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Automated Coarse-Graining to Accelerate Conformational Searches of Large Systems

The conformational search of small molecules has become increasingly relevant in recent years after the significant speedups in computation chemistry, and the developments of new efficient algorithms for the task. In that regard, we recently published a new Global Optimization Algorithm (acronym GOAT)1, which has been shown to be among the best of its kind and can cover a wide range of systems, from organic drug-like molecules to metal complexes, to water clusters and even can deal with atomic clusters like nanoparticles.

In this work, we show a novel automatic algorithm for coarse graining of molecules, which allows for the use of such conformational search algorithms in much larger systems due to the reduced dimensionality. This algorithm automatically splits the system into chemically meaningful fragments using an efficient graph-based approach, and by projecting the gradient such that each fragment is treated as a rigid body with only translations and rotations, one can significantly reduce the dimension of the conformational search problem. Since these problems usually scale exponentially with the system size, the overall effect can be drastic, and systems with hundreds of atoms can be treated on a reasonable time scale, without losing too much accuracy since the full calculated gradient is still used.

We will show some results of the new approach, its advantages and shortcomings together with a general overview of the GOAT algorithm, which is already implemented in the ORCA software2, from version 6.0.

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