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Publication Date
2012-04-09

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Topology-based Visualization and Analysis of High-dimensional Data and Time-varying Data at the Extreme Scale

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Exascale/Big Data Challenges

- Complexity of simulation results already exceeds data analysis capabilities
- Gap between simulation complexity and data analysis capabilities likely to grow
- Aggressive improvements in data analysis necessary to derive new insights from future simulations
- *Important Approach:* General methods to extract features and analyze them

Research Agenda

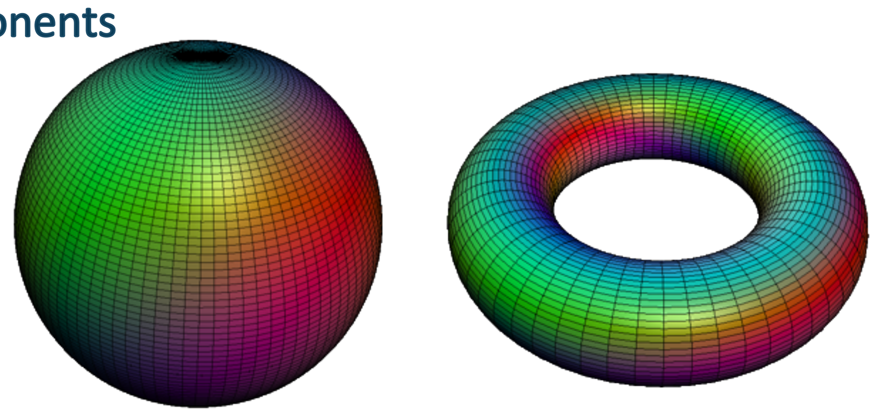
- Topological methods provide general feature definitions applicable to wide application range
- Extend and improve these techniques:
  - Implement topological methods at the extreme scale
  - Perform in-situ topological data analysis
  - Enable multidimensional and multivariate feature mining using topological methods

Topological Methods at the Extreme Scale

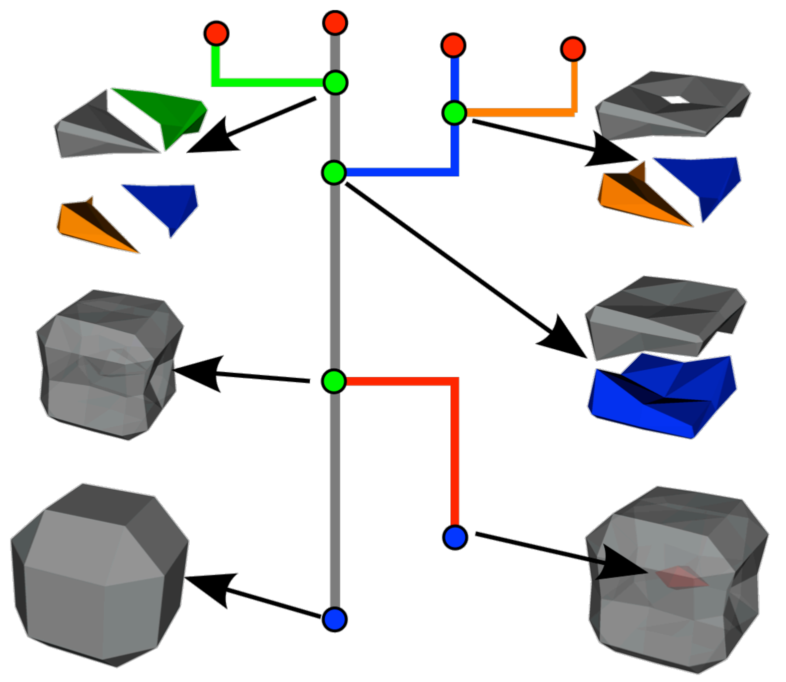
- Develop algorithms that implement current (3D) topological analysis methods on massively parallel architectures
- Determine required computational resources for topological analysis of extreme scale simulation
- Identify bottlenecks in scaling and address them
- **Goal:** Provide practical means of applying topological data analysis to hero run results

Topology of Surfaces

- Properties that remain invariant under elastic deformation
- Topology of compact surface, e.g., defined by:
  - Number of connected components
  - Genus (number of holes)



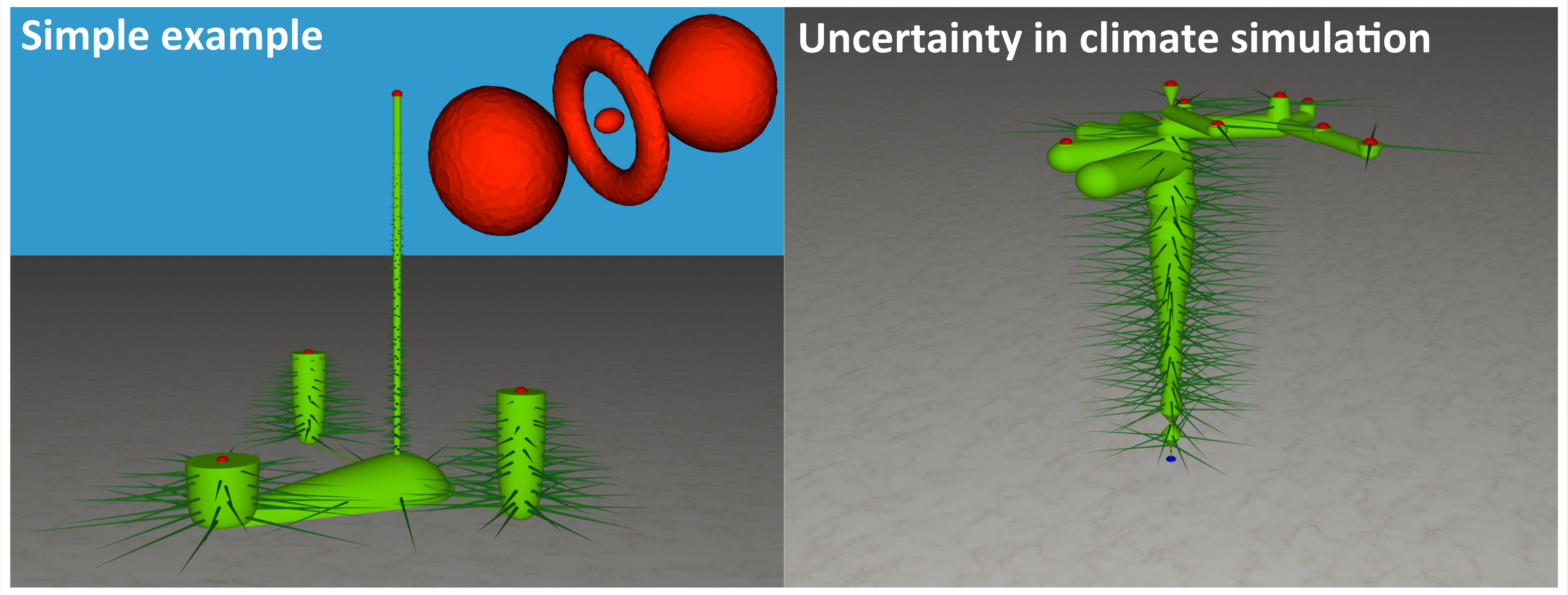
Contour Tree Encodes Isosurface Topology Changes



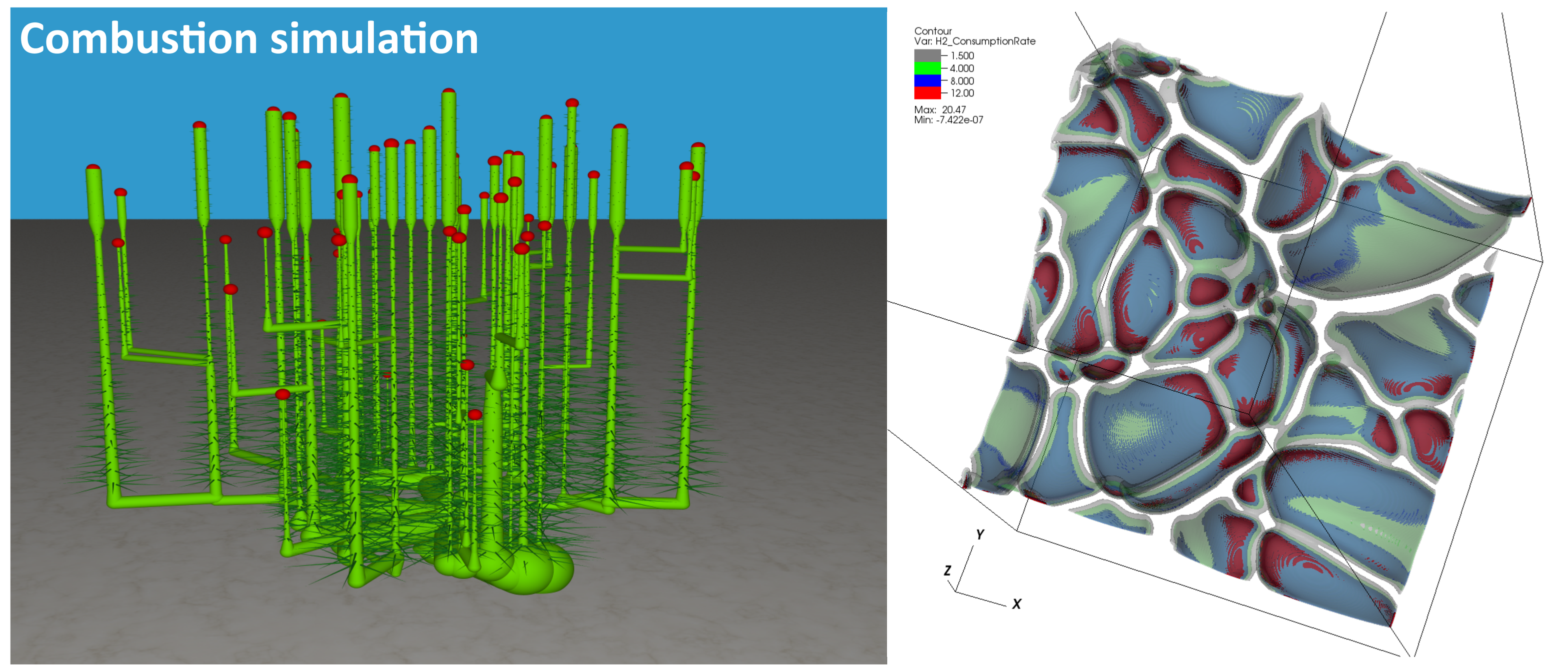
(Data courtesy of Hamish Carr, University of Leeds, UK)

Presenting Structural and Quantitative Information

- Isosurface extraction is versatile visualization and analysis method
- Common approaches provide two complementary types of information
- Structural information, e.g., number of connected components ➔ Contour tree
- Quantitative information, e.g., surface area, volume ➔ Contour spectrum
- **Goal:** Combine in single visualization ➔ Topological Cacti



- **Simple example:** Spatial probability distribution of the electron in an hydrogen atom, residing in a strong magnetic field. Branch width corresponds to cube root of volume and spike length to the square root surface area.
- **Uncertainty in climate simulation:** Average longwave energy output (FLUT) in the winter months of a 21 dimensional climate simulation ensemble comprising 1197 climate simulation. The width corresponds to cube root of vertex count–"volume" in parameter space. Spike length shows mean value of FLUT.



- **Combustion simulation:** Fuel consumption rate in a combustion simulation (one 4.3G time step from a coarse AMR simulation). We are interested in how the size of burning regions correlates with temperature variance. Thus, we map the cube root of volume – approximated as the number of vertices – to branch width and temperature variance to spike length.

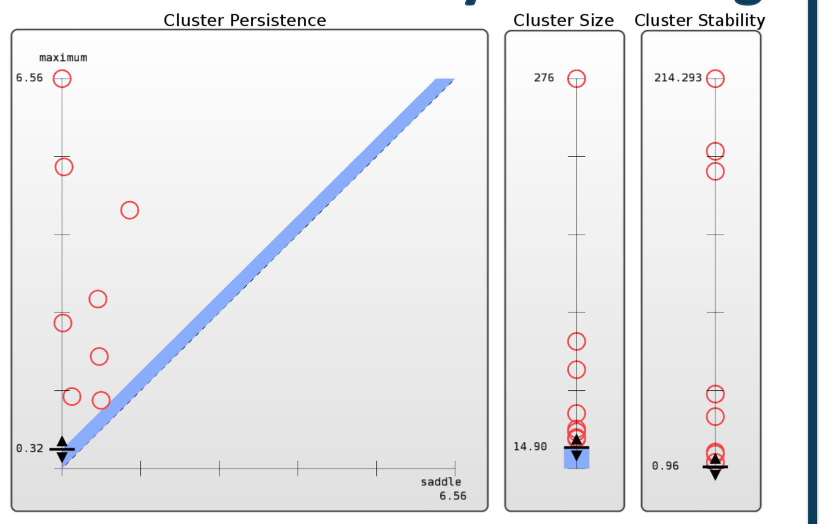
(Work with P.-T. Bremer and V. Pascucci, Combustion data: John Bell, Marc Day)

Multidimensional and Multivariate Feature Mining

- Utilize topological structures to define features in high-dimensional data
- Derive quantities (such as size distribution) from features
- Define visualization methods based on topological structures (graphs) and derived quantities
- **Goals:**
  - Show applicability of topological analysis to high-dimensional data
  - Identify commonalities in different areas ➔ general feature definitions

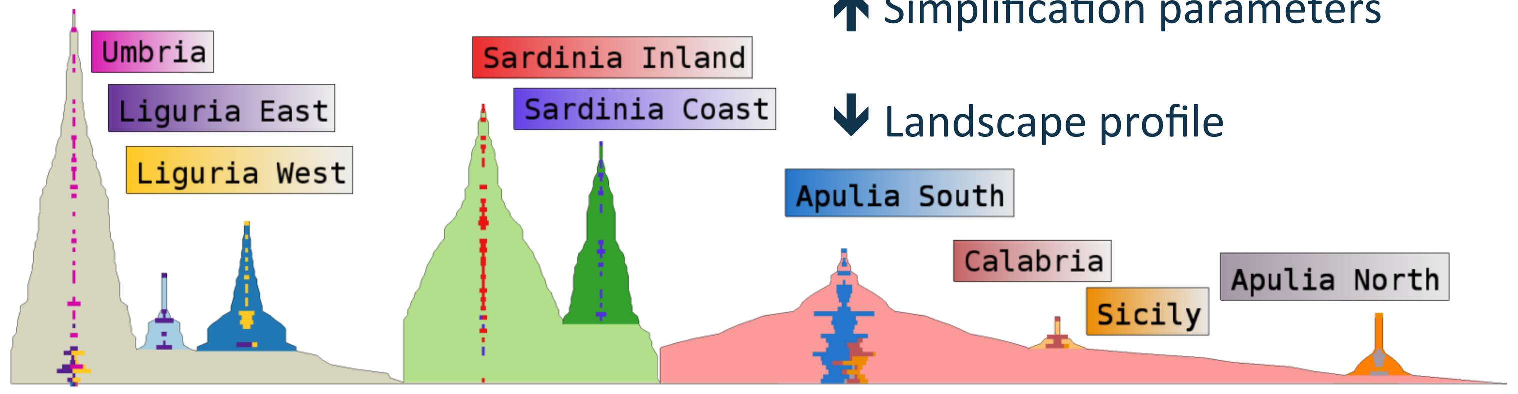
Topological Analysis of High-dimensional Density Clustering

- **Input:** Points in n-dimensional space
- Interested in clusters of high density
- Use merge tree to represent density function and identify clusters
- Present results as landscape profile
- Link to views showing simplification parameters
- Couple with parallel coordinate views and dimension reduction approaches



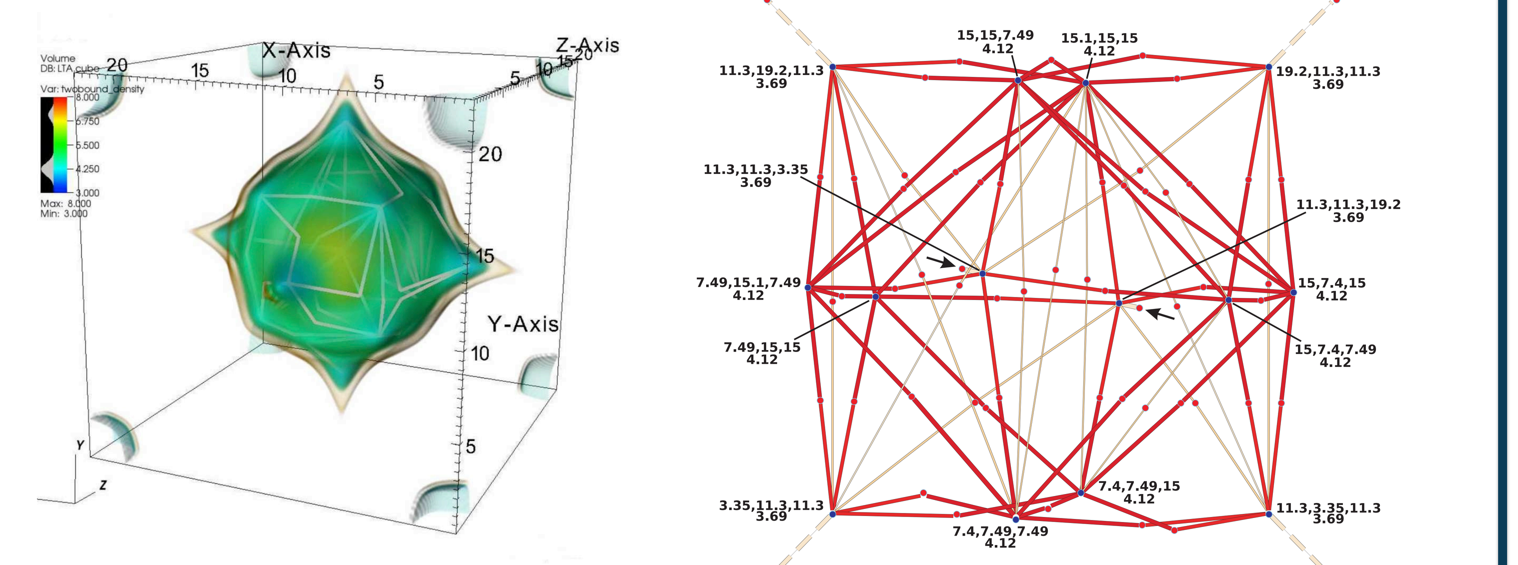
🡑 Simplification parameters

🡓 Landscape profile



(Work with Patrick Oesterling, Christian Heine and Gerik Scheuermann)

Analysis of Transformation Paths in Chemical Systems



- Transformation in chemical systems of fundamental interest
- Consider energy as function of coordinates of system components
- Lack of effective high-dimensional visualization techniques limits analysis to one or two coordinates at a time
- Comprehensive understanding requires showing relationship between *all* coordinates *at the same time*
- Combine concepts from topological analysis, multidimensional scaling and graph layout
- Enable energy function analysis for wide range of molecular structures
- Provide chemists with important tool for understanding complex reactions

(Work with K. Beketayev, M. Haranczyk, P.-T. Bremer, M. Hlawitschka, B. Hamann)

Acknowledgements

- This work is supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 through the "Scientific Data Management and Analysis at Extreme Scale" (DE-FOA-0000256) program.
- We thank the members of the
  - Visualization and Analytics Center for Enabling Technologies (VACET)
  - Center for Computational Sciences and Engineering (CCSE)
  - LBNL Scientific Computing Group

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