

ICE

Orientation

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PACE

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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

- ***ICE accounts are created by a hook to the registrar for most students.***
- ***Instructors and TAs are added manually.***
- ***The CRS handles this for most classes, but we communicate it to the CSR.***

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

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COC David Mercer

ECE Keith May

Chbe Kevin Guger

COS Mack Jenkins

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Note

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

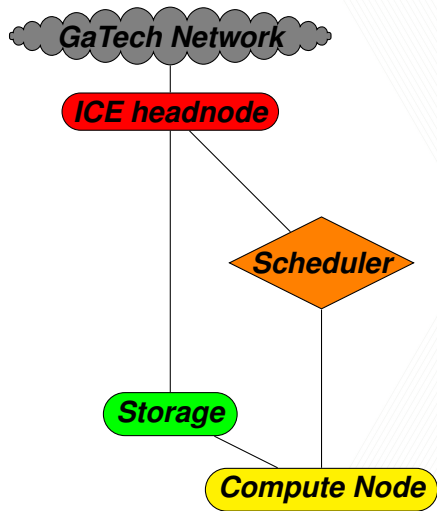
Accessing Clusters

- *The cluster are accessed using the SSH protocol.*
- *The login-nodes for the each cluster is*
 - ▶ *pace-ice.pace.gatech.edu*
 - ▶ *coc-ice.pace.gatech.edu*
- *There are multiple SSH clients which may be used, according to the user's OS.*

Structure of a Computational Cluster

A computational cluster is composed of

- *Head nodes*
- *Computational nodes*
- *Storage Servers*
- *Scheduler*



Head Nodes

A head node is the part of the cluster that users

- ***Connect to submit jobs.***
- ***Can code and compile small-scale programs.***
- ***Access their files and storage.***

Computational Nodes

Computational nodes are the nodes which the heavy work is performed. Computational nodes

- ***are accessed using the scheduler only.***
- ***have access to the storage server.***
- ***may vary in their computational capability.***

Storage Servers

- ***The storage for the system is handled via a centralized NetApp storage.***
- ***Each user has a quota of 10 GB.***
- ***Professors and others can request larger quotas.***

Accessing Software

- ***Computational clusters often have many software packages, which may have conflicting names and versions.***
- ***A module system can be used to handle this.***
- ***The module system handles setting up the environment.***
- ***The module system has been prepared to handle dependencies so only loadable software is shown.***

module commands

<i>Command</i>	<i>Meaning</i>
<i>module avail</i>	<i>Show the currently available modules</i>
<i>module spider name</i>	<i>Search for a module</i>
<i>module load name</i>	<i>Load the module</i>
<i>module list</i>	<i>See the currently loaded modules</i>
<i>module remove name</i>	<i>Remove the named module</i>
<i>module purge</i>	<i>Remove all loaded modules</i>

Scheduler

The scheduler/resource manager handles

- ***placing jobs on computational resources***
- ***ensuring that all users have appropriate access what they need***
- ***abstracts knowing which computational node has what is needed***

Accessing Computational Resources

- ***Since the system has multiple resources, queues are used to determine access.***
- ***Depending on the systems, there are different queues to control how the resources are used.***

PACE-ICE Queues

<i>Name</i>	<i>Max. Proc.</i>	<i>Walltime</i>	<i>Avail.</i>	<i>Notes</i>
<i>pace-ice</i>		<i>12:00:00</i>	<i>All</i>	
<i>pace-ice-gpu</i>		<i>16:00:00</i>	<i>All</i>	<i>GPU available</i>

COC-ICE Queues

<i>Name</i>	<i>Max. Proc.</i>	<i>Walltime</i>	<i>Avail.</i>	<i>Notes</i>
<i>coc-ice</i>	<i>28</i>	<i>2:00:00</i>	<i>All</i>	
<i>coc-ice-gpu</i>	<i>28</i>	<i>2:00:00</i>	<i>All</i>	<i>GPUs</i>
<i>coc-ice-multi</i>	<i>128</i>	<i>00:30:00</i>	<i>All</i>	<i>MPI</i>
<i>coc-ice-long</i>	<i>28</i>	<i>08:00:00</i>	<i>All</i>	
<i>coc-ice-devel</i>	<i>128</i>	<i>08:00:00</i>	<i>All</i>	
<i>coc-ice-grade</i>	<i>128</i>	<i>12:00:00</i>	<i>Fac,TA</i>	

Methods for accessing Computational Resources

- ***Scheduler directives***
- ***pace-vnc-job wrapper***
- ***pace-jupyter-notebook wrapper***
- ***batch jobs***

Scheduler directives

<i>Directive</i>	<i>Meaning</i>	<i>Example</i>
<code>-q <name></code>	<i>Use queue named</i>	<code>-q pace-ice</code>
<code>-l nodes=<nodes>:ppn=<ppn></code>	<i>Number of processors and processors per node</i>	<code>-l nodes=2:ppn=4</code>
<code>-l walltime=HH:DD:SS</code>	<i>Requested walltime</i>	<code>-l walltime=12:00:00</code>
<code>-l nodes=1:ppn=1:gpus=<ngpus></code>	<i>Request ngpus GPU</i>	<code>-l nodes=1:ppn=1:gpus=1</code>
<code>-N</code>	<i>job name</i>	<code>-N myjob</code>
<code>-o</code>	<i>output</i>	<code>-o myjob.out</code>
<code>-j oe</code>	<i>join the output and error</i>	<code>-j oe</code>

Interactive CLI Sessions

An interactive session on the command line can be created using

```
$ qsub -l nodes=1:ppn=4 -l walltime=04:00:00 \  
-q pace-ice -I
```

This will create a BASH session on one or more compute nodes.

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Note

The user must wait for the job to start in real-time.

A graphical session on a compute node can be created using the command

```
$ pace-vnc-job
```

This does require that the `vncpasswd` have been run before. Full details are found at [http:](http://docs.pace.gatech.edu/interactiveJobs/setupVNC_Session/)

[// docs.pace.gatech.edu/interactiveJobs/setupVNC_Session/](http://docs.pace.gatech.edu/interactiveJobs/setupVNC_Session/)

Jupyter Notebooks

- ***Jupyter notebooks provide a useful interface for interactive computing in various programming languages, especially Python.***
- ***There is a wrapper that handles submitting and creating a tunnel to allow users to use Jupyter notebook web interface on their local computer.***
- ***Full instructions are found at***
<http://docs.pace.gatech.edu/interactiveJobs/jupyterInt/>

Batch Script

- ***For longer jobs, the time it takes the system to find resources***
- ***This is the most traditional way to perform calculations on HPC cluster.***

```
#!/bin/bash
#PBS -N myjob
#PBS -l nodes=2:ppn=4
#PBS -l walltime=04:00:00
#PBS -q pace-ice

module load gcc mvapich2
cd $PBS_OW_WORKDIR
mpirun ./a.out
#End of script.
```


Full documentation

Fuller documentation of how to use ICE and similar clusters is found at <https://docs.pace.gatech.edu>