High-Performance and Mobile Computing Platform for Drug Comparisons on NVIDIA Jetson TK1

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A. Background and Motivation

Compound comparison is an important task for computational chemistry. In most of works, molecules can be represented as fingerprints and ***SMILES***, and then the work of compound comparison can be seen as the ***string comparison***. However, it will be time-consuming when comparing with a large amount of compounds, such as ZNIC and GDB-13 database.

B. Goal and Method

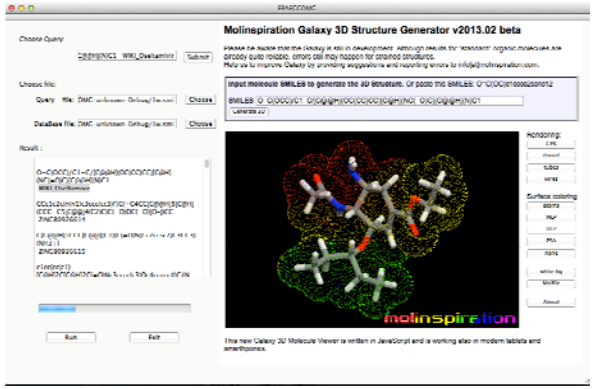
We proposed a GPU-based parallel algorithm for multiple compound comparisons (O2A and A2A) on NVIDIA Jetson TK1. In this algorithm, the goal is to compare two sets of compounds listed as *Query* and *Database* at first, and then find the compounds in *Database* with more than 0.85 Tanimoto coefficient for each compound in *Query*.

For each compound in *Query* and *Database*, it should be fragmented into a set of *q*-Lingos, respectively. a ***preprocessing phase*** is designed to do this procedure on CPU. After this phase, ***a GPU implementation of comparison phase*** is designed in order to accelerate the computation speed. In our algorithm, a compound in *Query* will be used to compare with all compounds in *Database* by all threads on GPUs when executing the kernel function once. A load-balancing strategy by considering four LINGO types can be used to accelerate the computation speed for single GPU and multiple GPUs. All of compounds in *Database* with more than 0.85 Tanimoto coefficient for each compound in *Query* are reported in the ***output phase*** on CPU.

C. Results

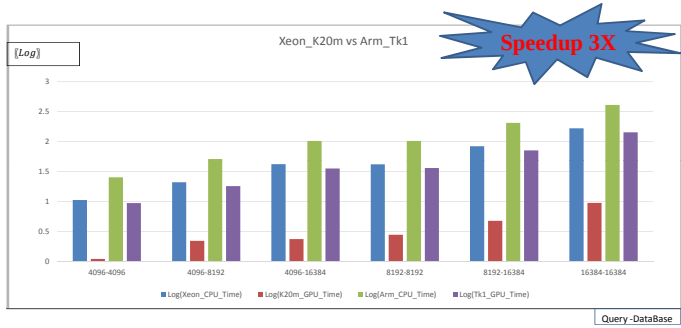
C.1 User interface

Oseltamivir (Tamiflu)
SMILE:
O=C(OCC)/C1=C/[C@@H](OC(CC)CC)[C@H](NC(=O)C)[C@@H](N)C1

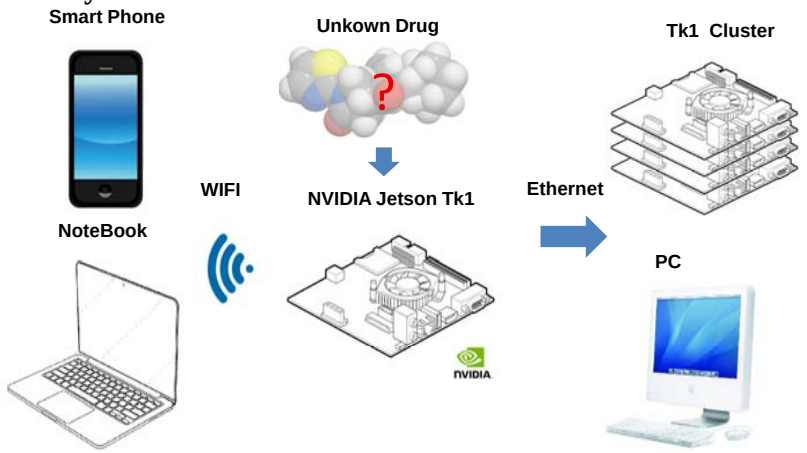


C.2 Experimental Results

Two test sets:
(s1) ten thousand compounds in *Query* and *Database*, respectively,
(s2) thirty thousand compounds in *Query* and *Database*, respectively.
Environment:
Machine 1: CPU: Intel Xeon E5-2650 2.0GHz, 32 processors, 125.87GB RAM.
GPU: Tesla K20m (4 cards), 13 Multiprocessors, 2496 CUDA Cores (192 CUDA Cores/MP, 706MHz), 4.8 GB RAM.
Jetson TK1: CPU: 4 core Cortex-A15 (2.32GHz).
GPU: Kepler GK20a, 1 Multiprocessors, 192 CUDA Cores/MP (852MHz).
Memory: 1.7GB RAM. (OS: L4T R21.1)



C.3 System Architecture



Contribution:

1. Mobile platform.
2. High performance computing.
3. Power saving.
4. Drug design:
   a. shorten the synthesis procedures.
   b. generic drugs.
5. Scalability

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