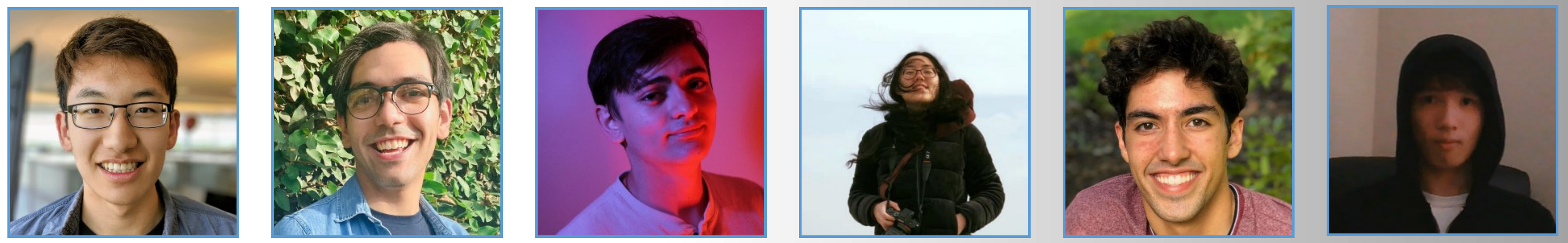
BOSTON UNIVERSITY

MIT

SPARK!

Mentored by
Kurt Keville

BUHPC @ SC20



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Our Team (+Cluster)

BU HPC

We are team **BU HPC** from Boston University where engineers and computer scientists love to work together! Coming from diverse backgrounds around the world and a variety of majors from CS to Biomedical Engineering, we are bonded by the same enthusiasm for high speed computing and algorithm optimization. All levels of expertise are welcomed here, with members of all class years, as our primary goal is to learn. Our team would like to explore the full potential of parallel computing during the competition. Hope to see you there!

ACKNOWLEDGEMENTS

A huge thank you to the **SC20 Organizers** for inviting us to compete and hosting the competition, even with all the difficulties organizing during the global pandemic!

We would like to acknowledge the Boston University **SPARK! Ignite Council** for funding our club and providing resources to facilitate our growth.

We would also like to give thanks to our competition advisor **Kurt Keville** from MIT and our club advisor **Martin Herbordt** from BU. We could not have made it this far without your guidance!

Our Unique Team of 6: BUHPC

From 4 Countries

With 5 Majors

OUR SYSTEM

For **CPU VMs**, we decided to go with the HB-series, because it is optimized for memory bandwidth workload for challenges that are memory intensive such as CESM. We chose **HB** over HBv2 mainly because of cost and we hope to evenly distribute our budget for challenges in which we can utilize GPU-acceleration such as GROMACS.

In terms of **GPU VM** solutions, we decided to go with VMs from the NCv3-series based on the benchmark results of Tesla V100 vs P100. We think that the **Tesla V100** will yield better performance for large jobs.

We will benchmark various **compiler optimizations** during the training periods to match our hardware strengths.

Azure VM Types

	General Purpose	Compute Optimized	Memory Optimized	Storage Optimized	GPU	High Performance Compute
Type	Av2, B, DCsv2, Dv2, Dsv2, Dv3, Dsv3, Dav4, Dasv4, Ddv4, Ddsv4,Dv4, Dsv4	Fsv2	M, Mv2, Dv2, DSv2, Ev3, Esv3, Eav4, Easv4, Ev4, Esv4, Edv4, Edsv4	Lsv2	NC, NCv2, NCv3, ND, NDv2, NV, NVv3, NVv4	H, HBv2, HC, HB
Description	Balanced CPU and memory	High ratio of compute to memory	High ratio of memory to compute	High disk throughput and IO	Specialized with single or multiple NVIDIA GPUs	High memory and compute power – fastest and most powerful
Uses	Testing and development, small-medium databases, low-medium traffic web servers	Medium traffic web servers, network appliances, batch processing, app servers	Relational database services, analytics, larger caches	Big Data, SQL, NoSQL databases	Compute intensive, graphics-intensive, visualization workloads	Batch processing, analytics, molecular modeling, fluid dynamics, low latency RDMA networking

Note the differences between the VMs available in Azure!

Source: *ParkMyCloud*

Why We'll Win

OUR PREPARATION

Our team prepared extensively during the **Summer and Fall** semesters, leading workshops on Cloud VMs, Parallelization, Optimization, Cluster Configurations, Benchmarking, and Large-scale Simulations. Each member of our team was specialized in one of the competition applications, leading research and optimization efforts in accordance with their skills & background.

After setting up Azure VMs, we **researched** what configurations were most efficient, what code implementations were best tailored for the specific hardware, and optimized for performance vs. cost improvements. During the weeks preceding the competition, our team setup **cloud training environments** with configurations similar to the selected competition hardware to emulate as best as possible the performance optimizations we hope to achieve.

OUR STRENGTHS

Team BUHPC brings together a diverse group of students with a variety of skills developed through personal interest and our computer science and engineering backgrounds. As a team, we have shared our strengths, learned from one another, and amalgamated our knowledge to build a well rounded and competitive group. We are prepared. We have a concrete strategy. But most importantly, we can depend on one another for support and cooperation. With our combined expertise, we know **we can solve any HPC problem thrown at us efficiently and optimally.**

OUR STRATEGY

During the training period, it is imperative that the performance per dollar cost of each VM SKU is understood and measured. To achieve this, the team will be deploying applications on various cluster configurations to understand the pros and cons of each of Azure's HPC offerings. Due to the use of **CycleCloud** as the deployment manager, clusters can be easily deployed and scrapped and deployed again. The goal of this would be to figure out which set of VMs best achieves a price to performance ratio that the team is comfortable with having as a ceiling for competition.

Management of the cluster will be done using **SLURM**, an open-source job scheduler for Linux, which can optimize the locality of task assignments, providing an efficient framework for executing workloads. Using a task scheduler will ensure minimal downtime during the precious hours of the competition. Ideally, any process started on the cluster will execute without failure. However, it is likely that there will be issues. SLURM will also be set up to notify the team members of a job failure so that it can be diagnosed and rescheduled appropriately.

Application

OPTIMIZATION TECHNIQUES

The initial plan is to perform some **preliminary analysis** of the executions of the competition applications. This would determine where various bottlenecks occur and how best to solve them. Afterwards, **performance tuning** can be done to find out exactly what SKU will work the best, whether it is the one we have decided on, or that we need to pivot. Finally, **validation** will need to be done to ensure that the system chosen works well against the budget constraint.

In terms of optimization, each application lends itself to being split across multiple executions units. This is what the team is most comfortable with, and it will be the focus for the one-month period leading up to the competition. This will be the hardest part of warming up to the competition, but it also where there is the most room for improvement.

Preliminary Analysis → Performance Tuning → Validation

Apps and Benchmarks

LINPACK: The HPC benchmark for dense linear equations. Based on our research, our set-up with the NVIDIA Tesla V100 should accelerate the performance. Additionally, we plan to profile and optimize our system with Arm Forge to improve our results from the benchmarks.

HPCG: A broad test on Conjugate Gradient for ranking top systems. The GPU focus on our budget should yield strong results.

CESM: The Community Earth System Model (CESM) is a state-of-the-art climate model developed by the National Center for Atmospheric Research. Single core high speed and I/O are critical for this application.

GROMACS: GROMACS is a versatile package to perform molecular dynamics. Our focus on GPU and single core speed is critical for performance in applications like GROMACS.

IO500: The IO500 benchmark is a benchmark suite for High-Performance IO. For our filesystem we plan to use BeeGFS as it is robust and easy to deploy. Based on the benchmark results of other supercomputers, we think BeeGFS is competitive compared to other filesystems.

MEMXCT (Reproducibility): MemXCT uses an optimized SpMV implementation with two-level pseudo-Hilbert ordering and multi-stage input buffering to study the internal morphology of materials at high resolution. We plan to optimize the GPU algorithms of this code and use smart compilers (*OpenACC*).