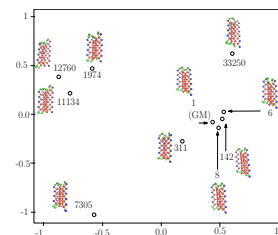


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POST-DOC POSITION PROPOSAL

MODELING ENERGY LANDSCAPES, WITH APPLICATIONS IN BIOPHYSICS

Context. The Algorithms-Biology-Structure project-team develops a synergy at the interface between Computer Science and Biophysics. Three themes are explored, namely (I) Modeling protein complexes (atomic level models of complexes and their interfaces, models for large biological assemblies), (II) Modeling macromolecular flexibility (modeling energy landscapes, designing collective coordinates), and (III) Algorithmic foundations (computational geometry and topology, data analysis). The developments undertaken are accompanied by high standards software developments, made available to the community. This post-doc falls in the realm of the second topic.

Goals. Protein functions are often associated with large amplitude - low frequency conformational changes, since such changes allow them to switch between active and inactive conformations. From a modeling perspective, predicting such changes requires two steps [Wal03, SJ09]. The first one is the exploration of the energy landscape of the system scrutinized, for which various Monte Carlo and molecular dynamics based methods have been developed. The second one, given a collection of conformations and/or critical points generated by a sampling method, consists in modeling kinetic and thermodynamic properties [BRM⁺10, RZMC11].

The goal of this post-doc will be to extend recent work on the problem on modeling energy landscapes [CDM⁺15, CM15], to improve sampling algorithms as well as collective coordinates designs. Validations will be carried out on simplified protein models, and on flexible antibody - antigen complexes.

Background. PhD in Biophysics (computational or experimental) with good background in computer science or applied mathematics, or PhD in Computer science (algorithms) or applied mathematics with interests in biophysics / chemistry.

Duration. 12 months, extensible to 24 months.

Gross salary. 2621 euros / month.

Constraint and timeline. The PhD thesis must have been defended in 2014 or before the recruitment date. The position will start in the fall of 2015.

Applying. From <http://www.inria.fr/en/institute/recruitment/offers/post-doctoral-research-fellowships/post-doctoral-research-fellowships/campaign-2015>, find the topic MODELING ENERGY LANDSCAPES AND APPLICATIONS IN BIOPHYSICS.

References

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