New, Efficient Method for Locating Saddle Points Demonstrated

Scientific Achievement

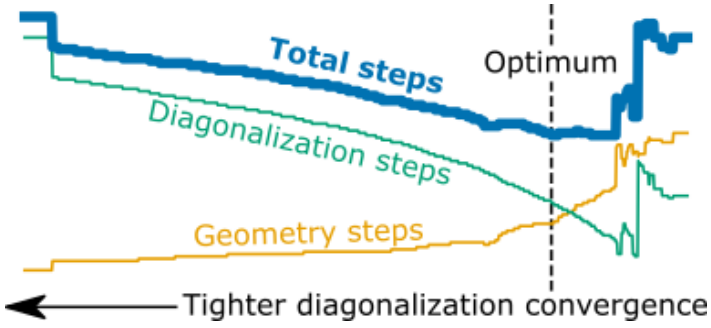
A new method has been developed for locating saddle points on potential energy surfaces in atomistic simulations using iterative Hessian diagonalization. Our method scales better with respect to system size and converges more reliably than traditional approaches. The method is implemented in a new open-source software package, `Sella`, which provides a convenient way to use our method in combination with more than 40 electronic structure packages for molecules, solids and other atomic systems.

Significance and Impact

Automated workflows to explore reactive potential energy landscapes combined with current peta- and upcoming exascale computing resources promise an unprecedented acceleration of the rate at which we can understand complex chemical phenomena at the atomic scale. Robust and efficient optimizers are the linchpins of these frameworks. Especially difficult in this context is to have reliable search methods for first order saddle points, these lowest energy passage points between the intermediates of a reaction networks, which ultimately determine the importance and rate of the various chemical processes.

Research Details

We use iterative diagonalization to update an approximate Hessian. Efficiency is gained by using it both to progress towards the saddle point and as a preconditioner for subsequent Hessians. Balancing the cost of diagonalization and the desired accuracy to make the right geometry steps results in a substantial reduction in the total cost of optimization compared to other low-scaling algorithms. `Sella` is being incorporated into automated potential energy landscape exploration codes, including `KinBot` (for gas-phase molecules) and the newly-developed `pynta` (for heterogeneous catalysis).



Eric D. Hermes, Khachik Sargsyan, Habib N. Najm, and Judit Zádor, Journal of Chemical Theory and Computation, 2019, 15, 6536-6549.
https://github.com/zadorlab/sella

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