Finding Hidden Shapes: Topology for Feature-Based Reasoning

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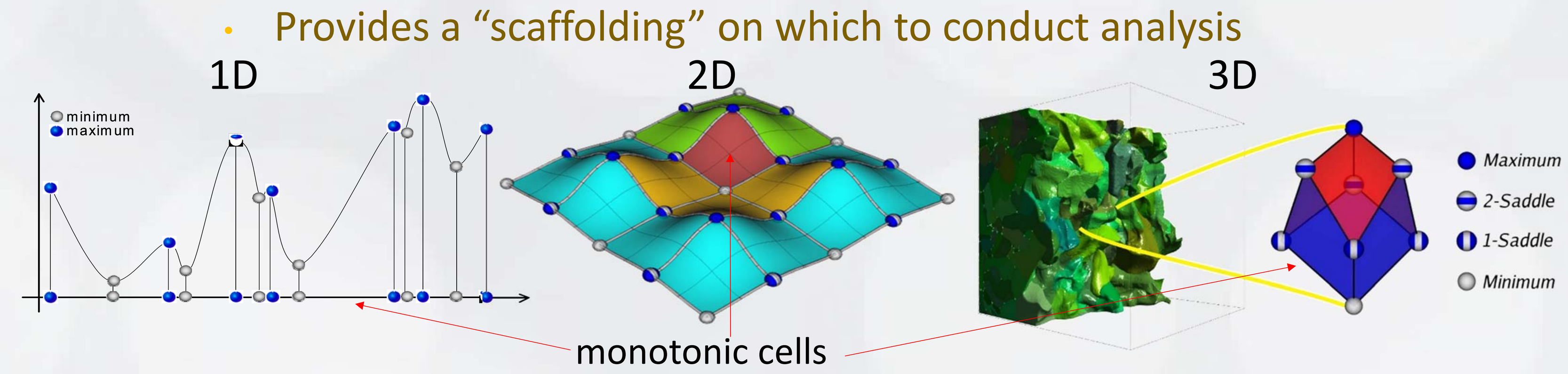
Introduction - Fundamental to rigorous study of physical phenomena is our ability to *describe* what it is we are looking for. For example, how would you describe how a lithium ion can diffuse in a battery material? Or how do you quantify the region of space a burning flame affects? How would you define the surface of a sponge? Topology is the study of the *shape* and *connectedness* of things. When applied to scientific data, it provides a *language* for defining, and reasoning with features. We use computational topology to solve complex problems in a wide range of scientific disciplines.

The core technologies represented in MSCEER are feature based techniques defining features in terms of gradient flow structures of a scalar field. In particular, MSCEER utilizes the Morse-Smale complex, a topological representation that enables multi-scale analysis.

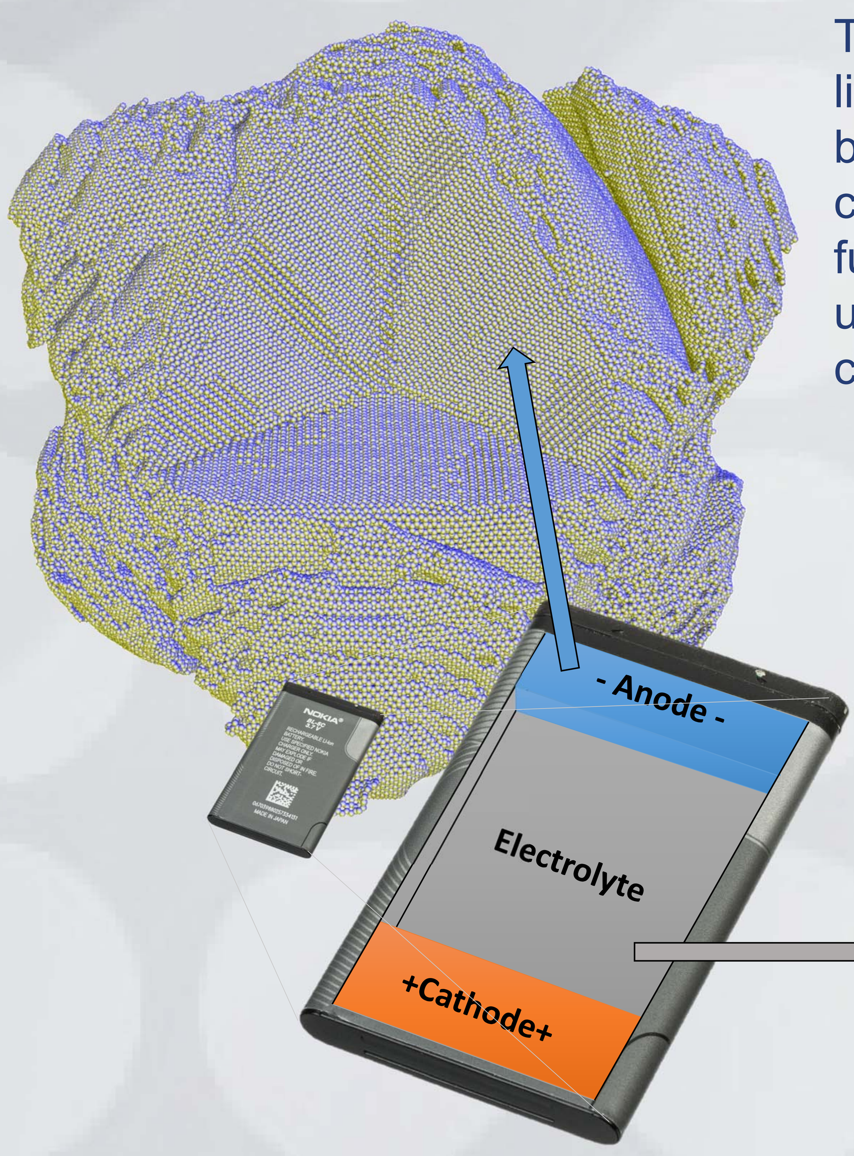
- Generalized monotonic decomposition of domain
- Provides a "scaffolding" on which to conduct analysis

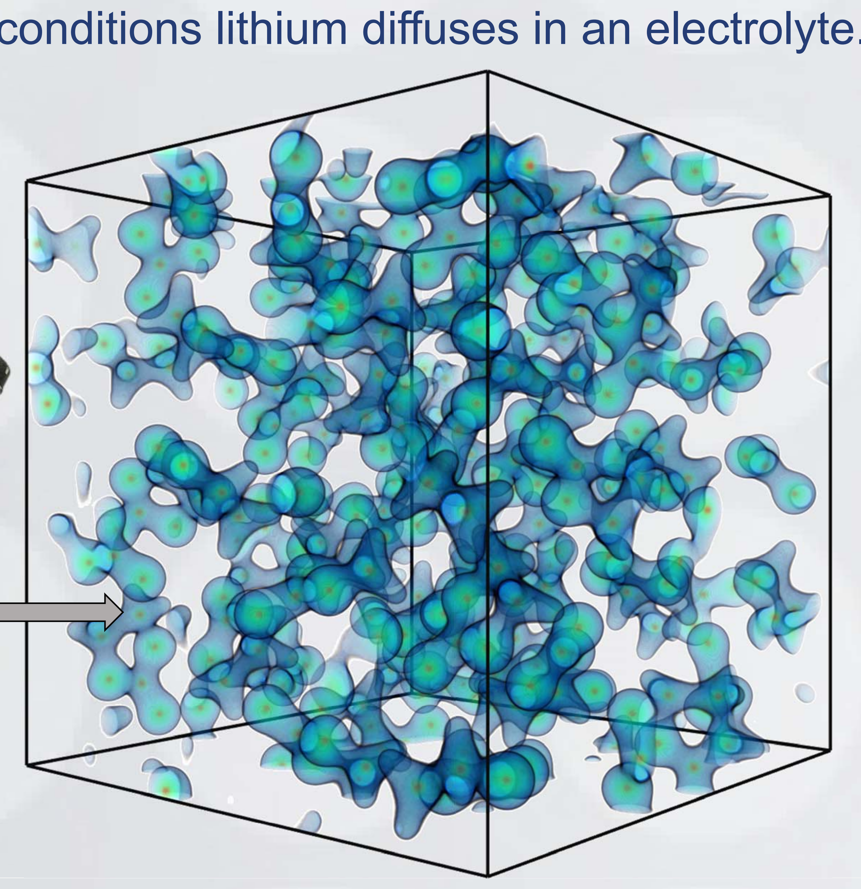


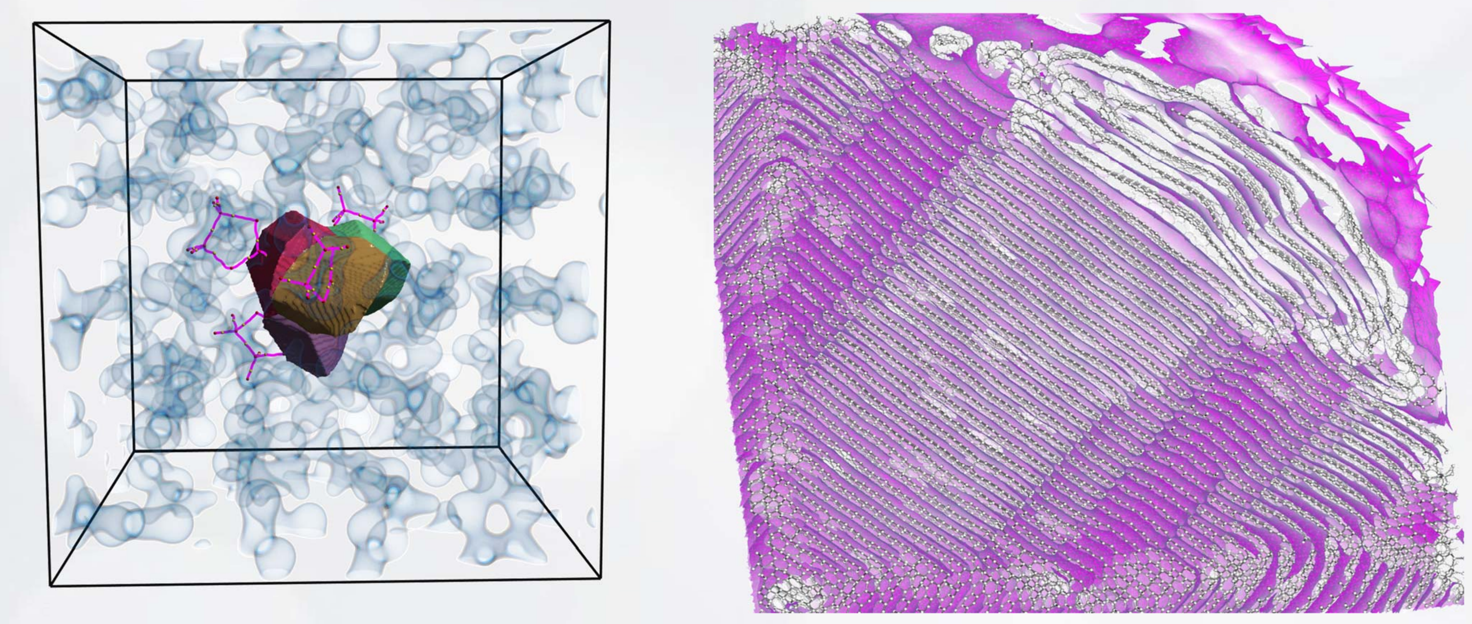
MSCEER – Morse-Smale Complex Extraction, Exploration, and Reasoning

Lithium Dynamics

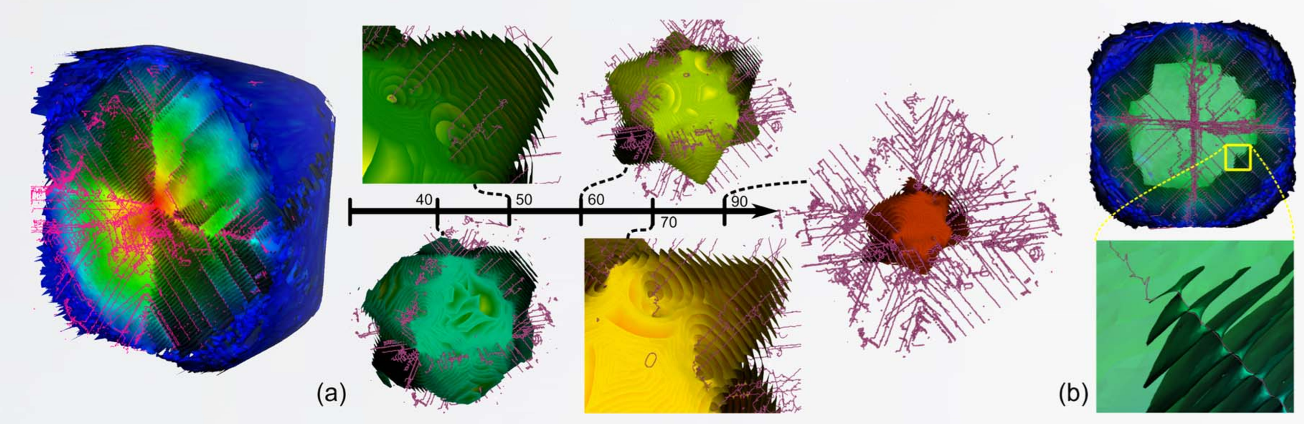
The dynamics governing the motion of lithium determine the performance of a battery material. We quantify *where* lithium can diffuse in graphitic carbon, and furthermore measure *how fast*. We also use topology to understand under what conditions lithium diffuses in an electrolyte.



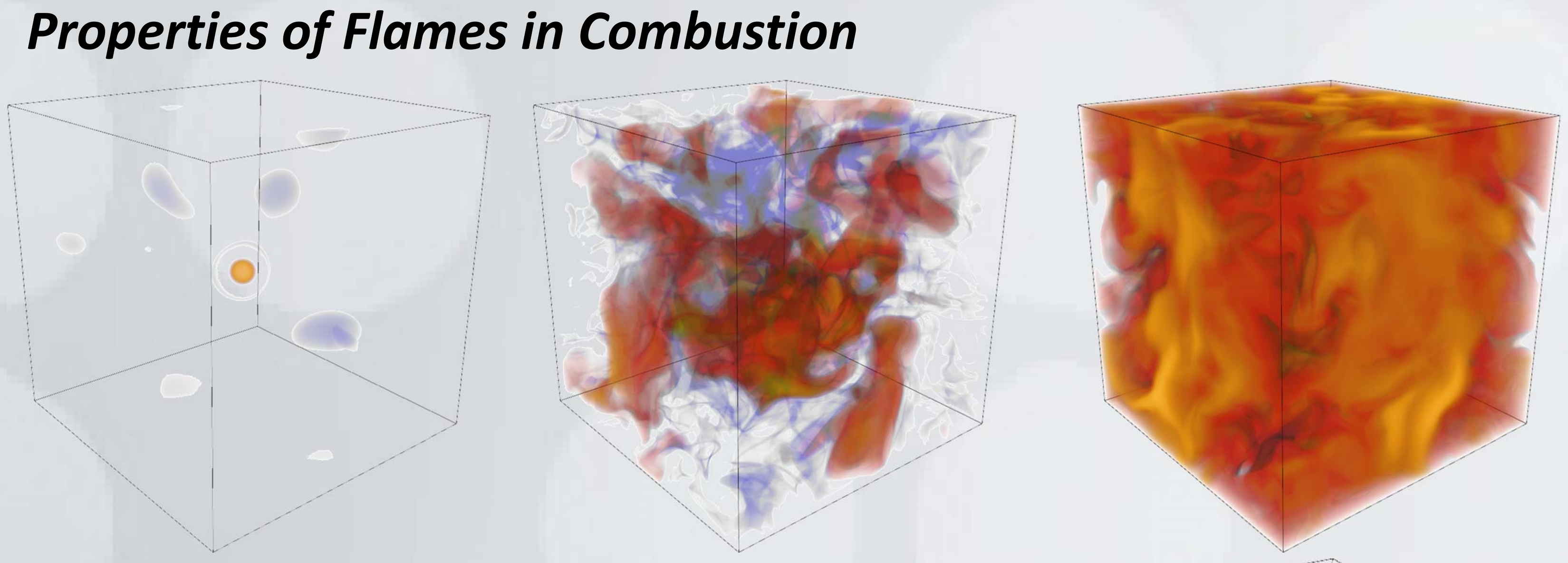




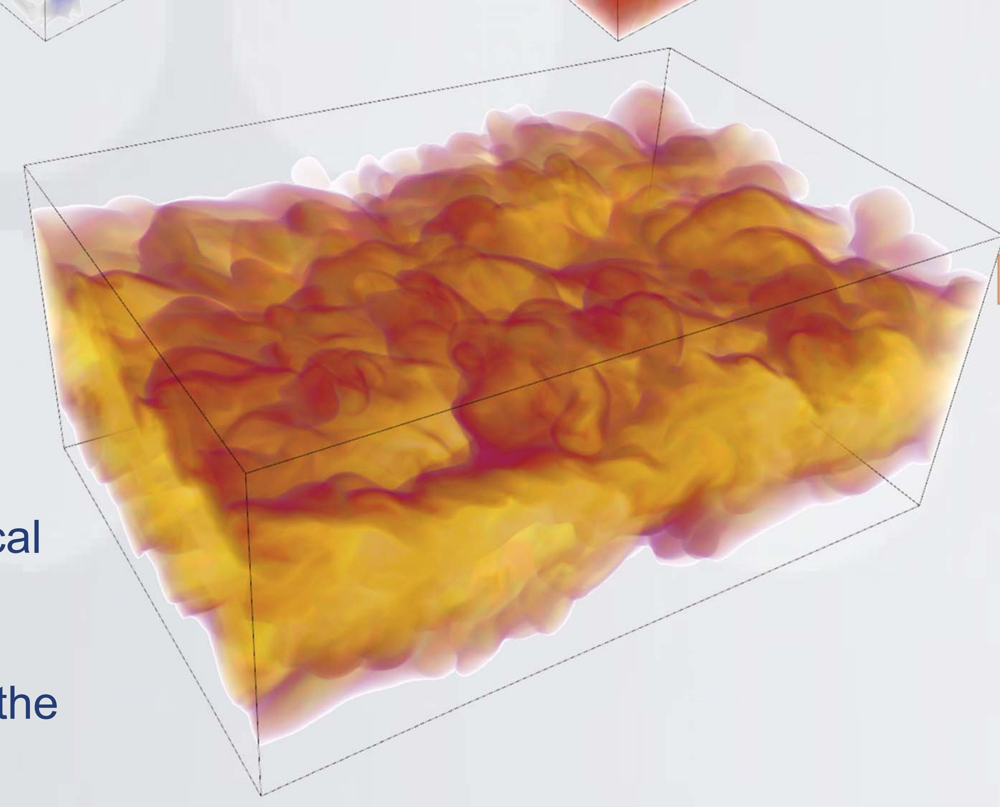
(Top Left) Basins of the Morse-Smale complex are used to measure the configuration of charge densities of molecules surrounding a lithium atom. 2D surfaces (Top Right) determine where lithium can diffuse in a carbon nanosphere, and are used to measure the saturation over time (Bottom).

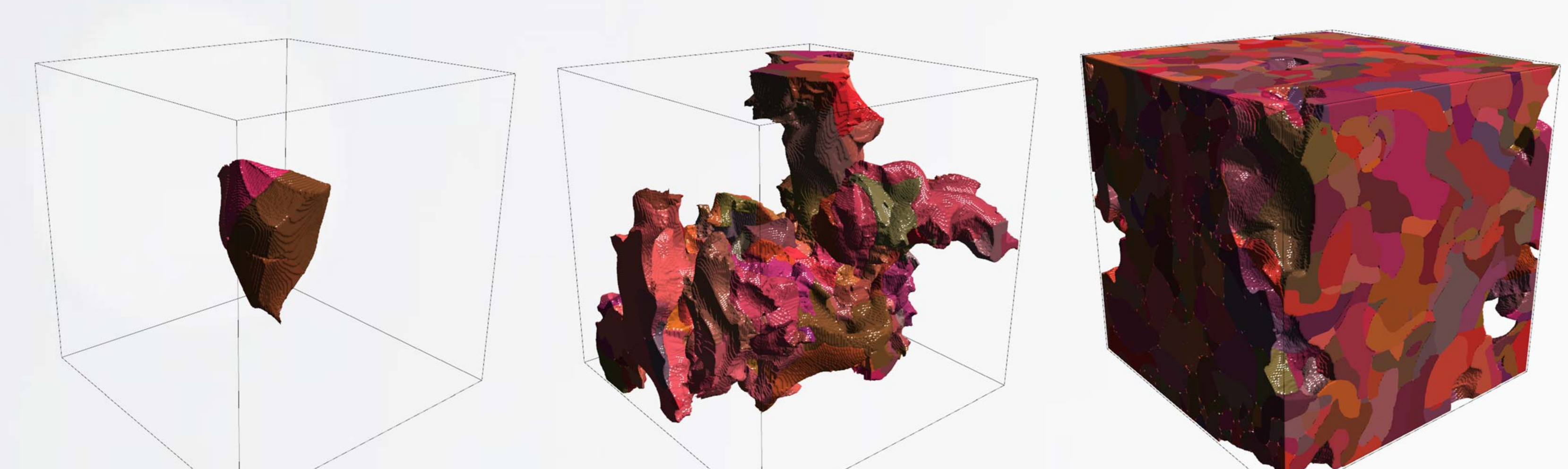


Properties of Flames in Combustion

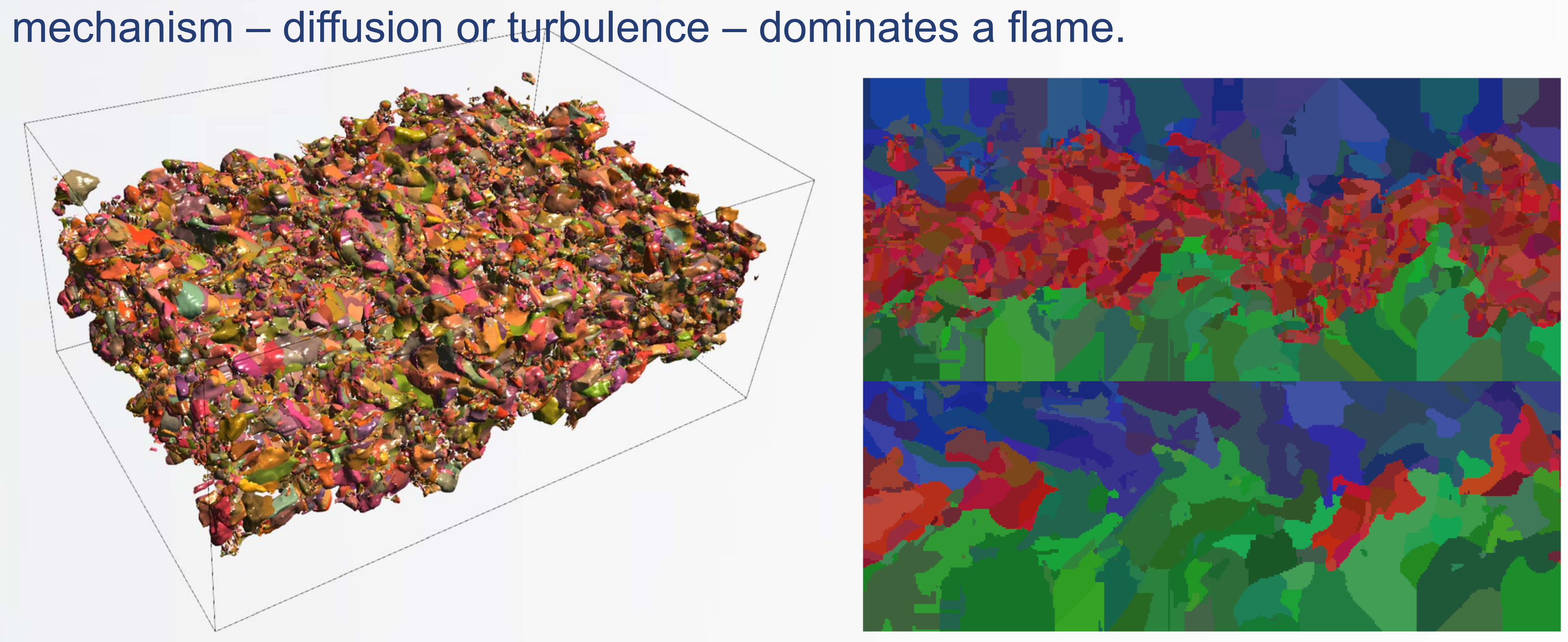


The transport and diffusion of byproducts affects the cycling characteristics of a combustion engine. *Dissipation elements* determine the physical extent of local diffusive processes, and determine which regions of space have been directly exposed to explosive chemistry. The topological cells of the Morse-Smale complex provide a robust mechanism to extract such structures and study the phenomena when varying scales.

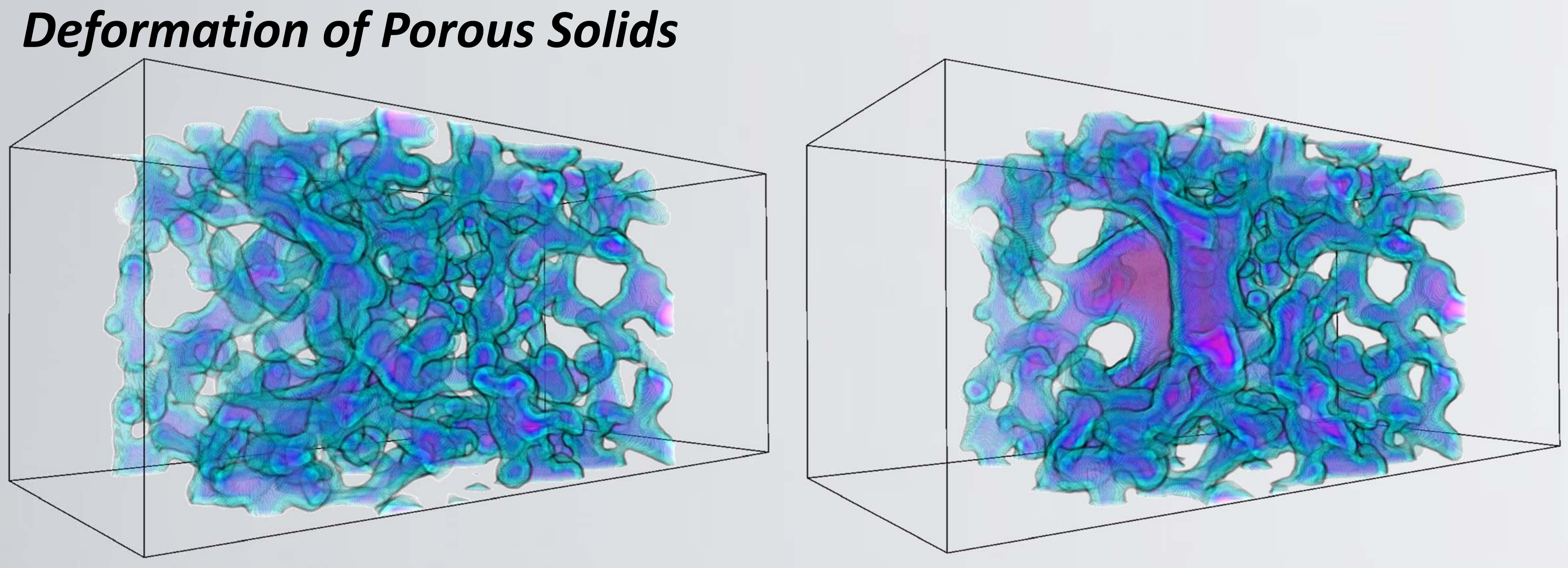




(Top) 3D cells of the Morse-Smale complex determine the extent, over time, of explosive combustion. Together with turbulence mechanisms, they control the speed of a flame. The stability of these features (Bottom) predicts which mechanism – diffusion or turbulence – dominates a flame.



Deformation of Porous Solids



How an aerogel deforms is crucial in investigating its usability for spacecraft insulation. When a copper foam is struck by a micrometeoroid, a scientist wants to measure the loss in porosity and structural integrity of the material.

The 1-skeleton of the Morse-Smale complex provides a structural view of a porous solid. Tracking this structure over time highlights local deformations, and is further used to study the connectivity after impact.