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GPU-Accelerated Search for Interacting Atoms in a Scoring Function

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In this study, we consider a scoring function [1] for evaluating the interaction energy of protein-protein complexes composed of two all-atom proteins. During the initial stage of interaction energy evaluation within a scoring function, interatomic distances are computed for all atom pairs located within a predefined cutoff threshold, prior to the calculation of potential energy terms. This stage can be formally formulated as follows.

Let A and B be datasets in three-dimensional space, containing n and m points, respectively. A distance similarity search, for a query point $q \in B$, consists of finding all points $a_i \in A$ such that $d(q, a_i) < \varepsilon$, where $d(\cdot, \cdot)$ denotes the Euclidean distance function and ε is a specified threshold. The process of identifying all pairs of points from two sets that lie within a specified threshold distance corresponds to performing a distance similarity join, with the resulting pairs stored in a result set.

In the simplest case, the task requires an exhaustive comparison of all point pairs with distance computation, resulting in a time complexity of $O(n \times m)$. Various approaches can be employed to construct the exact set of matching pairs, including tree-based data structures such as k-d trees and AABB trees, as well as specialized algorithms designed for this task, such as Super-EGO [2].

In this work, we consider an approach based on exhaustive pairwise comparison, accelerated using a graphics processing unit (GPU). This choice is motivated by the fact that GPU-based computations are also utilized in subsequent stages of scoring function evaluation. We present several GPU-based implementations employing both general-purpose CUDA cores and specialized Tensor cores which are a compelling alternative to CUDA cores, particularly with given dimension [3]. The problem formulation, implementation, and supplementary materials are available in the repository [4].

1. S. V. Poluyan, D. A. Nikulin, and N. M. Ershov, Development and Verification of a Score Function for Estimation of Intermolecular Interactions in Protein-Protein Complexes, in Proc. Int. Conf. on ITTMM, Moscow, Russia, April 17-21, 2023 (RUDN Univ., Moscow, 2023), pp. 231-235.
2. D. V. Kalashnikov, Super-EGO: Fast multi-dimensional similarity join, The VLDB Journal, 2013, doi: 10.1007/s00778-012-0305-7
3. B. Gallet and M. Gowanlock, Leveraging GPU Tensor Cores for Double Precision Euclidean Distance Calculations, 29th IEEE International Conference on High Performance Computing, Data, and Analytics, 2022, doi: 10.48550/arXiv.2209.11287
4. Supplemental materials - URL: https://vcs.uni-dubna.ru/dsj/test

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