New, Improved Method for Optimizing Molecular Geometries

Scientific Achievement

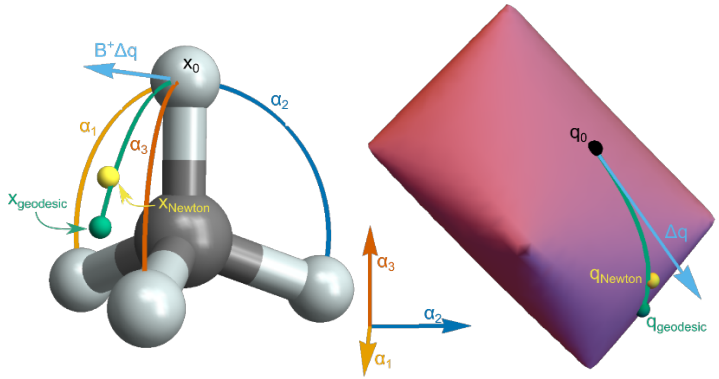
Optimization of molecular geometries is best done in internal coordinates: bonds lengths, bond angles, and dihedral angles. However, these coordinates are coupled, creating complicated constraints and consequently loss of efficiency for widely used optimization algorithms. Our new optimization strategy interprets the space of all possible molecular geometries as a manifold, and molecular geometry displacements are taken along the geodesics on these manifold, inherently satisfying the necessary constraints. Compared to the traditional approach, this substantially reduces the number of steps required to reach convergence on a molecular geometry optimization benchmark

Significance and Impact

Geometry optimization is a key aspect in any computational study of molecules. This step may be rate-limiting in automatic potential energy surface exploration frameworks suitable for use on exascale computational resources. Our geodesic optimization method dramatically speeds up optimization of molecules, thereby increasing the throughput in such applications.

Research Details

- Our method has been implemented in our open-source geometry optimization code, Sella.
- The method is a drop-in replacement for existing optimization codes using redundant internal coordinates.
- It can also be used in saddle point optimization for reaction network exploration.



Eric D. Hermes, Khachik Sargsyan, Habib N. Najm, and Judit Zádor, The Journal of Chemical Physics, *accepted, doi: 10.1063/5.0060146*