

Qi Shao

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EDUCATION

Shandong University (SDU) (985, 211)

Master of Software Engineering

Sept. 2019 - Jul. 2022

GPA: 84.6 / 100

- Supervisor: Prof. Weiguo Liu, Associate Dean of the School of Software Engineering

Shandong University (SDU) (985, 211)

Bachelor of Software Engineering

Sept. 2015 - Jul. 2019

GPA: 87.0 / 100

PROFESSIONAL EXPERIENCE

Long Term Intern, Biomaterial Department, R&D Center, National Supercomputing Center in Wuxi

Jul. 2020 - Jul. 2022

- Led the development of long-range interaction of molecular dynamics simulation on the Sunway TaihuLight
- Key contributor to the specific molecular dynamics simulation for the Sunway TaihuLight

Lecturer, ACM-China International Parallel Computing Challenge

Apr. 2021 - Nov. 2021

- Provided technical education, training and support to 150 participating teams during the competition (6 hrs/day)

Long Term Intern, Biomaterial Department, R&D Center, National Supercomputing Center in Wuxi

May. 2019 - Sept. 2019

- Familiarized with the Sunway architecture, ported and optimized scientific computing software
- Successfully ported, optimized and deployed molecular dynamics simulation application on the Sunway TaihuLight
- Developed and optimized the N-body simulation application on the Sunway TaihuLight

RESEARCH EXPERIENCE

- **SW-MSM: Efficient Multilevel Summation Method for Long-range Electrostatic Interaction on Sunway Manycore Architecture (Jun. 2020 - present, National Key R&D Program of China 2019YFA0709400, PI: Prof. Guohui Li, role: lead contributor)**

Based on the Multilevel Summation Method (MSM), SW-MSM is a long-range evolution method designed for the Sunway architecture. As the lead contributor, I have proposed specific strategies to improve performance, including reorganizing the process of MSM, decoupling dependencies of methods, implementing a preemptive framework by assembly language on computing processor elements, designing static partition method based on workload and dynamics dispatch method to solve load imbalance, optimizing the convolution by directly optimized convolution method and convolution theorem(convolution computation using Fast Fourier Transform). Based on these optimizations, SW-MSM achieved a speedup of about 190 on one SW26010 processor. As for scalability, the simulation of 77.2 million atoms can achieve 2.98ns/day with 512 core groups (33280 cores), and the efficiency of weak scalability is up to 99%.

- **Bio-ESMD: A Data Centric Implementation for Large-Scale Biological System Simulation on Sunway TaihuLight Supercomputer (Jun.2020 - Aug.2021, National Key R&D Program of China 2019YFA0709400, PI: Prof. Guohui Li, role: key contributor)**

Bio-ESMD is a biological system simulator designed for Sunway processors, which extended ESMD, a cell-list based performance proxy application, to support bonded forces. We have reorganized the data and added guest atoms in cells. We have designed the cell list with skin to reduce the cell-list reconstruction. As for force computation, We have fused all bonded interactions into one computational kernel and used local masks for exclusion, and estimated the cost of each cell by linear regression to achieve static load balance in non-bonded interaction. As a result, Bio-ESMD has $2\times$ performance of SW_GROMACS on the Sunway TaihuLight supercomputer. Bio-ESMD can scale almost linearly on TaihuLight, and can simulate 308.8 million atoms at 1.33 ns/day or 14.44 million atoms at 17.28 ns/day.

- **PhotoNs-2.0: Simulation of the N-body system in Universe (Jul. 2019 - Sept. 2019, supported by National Supercomputing Center in Wuxi, PI: Prof. Weiguo Liu, role: principal software developer)**

PhotoNs-2.0 is software to perform simulation of the N-body system in universe based on the Sunway TaihuLight. As the major developer of this project, I have separated the communication and computing to solve the imbalance of computing. I have organized a queue of pairs of computation elements to ensure the load balance of computing nodes, and I used the polynomial fitting and vectorize polynomial calculations to eliminate the global load/store operations, achieving higher efficiency. I have also designed a double-end update strategy to remove computational redundancy. Results have shown that it achieved 80-100 times acceleration compared to the benchmark program under 8 processes, 64 processes, and 512 processes.

- **SW_GROMACS: Accelerate GROMACS on Sunway TaihuLight (May. 2019-Jul. 2019, National Natural Science Foundation of China No. U1806205, 51761135015 and National Key R&D Program of China 2017YFA0604500, PI: Prof. Weiguo Liu, role: principal software developer)**

SW_GROMACS is GROMACS-based molecular dynamics simulation software ported and optimized for the Sunway architecture. I have implemented a package strategy, a software cache method to strengthen data transfer, double-end updates to reduce computation, and delayed updates with masks to efficiently solve write-conflict, and carried out all experiments presented in the paper accepted by SC19. My work has led to short-range evolution achieving 60 speedups and the entire simulation 30 speedups.

HONORS AND AWARDS

- Silver Medal of China Parallel Application Challenge on Domestic CPU (**2nd/150**), 2020, CCF TCHPC
- Graduate Academic Scholarship (**3 times**), 2019, 2020, 2021, Shandong University
- Silver Medal of China Parallel Application Challenge on Domestic CPU (**2nd/181**), 2019, CCF TCHPC
- The Third prize of the 10th National Undergraduate Software Innovation Competition (Aim to Deep Learning) (**13th/150**), 2017, Ministry of Education
- Outstanding Graduate of Shandong Province, 2019, People's Government of Shandong Province
- Outstanding Graduate of Shandong University, 2019, Shandong University
- Undergraduate Academic Scholarship (**2 times**), 2017, 2018, Shandong University

PROFESSIONAL MEMBERSHIPS

- Professional Member of High Performance Computing Committee of China Computer Federation

PROFESSIONAL ACTIVITIES

- 2021, IPCC Lecturer, CCF National Annual Conference on High Performance Computing
- 2020, CPC Team Member, CCF National Annual Conference on High Performance Computing
- 2019, CPC Team Member, CCF National Annual Conference on High Performance Computing

SKILLS

- **Programming Languages:** C/C++, Python, Java, Android

RESEARCH INTERESTS

- Scientific Computing, Computational Biology
- High Performance Computing, Parallel Computing
- Machine Learning, Deep Learning, Artificial Intelligence

PUBLICATIONS

Conference Papers:

- Zhang T., Li Y., Gao P., **Shao Q.**, Shao M., Zhang M., Zhang J., Duan X., Liu Z., Gan L., Fu H., Xue W., Liu W., and Yang G. SW_GROMACS: accelerate GROMACS on Sunway TaihuLight. Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC'19). 2019

Journal Papers:

- **Shao Q.**, Duan X., Liu W., and Bertil S. SW-MSM:Efficient Multilevel Summation Method for Long-range Electrostatic Interaction on Sunway Manycore Architecture. IEEE Transactions on Parallel and Distributed Systems (TPDS). (under review)
- Duan X., **Shao Q.**, Liu W., and Bertil S. Bio-ESMD: A Data Centric Implementation for Large-Scale Biological System Simulation on Sunway TaihuLight Supercomputer. IEEE Transactions on Parallel and Distributed Systems. (under review)

Patents:

- Liu W.(Supervisor), Wang Q., **Shao Q.**, Shao M., and Zhang T. 2022. Universe N body numerical simulation optimization method and system based on Shenwei framework. Patent CN111368484B, filed March 9, 2020 and issued April 15 2022.
- Liu W.(Supervisor), **Shao Q.**, and Zhang T. Acceleration Optimization Method and System for Parallel PME of Molecular Dynamics Simulation Software. Patent CN111444134A, filed March 24, 2020. Patent pending.