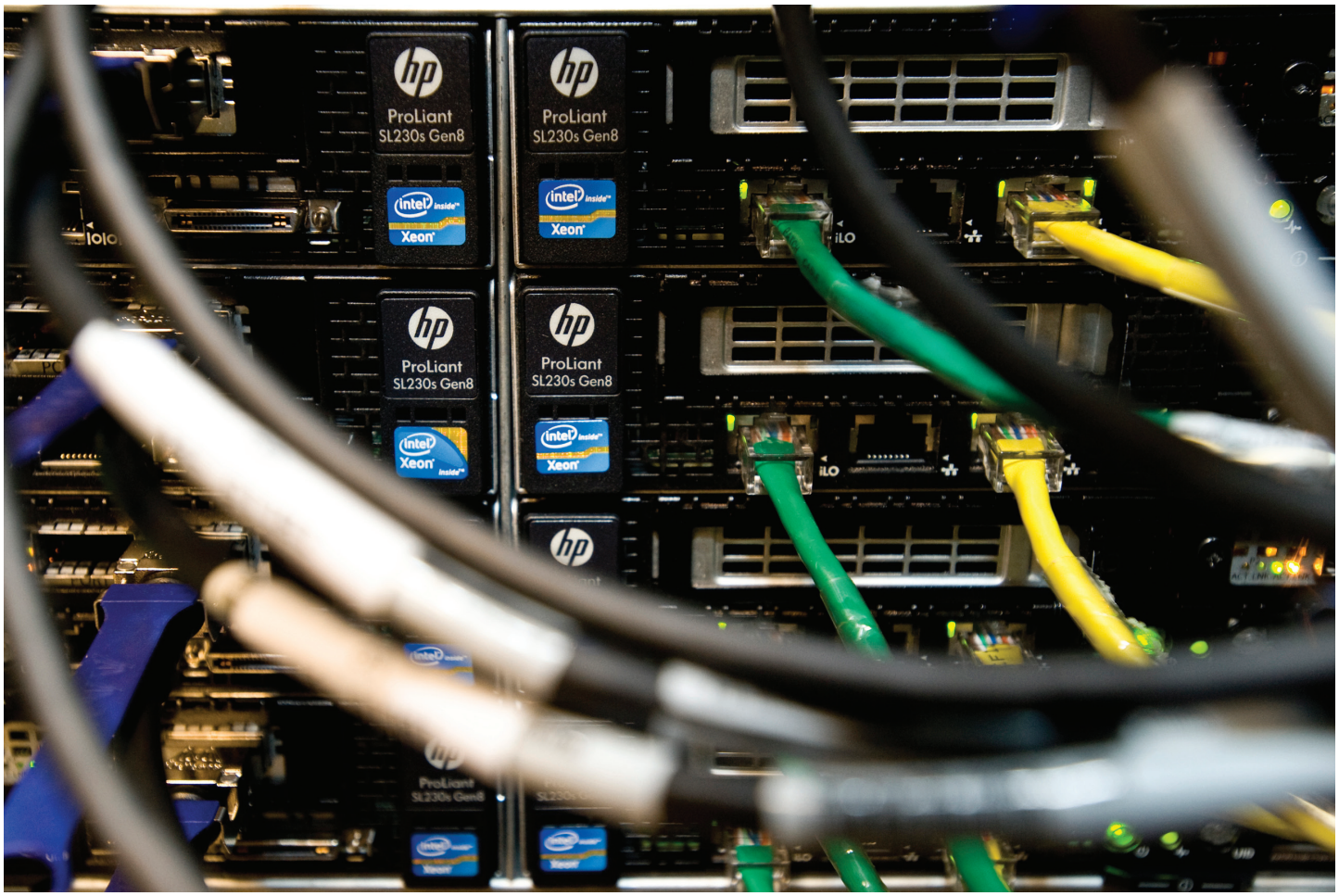
PURDUE UNIVERSITY

PURDUE
UNIVERSITY

RESEARCH COMPUTING



COMMUNITY CLUSTER PROGRAM

Fall 2013

COMMUNITY CLUSTERS AT PURDUE UNIVERSITY

PURDUE UNIVERSITY

ABOUT THE COMMUNITY CLUSTERS

Information Technology at Purdue (ITaP) operates a significant shared cluster computing infrastructure developed over several years through focused acquisitions using funds from grants, faculty startup packages, and institutional sources.

These "community clusters" are now at the foundation of Purdue's research cyberinfrastructure.

We strongly encourage any Purdue faculty or staff with computational needs to join this growing community and enjoy the enormous benefits this shared infrastructure provides:

PEACE OF MIND **LOW OVERHEAD** **COST EFFECTIVE** **FLEXIBLE**

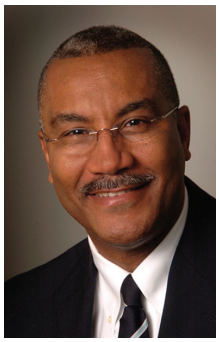
Peace of Mind	ITaP system administrators take care of security patches, software installation, operating system upgrades, and hardware repair so faculty and graduate students can concentrate on research. Research support staff are available to support your research by providing consulting and software support.
Low Overhead	The ITaP data center provides infrastructure such as racks, floor space, cooling, and power; networking and storage are more of the value that you get from the Community Cluster Program for free. In addition, the clusters are built with a lifespan of five (5) years, and ITaP provides free support the entire time.
Cost Effective	ITaP works with vendors to obtain the best price for computing resources by pooling funds from different disciplines to leverage greater group purchasing power and provide more computing capability for the money than would be possible with individual purchases. Through the Community Cluster Program, Purdue affiliates have invested several million dollars in computational and storage resources since 2006 with great success in both the research accomplished and the money saved on equipment purchases.
Flexible	Partners in a community cluster always have ready access to the capacity they purchase and potentially to much more, if they need it. The Community Cluster Program shares compute nodes among cluster partners when the nodes are idle. This allows each partner to get more computational value per dollar than could be on his or her own.

ADDITIONAL BENEFITS

- **Parallel Filesystem**: Each cluster includes access to large-scale, high-performance, parallel scratch for running jobs.
- **Archive**: Each community cluster user gets access to the high-performance HPSS Archive system "Fortress", for long-term storage of research data.
- **Persistent Group Storage**: Each research group is provided with expandable space to empower the group to:
  - Share data and results
  - Centrally install and manage the group's applications
  - Define and manage access to custom UNIX groups for easy project-based collaboration
- **Web Applications:** Easily deploy research portals that integrate with community cluster or storage resources.
- **Data Sharing Services**: Connect domain-specific data sharing services to research storage resources.
- **Computational Interfaces:** Work with ITaP staff to create custom or dedicated interfaces to community cluster resources.

COMMUNITY CLUSTERS AT PURDUE UNIVERSITY

PURDUE UNIVERSITY



"I wouldn't have been elected to the National Academy of Sciences without these clusters. Having the clusters, we were able to set a very high standard that led a lot of people around the world to use our work as a benchmark, which is the kind of thing that gets the attention of the National Academy."

Joseph Francisco
William E. Moore Distinguished Professor of Chemistry
Member, National Academy of Sciences, 2013

"I'm worry free. I'm sure if something goes wrong someone will be there to fix the problem. I might be able to do it, but it costs me more time and that's not very productive. It's better to have a professional do it."

Qingyan Chen
Vincent P. Reilly Professor of Mechanical Engineering

"We do extremely intensive calculations requiring computation at a magnitude that has been impossible because of the lack of sufficiently powerful computers. The availability of such large-scale machines and the codes that can utilize them enables us to move nano science to nano engineering."

Gerhard Klimeck
Professor of Electrical and Computer Engineering, director of the Network for Computational Nanotechnology and nanoHUB.org

FACULTY PARTNERS BY CLUSTER

STEELE
18 departments
62 faculty

COATES
25 departments
81 faculty

ROSSMANN
16 departments
36 faculty

HANSEN
11 departments
22 faculty

CARTER
2 Purdue campuses
26 departments
60 faculty
Commercial users

COMMUNITY CLUSTERS AT PURDUE UNIVERSITY

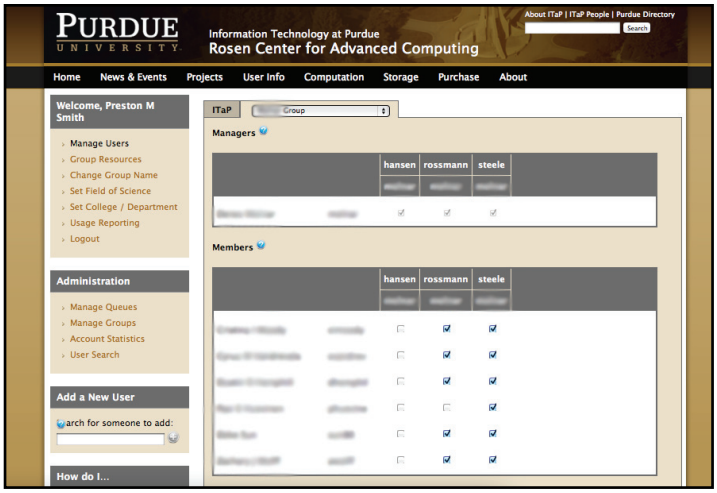
PURDUE UNIVERSITY

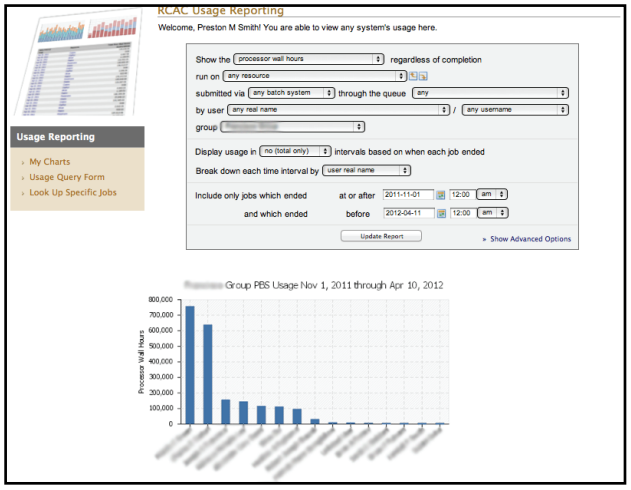
SELF-SERVICE TOOLS

MANAGE YOUR QUEUES

You or your delegate can enable or remove access for any student, researcher, or collaborator on any queue on any cluster that you own.

Create and define UNIX groups for students and collaborators.





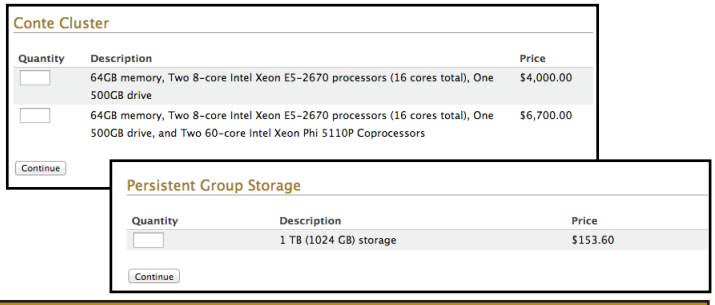
TRACK YOUR USAGE

Monitor up-to-near-time historical usage of your queues.

Track which students use the most computing, generate reports for sponsors, and monitor trends in your group's resource usage.

ADD NEW RESOURCES

Easily purchase additional nodes or persistent storage space for your research group.



APPLICATIONS AND ENGAGEMENT

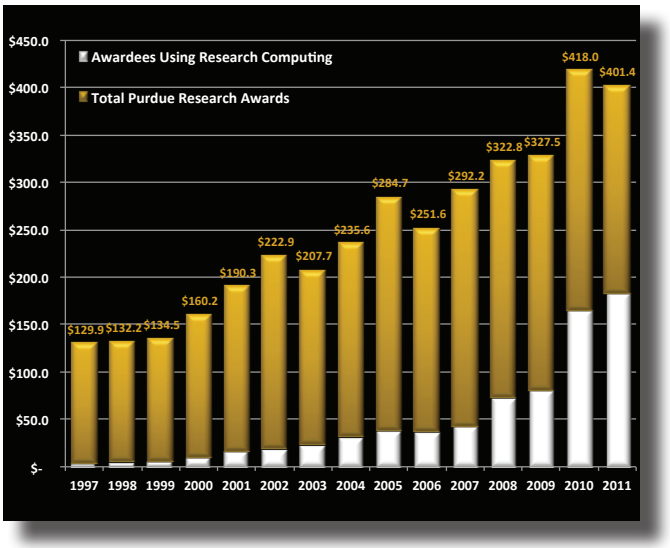
In addition to the peace of mind gained from professional systems engineering staff, community cluster partners can draw from the expertise of ITaP's experienced application and engagement staff, software engineers, and visualization experts.

ITaP application and engagement team members are experienced users of computational scientists, with advanced degrees in Engineering, Biology, Chemistry, and Physics. Engagement staff can help with a wide range of issues: from answering user questions and providing training, to code development, software installation, designing effective workflows, and performance analysis.

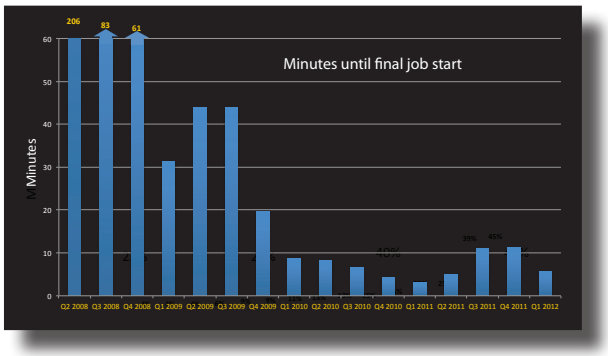
COMMUNITY CLUSTERS AT PURDUE UNIVERSITY

PURDUE UNIVERSITY

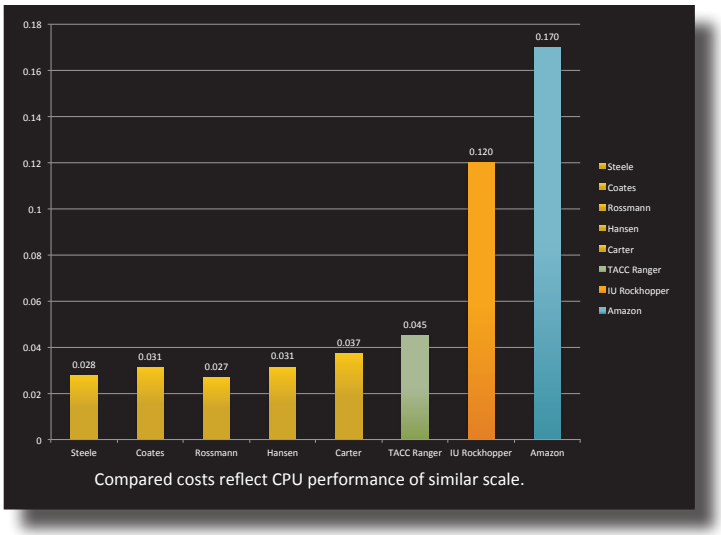
EXTERNAL GRANTS TO HPC USERS



RAPID TIME TO SCIENCE



COST-EFFECTIVE



NODE PRICES

Steele (8)	$2014 - $27.02/GFlop
Coates (8)	$1746 - $21.84/GFlop
Rossmann (24)	$3341 - $16.58/GFlop
Hansen (48)	$5862 - $13.28/GFlop
Carter (16)	$3300 - $10.52/GFlop
Conte (16)	***$6700 - $2.86/GFlop***

Numbers in parentheses are the numer of cores per node.

CAMPUS SUPERCOMPUTER RANKINGS

June 2013

1. ***Conte*** **- Purdue University (#28 - .962 TF)**
2. *Big Red II* - Indiana University (#46 - .597 TF)
3. *HPCC* - University of Southern California (#53)
4. *Blue Gene/Q* - Rensselaer Polytechnic Institute (#76)
5. *Palmetto* - Clemson University (#115)
6. *Blue Gene/Q* - University of Rochester (#170)
7. ***Carter*** **- Purdue University (#175)**
8. *Janus* - University of Colorado (#239)

COMMUNITY CLUSTERS AT PURDUE UNIVERSITY

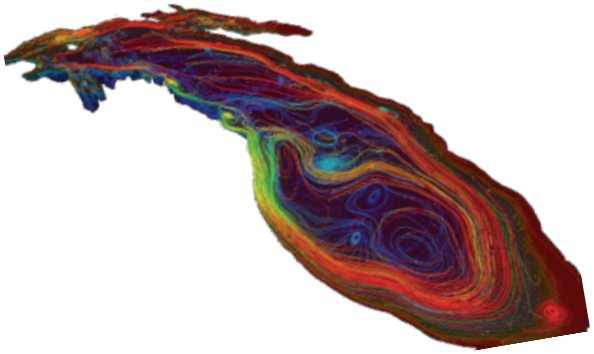
PURDUE UNIVERSITY

VISUALIZATION

The Envision Center for Data Perceptualization provides novel solutions to effectively communicate complex research concepts. Computer graphics, advanced visualization, auditory, touch, and multimodal interaction assist researchers, instructors, and leaders in their quest for new knowledge and innovative products.

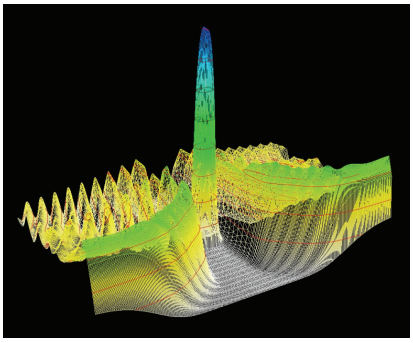
The expert staff and facilities at the Envision Center assist faculty in research and teaching to:

- **Develop** a visual pathway into your research data to discover and communicate innovative results.
- **Create** new virtual environments for training and simulation deployable to mobile devices, web, and the VR Theater.
- **Capture** and track body movements, recognize gestures, and integrate touch-feedback into your research.
- **Produce** high-fidelity renderings for educational, training, and publication purposes.



Visualization of Hydrodynamic flow in Lake Michigan

VISUALIZATION FACILITIES



- Virtual reality theater for display of 3-D stereoscopic images on a 30x8 foot screen or in a semi-enclosed "room" with three walls to create an immersive environment
- Motion-capture system for recording human movement and converting it to an accurate 3-D digital representation for use in analysis and animationVideo Conferencing Meeting Facility
- Video-conferencing and collaboration room with an 18x5 foot screen for displaying interactive feeds from multiple sites, including internationally
- Tiled wall with a 7x12 foot high-resolution display area and 2-D, 3-D and stereo capabilities

CASE STUDY - VIRTUAL CLEAN ROOM

Pharmacy clean rooms are sterile environments where pharmacists and pharmacy technicians prepare materials that need to be guaranteed contamination free, said Steve Abel, assistant dean for clinical programs in the Purdue School of Pharmacy and Pharmaceutical Sciences. Researchers from the Rosen Center for Advanced Computing, the School of Pharmacy and Pharmaceutical Sciences, and the School of Industrial Engineering have created a virtual version of a standard hospital clean room.

The virtual clean room is designed to give pharmacy students plenty of "stick time" — in the vernacular of pilots, who do a lot of virtual flight training on computerized simulators — even before they set foot in a real clean room.

COMMUNITY CLUSTERS AT PURDUE UNIVERSITY

PURDUE UNIVERSITY

SERVICES AND SOLUTIONS

ITaP provides research services and solutions to develop faculty partnerships to support and advance the research agenda at Purdue. Faculty in need of software solutions and consulting for research projects may leverage ITaP research scientists with experience in high performance computing, data-intensive and high throughput computing, and science gateways that make it easier for a community of researchers to access advanced cyberinfrastructure and resources.

DISTRIBUTED COMPUTING SUPPORT

Expertise is available to support projects that can make use of distributed computing resources, through DiaGrid. DiaGrid provides easy access to high-throughput computing applications through an easy-to-use interface.

PARTNERSHIPS ON GRANT PROPOSALS

ITaP Research Scientists collaborate with faculty on grant proposals and support them by providing cyberinfrastructure solutions to funded projects. Our staff can also assist in creating your data management plan and provide requested text on ITaP equipment and facilities.

ACCESS TO NATIONAL RESOURCES

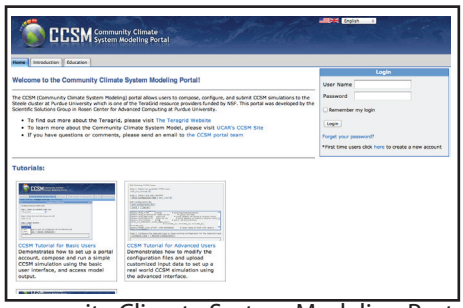
SCIENCE GATEWAY SUPPORT

SOFTWARE DESIGN AND DEVELOPMENT

Bring in expertise to help your researchers create or modify software to take advantage of the latest in advanced computation, web frameworks, data analysis, visualization, sharing, and management. Our software developers can be funded through grant awards or contracts based on developer time.

DATA MANAGEMENT SUPPORT

ITaP Research Scientists partner with faculty to create solutions for their data management needs, such as publishing data and metadata, creating a Web interface for data discovery and analysis, or integrating data access into tools and simulations.



Community Climate System Modeling Portal

SERVICES AND PROJECTS

CESM science gateway for online climate modeling and data publishing: an easy-to-use Web interface for running Community Earth System Model simulations and managing output data on HPC resources.

Diagrid: No Forms. No waiting. Just instant access to high-throughput computing applications. BLAST, R, CESM, and SWATShare applications available today, or share your own tools.

DRINET Drought Research portal: a research environment for collecting and disseminating local- to regional-scale drought information.

Dataset storage and metadata management

LARS remote sensing data
NEXRAD Level 2 radar data
Climate Simulation Model data
Satellite data

COMMUNITY CLUSTERS AT PURDUE UNIVERSITY

PURDUE UNIVERSITY

WANT TO LEARN MORE?

CONTACT US:

EMAIL:
rcac-cluster-purchase@lists.purdue.edu

SUPPORT QUESTIONS:
rcac-help@purdue.edu

BUSINESS ADDRESS:

ITaP - Young Hall
155 S Grant Street
West Lafayette, IN 47907-2114

PURCHASING QUESTIONS:
Donna Cumberland
Phone: 765.494.7931
Email: donnac@purdue.edu

TECHNICAL QUESTIONS:
Preston Smith
Phone: 765.494.9729
Email: psmith@purdue.edu

FIND US ONLINE:

ITaP: http://www.itap.purdue.edu
ITaP Research Computing (RCAC):
http://www.rcac.purdue.edu
Community Cluster Program:
http://www.rcac.purdue.edu/userinfo/communityclusters.cfm

facebook.com/PurdueRCAC
Twitter: @PurdueRCAC
youtube.com/PurdueRCAC

Photo Credits - Front: Purdue University photo/Andrew Hancock Page 2: Patrick Finnegan
Back: Patrick Finnegan (bottom)