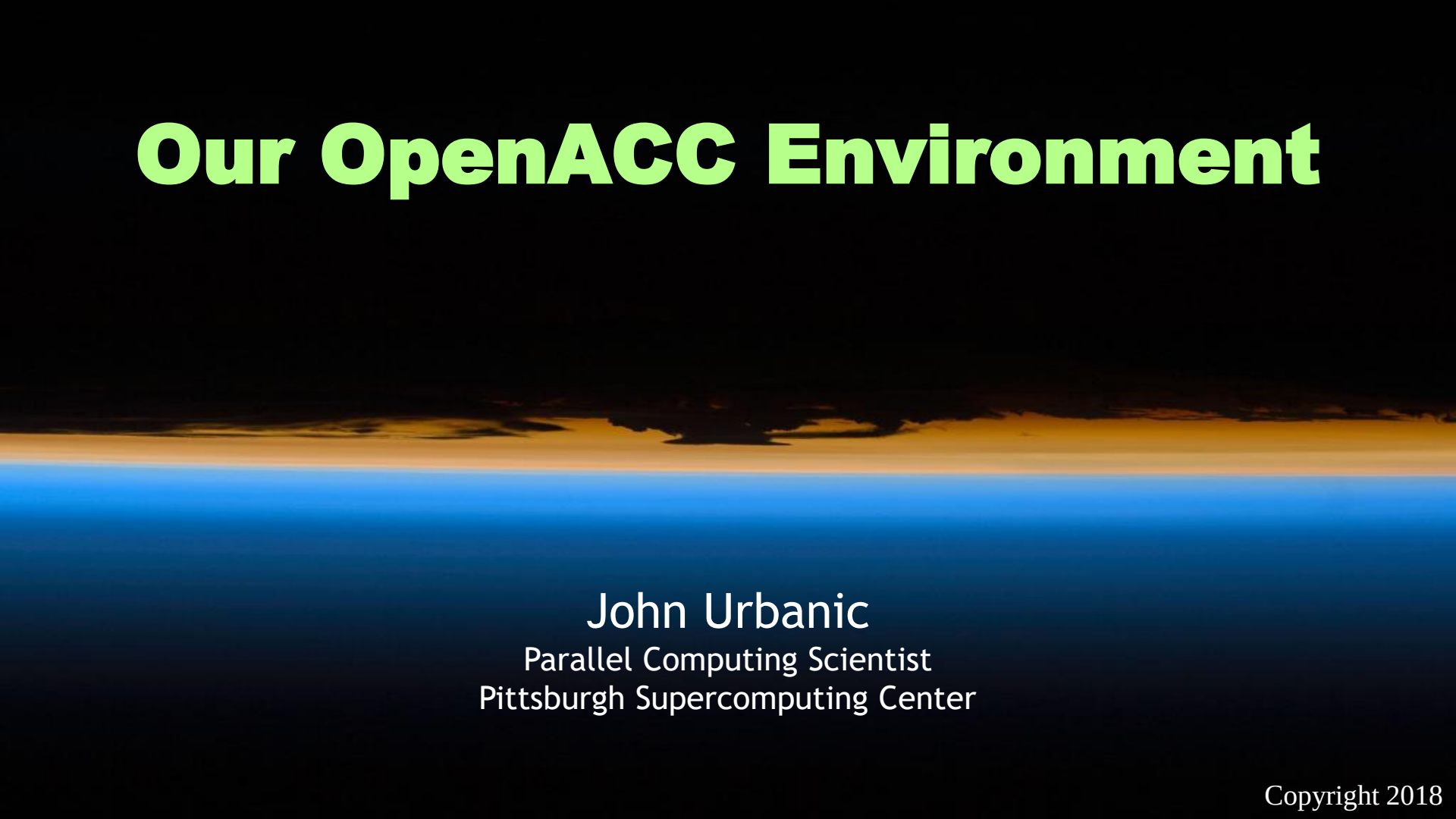
Our OpenACC Environment



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Our Environment Today

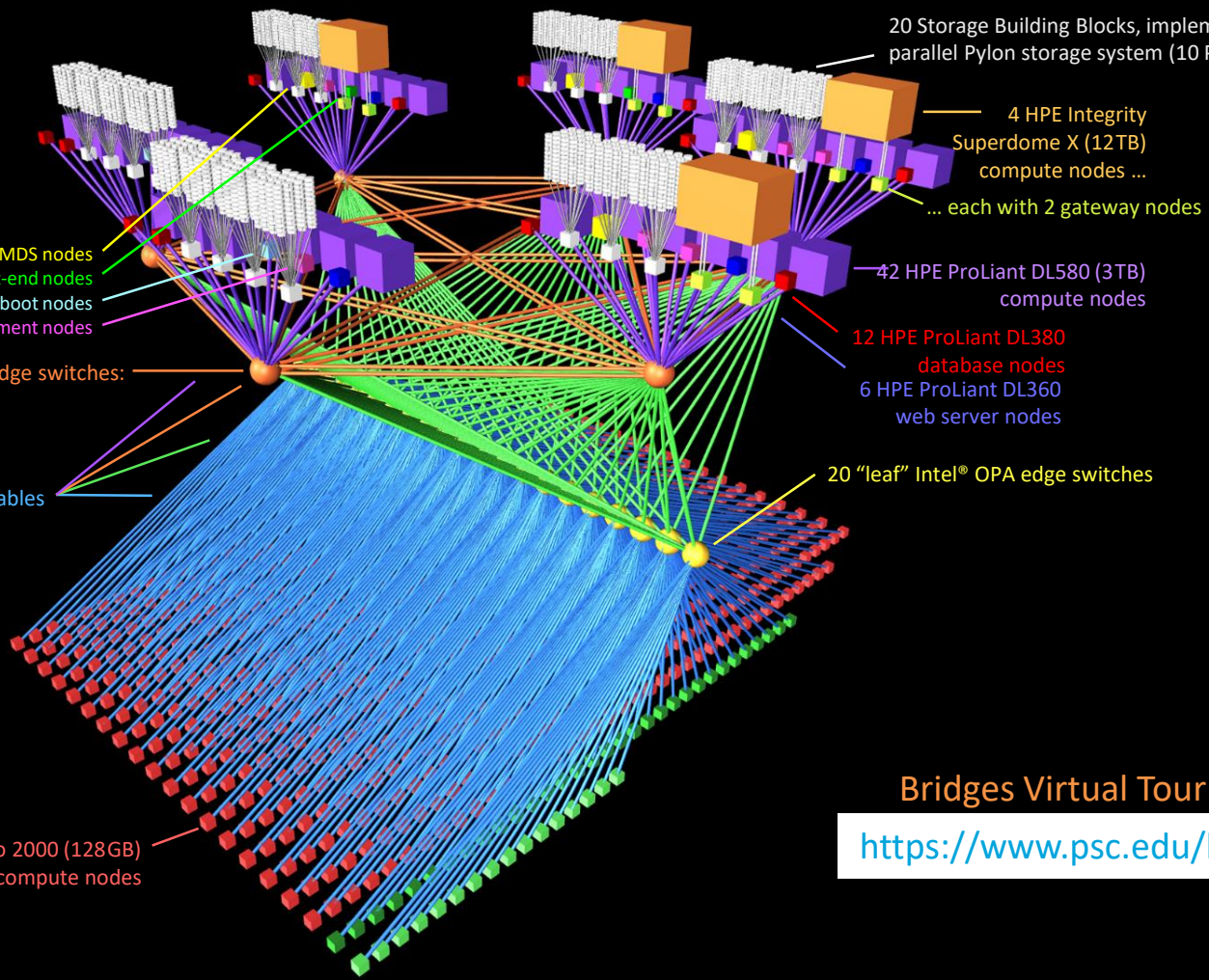
- Your laptops or workstations: only used for portal access
- Bridges is our HPC platform

We will here briefly go through the steps to login, edit, compile and run before we get into the real materials.

We want to get all of the distractions and local trivia out of the way here. Everything *after* this talk applies to any HPC environment you will encounter.

BRIDGES

A PITTSBURGH SUPERCOMPUTING CENTER RESOURCE



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

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.

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Bridges Node Types

Type	RAM[a]	Phse.	n	CPU / GPU / other	Server
ESM	12TB	1	2	16 × Intel Xeon E7-8880 v3 (18c, 2.3/3.1 GHz, 45MB LLC)	HPE Integrity Superdome X
		2	2	16 × TBA	
LSM	3TB	1	8	4 × Intel Xeon E5-8860 v3 (16c, 2.2/3.2 GHz, 40 MB LLC)	HPE ProLiant DL580
		2	34	4 × TBA	
RSM	128GB	1	752	2 × Intel Xeon E5-2695 v3 (14c, 2.3/3.3 GHz, 35MB LLC)	HPE Apollo 2000
RSM-GPU	128GB	1	16	2 × Intel Xeon E5-2695 v3 + 2 × NVIDIA K80	
		2	32	2 × Intel Xeon E5-2695 v3 + 2 × NVIDIA P100 GPU	
DB-s	128GB	1	6	2 × Intel Xeon E5-2695 v3 + SSD	HPE ProLiant DL360
DB-h			6	2 × Intel Xeon E5-2695 v3 + HDDs	HPE ProLiant DL380
Web	128GB	1	6	2 × Intel Xeon E5-2695 v3	HPE ProLiant DL360
Other[b]	128GB	1	14	2 × Intel Xeon E5-2695 v3	HPE ProLiant DL360, DL380
Total					

a. All RAM in these nodes is DDR4-2133
b. Other nodes = front end (2) + management/log (8) + boot (2) + MDS (4)

Getting Connected

- The first time you use your account sheet, you must go to apr.psc.edu to set a password. 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 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. To get a single GPU use “interact –p GPU”:

```
[urbanic@br006 ~]$ interact -p GPU
[urbanic@gpu016 ~]$
```

- **But wait!**

Executing Class Exercises

During the class itself, we may have too many of you to let you squat on nodes. So we will use the queueing system to keep things moving during the actual class. We will keep it very simple:

```
[urbanic@br006 ~]$ sbatch gpu.job
```

This is a jobscript in Exercises/OpenACC. It is fairly basic, and you may choose to ignore the details:

```
#!/bin/bash
#SBATCH -N 1
#SBATCH -p GPU-shared
#SBATCH --ntasks-per-node 7
#SBATCH --gres=gpu:p100:1
#SBATCH -t 5
#SBATCH -A ac560tp
#SBATCH --reservation=ihsstu
echo "4000" | ./a.out
```

However, due to annoying limitations of the Slurm queue system, we will need to use a different reservation name for our second day - tomorrow. I will update the jobscript in ~training, or you may simply edit the reservation line yourself to:

```
#SBATCH --reservation=ihssmo
```

After we wrap up the second day of exercises, you can just use interactive mode from there on out.

Editors

For editors, we have several options:

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

Compiling

We will be using standard Fortran and C compilers. They should look familiar.

- pgcc for C
- pgf90 for Fortran

Note that on Bridges you would normally have to enable this compiler with

```
module load pgi
```

I have put that in the .bashrc file that we will all start with.

Multiple Sessions

There is no reason not to open other sessions (windows) to the login nodes for compiling and editing. You may find this convenient. Feel free to do so.

Our Setup For This Workshop

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

```
/Exercises
        /Test
        /OpenMP
                laplace_serial.f90/c
                /Solutions
                /Examples
                /Prime
        /OpenACC
        /MPI
```

Preliminary Exercise

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

- Log on to apr.psc.edu and set an initial password.
- Log on to Bridges.

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

- Copy the exercise directory from the training directory to your home directory, and then copy the workshop shell script into your home directory.

```
cp  -r ~training/Exercises .
cp  ~training/.bashrc  .
```

- Logout and back on again to activate this script. You won't need to do that in the future.
- Edit a file to make sure you can do so. Use emacs, vi or nano (if the first two don't sound familiar).
- cd into your exercises/test directory and compile (C or Fortran)

```
cd Exercises/Test
pgcc test.c
pgf90 test.f90
```

- Run your program

```
sbatch gpu.job
```

(Wait a minute, or see how your job is doing with *squeue –u username*)

- Look at the results

```
more slurm-55838.out        (The exact job number will differ)
```

It should say *"Congratulations!"*