CLOUDY WITH A CHANCE OF HPC

TEXAS A&M AG-JAG CLUSTER TEAM

SC20 Everywhere we are | more than hpc.

AG-JAG CLUSTER

INTRODUCTION

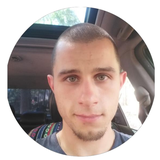
THE TEAM

The Texas A&M Ag-Jag Cluster cross-institutional team consists of three students from Texas A&M University (TAMU), College Station, and three students from Texas A&M University-San Antonio (TAMU-SA). The members of the Ag-Jag Cluster team are a diverse group of experienced college students whose educational backgrounds include Computer Science, Cyber Security, Computer Engineering, and Technology Management. The team members expertise ranges across different aspects of computing including Linux, system administration, cloud computing (AWS/GCP), computer programming, computer networking, and Cisco infrastructures. All members of the Ag-Jag Cluster team have a strong interest in HPC, cyber security and cloud computing.

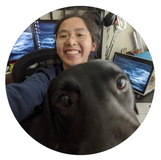
DR. LISA M. PÉREZ
Computational Chemistry & HPC
Team Advisor – TAMU

MICHAEL K. LAU
Computer Science
CESM2, Reproducibility

DR. SMRITI BHATT
Computing & Cyber Security
Team Advisor – TAMU-SA



PETAR LACHKOV
Computing & Cyber Security
CESM2, Mystery



SHAINA D. LE
Computer Engineering
GROMACS, Reproducibility, Mystery

DYLAN M. RODRIGUEZ
Technology Management
GROMACS, Mystery

JONATHAN ROSETT
Information Assurance & Cyber Security
CESM2, Reproducibility

SELINA L. URIAS
Computing & Cyber Security
GROMACS, CESM2, Reproducibility

ENHANCING DIVERSITY

- Members of the team possess cultures from three continents: North America, Europe, and Asia.
- Team is led by two women.
- Members have a healthy mix of career interest post-graduation.
- Two team members were instructors and counselors for Texas A&M's Summer Computing Academy for K-12 students.

WHY WE WILL SUCCEED

- System administrators and User Support specialists at TAMU High Performance Research Computing (HPRC) offered expert guidance.
- The team received support from experts in CESM2 (Abishek Gopal, TAMU iHESP) and GROMACS.
- TAMU HPRC provided access to on-campus computing resources, like the Ada and Terra clusters for preliminary application testing in the early stages of the competition.
- Dell provided resources to prepare for the competition through the Dell Innovation Lab.
- Working in teams created redundancy with application knowledge, ensuring everyone was knowledgeable in multiple applications.
- Three team members work at Texas A&M High Performance Computing Research.
- Team members gained invaluable experience from Student Cluster Competition SC18, Asia Supercomputing Community Student Challenge, cyber security capture-the-flag events, hackathons, and other programming competitions.

CLOUD CLUSTERS

INFRASTRUCTURE

CPU Dense Cluster 1 – x nodes of HC44rs
CPU Dense Cluster 2 – x nodes of HB120rs v2
GPU Dense Cluster – x nodes of ND40rs v2
x will vary depending on the size of the problem/database and the budget available.

SOFTWARE

Operating System	CentOS 8
Compiler	Intel or GNU
Interconnect	IB/RDMA
I/O	BeeOND
HPC & Budget Control	CycleCloud CLI
GPU Runtime	CUDA
MPI	OpenMPI, IntelMPI

DRIVING FACTORS: BUDGET & PERFORMANCE

- The hardware was chosen in consultation with experts in the applications and our sponsors with regards to feasibility of budget management with optimal performance.
- H8 Promo may be used as the head node in order to take advantage of its lower price.
- HC44rs vs HB120rs v2 application specific benchmarking for Intel vs AMD.
- Spot pricing can also be taken advantage of during checkpointed runs
- SLURM queueing system integration to auto-scale the cluster size.

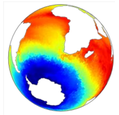
APPLICATIONS & OPTIMIZATION STRATEGIES

BENCHMARKS

HPL & HPCG: Automated runs to determine optimum input parameters for various cluster configurations to stay in budget.

IO500: Tune the number of MPI workers per node and use the fast BeeOND filesystem.

CESM2

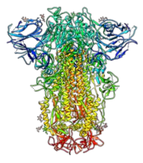


Using the CESM Load Balancing Tool along with multiple manual load balancing exercises to determine the most optimal PE layout for the chosen cluster configuration.

GROMACS

GROMACS FAST. FLEXIBLE. FREE.

- Determine the algorithms and their implementations for the provided dataset to tune the run parameters accordingly.



- Enabling multi-level parallelization with MPI and OpenMP to acquire speedup for highly-parallel portions of the simulations, such as PME, and disable it if called for by the architecture to reduce overhead.
- Allow simulations to run hybrid acceleration to balance the load between CPUs and GPUs, and keep costs in check by not running the simulations on a single type of processor.

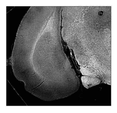
MYSTERY APPLICATION

Preparation included referencing applications in this category from previous years. As team members worked on the listed applications, we maintained notes on the build process. These documented processes, along with previous experience building software on Linux distributions contribute to our confidence with regards to the Mystery Application.

CHECKPOINTING

- Checkpointing during runs lessens the risk of data loss.
- Saves time in event of disruptions
- Application state is periodically written to disk so it can be resumed later
- GROMACS and CESM2 have integrated checkpointing

REPRODUCIBILITY CHALLENGE: MEMXCT



Leverage the ARM Forge parallel profiler to identify bottlenecks in various portions of the program, and acting accordingly to optimize the code.

TEXAS A&M UNIVERSITY | DELL EMC | High Performance Research Computing, DIVISION OF RESEARCH | Microsoft | TEXAS A&M UNIVERSITY SAN ANTONIO