High Performance Computing Center

SPRING 2015 NEWSLETTER

TECH TIPS

EXPRESS QUEUE

- ✓ Short Jobs
- ✓ Testing/debugging scripts
- ✓ Less than 1 hour wall time

SCRATCH DIRECTORY

- ✓ /scratch/<username>
- ✓ Large files
- ✓ Large Collections of Files
- ✓ Not backed up
- ✓ Actively used files ONLY

MARK YOUR CALENDARS

New user Training
March 12 @ 2:00 – 3:30 p.m.
CLBN 403

State of the HPC
(all users invited)
March 26th 9:30 – 11:00 a.m.
SU416 – Case Study 2

For more information go to *hpcc.okstate.edu* for updates!

ACKNOWLEDGING THE HIGH PERFORMANCE COMPUTING CENTER

The High Performance Computing Center exists to facilitate research, development and test activities. Our best measurement of continued needs and benefits remains publications, dissertations and grants facilitated by the users of our resources. Please remember to always acknowledge use of OSU's High Performance Computing center resources and/or personnel in publications. For a quick reference guide for acknowledging please visit the Acknowledging page on our website.

Don't forget to email dana.brunson@okstate.edu to inclusion in our publication listings. For a list of all the extensive list of facilitated publications the HPCC has helped contribute to in the past visit the Scholarly Publications page on our website.

COMPUTATIONAL CHEMISTRY – BY CHRISTOPHER FENNELL

Hired to the faculty in the OSU Chemistry Department in 2013, Dr. Fennell specializes in molecular simulation of condensed phase systems. His research involves characterizing the driving forces for molecular transfer, association, and solvation. Uncovering the whys behind the collective behavior of molecules in complex systems provides critical knowledge and power for rational design of targeted therapeutics, materials with specific physical properties, and self-organizing and assembling systems.

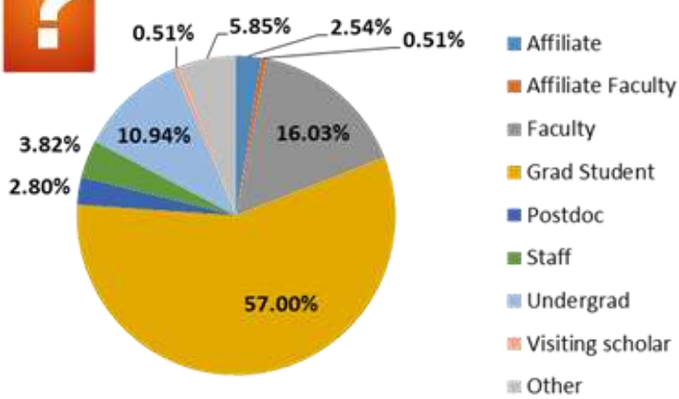
Tackling problems in complex molecular systems requires extensive sampling of system states. Fortunately, molecular mechanics simulations lend themselves quite well to parallel computing environments. As part of Dr. Fennell coming to OSU, he purchased a subsystem of compute nodes that were recently integrated into the Cowboy Cluster.

In addition to 24 CPU cores, these nodes each contain four Intel Xeon Phi cards. Each Phi card contains 228 simultaneous multithreading pipelines, and this hardware provides new capabilities that are not available on standard Cowboy compute nodes. When used fully, these Phi nodes can give upwards of a 1000-fold improvement in performance over a single core calculation.

OSU HPCC supports researchers that want to take advantage of this newly available compute hardware.

DID YOU KNOW ?

OSU – HPCC USERS BREAKOUT



Do you have a research item, tech tip or other suggestion for making our quarterly newsletter even better? Please send them to hpcc@okstate.edu.

QUESTIONS: hpcc@okstate.edu
WEBSITE: https://hpcc.okstate.edu