

What is Topological Data Analysis?

- Context
 - Data
 - On "meshes", or "meshable" things

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What is Topological Data Analysis?

- Context
 - Data
 - On "meshes", or "meshable" things
- Topological data analysis
 - Recover **structures** in data

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Towards a "data map"

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Towards a “data map”



Raw data



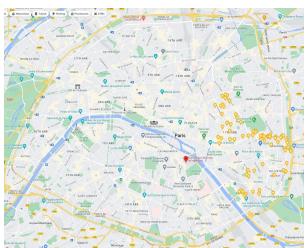
Feature extraction

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Towards a “data map”



Raw data



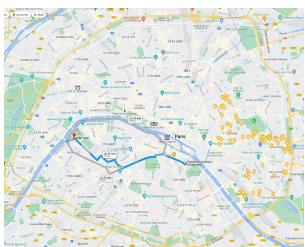
Structural data representation

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Towards a “data map”



Raw data



Structure extraction

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Towards a “data map”



Raw data



Structure extraction & selection

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Towards a “data map”



Raw data



Structure extraction & derived indicator

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Towards a “data map”



Raw data



Structure comparison

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Towards a “data map”



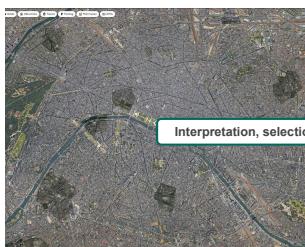
Raw data



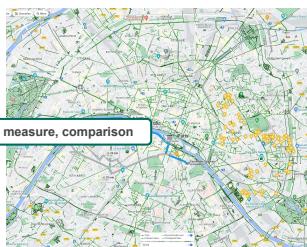
Structure comparison

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Towards a “data map”



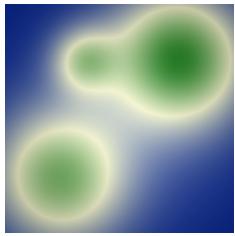
Raw data



Structure comparison

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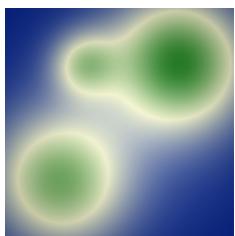
Towards a “data map”



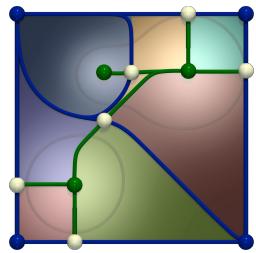
Raw data

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Towards a “data map”



Raw data



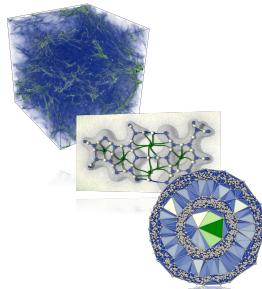
Structural representation

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What is Topological Data Analysis?

- **Context**
 - Data
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- **Topological data analysis**
 - Recover **structures** in data
 - Swiss-army knife
 - Feature extraction
 - Feature comparison

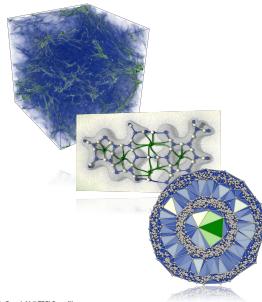


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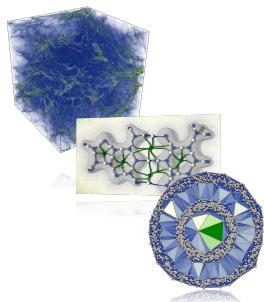
- **Topological data analysis**
 - Recover **structures** in data
 - Swiss-army knife
 - Feature extraction
 - Feature comparison
 - Robust algorithms
 - Combinatorial, multi-scale



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Input data

- Piecewise linear scalar field
 - $f : \mathcal{M} \rightarrow \mathbb{R}$



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Input data

- Piecewise linear scalar field
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 - \mathcal{M} : simplicial complex



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Input data

- Piecewise linear scalar field
 - $f : \mathcal{M} \rightarrow \mathbb{R}$
 - \mathcal{M} : simplicial complex
 - Triangulated surface
 - Tetrahedral volume
 - 2D pixel image
 - 3D voxel image
 - Point cloud data



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Topological abstractions

- Piecewise linear scalar field
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Critical points

- Piecewise linear scalar field
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Critical points

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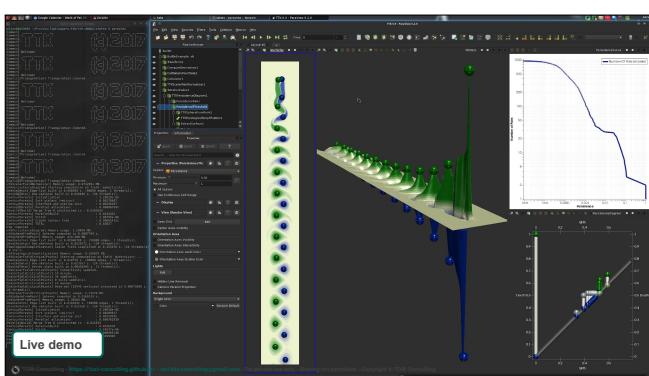
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Critical points

- Local link inspection
 - Banchoff 1970



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Persistence diagram

- Piecewise linear scalar field
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Persistence diagram

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Persistence diagram

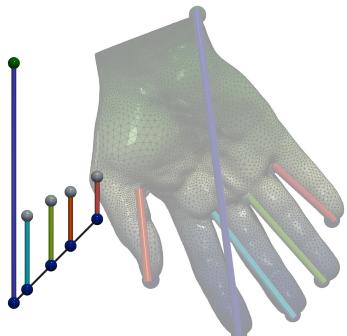
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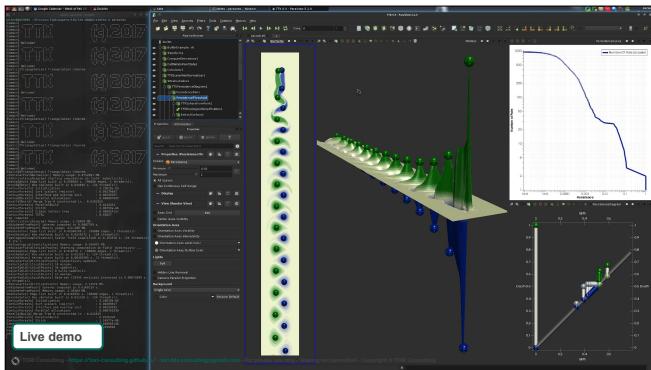
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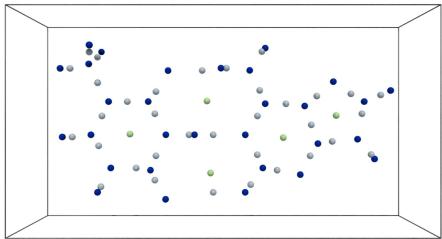


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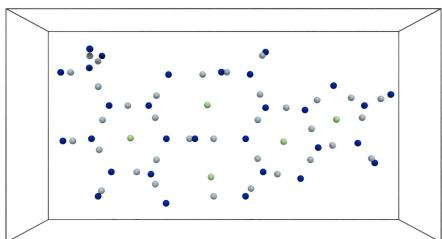
Persistence diagram

- Beyond connected components



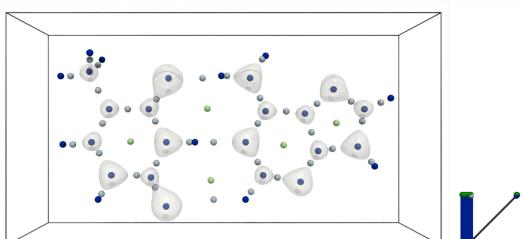
Persistence diagram

- Beyond connected components



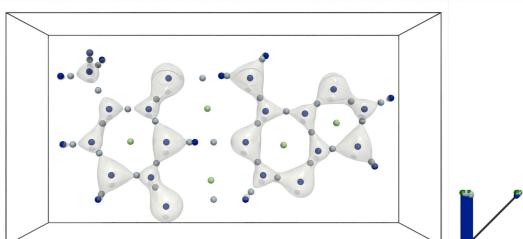
Persistence diagram

- Beyond connected components



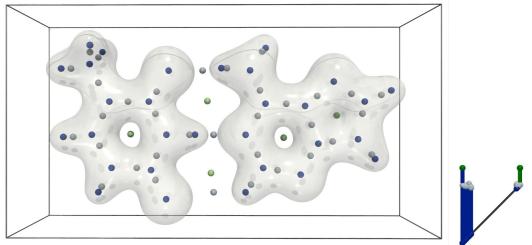
Persistence diagram

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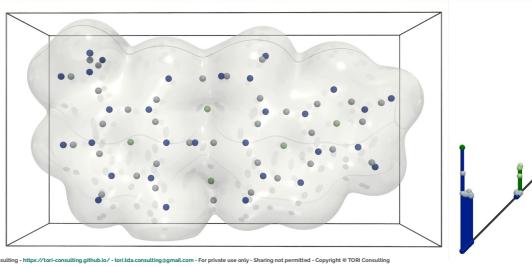
Persistence diagram

- Beyond connected components



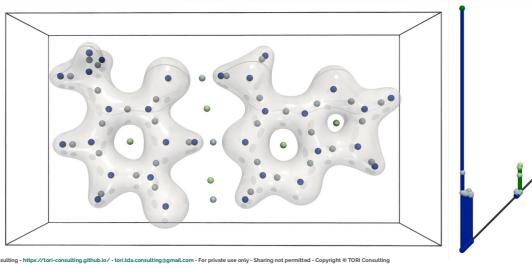
Persistence diagram

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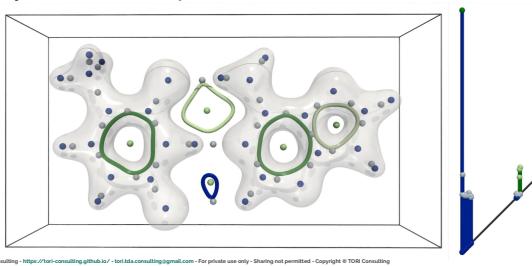
Persistence diagram

- Beyond connected components



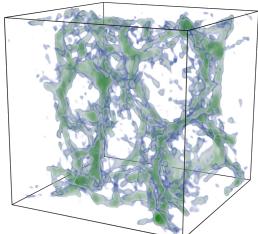
Persistence diagram

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Persistence diagram

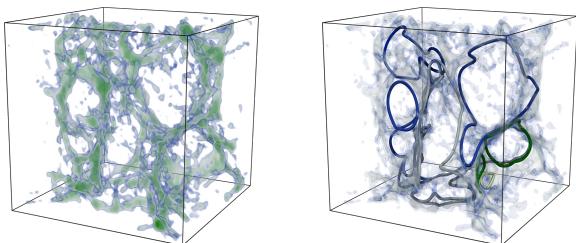
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Persistence diagram

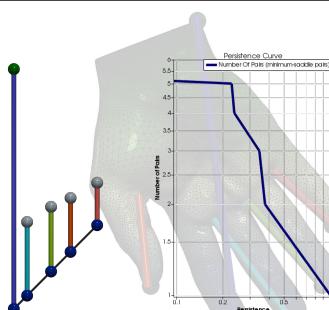
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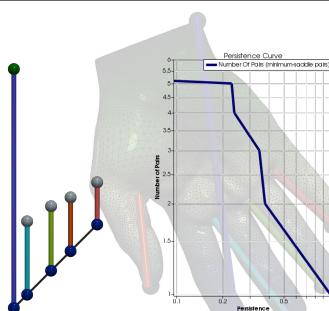
- Piecewise linear scalar field
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Persistence diagram

- Arbitrary dimension
 - Boundary matrix reduction
 - Edelsbrunner et al. 2002

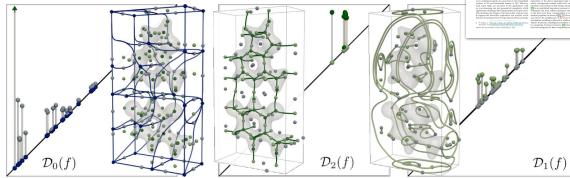


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- Low-dimensions
 - Union-Find data structures
 - Gueunet et al. 2017
 - Discrete Morse Theory
 - Guillou et al. 2023

Persistence diagram

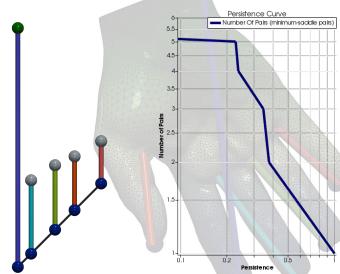
- Latest backend!
 - "Discrete Morse Sandwich"
 - <https://arxiv.org/abs/2206.13932>



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Persistence diagram

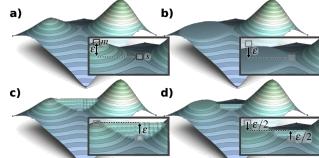
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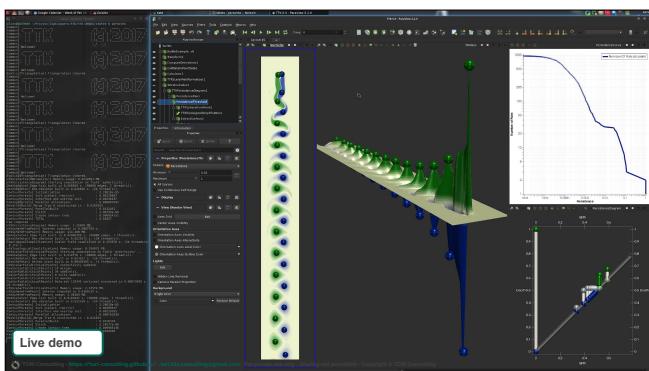
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Persistence simplification

- Simplify the data
 - Retain only persistent features
- Algorithms
 - Edelsbrunner et al. 2006, Attali et al. 2009, Tierny and Pascucci 2012, Bauer et al. 2012, Lukasczyk et al. 2020



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Statistical analysis with persistence diagrams

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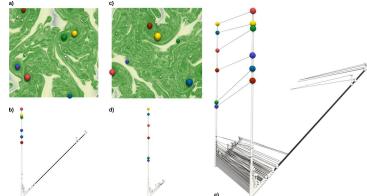
Statistical analysis with persistence diagrams

- Metric
 - Optimal transport
 - Computable, stable
 - Diagram
 - Concise descriptor

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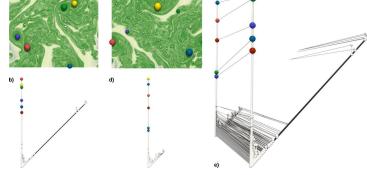


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Statistical analysis with persistence diagrams

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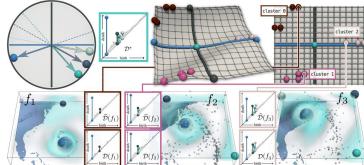
- Statistical tools
 - Geodesics (morphings)
 - Fréchet means (k-means)
 - [Vidal et al. 2019](#)
 - Principal geodesic analysis
 - [Pont et al. 2023](#)



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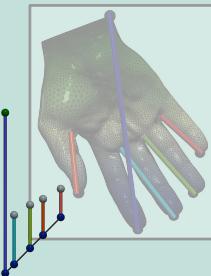


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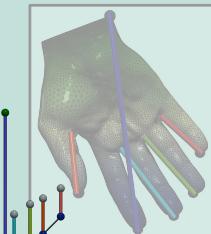
Recap on Persistence diagrams

- What do they encode?
 - Individual topological structures
 - Components
 - Cycles
 - Voids
 - Along with their "importance"



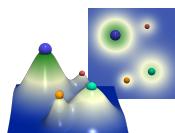
Recap on Persistence diagrams

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Topological abstractions

- Piecewise linear scalar field
 - $f : \mathcal{M} \rightarrow \mathbb{R}$

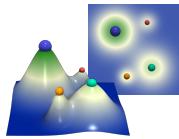


- Topological abstractions
 - Critical points
 - Persistence diagrams
 - Persistence curves

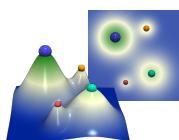
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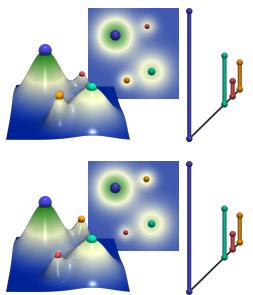
- Topological abstractions
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Topological abstractions

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- Topological abstractions
 - Critical points
 - Persistence diagrams
 - Persistence curves

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Reeb graphs

- Piecewise linear scalar field
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Reeb graphs

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Reeb graphs

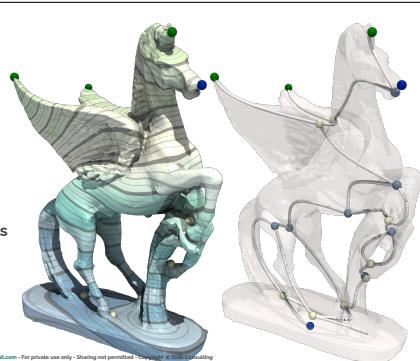
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Reeb graphs

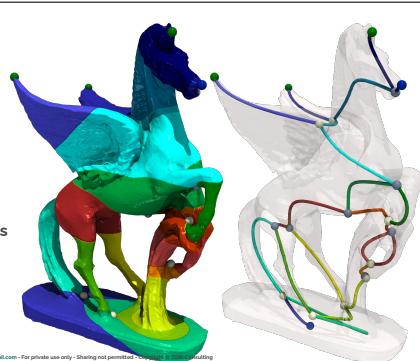
- Piecewise linear data
 - $f : \mathcal{M} \rightarrow \mathbb{R}$



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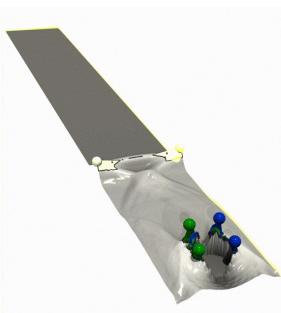
Reeb graphs

- Piecewise linear data
 - $f : \mathcal{M} \rightarrow \mathbb{R}$



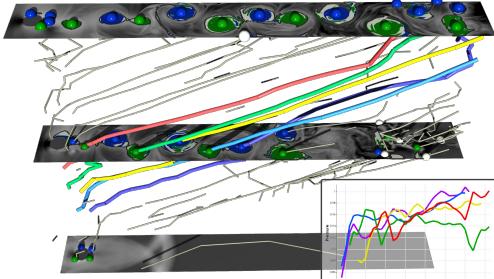
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Vortex extraction

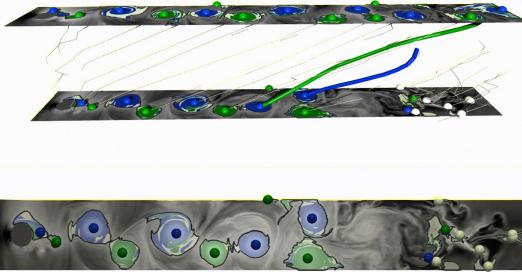


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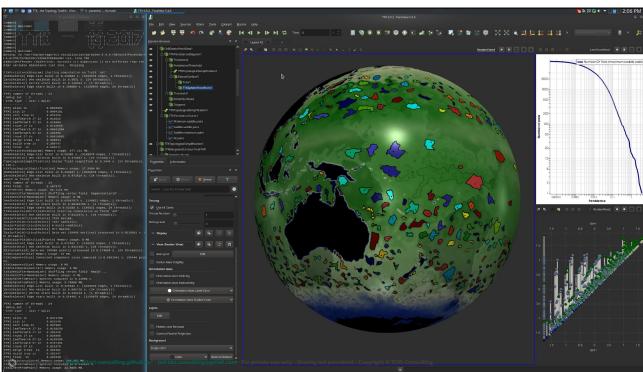
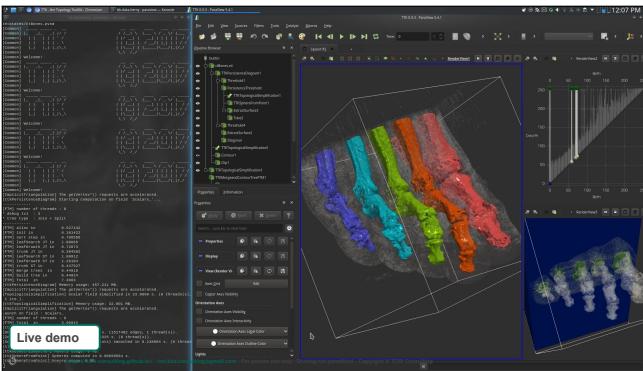
Vortex trajectory analysis



Vortex tracking



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Reeb graphs

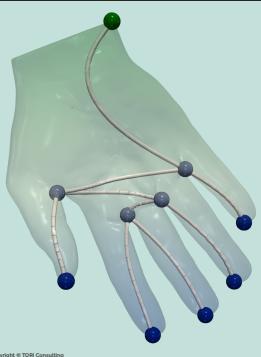
- Vertex based contouring
 - Shinagawa and Kuni 1991
- Quantized range contouring
 - Biasotti et al. 2000, Hilaga et al. 2001, Wood et al. 2004
- Critical contouring
 - Patane et al. 2008, Tierny et al. 2009, Doraiswamy and Natarajan 2013, Hajij and Rosen 2018
- Dynamic connectivity
 - Cole-McLaughlin et al. 2003, Pascucci et al. 2007, Doraiswamy and Natarajan 2009, Parsa 2013, Gueunet et al. 2019



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Recap on Reeb graphs

- What do they encode?
 - Structural skeleton
 - Connectivity of contours



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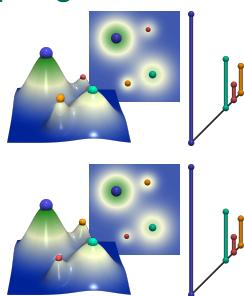
Recap on Reeb graphs

- What do they encode?
 - Structural skeleton
 - Connectivity of contours
- What are they useful for?
 - Skeleton-based signature
 - Regions of influence (e.g. vortices)
 - Structure comparison and statistics
 - Research in progress...

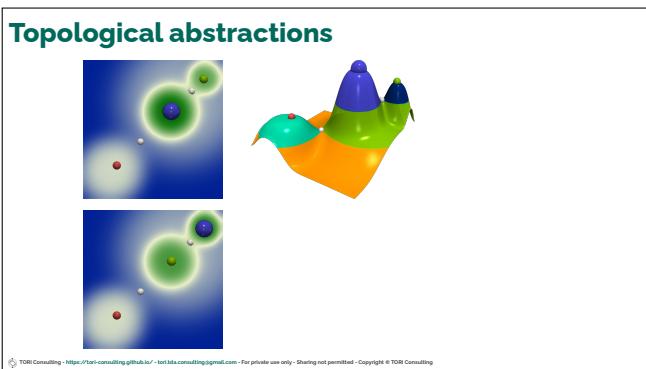
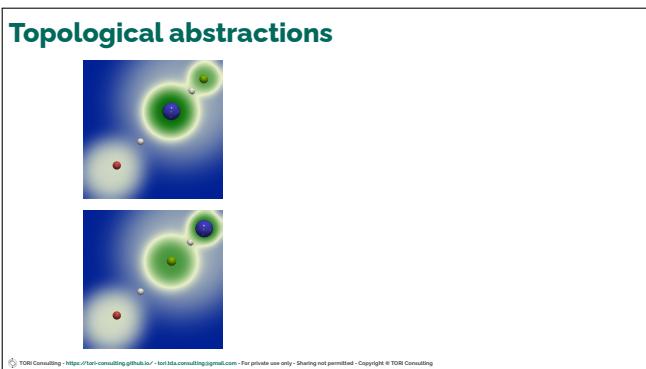
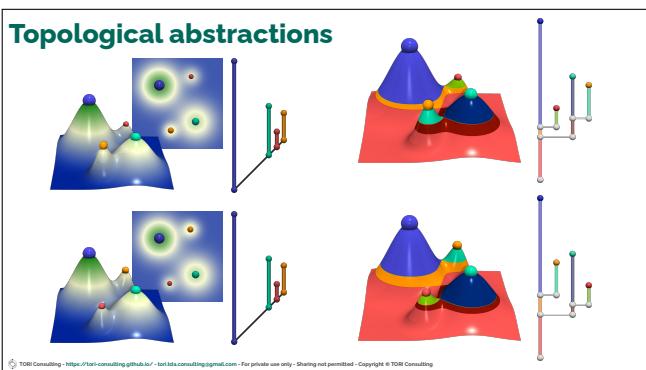
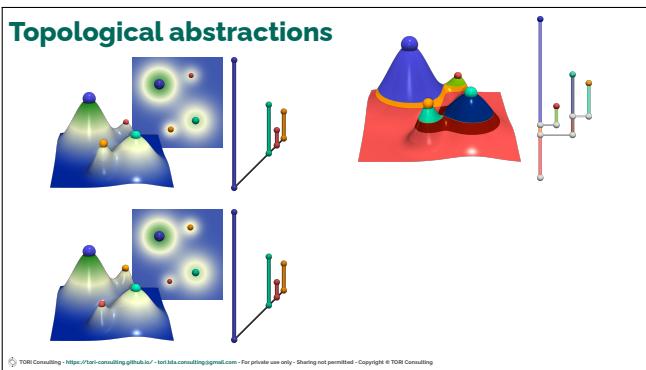


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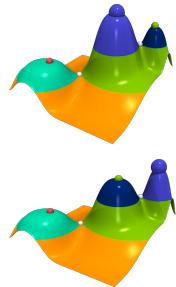
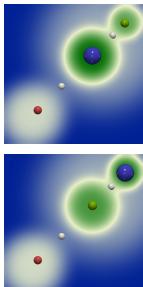
Topological abstractions



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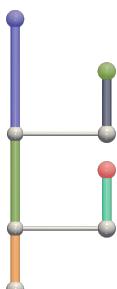
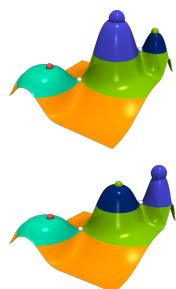
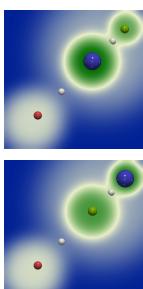


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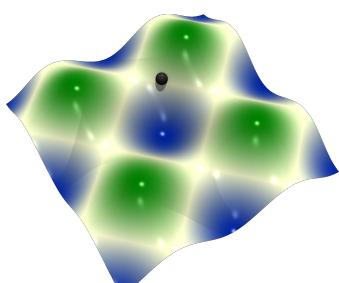
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Morse-Smale complex

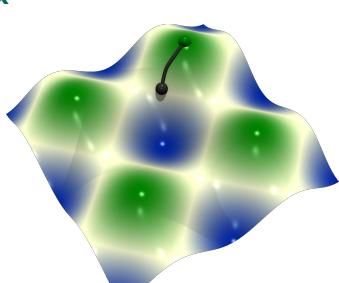
- Key idea
 - Integration equivalence



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Morse-Smale complex

- Key idea
 - Integration equivalence

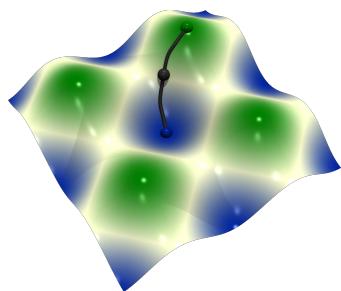


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Morse-Smale complex

- Key idea

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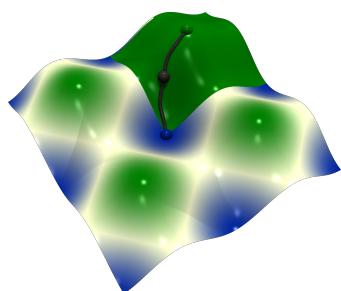


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Morse-Smale complex

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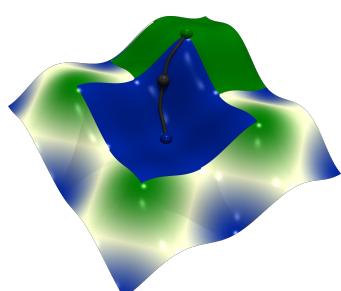


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Morse-Smale complex

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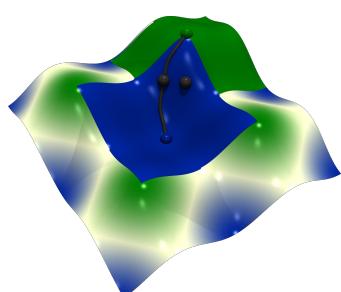


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Morse-Smale complex

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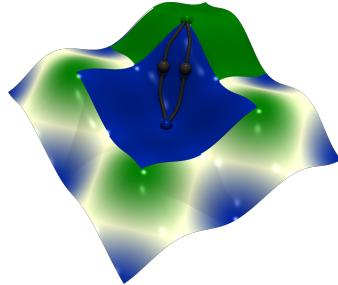


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Morse-Smale complex

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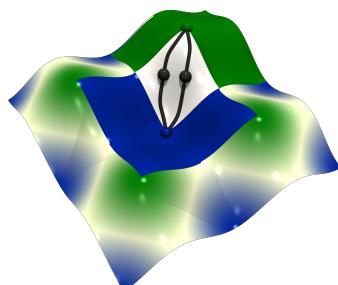


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Morse-Smale complex

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- Integration equivalence

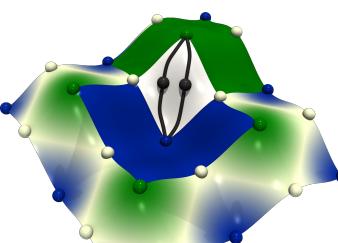


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Morse-Smale complex

- Key idea

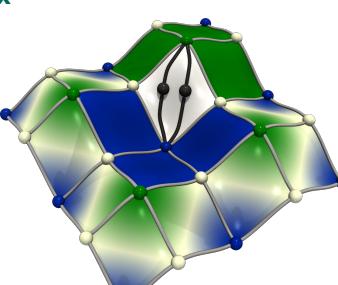
- Integration equivalence



Morse-Smale complex

- Key idea

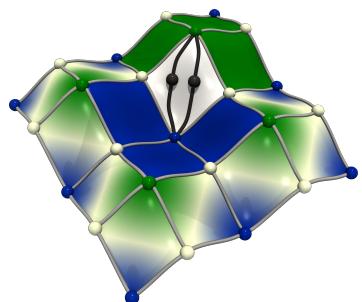
- Integration equivalence



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Morse-Smale complex

- Key idea
 - Integration equivalence
 - Challenging PL computation

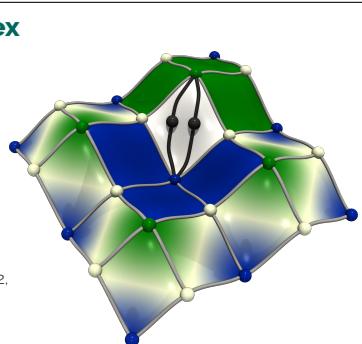


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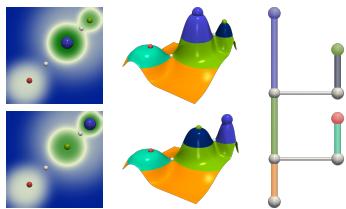
- Key idea
 - Integration equivalence
 - Challenging PL computation

- Discrete Morse theory
 - Forman 1998
 - Algorithms
 - Gyulassy 2008, Robins 2011, Shivashankar and Natarajan 2012, Tierny et al. 2017



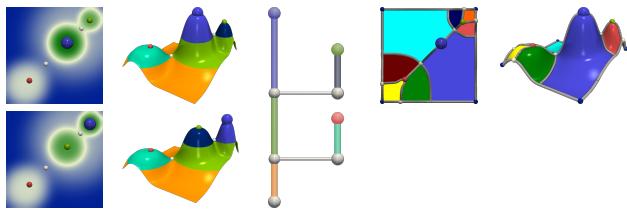
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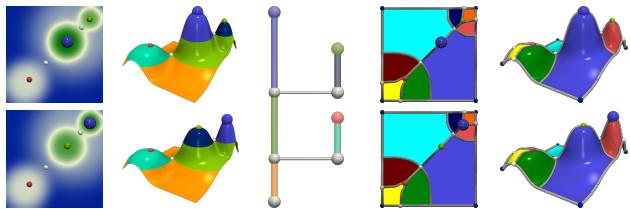
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Topological abstractions

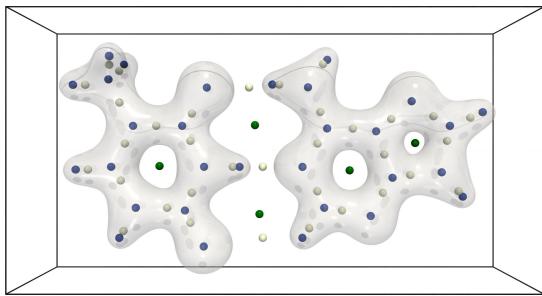


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Applications of the Morse-Smale complex

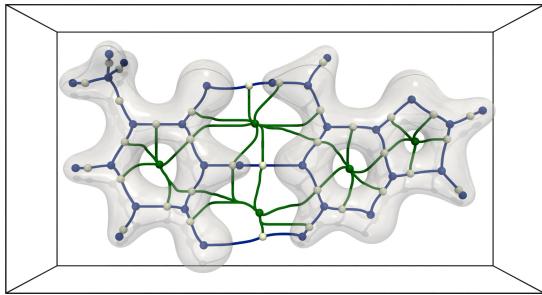
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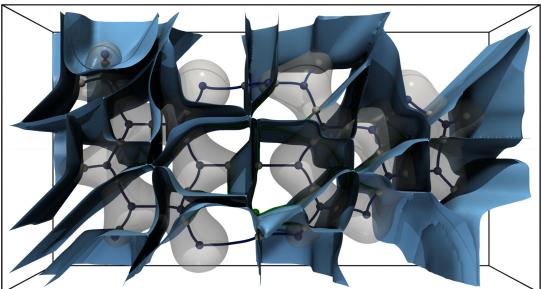
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Applications of the Morse-Smale complex



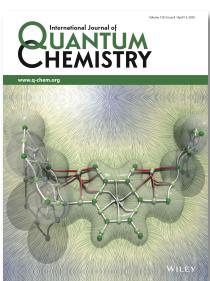
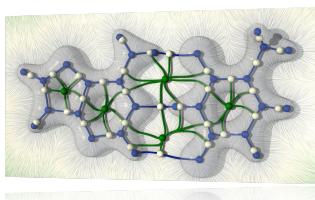
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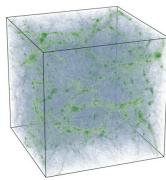
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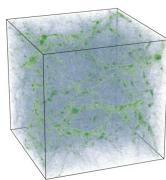
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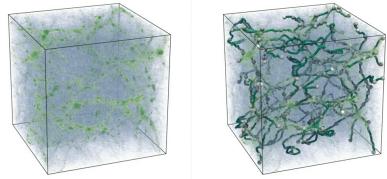
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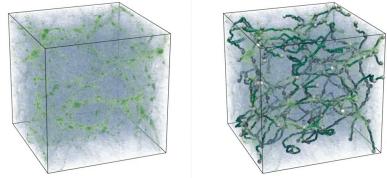
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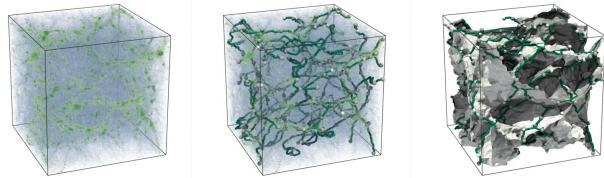
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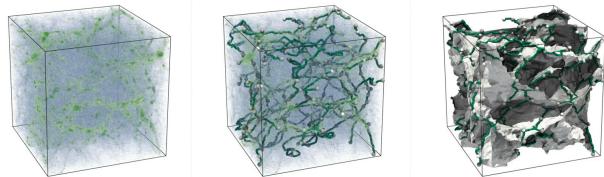
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Application of the Morse-Smale complex

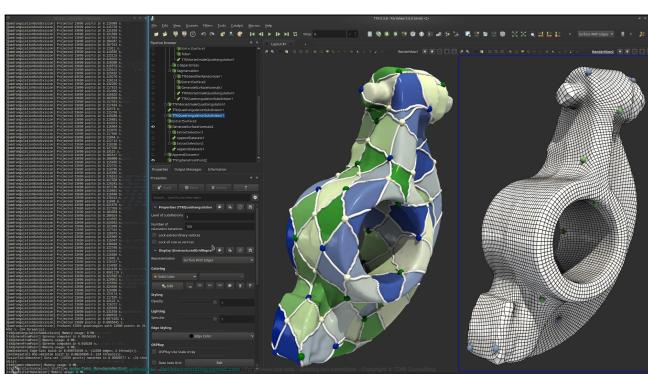
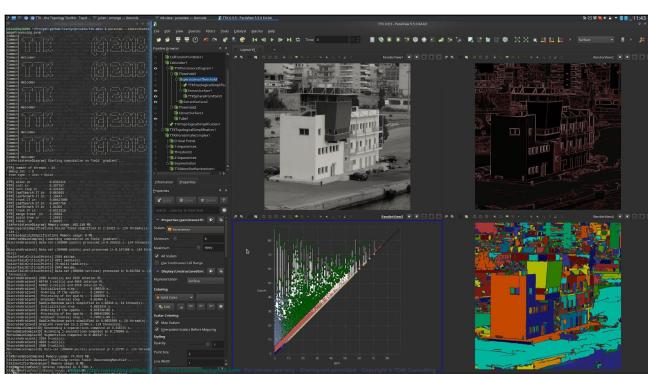
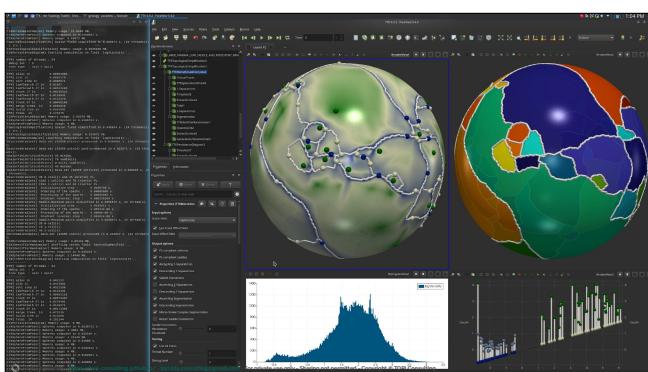
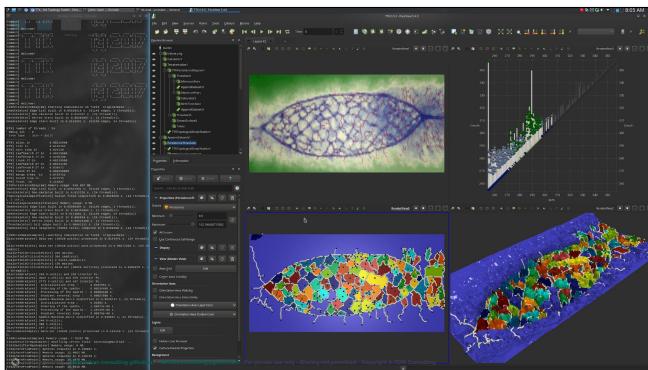


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Application of the Morse-Smale complex

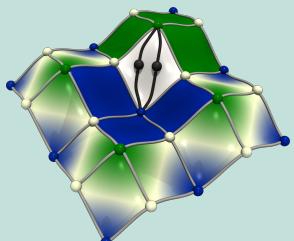


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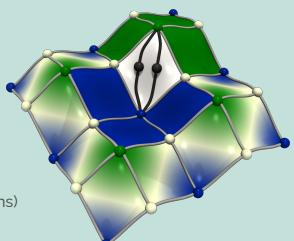
Recap on Morse-Smale complexes

- What do they encode?
 - Richest topological representation
 - Cellular decomposition



Recap on Morse-Smale complexes

- What do they encode?
 - Richest topological representation
 - Cellular decomposition
- What are they useful for?
 - Filament-like structures (e.g. cosmic web)
 - Honeycomb-like compartments (e.g. basins)



So far

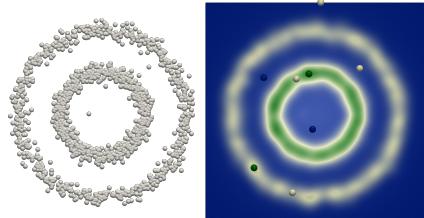
- TDA for low dimensional fields
 - Data reduction by feature extraction
 - Critical points (e.g. vortex centers)
 - Cycles (e.g. molecular rings)
 - Regions of interest (vortices)
 - 1-Separatrices (filament structures)
 - 2-Separatrices (walls)
- How about point cloud data?
 - Dimension reduction, then TDA
 - TDA, then dimension reduction



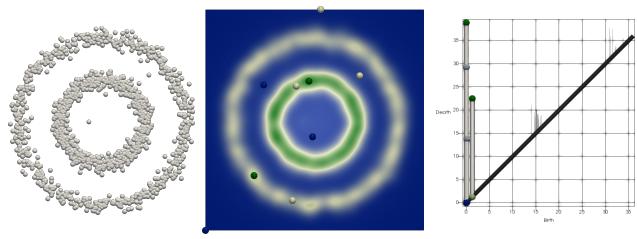
What about point cloud data? (low)



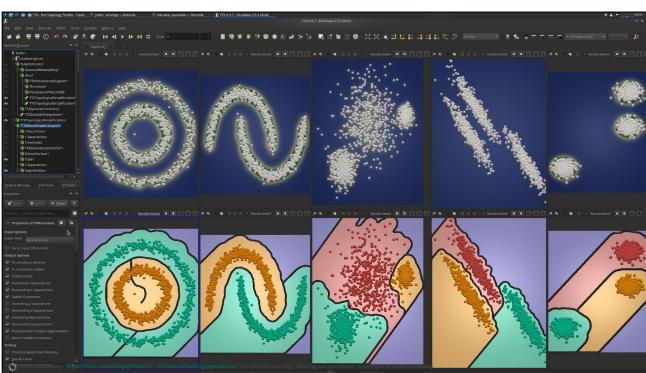
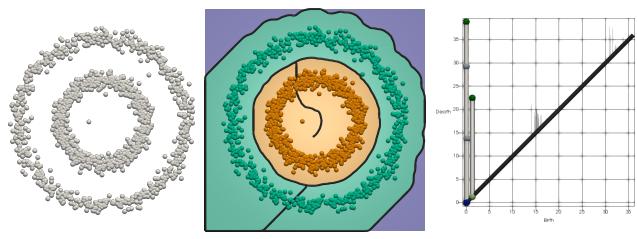
What about point cloud data? (low)



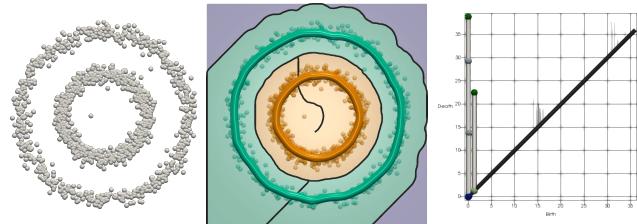
What about point cloud data? (low)



What about point cloud data? (low)



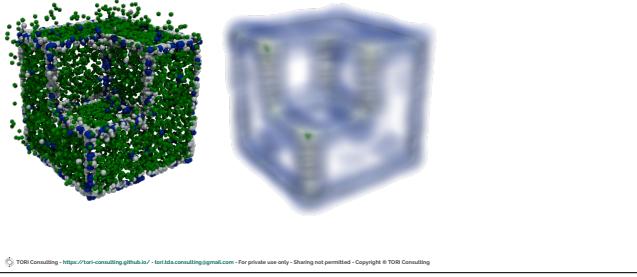
What about point cloud data? (low)



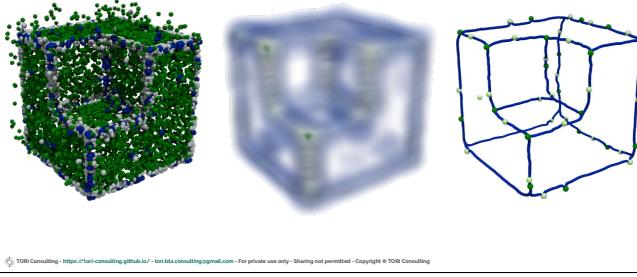
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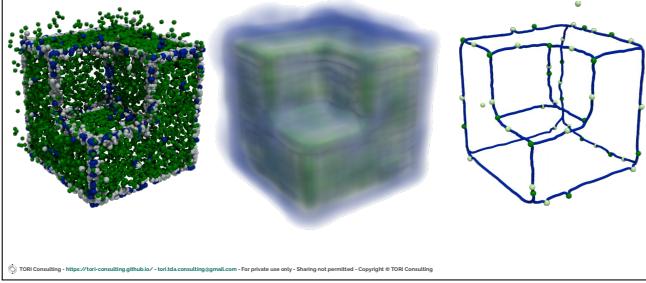
What about point cloud data? (low)



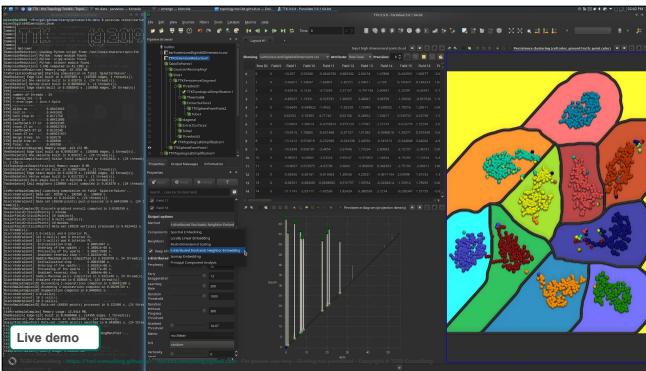
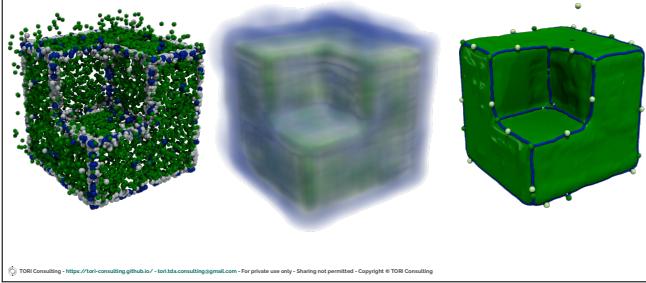
What about point cloud data? (low)



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What about point cloud data? (low)

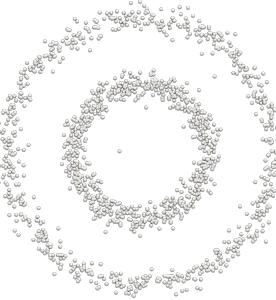


What about point cloud data? (high)

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What about point cloud data? (high)

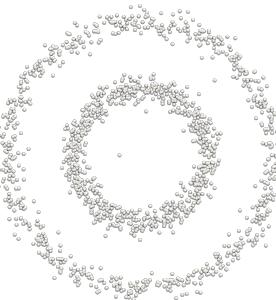
- Rips complex



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What about point cloud data? (high)

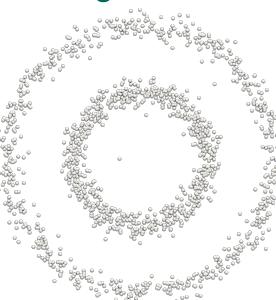
- Rips complex
- Inputs
- Target distance ε -max
- Target dimension d-max



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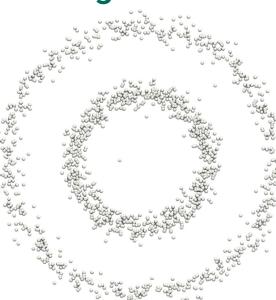
- Rips complex
- Inputs
- Target distance ε -max
- Target dimension d-max
- Construct all d-simplices
- With d smaller than d-max
- With all edges smaller than ε -max



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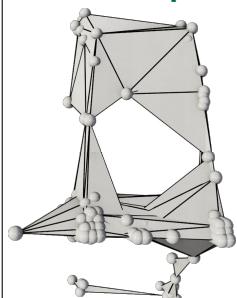
What about point cloud data? (high)

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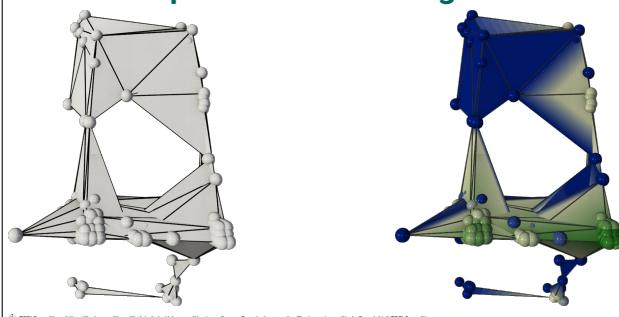
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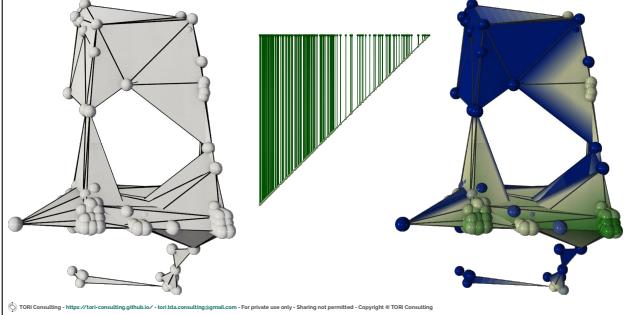
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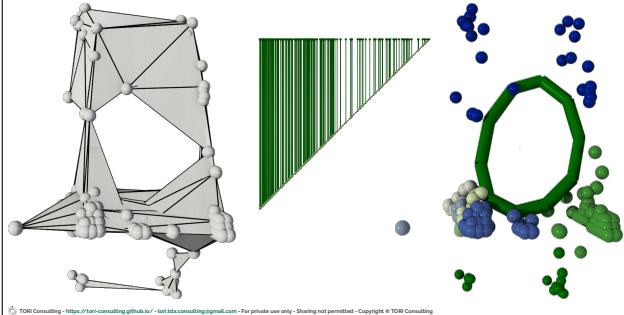


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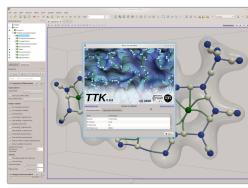


What about point cloud data? (high)



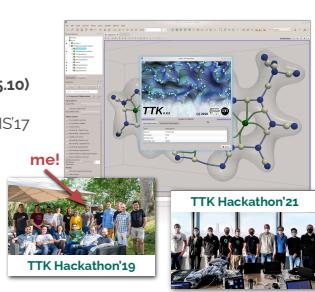
The Topology ToolKit (TTK)

- Open-source TDA library
 - ~170k lines in C++, BSD license
 - Python bindings, binary packages
 - Officially integrated in ParaView (>=5.10)
 - <http://topology-tool-kit.github.io>
 - Best paper honorable mention IEEE VIS17



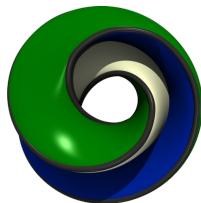
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What's next in TTK?

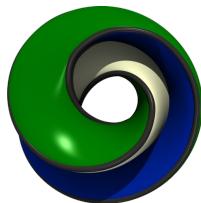


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What's next in TTK?

- **Computation at scale**

- Continuing shared-memory efforts (OpenMP)
- New distributed infrastructure (MPI), available soon



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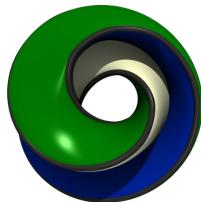
What's next in TTK?

- **Computation at scale**

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- New distributed infrastructure (MPI), available soon

- **Ensemble data**

- More statistical tools
- Data reduction and compression



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What's next in TTK?

- **Computation at scale**

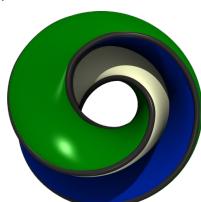
- Continuing shared-memory efforts (OpenMP)
- New distributed infrastructure (MPI), available soon

- **Ensemble data**

- More statistical tools
- Data reduction and compression

- **High-dimensional data**

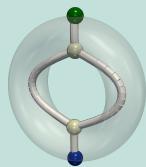
- New dimensionality reduction approaches
- Approximate methods



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Take-home messages

- **Data on meshes, or meshable data?**
 - Features of interest?
 - Recover/analyze/compare 'structural' information
- ⇒ Topological Data Analysis
 - Robust, multiscale
 - Successful in applications
 - Available in ParaView!



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Relevant references/links

- Applications of TDA
 - Quantum chemistry
 - Topological Data Analysis of Vortices in the Magnetically-induced Current Density in LiH Molecule
 - A Topological Data Analysis Perspective on Non-Covalent Interactions in Relativistic Calculations
 - Characterizing Molecular Interactions in Chemical Systems
 - Fluid dynamics
 - Topological Analysis of Ensembles of Hydrodynamic Turbulent Flows -- An Experimental Study
 - Topological Analysis of High Velocity Turbulent Flow
 - Material sciences
 - Ranking Viscous Finger Simulations to an Acquired Ground Truth with Topology-Aware Matchings
 - Visualizing Ensembles of Viscous Fingers
- Introduction to TDA
 - Topological Data Analysis for Scientific Visualization

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TTK Resources

- Website
 - <http://topology-tool-kit.github.io>
- Examples
 - <https://topology-tool-kit.github.io/examples>
- Source code
 - <https://github.com/topology-tool-kit/ttk>
- Questions?

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