ICE Orientation

PACE Instructional Cluster Environments: PACE-ICE and COC-ICE

Michael Weiner, PhD
Partnership for an Advanced Computing Environment

- PACE provides faculty participants sustainable leading-edge advanced research computing resources with technical support services, infrastructure, software, and more.
  - Interested in using PACE's research clusters? Free tier provides any GT academic or research faculty the equivalent of 10,000 CPU-hours per month on a 192GB compute node and 1 TB of project storage at no cost on Phoenix

- Virtual tour of Coda datacenter hosting PACE clusters, including PACE-ICE and COC-ICE: https://pace.gatech.edu/coda-datacenter-360-virtual-tour

Sign up for our hands-on workshops taught by PACE Research Scientists: Linux 101, Linux 102, Python 101: Intro to Data Analysis with NumPy, Git 101, Optimization 101, and Applications of Machine Learning

https://pace.gatech.edu/training
ICE access

- Apply for your class to use ICE
  - Classes outside of CoC → PACE-ICE: http://docs.pace.gatech.edu/training/pace-ice/
  - Classes in CoC → COC-ICE: Contact David Mercer (CoC TSO)
- Students are automatically given access as registrar records course enrollment, once course is enabled for ICE
- Instructors and TAs added manually by PACE or School IT
Tiered Support Structure

- PACE provides training to instructors and TAs
- **Students** seek help from instructors and TAs. Due to the large number of students and PACE’s staffing, *students may not open support tickets directly with PACE.*
- **Instructors and TAs** may seek help from PACE through support tickets, by emailing *pace-support@oit.gatech.edu* at any time.
- In some schools/colleges, local IT professionals also provide support to instructors and TAs:
  - CoC: David Mercer and TSO (*david.mercer@cc.gatech.edu*)
  - ECE: Keith May and ECE IT (*keith.may@ece.gatech.edu*)
  - CoS: ARCS (*https://arcs.gatech.edu/gethelp*)
- Much of PACE documentation applies to ICE as well: *docs.pace.gatech.edu*
Head Nodes vs. Compute Nodes

- **Head Nodes:** The machines you use to log in
  - Good for compiling, editing, debugging, etc.
  - Not good for actual computations or visualizations!
  - Named like “pace-ice.pace.gatech.edu”

- **Compute Nodes:** The machines that run all computations
  - No direct access by users
  - Allocated per-job by the scheduler
ICE Nodes

- **PACE-ICE**: 16 nodes with 6 GPU cards
  - 13 nodes with 24 CPUs and 192GB RAM
  - 3 nodes with 24 CPUs, 384 GB RAM, and 2 Tesla V100 GPUs

- **COC-ICE**: 45 nodes with 60 GPU cards
  - 17 nodes with 24 CPUs and 192 GB RAM
  - 1 node with 24 CPUs and 384 GB RAM
  - 5 nodes with 24 CPUs and 768 GB RAM
  - 6 nodes with 24 CPUs, 192 GB RAM, and 4 RTX6000 GPUs
  - 4 nodes with 40 CPUs, 192 GB RAM, and 1 V100 GPU
  - 4 nodes with 40 CPUs, 192 GB RAM, and 4 V100 GPUs
  - 8 nodes with 24 CPUs, 384 GB RAM, and 2 V100 GPUs
Accessing Clusters

- You will need an SSH Client (a.k.a. terminal). Recommended options:
  - Windows: **Powershell** (built-in on Windows 10) or Windows Subsystem for Linux (WSL)
  - MacOS: **Terminal** (built-in)
  - Linux: System-default **terminal** (gnome/KDE)

- SSH access to PACE clusters:
  
  ```bash
  ssh <GT_username>@<headnode>.pace.gatech.edu
  PACE-ICE: pace-ice.pace.gatech.edu
  COC-ICE: coc-ice.pace.gatech.edu
  ```

- You need to be connected to Georgia Tech’s VPN to access the resources
  - Either Cisco AnyConnect or GlobalProtect – both work

For information VPN access, see [http://docs.pace.gatech.edu/gettingStarted/vpn/](http://docs.pace.gatech.edu/gettingStarted/vpn/)
Storage and Quotas

• Your data are accessible from all nodes (head and compute nodes)
• Each user has a **15 GB** home directory on NetApp storage, backed up daily
• `pace-quota` command can be used to check quota utilization
• Extra space for individual users may be requested.
• Shared space for posting course materials or software upon request
• Data transfer in/out via **scp** or **sftp**
  • `scp -r ~/mylocalstuff <username>@<login-node>.pace.gatech.edu:~/
• Any **SFTP** client will work with ICE
  • FileZilla is a free FTP tool for Windows, macOS, and Linux
  • Use “<login-node>.pace.gatech.edu” for configuring any of these clients
• The scheduler (Moab) allows a fair use of shared resources within a queue (dynamic priorities, limits on walltime, CPU and RAM)

• Users make requests specifying the requirements of the code:
  • The number of Nodes and/or Cores per node.
  • The total Memory or Memory-per-core.
  • An estimated Runtime (walltime, not CPU time)
  • Specific hardware resources, e.g. GPU

• Allocated resources can only be used by the user for the duration of requested walltime. This is the only time users can directly login to compute nodes.
## ICE Queues

<table>
<thead>
<tr>
<th>PACE-ICE</th>
<th>Max CPU per Job</th>
<th>Max walltime</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>pace-ice</td>
<td>80</td>
<td>8:00:00</td>
<td></td>
</tr>
<tr>
<td>pace-ice-gpu</td>
<td>48</td>
<td>8:00:00</td>
<td>Max 2 GPUs per job</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>COC-ICE</th>
<th>Max CPU per Job</th>
<th>Max walltime</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>coc-ice</td>
<td>28</td>
<td>2:00:00</td>
<td>Higher priority</td>
</tr>
<tr>
<td>coc-ice-gpu</td>
<td>28</td>
<td>2:00:00</td>
<td>For GPU jobs, higher priority</td>
</tr>
<tr>
<td>coc-ice-multi</td>
<td>128</td>
<td>0:30:00</td>
<td>For MPI jobs, lower priority</td>
</tr>
<tr>
<td>coc-ice-long</td>
<td>28</td>
<td>8:00:00</td>
<td>Lower priority</td>
</tr>
<tr>
<td>coc-ice-devel</td>
<td>128</td>
<td>8:00:00</td>
<td>Limited access, lowest priority</td>
</tr>
<tr>
<td>coc-ice-grade</td>
<td>128</td>
<td>12:00:00</td>
<td>Instructors/TAs only, highest priority</td>
</tr>
</tbody>
</table>
Steps to Use the PACE Clusters

1. Connect to GT VPN
2. Login to headnode using SSH
3. Submit jobs to Moab using “qsub” command
4. Moab decides which compute node to use
5. Your job starts on the node that Moab picks
Two modes of operation:

- **Batch**: Submit & forget. Job waits in the queue until resources become available, runs, emails user on exit.

- **Interactive**: Allows interactive use, no different than remotely using any workstation.
  - Required for using GUI, such as MATLAB, R, COMSOL, ANSYS, visualization, etc.
Submitting Batch Jobs

- Everything needs to be scripted. Not for codes that require user interaction (e.g. press ‘y’ to continue).
- A ‘PBS script’ that includes resource requirements, environmental settings, and tasks.
- Use ‘qsub’ to submit the job.
  
  ```
  qsub example_PBS_Script.pbs
  ```
- The output and error logs are printed on files, as they would appear on the screen.
PBS Script Example

```plaintext
# This is an example PBS script
#PBS -N hello
#PBS -l nodes=2:ppn=4
#PBS -l pmem=2gb
#PBS -l walltime=1:00:00
#PBS -q pace-ice
#PBS -j oe
#PBS -o myjob.out
#PBS -m abe
#PBS -M youremail@gatech.edu

cd $PBS_O_WORKDIR
echo "Started on `/bin/hostname`"
module purge
module load gcc/4.9.0 mvapich2/2.1
mpirun -np 8 ./hello
```

# A name for this run, can be anything
# 2 nodes, 4 cores in each
# 2GB memory per core (16GB total)
# 1 hr “max”, after which job is killed!!
# submitting to queue named “pace-ice”
# Put output and error files in specified format
# Event notifications set to start, finish or error, via email

Actual Computation
Interactive Command-Line Jobs

• Same PBS commands, but this time on the command line:

```bash
qsub -l -q pace-ice -l nodes=2:ppn=4,walltime=4:00:00,pmem=2gb
```
• ‘,’ are for binding multiple values for a parameter (-l)

• The scheduler logs the user onto a compute node when the resources become available
• User waits in real-time until space is assigned
• Session is terminated:
  • The user exits
  • The terminal is closed
  • The walltime is exceeded
Graphical Interactive Jobs

• Virtual Network Computing (VNC) allows you to access a graphical desktop on a PACE compute node

• Use the `pace-vnc-job` command to launch a VNC job on the scheduler:
  `pace-vnc-job -q pace-ice`

• You will need a VNC client installed on your computer to access the session by following the 3 steps provided on the terminal

• Documentation: https://docs.pace.gatech.edu/software/setupVNC_Session/

Using PuTTY or another client for VNC or Jupyter?
See instructions at http://docs.pace.gatech.edu/software(pf_3rd_party_ssh/)

• For Python and other languages, you can use a Jupyter notebook.

• Use the `pace-jupyter-notebook` command to launch a Jupyter job on the scheduler
  `pace-jupyter-notebook -q pace-ice`

• No client necessary – just use a browser!

• Documentation: https://docs.pace.gatech.edu/software/jupyter/
Monitoring Jobs

`qstat` lists your queued jobs and their state:

```
qstat -u <UserName> -n
```

sched-torque.pace.gatech.edu:

<table>
<thead>
<tr>
<th>Job ID</th>
<th>Username</th>
<th>Queue</th>
<th>Jobname</th>
<th>SessID</th>
<th>NDS</th>
<th>TSK</th>
<th>Req'd Memory</th>
<th>Req'd Time</th>
<th>S</th>
<th>Elap Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>95521.sched-torque.pace-atl1-1-02-010-14-l</td>
<td>ssarajlic3</td>
<td>inferno</td>
<td>pace-vnc-job.pbs</td>
<td>337870</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>01:00:00 R</td>
<td>00:01:42</td>
<td></td>
</tr>
<tr>
<td>95522.sched-torque.pace-atl1-1-02-010-14-l</td>
<td>ssarajlic3</td>
<td>inferno</td>
<td>pace-vnc-job.pbs</td>
<td>339184</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>01:00:00 R</td>
<td>00:01:08</td>
<td></td>
</tr>
<tr>
<td>95526.sched-torque.pace-atl1-1-02-010-14-l</td>
<td>ssarajlic3</td>
<td>inferno</td>
<td>pace-jupyter-not</td>
<td>340707</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>01:00:00 R</td>
<td>00:00:34</td>
<td></td>
</tr>
</tbody>
</table>

• Cancelling a submitted job

```
qdel <jobID>
```

• Querying for specific users/queues also available with `showq`
Checking the Queue Status

• Summarizes the utilization of each queue

```plaintext
pace-check-queue pace-ice-gpu
```

```plaintext
=== pace-ice-gpu Queue Summary ====

<table>
<thead>
<tr>
<th>Last Update</th>
<th>08/13/2021 10:45:01</th>
</tr>
</thead>
<tbody>
<tr>
<td>Next Maintenance Start</td>
<td>11/03/2021 06:00:00</td>
</tr>
<tr>
<td>Number of Nodes (Accepting Jobs/Total)</td>
<td>3/3 (100.00%)</td>
</tr>
<tr>
<td>Number of Cores (Used/Total)</td>
<td>0/72 (0.00%)</td>
</tr>
<tr>
<td>Amount of Memory (Used/Total) (GB)</td>
<td>15/1152 (1.30%)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>atl1-1-02-009-31</td>
<td>0/24</td>
<td>0.13</td>
<td>0/2</td>
<td>5/ 0/ 384</td>
<td>1.30</td>
<td>12/ 0/1708</td>
<td>0.70</td>
<td>Yes</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>atl1-1-02-009-32</td>
<td>0/24</td>
<td>0.17</td>
<td>0/2</td>
<td>5/ 0/ 384</td>
<td>1.30</td>
<td>12/ 0/1708</td>
<td>0.70</td>
<td>Yes</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>atl1-1-02-009-33</td>
<td>0/24</td>
<td>0.00</td>
<td>0/2</td>
<td>5/ 0/ 384</td>
<td>1.30</td>
<td>12/ 0/1708</td>
<td>0.70</td>
<td>Yes</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
```
PACE Software Stack

• Licensed software packages:
  • Common license: Matlab, Mathematica, ...

• Open source packages and HPC libraries:
  • BLAS, PETSc, NAMD, NetCDF, FFTW, BLAST, LAMMPS, ...

• Compilers:
  • C/C++ & Fortran: GNU, Intel, PGI, NAG
  • Parallel Compilers: OpenMP, MPICH, MPICH2, MVAPICH
  • GPU Compilers: CUDA, PGI

• Scripting Languages: Python, Perl, R, ...
### Modules: How to Access Software on PACE

- **Painless configuration for software environment and switching between different versions:**
- **Main commands:**
  - `module spider`: Lists all software and its available versions on cluster
  - `module avail`: Lists all available modules that can be loaded with current environment
  - `module list`: Displays all the modules that are currently loaded
  - `module load`: Loads a module to the environment
  - `module rm`: Removes a module from the environment
  - `module purge`: Removes all loaded modules

  ```bash
  $ module load matlab/r2020a
  ```

- **Example PBS batch scripts command line utility (pace-getexample) for downloading example batch scripts for frequently used PACE software modules**
  - `pace-getexample --list`: Displays a list of currently available examples
  - `pace-getexample --help`: Instructions on how to download and submit an example job to the queue

- **Must-Read:** PACE-specific use cases and examples
  - [http://docs.pace.gatech.edu](http://docs.pace.gatech.edu)
Thank You

- Documentation: [http://docs.pace.gatech.edu](http://docs.pace.gatech.edu)
- Support for Instructors and TAs: [pace-support@oit.gatech.edu](mailto:pace-support@oit.gatech.edu)
- PACE Training workshops: [https://pace.gatech.edu/training](https://pace.gatech.edu/training)

Welcome to ICE!