated by the previous discussion, modeling macro-molecules touches upon biology, physics and chemistry, as well as mathematics and computer science. In the following, we present the topics investigated within ABS .

3. Research Program

3.1. Introduction

The research conducted by ABS focuses on three main directions in Computational Structural Biology (CSB), together with the associated methodological developments:

- Modeling interfaces and contacts,
- Modeling macro-molecular assemblies,
- Modeling the flexibility of macro-molecules,

(a) (b) (c)

Figure 1. Geometric constructions in computational structural biology. (a) An antibody-antigen complex, with interface atoms identified by our Voronoi based interface model [8], [1]. This model is instrumental in mining correlations between structural and biological as well as biophysical properties of protein complexes. (b) A diverse set of conformations of a backbone loop, selected thanks to a geometric optimization algorithm [10]. Such conformations are used by mean field theory based docking algorithms. (c) A tolerated model (TOM) of the nuclear pore complex, visualized at two different scales [9]. The parameterized family of shapes coded by a TOM is instrumental to identify stable properties of the underlying macro-molecular system.

– Algorithmic foundations.

3.2. Modeling Interfaces and Contacts

Keywords: Docking, interfaces, protein complexes, structural alphabets, scoring functions, Voronoi diagrams, arrangements of balls.

The Protein Data Bank, <http://www.rcsb.org/pdb>, contains the structural data which have been resolved experimentally. Most of the entries of the PDB feature isolated proteins ¹, the remaining ones being protein - protein or protein - drug complexes. These structures feature what Nature does —up to the bias imposed by the experimental conditions inherent to structure elucidation, and are of special interest to investigate non-covalent contacts in biological complexes. More precisely, given two proteins defining a complex, interface atoms are defined as the atoms of one protein *interacting* with atoms of the second one. Understanding the structure of interfaces is central to understand biological complexes and thus the function of biological molecules [4348]. Yet, in spite of almost three decades of investigations, the basic principles guiding the formation of interfaces and accounting for its stability are unknown [4351]. Current investigations follow two routes. From the experimental perspective [4334], directed mutagenesis enables one to quantify the energetic importance of residues, important residues being termed *hot* residues. Such studies recently evidenced the *modular* architecture of interfaces [4345]. From the modeling perspective, the main issue consists of guessing the hot residues from sequence and/or structural informations [4340].

The description of interfaces is also of special interest to improve *scoring functions*. By scoring function, two things are meant: either a function which assigns to a complex a quantity homogeneous to a free energy change ², or a function stating that a complex is more stable than another one, in which case the value returned is a score and not an energy. Borrowing to statistical mechanics [4329], the usual way to design scoring functions is to mimic the so-called potentials of mean force. To put it briefly, one reverts Boltzmann's law, that is, denoting $p_i(r)$ the probability of two atoms —defining type i — to be located at distance r , the (free) energy assigned to the pair is computed as $E_i(r) = -kT \log p_i(r)$. Estimating from the PDB one function $p_i(r)$ for each type of pair of atoms, the energy of a complex is computed as the sum of the energies of the pairs located within a distance threshold [4349], [4336]. To compare the energy thus obtained to a reference state, one may compute $E = \sum_i p_i \log p_i/q_i$, with p_i the observed frequencies, and q_i the frequencies stemming from an a priori model [4341]. In doing so, the energy defined is nothing but the Kullback-Leibler divergence between the distributions $\{p_i\}$ and $\{q_i\}$.

Describing interfaces poses problems in two settings: static and dynamic.

¹For structures resolved by crystallography, the PDB contains the asymmetric unit of the crystal. Determining the biological unit from the asymmetric unit is a problem in itself.

²The Gibbs free energy of a system is defined by $G = H - TS$, with $H = U + PV$. G is minimum at an equilibrium, and differences in G drive chemical reactions.

In the static setting, one seeks the minimalist geometric model providing a relevant bio-physical signal. A first step in doing so consists of identifying interface atoms, so as to relate the geometry and the bio-chemistry at the interface level [8]. To elaborate at the atomic level, one seeks a structural alphabet encoding the spatial structure of proteins. At the side-chain and backbone level, an example of such alphabet is that of [4330]. At the atomic level and in spite of recent observations on the local structure of the neighborhood of a given atom [4350], no such alphabet is known. Specific important local conformations are known, though. One of them is the so-called dehydron structure, which is an under-desolvated hydrogen bond—a property that can be directly inferred from the spatial configuration of the C_α carbons surrounding a hydrogen bond [4333].

In the dynamic setting, one wishes to understand whether selected (hot) residues exhibit specific dynamic properties, so as to serve as anchors in a binding process [4344]. More generally, any significant observation raised in the static setting deserves investigations in the dynamic setting, so as to assess its stability. Such questions are also related to the problem of correlated motions, which we discuss next.

3.3. Modeling Macro-molecular Assemblies

Keywords: Macro-molecular assembly, reconstruction by data integration, proteomics, modeling with uncertainties, curved Voronoi diagrams, topological persistence.

3.3.1. Reconstruction by data integration

Large protein assemblies such as the Nuclear Pore Complex (NPC), chaperonin cavities, the proteasome or ATP synthases, to name a few, are key to numerous biological functions. To improve our understanding of these functions, one would ideally like to build and animate atomic models of these molecular machines. However, this task is especially tough, due to their size and their plasticity, but also due to the flexibility of the proteins involved. In a sense, the modeling challenges arising in this context are different from those faced for binary docking, and also from those encountered for intermediate size complexes which are often amenable to a processing mixing (cryo-EM) image analysis and classical docking. To face these new challenges, an emerging paradigm is that of reconstruction by data integration [4328]. In a nutshell, the strategy is reminiscent from NMR and consists of mixing experimental data from a variety of sources, so as to find out the model(s) best complying with the data. This strategy has been in particular used to propose plausible models of the Nuclear Pore Complex [4327], the largest assembly known to date in the eukaryotic cell, and consisting of 456 protein *instances* of 30 *types*.

3.3.2. Modeling with uncertainties and model assessment

Reconstruction by data integration requires three ingredients. First, a parametrized model must be adopted, typically a collection of balls to model a protein with pseudo-atoms. Second, as in NMR, a functional measuring the agreement between a model and the data must be chosen. In [4326], this functional is based upon *restraints*, namely penalties associated to the experimental data. Third, an optimization scheme must be selected. The design of restraints is notoriously challenging, due to the ambiguous nature and/or the noise level of the data. For example, Tandem Affinity Purification (TAP) gives access to a *pullout* i.e. a list of protein types which are known to interact with one tagged protein type, but no information on the number of complexes or on the stoichiometry of proteins types within a complex is provided. In cryo-EM, the envelope enclosing an assembly is often imprecisely defined, in particular in regions of low density. For immuno-EM labelling experiments, positional uncertainties arise from the microscope resolution.

These uncertainties coupled with the complexity of the functional being optimized, which in general is non convex, have two consequences. First, it is impossible to single out a unique reconstruction, and a set of plausible reconstructions must be considered. As an example, 1000 plausible models of the NPC were reported in [4326]. Interestingly, averaging the positions of all balls of a particular protein type across these models resulted in 30 so-called *probability density maps*, each such map encoding the probability of presence of a particular protein type at a particular location in the NPC. Second, the assessment of all models (individual and averaged) is non trivial. In particular, the lack of straightforward statistical analysis of the individual models and the absence of assessment for the averaged models are detrimental to the mechanistic exploitation of the reconstruction results. At this stage, such models therefore remain qualitative.

3.4. Modeling the Flexibility of Macro-molecules

Keywords: Folding, docking, energy landscapes, induced fit, molecular dynamics, conformers, conformer ensembles, point clouds, reconstruction, shape learning, Morse theory.

Proteins in vivo vibrate at various frequencies: high frequencies correspond to small amplitude deformations of chemical bonds, while low frequencies characterize more global deformations. This flexibility contributes to the entropy thus the free energy of the system *protein - solvent*. From the experimental standpoint, NMR studies generate ensembles of conformations, called *conformers*, and so do molecular dynamics (MD) simulations. Of particular interest while investigating flexibility is the notion of correlated motion. Intuitively, when a protein is folded, all atomic movements must be correlated, a constraint which gets alleviated when the protein unfolds since the steric constraints get relaxed³. Understanding correlations is of special interest to predict the folding pathway that leads a protein towards its native state. A similar discussion holds for the case of partners within a complex, for example in the third step of the *diffusion - conformer selection - induced fit* complex formation model.

Parameterizing these correlated motions, describing the corresponding energy landscapes, as well as handling collections of conformations pose challenging algorithmic problems.

At the side-chain level, the question of improving rotamer libraries is still of interest [4332]. This question is essentially a clustering problem in the parameter space describing the side-chains conformations.

At the atomic level, flexibility is essentially investigated resorting to methods based on a classical potential energy (molecular dynamics), and (inverse) kinematics. A molecular dynamics simulation provides a point cloud sampling the conformational landscape of the molecular system investigated, as each step in the simulation corresponds to one point in the parameter space describing the system (the conformational space) [4347]. The standard methodology to analyze such a point cloud consists of resorting to normal modes. Recently, though, more elaborate methods resorting to more local analysis [4343], to Morse theory [4338] and to analysis of meta-stable states of time series [4339] have been proposed.

3.5. Algorithmic Foundations

Keywords: Computational geometry, computational topology, optimization, data analysis.

Making a stride towards a better understanding of the biophysical questions discussed in the previous sections requires various methodological developments, which we briefly discuss now.

3.5.1. Modeling interfaces and contacts

In modeling interfaces and contacts, one may favor geometric or topological information.

On the geometric side, the problem of modeling contacts at the atomic level is tantamount to encoding multi-body relations between an atom and its neighbors. On the one hand, one may use an encoding of neighborhoods based on geometric constructions such as Voronoi diagrams (affine or curved) or arrangements of balls. On the other hand, one may resort to clustering strategies in higher dimensional spaces, as the p neighbors of a given atom are represented by $3p - 6$ degrees of freedom —the neighborhood being invariant upon rigid motions. The information gathered while modeling contacts can further be integrated into interface models.

On the topological side, one may favor constructions which remain stable if each atom in a structure *retains* the same neighbors, even though the 3D positions of these neighbors change to some extent. This process is observed in flexible docking cases, and call for the development of methods to encode and compare shapes undergoing tame geometric deformations.

3.5.2. Modeling macro-molecular assemblies

In dealing with large assemblies, a number of methodological developments are called for.

³Assuming local forces are prominent, which in turn subsumes electrostatic interactions are not prominent.

On the experimental side, of particular interest is the disambiguation of proteomics signals. For example, TAP and mass spectrometry data call for the development of combinatorial algorithms aiming at unraveling pairwise contacts between proteins within an assembly. Likewise, density maps coming from electron microscopy, which are often of intermediate resolution (5-10Å) call the development of noise resilient segmentation and interpretation algorithms. The results produced by such algorithms can further be used to guide the docking of high resolutions crystal structures into maps.

As for modeling, two classes of developments are particularly stimulating. The first one is concerned with the design of algorithms performing reconstruction by data integration, a process reminiscent from non convex optimization. The second one encompasses assessment methods, in order to single out the reconstructions which best comply with the experimental data. For that endeavor, the development of geometric and topological models accommodating uncertainties is particularly important.

3.5.3. Modeling the flexibility of macro-molecules

Given a sampling on an energy landscape, a number of fundamental issues actually arise: how does the point cloud describe the topography of the energy landscape (a question reminiscent from Morse theory)? Can one infer the effective number of degrees of freedom of the system over the simulation, and is this number varying? Answers to these questions would be of major interest to refine our understanding of folding and docking, with applications to the prediction of structural properties. It should be noted in passing that such questions are probably related to modeling phase transitions in statistical physics where geometric and topological methods are being used [4342].

From an algorithmic standpoint, such questions are reminiscent of *shape learning*. Given a collection of samples on an (unknown) *model*, *learning* consists of guessing the model from the samples —the result of this process may be called the *reconstruction*. In doing so, two types of guarantees are sought: topologically speaking, the reconstruction and the model should (ideally!) be isotopic; geometrically speaking, their Hausdorff distance should be small. Motivated by applications in Computer Aided Geometric Design, surface reconstruction triggered a major activity in the Computational Geometry community over the past ten years [5]. Aside from applications, reconstruction raises a number of deep issues: the study of distance functions to the model and to the samples, and their comparison; the study of Morse-like constructions stemming from distance functions to points; the analysis of topological invariants of the model and the samples, and their comparison.

3.6. LaTeX Test Page

Exemples d'équations :

- Equation en mode “mathématique” :
 $y = x^2$
- Equation en environnement “equation” :

$$P \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_r \end{pmatrix} = Q + R, \quad (1)$$

- Equation en environnement “displaymath” :

$$\sum_0^{\infty} y = x^4$$

- Autre exemple :

$$\forall f \in C^\infty \left(\left[-\frac{T}{2}; \frac{T}{2} \right] \right), \forall t \in \left[-\frac{T}{2}; \frac{T}{2} \right], f(\tau) = \sum_{k=-\infty}^{+\infty} e^{2i\pi \frac{k}{T} t} \times \underbrace{\frac{1}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} f(t) e^{-2i\pi \frac{k}{T} t} dt}_{a_k = \tilde{f}\left(\nu = \frac{k}{T}\right)}$$

Exemple de caractères spéciaux :

math pi : π

lettres : æ Æ à À â Â ä Ä ç Ç é É è È ê Ê ë Ë î Î ï Ï ô Ô ö Ö ù Û û Ü ü Þ ð

Exemples d'images :

- Image en jpeg : voir image 2

Figure 2. An example of a jpeg image

- Image en eps : voir figure 3

Figure 3. An example of an eps file

- Image en pdf : voir image 4

Figure 4. An example of a pdf file

4. Application Domains

4.1. Domain 1

5. New Software and Platforms

5.1. Software

This section briefly comments on all the software distributed by ABS . On the one hand, the software released in 2013 is briefly described as the context is presented in the sections dedicated to new results. On the other hand, the software made available before 2013 is briefly specified in terms of applications targeted.

In any case, the website advertising a given software also makes related publications available.

5.1.1. *addict: Stoichiometry Determination from Mass Spectrometry Data*

Participants: Deepesh Agarwal, Frédéric Cazals, Noël Malod-Dognin.

Context. Given the individual masses of the proteins present in a complex, together with the mass of that complex, *stoichiometry determination* (SD) consists of computing how many copies of each protein are needed to account for the overall mass of the complex. Our work on the stoichiometry determination (SD) problem for noisy data in structural proteomics is described in []. The `addict` software suite not only implements our algorithms `DP++` and `DIOPHANTINE`, but also important algorithms to determine the so-called Frobenius number of a vector of protein masses, and also to estimate the number of solutions of a SD problem, from an unbounded knapsack problem.

Distribution. Binaries for the `addict` software suite are made available from <http://team.inria.fr/abs/software/addict/>.

5.1.2. *vorpatch and compatch: Modeling and Comparing Protein Binding Patches*

Participants: Frédéric Cazals, Noël Malod-Dognin.

Context. Modeling protein binding patches, i.e. the sets of atoms responsible of an interaction, is a central problem to foster our understanding of the stability and of the specificity of macro-molecular interactions. We developed a binding patch model which encodes morphological properties, allows an atomic-level comparison of binding patches at the geometric and topological levels, and allows estimating binding affinities—with state-of-the-art results on the protein complexes of the binding affinity benchmark. Given a binary protein complex, `vorpatch` identifies the binding patches, and computes a topological encoding of each patch, defined as an *atom shelling tree* generalizing the core-rim model. The program `compatch` allows comparing two patches via the comparison of their atom shelling trees, by favoring either a geometric or a topological comparison.

Distribution. Binaries for `VORPATCH` and `COMPATCH` are available from <http://team.inria.fr/abs/software/vorpatch-compatch>.

5.1.3. *voratom: Modeling Protein Assemblies with Toleranced Models*

Participants: Frédéric Cazals, Tom Dreyfus.

Context. Large protein assemblies such as the Nuclear Pore Complex (NPC), chaperonin cavities, the proteasome or ATP synthases, to name a few, are key to numerous biological functions. Modeling such assemblies is especially challenging due to their plasticity (the proteins involved may change along the cell cycle), their size, and also the flexibility of the sub-units. To cope with these difficulties, a reconstruction strategy known as Reconstruction by Data Integration (RDI), aims at integrating diverse experimental data. But the uncertainties on the input data yield equally uncertain reconstructed models, calling for quantitative assessment strategies.

To leverage these reconstruction results, we introduced Toleranced Model (TOM) framework, which inherently accommodates uncertainties on the shape and position of proteins represented as density maps — maps from cryo electron-microscopy or maps stemming from reconstruction by data integration. In a TOM, a fuzzy molecule is sandwiched between two union of concentric balls, the size of the region between these two unions conveying information on the uncertainties.

The corresponding software package, `VORATOM`, includes programs to (i) perform the segmentation of (probability) density maps, (ii) construct toleranced models, (iii) explore toleranced models (geometrically and topologically), (iv) compute Maximal Common Induced Sub-graphs (MCIS) and Maximal Common Edge Sub-graphs (MCES) to assess the pairwise contacts encoded in a TOM.

Distribution. Binaries for the software package `VORATOM` are made available from <http://team.inria.fr/abs/software/voratom/>.

5.1.4. *intervor: Modeling Macro-molecular Interfaces*

Participant: Frédéric Cazals.

In collaboration with S. Lorient (The GEOMETRY FACTORY)

Context. Modeling the interfaces of macro-molecular complexes is key to improve our understanding of the stability and specificity of such interactions. We proposed a simple parameter-free model for macro-molecular interfaces, which enables a multi-scale investigation—from the atomic scale to the whole interface scale. Our interface model improves the state-of-the-art to (i) identify interface atoms, (ii) define interface patches, (iii) assess the interface curvature, (iv) investigate correlations between the interface geometry and water dynamics / conservation patterns / polarity of residues.

Distribution. The following website <http://team.inria.fr/abs/software/intervor> serves two purposes: on the one hand, calculations can be run from the website; on the other hand, binaries are made available. To the best of our knowledge, this software is the only publicly available one for analyzing Voronoi interfaces in macro-molecular complexes.

5.1.5. *vorlume: Computing Molecular Surfaces and Volumes with Certificates*

Participant: Frédéric Cazals.

In collaboration with S. Loriot (The GEOMETRY FACTORY, France)

Context. Molecular surfaces and volumes are paramount to molecular modeling, with applications to electrostatic and energy calculations, interface modeling, scoring and model evaluation, pocket and cavity detection, etc. However, for molecular models represented by collections of balls (Van der Waals and solvent accessible models), such calculations are challenging in particular regarding numerics. Because all available programs are overlooking numerical issues, which in particular prevents them from qualifying the accuracy of the results returned, we developed the first certified algorithm, called `vorlume`. This program is based on so-called certified predicates to guarantee the branching operations of the program, as well as interval arithmetic to return an interval certified to contain the exact value of each statistic of interest—in particular the exact surface area and the exact volume of the molecular model processed.

Distribution. Binaries for `Vorlume` is available from <http://team.inria.fr/abs/software/vorlume>.

5.1.6. *ESBTL: the Easy Structural Biology Template Library*

Participant: Frédéric Cazals.

In collaboration with S. Loriot (The GEOMETRY FACTORY, France) and J. Bernauer (Inria AMIB, France).

Context. The ESBTL (Easy Structural Biology Template Library) is a lightweight C++ library that allows the handling of PDB data and provides a data structure suitable for geometric constructions and analyses, such as those proposed by `INTERVOR`, `VORPATCH` and `COMPATCH`.

Distribution. The C++ source code is available from <http://esbtl.sourceforge.net/http://esbtl.sourceforge.net/>.

5.2. Platforms

5.2.1. Platform A

...

5.2.2. Platform B

...

6. New Results

6.1. Highlights of the Year

6.2. New result 1

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Contracts with Industry

7.2. Bilateral Grants with Industry

8. Partnerships and Cooperations

8.1. Regional Initiatives

...

8.2. National Initiatives

8.2.1. *Projets Exploratoires Pluridisciplinaires from CNRS/Inria/INSERM*

Title: Modeling Large Protein Assemblies with Toleranced Models

Type: Projet Exploratoire Pluri-disciplinaire (PEPS) CNRS / Inria / INSERM

Duration: two years

Coordinator: F. Cazals (Inria, ABS)

Others partners: V.Doye (Inst. Jacques Monod)

Abstract: Reconstruction by Data Integration (RDI) is an emerging paradigm to reconstruct large protein assemblies, as discussed in section [5.1.3](#).

Elaborating on our Toleranced Models framework, a geometric framework aiming at inherently accommodating uncertainties on the shapes and positions of proteins within large assemblies, we ambition within the scope of the two year long PEPS project entitled *Modeling Large Protein Assemblies with Toleranced Models* to (i) design TOM compatible with the flexibility of proteins, (ii) develop graph-based analysis of TOM, and (iii) perform experimental validations on the NPC.

8.3. European Initiatives

8.3.1. *FP7 & H2020 Projects*

8.3.2. *Collaborations in European Programs, except FP7 & H2020*

8.3.3. *Collaborations with Major European Organizations*

8.4. International Initiatives

8.4.1. *Inria International Labs*

8.4.2. *Inria Associate Teams*

8.4.3. Inria International Partners

8.4.3.1. *Declared Inria International Partners*

8.4.3.2. *Informal International Partners*

8.4.4. Participation In other International Programs

8.5. International Research Visitors

8.5.1. Visits of International Scientists

8.5.1.1. *Internships*

8.5.2. Visits to International Teams

8.5.2.1. *Sabbatical programme*

8.5.2.2. *Explorer programme*

8.5.2.3. *Research stays abroad*

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific events organisation

9.1.1.1. *general chair, scientific chair*

9.1.1.2. *member of the organizing committee*

9.1.2. Scientific events selection

9.1.2.1. *responsible of the conference program committee*

9.1.2.2. *member of the conference program committee*

9.1.2.3. *reviewer*

9.1.3. Journal

9.1.3.1. *member of the editorial board*

9.1.3.2. *reviewer*

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

E-learning

Mooc, SPOC, etc. : Enseignant ou auteur, titre du cours, durée en nombre de semaine, plate-forme, établissement porteur du cours, public ciblé, formation initiale ou continue, nombre d'inscrits

Pedagogical resources : enseignant, titre, type (video, pdf, exercice, ou autre), niveau, url

9.2.2. Supervision

9.2.3. Juries

9.3. Popularization

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