



Contribution ID: 3

Type: **Talk**

Hybrid methods for analyzing conformational variability in cryo-EM and cryo-ET data

Monday, 12 February 2024 17:30 (25 minutes)

The elucidation of different conformations of biomolecular complexes is the key to understand the molecular mechanisms behind the biological functions of the complexes and the key to novel drug discovery. Single-particle cryo electron microscopy (cryo-EM) allows 3D reconstruction of multiple conformations of purified biomolecular complexes from their 2D images. Cryo electron tomography (cryo-ET) allows obtaining information on the conformational variability of the complexes in their cellular environment. My group is developing hybrid methods for analyzing continuous conformational changes of biomolecules from cryo-EM and cryo-ET data, which integrate image processing, molecular dynamics simulations, and deep learning approaches. These methods are made available publicly via our open-source, ContinuousFlex software package (a plugin of Scipion, the software largely used in the cryo-EM/ET field). In this talk, I will present our recent work regarding these methodological developments.

Submitting to:

Integrative Computational Biology workshop

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Session Classification: Computational Methods and Deep Learning