

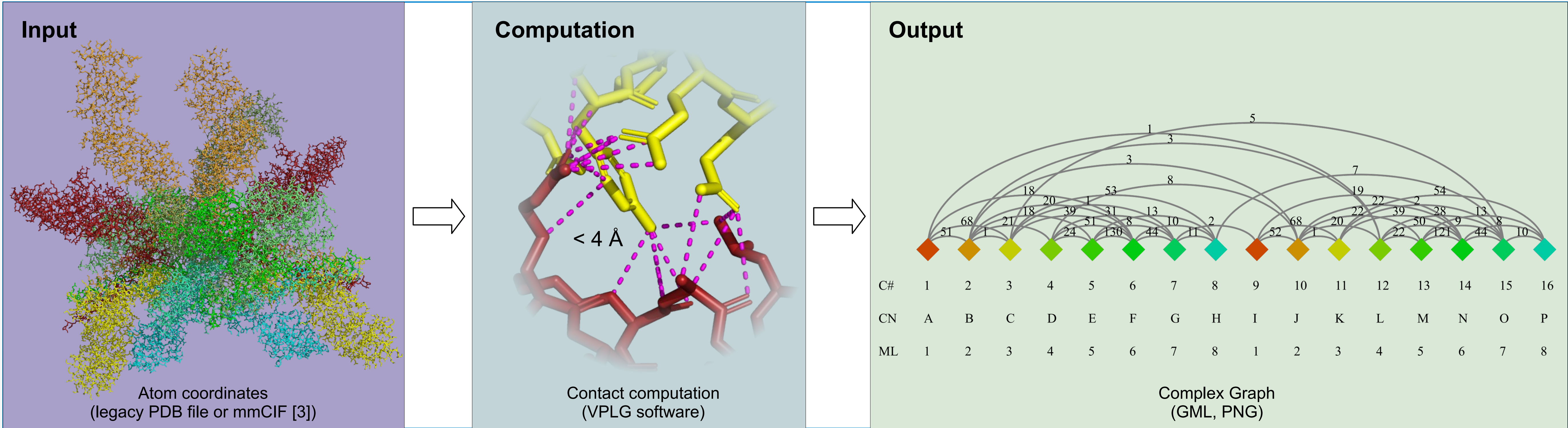
Graph-theoretical analysis of the topology of large protein complexes based on cryo-EM data

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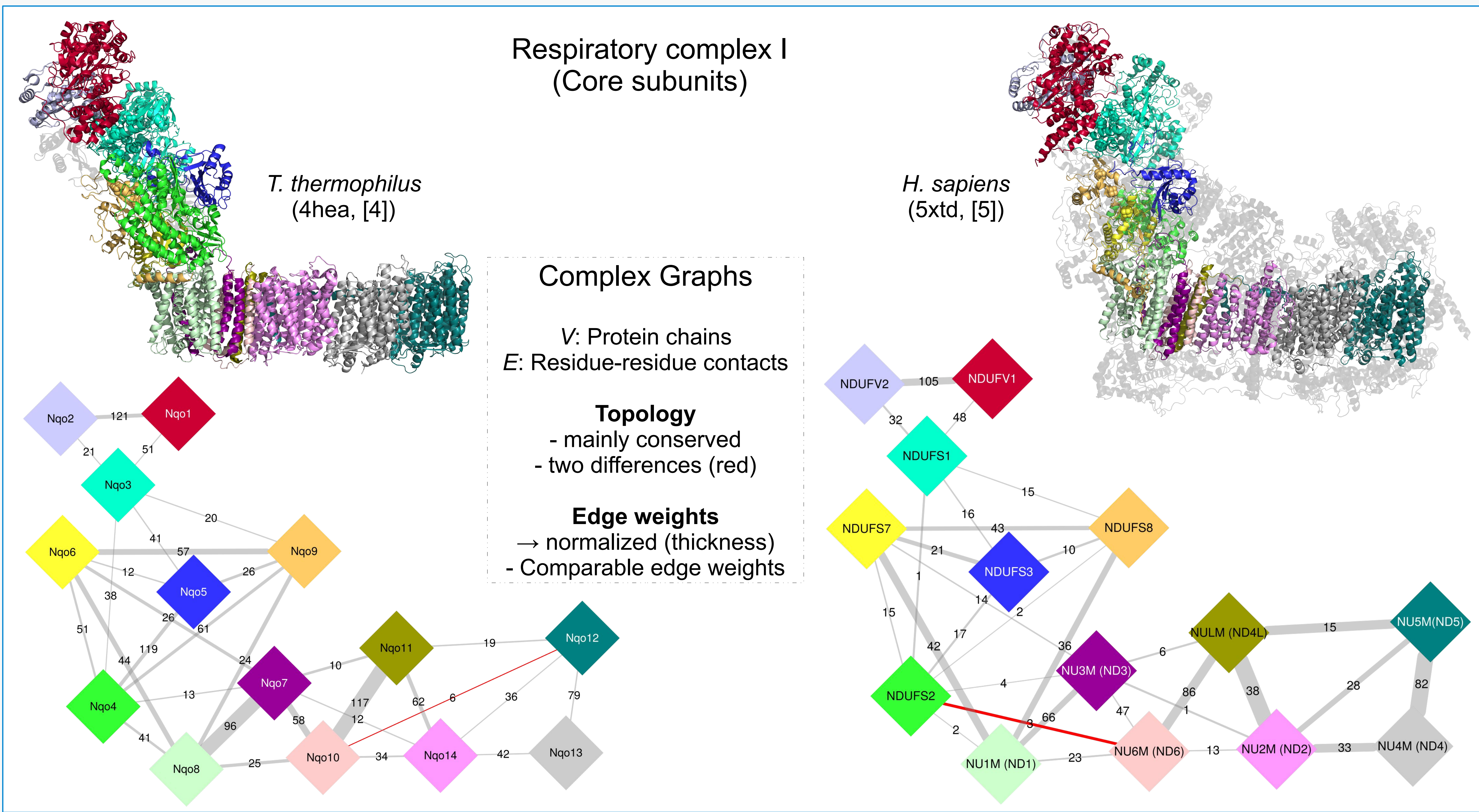
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Proteins often interact with each other by forming complexes. Cryo-EM is capable of resolving the three-dimensional structures of complete complexes. The Protein Data Bank [1] currently stores over 1,200 structures of more than 99,999 atoms or 62 chains (large structures). We abstracted protein complexes to graphs to cope with the large number of data. We defined Complex Graphs depicting the chain topology of a complex. We showed for an example, respiratory complex I, that Complex Graphs enable the comparison of structural topologies between, e.g., different organisms. Our online Protein Topology Graph Library [2,3] stores Complex Graphs of 921 large structures.

Methods

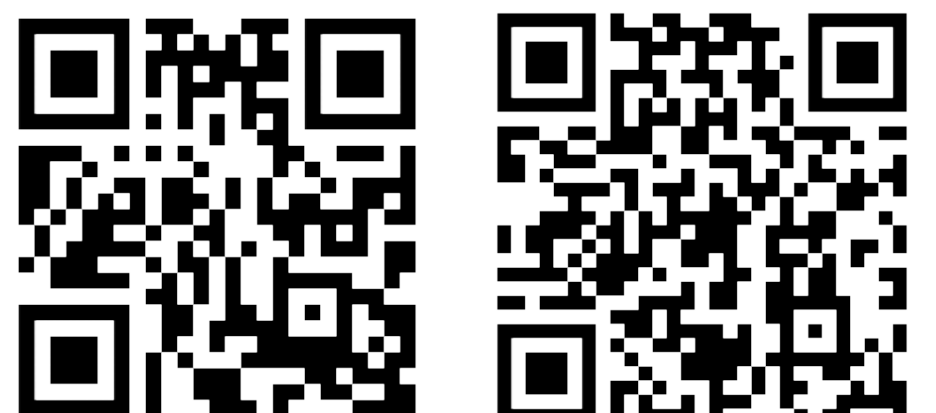


Results



Conclusion

- Model large structures as graphs
- Fast automated computation and analysis
- Identify conserved topologies
- Classification of protein complexes
- Outlook: derive assembly pathway and biological modules from Complex Graphs
- Protein topology graph library <http://ptgl.uni-frankfurt.de>
- Source code <https://github.com/MolBIFFM/vplg>



References

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