High Performance Computing Center

SUMMER 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

Software Carpentry
May 27, 28, 2015
9:00 a.m. – 4 p.m.

Sign Up:
http://ouinformatics.github.io/2015-05-27-osu/

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

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.

HPCC GRANT AND PUBLICATION WRITING

Writing a grant? We can help!
We have boilerplates for facilities and service sections that can help take the stress off of you. Please contact us if you require assistance, and we can provide documentation to support your efforts. The High Performance Computing Center exists to facilitate research, development and test activities.

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 for inclusion in our publication listings.

COMPUTATIONAL OPTIMIZATION – BY BASKI BALASUNDARAM

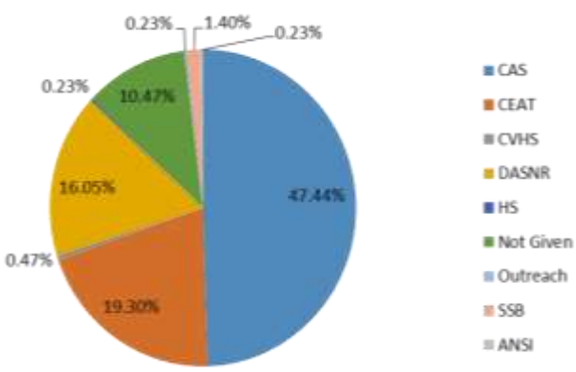
Dr. Balasundaram is an Associate Professor (http://baski.okstate.edu/) in the School of Industrial Engineering & Management (IEM) who specializes in computational optimization, specifically with network models and graph theoretic approaches. His basic research focuses on the development of theory and algorithms to solve combinatorial optimization problems that are motivated by graph-based data mining, social network analysis, computational biology, and other fields.

The problems he studies range from seeking specific patterns or substructures in networks to designing networks to have optimal structural properties like robustness and reachability. Even when the structural properties or patterns are simple to describe, the resulting optimization problems are often computationally intractable requiring an intelligent use of decomposition techniques in algorithm design, and the power of high performance parallel computing to solve.

Dr. Balasundaram and several other faculty from IEM that work broadly in the field of Operations Research, with help from OSU HPCC acquired cluster "Cimarron." This large-memory cluster consists 10 compute nodes with dual quad core Intel E5620 processors, 6 of which have 96 GB RAM and 4 have 144 GB RAM. The cluster also hosts high-performance optimization packages like CPLEX and Gurobi. Since his research often employs worst-case exponential algorithms, such high-memory nodes and parallel computing are particularly advantageous to his group's research, enabling optimal resolution on massive power-law networks with several million nodes that were previously unsolved.

DID YOU KNOW ?

OSU – HPCC Schools Breakdown



CONGRATS!

Cassidy Gierhart is a Freshman Research Scholar mentored by Christopher Fennell, who "won" the OSU Scholar Development Undergraduate Research Symposium with the Best Overall Presentation. Her project was titled "Organized Disorder: Packing in Microscopic and Macroscopic Systems". Cassidy used Cowboy to study 4 different variants of pentane, each involved a single long (10 ns) liquid simulation and 201 short (100 ps) glass quenching simulations derived from the liquid state trajectory, so 808 separate computer simulations. She then compared this work with Runts candy packing and she uncovered direct correspondence between the macroscopic candy models and microscopic molecular simulation models. As part of this honor, Cassidy will represent OSU at next year's National Conference on Undergraduate Research. Congratulations, Cassidy, and OSU HPCC is proud to support novel undergraduate research.