

High-Performance Cluster Computing:

Teaching Young Scientists and Engineers Future Computing Methodologies

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What is High Performance Computing:

- High-Performance Computing is the application of Computational Science using "supercomputers", large clusters
 of computers working together capable of <u>hundreds of quadrillions of Floating Point Operations Per Second</u>
 (FLOPs).
- Computational Science is a rapidly growing multidisciplinary field that uses advanced computing capabilities to
 understand and solve complex problems. Computational Science involves the development of models and
 simulations to understand natural systems. ALL science is moving towards using computational methods!

Student Cluster Competition:

- An international cluster computing competition for students from all over the world.
- Held at Supercomputing, a top tier conference, provides excellent opportunities to learn from and network with experts in the field.
- Teams run a set of HPC applications and complete a set of goals with each application.
- Achieving the best performance on our cluster setup we gain more points and a higher ranking.
- Provides invaluable experience working with large amounts HPC resources and commonly used HPC workloads.

Competition Experience, Fall 2020

In Fall 2020, 6 CI competed in the Virtual Student Cluster Competition. We ran applications on Azure Cyclecloud; spending a combined budget of \$61,300 of cloud credits during the competition. The Clemson Team placed 15th overall, posted a High Performance Linpack Score of 32.6 TeraFlops. We also completed all tasks for the Mystery Application miniVite, an ECP Proxy Application used for community detection over a graph. Our critique written for the reproducibility challenge on a paper from SC'19 is being considered publication in a special edition of the IEEE Transactions on Parallel and Distributed Systems on reproducibility.



Example Applications and Benchmarks from 2020	
Gromacs	Molecular dynamics simulator
High Performance Linpack	Performance Benchmark
HPCG	Performance Benchmark

Raspberry Pi Clusters

- Each student assembled their own 4 node Raspberry Pi Cluster.
- Pi Clusters contain resources similar to that in supercomputers at a fraction of the cost.
- Building these clusters students we investigate HPC concepts such as strong and weak scaling.
- By constructing their own clusters, students have the freedom to experiment with software configurations and applications
- Learning how to install software on these systems also helps students prepare for the Student Cluster Competition.



Figure 1: A Student's cluster, made from Raspberry Pi's

Soft	ware
Ubuntu 20.04.2 LTS	Operating System
MPICH 3.3.2	Message Passing Interface
NFS 4.2	Shared File System

64 GB USB 3.1 Flash Drive
4x Cat 6 Patch cables
5 port network switch
4x 32 GB micro SD card
4x Type C charge cables

4 node Pi rack

4 port usb power supply

Hardware

4x Raspberry Pi 4

Applications of High Performance Computing:

Gromacs is a molecular

dynamics simulation tool

Researchers perform

intensive and complex

biomechanical systems

used to research

biomechanics.

computationally

and free energy

calculations

Gromacs:

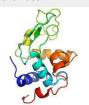


Figure 2: Lysozyme in Water

MemXCT:



Figure 3: Reconstructed scan of a Shale Rock Sample using MemXCT MemXCT is a massively parallel application for reconstruction of X-ray computed tomography reconstruction featured as the Reproducibility Application at the SC'20 Virtual Student Cluster Competition