Yuejiang Yu

yuyuejiang.yyj@gmail.com | (+86) 13761350801

EDUCATION BACKGROUND

PEKING UNIVERSITY   2019.9-Present
School of Electronics Engineering and Computer Science   *Beijing, China*
B.S. in Computer Science
Expected Date of Graduate: 2023.7, Overall GPA 3.59/4.00, TOEFL 108

EXPERIENCE

ASC20-21 Student Supercomputer Challenge   2021.5 | *Shenzhen, China*
- Participate in the competition as a representative of Peking University and win First Prize (team best)
    - Contribution: responsible for PRESTO Challenge - 29-times speedup of a CPU-intensive scientific pulsar-searching toolkit using MPI, OpenMP, Ramdisk and Math kernel library (MKL) SIMD strategies
    - Skills: 1) team training of CUDA, MPI, and VTune, etc. in the broad field of parallel computing and program profiling; 2) specific optimization methodology towards CPU and IO-intensive application; 3) on-site heterogeneous cluster configuration and power control
    - Teamwork: cooperation of profiling and optimization; on-the-spot adaptability of ultra-large datasets

Internship at DP Technology as Algorithm Researcher   2021.10-Present | *Beijing, China*
- Design and develop Uni-Dock, a GPU-accelerated molecular docking software, integrated in advanced industrial computer-aided drug design (CADD) product
    - Contribution: design and implementation of molecular docking software achieving more than **1600** times acceleration on GPU compared to CPU, enabling billion-scale virtual screening
    - Skills: C++/CUDA programming and tuning techniques, especially in Monte Carlo searches; proficient in profiling hotspots, memory bounds and IO bounds associated with hardware features
    - Usability: engineering algorithmic projects to production, mastering tools such as docker, CI/CD, and unit-test
- Uni-Dock + ML: combine physical force fields of Uni-Dock with pre-trained molecular representation ML framework, improving molecular docking pose accuracy from 69% to 86%
    - Contribution: 1) design correction of physical force fields using ML to enhance the accuracy of Monte Carlo searches of poses, patented as an invention; 2) improve the probability of hit compound identification in early virtual screening

EXTRACURRICULAR ACTIVITY

ADA Innovation Fair 2020   2020.8 | *Online, Toronto*
- Develop an application prototype called E-PEDIA for college students course selection during the epidemic

Contemporary Undergraduate Mathematical Contest in Modeling 2020   2020.9 | *Online, China*
- Win the Second Prize of Beijing division

The 3rd Priority Research Application Competition   2022.8-2022.10 | *Beijing, China*
- Win the Third Prize in AI for Science track as team leader: migration of Uni-Dock from NVIDIA Volta to ROCm architecture hardware with linear scalability on 1000+ nodes

PUBLICATION

Yu, Y., Cai C., Zhu Z., Zheng H., 2022. Uni-Dock: A GPU-Accelerated Docking Program Enables Ultra-Large Virtual Screening. DOI: 10.26434/chemrxiv-2022-5t5ts

AWARDS AND CERTIFICATES

- Computer software copyright of Uni-Dock, *National Copyright Administration*   2022.5 | *Beijing,China*
- Second Class Scholarship, *Peking University*   2021.9 | *Beijing,China*
- Ubiquant Investment Scholarship, *Peking University*   2022.9 | *Beijing,China*
- Learning Excellence Award, *Peking University*   2021.9 | *Beijing,China*
- Outstanding Scientific Research Award, *Peking University*   2022.9 | *Beijing,China*

SKILLS AND HOBBIES

- Languages   Mandarin (Native), English Fluent (TOEFL 108 S25, GRE 328+4.0)
- Programming Languages   C/C++, CUDA, Python, Bash, JavaScript, HTML
- High Performance Computing   Performance profiling & optimizations, MPI, OpenMP, OpenACC