ICE Orientation

Chris Blanton, Ph.D.

PACE

Spring 2020
Introduction

Access

Queues

Storage

Software

Important Notes
Introduction
What is PACE

**Definition**

*Partnership for an Advanced Computing Environment.*

**PACE’s mission is to**

- *provide faculty and researchers vital tools to accomplish the Institute’s vision to define the technological research university of the 21st century.*
- *create a strong HPC and HTC environment via a tight partnership with our world-class students, researches, and innovators to help them make the greatest impact with their work.*
ICE Accounts

- Automated based on class enrollments.
- Departments manage access groups without PACE’s involvement.
- COC has their own resources (coc-ice), other departments share PACE resources (pace-ice).
Tiered Help Structure

Support Structure

Due to the large number of users in the classes, we must use a tiered support structure.

Students reach out to Instructors/TAs (no direct tickets to PACE)

Instructors/TAs can contact their departmental contacts

Instructors, TAs and department contacts can open tickets:
pace-support@oit.gatech.edu
Due to the large number of users in the classes, we must use a tiered support structure.

**Students** reach out to Instructors/TAs (no direct tickets to PACE)

**Instructors/TAs** can contact their departmental contacts

- **COC**  David Mercer
- **ECE**  David Webb
- **Chbe**  Kevin Guger
- **COS**  Mack Jenkins

**Instructors, TAs and department contacts** can open tickets:

pace-support@oit.gatech.edu
Tiered Help Structure

**Support Structure**

*Due to the large number of users in the classes, we must use a tiered support structure.*

**Students** reach out to Instructors/TAs *(no direct tickets to PACE)*

**Instructors/TAs** can contact their departmental contacts

**Instructors, TAs and department contacts** can open tickets: `pace-support@oit.gatech.edu`

**Note**

*Please make sure to include ICE in the subject line as well as course, department, and number in the body.*
Access
Accessing Clusters

- **The clusters are accessed using a SSH client**
  - **Windows** MobaXterm, Putty, Xming (for X11), X-win32 (for X11), PowerShell, WSL
  - **MacOSX** iTERM2, Terminal, XQuartz (for X11)
  - **Linux** various terminals, X11 windowing system for X11 forwarding

- **The command is**
  
  $ ssh -XY <GT_user_id>@pace-ice.pace.gatech.edu
  $ ssh -XY <GT_user_id>@coc-ice.pace.gatech.edu

- **The user must be on campus or connected via VPN.**
Accessing Clusters

- **The clusters are accessed using a SSH client**
  - **Windows** MobaXterm, Putty, Xming (for X11), X-win32 (for X11), PowerShell, WSL
  - **MacOSX** iTerm2, Terminal, XQuartz (for X11)
  - **Linux** various terminals, X11 windowing system for X11 forwarding

- **The command is**
  
  $ ssh -XY <GT_user_id>@pace-ice.pace.gatech.edu
  
  $ ssh -XY <GT_user_id>@coc-ice.pace.gatech.edu

- **The user must be on campus or connected via VPN.**

**Note**

For information on VPN access, see
https://faq.oit.gatech.edu/content/how-do-i-get-started-campus-vpn
The PBS (Torque/MOAB) scheduler and resource manager

- **Users make requests to the MOAB scheduler specifying the requirements of their computation**
  - The number of nodes and/or cores per node.
  - The total memory or memory-per-code.
  - An estimated runtime (walltime, not CPU time).
  - Other specific requirements, such as GPU.

- **Allocated resources can only be used by the user for the duration of the requested walltime. This is the only time users can directly login to compute nodes.**
Operation Modes

There are two modes of operations on the ICE clusters:

**Batch:** Jobs are submitted and run as resources become available, which may take some time. The jobs must run without interaction from a user.

**Interactive:** The user enters commands after compute resources have been acquired. There are a few ways to do this:

- **Manual** Use of the `–I` flag on `qsub`.
- **pace-interact** A wrapper to do the above. Encouraged.
- **pace-vnc-job** A simplified wrapper to run VNC (graphical jobs).
- **pace-jupyter-notebook** A wrapper to run JuPyteR notebooks.
Submitting batch jobs

- *Everything needs to be scripted. Not for codes that require user interaction.*
- *A PBS script includes resources requirements, environmental settings, and task.*
- *The qsub command is used to submit the job:*

  ```
  $ qsub example_pbs_script.pbs
  ```
PBS script example

# This is an example PBS script
#PBS -N hello
#PBS -l nodes=2:ppn=4
#PBS -l pmem=2gb
#PBS -l walltime=09:00:00
#PBS -q coc-ice
#PBS -j oe
#PBS -o myjob.out
#PBS -m abe
#PBS -M userid@gatch.edu

cd $PBS_O_WORKDIR
module load gcc/7.2.0
./a.out > myoutput
#End of file—need a blank line or comment for safety.
PBS script example

# This is an example PBS script
#PBS -N hello
#PBS -l nodes=2:ppn=4
#PBS -l pmem=2gb
#PBS -l walltime=09:00:00
#PBS -q coc-ice
#PBS -j oe
#PBS -o myjob.out
#PBS -m abe
#PBS -M userid@gatch.edu

cd $PBS_O_WORKDIR
module load gcc/7.2.0
./a.out > myoutput
#End of file—need a blank line or comment for safety.

More about PBS jobs

http://docs.pace.gatech.edu/scheduler/job_submission/
Requesting GPU nodes

- **Available on** `coc-ice` and `pace-ice`.
- **Add the directive to your script as**
  
  ```bash
  #PBS -l nodes=1:ppn=4:gpus=2:exclusive_process
  ```

  for an appropriate queue. You can use this request in interactive mode as well.

- **You can use request a particular model**
  
  - **For Tesla K40**
    
    ```bash
    #PBS -l nodes=1:ppn=4:gpus=2:teslak40:exclusive_process
    ```

  - **For Tesla P100**
    
    ```bash
    #PBS -l nodes=1:ppn=4:gpus=1:teslap100:exclusive_process
    ```
Manual interactive sessions

- The best practice for interactive compute is to get a session on the compute nodes.
- This can be done with the `-I` flag.
- As an example,

  ```
  $ qsub -I -X -l walltime=02:00:00 -l nodes=2:ppn=4 -l pmem=2gb -q pace-ice
  ```
The wrapper `pace-interact` can be used to simplify the start of interactive jobs on the compute nodes.

The usage of the wrapper is

```
$ pace-interact -l walltime=02:00:00 -l nodes=2:ppn=4 -q pace-ice
```

The only required component is the `-q`. There are defaults of 1 hours with 1 node and 1 processor.
**pace-vnc-job**

- **Virtual Network Computing (VNC) is a method for using desktop and GUI-based programs which leverages the Remote Frame Buffer protocol.**
- **VNC performs much better than X11 forwarding.**
- **The new pace-vnc-job wrapper greatly simplifies the process of creating a VNC session**
- **Full instructions are available at**
  
  http://docs.pace.gatech.edu/interactiveJobs/setupVNC_Session/
Jupyter notebooks allow you to create and share documents that contain live code, equations, visualizations, and narrative text.

The `pace-jupyter-notebook` command simplifies the creation Jupyter sessions on the PACE system.

Full instructions are available at
http://docs.pace.gatech.edu/interactiveJobs/jupyterInt/
Queues
COC-ICE Queues

Login Node

coc-ice.pace.gatech.edu

- **coc-ice**: (All nodes, 2 hr walltime, 4 max procs; All users)
- **coc-ice-gpu**: (Only GPU nodes, 2 hr walltime, 4 max procs; All users)
- **coc-ice-multi**: (All nodes, 30 min walltime, 16 max procs; All users)
- **coc-ice-long**: (All nodes, 8 hr walltime, 2 max procs; All users)
- **coc-ice-grade**: (All nodes, 12 hr walltime, 16 max procs; Faculty, TAs, and Admins)
- **coc-ice-devel**: (All nodes, 8 hr walltime, 16 max procs; Faculty TAs Admins)

Chris Blanton, Ph.D. (PACE)
COC-ICE Resources

The available resources and their current status may be checked using `pace-check-queue coc-ice`

```
[root@coc-ice ~]# pace-check-queue coc-ice

** NEW FEATURE : add '-s' to pace-check-queue to list
** scheduler features for each node

=== coc-ice Queue Summary: =====
Last Update : 01/09/2020 15:00:07
Number of Nodes (Accepting Jobs/Total) : 49/49 (100.00%)
Number of Cores (Used/Total) : 0/892 ( 0.00%)
Amount of Memory (Used/Total) (MB) : 149135/7974738 ( 1.87%)
```

<table>
<thead>
<tr>
<th>Hostname</th>
<th>tasks/rp</th>
<th>Cpu%</th>
<th>loadavg%</th>
<th>used/totmem(MB)</th>
<th>Mem%</th>
<th>Accepting Jobs?</th>
</tr>
</thead>
<tbody>
<tr>
<td>rich133-h35-15-r</td>
<td>0/28</td>
<td>0.0</td>
<td>0.6</td>
<td>3530/131126</td>
<td>2.7</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-h35-16-l</td>
<td>0/28</td>
<td>0.0</td>
<td>0.5</td>
<td>4546/131126</td>
<td>3.5</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-h35-16-r</td>
<td>0/28</td>
<td>0.0</td>
<td>0.4</td>
<td>3227/131126</td>
<td>2.5</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-h35-17-l</td>
<td>0/28</td>
<td>0.0</td>
<td>0.8</td>
<td>4262/518966</td>
<td>0.8</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-h35-17-r</td>
<td>0/28</td>
<td>0.0</td>
<td>0.8</td>
<td>5653/518966</td>
<td>1.1</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-h35-18-l</td>
<td>0/28</td>
<td>0.0</td>
<td>0.35</td>
<td>5596/518966</td>
<td>1.1</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-h35-18-r</td>
<td>0/28</td>
<td>0.0</td>
<td>0.9</td>
<td>3802/518966</td>
<td>0.7</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k33-17</td>
<td>0/8</td>
<td>0.0</td>
<td>0.2</td>
<td>4175/260408</td>
<td>1.6</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k40-17</td>
<td>0/8</td>
<td>0.0</td>
<td>0.4</td>
<td>21865/131128</td>
<td>16.7</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k40-18</td>
<td>0/8</td>
<td>0.0</td>
<td>1.9</td>
<td>3173/131128</td>
<td>2.4</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k40-20-l</td>
<td>0/28</td>
<td>0.0</td>
<td>0.5</td>
<td>3195/131126</td>
<td>2.4</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k40-20-r</td>
<td>0/28</td>
<td>0.0</td>
<td>1.1</td>
<td>3260/131126</td>
<td>2.5</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k40-21-l</td>
<td>0/28</td>
<td>0.0</td>
<td>1.0</td>
<td>3143/131126</td>
<td>2.4</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k40-21-r</td>
<td>0/28</td>
<td>0.0</td>
<td>0.7</td>
<td>3242/131126</td>
<td>2.5</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k40-22-l</td>
<td>0/28</td>
<td>0.0</td>
<td>1.1</td>
<td>3022/131126</td>
<td>2.3</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k40-22-r</td>
<td>0/28</td>
<td>0.0</td>
<td>0.7</td>
<td>3339/131126</td>
<td>2.5</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k40-23-l</td>
<td>0/28</td>
<td>0.0</td>
<td>0.6</td>
<td>3262/131126</td>
<td>2.5</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k40-23-r</td>
<td>0/28</td>
<td>0.0</td>
<td>1.3</td>
<td>3161/131126</td>
<td>2.4</td>
<td>Yes (free)</td>
</tr>
<tr>
<td>rich133-k40-24-l</td>
<td>0/28</td>
<td>0.0</td>
<td>0.6</td>
<td>3108/131126</td>
<td>2.4</td>
<td>Yes (free)</td>
</tr>
</tbody>
</table>
PACE-ICE Queues

The login-node is `pace-ice.pace.gatech.edu`

The queues are

- **pace-ice** 12:00:00 max walltime, 98 cores max job, everyone has access
- **eas-pace-ice** 48:000:00 max walltime, 90 cores max job, only TAs, admins, and Faculty have access
- **pace-ice-gpu** 16:00:00 max walltime

- Walltime can be adjusted per request.
- `pace-check-queue` shows all nodes and cores, but submissions with greater...
Storage
Storage Space on ICE

- **COC-ICE** has 41TB total capacity owned by the departments, 10GB per student.
- **PACE-ICE** has 10GB per student (provided by PACE).
- All data are accessible from all nodes (login and compute nodes).
- Complete (orthogonal) separation from the rest of PACE (your standard PACE account is completely different).
Mounter applications mount remote storage so you can drag/drop or edit in place as if the files are on the local machine may be used.

- **Windows** webdrive
- **MAC OSX** macfusion
- **Linux** SSHFS, autofs

Any SFTP client will work with PACE. FileZilla is a free SFTP tool available for major OSs.

Use the login nodes as the server for configuring any of these clients.
Software
PACE Software Stack

- **PACE-ICE and COC-ICE share the same base software stack as the standard PACE machines.**
- **Licensed software package, such as Matlab, Fluent, Mathematica, Abaqus, Comsol, ...**
- **Open source packages and standard HPC, such as BLAS, PETSc, NAMD, NetCDF, BLAST, LAMMPS, ...**
- **Compilers:**
  - **C/CC++ and Fortran:** GNU, Intel, PGI, NAG
  - **Parallel:** OpenMP, MPICH, MPICH2, MVAPICH, Intel MPI
  - **GPU:** CUDA, PGI
- **Scripting and Interactive Languages:** Python, Perl, R, ...
**Modules**

- **Painless configuration for software environment and switching between different versions** (no need to much about with PATH, LD_LIBRARY_PATH etc!)

- **Main commands**
  - `module avail` List all available modules that can be loaded.
  - `module list` List all the module that are currently loaded.
  - `module load xxx` Loads the XXX module to the environment.
  - `module rm xxx` Removes the XXX module from the environment.
  - `module purge` Removes all the modules from the environment.
Maintenance Periods

Important

PACE maintenance period will be 2/27/2020-2/29/2020. Resources will be unavailable during this period, so please plan accordingly.
Thank you!