ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

DIPARTIMENTO
DI FARMACIA
E BIOTECNOLOGIE

AVVISO DI SEMINARIO

Il giorno **23 Gennaio 2025**
alle ore **10:00**

Dr. Riccardo Capelli

Assistant Professor, Department of Biosciences, University of Milan
(ospite di Prof. Francesco Musiani)

terrà un seminario in lingua inglese dal titolo:

Multi-eGO: a structure-based framework for molecular simulations

Area tematica:
Computational biophysics

in presenza:
Aula 1, Via Belmeloro 6, Bologna BO

e in streaming:
https://teams.microsoft.com/l/meetup-join/19%3aN09c0NIyEssBnF7ObCyDOQwkgDWm1qdd9f7F2nJV9fw1%40thread.tacv2/1631519544944?context=%7b%22Tid%22%3a%22e99647dc-1b08-454a-bf8c-699181b389ab%22%2c%22Oid%22%3a%225a941351-ef41-4aa4-8771-fa50a6d62ca1%22%7d

Colleghi e studenti sono cordialmente invitati

ABSTRACT

Efficient and accurate molecular simulations remain a key challenge in computational structural biology. Recently, we introduced multi-eGO, a hybrid structure-based approach that addresses this need by integrating information from classical molecular dynamics (MD) simulations into a simplified potential via a Bayesian approach. This combination results in a versatile framework that maintains atomic resolution while reducing computational cost.

In this seminar, I will present the broad potential of multi-eGO for modeling diverse biomolecular processes. Using examples ranging from ligand binding and protein folding to self-assembly, I will illustrate how our framework achieves an effective balance between speed and accuracy. I will also discuss ongoing refinements that extend its applicability to a wide range of systems, including well-structured proteins and intrinsically disordered peptides, opening up avenues previously inaccessible to conventional MD methods. In doing so, multi-eGO advances the use of structure-based frameworks and brings us closer to a realistic computational microscope.

BIOGRAPHICAL SKETCH

Dr. Riccardo Capelli is an assistant professor in Applied Physics at the Department of Biosciences, University of Milan. He earned his PhD in Physics at the same university, focusing on in silico structural vaccinology and advancing free energy calculation techniques. He then held a postdoctoral position at Forschungszentrum Jülich in Germany, where he worked on calculating ligand binding kinetics using classical molecular dynamics (MD). This was followed by a postdoctoral role at the Polytechnic University of Turin, where he developed coarse-grained models for self-assembling systems. Now in a tenure-track position, his research spans the development of computational methods such as structure-based models and enhanced sampling techniques, as well as their application to biomolecular systems, mainly on G Protein-Coupled Receptors activation and dynamics.