BRIDGES

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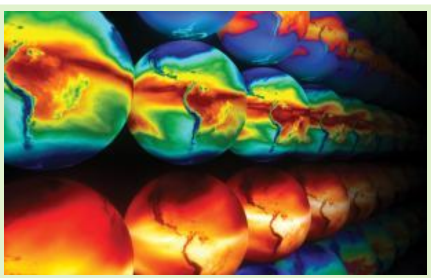
A Big Big Data Platform

John Urbanic, Parallel Computing Scientist

The Shift 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

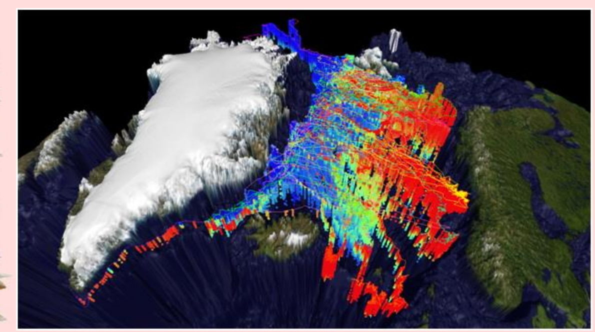
Social networks and the Internet


Video
Wikipedia Commons

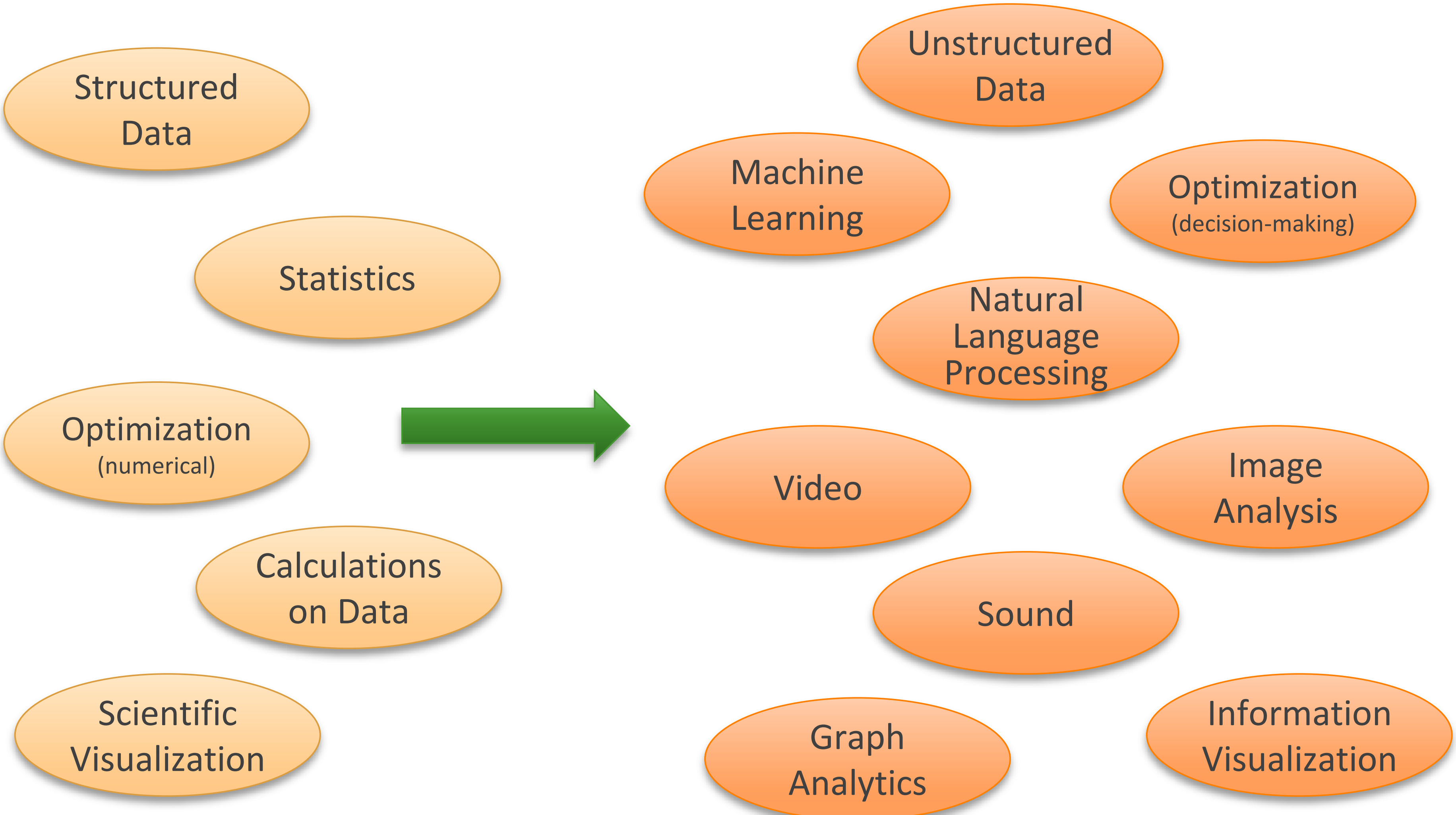

Library of Congress stacks
https://www.flickr.com/photos/danlem2001/6922113091/


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

Challenges and Software are Co-Evolving



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Motivating Use Cases

- Data-intensive applications & workflows
- Gateways – the power of HPC without the programming
- Shared data collections & analyses: cross-domain analytics
- Deep learning
- Graph analytics, machine learning, genome sequence assembly, and other large-memory applications
- Scaling beyond the laptop
- Scaling research to teams and collaborations
- In-memory databases
- Optimization & parameter sweeps
- Distributed & service-oriented architectures
- Data assimilation from large instruments & Internet
- Leveraging an extensive software collection

Research areas that haven't used HPC

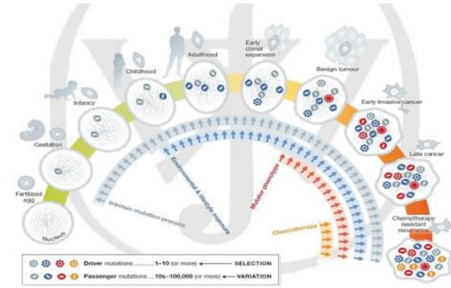
Nontraditional HPC approaches to fields such as the physical sciences

Coupling applications in novel ways

Leveraging large memory and high bandwidth

Objectives

- 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* has 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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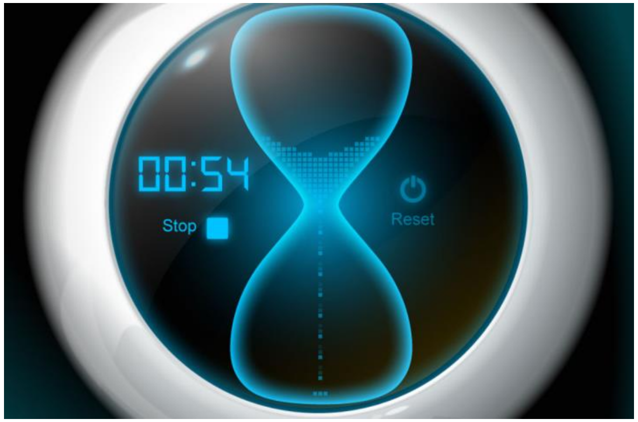
Interactivity

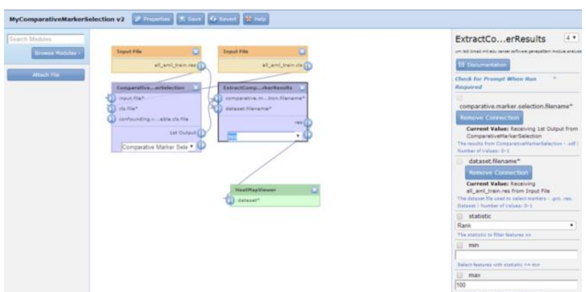
- *Interactivity is the feature most frequently requested by nontraditional HPC communities.*
- Interactivity provides immediate feedback for doing exploratory data analytics and testing hypotheses.
- *Bridges* offers interactivity through a combination of virtualization for lighter-weight applications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

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Virtualization and Containers

- Virtual Machines (VMs) enable flexibility, security, customization, reproducibility, ease of use, and interoperability with other services.
- User demand is for *custom database and web server installations* to develop data-intensive, distributed applications and *containers* for custom software stacks and portability.
- Bridges leverages OpenStack to provision resources, between interactive, batch, Hadoop, and VM uses.

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.

High-Productivity Programming

Supporting languages that communities already use is vital for them to apply HPC to their research questions.

Spark, Hadoop & Related Approaches

Bridges' large memory is great for Spark!

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

hadoop

Spark

HIVE

Cassandra

APACHE HBASE

PROJECT PEGASUS

mahout

PETUUM

Deep Learning Frameworks on *Bridges*

Caffe

PYTORCH

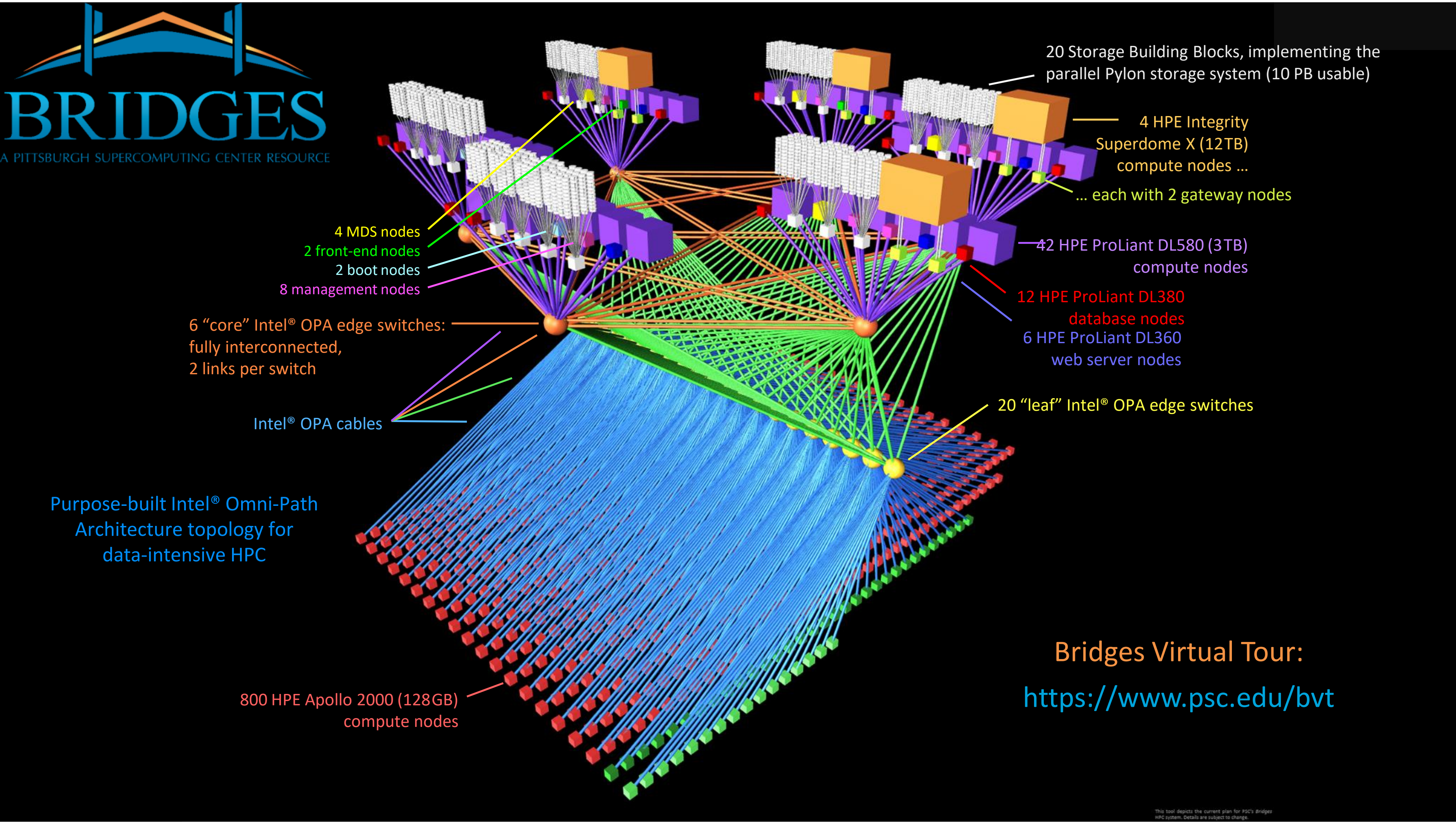
K

TensorFlow

torch

NVIDIA
DIGITS

theano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20 Storage Building Blocks, implementing the parallel Pylon storage system (10 PB usable)
4 HPE Integrity Superdome X (12TB) compute nodes …
… each with 2 gateway nodes
42 HPE ProLiant DL580 (3TB) compute nodes
12 HPE ProLiant DL380 database nodes
6 HPE ProLiant DL360 web server nodes
4 MDS nodes
2 front-end nodes
2 boot nodes
8 management nodes
6 "core" Intel® OPA edge switches: fully interconnected, 2 links per switch
Intel® OPA cables
20 "leaf" Intel® OPA edge switches
Purpose-built Intel® Omni-Path Architecture topology for data-intensive HPC
800 HPE Apollo 2000 (128GB) compute nodes
Bridges Virtual Tour:
https://www.psc.edu/bvt

Node Types

Type	RAM	Phase	n	CPU / GPU / other	Server
ESM	12TB[b]	1	2	16 × Intel Xeon E7-8880 v3 (18c, 2.3/3.1 GHz, 45MB LLC)	HPE Integrity Superdome X
	12TB[c]	2	2	16 × Intel Xeon E7-8880 v4 (22c, 2.2/3.3 GHz, 55MB LLC)	
LSM	3TB[b]	1	8	4 × Intel Xeon E7-8860 v3 (16c, 2.2/3.2 GHz, 40 MB LLC)	HPE ProLiant DL580
	3TB[c]	2	34	4 × Intel Xeon E7-8870 v4 (20c, 2.1/3.0 GHz, 50 MB LLC)	
RSM	128GB[b]	1	752	2 × Intel Xeon E5-2695 v3 (14c, 2.3/3.3 GHz, 35MB LLC)	HPE Apollo 2000
RSM-GPU	128GB[b]	1	16	2 × Intel Xeon E5-2695 v3 + 2 × NVIDIA Tesla K80	
	128GB[c]	2	32	2 × Intel Xeon E5-2683 v4 (16c, 2.1/3.0 GHz, 40MB LLC) + 2 × NVIDIA Tesla P100	
DB-s	128GB[b]	1	6	2 × Intel Xeon E5-2695 v3 + SSD	HPE ProLiant DL360
DB-h	128GB[b]	1	6	2 × Intel Xeon E5-2695 v3 + HDDs	HPE ProLiant DL380
Web	128GB[b]	1	6	2 × Intel Xeon E5-2695 v3	HPE ProLiant DL360
Other[a]	128GB[b]	1	16	2 × Intel Xeon E5-2695 v3	HPE ProLiant DL360, HPE ProLiant DL380
Gateway	64GB[b]	1	4	2 × Intel Xeon E5-2683 v3 (14c, 2.0/3.0 GHz, 35MB LLC)	HPE ProLiant DL380
	64GB[c]	2	4	2 × Intel Xeon E5-2683 v3	
Storage	128GB[b]	1	5	2 × Intel Xeon E5-2680 v3 (12c, 2.5/3.3 GHz, 30 MB LLC)	Supermicro X10DRi
	256GB[c]	2	15	2 × Intel Xeon E5-2680 v4 (14c, 2.4/3.3 GHz, 35 MB LLC)	
Total	**281.75TB**		**908**		

a. Other nodes = front end (2) + management/log (8) + boot (4) + MDS (4)
b. DDR4-2133
c. DDR4-2400

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

(examples)

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

GPU Nodes

Bridges' GPUs are accelerating both deep learning and simulation codes

Phase 1: 16 nodes, each with:

- **2 × NVIDIA Tesla K80 GPUs (32 total)**
- 2 × Intel Xeon E5-2695 v3 (14c, 2.3/3.3 GHz)
- 128GB DDR4-2133 RAM

Phase 2: +32 nodes, each with:

- **2 × NVIDIA Tesla P100 GPUs (64 total)**
- 2 × Intel Xeon E5-2683 v4 (16c, 2.1/3.0 GHz)
- 128GB DDR4-2400 RAM

Kepler architecture

2496 CUDA cores (128/SM)

7.08B transistors on 561mm^2 die (28nm)

2×24 GB GDDR5; 2×240.6 GB/s

562 MHz base – 876 MHz boost

2.91 Tf/s (64b), 8.73 Tf/s (32b)

Pascal architecture

3584 CUDA cores (64/SM)

15.3B transistors on 610mm^2 die (16nm)

16GB CoWoS® HBM2 at 720 GB/s w/ ECC

1126 MHz base – 1303 MHz boost

4.7 Tf/s (64b), 9.3 Tf/s (32b), 18.7 Tf/s (16b)

Page migration engine improves unified memory

64 P100 GPUs → 600 Tf/s (32b)

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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 (OPA)

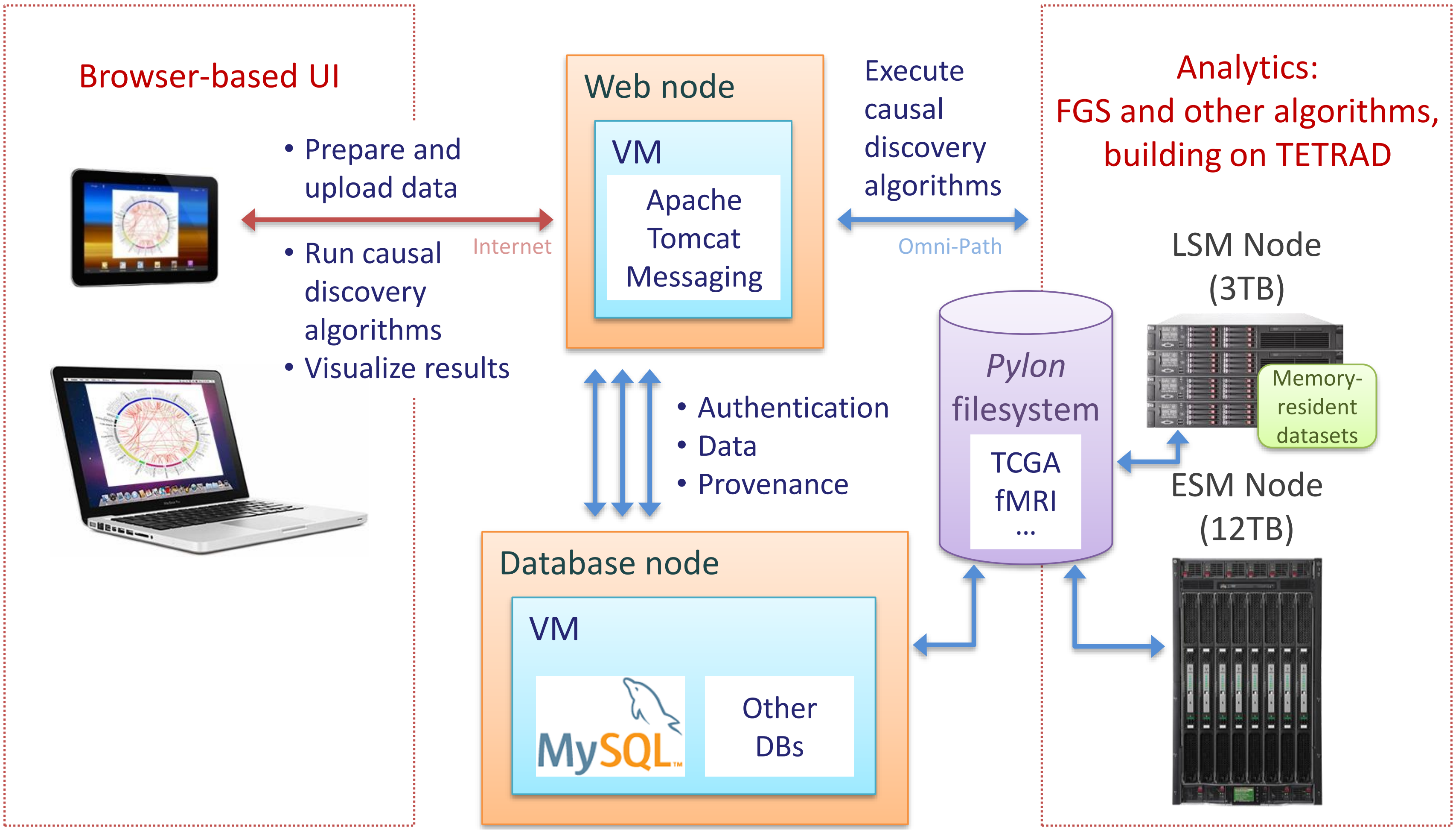
- *Bridges* is the first production deployment of Omni-Path
- Omni-Path connects all nodes and the shared filesystem, providing *Bridges* and its users with:
  - 100 Gbps line speed per port;
    25 GB/s bidirectional bandwidth per port
  - Observed <0.93µs latency, 12.36 GB/s/dir
  - 160M MPI messages per second
  - 48-port edge switch reduces interconnect complexity and cost
  - HPC performance, reliability, and QoS
  - OFA-compliant applications supported without modification
  - Early access to this new, important, forward-looking technology

- *Bridges* deploys OPA in a two-tier island topology developed by PSC for cost-effective, data-intensive HPC

Center for Causal Discovery

Example: Causal Discovery Portal

Center for Causal Discovery, an NIH Big Data to Knowledge Center of Excellence



Carnegie Mellon Yale PSC PITTSBURGH SUPERCOMPUTING CENTER BRIDGES A PITTSBURGH SUPERCOMPUTING CENTER RESOURCE

Some of the Deep Learning Projects Using *Bridges*

Deep Learning of Game Strategies for RoboCup, Manuela Veloso (CMU)

Automatic Building of Speech Recognizers for Non-Experts, Florian Metze (CMU)

Automatic Evaluation of Scientific Writing, Diane Litman (U. of Pittsburgh)

Image Classification Applied in Economic Studies, Param Singh (CMU)

Exploring Stability, Cost, and Performance in Adversarial Deep Learning, Matt Fredrikson (CMU)

Enabling Robust Image Understanding Using Deep Learning, Adriana Kovashka (U. of Pittsburgh)

Optimal Data Representation for Deep Learning for Computational Chemistry, Garrett Goh (Pacific Northwest National Laboratory)

Petuum, a Distributed System for High-Performance Machine Learning, Eric Xing (CMU)

Deep Learning the Gene Regulatory Code, Shaun Mahony (Penn State)

Developing Large-Scale Distributed Deep Learning Methods for Protein Bioinformatics, Junbo Xu (Toyota Technological Institute at Chicago)

Education Allocation for the Course Unstructured Data & Big Data: Acquisition to Analysis, Dokyun Lee (CMU)

Deciphering Cellular Signaling System by Deep Mining a Comprehensive Genomic Compendium, Xinghua Lu (U. of Pittsburgh)

Quantifying California Current Plankton Using Machine Learning, Mark Ohman (Scripps Institution of Oceanography)

Automatic Pain Assessment, Michael Reale (SUNY Polytechnic Institute)

Learning to Parse Images and Videos, Deva Ramanan (CMU)

Deep Recurrent Models for Fine-Grained Recognition, Michael Lam (Oregon State)

Some of the Deep Learning Projects Using *Bridges*

Live Song Identification Using Semantic Features, Timothy Tsai (Harvey Mudd College)

Inverse Graphics Engines for Visual Inference, Ioannis Gkioulekas (CMU)

Development of a Hybrid Computational Approach for Macroscale Simulation of Exciton Diffusion in Polymer Thin Films, Based on Combined Machine Learning, Quantum-Classical Simulations and Master Equation Techniques, Peter Rossky (Rice U.)

Summarizing and Learning Latent Structure in Video, Jeff Boleng (CMU)

Machine Learning for Medical Image Analysis, Mai Nguyen (UCSD)

Deep Learning for Drug-Protein Interaction Prediction, Gil Alterovitz (Harvard Medical School/Boston Children's Hospital)

CMU course Deep reinforcement Learning, Aikaterini Fragkiadaki (CMU)

Course 11-364: Introduction to Deep Learning, James Baker (CMU)

Deep Recurrent Models for Fine-Grained Recognition, Michael Lam (Oregon State University)

ARIEL: Analysis of Rare Incident-Event Languages, Ravi Starzl (CMU)

Aarti Singh, Deep Purple: Deep Purposeful Learning of Complex Dynamic Systems (CMU)

Deep Learning for Genomic Sequence Associated Study, Zhi Wei (New Jersey Institute of Technology)

Learning to Parse Images and Videos, Deva Ramanan (CMU)

Preparing Grounds to Launch All-US Students Kaggle Competition on Drug Prediction, Gil Alterovitz (Harvard Medical School/Boston Children’s Hospital)

Modeling Enzymatic Carbohydrate Decomposition, Heather Mayes (U. of Michigan)

Gaining Access to *Bridges*

Bridges is allocated through XSEDE: https://www.xsede.org/allocations

- Starter Allocation
  - Can request *anytime*
  - Up to 50,000 core-hours on RSM and GPU (128GB) nodes and/or 10,000 TB-hours on LSM (3TB) and ESM (12TB) nodes
  - Can request XSEDE ECSS (Extended Collaborative Support Service

XSEDE calls these "Service Units" (SUs)

- Research Allocation (XRAC)
  - Appropriate for larger requests; can request ECSS
  - Can be up to millions to tens of millions of SUs
  - Quarterly submission windows: ***March 15–April 15***, *June 15–July 15*, etc.
- Coursework Allocations
  - To support use of *Bridges* for relevant courses
- Community Allocations
  - Primarily to support gateways

Up to 10% of *Bridges*' SUs are available on a discretionary basis to industrial affiliates, Pennsylvania-based researchers, and others to foster discovery and innovation and broaden participation in data-intensive computing.

For Additional Information

Project website: www.psc.edu/bridges

Questions: bridges@psc.edu

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Co-PIs: Michael J. Levine
Ralph Roskies
J Ray Scott

Project Manager: Robin Scibek

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