2017 Community Cluster
Since Steele in 2008, Research Computing has deployed many world-class offerings in computation
## 9 HPC SYSTEMS

<table>
<thead>
<tr>
<th>System</th>
<th>Cores</th>
<th>Installation Date</th>
<th>Departments</th>
<th>Faculty Investors</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEELE</td>
<td>7,216</td>
<td>May 2008</td>
<td>24</td>
<td>61</td>
<td>Retired Nov. 2013</td>
</tr>
<tr>
<td>COATES</td>
<td>8,032</td>
<td>May 2008</td>
<td>24</td>
<td>61</td>
<td>Retired Sep. 2014</td>
</tr>
<tr>
<td>ROSSMANN</td>
<td>11,088</td>
<td>Sept. 2010</td>
<td>17</td>
<td>37</td>
<td>Retired Sep. 2015</td>
</tr>
<tr>
<td>CARTER</td>
<td>10,368</td>
<td>April 2012</td>
<td>26</td>
<td>60</td>
<td>#54 on June 2012 Top 500</td>
</tr>
<tr>
<td>CONTE</td>
<td>9,280</td>
<td>Aug 2013</td>
<td>26</td>
<td>62</td>
<td>#28 on June 2013 Top 500</td>
</tr>
<tr>
<td>DATA DEPOT</td>
<td>2.5 PB of disk storage</td>
<td>Nov. 2014</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RICE</td>
<td>13,200</td>
<td>May 2015</td>
<td>23</td>
<td>69</td>
<td></td>
</tr>
<tr>
<td>HALSTEAD</td>
<td>10,160</td>
<td>Dec 2016</td>
<td>25</td>
<td>62</td>
<td></td>
</tr>
</tbody>
</table>

**DATA DEPOT**
- 2.5 PB of disk storage
- Installed Nov. 2014
- 400+ faculty investors from every academic college

**RICE**
- 13,200 cores
- Installed May 2015
- 23 departments
- 69 faculty investors

**HALSTEAD**
- 10,160 cores
- Installed December 2016
- 25 departments
- 62 faculty investors
- Halstead-GPU Expansion: May 2017
### FACULTY DEMOGRAPHICS

<table>
<thead>
<tr>
<th>Department</th>
<th>Cores</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aeronautics and Astronautics</td>
<td>5740</td>
</tr>
<tr>
<td>Mechanical Engineering</td>
<td>5556</td>
</tr>
<tr>
<td>CMS Tier2</td>
<td>5440</td>
</tr>
<tr>
<td>Electrical and Computer Engineering</td>
<td>4344</td>
</tr>
<tr>
<td>Earth, Atmospheric, and Planetary Sciences</td>
<td>2540</td>
</tr>
<tr>
<td>Materials Engineering</td>
<td>2064</td>
</tr>
<tr>
<td>Nuclear Engineering</td>
<td>1564</td>
</tr>
<tr>
<td>Other College of Engineering</td>
<td>980</td>
</tr>
<tr>
<td>Chemistry</td>
<td>824</td>
</tr>
<tr>
<td>Physics and Astronomy</td>
<td>820</td>
</tr>
<tr>
<td>Biomedical Engineering</td>
<td>640</td>
</tr>
<tr>
<td>Other Executive Vice President for Research and Partnerships</td>
<td>600</td>
</tr>
<tr>
<td>Statistics</td>
<td>512</td>
</tr>
<tr>
<td>Chemical Engineering</td>
<td>424</td>
</tr>
<tr>
<td>Agricultural and Biological Engineering (Biological Engineering)</td>
<td>368</td>
</tr>
<tr>
<td>Biological Sciences</td>
<td>356</td>
</tr>
<tr>
<td>Industrial Engineering</td>
<td>296</td>
</tr>
<tr>
<td>Civil Engineering</td>
<td>276</td>
</tr>
<tr>
<td>Computer and Information Technology</td>
<td>248</td>
</tr>
<tr>
<td>Medicinal Chemistry and Molecular Pharmacology</td>
<td>248</td>
</tr>
<tr>
<td>Mathematics</td>
<td>232</td>
</tr>
<tr>
<td>Bioinformatics Core</td>
<td>200</td>
</tr>
<tr>
<td>Intelligent Bioenergy</td>
<td>180</td>
</tr>
<tr>
<td>ITaP</td>
<td>176</td>
</tr>
<tr>
<td>Computer Science</td>
<td>156</td>
</tr>
<tr>
<td>Horticulture and Landscape Architecture</td>
<td>156</td>
</tr>
<tr>
<td>Cancer Center</td>
<td>96</td>
</tr>
<tr>
<td>Forestry and Natural Resources</td>
<td>96</td>
</tr>
<tr>
<td>Biochemistry</td>
<td>40</td>
</tr>
<tr>
<td>Agricultural and Biological Engineering (Biological Engineering)</td>
<td>40</td>
</tr>
<tr>
<td>Industrial and Physical Pharmacy</td>
<td>40</td>
</tr>
<tr>
<td>Brian Lamb School of Communication</td>
<td>32</td>
</tr>
<tr>
<td>Agricultural Economics</td>
<td>20</td>
</tr>
<tr>
<td>Animal Sciences</td>
<td>20</td>
</tr>
<tr>
<td>Food Science</td>
<td>20</td>
</tr>
<tr>
<td>Health Sciences</td>
<td>20</td>
</tr>
<tr>
<td>Other College of Pharmacy</td>
<td>20</td>
</tr>
<tr>
<td>Agricultural and Biological Engineering (Agricultural Systems Mgmt)</td>
<td>16</td>
</tr>
</tbody>
</table>

287M hours delivered in 2016

Almost 200 investors from 36 departments, from every College, and 3 Purdue campuses

The gold standard for condo-style computing

Today, the program is part of departments’ faculty recruiting process.

*A selling point to attract people to Purdue!*
Open bid process requesting:
- Quantity 500 nodes
- Included various interconnects (EDR/HDR Infiniband, OmniPath)
- “Broadwell” or “Sky Lake” processors, 2.4 GHz or better
- At least 128GB memory per node
- SSD boot drive, 250G or better
- Optional uplift for one Nvidia P100 GPU per node

Responses ranged from $4,400-4,800 for a node like Halstead, or $6,000-7,700 per node for the latest Intel CPU.
Base node: Dell R640
- 24-core node, 2.6 GHz Intel Xeon Gold “Sky Lake” processors (Xeon Gold 6126)
  - Higher node price, but 50% faster processors
  - 32 Flops per cycle!
- 96 GB DDR4 memory
  - 384 GB, 768 GB & 1536 GB options
  - Memory prices are high world-wide
  - (More on this later!)
- EDR Infiniband interconnect
  - 100 Gbps, 3:1 fat tree – very similar in speed to Halstead
  - Converged fabric – IP traffic uses Infiniband rail

Also bid systems for provost equipment program, leading to substantial savings!
Halstead
- 1 PB GPFS
- 22 GB/sec bandwidth
- 100k IOPS

Brown
- 3 PB Lustre
- 40 GB/sec bandwidth
- 400k IOPS
For codes used by community cluster partners

- Ansys Fluent: 1.6x faster
- Converge CFD: up to 1.29x faster
- Gaussian: 1.25x faster
- LAMMPS: Up to 2.4x faster
- GROMACS: Up to 2x faster
- VASP: Up to 1.9x faster
- AMBER: Up to 1.73x faster
- NAMD: 1.67x faster
- HOMME: Up to 1.67x faster
- WRF: Up to 1.41x faster
- HS06: 675.27
Halstead had 128G RAM per node -

Why 96GB for Brown?

<table>
<thead>
<tr>
<th>Cluster</th>
<th>95th Percentile</th>
<th>99th Percentile</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rice</td>
<td>17.2</td>
<td>36.6</td>
</tr>
<tr>
<td>Conte</td>
<td>27.3</td>
<td>44.7</td>
</tr>
<tr>
<td>Snyder</td>
<td>184</td>
<td>510.4</td>
</tr>
</tbody>
</table>

GB/node per job
Brown: A traditional HPC system

The same, familiar model:
- New cluster acquisition every year
- Service through October of 2022

Improved floating point performance
Vastly improved I/O subsystem

Great for most science and engineering codes
550 Nodes of Brown:
1.1 PF peak

Equivalent to all of Conte, including Xeon Phi Accelerators!
Base node option, plus

- Node with 3 Nvidia GPUs
- Large memory options, also with 768 GB and 1.5 TB configurations available.

<table>
<thead>
<tr>
<th></th>
<th>96G Brown Node</th>
<th>384G Snyder Node</th>
<th>3-GPU Brown Node</th>
</tr>
</thead>
<tbody>
<tr>
<td>Price</td>
<td>$5,599.00</td>
<td>$9,500.00</td>
<td>$18,325.00</td>
</tr>
</tbody>
</table>
Requests for GPU for accelerating simulations, computer architecture research, or deep learning.

12 researchers are currently evaluating Halstead’s GPU partition

With Brown:

Plans are for a 16-node GPU partition, with 3 Nvidia P100 GPUs per node.

Annual subscription to access to GPU nodes:
$2,500 per year
Community Cluster Program - Price per Node and Dollars per GFlop

- **Steele**, **Coates**, **Rossmann**, **Hansen**, **Carter**, **Conte**, **Rice**, **Halstead**, **Brown**
- **Cost per Node** (Dollars per Node)
- **Dollars per GFlop**

**Legend**:
- Blue: Cost per Node
- Red: Dollars per GFlop
General implementation schedule:
- Facilities preparation already in progress - in the POD modular datacenter.
- Plan is for early access and burn-in early October
- Top 500 benchmark run week of Oct 16

- General availability Oct 30

- *No install event this year.*
RESEARCH
DATA STORAGE
DATA IS HUGE!

AND GROWING

Fortress Archive Growth

TB

9,000.00
8,000.00
7,000.00
6,000.00
5,000.00
4,000.00
3,000.00
2,000.00
1,000.00
-

Mar-97
Dec-97
Sep-98
Jun-99
Mar-00
Dec-00
Sep-01
Jun-02
Mar-03
Dec-03
Sep-04
Jun-05
Mar-06
Dec-06
Sep-07
Jun-08
Mar-09
Dec-09
Sep-10
Jun-11
Mar-12
Dec-12
Sep-13
Jun-14
Mar-15
Dec-15
Sep-16
Jun-17

0.24
550.15
1,002.30
2,109.91
3,273.25
8,331.98
At $75/TB per year:

- Storage oriented around your research lab, with
  - Snapshots
  - Multi-site copies of your data
  - Disaster protection
  - A scalable, expandable storage resource optimized for HPC
- Access to Globus data transfer service, and endpoint sharing
To buy 1 or more TB of space,
Or to set up a trial for your lab

Order online:
https://www.rcac.purdue.edu/purchase/
A hit!

- Over 400 research labs are Depot partners!
  - Many are not HPC users!
  - Thousands of individual users

- 1.25 PB sold

- A research group purchasing space has purchased, on average, nearly 10 TB.

- Other institutions looking to Purdue for leadership from our Depot storage service
Transfer and share large datasets....

.... With dropbox-like characteristics ....

.... Directly from your own storage system!
• Last 12 months:
  • 2.4 PB transferred (388TB in March!)
  • Average of 185 TB, 84 unique users per month

Fortress: 1.74PB since Aug ‘15!
RESEARCH SERVICES

OTHER SERVICES YOU MIGHT BE INTERESTED IN
### Non-Traditional HPC Researchers

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Agriculture</td>
<td>48</td>
<td>111</td>
<td>63</td>
<td>131%</td>
</tr>
<tr>
<td>Engineering</td>
<td>161</td>
<td>265</td>
<td>104</td>
<td>65%</td>
</tr>
<tr>
<td>Science</td>
<td>199</td>
<td>227</td>
<td>28</td>
<td>14%</td>
</tr>
<tr>
<td>Education</td>
<td>1</td>
<td>7</td>
<td>6</td>
<td>600%</td>
</tr>
<tr>
<td>Liberal Arts</td>
<td>1</td>
<td>9</td>
<td>8</td>
<td>800%</td>
</tr>
<tr>
<td>Management</td>
<td>20</td>
<td>24</td>
<td>4</td>
<td>20%</td>
</tr>
<tr>
<td>Pharmacy</td>
<td>5</td>
<td>9</td>
<td>4</td>
<td>80%</td>
</tr>
<tr>
<td>Polytechnic</td>
<td>13</td>
<td>21</td>
<td>8</td>
<td>62%</td>
</tr>
<tr>
<td>Health and Human Sciences</td>
<td>14</td>
<td>28</td>
<td>14</td>
<td>100%</td>
</tr>
<tr>
<td>Veterinary Medicine</td>
<td>0</td>
<td>5</td>
<td>5</td>
<td></td>
</tr>
</tbody>
</table>
DATA WORKBENCH

WE HAVE THE PARTS

But not wrapped up in a package
DATA ANALYTICS

IN THE BROWSER

Jupyterhub (Python)

Rstudio
• Approx. $150 annual charge for access
• Easy access to data analysis tools
• Run virtual private Windows desktops
• Run virtual private Linux images in containers
• Integrate with RCAC services
  • Depot, Fortress, Globus, Github, Self Service, etc.
• Grow to batch HPC as your needs grow!
• Add same interactive capabilities to community cluster frontends
DOMAINS

Chemistry
Physics
Astrophysics
Earth and Atmospheric Sciences
Computer Science
Chemical Engineering
Electrical and Computer Engineering
Cell and Molecular Biology
Agriculture

APPLICATION SPACES

Molecular Dynamics
Image Processing
Quantum Chemistry
Weather Modeling
Machine Learning
Big Data
Computer Architecture
Finite Element Analysis

Statistics
Bioinformatics
Geospatial
Remote Sensing
Visualization
NEED HELP?

- Hard to solve problems with HPC?
- Need help building your software or optimizing your workflow?
- Need to learn what resources are available?

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
Need to teach students to use HPC or work with big data in a course?

Scholar cluster is available to any instructor at no cost.

Spring 2016:
- EAPS
- CS
- STAT
- CHEM
- AAE
- ANSC
- ME

Just add your CRN
VERSION CONTROL

COLLABORATE ON CODE OR DOCUMENTATION

Local-to-Purdue Github repositories for your lab, managed by you!
Fall kick-off meeting Wednesday, August 30th 12:00-1:00PM in RAWL 2082.

Our invited speaker: Dr. Beth M. Holloway, Director of the Women in Engineering program and Assistant Dean of Undergraduate Education, College of Engineering.

Join WHPC for computing scholarship, networking, and mentorship opportunities!
Big data research with Hadoop and Spark
XSEDE Workshop
September 12 & 13, 2017  11:00am – 5:00pm

Unix 101
September 19 & 21, 2017

Jetstream cloud resource for science and engineering
September 20, 2017  1:30pm – 4:30pm

Unix 201
October 3 & 5, 2017

XSEDE HPC Monthly Workshop Series - MPI Day 1
October 3& 4, 2017  11:00am – 5:00pm

Clusters 101
October 17 & 19, 2017

XSEDE HPC Monthly Workshop Series - GPU Programming Using OpenACC
November 7, 2017  11:00am – 5:00pm

Upcoming but not yet scheduled:

NVIDIA GPU - Deep learning and CUDA programming
Software Carpentry – Programming with Python
Software Carpentry - Programming with R
Software Carpentry - R for Reproducible Scientific Analysis
Software Carpentry - Programming with MATLAB