OSC Spring 2017

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April 2017 SUG General Meeting
General Agenda

• Organizational Update
• New Services
• Hardware Futures
• Committee Reports
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%)
469 Active Projects CY2016
Ohio Academic Resource Network (OARnet) Update

OARnet 100 Gigabit/second network backbone with connected partners

- **26** K-12 Schools
- **91** Higher Education
- **65** Healthcare Facilities
- **15** Broadcast Stations
- **35** Local Entities
- **543** State of Ohio Agency Sites
- **6** Research Facilities

- **2,240+** miles of high-speed network backbone
- **$8 million** savings to Ohio education
- **$47+ million** savings through virtualization program
- **300+** campuses of college, university, and branch partners
- **700+** schools in public K-12 sector
New Services

• Owens in full production (Dedication ceremony last week!)
• Expansion of GPU services with new NVIDIA P100s
• Expansion of data analytics services
• Interactive applications via the web
Owens Dedication

- March 29th, 2017
- Well attended, with representatives from major partners, vendors, and R1 institutions in Ohio
### OSC Supercomputer and Storage Services

#### #202 on the Top 500

<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>Theoretical Performance (TF)</td>
<td>~860</td>
<td>~144</td>
<td>~154</td>
</tr>
<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>
</tr>
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#### Storage

<table>
<thead>
<tr>
<th></th>
<th>Capacity (PB)</th>
<th>Bandwidth (GB/s)</th>
</tr>
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<tbody>
<tr>
<td>Home Storage</td>
<td>0.8</td>
<td>10</td>
</tr>
<tr>
<td>Project Storage</td>
<td>3.4</td>
<td>40</td>
</tr>
<tr>
<td>Scratch Storage</td>
<td>1.1</td>
<td>100</td>
</tr>
<tr>
<td>Tape Library (backup &amp; archive)</td>
<td>5+</td>
<td>3.5</td>
</tr>
</tbody>
</table>
## Owens Node Configurations “side-by-side” Comparison

<table>
<thead>
<tr>
<th>Node Type</th>
<th>Compute</th>
<th>GPGPU</th>
<th>Data Analytics</th>
</tr>
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<tbody>
<tr>
<td>Node Count</td>
<td>648</td>
<td>160</td>
<td>16</td>
</tr>
<tr>
<td>Core Count</td>
<td>28</td>
<td>28</td>
<td>48</td>
</tr>
<tr>
<td>Core Type</td>
<td>Broadwell</td>
<td>Broadwell</td>
<td>Haswell</td>
</tr>
<tr>
<td>Memory</td>
<td>128 GB</td>
<td>128 GB</td>
<td>1500 GB</td>
</tr>
<tr>
<td>Disk</td>
<td>1 TB</td>
<td>1 TB</td>
<td>20 TB</td>
</tr>
<tr>
<td>GPU</td>
<td>N/A</td>
<td>P100</td>
<td>None</td>
</tr>
</tbody>
</table>
• Tradeoffs: very large number of compute cores, high bandwidth memory
• Model: NVIDIA “Pascal” P100
• Purchase Price: $770K
• Quantity: 160
• Expected Performance: ~750TF (will make Owens ~1.6PF)
• Customer availability now!
• 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
Owens Data Analytics Nodes

- Tradeoffs: very large memory, increased core count, large local storage
- Quantity: 16
- Cores: 48 / node (Intel Haswell)
- Memory: 1.5TB / node
- Local Disk: 24TB
Data Analytics Use Cases and Services

- 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
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
DDN Infinite Memory Engine (IME)

- “Burst Buffer” for /fs/scratch file system
- NVMe SSD based storage (same hardware as storage arrays, no spinning media)
- Logically sits between compute nodes, and file system
- Acts as write-back/read cache, or temporary storage
  - Additional tier in storage hierarchy
  - Can smooth peak demand on file system
  - Better suited for small, or unaligned writes than parallel file system
DDN IME Performance, and Status

- Capacity: ~40TB
  - Only ½ disk slots populated
- Methods for access
  - POSIX interface, /ime/scratch instead of /fs/scratch
  - Native API
  - MPI-IO (NetCDF, HDF5, etc)
- Data location management not completely automatic
- Still in testing, friendly user availability soon
Hardware Futures

• **Compute**
  – Oakley decommissioning, and replacement

• **Storage**
  – Performance and capacity upgrades for backups
  – Infrastructure storage upgrade
  – Project storage expansion, additional tier(s) when needed

• **Network**
  – Upgrade to 40Gb uplink to OARnet
Upcoming Events

• OSC Workshop: Computing Services to Accelerate Research and Innovation: Thursday, April 13th @ UC
• OSC Workshop: Big Data at OSC: Intro to Hadoop and Spark at OSC: Thursday, April 13th @ UC
• XSEDE Workshop: MPI: Tuesday April 18th & Thursday April 19th
• Scratch Policy public comment period closes: Friday, April 28th
• Client Survey currently open
• Office Hours at OSU’s Research Commons (alternating Tuesdays) – in person or remote
• OSC 30th Anniversary: TBD (Fall)
Committee Reports
Allocations Committee

• Allocations:
  – 7.7M+ RUs allocated
  – Reviewed 215 applications
    • 25 discovery-level
    • 14 major-level
    • 28 standard-level
    • 5 emerita
    • 25 classroom
    • 118 startup
  – 22 institutions allocated RUs

• Annual Allocations (for CY16):
  • 4.9M+ RUs allocated
  • 7 institutions

Resource Units consumed by Field of Science, CY16
Hardware Committee

John Heimaster, Committee Chair
• **New Purchase Discussion**
  - Comsol Server: provide non-OSU users
  - Debugger: Totalview vs. DDT

• **Third party hosting**
  - Matlab
    - Any academic users in Ohio can use Matlab on OSC as part of our license.

• **Renewal (Since Oct 2016 meeting)**
  - Abaqus, pgi, CSD, Gaussian, Intel Cluster (Capital), MDCS, Turbomole

• **Upcoming (during 2017 calendar year)**
  - Discontinue?: CSD (Cambridge Structural Database)
  - Capital purchase: Totalview, Ansys
  - Regular renewal: Amber, Comsol, Q-chem, Star-CCM+, Schrodinger, Allinea, abaqus, pgi, Gaussian