UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Modelling and simulation of complex macromolecular systems, in the age of machine learning

2223-113R-12

Title

Modelling and simulation of complex macromolecular systems, in the age of machine learning

Teacher(s)

Prof. Pietro Faccioli

Language

English

Short description

COURSE OBJECTIVES:
The problem of understanding the structural dynamics of macromolecular systems provides an ideal framework to develop and validate new paradigms for advanced multi-scale computing. In this short graduate-level course, I will discuss how the integration of advanced statistical mechanics techniques with machine learning algorithms and (very recently) quantum computing hardware is opening new research avenues in this field, paving the way to accurately simulating

complex transitions with an unprecedented level of accuracy and resolution.
STRUCTURE OF THE COURSE
The course consists in a set of 8 two-hour lectures intended to cover concepts in advanced statistical mechanics and theory of stochastic processes, embedded in the framework of molecular simulation of rare macromolecular transitions
PREREQUISITES:
A background in equilibrium statistical mechanics and basic (undergraduate level) quantum mechanics will be assumed.
SYLLABUS:

- LECT 1: Macromolecules as complex systems: classical and quantum degrees of freedom, frustration, metastability, and multi-scale rare event problems.
- LECT 2: Stochastic dynamics of macromolecules: Langevin equation and Fokker-Plank Equation
- LECT 3: Renormalizing the Stochastic Dynamics: Markov State modelling
- LECT 4: Stochastic path integrals and their applications to macromolecular systems. Statistical mechanics of transition paths
- LECT 5: Machine learning based enhanced sampling methods.
- LECT 6: Machine learning schemes for data reduction and intrinsic manifold exploration
- LECT 7: Introduction to quantum annealing and QUBO
- LECT 8: Quantum encoding and quantum computing of paradigmatically hard statistical mechanical problems

CFU / Hours

2 CFU / 16 hours

Teaching period

March

Sustainable Development Goals