HPCXXL - Site Update
Indiana University

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Research Technologies
Indiana University

April 2018
Content

• Overview Indiana University
• High Performance Computing at IU
• Interesting Projects
  – Jetstream
  – Research Desktop
  – HPC Tools
Indiana University
IU – Campuses and Medical School Centers

IU Campuses

IU School of Medicine campuses and clinics
IU Overview

Fall 2016

<table>
<thead>
<tr>
<th>Number</th>
</tr>
</thead>
</table>
| Undergraduate | 93,740  
| Graduate     | 12,397  
| Doctoral - Research | 4,323  
| Doctoral - Practice | 3,700  
| Total Students | 114,160  
| Staff        | 11,498  
| Faculty      | 9,005   
| Grand Total  | 134,633 |

Overall
- Operating budget - $3.5B
- Grant Awards of $614M in 2016

Centralized IT Org - UITS
- 700+ professional staff
  - 130 Research Technologies
- 500+ part time staff
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HPC @ IU - Compute

- **Big Red II** – Cray XE6/XK7
  - 1020 nodes, 1 PFLOPS
  - CPUs/GPUs
  - CLE 5 up 02
  - Torque/Moab
  - 22 LNET Routers (QDR)
  - 4 DVS nodes (10Gb)

- Available to all Faculty, Staff, and Graduate Students
- Support/consulting available
• **Big Red II+** – Cray XC30
  • 560 nodes, 286 TFLOPS
  • Only CPUs
  • CLE 6
  • SLURM
  • 6 LNET Routers (2x FDR)
  • 2 DVS Nodes (40Gb)
  • Available to Grand Challenge Projects
  • Jobs >= 256 node desired
HPC @ IU - Compute

- **Karst** – standard cluster available for expansion
  - General purpose Intel Linux cluster
  - Condo nodes may be purchased for special needs or greater response

- Started at ~275 nodes -> ~400
- Upgrade in progress
- First nodes installed in Fall 2014
- NextScale nx360 M4 & M5
- 10/40Gb networking
- Memory profiles from 32GB -> 1024GB
- Using xCAT
- RHEL6
HPC @ IU - Compute

- **Carbonate** – large memory cluster
  - Supports high-performance, data-intensive computing
  - Available to all IU Faculty, Staff and Students
  - Condo nodes may be purchased for special needs or greater response
    - 72 nodes with 256 GB RAM
    - 8 high-mem nodes with 512 GB RAM
    - NextScale nx360 M5
    - Two 12-core Intel Xeon E5-2680 v3 CPUs
    - Four 480 GB solid-state drives
    - Using xCAT
    - RHEL7
HPC @ IU - Storage

Data Capacitor 2, DC-WAN, DC-RAM
- Data storage on disk, **not backed up** (scratch & projects)
- Temporary storage of research data – purged regularly
- 5 PB DCII (16 x FDR IB) / 1.1 PB DC-WAN (4 x 40Gb Ethernet)
- Lustre file system backed with LDISKFS

Slate, Slate-Condo
- *Persistent* high performance disk storage (not purged), **not backed up**
- 4 PB Slate (8 x EDR IB) / 8 PB Condo (16 x EDR IB)
- Lustre file system backed with ZFS

Wrangler (XSEDE dual-site 20 PB environment with TACC)
Research File System (RFS) / Computational Home Dirs

- Centralized disk storage designed to support researchers
- Home Dirs backed up regularly – 2 copies (IUB and IUPUI)
- Open to IU community – undergrads/non-IU must have sponsor
- HIPAA-aligned
- GPFS v4 with encryption and asynchronous replication
HPC @ IU - Storage

Scholarly Data Archive (SDA)

- Distributed tape storage for large-scale archival/near-line storage
- Mirrored – 2 copies (IUB and IUPUI)
- Open to IU community – undergrads/non-IU must have sponsor
- Supports collaborative activities

- 59 PB of tape storage capacity
- Supports SFTP, HSI, HPSS API
- HIPAA-aligned
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  – Research Desktop
  – HPC Tools
What is “the” Jetstream?

- Fast moving air currents
- Hot/Cold air boundaries
- Cloud resource funded by National Science Foundation

- NASA's Suomi NPP satellite collected this natural-color image using the VIIRS (Visible Infrared Imaging Radiometer Suite) instrument on Sept. 4, 2017. Actively burning areas are outlined in red. NASA image courtesy Jeff Schmaltz LANCE/EOSDIS MODIS Rapid Response Team, GSFC
What is Jetstream and why does it exist?

- NSF’s first production cloud facility
- Focus on ease-of-use, broad accessibility
- Encourage collaboration and community development
- User-selectable library of preconfigured virtual machines
- Provides on-demand *interactive* computing and analysis or persistent services such as gateways (e.g. SEAGrid, Galaxy, GenApp, and others)
- Enables *configurable* environments and *programmable cyberinfrastructure*
- Reproducibility: Share VMs and then store, publish via IU Scholarworks (DOI)
Jetstream System Overview

IU Cyberinfrastructure
Jetstream (production)
- 320 Nodes
- 7,680 Cores
- 40 TB RAM
- 640 TB local disk
- 4x40 Gbps

TACC Cyberinfrastructure
Jetstream (production)
- 320 Nodes
- 7,580 Cores
- 40 TB RAM
- 640 TB local disk
- 4x40 Gbps

U of Arizona Cyberinfrastructure
Jetstream (development)
- 16 Nodes
- 384 Cores
- 2 TB RAM
- 32 TB local disk

100 Gbps
100 Gbps
10 Gbps
10 Gbps

Internet2
XSEDE

funded by the National Science Foundation
Award #ACI-1445604

http://jetstream-cloud.org/
Platform Overview

- Atmosphere API
- Globus Auth
- Atmo Services
- XSEDE Accounting

OpenStack

Ceph

Indiana University

TACC
Jetstream usage highlights – March 2018

- 314 active XSEDE projects covering 72 fields of science and **2039 active users** representing **201 institutions**
- **86%** of Jetstream users new to XSEDE (at end of PY1 Ops)
- >104 million CPU hours allocated to XSEDE projects since June 2016
- 12 active science gateways
- 43 education/teaching allocations serving almost 700 students
- Averaging 1230 concurrent Active VMs in February 2018
- **100%** system availability, **99.4%** cap availability
- **97.7%** “job” completion (at end PY1)
Not just the usual suspects...

- Physics, chemistry, and other “usual” HPC suspects are represented, but Jetstream also is home to projects on:
  - Financial analysis / Economics
  - Political science
  - Humanities / Text analysis
  - Network analysis
  - Computer Science / Machine learning
  - Satellite data analysis
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  – HPC Tools
Research Desktop – The Idea

- A way to make supercomputing more user friendly
- A new way to login and interact with IU HPC systems
- A GUI/desktop instead of a terminal

- Based on ThinLinc, a Linux remote desktop solution using VNC and SSH
Research Desktop - Architecture

User Desktop/Laptop

Load Balancing Gateway

25 Nodes, 32 or 48 cores, 256 GB of Memory
Research Desktop - Features

- More user friendly interface than a terminal
  - A new front end to HPC, with new capabilities
  - Filesystem browser and file editors/viewers
- Graphical access to compute nodes (indirectly)
- Works more seamlessly compared to X forwarding
  - Addresses latency issues, really great for GUI based applications
- Convenient data transfer/share options
- Supports long running tasks (disconnect / reconnect)
- Supports ssh keys and two factor authentication
- Hands on user support
Research Desktop – Use Cases

- Running mathematical and statistical applications
- GUIs of HPC applications such as Vampir, Allinea MAP, TotalView
- Visualization (VMD, ParaView…)
- COMSOL Multiphysics Client/Server
- Data Enclave
- Desktop environment for crystallography tool suite
- Easy access to compilers for classes
- Long running data movement jobs
- Facilitates collaboration
Dr. Franco Pestilli’s research group has collaborators in Argentina, Japan, Europe and the US.
Research Desktop – User Survey

• 900 users contacted
• 162 responses received (18% response rate)
  – 83% of the respondents said that, in general, a desktop point-and-click interface is extremely or moderately important for their research. Only 7% said it is of low or no importance.
  – 82% of the respondents said that, in particular, Karst Desktop is extremely or moderately important for their ability to use HPC resources at IU. Only 8% said that it is of low or no importance.
  – 82% of the respondents said that they are extremely satisfied or satisfied with the Karst Desktop service. Only 3% said that they are dissatisfied or extremely dissatisfied.
• Karst Desktop brought in 268 new users to the HPC environment in 2017. (users who never submitted a traditional batch job)
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  – HPC Tools (Pathfinder, Dashboard, Job GUI)
HPC Pathfinder

• Help new users identify the machine to start with.
• Provide direct links to relevant knowledge base articles and how to create an account.
At IU, how can I get help determining which research supercomputer I should use?

As a researcher at Indiana University, you have access to several robust, reliable, world-class supercomputing systems managed by the Research Technologies division of UITS. To help determine which system best suits the needs of your project and/or your level of experience working with high-performance computing (HPC) systems, use the UITS Supercomputing Pathfinder.

To use the Supercomputing Pathfinder, just answer Yes or No to each of the statements. Some statements have additional information you can reveal by clicking the Information icon (🔍). When you're finished, click Submit to see which IU supercomputing system is the best match, based on your responses.

If you are unsure about a particular response or need further guidance, contact the UITS Scientific Applications and Performance Tuning (SciAPT) team.

Related documents

- What statistical and mathematical software packages are available on IU's supercomputers?
- Research computing support at IU
- UITS Research Technologies systems and services for researchers working with data containing HIPAA-regulated PHI
# Supercomputing Pathfinder

As a researcher at Indiana University, you have access to several world class supercomputing and storage resources. The Pathfinder attempts to guide you toward the optimal compute resources for your research based on your responses to the set of questions below. If you are unsure about the answer to a question, then please leave that response unselected. Please contact sciapt@iu.edu if you have any questions about Pathfinder.

1. I am an undergraduate student.  
2. I need to run a Windows application.  
3. I am new to using supercomputers.  
4. My application uses a programming language like Java, Python, Perl or Matlab.  
5. I intend to use the computing resources interactively. I expect to obtain results within minutes.  
6. My application needs more than 32 GB of computer memory.  
7. I need an interactive desktop type environment.  
8. My application is designed for a single CPU and does not support parallel processing.  
9. My application uses MPI (Message Passing Interface) for distributed parallel computing.  
10. My application takes advantage of GPUs to accelerate computation.

[Submit]
Supercomputing Pathfinder

Big Red II
Karst
Karst Desktop
Carbonate

Karst’s key properties matches 70% of your needs.

5. I intend to use the computing resources interactively. I expect to obtain results within minutes.  
   True

Supercomputers are optimized for serving large amounts of users and workloads. They are not designed for short response times. Interactive testing is enabled by an 'interactive queue', but large compute workloads should be run through the batch reservation system.

For More Information
- KB: What is a batch job?
- KB: On Big Red II, Carbonate, or Karst at IU, why is my job sitting in the queue, and when will it run?
- KB: How do I run batch jobs on Big Red II at IU?
- KB: Getting started on Carbonate #Running jobs
- KB: Getting started on Karst #Running jobs
- KB: How do I run interactive jobs on Big Red II at IU?

7. I need an interactive desktop type environment.  
   True

You may need a system that is similar to a standard Linux desktop computer. Karst Desktop provides precisely this. To use it, you have to install a client application on your desktop.
HPC Dashboard

HPC Tools
- Pathfinder: Determine which IU computing cluster best fits your HPC needs
- MyHPC: Monitor your running and queued HPC jobs
- Wait-time Visualizer: Visualize available resources and minimize your wait times
- Script Generator: Generate a custom HPC Job script
- Access Management: Manage your existing accounts and request access
- Status: IU: Current status updates for IITS systems and services

HPC Resources
- Big Red II
- Carbonate
- Karst
- 5 active users
- 423 running jobs
- 1485 queued jobs
HPC Dashboard – Wait-time Visualizer

Wait-time Visualizer

Compute Resource
- Big Red II
- MOTID

Queue
- cpu (normal)
- Time Limit: 2 days
- Node Limit: 328
- Cores per Node: 32

Number of Nodes: 64

Waittime (D:H:M): 08:00

Job expected to start in 10 hours

Generate Script
Job GUI

• Using Zenity
## Job GUI – Job Listing

Select items from the list below.

<table>
<thead>
<tr>
<th>Job ID</th>
<th>Username</th>
<th>Queue</th>
<th>Jobname</th>
<th>SessID</th>
<th>NDS</th>
<th>TSK</th>
<th>Req'd Memory</th>
<th>Req'd Time</th>
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<th>Elap</th>
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<td>pbsname</td>
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<td>1</td>
<td>1</td>
<td>20gb</td>
<td>40:00:00</td>
<td>Q</td>
<td>..</td>
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<td>27360</td>
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<td>6</td>
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<td>6</td>
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<td>normal</td>
<td>_main</td>
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<td>6</td>
<td>16gb</td>
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<td>28297</td>
<td>1</td>
<td>8</td>
<td>16gb</td>
<td>04:00:00</td>
<td>R</td>
<td>00:1</td>
</tr>
</tbody>
</table>
Job GUI – Interactive Job

Your job is waiting for resources and has not started. It has been in the Queue for 15 second(s).

An interactive job can be submitted by executing the following command:

```
qsub -I -X -q interactive -l nodes=1:ppn=4 -l walltime=04:00:00 -N job_name
```

Information:
- Queue: interactive
- Nodes: 1
- PPN: 4
- Req'd Memory: --
- Req'd Time: 04:00:00

On Carbonate, you currently have 0 Running Job(s), 1 Queued Job(s), 0 Waiting Job(s) and 0 Completed Job(s).

Press Cancel to close this window (this will not cancel your job).
And there is Tableau....

Big Red II

Total Jobs Per Month

<table>
<thead>
<tr>
<th>Month</th>
<th>2015</th>
<th>2016</th>
<th>2017</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jan</td>
<td>4,486</td>
<td>6,702</td>
<td>6,424</td>
</tr>
<tr>
<td>Feb</td>
<td>4,822</td>
<td>6,206</td>
<td>4,914</td>
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<tr>
<td>Mar</td>
<td>5,003</td>
<td>6,437</td>
<td>6,104</td>
</tr>
<tr>
<td>Apr</td>
<td>6,856</td>
<td>6,596</td>
<td>5,901</td>
</tr>
<tr>
<td>May</td>
<td>7,930</td>
<td></td>
<td>9,575</td>
</tr>
</tbody>
</table>

Top Users

Big Red II’s Active Users 2015-2017

<table>
<thead>
<tr>
<th>Year</th>
<th>2015</th>
<th>2016</th>
<th>2017</th>
</tr>
</thead>
<tbody>
<tr>
<td>Active Users</td>
<td>469</td>
<td>595</td>
<td>619</td>
</tr>
<tr>
<td>Avg Queued Time (Hours)</td>
<td>7</td>
<td>13</td>
<td>24</td>
</tr>
<tr>
<td>Total Jobs Run</td>
<td>393,401</td>
<td>343,685</td>
<td>408,966</td>
</tr>
<tr>
<td>Avg Job Duration (Hours)</td>
<td>5</td>
<td>7</td>
<td>10</td>
</tr>
<tr>
<td>Total Hours Duration</td>
<td>2,098,084</td>
<td>2,389,710</td>
<td>3,876,456</td>
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<tr>
<td>Avg Task Count Per Job</td>
<td>59</td>
<td>56</td>
<td>55</td>
</tr>
<tr>
<td>Avg Core Hours Per Job</td>
<td>377</td>
<td>459</td>
<td>394</td>
</tr>
<tr>
<td>Total Core Hours</td>
<td>148,478,337</td>
<td>157,672,832</td>
<td>160,459,990</td>
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</tbody>
</table>

Total Core Hours

<table>
<thead>
<tr>
<th>Year</th>
<th>2015</th>
<th>2016</th>
<th>2017</th>
</tr>
</thead>
<tbody>
<tr>
<td>0M</td>
<td>148,478,337</td>
<td>157,672,832</td>
<td>160,459,990</td>
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<td>100M</td>
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</table>
And there is Tableau....
Thank you!

Questions?