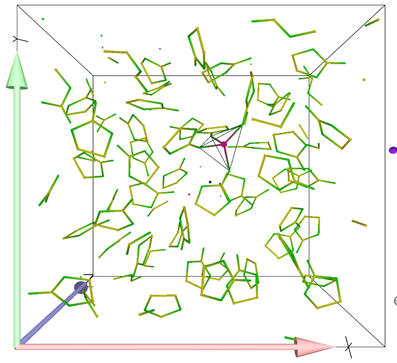
Topological Analysis for Molecular Dynamics

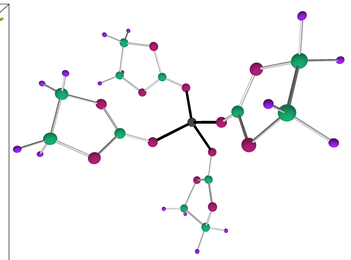
Harsh Bhatia
Data Analysis Group, Center for Applied Scientific Computing (CASC), LLNL

with Peer-Timo Bremer, Mitchell Ong, Vincenzo Lordi, Erik Draeger, & John Pask (LLNL); Attila Gyulassy & Valerio Pascucci (The University of Utah)

The importance of lithium-ion batteries cannot be overstated

- Solvation and diffusion of lithium strongly influences the battery performance
- New tools and techniques are needed to explore the phenomena affecting lithium's motion and bonding behavior
- Understanding local and global structures may highlight bottlenecks in the system potentially restricting battery performance





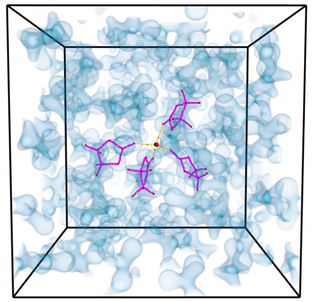
Simulation of a lithium salt in a liquid electrolyte. Lithium (gray) bonds with 4 electrolyte molecules through oxygen (magenta).

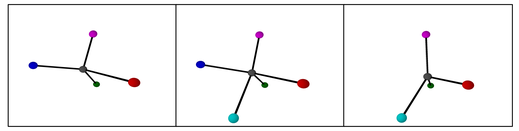
Analysis of molecular dynamics data poses challenges

- First-principles molecular dynamics simulations are computationally expensive, and often yield only few events of interest
- Lack of interactivity, numerical robustness, and specialized tools often slow down progress

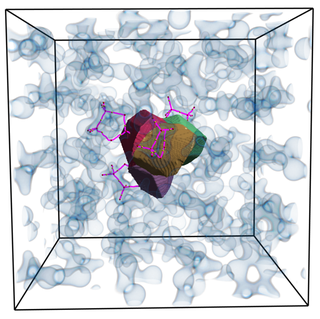
Robust detection of bonds

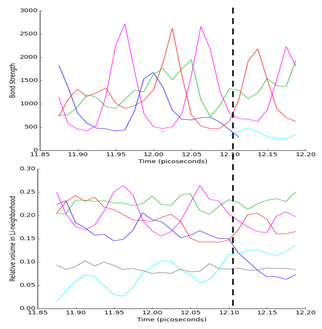
- The topology of electron charge density gives a robust way of detecting bonds [Bader, 1990]
- Such bonds are more reliable for unstable cases, especially, during reconnections





Lithium (gray) gains a bond with cyan oxygen, creating an unstable configuration, causing it to shed the blue oxygen. Plots of topological properties help understand reconnection events.

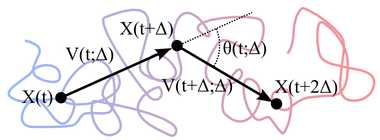




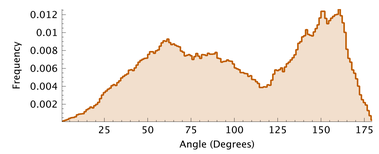
- Topological properties appear to foretell reconnection events
- Check-pointing and branching simulations at unstable configurations may create more events of interest

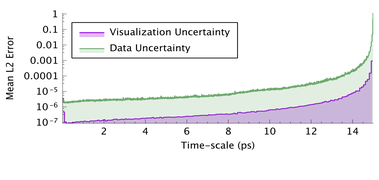
Compact characterization of ionic trajectories

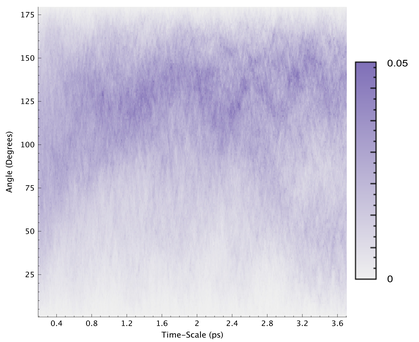
- Ionic/atomic trajectories capture complex dynamics
- Statistical characterization is desired to compactly represent the phenomena captured by atomic motion



Distribution of relative-angle [Burov et al, 2013] studies the directional motion and can classify it as Brownian vs. non-Brownian.



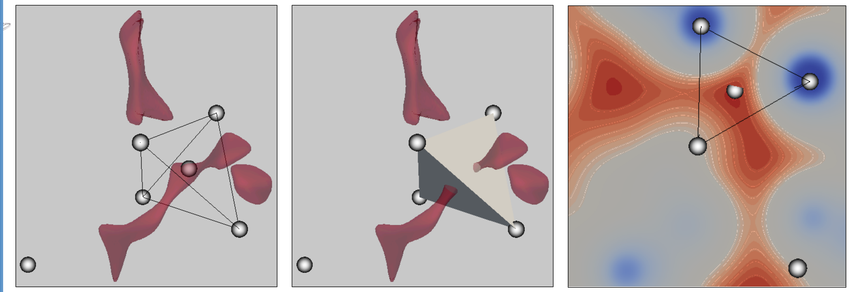




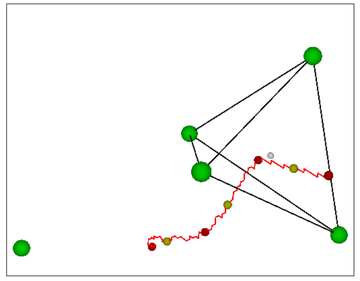
- Interactive visualization tool enables identification of the "caging" effect and reduces exploration time by orders of magnitudes
- Uncertainty visualization provides increased confidence in the results

Exploration of "tunnels" in the diffusion environment

- The diffusion environment contains "tunnels" in which lithium moves
- *Hypothesis:* The tunnels are created by the environment, not by lithium



Visualization of tunnels, i.e., contours of electrostatic potential without lithium. Position of lithium is at the center, surrounded by five oxygen atoms.



Topology of the electrostatic potential shows tunnels around lithium (gray) and oxygen (green). Red and brown spheres denote minima and 1-saddles, and red lines denote ridges connecting them.

- The tunnels appear to be "too shallow" to substantially affect lithium's motion
- Further exploration is needed to study how lithium affects the tunnels and/or makes it way through the environment

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