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A Particle Swarm Optimization Algorithm with Random Learning Mechanism and Levy Flight for Optimization of Atomic Clusters

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Abstract

Swarm intelligence optimization algorithms are mainstream algorithms for solving complex optimization problems. Among these algorithms, the particle swarm optimization (PSO) algorithm has the advantages of fast computation speed and few parameters. However, PSO is prone to premature convergence. To solve this problem, we develop a new PSO algorithm (RPSOLF) by combining the characteristics of random learning mechanism and Levy flight. The RPSOLF algorithm increases the diversity of the population by learning from random particles and random walks in Levy flight. On the one hand, we carry out a large number of numerical experiments on benchmark test functions, and compare these results with the PSO algorithm with Levy flight (PSOLF) algorithm and other PSO variants in previous reports. The results show that the optimal solution can be found faster and more efficiently by the RPSOLF algorithm. On the other hand, the RPSOLF algorithm can also be applied to optimize the Lennard-Jones clusters, and the results indicate that the algorithm obtains the optimal structure (2-60 atoms) with an extraordinary high efficiency. In summary, RPSOLF algorithm proposed in our paper is proved to be an extremely effective tool for global optimization.

Keywords: Random Learning Mechanism; Levy Flight; RPSOLF Algorithm; Lennard-Jones Cluster

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