

# 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

# 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



# 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 10-11 *HPC Monthly Workshop: Big Data*
- September 14-15 *HPC Monthly Workshop: MPI*
- October 5-6 *HPC Monthly Workshop: Big Data*
- November 3 *HPC Monthly Workshop: OpenMP*
- December 7-8 *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.

# Agenda

Tuesday, Dec 7

- 11:00 Welcome
- 11:25 A Brief History of Big Data
- 12:20 Intro to Spark
- 1:00 Lunch Break
- 2:00 More Spark and Exercises
- 3:00 Intro To Machine Learning
- 5:00 Adjourn

Wednesday, Dec 7

- 11:00 Machine Learning: A Recommender System
- 1:00 Lunch break
- 2:00 Deep Learning with TensorFlow
- 5:00 The Big Picture
- 5:30 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.
- 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: <https://www.psc.edu/resources/training/hpc-workshop-series/>

Copying code from PDFs is very error prone. Subtle things like substituting “-” for “-” are

## The YouTube Channel Has Arrived!

Due to overwhelming demand, we have begun to post workshop videos on the XSEDE Monthly Workshop Training Channel:

*XSEDETraining*

They will be incrementally updated. Subscribe and give us feedback.

ded online  
directory  
. I strongly  
here if you

# *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](mailto:akli@sura.org))
  - Lizanne Destefano, Georgia Tech ([lizanne.destefano@ceismc.gatech.edu](mailto:lizanne.destefano@ceismc.gatech.edu))
  - Ken Hackworth, Pittsburgh Supercomputing Center ([hackworth@psc.edu](mailto:hackworth@psc.edu))
  - Bryan Snead, Texas Advanced Computing Center ([jbsnead@tacc.utexas.edu](mailto:jbsnead@tacc.utexas.edu))
- Anonymous reporting form available at <https://www.xsede.org/codeofconduct>.

# Terminology Statement

In line with XSEDE's Code of Conduct, XSEDE is committed to providing training events that foster inclusion and show respect for all. This commitment applies not only 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.

XSEDE instructors strive to keep inclusive language at the forefront. In the event that we have included inappropriate materials, verbal or written, please let us know at [terminology@xsede.org](mailto:terminology@xsede.org). While XSEDE has no control over external third-party documentation, we are taking steps to effect change by contacting the relevant organizations; we hope this will be addressed by all third-parties 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](mailto:terminology@xsede.org)*



## **Check your email later 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: Tonya Miles, [toamiles@iu.edu](mailto:toamiles@iu.edu), or Lizanne DeStefano, [ldestefano6@gatech.edu](mailto:ldestefano6@gatech.edu)

# 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 [bridges2.psc.edu](http://bridges2.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 “bridges2-login012”. 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 “v32”.

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*

```
singularity shell --nv /ocean/containers/ngc/tensorflow/tensorflow_21.02-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

- 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.



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-2.

```
ssh username@bridges2.psc.edu
```

- Run the setup script that will copy over the BigData directory we will all use..

```
~training/Setup
```

- 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
```