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S E M I N A I R E

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"Using the contact map in the MARTINI and Elastic Network models to study large conformation changes in proteins"

We combine the contact map with two different popular coarse-grained models for proteins, namely the MATINI force-field and the Elastic Network (EN) model. Our approach enables the study of systems involving large conformation transitions in proteins, for example, folding and thermal unfolding, and stretching. In the case of the MARTINI force-field for proteins, we substitute the ELNEDIN approach with the contact map based on the overlap criterion and rCSU contacts.[1] In the case of the EN model, residues within a certain cutoff form harmonic bonds as in the standard EN model, while contacts at a larger distance interact by means of a harmonic approximation of a Lennard—Jones (LJ) potential or (LJ) interactions based on the contact map as in standard Go models.[2] We anticipate that our work will provide new venues in a broader range of problems involving large conformation changes of proteins.

[1] A. B. Poma, M. Cieplak, P.E. Theodorakis, J. Chem. Theory Comput. 13, 1366 (2017)
[2] A. B. Poma, P. E. Theodorakis (under review)

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Salle des conférences