

# Welcome to the XSEDE Big Data Workshop

John Urbanic

Parallel Computing Scientist  
Pittsburgh Supercomputing Center

# Who are we?

*Your hosts:*  
Pittsburgh Supercomputing Center

*Our satellite sites:*

Tufts University  
Lehigh University  
Howard University  
University of Iowa  
Purdue University  
Harvey Mudd College  
University of Delaware  
Old Dominion University  
Georgia State University  
George Mason University  
Louisiana State University  
Michigan State University  
Oklahoma State University  
Kennesaw State University  
Ohio Supercomputer Center  
Pennsylvania State University  
University of Nebraska-Lincoln  
University of Texas at El Paso  
San Diego Supercomputer Center  
University of Houston - Clear Lake  
University of California, Los Angeles  
North Carolina A&T State University  
Yale Center for Research Computing  
National Center for Supercomputing Applications  
University of Tennessee, Knoxville - National Institute for Computational Sciences

# XSEDE

Extreme Science and Engineering  
Discovery Environment

# 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

Primarily for XSEDE platforms. Mostly to extreme scalability.

# XSEDE

Extreme Science and Engineering  
Discovery Environment



# XSEDE HPC Monthly Workshop Schedule

- June 6-9 *Summer Boot Camp*
- August 15 *HPC Monthly Workshop: OpenMP*
- September 12-13 *HPC Monthly Workshop: Big Data*
- October 3-4 *HPC Monthly Workshop: MPI*
- November 7 *HPC Monthly Workshop: OpenACC*
- **December 5-6** ***HPC Monthly Workshop: Big Data***
- January 9 *HPC Monthly Workshop: OpenMP*
- February 7-8 *HPC Monthly Workshop: Big Data*
- March 6 *HPC Monthly Workshop: OpenACC*
- April 3-4 *HPC Monthly Workshop: MPI*
- May 1-2 *HPC Monthly Workshop: Big Data*
- June 4-7 *Summer Boot Camp*
- August 7 *HPC Monthly Workshop: OpenMP*
- September 5-6 *HPC Monthly Workshop: Big Data*
- October 2-3 *HPC Monthly Workshop: MPI*
- November 6 *HPC Monthly Workshop: OpenACC*
- December 4-5 *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
  - This is the **Wide Area Classroom**  
so raise your expectations

# Agenda

Tuesday, December 5

11:00 Welcome  
11:25 Intro To Big Data  
12:00 Hadoop  
12:30 Intro to Spark  
1:00 Lunch Break  
2:00 Spark  
3:30 Spark Exercises  
4:30 Spark  
5:00 Adjourn

Wednesday, December 6

11:00 Machine Learning: A Recommender System  
1:00 Lunch break  
2:00 Deep Learning with Tensorflow  
4:30 A Big Big Data Platform  
5:00 Adjourn

# *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.
- Three 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.
  - We are going to assume you will use your extended access to do exercises. Usually this is just a bonus.
  - Worked last time.

# Resources

Your local TAs

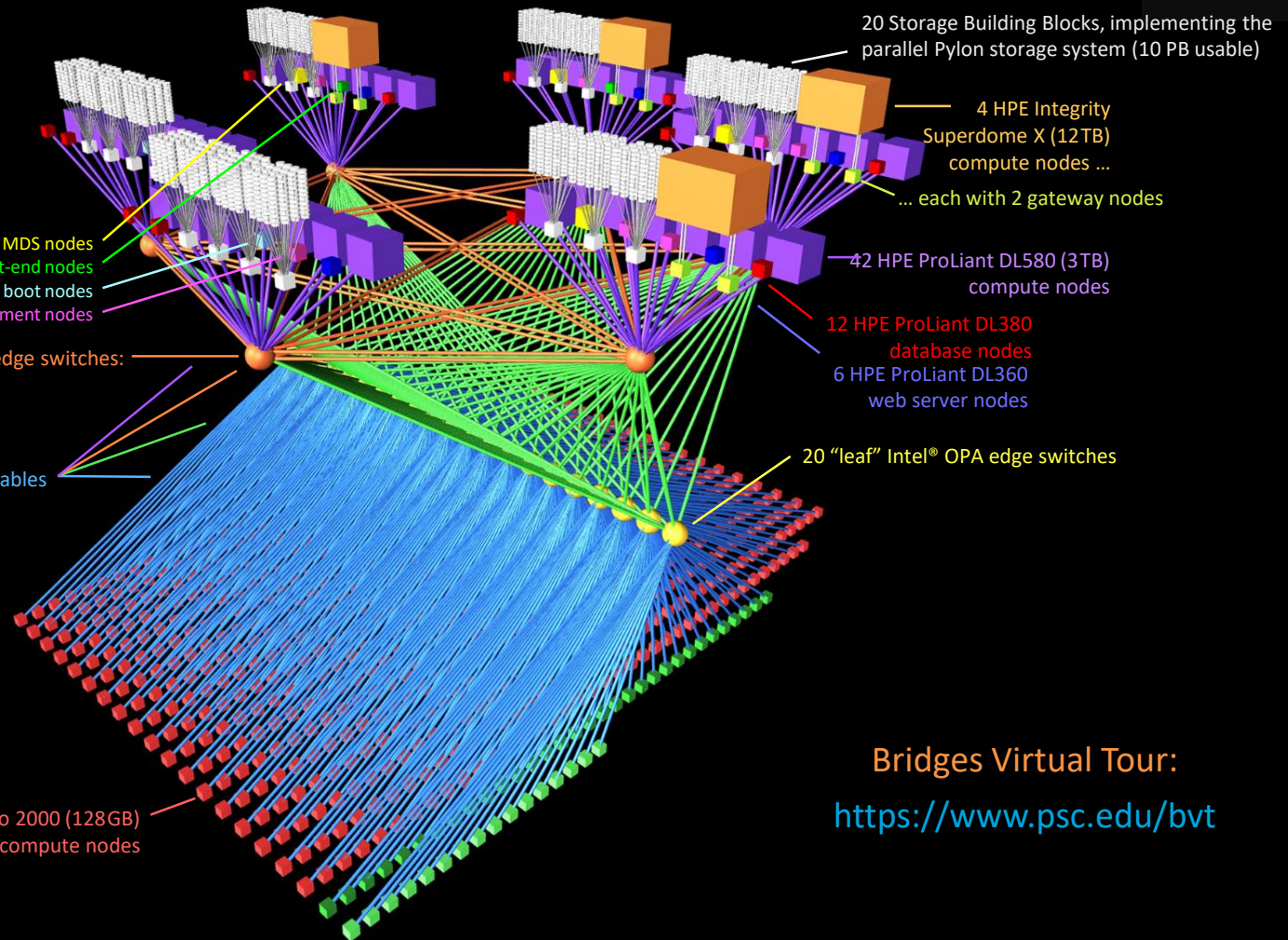
Questions from the audience

On-line talks

[bit.ly/XSEDEWorkshop](https://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.





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

Bridges Virtual Tour:  
<https://www.psc.edu/bvt>

# Node Types

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

a. Other nodes = front end (2) + management/log (8) + boot (4) + MDS (4)

b. DDR4-2133

c. DDR4-2400

# *Getting Time on XSEDE*

# XSEDE

Extreme Science and Engineering  
Discovery Environment

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

# Getting Connected

- The first time you use your account sheet, you must go to [apr.psc.edu](http://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](http://bridges.psc.edu). Use an ssh client (a Putty terminal, for example), to ssh to the machine.
- If you are already an active Bridges user, then to take advantage of the higher-priority training queue we are using for this workshop you will have to change to the training group account that is also available to you:
  - `newgrp tr561bp`
  - You can see what groups you are in with the “id” command, and which group you are currently using with “id -gn”
- You will want to use the training group today. With hundreds of us on the machine, the normal interact access time might leave you waiting for a bit.

# Getting Connected

At this point you are on a login node. It will have a name like “br001” or “br006”. 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.

You can load the two packages we will be using as

## *Spark*

```
module load spark
```

## *Tensorflow*

```
module load tensorflow/1.1.0  
source $TENSORFLOW_ENV/bin/activate
```

The Tensorflow one is atypical and reflects the complexities of its installation. If you find either of these tedious to repeat, feel free to put them in your `.bashrc`.

# 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

- 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, etc. you should be fine.



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.



# 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
```