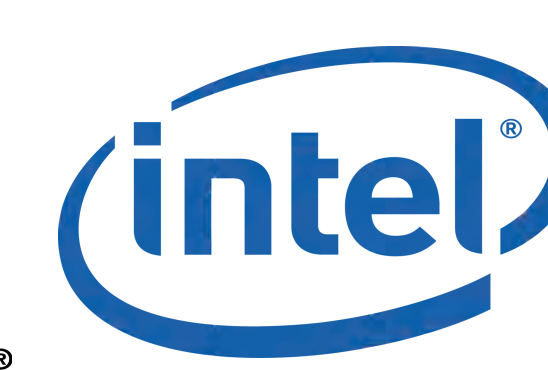
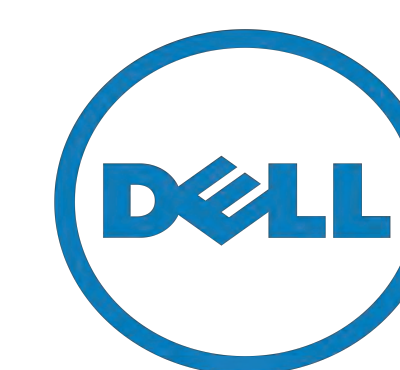


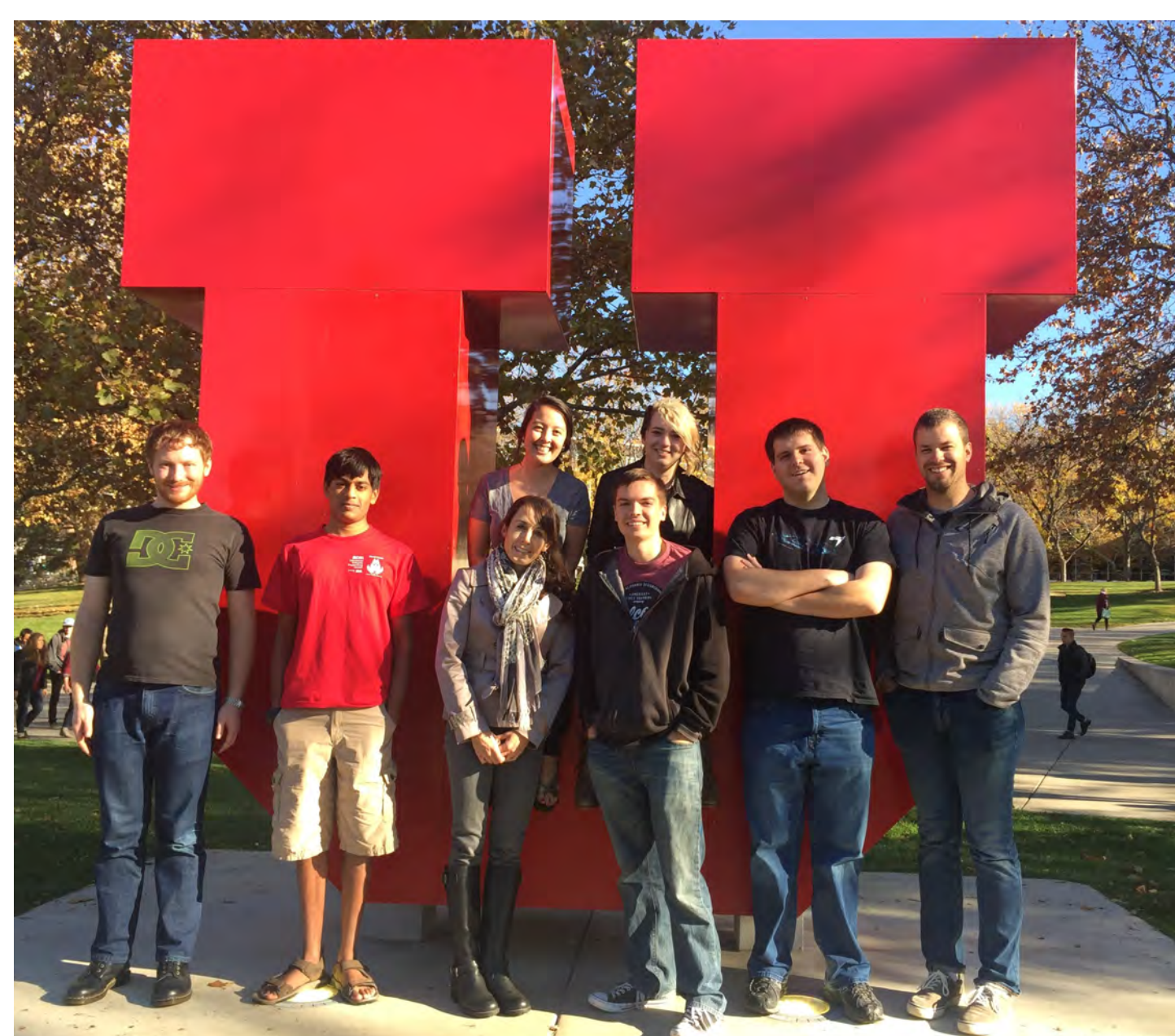
Team SupercompUtes

Mark Baranowski, Braden Caywood, Hannah Eyre, Janaan Lake, Kevin Parker, Kincaid Savoie



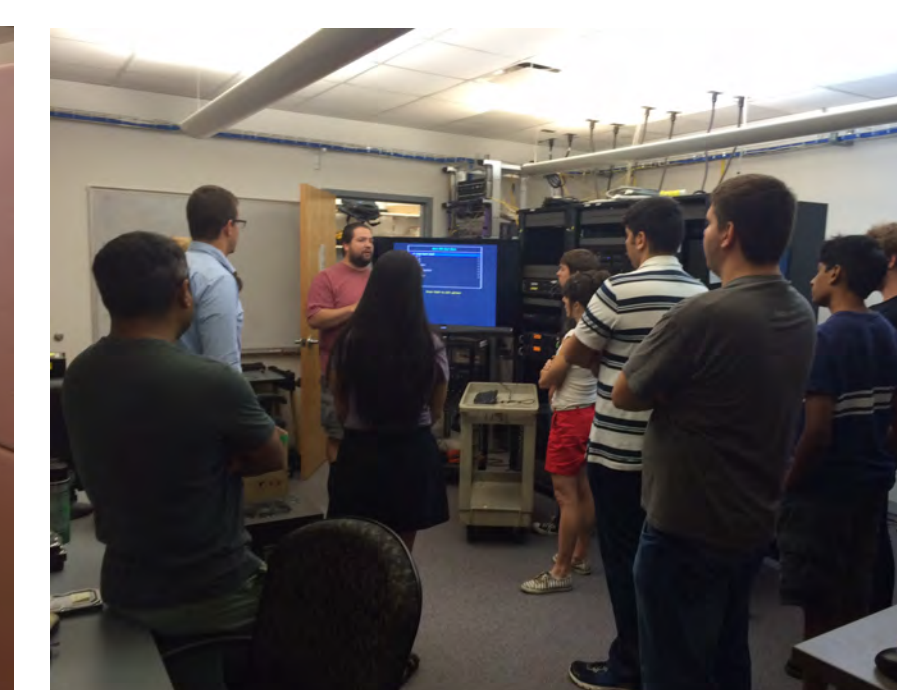
ABOUT OUR TEAM

- Our team was selected from a special topics class taught by two professors active in the SC community
- To recruit students for the class, the female professor advertised in classrooms and an ACM chapter meeting and asked other professors for suggestions to encourage diverse involvement
- On our team of six, two are female; in contrast, our undergraduate CS/CE majors are only represented by 11% females
- The team is comprised of Computer Science, Computer Engineering and Mathematics undergraduates with expertise in biology, the arts, business, finance, Spanish, and several have significant work experience
- At the beginning of the semester we worked in groups to build and run the applications, but over time the tasks have become individualized to leverage expertise and interest



COMPETITION PREPARATION

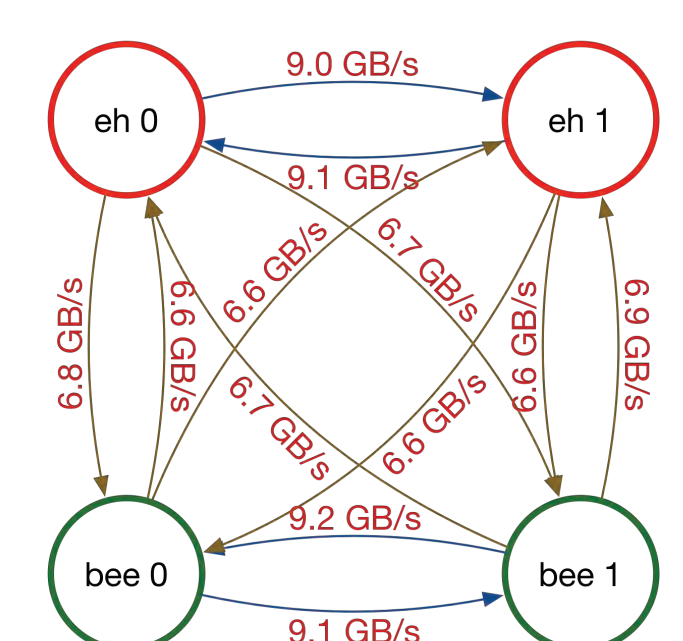
- We began meeting in the summer to tour the Data Center, learn about the competition, and start looking at the applications
- In a special topics course in the fall, we acquired broad knowledge of HPC foundations, scaling and performance, and hardware and software technologies
- HPC-oriented faculty and Center for High Performance Computing staff guided us on underlying concepts and competition preparation
- Experts on the applications and technologies provided guest lectures and met with us individually to assist in bringing up the applications on the cluster
- During many afternoons, we could be found gathering at the Center for High Performance Computing office which housed our cluster. The CHPC was critical in our preparation for the conference, providing us with space to work, and around the clock assistance
- Mystery application preparation included practicing using HPGMG in a competition setting, learning how to use checkpointing in OpenMPI, and using Allinea to profile the mystery application



SOFTWARE AND HARDWARE SYSTEM

HARDWARE CONFIGURATION OVERVIEW

- Our cluster has two Dell C4130 nodes, called Eh and Bee, each with a 128GB SSD drive attached, for a total of 40 cores and 256GB RAM
- Each node has two 2.4 GHz Intel Xeon E5-2640 v4 CPUs each with 10 cores and 64GB 2133MHz DDR4 memory
- The cluster incorporates eight Nvidia Tesla P100 (Pascal) GPUs attached through PCIe slots and rated at 4.7 TFlops per card for double precision computations
- Each node has an Omni-Path Fabric adapter 100 Series supporting up to 100 Gbps per port, effectively increasing the bandwidth between the two nodes and enabling us to design a fully-connected topology



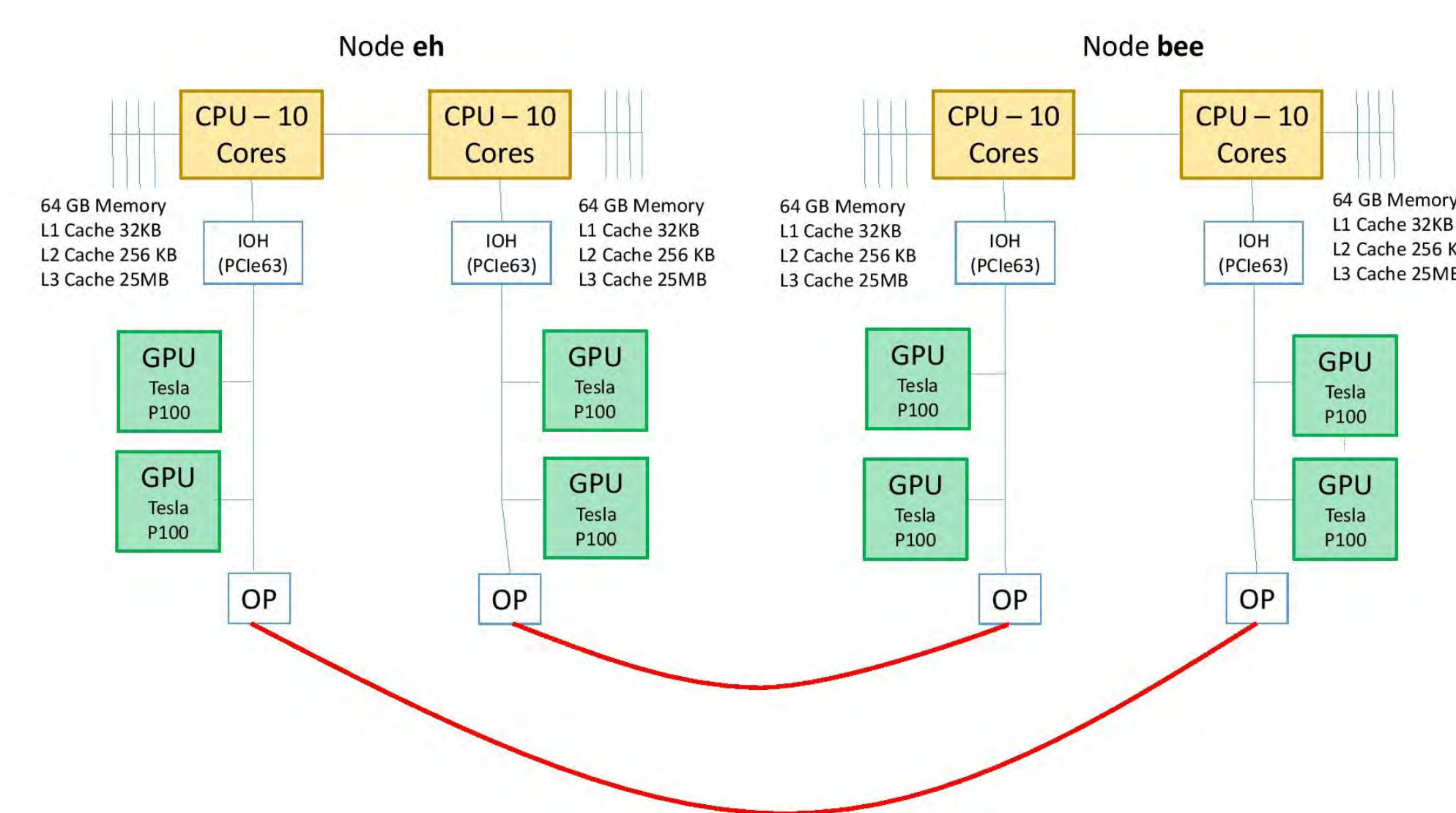
Omni-Path Bandwidth Measurements

JUSTIFICATION OF HARDWARE CONFIGURATION

- Our cluster is comprised of two fat multi-core nodes populated with GPUs and a high bandwidth interconnect
- A GPU-centric architecture was motivated by the applications and the power constraints, which could exploit the higher parallelism and memory bandwidth in a more power-efficient package (all but ParConnect can exploit GPUs)
- From the machine balance calculations below, the GPUs are capable of more computation relative to memory bandwidth

Machine Balance

- Xeon E5-2640 v4: $(400 \text{ GFlops}) / (89 \text{ GBytes/s}) = 4.49$
- P100: $(4.7 \text{ TFlops}) / (495 \text{ GBytes/s}) = 9.49$



SOFTWARE

- We adopted most of the software stack that was already installed on the CHPC clusters to make it easier for us to get help on configuration issues
- Operating System: Centos 7 flavor of Linux
- Compilers: Gnu Compiler Collection (GCC) 4.8.5 and Intel C++ compiler ICC v16.0.3
- OpenMP: v3.1
- CPU BLAS: Intel MKL v11.3.2
- MPI : Intel MPI v5.1.3, OpenMPI 1.6.5
- Modules: Lmod framework from TACC to easily switch between different software packages and dependencies
- Profiling: Allinea profiler
- The Intel MPI implementation is optimized for OmniPath and we use OpenMPI with built-in checkpointing to prepare for power outages
- The GPUs use Nvidia CUDA Toolkit (v8.0, v7.5 and v7.0) and the latest implementation of HPL and HPCG provided by Nvidia

OPTIMIZATION STRATEGY

- To best allocate our time we will complete ParaView and ParConnect on the first day
- We will then divide our time between HashCat and the mystery application

HPL

- Used optimized benchmark implementation from Nvidia
- Autotuning to identify the best values for problem size, block size, and 12 other variables
- Graphs and charts were created to help us steer the autotuning in the right direction

HPCG

- Used optimized benchmark implementation from Nvidia
- Autotuning to identify the best problem size and MPI implementation
- Ran HPCG at all sizes within the scope of the competition and created graphs to determine the best run

Distributed Password Auditing/Recovery

- The entire class experimented with different approaches to the problem
- Researched password security and what a typical password looks like
- Scraped different websites and password breaches to create dictionaries

ParaView

- Built Paraview so it can run on either multiple or a single GPU, and we can specify exactly which GPU each job runs on
- Plan to break out frames into many jobs spread across multiple GPUs

ParConnect

- Investigated various MPI implementations for the lowest overhead
- Scripting to extract compute and communication times from ParConnect runs

WHY WE COULD WIN

- Diversity of our team, with respect to gender, age, skill sets, and background
- State-of-the-art hardware due to working with great engineers from three renowned companies
- Optimized HPL and HPCG implementations from Nvidia
- Input and excellent advice from many experts
- OpenTuner used for autotuning in order to improve benchmark results



ACKNOWLEDGMENTS

We are grateful to our sponsors Dell, Nvidia and Intel, and to the many people who helped prepare us for this competition: professors of our class, Mary Hall and Hari Sundar; Center for High Performance Computing staff, especially Brian Haymore, but also Anita Orendt, Martin Cuma; guest lecturers who were experts on specific technologies including Ganesh Gopalakrishnan (MPI), Alan Humphrey (Allinea), Aaron Knoll (Paraview), Kelly Genessy and Nate Henne from Utah Education Network (Hashcat) and Tharindu Rusira (OpenTuner).