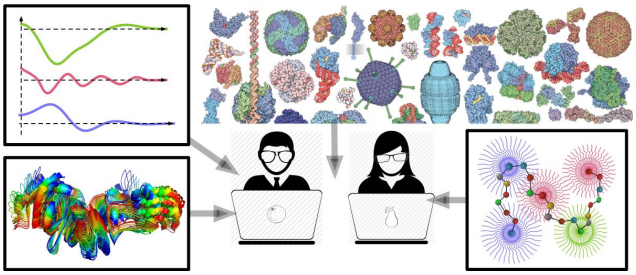

Contribution ID: **27** Type: **Talk**

Spectral partitioning into protein structural domains

Tuesday, 13 February 2024 09:00 (25 minutes)

The decomposition of a biomolecular complex into domains is an important step to investigate biological functions, and is also relevant to ease structure determination. A successful approach to do so is the SPECTRUS algorithm, which provides a segmentation based on spectral clustering applied to a graph coding inter-atomic fluctuations derived from an elastic network model. We present a simplification and an extension of SPECTRUS, both straightforward and useful.
For single structures, we show that high quality partitioning can be obtained from a graph Laplacian derived from pairwise interactions, without the use of normal modes. For sets of homologous structures, we introduce a Multiple Sequence Alignment mode, exploiting both the sequence based information (MSA) and the geometric information embodied in experimental structures.
The algorithm compares favorably with the original SPECTRUS as well as state-of-the-art deep approaches such as Chainsaw.

Submitting to:

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