Our Workshop Environment

John Urbanic
Parallel Computing Scientist
Pittsburgh Supercomputing Center
Our Environment This Week

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

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

\(^a\) Other nodes = front end (2) + management/log (8) + boot (4) + MDS (4)
\(^b\) DDR4-2133
\(^c\) DDR4-2400
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 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 8 processors on a node use “interact”:

  [urbanic@br006 ~]$ interact -n 8
  [urbanic@r590 ~]$ 

- You can tell you are on a regular memory compute node because it has a name like “r590” or “r101”.

- Do make sure you are working on a compute node. Otherwise your results will be confusing.
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 this week. They should look familiar.

- pgcc (aka mpicc) for C
- pgf90 (aka mpif90) for Fortran

We will slightly prefer the PGI compilers (the Intel or gcc ones would also be fine for most of our work, but not so much for OpenACC). There are also MPI wrappers for these called mpicc and mpif90 that we will use. 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

You are limited to one interactive compute node session for our workshop. However, 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
   /OpenACC
   /MPI

laplace_serial.f90/c
laplace_template.f90/c
/Solutions
/Examples
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 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).

- Start an interactive session.
  
  ```
  interact -n 8
  ```

- cd into your exercises/test directory and compile (C or Fortran)
  
  ```
  cd Exercises/Test
  pgcc test.c
  pgf90 test.f90
  ```

- Run your program
  
  ```
  a.out  (You should get back a message of “Congratulations!”)
  ```