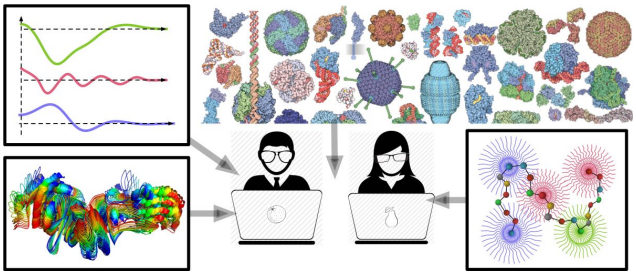

Contribution ID: **45** Type: **Talk**

Integrative modeling meets deep learning: applications to crosslinking mass spectrometry

Monday, 12 February 2024 13:40 (25 minutes)

Recent progress in protein structure prediction significantly enhanced integrative structure modeling of large macromolecular assemblies by providing improved structural coverage for individual proteins and protein-protein interactions. However, direct prediction of large protein assemblies remains a challenge. I will introduce CombFold, a hierarchical and combinatorial assembly algorithm designed to predict structures of large protein complexes utilizing pairwise interactions between subunits predicted by AlphaFold2. Distance restraints based on cross-linking mass spectrometry can be directly integrated into the assembly algorithm, further improving the accuracy. To optimize the integration of information from cross-linking experiments, we propose a deep-learning model to predict the optimal distance range for crosslinked residue pairs based on their structural neighborhoods. Despite the availability of high-throughput approaches for identifying protein-protein interactions and crosslinks in whole-cell crosslinking experiments, applying integrative modeling to these datasets poses challenges. One major obstacle is the need for methods to decipher temporal and spatial composition and stoichiometry of the cellular assemblies.

Submitting to:

Integrative Computational Biology workshop

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