CeNT CENTRE OF NEW TECHNOLOGIES

UNIVERSITY OF WARSAW

invites to a seminar by

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On Some Aspects Of Computational Predictions Of Protein Structure and Organization

9th October 2017 at 10:00 a.m.

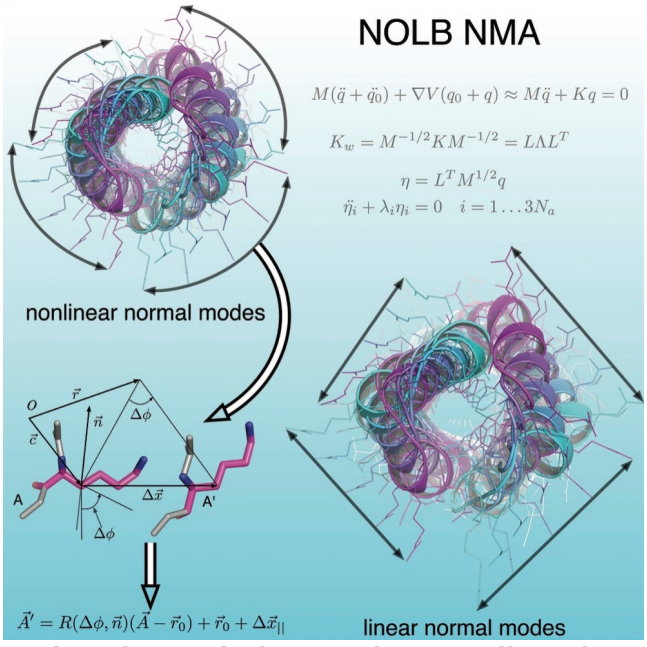
Venue: Centre of New Technologies, Banacha 2C,
Seminar room 4050 (4th floor)

Host: Ass. Prof. Joanna I. Sułkowska

In my talk I will cover two aspects of protein structure and organization, their symmetrical assemblies and their intrinsic flexibility.

First, I will present the method of symmetrical protein assembling and for the symmetry detection. Large symmetrical protein structures have evolved in many organisms because they carry specific morphological and functional advantages compared to small individual protein molecules. There is therefore considerable interest in studying and modelling the structures of these large bio-molecular complexes. I will talk about a novel ab-initio protein docking algorithm for protein complexes with arbitrary point group symmetry and report on a very fast analytical method for the analysis of symmetric protein assemblies.

In the second part of my talk, I will present Normal mode analysis (NMA), a well–established technique that is able to compute low-frequency motions which are commonly assumed to give insight into protein function, dynamics and conformational transitions. I will present a new conceptually simple and computationally efficient method for nonlinear normal mode analysis called NOLB. It relies on the rotations-translations of blocks (RTB) theoretical basis developed by Y.-H. Sanejouand and colleagues.



Overall, the NOLB method produces better structures compared to the standard approach, especially at large deformation amplitudes. Also, the NOLB method is scalable and can be applied to very large molecular systems, such as ribosomes. Further, I will show a computational scheme that uses the NOLB modes as a low-dimensional representation of the protein motion subspace and optimizes protein structures guided by the small-angle X-ray scattering (SAXS) profiles. I will demonstrate an interactive graphical user interface created in the SAMSON software platform (https://www.samson-connect.net), where a user can activate a combination of modes with different phases or apply these to opening the binding pockets. Finally, I will present some application of NMA for protein-protein docking and Cryo-EM fitting.