RESEARCH COMPUTING
AT PURDUE UNIVERSITY
• 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.
• RCAC also conducts its own research and development to enhance the capabilities of these resources.
A BRIEF HISTORY
OF RESEARCH COMPUTING AT PURDUE
1962: First Computer Science Department in USA
Faculty: Samuel Conte, Saul Rosen, Richard Kenyon, L. Duane Pyle, Robert Korfhage

1985: 2nd .edu domain on the Internet
cmu.edu, purdue.edu, rice.edu, ucla.edu, and berkeley.edu

Today: many programs in computational science
- Computer Science
- Computer Engineering
- Computer and Information Technology
- Electrical and Computer Engineering Technology
- Interdisciplinary computational science and engineering (computational biology, atmospheric science, physics, chemistry, etc)
In 1967, Purdue became one of the first academic institutions with a supercomputer, a Control Data Corp 6500 (which had a performance of 1/3 of a megaflop).
In spring of 1983 Purdue acquired a Cyber 205 – one of the most powerful systems operated by a university.

Subsequent systems in the CDC family included an ETA10 running System V UNIX.
In the early 90s, Purdue operated an Intel Paragon XPS system.
In the 1990s the Computing Center ran a cluster of IBM RS/6000 systems, and then by 1995 ran an IBM SP/2.
By the early 2000s, research computing had taken to using Linux clusters, and a general purpose resource made from retired computer lab systems was in production.
• By this point the centrally-funded IBM SP was ~7 years old.

• Condor is great for one specific type of work
  – Monte Carlo runs, opportunistic access

• We have an inexhaustible supply of PCs to make recycled clusters, but…
  – PCs are not designed to do HPC
  – The PCs are already 3+ years old by the time they become cluster nodes!

The University was not inclined to make a large capital purchase to build a general-purpose supercomputer system.
COMMUNITY CLUSTERS
A BUSINESS MODEL FOR HPC AT PURDUE UNIVERSITY
• 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!
“As our lab's cluster aged, it developed serious maintenance issues and it started to hamper our ability to do research. As we looked for alternatives, the Community Cluster Program was appealing because it is an effective use of resources—and it gets us out of the computer maintenance business.”

Scott Sudhoff
professor, electrical and computer engineering

THE FIRST COMMUNITY CLUSTERS

PROFESSIONAL MAINTENANCE
• 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!
This model worked well... Well, mostly...

Not everything:

• Acquisition was fairly ad-hoc, resulting in very heterogeneous clusters.

• Opportunistic use by preemption was a good theory, but in practice, it didn’t work terribly well.

• If a faculty member didn’t have funds right when the purchase was made, they missed out.
  • As a result “community clusters” of one or two communities sprouted up. Economy of scale is lost.
• 5 Year cycle
  • Build a cluster every year!
  • Vendors provide 5 year warranty
  • After 5 years, MOU with faculty says that the cluster will be retired
  • Faculty get credit for the residual value of their nodes, towards the next cluster.
  • Community clusters now appear to funding agencies as paying for a service – not a capital purchase.

• No more preemption
  • Replace with “standby” queue
    - You can run all the jobs you want beyond what your queue would let you, but you’re subject to a time limit of 4 hours.
• Further refine what is centrally funded vs. what the faculty buy
  • **Purdue**: Data center space, storage, networking,
    • Software, admin staff, university user accounts, support process
  • **Faculty**: Just the nodes

• Machine selection
  • RFP sent to interested vendors
  • Benchmarking
  • Price guarantee for ~6 months (lets faculty continue to buy in)
    - Also, the rest of the university gets to use our pricing!
  • Selection
    - (Usually works out as “what is cheapest”)

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*Purdue University*
• Cost savings were enough that Gen 1 community clusters were retired and consolidated into a new system – Steele.

• **Install Day**: partners and IT staff from all over campus joined together to unpack, start and bring Steele into production in one day.
<table>
<thead>
<tr>
<th>Cluster</th>
<th>Architecture</th>
<th>Cores</th>
<th>Installed</th>
<th>Departments</th>
<th>Faculty</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEELE</td>
<td>Dell/Intel/GigE</td>
<td>7,216</td>
<td>May 2008</td>
<td>18</td>
<td>62</td>
</tr>
<tr>
<td>COATES</td>
<td>HP/AMD/10GbE</td>
<td>8,032</td>
<td>July 2009</td>
<td>25</td>
<td>81</td>
</tr>
<tr>
<td>ROSSMANN</td>
<td>HP/AMD/10GbE</td>
<td>11,088</td>
<td>Sept. 2010</td>
<td>16</td>
<td>36</td>
</tr>
<tr>
<td>HANSEN</td>
<td>Dell/AMD/10GbE</td>
<td>9,120</td>
<td>Sept. 2011</td>
<td>11</td>
<td>22</td>
</tr>
<tr>
<td>CARTER</td>
<td>HP/Intel/Mellanox FDR Infiniband</td>
<td>10,368</td>
<td>April 2012</td>
<td>Managed by Torque and Moab</td>
<td></td>
</tr>
</tbody>
</table>
Conte Cluster Purchasing System – Create New Order

Select Nodes > Enter Account Numbers > Additional Information > Order Submitted

To place an order for access to nodes in the new Conte cluster, please enter the quantity of each node to be purchased under the Conte Cluster heading below.

The Conte cluster consists of HP SL250 compute nodes with two (2) 8-core Intel Sandy Bridge processors (16 cores per node). All nodes have FDR10 InfiniBand interconnects and a 5-year warranty.

Once your order is ready, click “Continue” to go to the next page, where you will be able to add account numbers and other details to the order. If you have questions about any of the configurations, please send an email to rcac-cluster-purchase@lists.purdue.edu.

Conte Cluster

Nodes in Conte are available to Purdue researchers at two price levels:

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Description</th>
<th>Price</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>64GB memory, Two 8-core Intel Xeon E5-2670 processors (16 cores total) <em>For researchers whose codes do not make use of Phi accelerators. Phi acceleration can be purchased as an add-on later if a researcher’s codes become capable of taking advantage of it.</em></td>
<td></td>
</tr>
<tr>
<td></td>
<td>64GB memory, Two 8-core Intel Xeon E5-2670 processors (16 cores total), and Two 60-core Intel Xeon Phi 5110P Coprocessors <em>For researchers whose codes can take advantage of Intel Phi accelerators to greatly reduce time to results and enable far more extensive computations, or whose codes will be Phi ready soon.</em></td>
<td></td>
</tr>
</tbody>
</table>
COMMUNITY CLUSTERS

EMPOWERING THE FACULTY – USAGE REPORTING

RCAC Usage Reporting

Welcome, Preston M. Smith! You are able to view any system’s usage here.

- Show the processor wall hours regardless of completion
- Run on any resource
- Submitted via any batch system through the queue any
- By user any real name / any username
- Group Indiana Group

Display usage in no (total only) intervals based on when each job ended

Break down each time interval by user real name

Include only jobs which ended at or after 2011-11-01 12:00 am and which ended before 2012-04-11 12:00 am

Group PBS Usage Nov 1, 2011 through Apr 10, 2012

PURDUE UNIVERSITY
COMMUNITY CLUSTERS

EMPOWERING THE FACULTY – QUEUE MANAGEMENT
CONTE CLUSTER

PURDUE'S 2013 COMMUNITY CLUSTER

SAMUEL CONTE

Founder of nation’s first degree program in Computer Science – at Purdue
• Purdue’s first PetaFLOP system
• 580 nodes, HP SL6500 platform
  – Dual 2.6 GHz Intel Xeon-E5 processors
  – 64 GB memory (essentially a Carter-B node)
  – 145 chassis in 25 racks
  – two Xeon Phi 5110P co-processors
• 40 Gbps FDR10 Infiniband
  – non-blocking fat tree
  – next-generation Mellanox IB adapters
• Intel software tools
  – Intel compiler, math library (MKL), MPI
  – All take advantage of AVX instructions
• 1.2 PB Lustre storage system
  – Connected via FDR10 IB
• 40 Gbps network connectivity
  – Provided through IB-to-10G Ethernet gateways
• 85% of compute capability comes from Phis!
OTHER
RESOURCES
BEYOND THE COMMUNITY CLUSTERS
• HPC Clusters primarily scheduled with PBS

• **Condor** is used to backfill behind PBS, and integrate with opportunistic access to machines all over campus
  
  • For **ANY** user on campus

A resource like this, built on existing hardware, provides 18M hours per year to the campus at no* additional cost!
• General purpose cluster: Radon
  • 32 nodes, 8 cores/node, GigE
• Dedicated instructional cluster: Scholar
  • 8 nodes, 16 cores/node, FDR InfiniBand
• Hadoop/MapReduce
• Research Storage
• Performance Engineering
• Science Gateways
• Visualization
IMPACT

HOW CAN WE MEASURE SUCCESS?
**FACULTY PARTNERS**

<table>
<thead>
<tr>
<th>By Department</th>
<th>Cores</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrical and Computer Eng.</td>
<td>6,552</td>
</tr>
<tr>
<td>Physics</td>
<td>6,352</td>
</tr>
<tr>
<td>Mechanical Engineering</td>
<td>5,752</td>
</tr>
<tr>
<td>Chemistry</td>
<td>2,024</td>
</tr>
<tr>
<td>Earth and Atmospheric Sciences</td>
<td>1,800</td>
</tr>
<tr>
<td>Materials Engineering</td>
<td>1,168</td>
</tr>
<tr>
<td>Aeronautics and Astronautics</td>
<td>1,008</td>
</tr>
<tr>
<td>Med. Chem./Molecular Pharmacy</td>
<td>936</td>
</tr>
<tr>
<td>Biological Sciences</td>
<td>928</td>
</tr>
<tr>
<td>Mathematics</td>
<td>416</td>
</tr>
<tr>
<td>Statistics</td>
<td>416</td>
</tr>
<tr>
<td>Civil Engineering</td>
<td>392</td>
</tr>
<tr>
<td>Ag. and Biological Engineering</td>
<td>360</td>
</tr>
<tr>
<td>Computer Science</td>
<td>280</td>
</tr>
<tr>
<td>Chemical Engineering</td>
<td>152</td>
</tr>
<tr>
<td>PTO/Ag. Econ/Entomology</td>
<td>88</td>
</tr>
<tr>
<td>Agronomy</td>
<td>72</td>
</tr>
<tr>
<td>Industrial Engineering</td>
<td>56</td>
</tr>
<tr>
<td>Management/Economics</td>
<td>48</td>
</tr>
<tr>
<td>Computer Graphics Technology</td>
<td>32</td>
</tr>
<tr>
<td>Electrical/Computer Eng. Tech.</td>
<td>8</td>
</tr>
<tr>
<td>Horticulture/Landscape Arch.</td>
<td>8</td>
</tr>
<tr>
<td>Communication</td>
<td>8</td>
</tr>
</tbody>
</table>
128% increase in total computational hours for 2011
18% increase in number of research groups for 2011
All Systems Usage
(Including Retired)

By Date Job Ended

Processor Wall Hours

Millions


PBS / SLURM
Condor
HPC USERS AND SPONSORED DOLLARS

Awardees Using Research Computing

Total Purdue Research Awards

<table>
<thead>
<tr>
<th>Year</th>
<th>Awardees Using Research Computing</th>
<th>Total Purdue Research Awards</th>
</tr>
</thead>
<tbody>
<tr>
<td>1997</td>
<td>$129.9</td>
<td>$182.0</td>
</tr>
<tr>
<td>1998</td>
<td>$132.2</td>
<td>$185.5</td>
</tr>
<tr>
<td>1999</td>
<td>$134.5</td>
<td>$187.8</td>
</tr>
<tr>
<td>2000</td>
<td>$160.2</td>
<td>$204.0</td>
</tr>
<tr>
<td>2001</td>
<td>$190.3</td>
<td>$222.9</td>
</tr>
<tr>
<td>2002</td>
<td>$207.7</td>
<td>$229.8</td>
</tr>
<tr>
<td>2003</td>
<td>$235.6</td>
<td>$247.5</td>
</tr>
<tr>
<td>2004</td>
<td>$294.7</td>
<td>$312.8</td>
</tr>
<tr>
<td>2005</td>
<td>$292.2</td>
<td>$322.8</td>
</tr>
<tr>
<td>2006</td>
<td>$298.2</td>
<td>$327.5</td>
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<tr>
<td>2007</td>
<td>$322.8</td>
<td>$340.0</td>
</tr>
<tr>
<td>2008</td>
<td>$327.5</td>
<td>$365.0</td>
</tr>
<tr>
<td>2009</td>
<td>$418.0</td>
<td>$431.4</td>
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<tr>
<td>2010</td>
<td>$401.4</td>
<td>$422.1</td>
</tr>
<tr>
<td>2011</td>
<td></td>
<td>$418.0</td>
</tr>
</tbody>
</table>
A wide range of disciplines are represented in the Community Cluster program.

Prof. Michael Delgado from Agricultural Economics uses Carter and DiaGrid for his research.

Work involves large data sets on global, country, and state scales and data covering individual industries and companies as well as individual pollutants.

Prof. Delgado’s work generates answers that help guide policymakers using real data.

“What I do can take a standard computer weeks [...] That's why I turn to a cluster computing environment where I can run things in parallel”
• Prof. Jeffrey Greeley from Chemical Engineering utilizes RCAC’s Carter cluster
• Greeley’s lab works to simulate and optimize the properties of various classes of heterogeneous catalysts
• His research is of critical importance for industrial processes ranging from petrochemicals processing to biomass reforming
• More recently, his group is studying the production of hydrogen from biomass, which involves large numbers of complex biomolecules and requires supercomputing.

"You don't have to spend months trying to get your cluster running. [...] We can focus more on the scientific problems, which are our primary interest."
• Prof. Charles Bouman from Biomedical Engineering and Electrical and Computer Engineering uses RCAC’s Conte cluster for his research

• Bouman’s lab focuses on new and improved ways to construct images of fundamental processes captured by instruments in many areas

• His group processes huge amounts of data from medical instruments, and scanners used in material science.

“We've been running things that would have taken months to run in a day”
• Purdue’s RCAC has a wide array of compute systems
  • Community Clusters
  • Instructional and computing resources open to campus
  • Science Gateways
• Main goal is batch-scheduled big science
  • Also useful for related areas:
    – Visualization, data analysis, algorithm development

We serve the campus-wide research community!
Questions?

Contact Us:
@PurdueRCAC
http://www.facebook.com/PurdueRCAC