Balanced Multi-process Parallel Algorithm for Chemical Compound Inference with Given Path Frequencies

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Abstract

To enumerate chemical compounds with given path frequencies is a fundamental procedure in Chemo- and Bio-informatics. The applications include structure determination, novel molecular development, etc. The problem complexity has been proven as NP-hard. Many methods have been proposed to solve this problem. However, most of them are heuristic algorithms. Fujiwara et al. propose a sequential branch-and-bound algorithm. Although it reaches all solutions and avoids exhaustive searching, the computation time still increases significantly when the number of atoms increases. Hence, in this paper, a parallel algorithm is presented for solving this problem. The experimental results showed that computation time was reduced even when more processes were launched. Moreover, the speed-up ratio for most of the test cases was satisfactory and, furthermore, it showed potential for use in drug design.

Keyword：Branch-and-bound algorithm, load-balancing, chemical compound, inference, drug design.