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Parallelization of Molecular Docking algorithms using CUDA for use in Drug Discovery

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ABSTRACT

Traditional drug discovery methodology uses a multitude of software packages to design and evaluate new drug-like compounds. While software packages implement a wide variety of methods, the serial (i.e. single core) implementation for many of these algorithms, prohibit large scale docking, such as proteome-wide docking (i.e. thousands of compounds with thousands of proteins). Several docking algorithms can be parallelized, significantly reducing the runtime of the calculations, thus enabling large-scale docking. Implementing algorithms that take advantage of the distributed nature of graphical processing units (GPUs) via the Compute Unified Device Architecture (CUDA) enables us to efficiently implement massively parallel algorithms. Two main algorithms of importance to us are knowledge based energy minimization and greedy clustering, both of which are used in our in-house docking software package, CANDOCK. We implemented and benchmarked the differences between the original (single core) and GPU accelerated versions of CANDOCK to demonstrate parallelizing these algorithms show a decrease in the overall runtime of both single target and proteome-wide docking. The presented parallel algorithms can be easily applied to other common drug design methods and packages.

KEYWORDS

Molecular Docking, Drug Discovery, CUDA, Parallel Algorithms, Software Simulation