PURDUE UNIVERSITY

Preston Smith

Director of Research Services

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INTRODUCTION TO RESEARCH SERVICES

RESEARCH COMPUTING
AT PURDUE UNIVERSITY

RCAC Staffing

https://www.rcac.purdue.edu/about/staff/

OVERVIEW

- IT Research Computing (RCAC)

- A unit of ITaP (Information Technology at Purdue) – the central IT organization at Purdue.

- RCAC provides advanced computational resources and services to support Purdue faculty and staff researchers.

Our goal: To be the one–stop provider of choice for research compu9ng and data services at Purdue –Delivering powerful, reliable, easy–to–use, service–oriented compu9ng and exper9se to Purdue researchers.

COMMUNITY

CLUSTERS

A BUSINESS MODEL FOR HPC AT PURDUE UNIVERSITY

THE POWER OF
SHARING

- Without a large capital acquisition by the university, providing cutting-edge computing capabilities for researchers was not possible.
- Many faculty were getting funding to acquire and operate HPC resources for themselves

- **Solution:** pool these funds to operate clusters for researchers!
    - The faculty no longer have to devote a grad student to managing their cluster!

- ## You get out at least what you put in
  - Buy 1 node or 100, you get a queue that guarantees access up to that many CPUs

- ## But wait, there's more!!
  - What if your neighbor isn't using his queue?
    - You can use it, but your job is subject to preemption if he wants to run.

- ## You don't have to do the work
  - Your grad student gets to do research rather than run your cluster.
    - Nor do you have to provide space in your lab for computers.
  - ITaP provides data center space, systems administration, application support.
  - Just submit jobs!

SIX COMMUNITY CLUSTERS

STEELE

7,216 cores

Installed May 2008

Re9red Nov. 2013

COATES

8,032 cores

Installed July 2009

24 departments 61

faculty   Re9red

Sep. 2014

ROSSMANN

11,088 cores

Installed Sept. 2010

17 departments 37

faculty

HANSEN

9,120 cores

Installed Sept. 2011

13 departments 26

faculty

CARTER

10,368 cores

Installed April 2012

26 departments 60

faculty

#175 on June 2013 Top 500

CONTE

9,280 Xeon cores
(69,600 Xeon Phi cores)

Installed August 2013

20 departments

51 faculty (as of Aug. 2014)

#39 on June 2014 Top 500

VITAL STATS

- 165 "owners"
- ~1200 active users
- 259M hours provided in 2014
- Nationally, the gold standard for condo-style computing

- Today, the program is part of many departments' faculty recruiting process.
  - *A selling point to attract people to Purdue!*
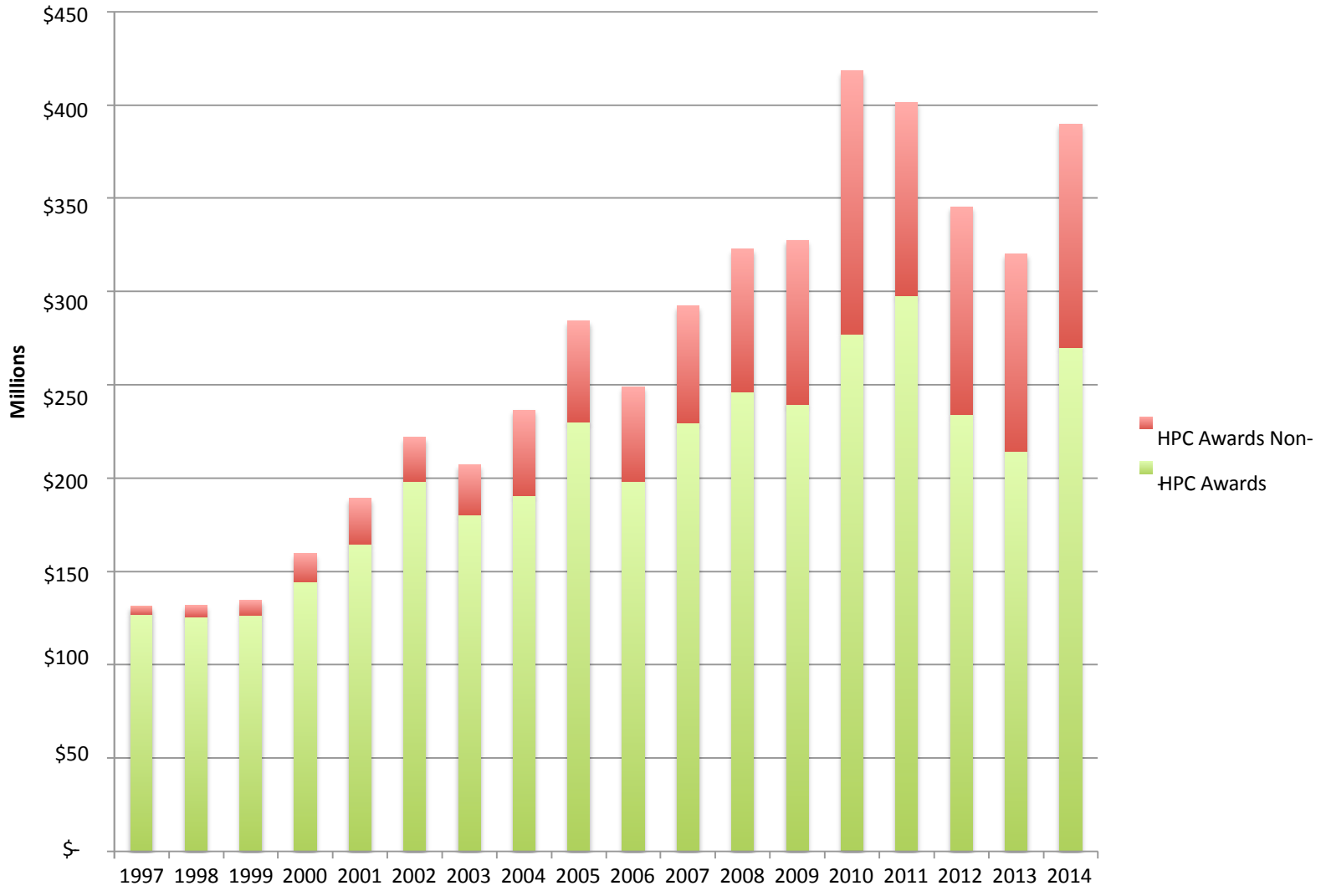 - *Please feel free and have your faculty candidates meet with us during recruitment!*

IMPACT

Department	Cores
Electrical and Computer Engineering	9816
OSG CMS Tier2	9168
Mechanical Engineering	7008
AeronauNcs and AstronauNcs	5048
Earth, Atmospheric, and Planetary Sciences	3632
Chemistry Materials	1936
Engineering Chemical	1504
Engineering Biological	1144
Sciences	1104
Medicinal Chemistry and Molecular Pharmacology	1104
MathemaNcs	720
Physics	664
Biomedical Engineering	640
StaNsNcs	520
Nuclear Engineering	492
Civil Engineering	448
Agricultural and Biological Engineering	416
Industrial and Physical Pharmacy	384
Commercial Partners	304
Computer Science	280
Other College of Agriculture	256
Agronomy	240
Forestry and Natural Resources	64

IMPACT

Millions

HPC Awards Non-

HPC Awards

$450
$400
$350
$300
$250
$200
$150
$100
$50
$-

1997 1998 1999 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014

COMPUTATION

Community Clusters to Cluster Communities
What neighborhoods are in our community?

HPC (Rice): MulNple cores or nodes, probably MPI. Benefit from high–performance network and parallel filesystem. The vast majority of campus –80% of all work!

HTC (Hammer): Primarily single core. CPU–bound. No need for high–performance network.

Life Science/Big Memory (Snyder): Use enNre node to get large amounts of memory. Less need for high–performance network. Needs large, fast storage.

DATA

STORAGE
INFRASTRUCTURE FOR RESEARCH DATA

DATA STORAGE

- Research computing has historically provided some storage for research data for HPC users:

    - Archive (Fortress)

    - Actively running jobs (Cluster Scratch - Lustre)

    - Home directories

… And Purdue researchers have PURR to package, publish, and describe research data.

THE SERVICE

HPC researchers can at last purchase storage!

A storage service for research to address many common requests:

- 100G available at no charge to research groups

- Mounted on all clusters and exported via CIFS to labs

- *Not scratch*: Backed up via snapshots, with DR coverage

- Data in Depot is owned by faculty member!

- Sharing ability – Globus, CIFS, and WWW

- Maintain group-wide copies of application software or shared data

A SOLUTION

Well received!

- In less than 7 months, over 105 research groups are participating.

    - *Many are not HPC users!*

- Half a PB in use since November

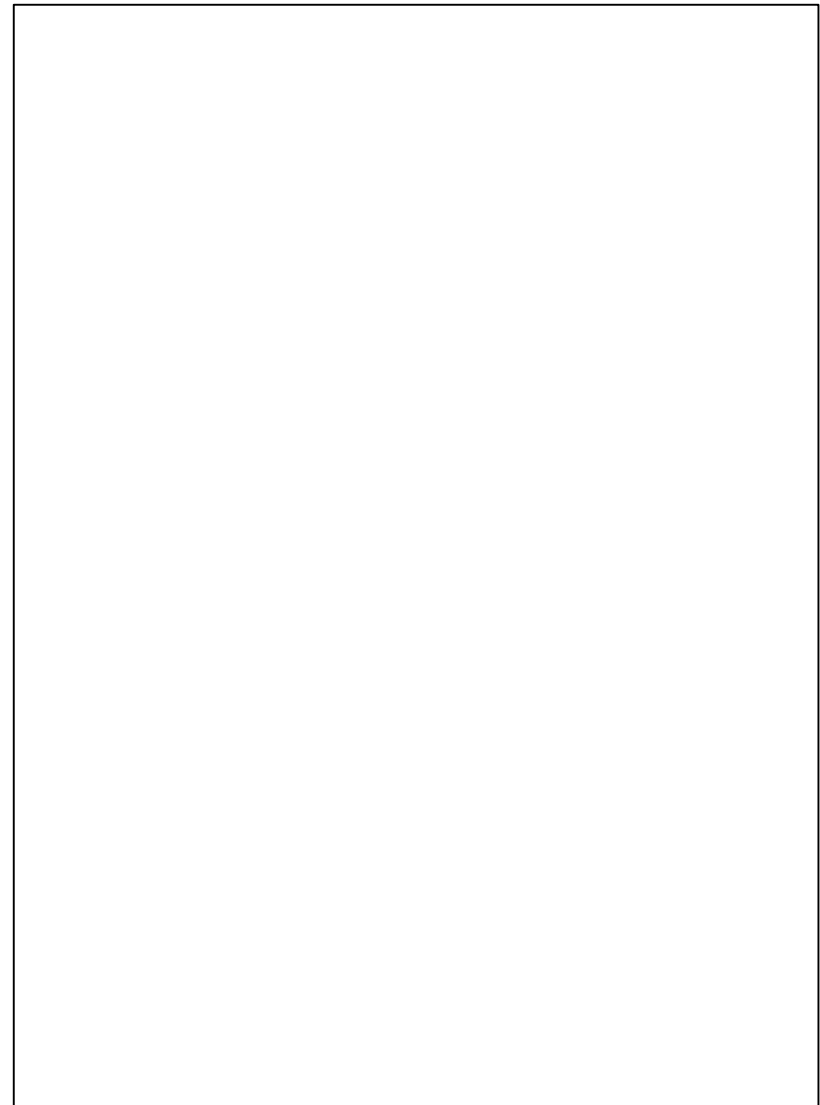- A research group purchasing space has purchased, on average, 8.6TB.

Approximately 2.25 PB of IBM GPFS

Hardware provided by a pair of Data Direct Networks SFA12k arrays, one in each of MATH and FREH datacenters

160 Gb/sec to each datacenter

5x Dell R620 servers in each datacenter

DESIGN TARGETS

The Research Data Depot Can do:

Depot Requirements	Previous solu9ons
At least 1 PB usable capacity	>1 PB
40 GB/sec throughput	**5 GB/sec**
< 3ms average latency, < 20 ms maximum latency	**Variable**
100k IOPS sustained	**55k**
300 MB/sec min client speed	**200 MB/sec max**
Support 3000 simultaneous clients	Yes
Filesystem snapshots	Yes
MulN--site replicaNon	**No**
Expandable to 10 PB	Yes
Fully POSIX compliant, including parallel I/O	**No**

DATA

- It's important to think of Depot as a "data service" – not "storage"
- It is not enough to just provide infrastructure
  - "Here's a mountpoint, have fun"

- Our goal: enabling the frictionless use and movement of data
  - *Instrument -> Depot -> Scratch -> Fortress -> Collaborators -> and back*
  - Continue to improve access to non-UNIX users

- Collaborations on multi-disciplinary grant proposals, both internal and external

- Developing customized Data Management Plans

- Organizing your data

- Describing your data

- Sharing your data

- Publishing your datasets

- Preserving your data

- Education on data management best practices

OTHER SERVICES

BEYOND THE COMMUNITY CLUSTERS

2014 network improvements

- 100 Gb/sec WAN connections

- Research Core

    - 160 Gb/sec core to each resource (up from 40)

    - 20 Gb/sec research core to most of campus

- Campus Core Upgrade

h l ps://www.rcac.purdue.edu/news/681

EVERYBODY NEEDS
TO SHARE

Globus:

Transfer and share large datasets….

…. With dropbox-like characteristics ….

…. *Directly from your own storage system!*

GLOBUS

Data moved in 2014:

13 TB in, 19TB out

200k files both directions

55 unique users

In progress:

Globus interface to Fortress

h" ps://transfer.rcac.purdue.edu

EDUCATION

- Programming practices – Software Carpentry

- Parallel Programming – MPI, OpenMP

- Big Data

- Matlab

- Accelerators – Xeon Phi, OpenACC, CUDA

- UNIX 101

- Effective use of Purdue research clusters

NEED HELP?

RESEARCH COMPUTING COFFEE BREAK CONSULTATIONS

Meet up with ITaP research computing staff and other researchers who use or are interested in High Performance Computing at Purdue. Join us for informal discussions of scientific computing along with any other topic that might spring up. We'll be meeting at different coffee shops around campus each week.

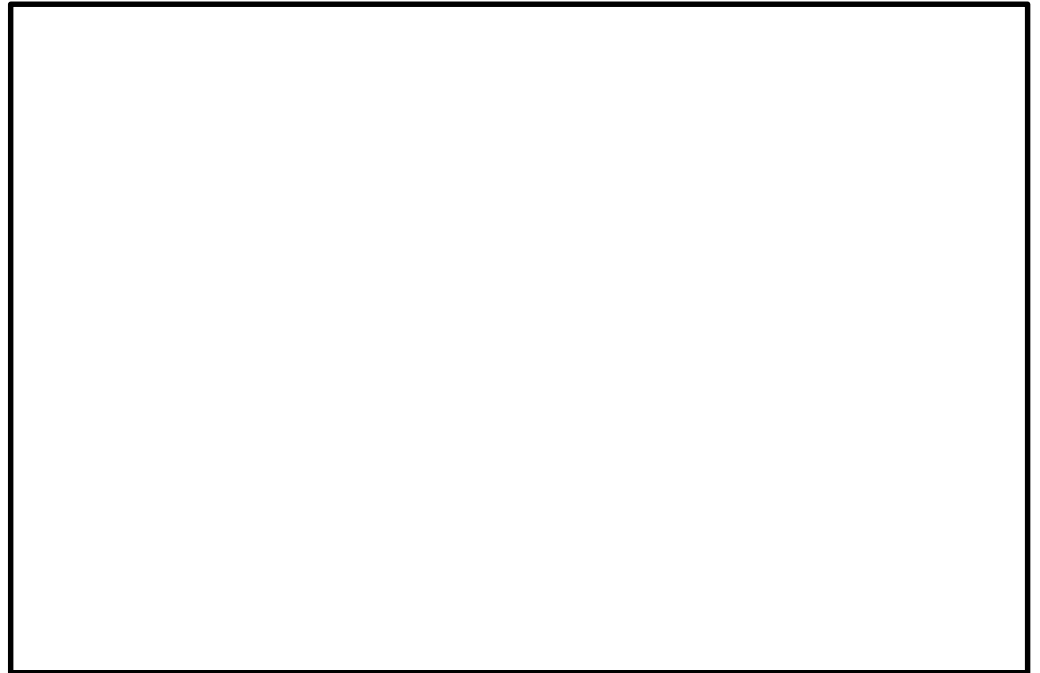Check the coffee web page to see this week's location and time.

rcac.purdue.edu/coffee

SCHOLAR

- Need to teach students to use HPC in a course?
- Scholar cluster is available to any instructor at no cost.

Spring 2015:   EAPS
CS   AGRY
STAT   ANSC
CHEM   ChemE

NEED A PROGRAMMER?

Bring in our expertise to help your researchers create or modify software to take advantage of the latest technology in advanced computation, web frameworks, data analysis, visualization, sharing, and management.

Our software development effort can be funded through grant awards or contracts based on developer time.