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Genetic whale optimization algorithm for minimizing molecular potential energy function

We propose a new hybrid algorithm by combining the whale optimization algorithm and the genetic algorithm in order to minimize a simplified model of the potential energy function of the molecule. The proposed algorithm is called Accelerated Whale Optimization Algorithm (AWOA). Also, we test the proposed algorithm with different molecule size with up to 200 dimensions to minimize the potential energy function. Moreover, we compared the proposed algorithm against 8 benchmark algorithms, in order to verify the efficiency of it for solving molecules potential energy function. The numerical experiment results show that the proposed algorithm is a promising and efficient algorithm and can obtain the global minimum or near global minimum of the molecular energy function faster than the other comparative algorithms in reasonable time. Moreover, we apply this algorithm on large scale unconstrained optimization problems and nonlinear systems.

----Joint Work with Ahmed F. Ali and Abdelmonem M. Ibrahim