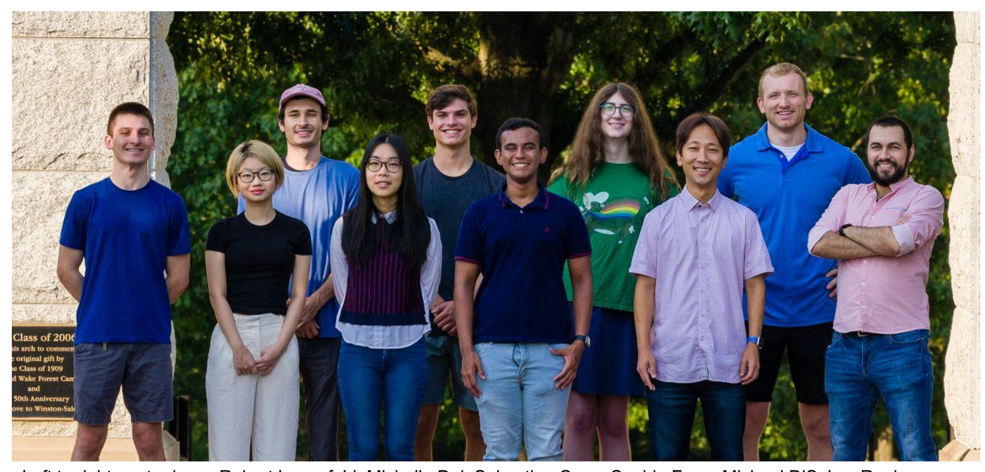
Sebastian Cave, Michelle Dai, Michael DiSalvo, Sophia Fang, Robert Langefeld, Raniery Mendes

Department of Computer Science, Wake Forest University, Winston-Salem, NC, 27109, USA

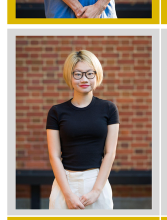
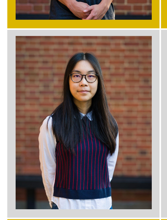
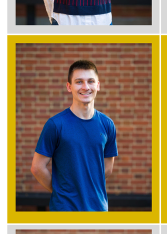
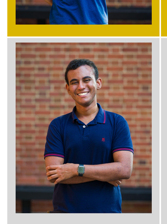
Primary Advisor: Samuel S. Cho (Depts. Computer Science and Physics)

Secondary Advisors: Sean Anderson(Information System), Adam Carlson (Information Systems) and Cody Stevens (Information Systems)

About our Team



Left to right, up to down: Robert Langefeld, Michelle Dai, Sebastian Cave, Sophia Fang, Michael DiSalvo, Raniery Mendes, Lucy McGinnis, Prof. Cho (Computer Science & Physics), Adam Carlson (Information Systems), Sean Anderson (Information Systems)

	**Name:** Sebastian Cave **Year:** Junior **Major:** Computer Science **Programming Languages:** C++, Python, Java, CUDA **Fluent Spoken Languages:** English **Research Interests:** Parallel Computation, Machine Learning
	**Name:** Michelle Dai **Year:** Senior **Major:** Computer Science and Mathematical Statistics **Programming Languages:** C, C++, Java, Python, R **Fluent Spoken Languages:** Chinese and English **Research Interests:** Neurocomputation/Bio-modeling
	**Name:** Michael DiSalvo **Year:** Junior **Major:** Mathematics and Computer Science **Programming Languages:** C, C++, Java, Python, Golang ,R **Fluent Spoken Languages:** English **Research Interests:** Computer Security, Machine Learning, Mathematical Modeling
	**Name:** Sophia Fang **Year:** Senior **Major:** Computer Science and Mathematical Statistics **Programming Languages:** C, C++, Java, Matlab, Python, R **Fluent Spoken Languages:** Chinese, English, Japanese **Research Interests:** Biostatistics
	**Name:** Robert Langefeld **Year:** Senior **Major:** Mathematics and Computer Science **Programming Languages:** C, C++, CUDA, Python, Matlab, R, Java **Fluent Spoken Languages:** English and Spanish **Research Interests:** Biostatistics, Machine Learning, Image Analysis
	**Name:** Raniery Mendes **Year:** Senior **Major:** Computer Science and Politics & International Affairs **Programming Languages:** C, C++, Java, Javascript, Python, R **Fluent Spoken Languages:** English, French, and Portuguese **Research Interests:** Cybersecurity, Latin America Democracy Studies

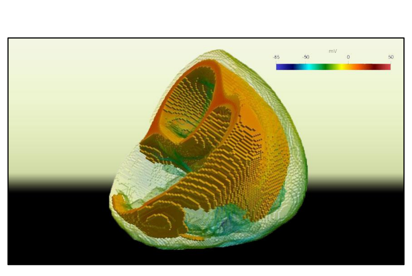
Our team consists of Computer Science, Mathematics/Mathematical Statistics, Applied Mathematics, and Engineering majors (half are double-majors) with minors in Biology, Computer Science, Economics, Japanese, and Neuroscience. Two of the students are returning veterans who participated in the previous SC20 SCC, and four are new students. Our students have taken a wide range of relevant prerequisite classes, including Data Structures I and II, Databases, Parallel Computing, GPU Programming, Numerical Linear Algebra, and Machine Learning, to name a few. Moreover, students have exposure to coding languages such as C/C++, Java, Python, MATLAB, R, CUDA, and SQL, among others. In addition, we have taken a wide array of upper-level mathematics and statistics courses, allowing us to leverage new and modern techniques for high performance computing, as well as adapt to applications from a wide range of fields. Our diverse background and wide range of skills will enable us to perform even better in the SC21 SCC.

Our team name is the "Daemon Deacons", a play on our university's mascot, the "Demon Deacons". In computing, a daemon is a process that works in the background and carries out critical processes.

While we tried to be as inclusive as possible but not target any specific group for increased representation, our team's diversity is manifested in several ways. In total, our "American" team has representatives from three different nations. Aside from English, which is spoken by everyone on the team, our team members fluently speak Spanish, Japanese, Mandarin Chinese, and Portuguese. Additionally, our team members have performed interdisciplinary computational research in disciplines including medicine, biophysics, biostatistics, neuroscience, and Latin America Democracy Studies. By having diverse backgrounds that focus on many different fields, our team can use different ideas from different fields to improve our approaches to solve problems in new, exciting ways.

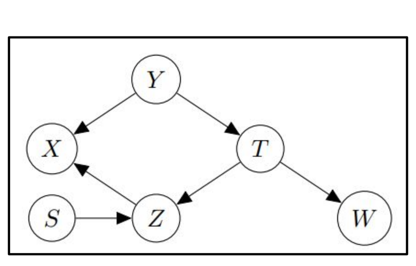
Wake Forest University is a liberal arts university with a predominantly undergraduate population currently listed on US World News Reports with a National Rank of #28. Located in North Carolina, Wake Forest University has about 5,000 undergraduate and 3,000 graduate students and prides itself on its low faculty-student ratio (1:10). Three years ago, we were the first school from North Carolina to ever participate in the SC Student Cluster Competition, and we finished 2nd among the 6 first time-competitors. Two years ago, we came 1st in the reproducibility challenge. This year, we will be the first to win (see below, right).

Applications and Optimizations



Cardioid

Cardioid is a clinical cardiac phenomena simulation program. It simulates how the electrical currents run through the heart tissue, triggering cell contractions that ultimately make the heart beat. In addition to simulating electrophysiological and mechanical organ-level simulations, a number of computed cardiac meshes can be computed, as well as torso ECG reconstructions and realistic cardiac fiber orientations can be generated. It utilizes BLAS and Lapack for mathematical modeling. Parallelization is achieved with MPI, with some code boosting performance from OpenMP. SIMD instruction sets are used for CPU architectures and CUDA for GPU architectures.

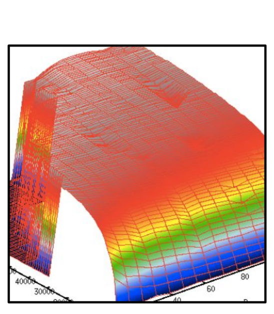


ramBLe

ramBLe is a high-performance parallel framework for computing large-scale bayesian networks. It is able to construct Bayesian networks that contains tens of thousands of variables and thousands of observations from real datasets in less than a minute on 1024 cores. The paper presents the result of parallelization on three algorithms, Grow-Shrink, Incremental Association MB, and Interleaved IAMB. We plan to reproduce similar trends of the strong scaling and weak scaling of ramBLe as on the original paper.

Quantum Espresso

Quantum Espresso is an open source suite of programs used for electronic structure analysis and materials modeling at the nanoscale. The program is based on the quantum mechanical structures of plane waves and pseudopotentials and uses density-functional theory on the computation side. We plan to utilize a GPU-enabled version of Quantum Espresso and tune the various levels of parallelism in the application.



HPL

The High Performance Linpack is the de-facto standard for comparing HPC systems. The computation it benchmarks is the solving of large dense linear algebra systems in double precision. Since we have received an optimized GPU version of linpack, we plan to utilize this on our hardware and explore the input space for configurations that can measure the full computational potential of our system.

HPCG

Short for High Performance Conjugate Gradients, this benchmark aims to provide context to HPL results. It tests access patterns that more closely reflect those of common HPC tasks, and this way incentivizes investment into their acceleration. As with HPL, HPCG can make use of GPU accelerators, allowing us to take advantage of our GPU nodes. Compared to HPL, the parameter space of HPCG is modest at 2 parameters, allowing us to use grid search to find the optimal parameter combination.

IO-500

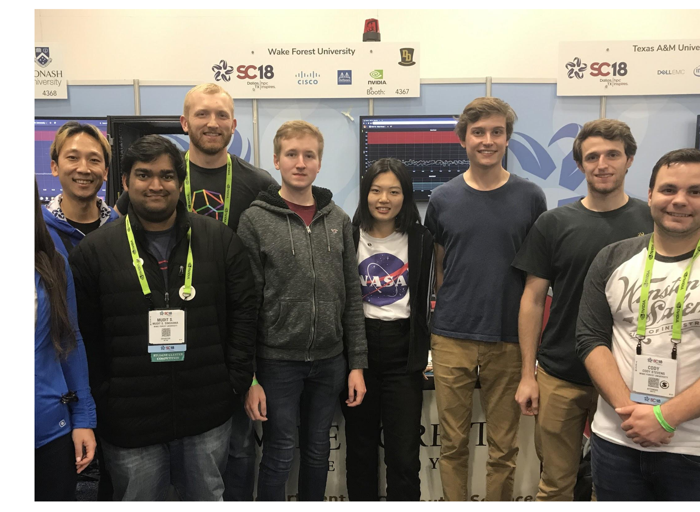
IO-500 is a benchmark measuring I/O characteristics consists of multiple subcomponents. It measure both the performance of I/O bandwidth and metadata with IOR and MDTEST respectively. For this competition, we will tune the parameters and different backends for optimal IO-500 overall performance.

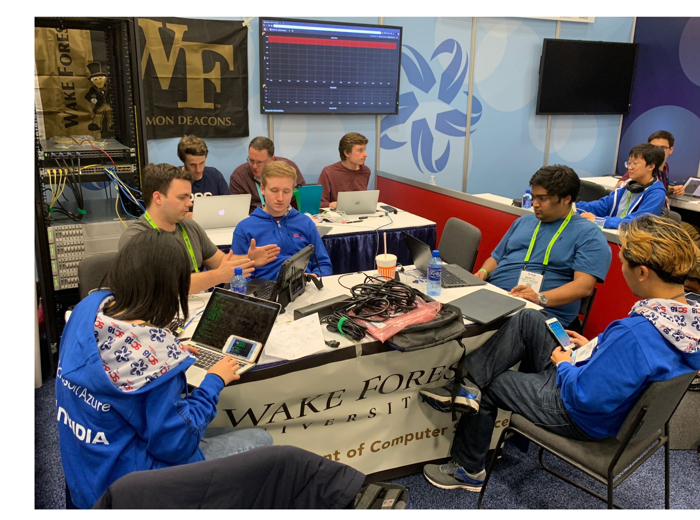
Team Preparation

To prepare for the competition, the Computer Science Department created a brand new High Performance Computing class in Fall 2017. It has been taught for ten (12) consecutive semesters by Prof. Samuel Cho (Associate Prof., Depts. Computer Science & Physics), who is the primary advisor for this team. Prof. Cho has extensive experience performing research and teaching classes in GPU Programming, Parallel Algorithms, Computational Biophysics, and Machine Learning. He has received funding from the National Science Foundation, National Institutes of Health, and NVIDIA, Inc. for research in those subjects. In addition, our team has three secondary advisors, Adam Carlson (Senior UNIX Systems Administrator), Cody Stevens (HPC UNIX Systems Administrator), and Dr. Sean Anderson (HPC UNIX System Administrator); together, they comprise the High Performance Computing Team at Wake Forest's DEAC Supercomputing Facility (4K CPU and 12K+ GPU cores). All advisors have extensive practical experience in compiling, running, benchmarking, and maintaining a variety of HPC applications and hardware.

Since Summer 2021, team members have worked independently or in groups on building the run-time environment for each application and communicated their progress to the rest of the team on a weekly basis. The installation and test-drive for each application was first done on local virtual machines, then moved to DEAC, Wake Forest's supercomputing facility, before being tested on NARF, our competition cluster.

To date, we have run all of the applications extensively using various inputs representing a wide range of possible scenarios. We have also monitored hardware and power usage throughout these runs to learn how to optimally partition these resources depending on the application inputs we are asked to run. Additionally, we have built and run several applications from previous competitions to prepare us for the mystery application.





Software Configuration and Usage

Ubuntu 21.04

Our nodes will run the Ubuntu 21.04 Server Linux operating system. This will provide a stable software platform with very recent software packages, including the GNU Compiler Suite, the oneAPI Base and HPC Toolkits, and the standard toolchain of cmake, autotools, Python, etc.

SPACK

Utilizing Spack, we will be able to have a very optimized set of applications ready to run for the competition. A tool for package management, it aims to simplify and automate the process of installing and setting up HPC applications and their dependencies. This allows us to quickly build out our software stack with a variety of dependency and optimization combinations. Ancillary libraries, such as the Intel/oneAPI MKL, Intel MPI and OpenMPI, CUDA, and a few other linear algebra, math, and utility libraries that are part of any standard HPC system will also be available for the mystery application.

SLURM

We will have the SLURM scheduler and resource manager to distribute the running of our applications so that we can allocate exclusive resources and prevent one application from taking over any one node. We have chosen SLURM as our resource manager because we have used it successfully in past competitions, and because it is also the scheduler used on DEAC. Further, we will monitor the execution of the application and limit the resources used by the applications to prevent our servers from exceeding the power usage limit. For monitoring, we plan to utilize the built in CIMC in combination with a metered PDU for power monitoring.

Slack

We have integrated SLURM and our power monitoring with Slack. This allows us to efficiently track when jobs finish and receive notifications based on current power consumption. It also integrates well with our team's current Slack communication workflow.

Hardware Configuration

For the competition, our team has recruited two vendors (Cisco Systems, Inc. and NVIDIA Corp.) to lend us equipment from September to December 2021, which will span the fall until the end of the competition in November at SC21..

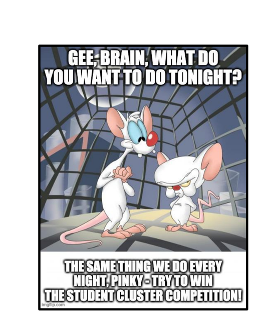
Cisco has provided two (2) C480ML-M5 servers with four (4) 12-core, 2.70GHz, Intel Xeon Gold 6226 CPUs, 384 GB DDR4 RAM, (4) 3.2TB NVME SSDs, and (4) 1600W Power Supplies in 3+1 redundancy each. For connectivity, the systems will be direct connected via one (1) dual-port Cisco 1495 VIC, which will be used to provide two 40GbE, low-latency usNIC direct connections to one another.

The main motivation for this configuration is that the C480 server will be capable of performing serial and parallel computations with the fastest communication possible, depending on the types of applications provided. The 40 GbE, usNIC connections will provide extremely fast and low-latency communication between nodes, while maintaining a simple, efficient configuration. We are hoping to maximize all of the Nvidia A100 GPUs for parallel processing, administered via software using the Open MPI framework.

We are hopeful that Nvidia will provide eight (8) Nvidia A100 GPUs with 40/80 GB memory in PCIe form factor; if disruption in the supply chain prevents the contribution of those A100s from happening, the HPC Team will reallocated eight (8) V100 GPU's (received from Nvidia as part of SCC19) from the DEAC Cluster to be used instead.

For highly parallelized GPU-enabled applications, we plan to use the NVIDIA A100 GPUs that have an ~11x speed-up when compared to the previous generation of V100 compute GPUs. With each node having four (4) NVIDIA GPUs, we will have thousands of cores that can perform parallel single-precision and double-precision computations for applications that are written in CUDA and can take advantage of the GPU architecture. Our approach is to assign a single MPI instance to a single CPU process, and that process is then mapped to individual GPUs, adjusting the process affinity and exploiting the available NUMA nodes for the lowest latency possible.

Why We Will Win



One of our secret sauces is **preparation**. We have invested a lot of time and resources to make sure that we have the strongest possible team. Three years ago, we finished 2nd out of the 6 first-time competitors. Two years ago, we came 1st in the reproducibility challenge. After the SC20 VSCC, the six undergraduate students who competed performed a SWOT (Strength, Weakness, Opportunity, Threats) analysis of their experience under the supervision of the primary advisor. From their SWOT analysis results, they identified a set of "action items" to be better prepared for the next competition. We spent the last year implementing them.

We are not only planning to win this year, we are also taking careful notes of the things that work and do not work so that we can learn to optimize ourselves too. We will overcome every failure and **persevere**. Why? We are already planning on winning next year too!

Acknowledgements

In addition to our team advisors and the Wake Forest University CS Department, we would like to thank Jeff Squyres from Cisco Systems Inc for his time spent and invaluable transfer of knowledge on OpenMPI. We would also like to thank Kevin McKenzie from Cisco Systems Inc for his time and effort securing hardware for this year's competition.