BRIDGES

A PITTSBURGH SUPERCOMPUTING CENTER RESOURCE

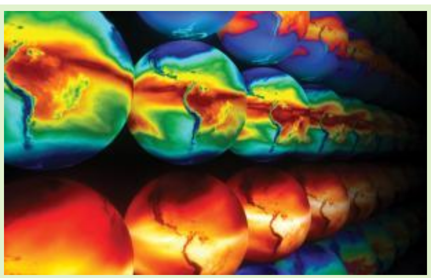
A Big Big Data Platform

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

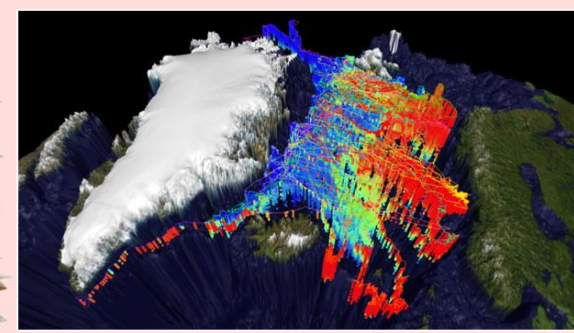
Social networks and the Internet

Video
Wikipedia Commons

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

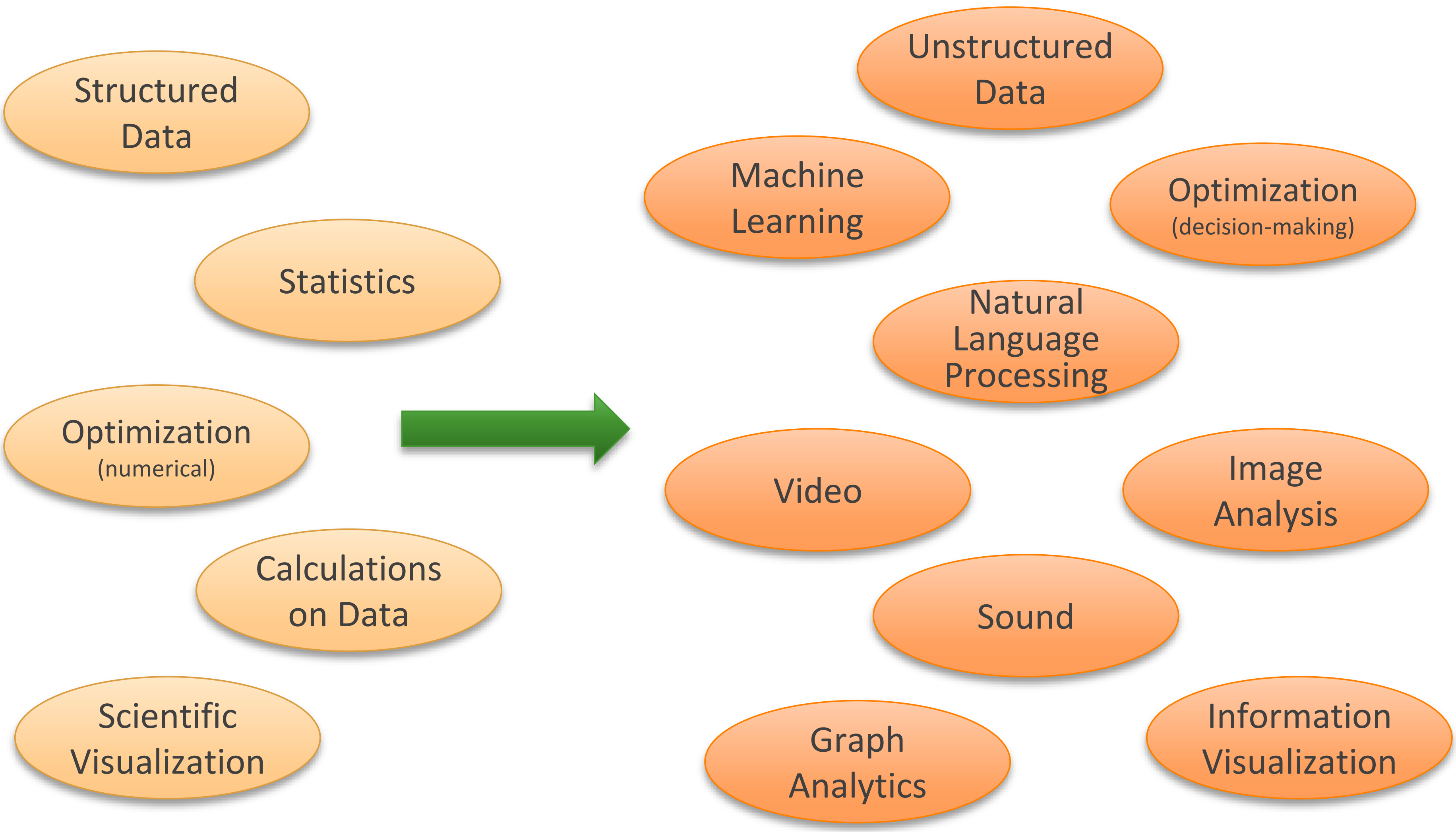
Collections
Horniman museum: http://www.horniman.ac.uk/get_involved/blog/bioblitz-insects-reviewed

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



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

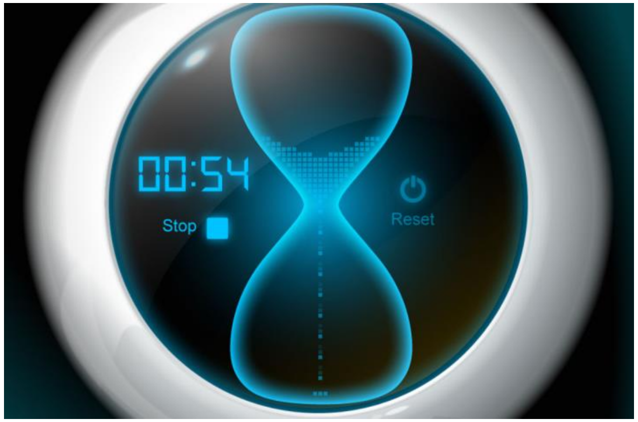
Nontraditional HPC approaches to fields such as the physical sciences

Coupling applications in novel ways

Leveraging large memory and high bandwidth

Interactivity

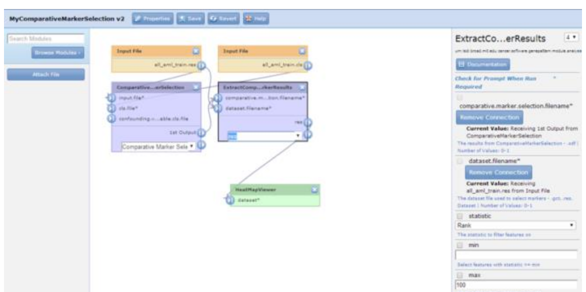
- *Interactivity is the feature most frequently requested by nontraditional HPC communities.*
- Interactivity provides immediate feedback for doing exploratory data analytics and testing hypotheses.
- *Bridges* offers interactivity through a combination of virtualization for lighter-weight applications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

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.

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.

Deep Learning Frameworks on *Bridges*

Caffe

PYTORCH

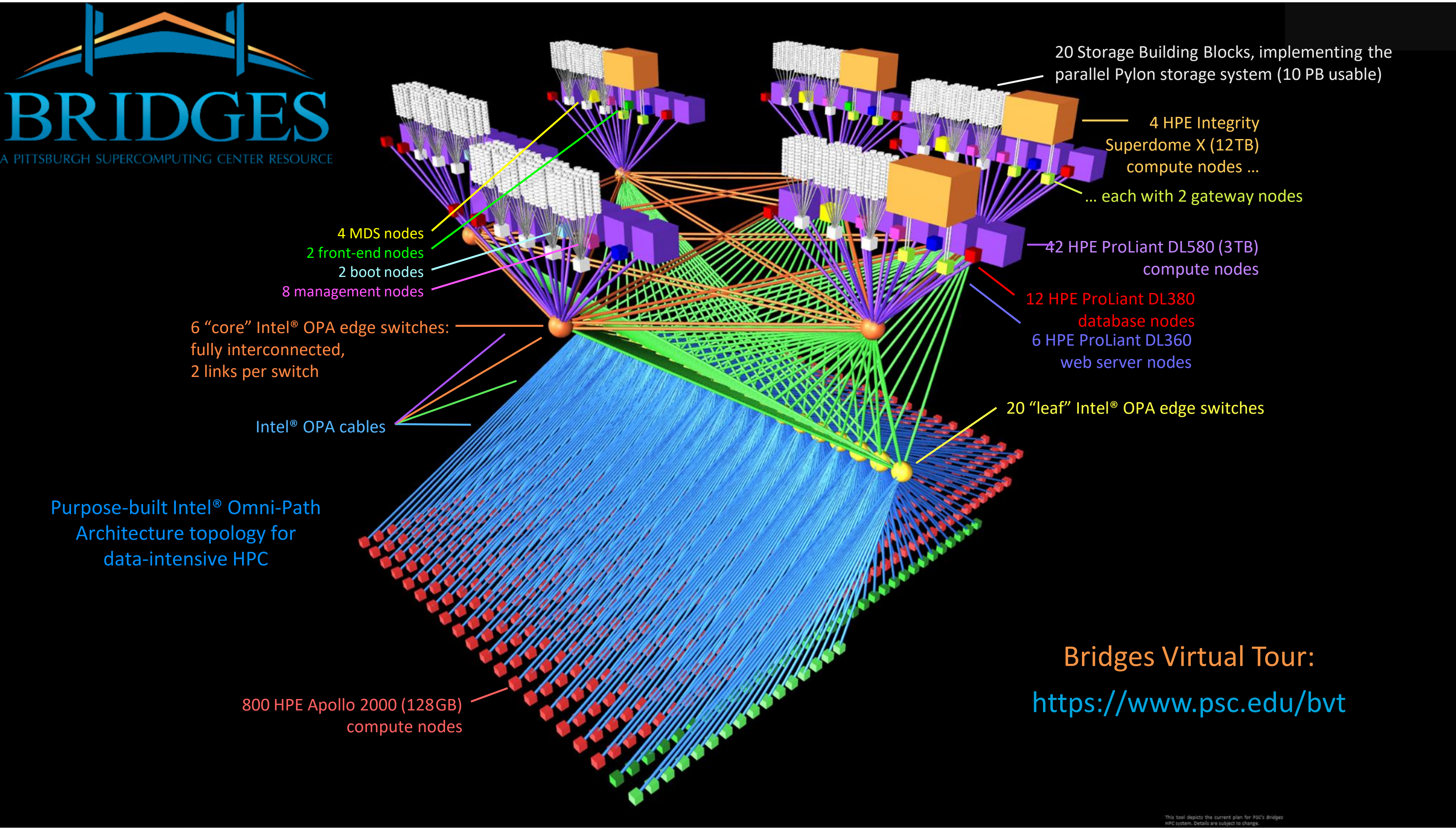
K

TensorFlow

torch

NVIDIA DIGITS

theano



BRIDGES
A PITTSBURGH SUPERCOMPUTING CENTER RESOURCE
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
20 “leaf” Intel® OPA edge switches
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
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
This tool depicts the current plan for PSC's Bridges HPC system. Details are subject to change.

Regular 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)

Bridges Hardware

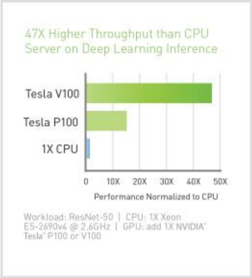
Bridges-DL

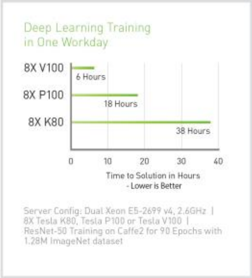
Type	RAM	#	CPU / GPU / SSD	Server
ESM	12 TB[b]	2	16 × Intel Xeon E7-8880 v3 (18c, 2.3/3.1 GHz, 45MB LLC)	HPE Integrity Superdome X
	12 TB[c]	2	16 × Intel Xeon E7-8880 v4 (22c, 2.2/3.3 GHz, 55MB LLC)	
LSM	3 TB[b]	8	4 × Intel Xeon E7-8860 v3 (16c, 2.2/3.2 GHz, 40 MB LLC)	HPE ProLiant DL580
	3 TB[c]	34	4 × Intel Xeon E7-8870 v4 (20c, 2.1/3.0 GHz, 50 MB LLC)	
RSM	128 GB[b]	752	2 × Intel Xeon E5-2695 v3 (14c, 2.3/3.3 GHz, 35MB LLC)	HPE Apollo 2000
RSM-GPU	128 GB[b]	16	2 × Intel Xeon E5-2695 v3 + 2 × NVIDIA Tesla K80	
	128 GB[c]	32	2 × Intel Xeon E5-2683 v4 (16c, 2.1/3.0 GHz, 40MB LLC) + 2 × NVIDIA Tesla P100	
GPU-AI16	1.5 TB[d]	1	16 × NVIDIA V100 32GB SXM2 + 2 × Intel Xeon Platinum 8168 + 8 × 3.84 TB NVMe SSDs	NVIDIA DGX-2 delivered by HPE
GPU-A8	192 GB[d]	9	2 × Intel Xeon Gold 6148 + 2 × 3.84 TB NVMe SSDs	HPE Apollo 6500 Gen10
DB-s	128 GB[b]	6	2 × Intel Xeon E5-2695 v3 + SSD	HPE ProLiant DL360
DB-h	128 GB[b]	6	2 × Intel Xeon E5-2695 v3 + HDDs	HPE ProLiant DL380
Web	128 GB[b]	6	2 × Intel Xeon E5-2695 v3	HPE ProLiant DL360
Other[a]	128 GB[b]	16	2 × Intel Xeon E5-2695 v3	HPE ProLiant DL360, DL380
Gateway	64 GB[b]	4	2 × Intel Xeon E5-2683 v3 (14c, 2.0/3.0 GHz, 35MB LLC)	HPE ProLiant DL380
	64 GB[c]	4	2 × Intel Xeon E5-2683 v3	
	96 GB[d]	2	2 × Intel Xeon	
Storage	128 GB[b]	5	2 × Intel Xeon E5-2680 v3 (12c, 2.5/3.3 GHz, 30 MB LLC)	Supermicro X10DRi
	256 GB[c]	15	2 × Intel Xeon E5-2680 v4 (14c, 2.4/3.3 GHz, 35 MB LLC)	
Total	286.5 TB	920		

a. Other nodes = front end (2) + management/log (8) + boot (4) + MDS (4)
b. DDR4-2133
c. DDR4-2400
d. DDR4-2666

The Heart of Bridges-DL: NVIDIA Volta

NVIDIA Tesla V100 SXM2 Module
with Volta GV100 GPU





Training ResNet-50 with ImageNet:
V100 : 1075 images/s[a]
P100 : 219 images/s[b]
K80 : 52 images/s[b]

a. https://devblogs.nvidia.com/tensor-core-ai-performance-milestones/
b. https://www.tensorflow.org/performance/benchmarks

NVIDIA.

New Streaming Multiprocessor (SM) architecture, introducing Tensor Cores, independent thread scheduling, combined L1 data cache and shared memory unit, and 50% higher energy efficiency over Pascal.

Tensor Cores accelerate deep learning training and inference, providing up to 12× and 6× higher peak flops respectively over the P100 GPUs currently available in XSEDE.

NVLink 2.0 delivering 300 GB/s total bandwidth per GV100, nearly 2× higher than P100.

HBM2 bandwidth and capacity increases: 900 GB/s and up to 32GB.

Enhanced Unified Memory and Address Translation Services improve accuracy of memory page migration by providing new access counters.

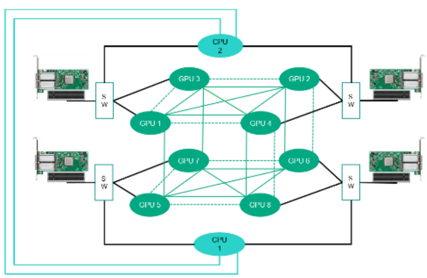
Cooperative Groups and New Cooperative Launch APIs expand the programming model to allow organizing groups of communicating threads.

Volta-Optimized Software includes new versions of frameworks and libraries optimized to take advantage of the Volta architecture: TensorFlow, Caffe2, MXNet, CNTK, cuDNN, cuBLAS, TensorRT, etc.

Balancing AI Capability & Capacity: HPE Apollo 6500

Hewlett Packard Enterprise

HPE Apollo 6500 Gen10 Server



HPE Apollo 6500 Gen10
hybrid cube-mesh topology

Bridges-DL adds 9 HPE Apollo 6500 Gen10 servers

Each HPE Apollo 6500 couples 8 NVIDIA Tesla V100 SXM2 GPUs

- 40,960 CUDA cores and 5,120 tensor cores

Performance: 1 Pf/s mixed-precision tensor, 125 Tf/s 32b, 64 Tf/s 64b

Memory: 128 GB HBM2, 7.2 TB/s aggregate memory bandwidth

2 × Intel Xeon Gold 6148 CPUs and *192 GB of DDR4-2666 RAM*

- 20c, 2.4–3.7 GHz, 27.5 MB L3, 3 UPI links

2 × 4 TB NVMe SSDs for user and system data

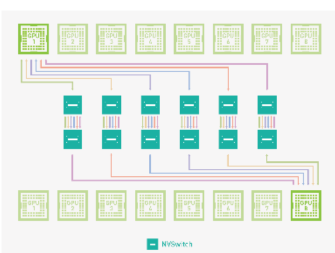
1 × Intel Omni-Path host channel adapter

Hybrid cube-mesh topology connecting the 8 V100 GPUs and 2 Xeon CPUs, using NVLink 2.0 between the GPUs and PCIe3 to the CPUs

Maximum DL Capability: NVIDIA DGX-2

NVIDIA

NVIDIA DGX-2



NVIDIA DGX-2 with NVSwitch internal topology

Couples 16 NVIDIA Tesla V100 SXM2 GPUs

- 81,920 CUDA cores and 10,240 tensor cores

Performance: 2 Pf/s mixed-precision tensor, 251 Tf/s 32b, 125 Tf/s 64b

Memory: 512 GB HBM2, 14.4 TB/s aggregate memory bandwidth

2 × Intel Xeon Platinum 8168 CPUs and *1.5 TB of DDR4-2666 RAM*

- 24c, 2.7–3.7 GHz, 33 MB L3, 3 UPI links

2 × 960 GB NVMe SSDs host the Ubuntu Linux OS

8 × 3.84 TB NVMe SSDs (aggregate ~30 TB) for user data

8 × Mellanox ConnectX adapters for EDR InfiniBand & 100 Gb/s Ethernet

The *NVSwitch* tightly couples the 16 V100 GPUs for capability & scaling

- Each of the 12 NVSwitch chips is an 18×18-port, fully-connected crossbar
- 50 GB/s/port and 900 GB/s/chip bidirectional bandwidths
- 2.4 TB/s system bisection bandwidth

The Center for Causal Discovery (CCD)

An NIH Big Data to Knowledge (BD2K) Center of Excellence

To help discover valid, novel, and significant causal relationships in big biomedical data that lead to new insights in health and disease.

- Develop highly efficient causal discovery algorithms that can be practically applied to very large biomedical datasets
- Conduct projects addressing 3 distinct biomedical questions (cancer driver mutations, lung fibrosis, brain causome) as a vehicle for algorithm development and optimization
- Disseminate causal discovery algorithms, software, and tools
- Train data scientists and biomedical investigators in the use of CCD tools
- Train data scientists and biomedical investigators to collaborate in the discovery of causality

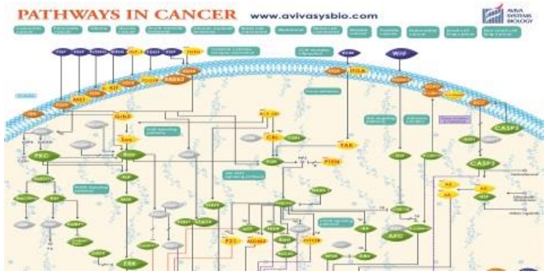
Supported by the NIH National Human Genome Research Institute under award number 5U54HG008540 ($11M).

Yale

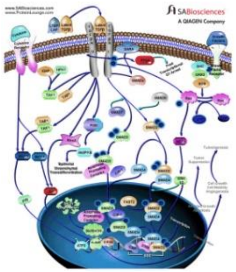
Carnegie Mellon University PSC University of Pittsburgh

Center for Causal Discovery

Driving Biomedical Projects



Discover cell signaling networks in cancer



Discover the mechanisms of disease onset and progression in chronic obstructive pulmonary disease and idiopathic pulmonary fibrosis

Discover the functional (causal) connectivity of regions of the human brain from fMRI data

Courtesy Greg Cooper (Pitt)

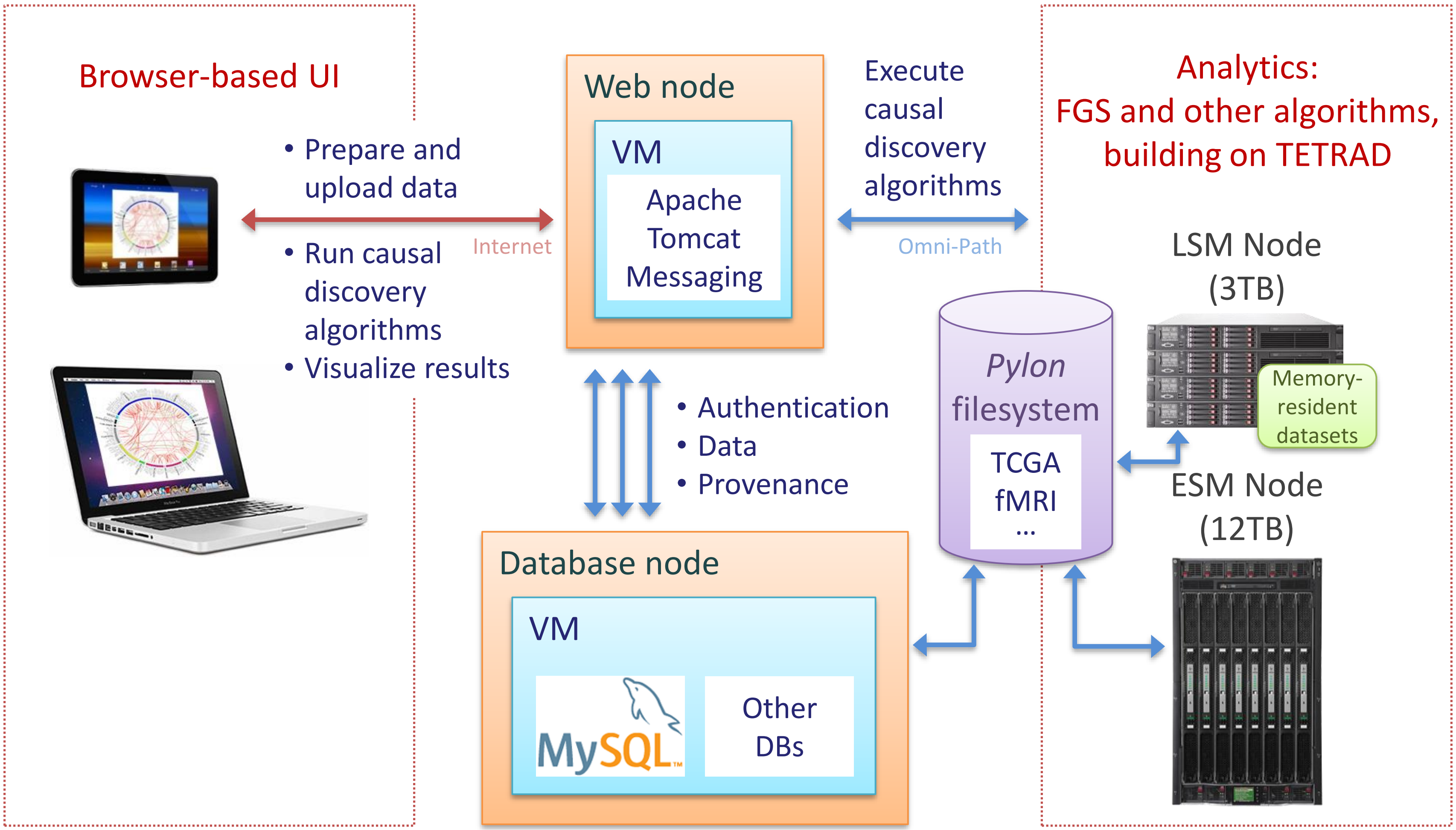
Yale

Carnegie Mellon University PSC University of Pittsburgh

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)

Accessing *Bridges*

	Open Research				Industry
	Pittsburgh Research Computing Initiative (PRCI)	XSEDE Extreme Science and Engineering Discovery Environment			PSC Corporate Program
		Startup	Research	Education	
Cost	No charge	No charge	No charge	No charge	Cost recovery
CPU-hours	50k	50k	Up to ~10^7	Up to ~10^6	Up to ~18M
GPU-hours	2500	2500	Up to ~10^5	Up to ~10^4	Up to ~180k
GPU-AI hours	1500	1500	Up to ~10^5	Up to ~10^4	Up to ~69k
TB-hours	1000	1000	Up to ~10^4	Up to ~10^4	Up to ~137k
Developer	-	Yes	Yes	(Yes)	Yes
Accepted	Any time	Any time	Quarterly	Any time	Any time
Awarded	~1-2 days	~1-2 days	Quarterly	~1-3 days	ASAP