A Hybrid LBFGS-DE Algorithm for Global Optimization of the Lennard-Jones Cluster Problem

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The Lennard-Jones cluster conformation problem is to determine a configuration of n atoms in three-dimensional space where the sum of the nonlinear pairwise potential

$$f(x,y,z) = \sum_{i<j} \frac{1}{r_{i,j}^{12}} - \frac{2}{r_{ij}^{6}}$$

function is at a minimum. In this formula, $r_{i,j}$ is the distance between atoms i and j. This optimization problem is a severe test for global optimization algorithms due to its computational complexity: the number of local minima grows exponentially large as the number of atoms in the cluster is increased. As a specific test case, a better cluster configuration than the previously published putative minimum for the 38-atom case was found in the mid-1990s.

Various algorithms have been tried for determining putative global minimum of Lennard-Jones clusters, for example, simulated annealing and genetic algorithm. There is a fast multistart two-step algorithm which can sometimes find the minimum potential energy clusters in seconds, but it works with a modified Lennard-Jones potential formula.

In this paper we present a hybrid limited memory BFGS (L-BFGS) algorithm and a modified differential evolution (DE) algorithm for determining the global minimum potential energy configurations of atom clusters using the unbiased or unmodified potential Lennard-Jones function. It performed with 100% reliability for clusters containing 2–50 atoms. The algorithm has excellent potential for solving other difficult global nonlinear optimization problems.

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