Two PhD positions in the framework of the H2020 ERC StG project VARIAMOLS

The University of Trento opens the call for position for the 33rd Cycle (Academic Year 2017/2018) of the Phd Programme in Physics jointly run with the National Institute for Nuclear Physics (INFN - Italy), within the project H2020-ERC StG 2017 VARIAMOLS (VAriable ResolutIon Algorithms for macroMOLecular Simulation-758588) reserved for the two topics described hereafter. The admission to the 3-year PhD Programme is by selection; research and training activities include attendance of courses and seminars. More information can be found on the project webpage https://sites.google.com/view/variamols.

PhD project A - Method development for protein modeling and simulation

The candidate will develop computational methods to study *in silico* large proteins and protein assemblies. The project aims at the design, implementation and usage of algorithms to model and efficiently simulate a biomolecule, and substantially involves scientific programming, modification and usage of existing software (in particular simulation suites e.g. LAMMPS), and AI applications (deep neural networks).
Mandatory prerequisites: solid background in statistical mechanics; proficiency in scientific programming (C, C++, Python) and competence in the usage of Unix-based systems.
Optional skills: experience in neural networks / deep neural networks (theory as well as software implementation); experience in molecular dynamics simulations and related software (GROMACS, NAMD, LAMMPS, etc.); basic knowledge of biophysics (molecular biophysics in particular). Basic knowledge of coarse-graining techniques.

PhD project B - Protein structure and function-oriented dynamics

The candidate will carry out a study focussing on the relationship between a protein's structure and its function-oriented dynamics. The project will require and extensive usage of bioinformatic tools and atomistic molecular dynamics simulations.
Mandatory prerequisites: good knowledge of molecular dynamics simulations and related software (GROMACS, NAMD, LAMMPS, etc.); basic to good knowledge of biophysics (molecular biophysics in particular); basic background in statistical mechanics.
Optional skills: proficiency in scientific programming (C, C++, Python) and competence in the usage of Unix-based systems; experience with bioinformatic tools (protein structure databases, sequence/structure alignment software, etc.).

Project overview

Within the broad spectrum of biological soft matter systems, large proteins and protein assemblies occupy a central role. These molecules are extremely versatile: they can catalyze chemical reactions, transport atoms and molecules across the cellular membrane, bind to foreign bodies to be destroyed, or combine into large molecular machines that perform a variety of different tasks. One of the most prominent problems in the computational study of these macromolecules is that the cost of using accurate atomistic models dramatically increases with system size. Simplified, coarse-grained representations offer an elegant and effective alternative to high-resolution models, and enable the simulation of large systems over extended time scales; the other side of the coin, however, is that the missing chemical detail often represents an insurmountable limitation to the realistic reproduction of the properties of interest.

The main goal of the VARIAMOLS project is to develop and apply novel computer-aided methods for the study of large molecular assemblies and their dynamics, thus bridging the existing gap between computational cost and chemical accuracy. Specifically, the research will unfold along two intertwined lines: 1) the development of non-uniform resolution models of the system, which optimize the balance between detail and efficiency; and 2) the study of dynamics-mediated properties of protein assemblies. The working philosophy of VARIAMOLS has two complementary and strictly interconnected aspects: on the one hand, the theoretical and algorithmic advancement of the methods currently employed to represent and simulate biomolecules; on the other hand, the systematic application of the developed methods to real-life case studies of great relevance for medical science and technology, with a particular focus on viruses and antibodies.