Topological feature directed data analysis and visualization

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Context: The SeRC MCP





Topology

- Study of connectivity of space.
 - Continuous deformations.
 - Geometry not considered.





Overview

- Large, complex data generated
 - Simulations
 - Imagining
- Application specific features
- Topology provides robust and efficient methods for feature based analysis





Channels and cavities in biomolecules

Acknowledgements:

- Vijay Natarajan (CSA, IISc)
- Sandhya Sankaran, Nagasuma Chandra (Bio Chem, IISc)



Features of interest



• Molecules given as a set of spheres, $S = \{(p_i, r_i)\}.$





Voronoi diagram

• Given a set of discs, $S = \{(p_i, r_i)\}.$

• Let
$$p \in \mathbb{R}^d$$
, $p_i \in S$, r_i radius of p_i
dist $(p_i, p) = |p - p_i|^2 - r_i^2$





Alpha Complex

• Tracks the changes in topology as the discs are grown in size.

•
$$r_i' = \sqrt{(r_i^2 + \alpha)}$$



Alpha Complex at $\alpha = 0$





Extraction of cavities





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Extraction of channels





Channel extraction pipeline









- Visualization and detailed exploration of channels.
- Comparison of channels.



Identifying and tracking cyclones

Acknowledgements:

- Wito Engelke, Ingrid Hotz (SciVis, LiU)
- Jakob Beran, Rodrigo Cabellaro (Stockholm University)



Cyclone tracking

- Cyclones are regions of deep pressure minima.
 - The threshold is latitude and season dependent.
 - Can be multi-centered.



Time step = 0



Cyclonic features



Time step = 1



Tracked features



Merge tree

- Given a scalar field $s: D \to \mathbb{R}$
- Merge tree tracks the topology of sub level sets.



Scalar field with critical points





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Analysis of electron density fields

Acknowledgements:

- Peter Steneteg, Martin Falk, Ingrid Hotz (SciVis, LiU)
- Elvis Jakobsson, Igor Abrikosov (Physics, LiU)



Analysis of lattice unit cells

- Electron density distribution within a lattice unit cells
 - Analysis
 - Atoms and bonds
 - Comparison





Morse-Smale complex





MS complex driven feature extraction



Input scalar field

Maxima-Saddle-Maxima Paths obtained from Morse-Smale complex Segmentation and connections

Atoms and Bonds



Analysis of lattice unit cells







Comparison of unit cells

MS complex skeleton computed for the two unit cells



Simulation with different input parameters: Two very similar but different unit cells Topology guided comparison of unit cells in "feature space"



Summary

- Complex feature-rich is being generated in various domains.
 - Many times heuristics and ad hoc methods employed.
- Topological methods:
 - Provide abstract representations.
 - Discrete and combinatorial.
 - Ideal for feature extraction, comparison and tracking.
 - Robust and sound mathematical foundations.
- Three use cases:
 - Alpha complex for channels and cavities in biomolecules.
 - Merge trees for cyclone tracking.
 - MS complex for electron density fields.







Thanks!

- Contact: <u>talha.bin.masood@liu.se</u>
- SciVis group at LiU: <u>http://scivis.itn.liu.se/</u>
- Topology Toolkit: <u>https://topology-tool-kit.github.io/</u>

