Annual Report 2014 - 2015

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May 18, 2015

Hardware Operations

This year I spent considerable effort to evaluate new management tools for the Frank cluster. I was tasked to learn evaluate alternative options for batch queue systems and cluster management packages. I worked with IBM representatives to learn how to install and operate the LSF queue package and PCM management package. It was determined that the cost of these packages was beyond what our budget could support. I was able to demonstrate that open source tools cluster management, Warewulf and Ansible, would be very effective in our cluster. In the spring of 2015 it was decided that CSSD staff will take over the responsibility of cluster management.

This year I begun working with the Pittsburgh Genome Resource Repository. The Center for Simulation and Modeling has been working closely with the Pittsburgh Supercomputing Center to provide disk storage for this project. My job, in coordination with CSSD staff, has been to ensure that the shared filesystem between SaM and PSC is operational.

Education and Training

In the spring of 2015 I taught a one-day Python workshop along with Esteban Meneses and Ben Albrecht.

Research

Working closely with graduate students from Ken Jordan's group we improved the conversion algorithms for the Quantum Monte Carlo (QMC) trail wavefunction generator in GAMESS. We plan to include the improved converter in the next GAMESS release. This fixes several bugs that were identified in the previous release and adds support for f-functions and multi-determinant trial wavefunctions.

Professional Development

- CASC Meeting Sept 16-19, 2014.

- ACS Regional Meeting Nov 29 - Oct 1, 2014

- CP2K workshop March 11, 2015. I help organize the workshop and helped the instructor prepare hands-on tutorials

- NVIDIA GPU Tech Conference March 17-20, 2015. I attended many hands-on CUDA development sessions.

- Pittsburgh Quantum Institute Symposium April 15-17 2015.

- Xeon Phi hands-on developer training April 28-29, 2015.