BRIDGES

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A GPU-Enabled HPC System for New Communities and Data Analytics

Nick Nystrom · Director, Strategic Applications & Bridges PI · nystrom@psc.edu

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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 is a new kind of converged HPC + Big Data system that will integrate advanced memory technologies to empower new communities, bring desktop convenience to HPC, connect to campuses, and intuitively express data-intensive workflows.

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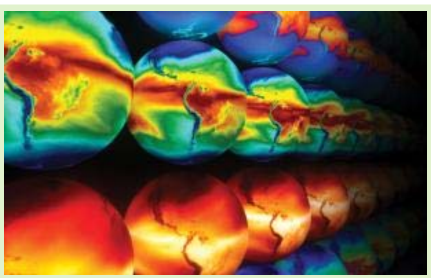
From HPC to Big Data

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

New Emphases

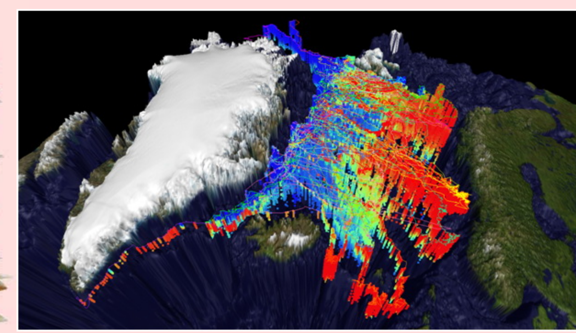
Social networks and the Internet

Video
Wikipedia Commons

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

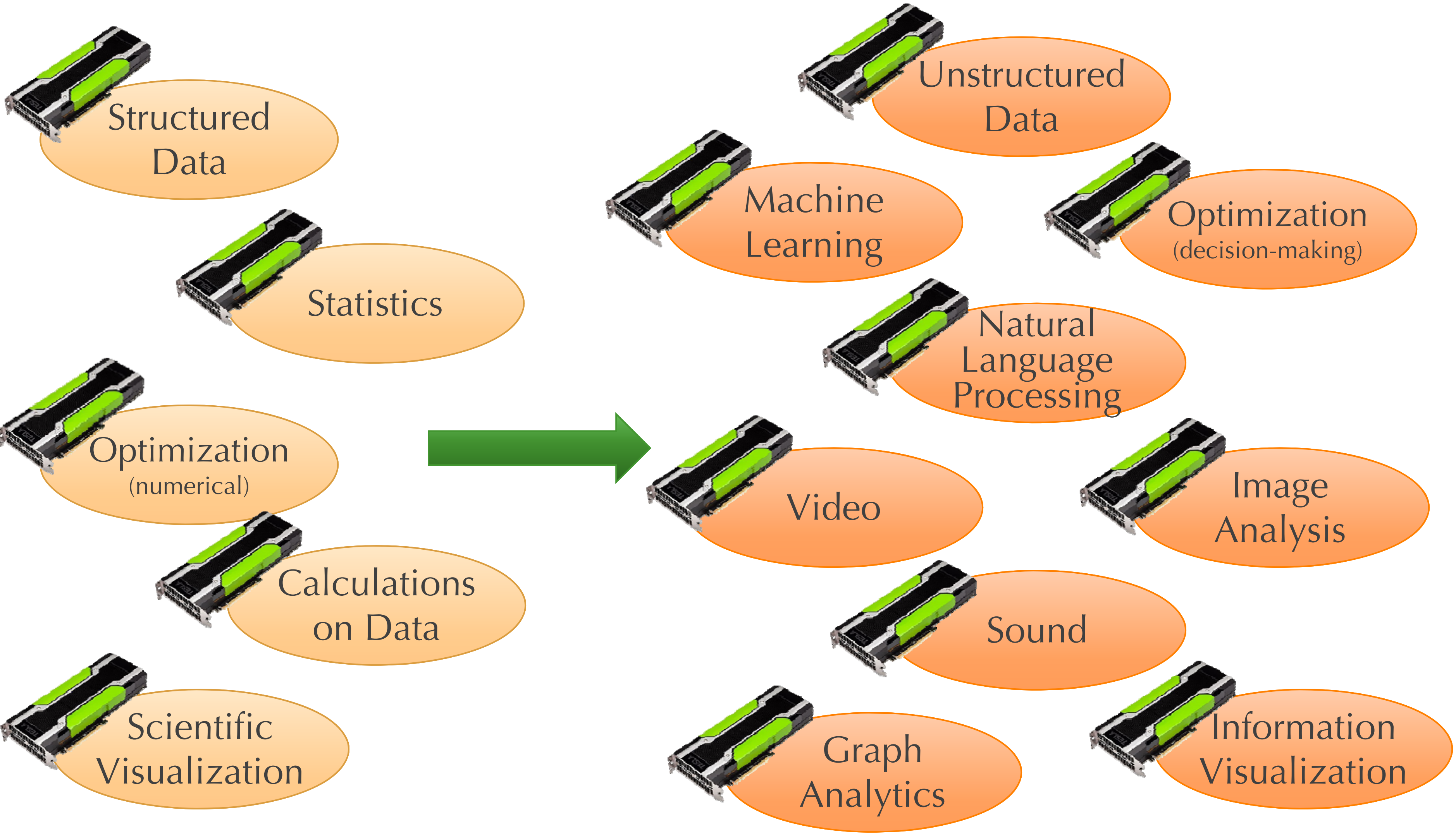
Collections
Horniman museum: http://www.horniman.ac.uk/get_involved/blog/bioblitz-insects-reviewed

Legacy documents
Wikipedia Commons



Environmental sensors: Water temperature profiles from tagged hooded seals
http://www.arctic.noaa.gov/report11/biodiv_whales_walrus.html

HPC → Big Data: Changing Algorithms



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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

Hewlett Packard Enterprise is delivering *Bridges*

Disclaimer: The following presentation conveys the current plan for *Bridges*. Details are subject to change.

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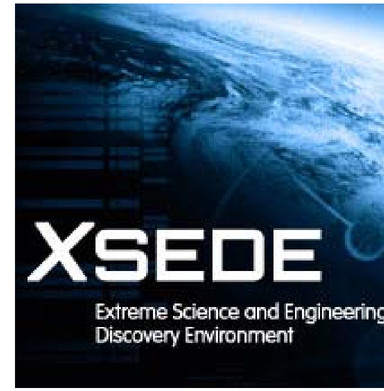
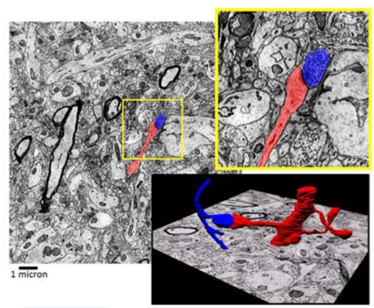
An Important Addition to the National Advanced Cyberinfrastructure Ecosystem

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



Reconstructing brain circuits from high-resolution electron microscopy

Social networks and the Internet

Data Infrastructure Building Blocks (DIBBs)
- Data Exacell (DXC)
- Integrating Geospatial Capabilities into HUBzero
- Building a Scalable Infrastructure for Data-Driven Discovery & Innovation in Education
- Other DIBBs projects

Other ACI projects

Carnegie Mellon University's Gates Center for Computer Science

Temple University's new Science, Education, and Research Center

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Motivating Use Cases
(examples)

Data-intensive applications & workflows

Gateways – the power of HPC without the programming

Shared data collections & related analysis tools

Cross-domain analytics

Graph analytics, machine learning, genome sequence assembly, and other large-memory applications

Scaling research questions beyond the laptop

Scaling research from individuals to teams and collaborations

Very large in-memory databases

Optimization & parameter sweeps

Distributed & service-oriented architectures

Data assimilation from large instruments and Internet data

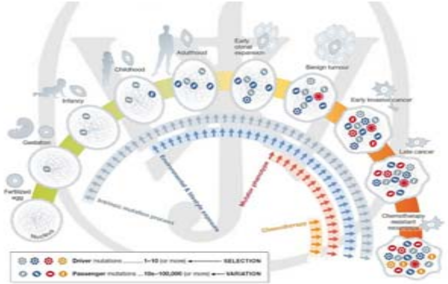
Leveraging an extensive collection of interoperating software

Potential Applications (*Examples*)

- Finding causal relationships in cancer genomics, lung disease, and brain dysfunction
- Analysis of financial markets and policies
- Improving the effectiveness of organ donation networks
- Assembling large genomes and metagenomes
- 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 corpora in the digital humanities
- Cross-observational analyses in astronomy & other sciences
- Data integration and fusion for history and related fields

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 streamline access and provide cloud-like burst capability.
- Leveraging PSC's expertise with shared memory, *Bridges* will feature 3 tiers of large, coherent shared-memory nodes: 12TB, 3TB, and 128GB.



EMBO Mol Med (2013) DOI: 10.1002/emmm.201202388: *Proliferation of cancer-causing mutations throughout life*

Alex Hauptmann et. al.: *Efficient large-scale content-based multimedia event detection*

- *Bridges* implements a uniquely flexible environment featuring interactivity, gateways, databases, distributed (web) services, high-productivity programming languages and frameworks, and virtualization, and campus bridging.

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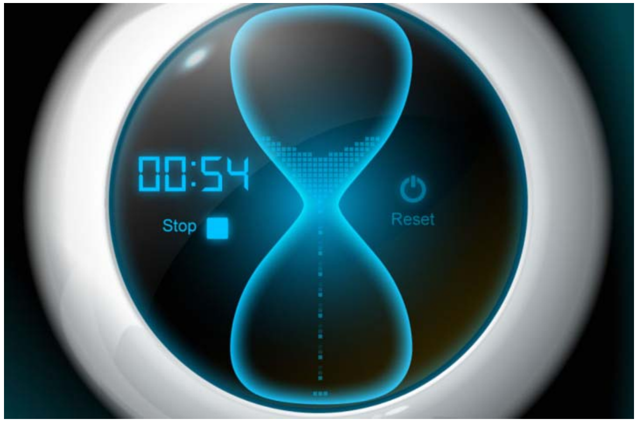
Interactivity

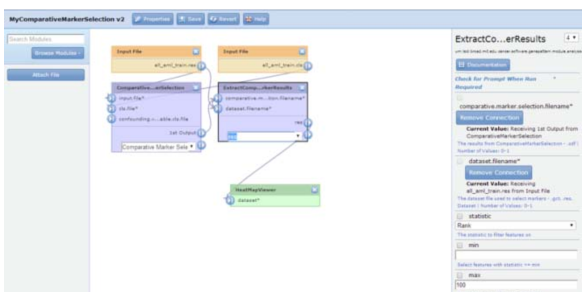
- *Interactivity is the feature most frequently requested by nontraditional HPC communities.*
- Interactivity provides immediate feedback for doing exploratory data analytics and testing hypotheses.
- *Bridges* will offer interactivity through a combination of virtualization for lighter-weight applications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



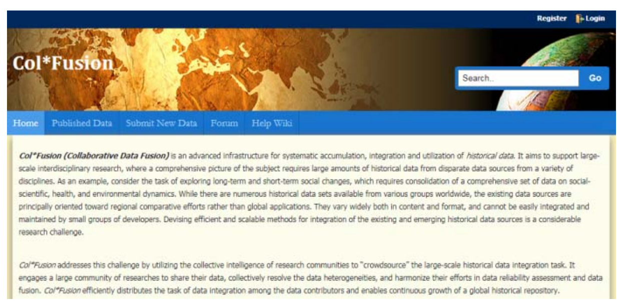
Gateways and Tools for Building Them

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

- *Extensive leveraging of databases and polystore systems*
- *Great attention to HCI is needed to get these right*



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

- Virtual Machines (VMs) will enable flexibility, customization, security, reproducibility, ease of use, and interoperability with other services.
- Early user demand on PSC's Data Exacell research pilot project has centered on VMs for custom database and web server installations to develop data-intensive, distributed applications and containers for reproducibility.
- Bridges leverages OpenStack to provision resources, between interactive, batch, Hadoop, and VM uses.

High-Productivity Programming

Supporting the languages that communities are already using is critical for successful application of HPC to their research questions.

Spark + Hadoop Ecosystem

Bridges' large memory is great for Spark!

Bridges enables workflows that integrate Spark/Hadoop, HPC, and/or shared-memory components.

Campus Bridging

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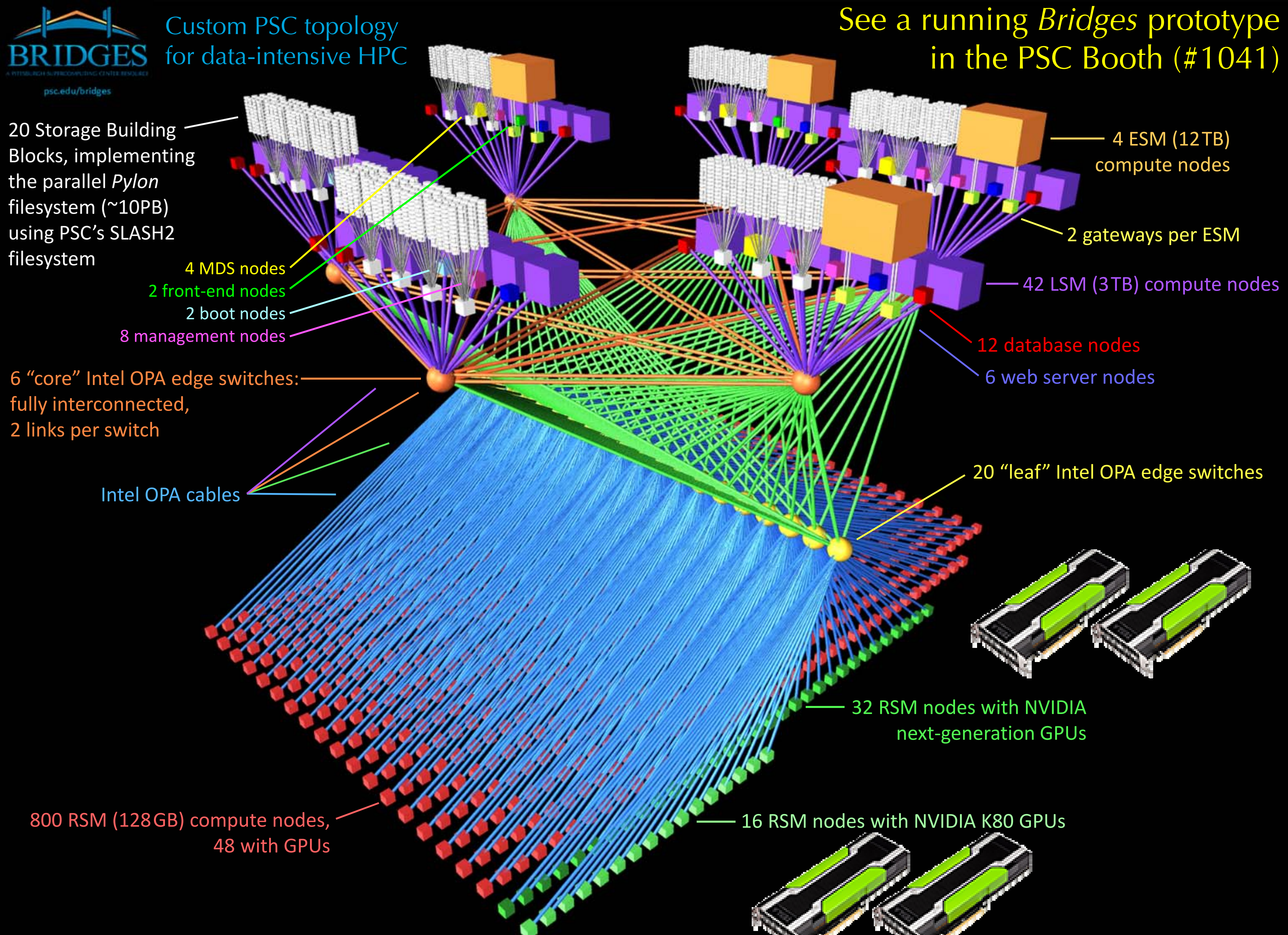
Federated identity management

Burst offload

http://www.temple.edu/medicine/research/RESEARCH_TUSM/

- 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.



This tool depicts the current plan for PSC's *Bridges* HPC system. Details are subject to change.

High-Performance, Data-Intensive Computing

3 tiers of large, coherent shared memory nodes

Memory per node	Number of nodes	Example applications
12 TB HPE Integrity Superdome X	4	Genomics, machine learning, graph analytics, other extreme-memory applications
3 TB HPE ProLiant DL580	42	Virtualization and interactivity including large-scale visualization and analytics; mid-spectrum memory-intensive jobs
128 GB HPE ProLiant DL580	800	Execution of most components of workflows, interactivity, Hadoop, and capacity computing

NVIDIA® Tesla® dual-GPU accelerators

Database and Web Server Nodes

- Dedicated database nodes will power persistent relational and NoSQL databases HPE ProLiant DL380
  - Support data management and data-driven workflows
  - SSDs for high IOPs; RAIDed HDDs for high capacity

(examples)

- Dedicated web server nodes HPE ProLiant DL360
  - Enable distributed, service-oriented architectures
  - High-bandwidth connections to XSEDE and the Internet

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

Supporting a Vast Number of Accelerated Applications and Tools

Deep Learning

Genomics

Neuroscience

Python

Speech

MATLAB

Video Analytics

Graph Analytics

Chemistry

Databases

Image Analytics

Rendering

Engineering

Materials Science

Physics

…

Getting Started on *Bridges*

- Starter Allocation https://www.xsede.org/allocations
  - Can request *anytime*… including *now!*
  - Can request XSEDE ECSS (Extended Collaborative Support Service)
- Research Allocation (XRAC) https://www.xsede.org/allocations
  - Appropriate for larger requests; can request ECSS
  - Quarterly submission windows; *Next: Dec. 15, 2015–Jan. 15, 2016*
- Early User Period
  - Users with starter or research proposals may be eligible for *Bridges'* Early User Period (starting late 2015)
- Questions?
  - See http://psc.edu/bridges
    or email Nick Nystrom at nystrom@psc.edu