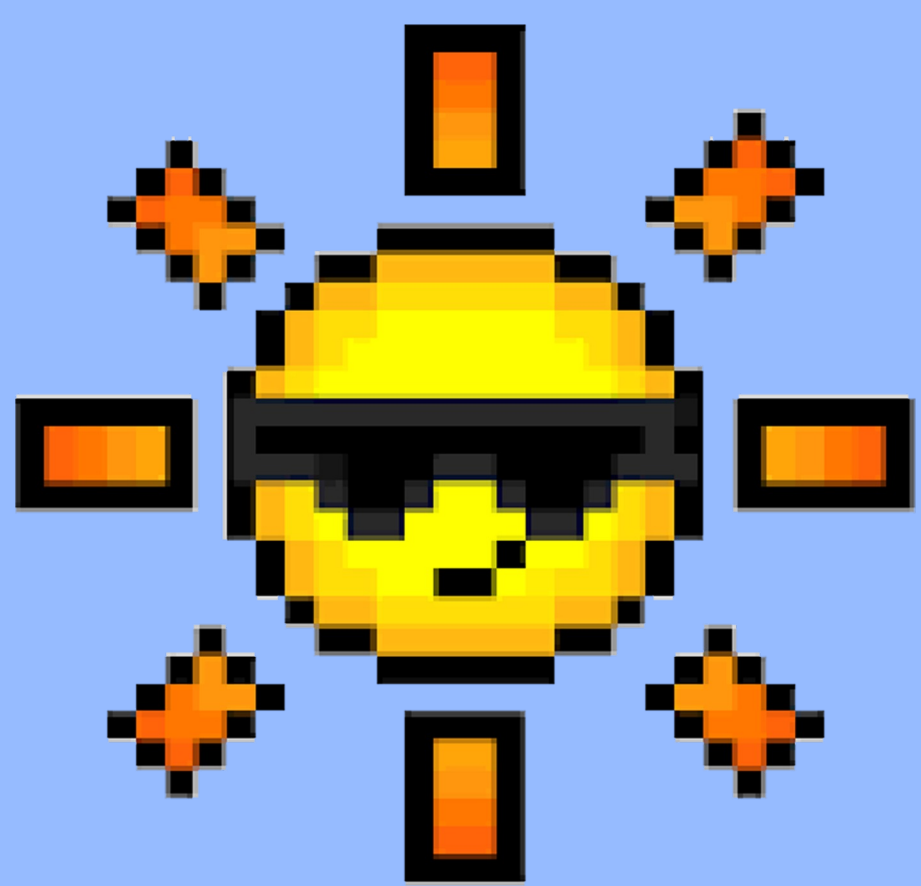




High Performance
Research Computing
DIVISION OF RESEARCH

Team Gig'Em Bytes

John Mason Ammon, Tanvi Aggarwal, Minh Nguyen,
Victoria Chen, Molly Jackson, Sophia Evanisko, and Dr. Lisa M. Pérez



Atlanta, GA
hpc creates.



Meet the Team!



John Mason Ammon
Major: Computer Science
Skills: Machine Learning,
Cloud Computing
Roles: Team Lead, HPL,
NAMD



Victoria Chen
Major: Computer Engineering
Skills: Software Development,
Linux/Bash
Roles: HPL, ICON



Tanvi Aggarwal
Major: Computer Engineering,
Physics Minor
Skills: Mathematics, Statistics
Roles: HPL, ICON



Molly Jackson
Major: Electrical Engineering
Skills: Computer Architecture,
Machine Learning
Roles: MLPerf, NAMD



Minh Nguyen
Major: Computer Science
Skills: Software Development,
Scripting
Roles: HPL, ICON



Sophia Evanisko
Major: Applied Mathematics,
Computer Science
Skills: Statistics,
Software Development
Roles: MLPerf, NAMD

Team Overview

The Gig'Em Bytes team possesses diversity in both the members' areas of study and cultural backgrounds. The team represents different areas of STEM, from computer & electrical engineering to applied mathematics and physics to statistics, which allows the team as a whole to tackle problems from any STEM discipline. The team's diversity allows for multiple perspectives and ways of thinking, a diversity in perspectives that will cultivate the flow of ideas and problem-solving methods that is perfect for the SCC. Each team member will work on specific applications with at least one overlap so that there is always one other team member that can be referenced when questions or issues arise. In addition to the 6 team members competing, we have an extended team of undergraduate members helping with programs such as NAMD, ICON, MLPerf Inference, and HPL.

Applications & Benchmarks

NAMD

NAMD is used for the efficient simulation of large-scale biomolecular systems. We have been given the amazing opportunity to receive guidance and support from experts in NAMD at Texas A&M's High Performance Research Computing (HPRC). We have access to NAMD on HPC systems allowing us to practice executing and tuning NAMD jobs on a wide variety of simulations.

ICON

An advanced climate modeling framework which uses weather pattern predictions to combat climate change and natural disasters. We plan on working to create and run real-world test cases to familiarize ourselves with the GPU centric ICON.

MLPerf Inference

A benchmark suite designed to measure the performance of machine learning systems during the inference phase, where trained models process inputs and produce results. MLPerf inference will benefit from the 192 GB of DDR5 memory per node.

HPL

HPL (High performance linpack) is a mobile and freely accessible implementation of a high-performance computing benchmark that is utilized to compute the peak performance of a HPC cluster. Through HPRC's system Grace, we were able to compile and run HPL on GPU nodes to gain experience with the code and learn to optimize the runs.

Reproducibility

We are leveraging the DataLife tool, which is available on GitHub, to reproduce and validate the results from the paper on Data Flow Lifecycles (DFLs). The tool provides a powerful framework for analyzing and optimizing complex scientific workflows by visualizing data movement and identifying bottlenecks. Our preparation involves practicing with a variety of workflows, using the DFL analysis to fine-tune task placement and data handling to achieve optimal performance.

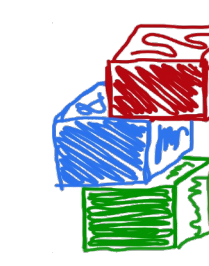
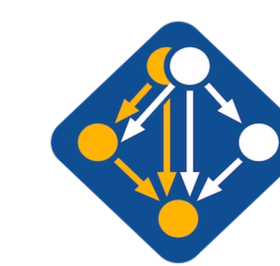
Mystery Application and Benchmark

Our hardware configuration is prepared for a CPU or GPU centric application and benchmark.

Software Configuration



OS: Rocky Linux 8.10



easybuild

Software Management: Spack and EasyBuild



Job Scheduling: slurm



File Management: BeeGFS

BeeGFS®

Hardware Configuration

Hardware Configuration

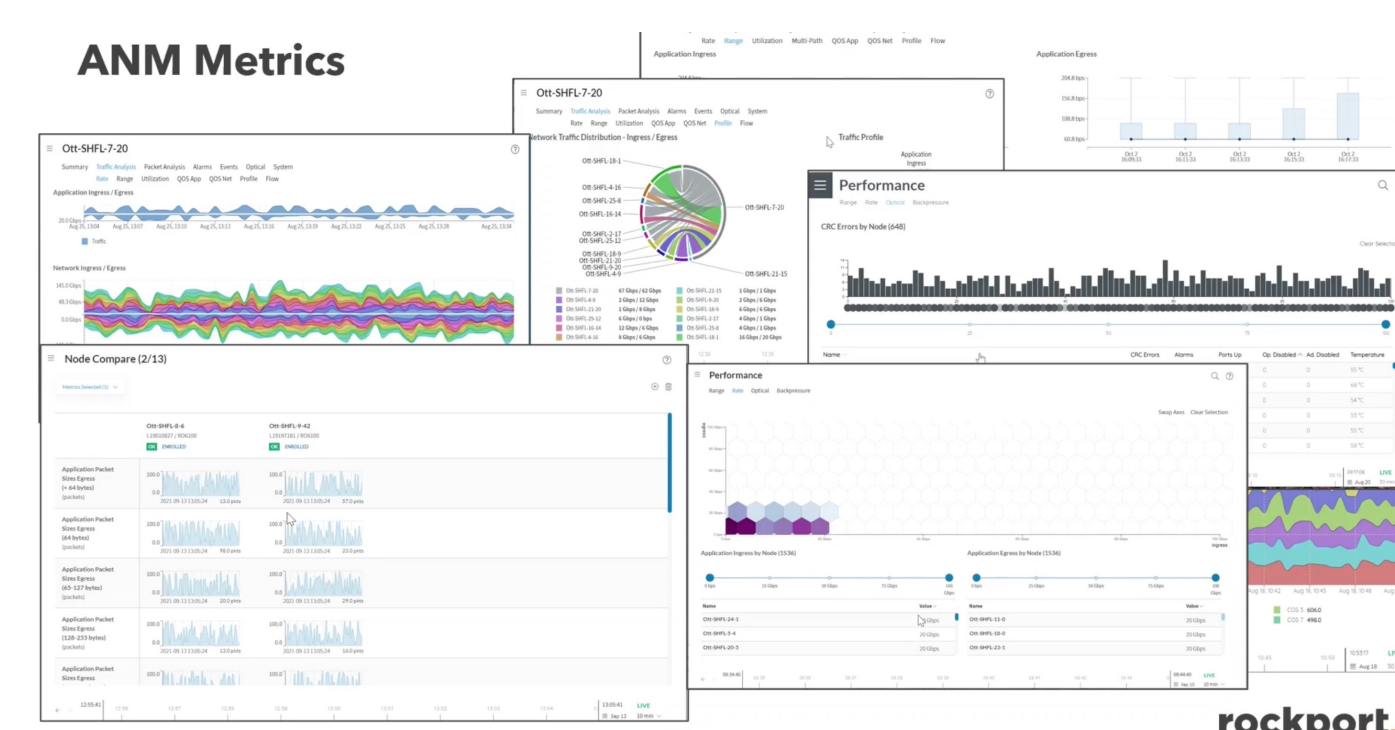
4 Dell PowerEdge R7625 servers, each with:

- Dual AMD 9534, 2.5GHz, 64C/128T processors
- 2 AMD Instinct MI210 64GB GPU
- 192 GB DDR5
- 2 480GB M.2 NVMe (Raid 1)
- 1.6TB NVMe

Network: Rockport Switchless Network
with Autonomous Network Manager
(ANM)

DELL Technologies

AMD
EPYC



Hardware Motivation

The Rockport Switchless Network by Cerio provides an amazing low power solution. Power consumption is lower than common HPC networks due to the switch being passive while the power is only consumed by the FPGA card. This network card has 12 bi-directional network connections, uses rockport Network Operating Software (rNOS), with a consumption of 34W at max load. The AMD Epyc 9534 CPU provides 64 cores and 128 threads, is extremely power efficient, and features 256MB of L3 cache per 4 cores. The AMD MI210 GPU cards provide the best balance of power consumption and performance with support for IEEE-compliant FP64 processing and a large 64GB High-bandwidth HBM2e memory. NVMe storage offer high performance and low power over traditional spinning disk.

Preparation & Strategy

Overview

The team has access to system administrators and user support specialists at HPRC and attends HPRC training session. The team meets weekly and completes application specific assignments on the HPRC systems.

Time Management

Our team is made up of members with diverse academic skill sets and strong learning abilities so we plan to each specialize on an aspect of the competition so that during the competition, we can all efficiently work. Smart scheduling of jobs via the slurm queueing system will allow the team to focus on problem solving and organization while jobs run. Checkpointing is critical in the event that there is an unexpected interruption or need to kill a running job.

Optimization Strategy

Since we have access to HPC hardware, we have compiled applications and benchmarks with various flags to maximize the performance. We also benchmark various system sizes to use the resources efficiently.

Power Limit

To control power usage, the team will utilize the rocm-smi tool to limit the power consumption of the AMD GPUs while still achieving optimal performance within the power constraints. For the AMD Epyc CPUs, we will make use of the cpupower utility to set the cpu frequency. Our use of Rockport network will conserve an immense amount of energy within the cluster due to its switchless fiber optic design. We will have cron jobs in place to monitor total and node level power consumption and automatically modify CPU and GPU power usage when needed.

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