



Team Members



Yicheng Xiao (He/Him/His)
Junior
 Department of Computer Science and Engineering
 First Prize Winner of ASC24
 Distributed System and Machine Learning



Qiwen Xiao (He/Him/His)
Junior
 Department of Computer Science and Engineering
 Automated Program Repair



Hemu Liu (He/Him/His)
Junior
 Department of Computer Science and Engineering
 First Prize Winner of ASC24
 Medical Image Processing & AI
 High-performance Computing



Bingzhen Wang (She/Her/Hers)
Senior
 Department of Computer Science and Engineering
 First Prize Winner of ASC22-23
 Compiler, Security



Haoyang Qin (He/Him/His)
Junior
 Department of Intelligent Medical Engineering
 First Prize Winner of ASC24
 Machine Learning, Computational Cognitive Neuroscience



Ziheng Wang (He/Him/His)
Sophomore
 Department of Computer Science and Engineering
 Participant of ASC24, ISC24
 Deep Learning and Medical Image Processing

About Us

We Are SuperSonicTech

The **SuperSonicTech (SST)** comprises SUSTech undergraduates who are interested in computational science and engineering. We aims to serve the HPC user community at SUSTech and practice our HPC skills.

Though most of the competing members are first-time participants of the IndySCC competition, our team members have interdisciplinary backgrounds and have experienced former participants as coordinators. One of our logistic coordinators, **Mr. Jiahua Zhao**, majors in Earth and Ocean sciences and is familiar with climate and ocean simulation software.

Our Strength

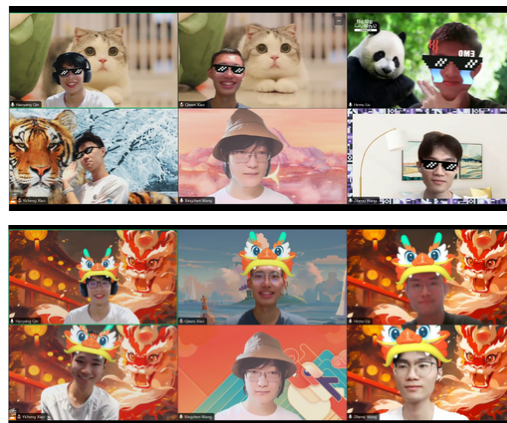
For **NAMD**, **Yicheng Xiao**, **Hemu Liu**, and **Qiwen Xiao** are all familiar with simulations.

For **ICON**, **Ziheng Wang**, **Bingzhen Wang**, and **Haoyang Qin** have relevant research background.

For **HPL** and **Mysterious Application**, all the team members are prepared to cope with the problems.

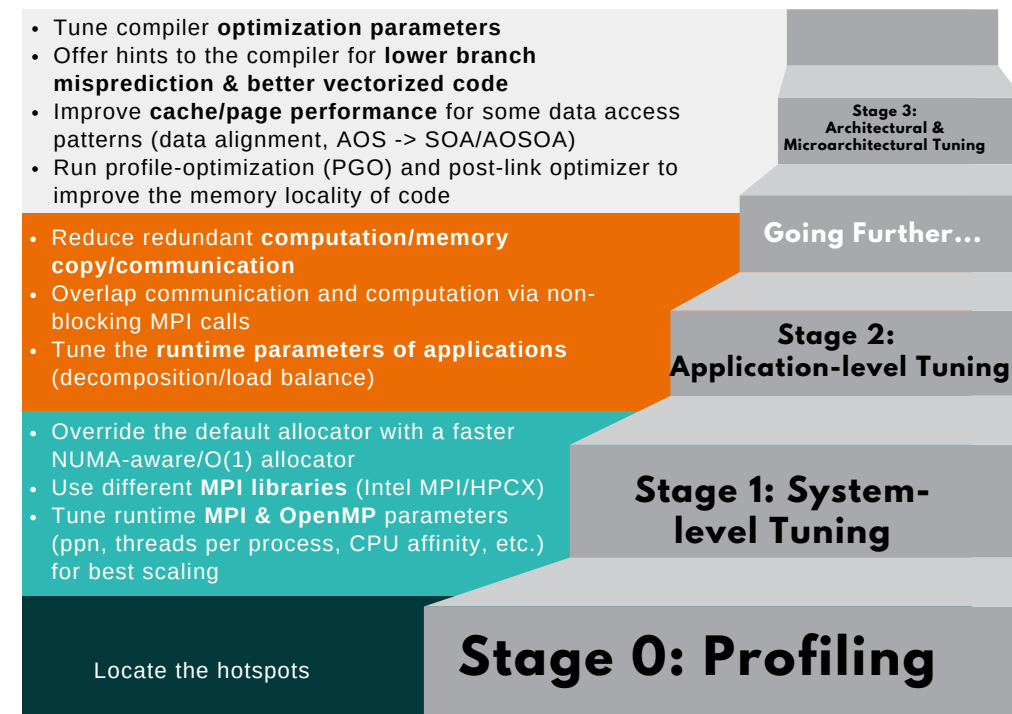
Our Diversity

SST is committed to **inclusivity** and dedicated to ensuring **equal participation** for students of all genders and ethnic backgrounds in the exploration and application of HPC technologies. Our team actively promotes diversity by recruiting members across **different departments** and **different minority groups**, allowing us to tackle challenges from multiple perspectives and devise comprehensive methods in the field of supercomputing.



Team Photo
 Bingzhen Wang, Yicheng Xiao, Qiwen Xiao,
 Hemu Liu, Haoyang Qin, Ziheng Wang

Optimization Strategy



NAMD

Speed-related:

- Patch size (*margin*), Patch shape (*twoAwayX/Y/Z*)
- PME offloading (*ldbUnloadPME*): Offloads long-range calculations to improve speed.
- Timestep (*timestep*), Multiple time stepping
- GPU acceleration (*GPUResident*)

Error-related:

- Cutoff 9.0
- PME grid spacing (*PMEGridSpacing 1.2*)

ICON

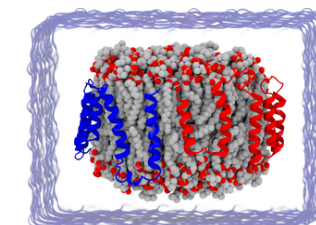
- Use different compilation flags to maximize the utilization the hardware.
- Apply more sufficient way the communication between CPUs and GPUs.
- Optimize the structure of data. Such as change the data structure like AOS and SOA. Use Parallel ,compress ,deferred I/O to accelerate the read and write of data.
- Profiling the software and parallelize, modularized, optimize the physical processes.

HPL

- Tune the **input parameters**, such as the problem size, in order to maximize performance based on the hardware configuration.
- Optimize compilation flags** based on CPU computing nodes' architecture and instruction set.
- Parallelization** of HPL benchmark testing.



- Deploy the application with different compilers and libraries using Spack
- Reserve resources for the mystery application according to the time budget/possible power limitation
- Analyze the scalability and computation/communication-intensity



Software Configuration

Package Manager Docker Job Scheduler	Modules & Conda & Mambaforge & Spack Singularity Slurm
Compiler	- AMD Optimizing C/C++ Compiler (AOCC) - Latest release of clang & polly & bolt - Some open source LLVM-based compilers for vectorization presented in recent
Profiler	- APS - AMD µProf - TAU
MPI BLAS Library Power Management	OpenMPI/MPICH BLIS, ACML (AMD Core Math Library) RAPL (Running Average Power Limit)



Team Preparation

- The Center for Computational Science and Engineering at SUSTech provides team members access to the **Qiming clusters**, enabling us to engage in coding practice, benchmarks/applications testing, and software configuration testing.
- We recognize the significance of **effective communication and collaboration**, therefore we have meetings every week to discuss about the applications and keep track of everyone's progress. During the meeting, our advisors and coordinators will give us instructions and suggestions on how to further optimize the applications.

- Our primary objective is to **foster deeper understanding of supercomputing** and seek to pay back to the community. We dedicate to identify and rectify performance bottlenecks. We focus on utilizing performance optimization tools and leveraging this platform to cultivate proficiency in programming, debugging, and comprehending codes.



Qiming Cluster
 Containing CPU nodes using Intel Xeon E5-2690 v3 @ 2.6GHz, 12 cores

