TEAM QUOKKA – AUSTRALIA

William Davey · Sandra Lee · Kai Dombrowski · Malin Sundberg · Samuel Evans-Powell

INTRODUCTION TO TEAM AND SCHOOL

Quokka at the Pawsey Centre's supercomputer cell

This is team Quokka, Quokkas are very small and smart marsupials found only on islands off the coast of Western Australia. It is Team Quokka's third year representing Australia at the Student Cluster Competition (SCC); brought together by Pawsey Supercomputing Centre.

The Pawsey Supercomputing Centre is a national high-performance computing facility in Perth, Western Australia. Pawsey is an unincorporated joint venture between CSIRO, Curtin University, Edith Cowan University, Murdoch University and The University of Western Australia and is supported by the Western Australian and Federal Government. Researchers across Australia have access to multiple systems at Pawsey, including Magnus, a 1 PFLOP machine and one of the largest supercomputers in the southern hemisphere. In addition to HPC resources, Pawsey provides researchers with infrastructure and support for visualization, cloud computing, and data storage.

Past SCC teams at Pawsey have typically been composed of students from several of Pawsey's partner institutions. However, this year's team is made up entirely of students from Murdoch University. Our students are all computer science majors, but are each focused on different aspects, including game design, mobile app development, system administration, and cyber-forensics. Also, our team has an international component, with students hailing from Australia, Germany, and Sweden.

HARDWARE DESCRIPTION

Our cluster is a Cray system made up of nine GreenBlade nodes. Each node contains two Intel Xeon "Haswell" CPUs. In addition, 2 of the nodes are hybrid nodes, each housing 2 NVIDIA Tesla K40 GPUs. The system has a total of 1.1 TB of RAM (128GB per node), and 2.25 TB of storage. Communication is handled on two different interconnects; an Ethernet network for system management, and a high-speed 56Gb/s Infiniband FDR network for inter-node communication.

System	Cray CS400-AC
Total Nodes	9
Total Cores	260
CPU	Intel E5-2695V3 x 14 (CPU Nodes) Intel E5-2698V3 x 4 (GPU Nodes)
Accelerator	NVIDIA Tesla K40 x 4
Memory	1152 GB DDR4-2133 (128 GB/node)
Interconnect	Mellanox FDR Infiniband 56Gb/s Brocade 6450 Ethernet 1Gb/s
Storage	2.25 TB (1x250GB SATA disk per node)

This hardware configuration was chosen as a balance between performance and the power demands of a GPU system. The NVIDIA K40s were chosen for MILC (using the QUDA library) and HPL. The rest of the applications will be run on the CPU-only nodes. As a whole, the system at full power exceeds the limit of 3120 watts. The students' strategy is to run on a subset of the machine, depending on the compute resources needed for the particular application, and use a job scheduler (PBS Pro) to handle simulation placement.

Our system on the floor in Wisconsin and a visualization of WRF practice dataset

PREPARATION

This team faced several challenges in preparing for the competition. The majority of the students had minimal Linux experience, and none had used a supercomputer. The initial preparation involved tutorials in Linux, HPC architecture, MPI & OpenMP, and software installation. Later work involved system administration topics (including node management tools such as XCat), job scheduling, and performance analysis with Allinea. All of this was done with the help of Pawsey staff members. The students were also given a basic introduction to the different areas of applied science, such as de novo assembly and QCD. Each student was expected to develop some general knowledge in all areas, and specialize in a few areas. For example, one student may focus more on WRF and using visualization tools (such as VisIt), while another student focused more on system administration and software installs.

Pawsey's Zeus system

Another challenge for the team was access to the hardware. Given the remote location of Perth, it was cost-prohibitive to ship our Cray system from the USA to Australia and back again. While the SCC system was being assembled, students trained on Pawsey's Zeus system. Zeus is an SGI cluster that is used for pre- and post-processing at Pawsey. It was chosen as it most closely resembles the proposed SCC architecture. It's uses SLES11 as an operating system (we're using CentOS), has the GNU and Intel compiler suites, and also has several nodes with NVIDIA Tesla and Quadro GPUS. The student's were also given access to Magnus, a Cray XC40, in order to work with larger scale jobs (Zeus has a limit of 2 node jobs).

GENERAL STRATEGIES FOR RUNNING AND OPTIMIZING THE APPS

The overall strategy was to become familiar with each application and how it performed at different scales, with less focus on actual code modifications. Allinea's MAP and Perfreport tools were used to see how applications behaved. Focus was given to examining how things like compiler options and job sizes would affect performance.

WHY WE WILL WIN

Mainly because we have a relaxed team spirit. The Pawsey team has had to deal with a number of issues, such as lack of hardware and personnel changes in the time leading up to the competition (the team is competing with only 5 students). As a result, we feel ready to handle anything the competition brings. We also feel we possess a very strong work ethic and sense of camaraderie that will help us in the competition.