Connecting Researchers, Data & HPC

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The Shift to Big Data

New Emphases

- **Social networks and the Internet**
- **Video**
- **Collections**
- **Legacy documents**
- **Environmental sensors: Water temperature profiles from tagged hooded seals**

**Pan-STARRS telescope**
http://pan-starrs.ifa.hawaii.edu/public/

**Genome sequencers**
(Wikipedia Commons)

**NOAA climate modeling**
http://www.oml.gov/info/omlreview/v42_3_09/article02.shtml

**Horniman museum**
http://www.horniman.ac.uk/get_involved/blog/bioblitz-insects-reviewed

**Library of Congress stacks**
https://www.flickr.com/photos/danlem2001/6922113091/

**Wikipedia Commons**
Algorithms and Applications Have Also Changed

- Structured Data
- Statistics
- Optimization (numerical)
- Calculations on Data
- Scientific Visualization

- Unstructured Data
- Machine Learning
- Optimization (decision-making)
- Natural Language Processing
- Video
- Image Analysis
- Sound
- Graph Analytics
- Information Visualization

BRIDGES
Pittsburgh is a city of bridges: from its history in steel to its leadership in computer science and biotechnology, between diverse neighborhoods housing its many universities, and at PSC, from science-inspired national cyberinfrastructure to researchers’ breakthroughs.

*Bridges* will be a new XSEDE resource that will integrate advanced memory technologies to empower new communities, bring desktop convenience to HPC, connect to campuses, and intuitively express data-intensive workflows.
The $9.65M Bridges acquisition is made possible by National Science Foundation (NSF) award #ACI-1445606:

Bridges: From Communities and Data to Workflows and Insight

HP is delivering Bridges
Disclaimer

The following presentation conveys PSC’s current plan for the *Bridges* supercomputer. Details are subject to change.
An Important Addition to the National Advanced Cyberinfrastructure Ecosystem

*Bridges* will be a new resource on XSEDE and will interoperate with other XSEDE resources, Advanced Cyberinfrastructure (ACI) projects, campuses, and instruments nationwide.

Examples:

- High-throughput genome sequencers
- Social networks and the Internet
- Reconstructing brain circuits from high-resolution electron microscopy
- Temple University’s new Science, Education, and Research Center
- Carnegie Mellon University’s Gates Center for Computer Science
- Data Infrastructure Building Blocks (DIBBs)
  - Data Exacell (DXC)
  - Other DIBBs projects
  - Other ACI projects
Meeting Research Needs – Examples

- Scaling research questions beyond the laptop
  - From individual researchers to teams & collaborations
  - Cross-domain analyses
  - Shared data collections & related analysis tools
- Workflows – HPC power without the programming
  - Large-memory applications & in-memory databases
- Optimization & parameter sweeps
  - Powerful collections of application & tools
- Modern, widely-used software environments
Potential Applications (Examples)

• Finding causal relationships underlying various diseases
• Assembling large genomes and metagenomes
• Analysis of financial markets and policies
• Improving the effectiveness of organ donation networks
• Recognizing events and enabling search for videos
• Understanding how the brain is connected from EM data
• Addressing societal issues from social media data
• Analyzing large bodies of work in the digital humanities
• Agent-based modeling for epidemiology
• Cross-observational analyses in astronomy & other sciences
• Data integration for history, political science & cultural studies
Objectives and Approach

- Bring HPC to nontraditional users and research communities.
- Allow high-performance computing to be applied effectively to big data.
- Bridge to campuses to ease access and provide burst capability.
- Leveraging PSC’s expertise with shared memory, Bridges will feature 3 tiers of large, coherent shared-memory nodes.

Bridges will leverage its large memory for interactivity and to seamlessly support applications through virtualization, gateways, familiar and productive programming environments, and data-driven workflows.
User-Friendly HPC & Data Analytics

- **Interactivity** is the feature most frequently requested by nontraditional HPC communities and for doing data analytics and testing hypotheses.

- **Gateways and tools for gateway building** will provide easy-to-use access to Bridges’ HPC and data resources.

- **Database and web server nodes** will provide persistent databases to enable data management, workflows, and distributed applications.

- **High-productivity programming languages & environments** will let users scale familiar applications and workflows.

- **Virtualization** will allow users to bring their particular environments and provide interoperability with clouds.
Interactivity

- *Interactivity is the feature most frequently requested by nontraditional HPC communities.*
- Interactivity provides immediate feedback for doing exploratory data analytics and testing hypotheses.
- *Bridges will offer interactivity through a combination of virtualization for lighter-weight applications and dedicated nodes for more demanding ones.*
Gateways and Tools for Building Them

Gateways will provide easy-to-use access to Bridges’ HPC and data resources, allowing users to launch jobs, orchestrate complex workflows and manage data from their web browsers.

Interactive pipeline creation in GenePattern (Broad Institute)

Col*Fusion portal for the systematic accumulation, integration, and utilization of historical data, from http://colfusion.exp.sis.pitt.edu/colfusion/

Download sites for MEGA-6 (Molecular Evolutionary Genetic Analysis), from www.megasoftware.net
Virtualization and Containers

Users will be able to import their entire computational environments into Bridges, conferring ease of use, reproducibility, and interoperability with cloud services.
High-Productivity Programming

*Bridges* will feature high-productivity programming languages and tools.
Hadoop Ecosystem

• *Bridges* will provide acceleration for Hadoop applications running on its 128GB nodes.
• Large memory will be great for Spark.
Campus Bridging

Through a pilot project with Temple University, the Bridges project will explore new ways to transition data and computing seamlessly between campus and XSEDE resources.

Federated identity management will allow users to use their local credentials for single sign-on to remote resources, facilitating data transfers between Bridges and Temple’s local storage systems.

Burst offload will enable cloud-like offloading of jobs from Temple to Bridges and vice versa during periods of unusually heavy load.

http://www.temple.edu/medicine/research/RESEARCH_TUSM/
High-Performance, Data-Intensive Computing

• 3 tiers of large, coherent shared memory nodes

<table>
<thead>
<tr>
<th>Memory per node</th>
<th>Number of nodes</th>
<th>Example applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 TB</td>
<td>Several</td>
<td>Genomics, machine learning, graph analytics, other extreme-memory applications</td>
</tr>
<tr>
<td>3 TB</td>
<td>Tens</td>
<td>Virtualization and interactivity including large-scale visualization and analytics; mid-spectrum memory-intensive jobs</td>
</tr>
<tr>
<td>128 GB</td>
<td>Hundreds</td>
<td>Execution of most components of workflows, interactivity, Hadoop, and capacity computing</td>
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• The latest Intel® Xeon® CPUs
• NVIDIA® Tesla® dual-GPU accelerators
Database and Web Server Nodes

• Dedicated database nodes will power persistent relational and NoSQL databases
  – Support data management and data-driven workflows
  – SSDs for high IOPs; RAIDed HDDs for high capacity

• Dedicated web server nodes
  – Enable distributed, service-oriented architectures
  – High-bandwidth connections to XSEDE and the Internet

(examples)
Data Management

• **Pylon**: A large, central, high-performance filesystem
  – Visible to all nodes
  – Large datasets, community repositories (~10 PB usable)
• **Distributed (node-local) storage**
  – Enhance application portability
  – Improve overall system performance
  – Improve performance consistency to the shared filesystem
• **Acceleration for Hadoop-based applications**
Intel® Omni-Path Architecture Fabric

• Omni-Path will connect all nodes and the shared filesystem, providing *Bridges* and its users with:
  – The highest-bandwidth internal network
  – Valuable optimizations for MPI and other communications
  – Early access to this new, important, forward-looking technology
High-Level Architecture

Service Nodes
- ESM Nodes: 12 TB each (several nodes)
- LSM Nodes: 3 TB each (10s of nodes)
- RSM Nodes: 128 GB each (100s of nodes)

Database Servers
Web Servers
Data Transfer

Intel® Omni-Path Fabric

XSEDE Campuses Instruments Clouds...

Pylon Filesystem

Compute Nodes

Web Servers

GPUs

Hadoop
Example: Causal Discovery

Browser-based UI
- Prepare and upload data
- Run causal discovery algorithms
- Visualize results

Web node
- VM
- Apache Tomcat

Execute causal discovery algorithms
- OmniPath

Analytics:
- TETRAD (FastGES, …) and related implementations

Database node
- VM
- MySQL
- Other DBs

1-10 GigE to Internet

LSM Node
(3TB)

ESM Node
(12TB)
Bridges Target Schedule

• Acquisition
  – Begins December 2014
  – Construction to begin October 2015
    • Will allow for including important new technologies
  – Early user period in late 2015

• Production
  – January 2016
For Additional Information

Project website: www.psc.edu/bridges

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