Hybrid Algorithms for Optimizing Molecular Structure

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Global optimization of molecular structures is still one of the challenges of computational chemistry. Various methods such as genetic algorithms, simulated annealing or differential evolution are used. Although most of them give good results in certain cases, they are still not efficient or universal enough to optimize big molecules. Moreover, these methods usually require setting numerous arbitrary parameters controlling their work, which proper choice strongly affects performance of the optimizing algorithm.

In this study we suggest two new ways of determinating optimal parameters of genetic algorithms used in chemistry. The first uses two stage genetic algorithm approach: a genetic algorithm is used for optimization of parameters of genetic algorithm supervising optimization of molecular structure. The other approach uses neural networks to establish optimum parameters of genetic algorithm later used in geometry optimization. In both cases, after each step of genetic evolution we use local gradient optimization algorithms which are the most efficient tool at finding the optimum within convex areas of design space.

Those two methods are used and compared for several medium-sized molecular systems like, e.g., met-enkephalin, n-alkanes and cyclopentadecanolide. Tests showed that those hybrid methods were more efficient than simple global and local methods.