Deploying a Software Ecosystem for Science and Engineering Applications at a Regional HPC Center

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Ohio Supercomputer Center
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Agenda

- Overview of Ohio Supercomputer Center
- Software resources and services
- Looking forward
About OSC

• 1987: Ohio Legislators Establish OSC
• Statewide resource for all universities in Ohio
  – high performance computing services
  – computational science expertise
  – “… propel Ohio's research universities and private industry to the forefront of computational based research.”
• Funded by and reporting line through the Ohio Department of Higher Education
• Fiscal agent is Ohio State University, offices on OSU’s west campus
Client Services CY2016

- 26 Ohio-based universities
- 41 companies
- 1,358 clients
- 218 trainees
- 8 training opportunities
- 218 awards made
- 533 projects served
- 31 academic courses used OSC’s supercomputers
Production Capacity CY2016

115,000,000+ core-hours consumed
3,400,000+ computational jobs
1,101 TB data stored
97.9% up-time (target: 96%)
Computing Usage by Field of Science CY2016

- Materials Research, 26.0%
- Engineering, 18.0%
- Chemistry, 23.0%
- Physics, 6.0%
- Geosciences, 10.0%
- Biological, Behavioral, and Social Sciences, 8.0%
- Computer and Information Science and Engineering, 6.0%
- Other, 3.0%
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<thead>
<tr>
<th></th>
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<tbody>
<tr>
<td># Nodes</td>
<td>824</td>
<td>240</td>
<td>692</td>
</tr>
<tr>
<td># CPU Cores</td>
<td>23,392</td>
<td>4,800</td>
<td>8,304</td>
</tr>
<tr>
<td>Total Memory (TB)</td>
<td>~120</td>
<td>~15.3</td>
<td>~33.4</td>
</tr>
<tr>
<td>Memory per Core (GB)</td>
<td>4.5</td>
<td>3.2</td>
<td>4</td>
</tr>
<tr>
<td>Interconnect Fabric (IB)</td>
<td>EDR</td>
<td>FDR/EN</td>
<td>QDR</td>
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<table>
<thead>
<tr>
<th>Capacity (PB)</th>
<th>Bandwidth (GB/s)</th>
</tr>
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<tbody>
<tr>
<td>Home Storage</td>
<td>0.8</td>
</tr>
<tr>
<td>Project Storage</td>
<td>3.4</td>
</tr>
<tr>
<td>Scratch Storage</td>
<td>1.1</td>
</tr>
<tr>
<td>Tape Library (backup &amp; archive)</td>
<td>5+</td>
</tr>
</tbody>
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## OSC Service Catalog

<table>
<thead>
<tr>
<th>Cluster Computing</th>
<th>Research Data Storage</th>
</tr>
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<tbody>
<tr>
<td>• High Performance Computing</td>
<td>• Project Storage</td>
</tr>
<tr>
<td>• High Throughput Computing</td>
<td>• Archival Storage</td>
</tr>
<tr>
<td>• Data-intensive Computing</td>
<td></td>
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<table>
<thead>
<tr>
<th>Client Services</th>
<th>Client Facilitation</th>
</tr>
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<tbody>
<tr>
<td>• 24x7 Call Center</td>
<td>• Consultation (in-person and online)</td>
</tr>
<tr>
<td>• Level 2 Engineering Support</td>
<td>• Training and Education</td>
</tr>
<tr>
<td></td>
<td>• Classroom accounts</td>
</tr>
</tbody>
</table>

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<thead>
<tr>
<th>Scientific Software Development</th>
<th>Web Software Development</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Software Development</td>
<td>• Software Development</td>
</tr>
<tr>
<td>• Software Parallelization</td>
<td>• Software Consulting</td>
</tr>
</tbody>
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<thead>
<tr>
<th>Partner on Proposals</th>
<th>Visualization &amp; Virtual Environments</th>
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</thead>
<tbody>
<tr>
<td>• Cyberinfrastructure solutions</td>
<td>• Visualization Services</td>
</tr>
<tr>
<td>• Modeling &amp; simulation for industry</td>
<td>• Virtual environments (DSL)</td>
</tr>
</tbody>
</table>
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• Overview of Ohio Supercomputer Center
• **Software resources and services**
• Looking forward
Deploying Software at OSC

- **Web and Interface Applications**
  - Open OnDemand
  - Federated Authentication
  - NoVNC, Apache
  - Ruby, Python, Node.js

- **Scientific Applications**
  - Software development tools: Compilers, debuggers, profilers, productivity languages
  - Communication, numerical and I/O libraries
  - Analysis and simulation frameworks and solvers

- **HPC Operations**
  - Tools for system administration
  - User facing: Red Hat Enterprise Linux, Torque/MOAB, Compilers, MPI
  - Federated Authentication
Scientific Applications Examples

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Software Resources for OSC Clients

- More than 150 software packages,
- https://www.osc.edu/resources/available_software
- Types of Software include compilers, development tools, numerical libraries, applications
- Mix of ISV, free and open source packages
- Agreements with ISVs are often challenging given our multi-institution and mixed academic/non-academic client base
- Molecular Dynamics (MD) Simulations
  - 3X - 7X faster than CPU
  - Materials Science, Biochemistry, Chemistry, Biophysics
  - Software: NAMD, LAMMPS, AMBER, GROMACS

- Machine Learning/Deep Learning
  - 4X - 10x faster for “training” than CPU
  - Wide range of disciplines
  - Software: Caffe, TensorFlow, Torch
Data Analytics Use Cases and Software

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<thead>
<tr>
<th>Statistics</th>
<th>MySQL</th>
<th>SPARK</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU vs Account</td>
<td>1.25 hour</td>
<td>5 sec</td>
</tr>
<tr>
<td>Walltime vs user</td>
<td>1.40 hour</td>
<td>5 sec</td>
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- Analytics on OSC Job data
  - Complex queries on historical job data
  - More than 700x faster than MYSQL query of same data
  - Software: Apache SPARK, PySpark

- Analysis of Simulation results
  - Large data sets from suite of simulation runs
  - Biochemistry/Bioinformatics
  - Software: VMD, R

- Other services: Hadoop, Statistical and mathematical software, high performance storage
OSC included in OSU site license
History: non-OSU clients using local licenses from campus servers when running at OSC
New terms allows for academic use of MATLAB on OSC systems by any OSC clients from educational institutions
Additionally, OSC has licenses for MATLAB DCS for multi-node parallel MATLAB
NSF funded “Automated, High Resolution Terrain Generation for XSEDE”

Howat, Noh – OSU, Tomko – OSC

Funding Source: National Science Foundation (NSF)

• Establish a service for on-demand polar Digital Elevation Model (DEM) production and distribution utilizing the XSEDE High Performance Computing framework and the NSF-funded Polar Geospatial Center (PGC) data services

• OSC is providing software engineering, code optimization and parallel software development for the project
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Improving Client Access with Open OnDemand

Message of the Day

2016-06-23 - SYSTEM DOWNTIME RESCHEDULED

UPDATE: Due to a bug identified on some of the center's systems, the June 26th downtime to upgrade project and scratch file systems will be postponed until July 12th.

A downtime is scheduled for all HPC systems starting July 12th, beginning at 7AM and scheduled to finish by 5PM. The downtime will affect all clusters and services. Login services and access to storage systems will not be available during this time.

Highlights include: * Migration of data to new Project and Scratch servers * Installation of new hardware in preparation for Owens Cluster

In preparation for the downtime the batch scheduler will begin holding jobs that cannot complete before 7AM July 12th. Jobs that are held will be scheduled after the system is returned to production status.

2016-06-17 - CHANGES TO HOME DIRECTORY ACCESS CONTROL LISTS (ACLs)

As of the June 7th downtime the Home Directory file system no longer supports POSIX ACLs. Due to the migration of the file system all previous ACLs were lost and will need to be reset using NFSv4 ACLs.

For more details on the change, including how to set NFSv4 ACLs, see: https://www.osc.edu/migration_to_nfs4_acls

Visit our website: https://osc.github.io/Open-OnDemand/
What can clients do with Open OnDemand?

- Supercomputer access
  - File Browser, File Editor, Terminal
  - Job Constructor, Job Status, System Status
- Virtual Desktop Interface (VDI)
- Interactive HPC (iHPC)
- Web apps (AweSim AppKit)
  - Open OnDemand apps (Jobs, VDI, iHPC)
  - Workflow apps (Cantilever Beam example)
AppKit Example: Beam

• Classic cantilever beam problem
  – User specifies geometry, materials and load
  – App calculates displacement and stress
• 100% open-source back end
  – gmsh for geometry and mesh generation
  – Elmer for the analysis
  – Paraview to generate a WebGL file for results visualization
Engineers and non-expert designers use OSC simulation apps to run fully automated, on-demand and accurate crush tests of new bucket designs inexpensively and quickly.

Dan Meyer, Comet Solutions
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New Technology Example: DDN Infinite Memory Engine (IME)

- “Burst Buffer” for scratch file system
- NVMe SSD based storage, acts as write-back/read cache, or temporary storage
- Test and document use cases for client rollout
  - POSIX interface, /ime/scratch instead of /fs/scratch
  - Native API
  - MPI-IO (NetCDF, HDF5, etc)
- Still in testing, friendly user availability soon
Interactive Applications via Web Browser

- New capability not available at other supercomputer centers
- Accessible via a web browser with a few clicks through OSC OnDemand
- High performance computing live via a dedicated HPC node(s) (vs. local laptop)
- Currently in Beta testing: Rstudio, Jupyter Notebook for python, MATLAB
Client-Centric View

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