Quantifying Lithium Ion Diffusion With MSCEER for Improved Battery Design

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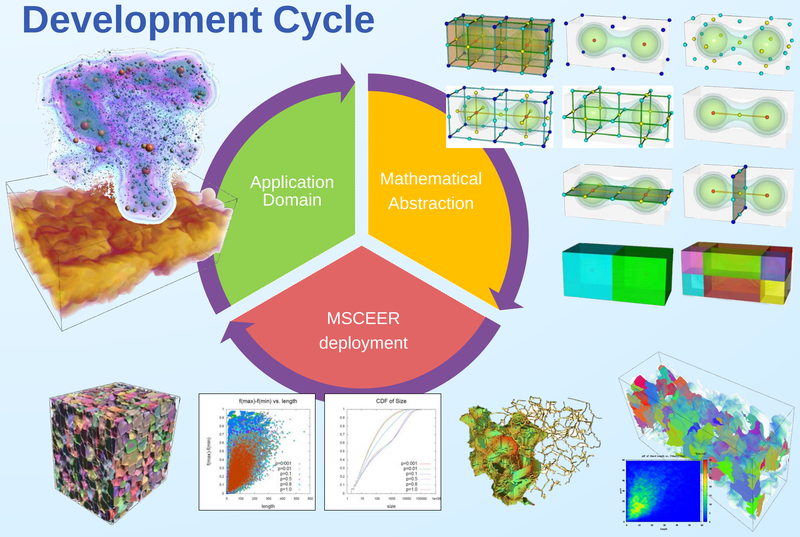
Overview

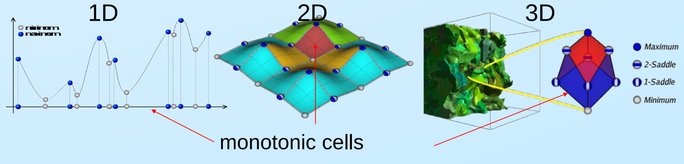
MSCEER (Morse-Smale Complex Exploration, Evaluation, and Reasoning) is a set of tools for delivering state-of-the art topology-based analytics to the scientific community. In particular, development of MSCEER has been an iterative process: individual scientific applications require custom analytics solutions; and the new analytics capabilities developed in addressing particular stakeholder problems opens new opportunities in often unrelated domains. Past successes of this design process include the deployment of new algorithms enabling new kinds of analysis for problems from material sciences, computational chemistry, combustion, and biological imaging.

Development Cycle



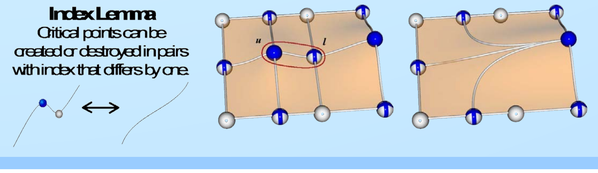
Morse-Smale Complex

The core technologies represented in MSCEER are feature based techniques, especially 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
- Topological simplification enables multi-scale analysis

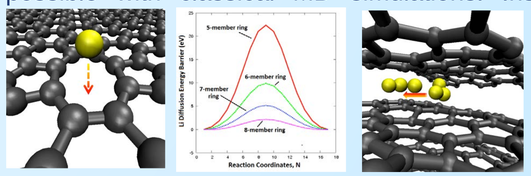
Index Lemma
Critical points can be created or destroyed in pairs with index that differs by one.



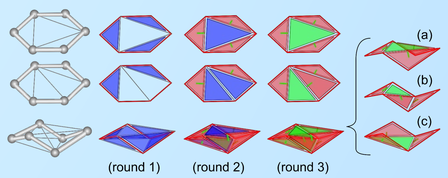
Case Studies from Basic Energy Science

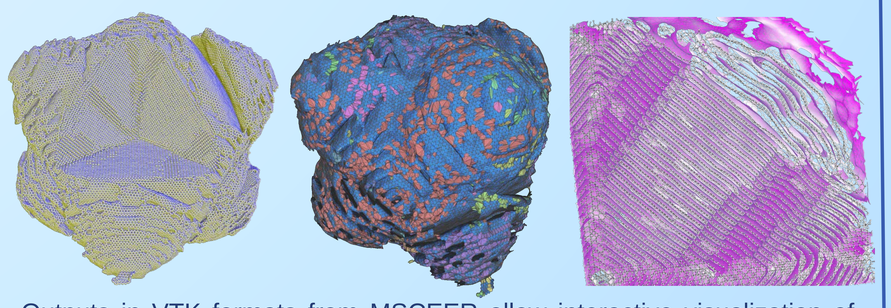
Lithium Diffusion in Carbon Nanospheres

Nanospheres of graphitic carbon show promise as a battery design, however understanding their cycling and capacity to store lithium is not possible with classical MD simulations. Instead, models for lithium diffusion are used where the valence of a carbon ring determines whether or not lithium is able to pass through

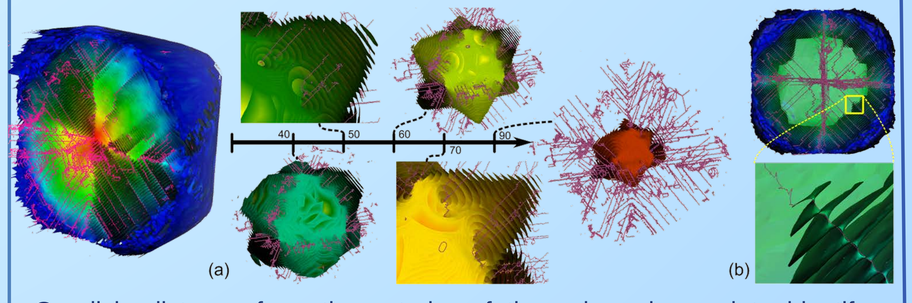


A new algorithm in MSCEER based on discrete Morse theory operates on a Delaunay triangulation, explicitly identifying ring structures and their valence



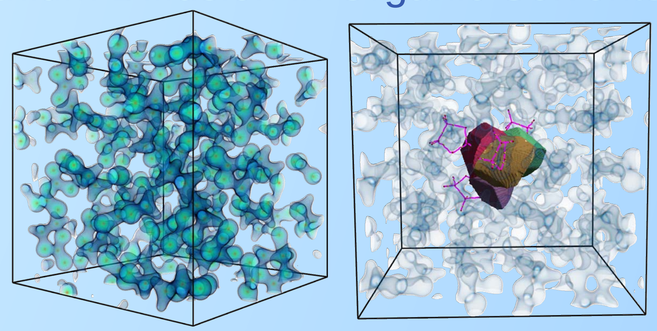


Outputs in VTK formats from MSCEER allow interactive visualization of blocking and non-blocking structures, for the first time showing the planes along which lithium can diffuse. Penetration into the nanosphere is dominated by large-scale dislocations.

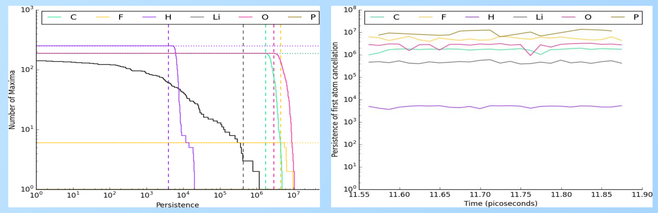


Geodisic distance from the exterior of the sphere is used to identify patterns in lithium diffusion.

Lithium Diffusion in Organic Solvents

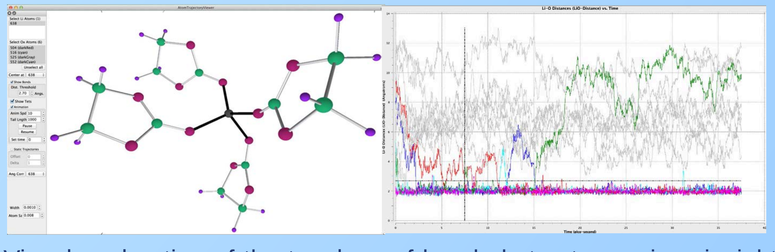


MSC of the charge density field allows detection of bonds. Various topological and geometric indicators derived from the MSC can help predict events where the solvation structure of Lithium ions changes.



Topological bond detection is effectively parameter-free as the detection is robust over a wide range of persistence – the only parameter for detection.

Lithium (gray ball in the center) can change bonded oxygens (colored balls) through a 4-3-4 state (left), or a 4-5-4 state (right).



Visual exploration of the topology of bonded structures gives insights into the unstable configurations, and can help understand the diffusion structure better. Such analysis can also help creating new configurations of interest, thus speeding up the exploration process.

SDAV Scalable Data Management, Analysis, and Visualization
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