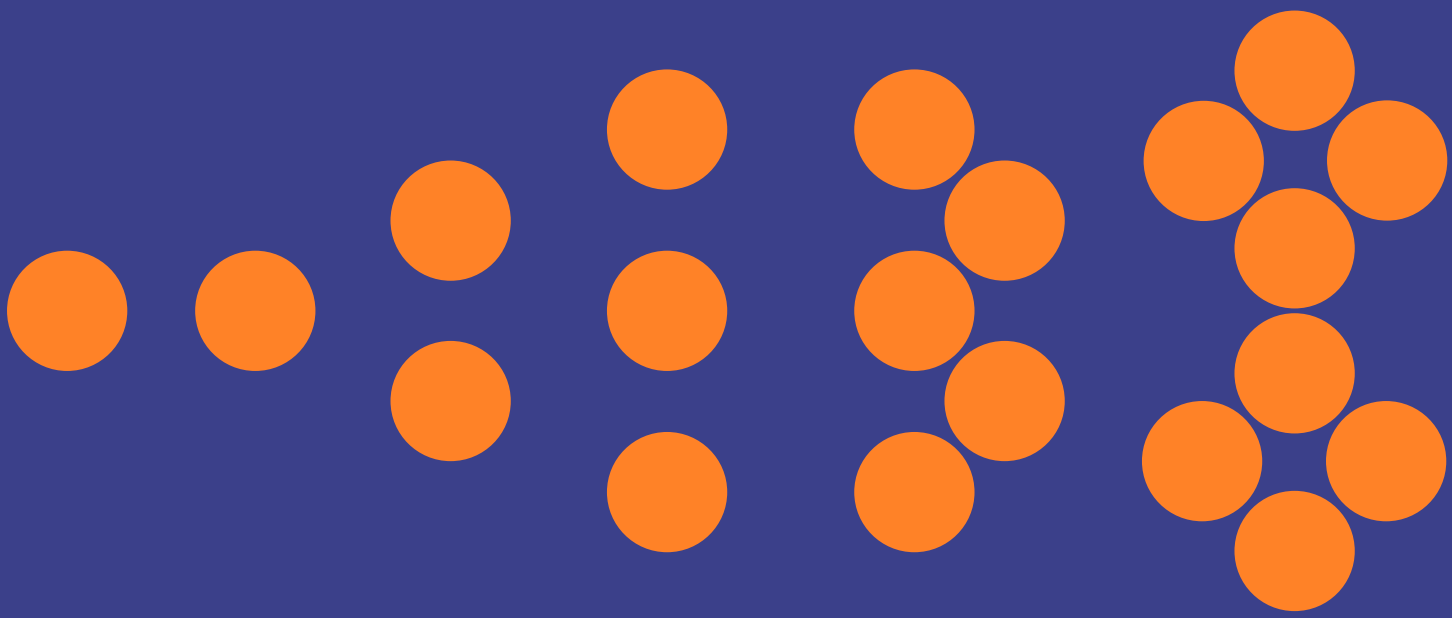
Statistical and Biological Physics group seminar

ARCTIC-3D: Automatic Retrieval and ClusTering of Interfaces in Complexes from 3D structural information

Speaker: Dr. Marco Giulini, Utrecht University

December 20, 2022 – 2:30 pm

Room A203 – Via Sommarive 5 – Povo (TN)



Abstract

The formation of a stable complex between two proteins lies at the core of a wide variety of biological processes, ranging from signal transduction to RNA translation. It is in this context that the enormous amount of structural information contained in the protein structural interactome can be employed to characterise and classify the existing biological interfaces. However, it is not immediate nor trivial to make sense of this information in an automatic procedure. We here propose a novel tool for the Automatic Retrieval and ClusTering of Interfaces in Complexes from 3D structural information - ARCTIC-3D, a fast and user-friendly data-mining software to gather the interface information associated with various kinds of protein input data, the latter being a sequence, a uniprot ID or a three-dimensional structure. The software automatically queries the PDBe SIFTS graph database and analyses and clusters the retrieved information, thus creating separated classes of interfaces, which are markedly different from a structural perspective. As an application example, we use ARCTIC-3D in the context of information-driven modelling of biomolecular complexes: For several candidate proteins from the Docking Benchmark 5 we automatically collect interface information, which is then fed into our docking software, HADDOCK. ARCTIC-3D is freely available as a standalone python3 package (https://github.com/haddocking/arctic3d).

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