# Graph-based analysis and visualization of structural topologies of MD simulation data

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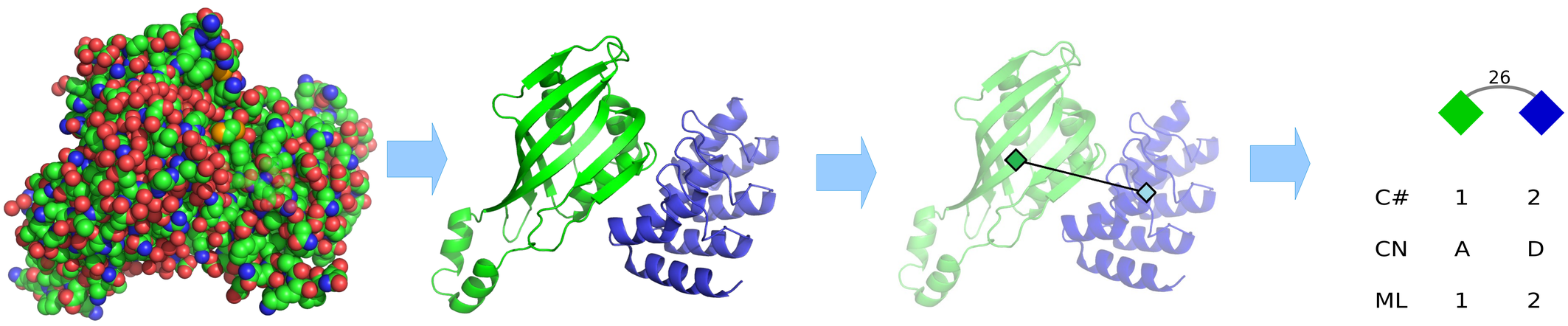
**Molecular dynamics (MD) simulations yield atom coordinates for multiple time steps. These snapshots can reach in order up to thousands. We developed a automated pipeline to investigate topological changes in MD simulation data with our Protein Topology Graph Library (PTGL) [1-3]. In PTGL, protein structures are modeled as undirected graphs indicating topological arrangements of protein chains in Complex Graphs (CGs). First, we compute CGs for different time steps of the MD simulation. Second, we compare edge topology and edge weights. Third, we compare observable changes in the CGs with the structure. We could observe changes of Complex I in the CGs.**

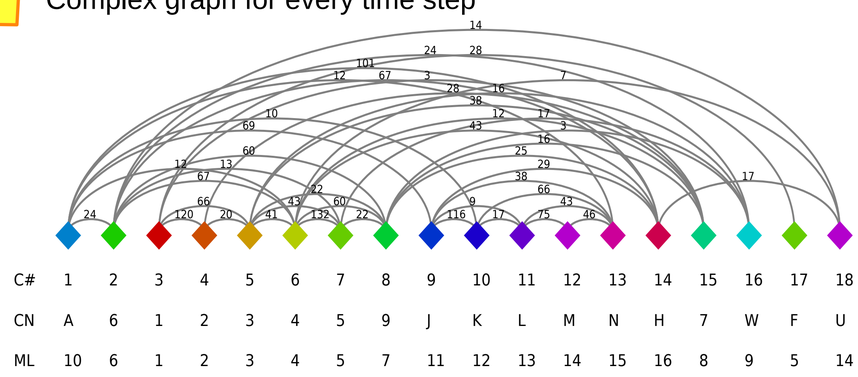
## Methods



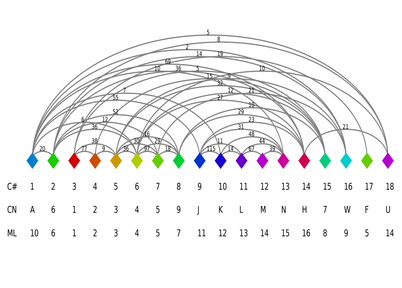

## Results

**2.** Complex graph for every time step

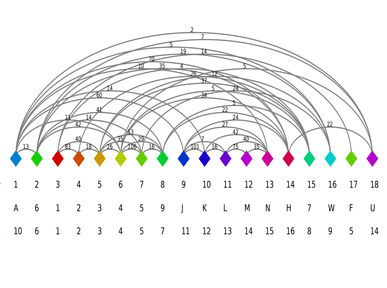
1 ns



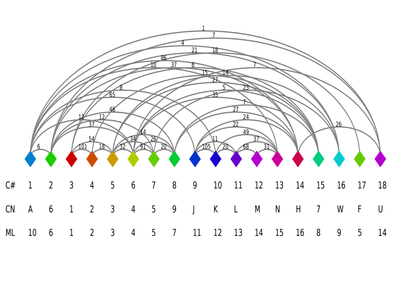

667 ns



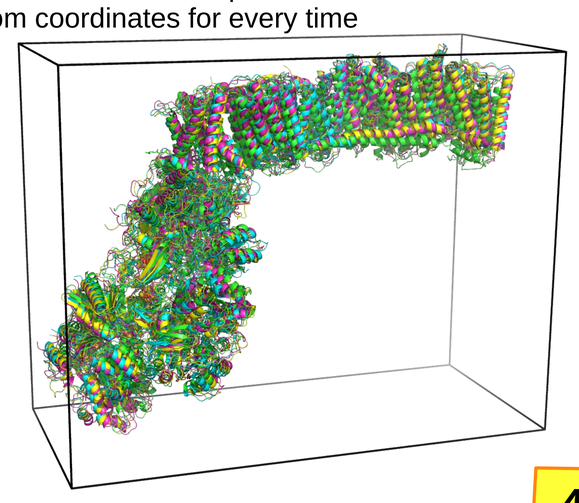
1334 ns



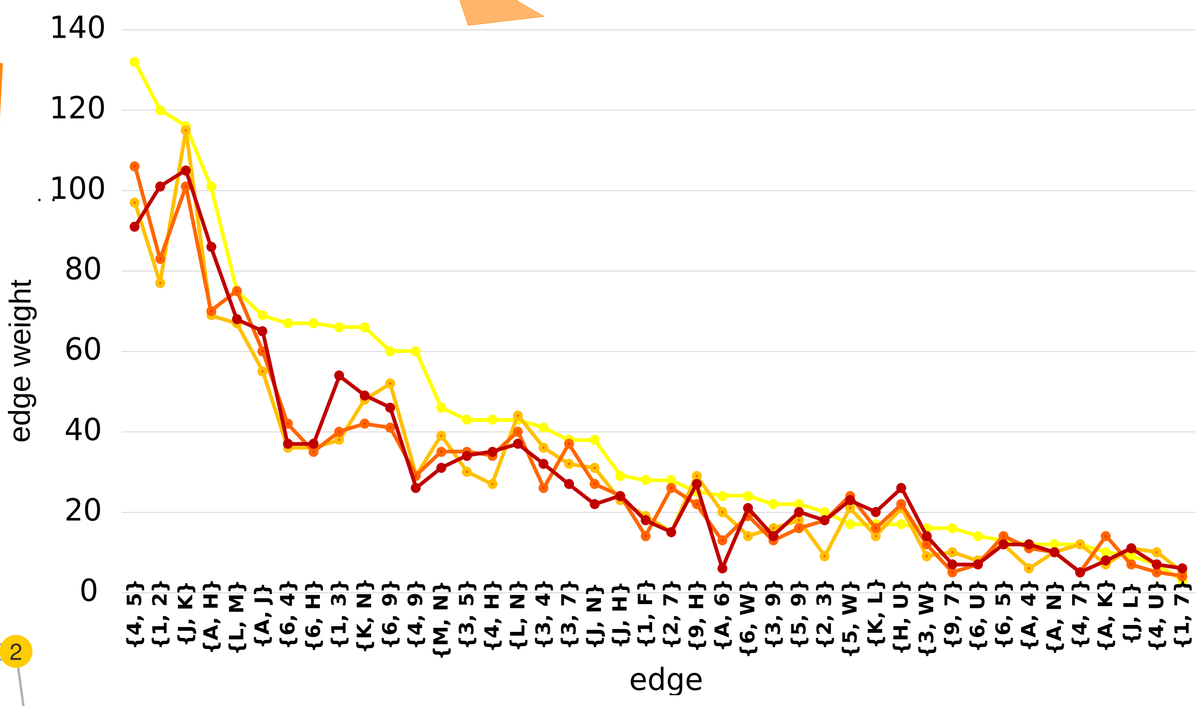
2000 ns



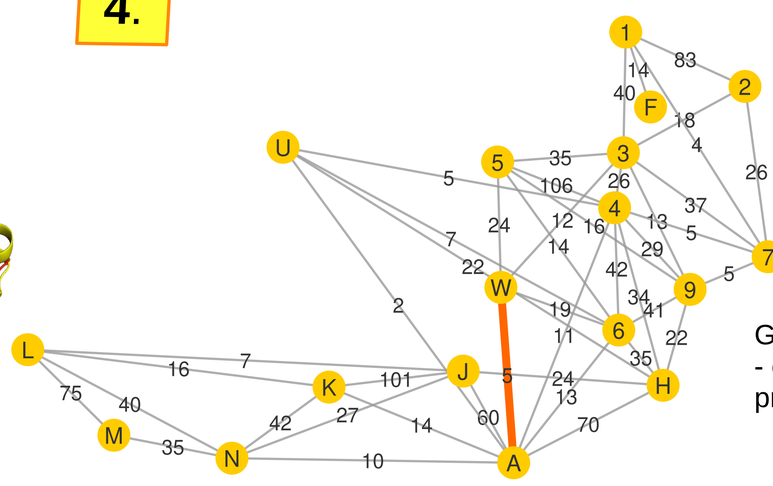
**1.** MD Simulation of Complex I
- atom coordinates for every time step



**3.**

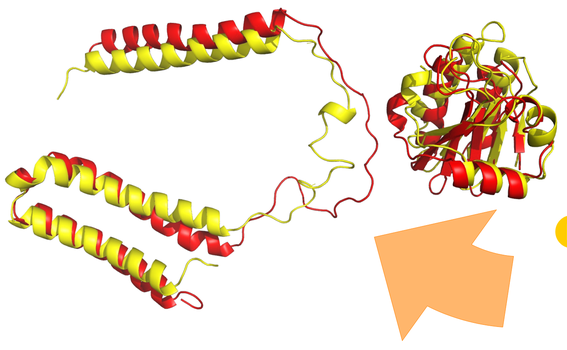



**4.**




Graph of 1334 ns
- orange edge not present in 1ns

**5.**
- yellow structure 1ns
- red structure 1334 ns



## Conclusion

- Fast detection of changes of simulated structures
- Automated analysis of MD simulation data
- Complex graph enables analysis of large protein complexes
- Extension of the pipeline for different abstraction levels is possible

Protein topology graph library:
http://ptgl.uni-frankfurt.de/

Source code:
https://github.com/dfsp-spirit/vplg

**References**

[1] J. N. Wolf, M. Kreßler, J. Ackermann and I. Koch, PTGL: extension to graph-based topologies of cryo-EM data for large protein structures. Bioinformatics, 2020.

[2] T. Schäfer, A. Scheck, D. Bruneß, P. Patrick and I. Koch. The new protein topology graph library web server. Bioinformatics, 32:474-476, 2016.

[3] I. Koch and T. Schäfer. Protein super-secondary structure topology: theoretical description and application. Current opinion in structural biology, 50:134–144, 2018.