



SCUOLA
NORMALE
SUPERIORE

SEMINARIO DI MATEMATICA

Giovedì 5 novembre 2020
ore 14:30

Scuola Normale Superiore
Pisa

Laurent Vuillon
(*Università di Savoie Mont Blanc*)

Terrà un seminario dal titolo:

“Data science for protein structures and molecular dynamics”

Abstract:

In this talk, we investigate the structure of proteins by considering the network associated with the adjacent amino acids according to a given cutoff. This network allows us to understand the protein structures and to study interfaces in polymers. We also use a dynamical version of these networks to study the allosteric paths in proteins. Indeed, elucidation of the allosteric pathways in proteins is a computational challenge that strongly benefits from combination of atomistic molecular dynamics (MD) simulations and coarse-grained analysis of the complex dynamical network of chemical interactions based on graph theory. Here, we introduce and assess the performances of the dynamical perturbation network analysis of allosteric pathways in a prototypical V-type allosteric enzyme. Dynamical atomic contacts obtained from MD simulations are used to weight the allosteric protein graph, which involves an extended network of contacts perturbed by the effector binding in the allosteric site. The outcome showed good agreement with previously reported theoretical and experimental extended studies and it provided recognition of new potential allosteric spots that can be exploited in future mutagenesis experiments. Overall, the dynamical perturbation network analysis proved to be a powerful computational tool, complementary to other network-based approaches that can assist the full exploitation of allosteric phenomena for advances in protein engineering and rational drug design.

Meet: 5 novembre 14:30, <https://meet.google.com/jby-iuhu-bmy>