Bridges and the Data Exacell: Database-Enabling Technologies for the National Research Community

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The Shift in Open Research to Big Data

New Emphases

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

Genome sequencers
(Wikipedia Commons)

NOAA climate modeling
http://www.ornl.gov/info/ornlreview/v42_3_09/article02.shtml

Social networks and the Internet

Video
Wikipedia Commons

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

Legacy documents
Wikipedia Commons

Library of Congress stacks
https://www.flickr.com/photos/danielm2001/6922113091/

Environmental sensors: Water temperature profiles from tagged hooded seals

Library of Congress stacks

Social networks and the Internet

Video
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Wikipedia Commons

Environmental sensors: Water temperature profiles from tagged hooded seals
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
Objectives and Approach

• Bring HPC to nontraditional users and research communities.
• Allow high-performance computing to be applied effectively to big data.
• Support diverse databases and high-productivity programming environments to allow the creation and execution of data-driven and data-intensive applications and workflows.
What’s Currently Available

• **Data Exacell (DXC)**
  – Couples analytic resources with innovative storage
  – PSC experts available to help develop applications
  – Research pilot; limited number research projects

• **Bridges**
  – National-scale (*large*), production resource (XSEDE)
  – DXC users can become early users on Bridges
  – Software developed for DXC will transition to Bridges

• *For open research, these resources are available at no charge.*
The Data Exacell (DXC)

- NSF Data Infrastructure Building Blocks (DIBBs) award #ACI-1261721
- A pilot project to create, deploy, and test software and hardware building blocks to enable data analytics in scientific research
- Application-driven: Pilot applications having diverse data analytic requirements motivate, test, and demonstrate the DXC’s capabilities
- Components:
  - Crucible: innovative, disk-based near-line storage system featuring low latency, high bandwidth, and high reliability for large-scale datasets
  - Blacklight: the world’s largest shared-memory supercomputer, capable of running Java and applications of 1-2048 threads using up to 16TB
  - Sherlock: a unique system for hardware- and software-optimized graph analytics, using either RDF/SPARQL for productivity or threaded C++ for very broad applicability
  - Hadoop and Spark: a cluster of nodes for the Hadoop ecosystem
  - Application, Database, and Web Server Nodes: cutting-edge technologies enable the development of powerful new application architectures
Bridges: Overview

*Bridges* will be a uniquely capable data-intensive HPC resource designed to empower new research communities, bring desktop convenience to supercomputing, expand campus access, and help researchers needing to tackle vast data to work more intuitively.

The $9.65M 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*

Target schedule:

- Oct–Dec 2015: Installation, testing, early user period, and acceptance
- January 2016: Begin production (allocated usage)
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
- Data Infrastructure Building Blocks (DIBBs)
  - Data Exacell (DXC)
  - Other DIBBs projects
- Other ACI projects

Carnegie Mellon University’s Gates Center for Computer Science

Temple University’s new Science, Education, and Research Center
Bridging to Nontraditional HPC Users and Enabling HPC + Big Data Workflows

Leveraging PSC’s expertise with shared memory, *Bridges* will feature 3 tiers of large, coherent shared-memory nodes – 12TB, 3TB, and 128GB – to support a uniquely flexible and user-friendly environment:

- **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, reaching large numbers of users who aren’t programmers.
- **Database and web server nodes** will provide persistent NoSQL and relational databases to enable data management, workflows, and distributed applications.
- **High-productivity programming languages & environments** (*R*, Python, MATLAB, Java, Hadoop, etc.) will let users scale familiar applications and workflows.
- **Virtualization** will allow users to bring their particular environments for portability, reproducibility, and security and provide interoperability with clouds.
- **Campus bridging** will streamline interoperation with campus resources and enable burst offload capability through a pilot project with Temple University.

Interest from new communities is already very high: examples include the digital humanities, machine learning, statistics, genomics, and radio astronomy.
**Bridges’ Architecture for High-Performance, Data-Intensive Computing (a very brief summary)**

- **3 tiers of large, coherent shared memory nodes** featuring the latest Intel® Xeon® CPUs and NVIDIA® Tesla® dual-GPU accelerators

<table>
<thead>
<tr>
<th>Node type</th>
<th>Example applications</th>
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<tbody>
<tr>
<td>12 TB</td>
<td>Genomics, machine learning, graph analytics, other extreme-memory applications</td>
</tr>
<tr>
<td>3 TB</td>
<td>Virtualization &amp; interactivity including large-scale vis and analytics; mid-range memory-intensive jobs</td>
</tr>
<tr>
<td>128 GB</td>
<td>Execution of most components of workflows, interactivity, Hadoop, and capacity computing</td>
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- **Database nodes and Web server nodes to enable persistent relational and NoSQL databases and enable distributed, service-oriented architectures**

- **Intel® Omni-Path Architecture Fabric** configured in a unique, PSC-developed topology to provide optimal communication and I/O performance

- **Data management:**
  - **Pylon**: A large, central, parallel, high-performance filesystem
  - **Node-local storage** for portability, performance, and performance consistency

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**High-Level Architecture of Bridges**

- **Service Nodes**
- **Database Servers**
- **Web Servers**
- **Data Transfer**
- **Intel® Omni-Path Fabric**
- **Pylon Filesystem**
- **Compute Nodes**
  - **ESM Nodes**: 12 TB each (several nodes)
  - **LSM Nodes**: 3 TB each (10s of nodes)
  - **RSM Nodes**: 128 GB each (100s of nodes)

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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
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.
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
Examples of Early Applications

- Finding causal relationships underlying cancer, chronic lung disease, and brain disorders (autism, schizophrenia)
- 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 public health issues from social media data
- Analyzing large bodies of work in the digital humanities
- Data integration for history, political science & cultural studies
- Cross-observational analyses in astronomy & other sciences
For Additional Information

Project website: [www.psc.edu/bridges](http://www.psc.edu/bridges)

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