Welcome to the XSEDE Big Data Workshop

John Urbanic
Parallel Computing Scientist
Pittsburgh Supercomputing Center

Who are we?

Your hosts:

Pittsburgh Supercomputing Center

XSEDE

Extreme Science and Engineering Discovery Environment

PITTSBURGH SUPERCOMPUTING CENTER

Who am I?

John Urbanic
Parallel Computing Scientist
Pittsburgh Supercomputing Center

What I mostly do:

Parallelize codes with

- MPI, OpenMP, OpenACC, Hybrid
- Big Data, Machine Learning

XSEDE
Extreme Science and Engineering Discovery Environment

PITTSBURGH SUPERCOMPUTING CENTER

XSEDE HPC Monthly Workshop Schedule

- September 3-4 *HPC Monthly Workshop*: MPI
- October 1-2 *HPC Monthly Workshop*: Big Data
- November 5 *HPC Monthly Workshop*: OpenMP
- December 3-4 *HPC Monthly Workshop*: Big Data
- January 21 *HPC Monthly Workshop*: OpenMP
- February 19-20 *HPC Monthly Workshop*: Big Data
- March 3 *HPC Monthly Workshop*: OpenACC
- April 7-8 *HPC Monthly Workshop*: Big Data
- May 5-6 *HPC Monthly Workshop*: MPI
- June 2-5 Summer Boot Camp
- August 4-5 *HPC Monthly Workshop*: Big Data
- September 1-2 *HPC Monthly Workshop*: MPI
- October 6-7 *HPC Monthly Workshop*: Big Data
- November 3 *HPC Monthly Workshop*: OpenMP
- December 1-2 *HPC Monthly Workshop*: Big Data

HPC Monthly Workshop Philosophy

- Workshops as long as they *should* be.
- You have real lives…
  in different time zones…
  that don't come to a halt.
- Learning is a social process
  - This is not a MOOC
  - But this is also not the Wide Area Classroom
    ...so bear with us.

PITTSBURGH SUPERCOMPUTING CENTER

Agenda

Tuesday, August 4

11:00	Welcome
11:25	A Brief History of Big Data
12:00	Hadoop
12:30	Intro to Spark
1:00	Lunch Break
2:00	More Spark and Exercises
3:00	Intro To Machine Learning
5:00	Adjourn

Wednesday, August 5

11:00	Machine Learning: A Recommender System
1:00	Lunch break
2:00	Deep Learning with TensorFlow
5:00	Adjourn

PITTSBURGH SUPERCOMPUTING CENTER

We do this all the time, but...

- This is a very ambitious agenda.
- We are going to cover the guts of a semester course.
- We may get a little casual with the agenda.
- The reasons we can attempt this now:
    - Tools have reached the point (Spark and TF) where you can do some powerful things at a high level.
    - Worked last time. Feedback is very positive.

Biggest Potential For Disappointment

- We absolutely, definitely, without question, wish we had more hands-on exercise time.
- This is by design and demand. The topics we cover are all greatly requested and attempts to delete any of them provoke outrage in our surveys. This demand has compressed our hands-on sessions.
- One solution is for you to use the remainder of our short days to do further work.
- We also assume you will use your extended access to do exercises. Usually this is just a bonus.
- Use your time wisely, and ask questions relentlessly.

Resources

Our TAs

Questions from the audience

On-line talks (no "pop ups")

bit.ly/XSEDEWorkshop

Copying code from PDFs is very error prone. Subtle things like substituting “-” for “-” are maddening. I have provided online copies of the codes in a directory that we shall shortly visit. I strongly suggest you copy from there if you are in a cut/paste mood.

The YouTube Channel Has Arrived!

Due to overwhelming demand, and a lot of editing, we have begun to post workshop videos on the XSEDE Monthly Workshop Training Channel:

XSEDETraining

They will be incrementally appearing in the coming months. Subscribe and give us feedback.

Getting Time on XSEDE

XSEDE

Extreme Science and Engineering
Discovery Environment

https://portal.xsede.org/web/guest/allocations

even simpler:

https://psc.edu/apply-for-an-xsede-startup-grant

Code of Conduct

XSEDE has an external code of conduct which represents our commitment to providing an inclusive and harassment-free environment in all interactions regardless of race, age, ethnicity, national origin, language, gender, gender identity, sexual orientation, disability, physical appearance, political views, military service, health status, or religion. The code of conduct extends to all XSEDE-sponsored events, services, and interactions.

Code of Conduct: https://www.xsede.org/codeofconduct

Contact:

- Event organizer: Tom Maiden (tmaiden@psc.edu)
- XSEDE ombudspersons:
  - Linda Akli, Southeastern Universities Research Association (akli@sura.org)
  - Lizanne Destefano, Georgia Tech (lizanne.destefano@ceismc.gatech.edu)
  - Ken Hackworth, Pittsburgh Supercomputing Center (hackworth@psc.edu)
  - Bryan Snead, Texas Advanced Computing Center (jbsnead@tacc.utexas.edu)
- Anonymous reporting form available at https://www.xsede.org/codeofconduct.

Content Warning

In line with the Code of Conduct, XSEDE is committed to providing training events that foster inclusion and show respect for all. This applies to how we interact during the event. It also applies to the training materials and presentation. It is not XSEDE's position to use, condone, or promote offensive terminology.

Unfortunately, the programming code we are presenting today includes terminology or code specifications that includes offensive terminology. We do not control the terminology and language in this code and its specification.

However, the XSEDE organization is taking steps to affect change by contacting the relevant organization; we hope this will be addressed soon.

If you see any terminology concerns in the following presentation or slides, we want to know!
Please contact the Terminology Task Force: terminology@xsede.org

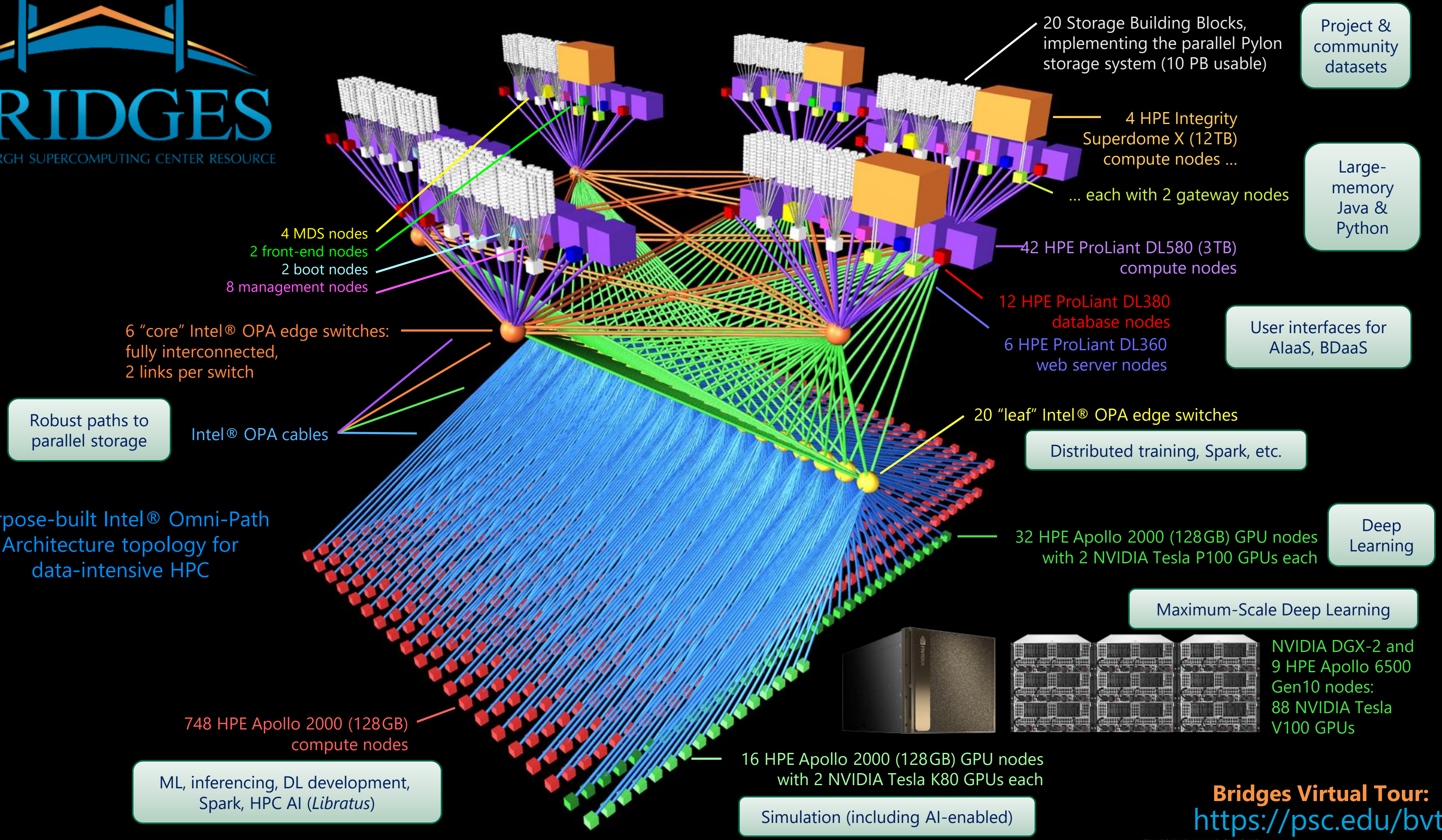
Check your email for the post-event survey.

Surveys are conducted by an external evaluation team. XSEDE staff will not know who said what. If you have questions regarding the evaluation please contact: Lorna Rivera, lorna.rivera@gatech.edu, or Lizanne DeStefano, ldestefano6@gatech.edu

BRIDGES

A PITTSBURGH SUPERCOMPUTING CENTER RESOURCE

Purpose-built Intel® Omni-Path Architecture topology for data-intensive HPC



Bridges Virtual Tour:
https://psc.edu/bvt

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

Bridges Hardware

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		

Bridges-DL

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

Getting Connected

The first time you use your account sheet, you must go to apr.psc.edu to set a password. You may already have done so, if not, we will take a minute to do this shortly.

We will be working on bridges.psc.edu. Use an ssh client (a Putty terminal, for example), to ssh to the machine.

At this point will be on a login node. It will have a name like "login001" or "login006". This is a fine place to edit and compile codes. However we must be on compute nodes to do actual computing. We have designed Bridges to be the world's most interactive supercomputer. We generally only require you to use the batch system when you want to. Otherwise, you get your own personal piece of the machine. For this workshop we will use

```
interact
```

to get a regular node of the type we will be using with Spark. You will then see name like "r251" on the command line to let you know you are on a regular node. Likewise, to get a GPU node, use

```
interact -gpu
```

This will be for our TensorFlow work tomorrow. You will then see a prompt like "gpu32".

Some of you may follow along in real time as I explain things; some of you may wait until exercise time, and some of you may really not get into the exercises until after we wrap up tomorrow. It is all good.

Modules

We have hundreds of packages on Bridges. They each have many paths and variables that need to be set for their own proper environment, and they are often conflicting. We shield you from this with the wonderful modules command or containers. You can load the two packages we will be using as

Spark

```
module load spark
```

Tensorflow

```
module load singularity
singularity shell --nv /pylon5/containers/ngc/tensorflow_20.02-tf2-py3.sif
```

Editors

For editors, we have several options:

- emacs
- vi
- nano: use this if you aren't familiar with the others

For this workshop, you can actually get by just working from the various command lines.

Programming Language

Warning! Warning!

Several of the packages we are using are very prone to throw warnings about the JVM or some python dependency.

We've stamped most of them out, but don't panic if a warning pops up here or there.

In our other workshops we would not tolerate so much as a compiler warning, but this is the nature of these software stacks, so consider it good experience.

- We have to pick something
- Pick best domain language
- Python
- But not "Pythonic"
- I try to write generic pseudo-code
    - If you know Java or C or R, etc. you should be fine.

Our Setup For This Workshop

After you copy the files from the training directory, you will have:

```
/BigData
        /Clustering
        /MNIST
        /Recommender
        /Shakespeare
```

Datasets, and also cut and paste code samples are in here.

Preliminary Exercise

Let’s get the boring stuff out of the way now.

- Log on to apr.psc.edu and set an initial password if you have not.
- Log on to Bridges.

```
ssh username@bridges.psc.edu
```

- Copy the Big Data exercise directory from the training directory to your home directory.

```
cp  -r ~training/BigData .
```

- Edit a file to make sure you can do so. Use emacs, vi or nano (if the first two don’t sound familiar).
- Start an interactive session.

```
interact
```