Introduction to GACRC Sapelo2 Cluster

CSP Lunch Seminar

Georgia Advanced Computing Resource Center (GACRC)

EITS/University of Georgia

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Outline

• What is Sapelo2 Cluster
• Work on Sapelo2 Cluster
• Request Sapelo2 User Account
• GACRC Wiki and Support
• Appendix
What is Sapelo2 Cluster

1. Cluster Overview

2. Storage Environment

3. Computing Resources

4. Software Environment
INTRODUCTION TO GACRC SAPelo2 CLUSTER

Please note:
You need to connect to the UGA VPN when accessing from outside of the UGA main campus.

1. ssh with MyID and password
2. Verify with Archpass Duo two-factor authentication

Node: Computer for a specific function on cluster, e.g., login node
Queue: Collection of compute nodes for specific computing need
Cluster: Nodes + Drives, all connected by network
Cluster Overview

1. Sapelo2 cluster is a Linux (64-bit Centos 7) high performance computing (HPC) cluster

2. You can log on to 2 nodes: Login node (sapelo2.gacrc.uga.edu) and Transfer node (xfer.gacrc.uga.edu)

3. From Login node, you can open Interactive node using qlogin command

4. You have 4 directories: Home, Global Scratch, Storage and Local Scratch

5. You can submit jobs to 4 computational queues: batch, highmem_q, gpu_q, grpBuyin_q

6. You can use more than 600 modules installed on cluster (as of 08/17/2018)
## Storage Environment – 4 Directories

<table>
<thead>
<tr>
<th>4 Directories</th>
<th>Role</th>
<th>Quota</th>
<th>Accessible from</th>
<th>Intended Use</th>
<th>Backed-up</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>/home/MyID</td>
<td>Home</td>
<td>100GB</td>
<td>Login</td>
<td>Static data: 1. Scripts, source codes 2. Local software</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>/lustre1/MyID</td>
<td>Global Scratch</td>
<td>No Limit</td>
<td>Transfer Interactive</td>
<td>Current job data: data being read/written by running jobs</td>
<td>No</td>
<td><strong>User to clean up!</strong> <em>Subject to deletion in 30 days</em></td>
</tr>
<tr>
<td>/project/abclab</td>
<td>Storage</td>
<td>1TB (initial)</td>
<td>Transfer</td>
<td>Temporary data parking: non-current active data</td>
<td>Yes</td>
<td>Group sharing possible</td>
</tr>
<tr>
<td>/scratch</td>
<td>Local Scratch</td>
<td>~200GB</td>
<td>Compute</td>
<td>Jobs with heavy disk I/O</td>
<td>No</td>
<td>1. <strong>User to clean up</strong> when job exits from the node! 2. <strong>Persistent data</strong></td>
</tr>
</tbody>
</table>
Storage Environment (Cont.) – Accessing Directories from Nodes

INTRODUCTION TO GACRC SAPELO2 CLUSTER

Login

Interactive

/home/MyID
/lustre1/MyID

Transfer

/project/abclab

Duo Authentication

User

log on using ssh

qlogin

exit

Duo Authentication

non-GACRC storage

log on using ssh

log on using ssh
## Computing Resources – 4 Computational Queues

<table>
<thead>
<tr>
<th>Queue</th>
<th>Node Feature</th>
<th>Total Nodes</th>
<th>RAM(GB)/Node</th>
<th>Max RAM(GB)/Single-node Job</th>
<th>Cores/Node</th>
<th>Processor Type</th>
<th>GPU Cards/Node</th>
<th>InfiniBand</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>batch</strong></td>
<td>Intel</td>
<td>30</td>
<td>64</td>
<td>62</td>
<td>28</td>
<td>Intel Xeon</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>42</td>
<td>192</td>
<td>188</td>
<td>32</td>
<td>Intel Xeon (Skylake)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>AMD</td>
<td>90</td>
<td>128</td>
<td>125</td>
<td>48</td>
<td>AMD Opteron</td>
<td>N/A</td>
<td>Yes</td>
</tr>
<tr>
<td>highmem_q</td>
<td>Intel/AMD</td>
<td>4/1</td>
<td>1024</td>
<td>997</td>
<td>28</td>
<td>Intel Xeon</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>AMD/Intel</td>
<td>4/1</td>
<td>512</td>
<td>503</td>
<td>48</td>
<td>AMD Opteron</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>gpu_q</strong></td>
<td>GPU</td>
<td>2</td>
<td>128</td>
<td>125</td>
<td>16</td>
<td>Intel Xeon</td>
<td>8 NVIDIA K40</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>2</td>
<td>96/80</td>
<td>92/76</td>
<td>12</td>
<td>Intel Xeon</td>
<td>7 NVIDIA K20</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4</td>
<td>192</td>
<td>188</td>
<td>32</td>
<td>Intel Xeon (Skylake)</td>
<td>1 NVIDIA P100</td>
<td></td>
</tr>
<tr>
<td>grpBuyin_q</td>
<td>variable</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

8/21/18

INTRODUCTION TO GACRC SAPELO2 CLUSTER
Software Environment

1. Software names are long and have a EasyBuild toolchain name associated to it

2. Complete module name: Name/Version-toolchain, e.g., Python/2.7.14-foss-2016b

3. Software names are case-sensitive!

   - `module avail`: List all available software modules installed on cluster
   - `module load moduleName`: Load a module into your working environment
   - `module list`: List modules currently loaded
   - `module unload moduleName`: Remove a module from working environment
   - `ml spider pattern`: Search module names matching a pattern (case-insensitive)
Work on Sapelo2 Cluster

1. Job Submission Workflow
2. How to Know Job Details
3. How to Know Node Details
4. qlogin Commands: Open Interactive Node for Running Interactive Tasks
5. Code Compilation
1. Log on to Login node using MyID and password, and two-factor authentication with Archpass Duo:

   \texttt{ssh MyID@sapelo2.gacrc.uga.edu}

2. On Login node, change directory to \texttt{global scratch} : \texttt{cd /lustre1/MyID}

3. Create a working subdirectory for a job : \texttt{mkdir ./workDir}

4. Change directory to \texttt{workDir} : \texttt{cd ./workDir}

5. Transfer data from local computer to \texttt{workDir} : use \texttt{scp} or \texttt{SSH File Transfer} to connect Transfer node

   Transfer data on cluster to \texttt{workDir} : log on to Transfer node and then use \texttt{cp} or \texttt{mv}

6. Make a job submission script in \texttt{workDir} : \texttt{nano ./sub.sh}

7. Submit a job from \texttt{workDir} : \texttt{qsub ./sub.sh}

8. Check job status : \texttt{qstat_me} or Cancel a job : \texttt{qdel JobID}
How to Know Job Details

Option 1: `qstat -f JobID` for running jobs or finished jobs in 24 hours

Option 2: Email notification from finished jobs (completed, canceled, or crashed), if using:

```
#PBS -M MyID@uga.edu
#PBS -m ae
```
Option 1: qstat -f JobID (running jobs or finished jobs in 24 hour)

$ qstat -f 12222
Job Id: 12222.sapelo2
  Job_Name = testBlast
  Job_Owner = zhuofei@10.56.200.51
  resources_used.cput = 00:00:00
  resources_used.vmem = 316864kb
  resources_used.walltime = 00:15:01
  resources_used.mem = 26780kb
  resources_used.energy_used = 0
  job_state = C
  queue = batch
  Error_Path = sapelo2-sub2.ecompute:/lustre1/zhuofei/examples/testBlast.e12222
  exec_host = n236/0-3
  Output_Path = sapelo2-sub2.ecompute:/lustre1/zhuofei/examples/testBlast.o12222
  Resource_List.nodes = 1:ppn=4:Intel
  Resource_List.mem = 20gb
  Resource_List.walltime = 02:00:00
  Resource_List.nodect = 1
  Variable_List = PBS_O_QUEUE=batch,PBS_O_HOME=/home/zhuofei,......
  PBS_O_WORKDIR=/lustre1/zhuofei/workDir,
Option 2: Email notification from finished jobs

BS Job Id: 12332.sapelo2   Job Name: bowtie2_test
Queue: batch
Exechost: n232/0
Message: Execution terminated
Details:
Exit_status=0
resources_used.cput=00:09:26
resources_used.vmem=755024kb
resources_used.walltime=00:09:51
resources_used.mem=1468676kb
resources_used.energy_used=0
Short reason: Execution terminated

PBS Job Id: 12331.sapelo2   Job Name: bowtie2_test
Queue: batch
Exechost: n235/0
Message: Execution terminated
Details:
Exit_status=271
resources_used.cput=00:02:58
resources_used.vmem=755024kb
resources_used.walltime=00:03:24
resources_used.mem=420712kb
resources_used.energy_used=0
Short reason: Execution terminated

Sender: dispatch_root
How to Know Node Details

Option 1: mdiag -v -n | grep [pattern] | ...
mdiag -v -n | grep batch | grep AMD
mdiag -v -n | grep batch | grep Intel
mdiag -v -n | grep highmem_q
mdiag -v -n | grep grpBuyin_q

Option 2: from login node, you can ssh to a compute node and run a command there!
ssh n72 lsmpu`
ssh n222 free -g`
ssh n237 "ps aux | grep '^MyID""
qlogin Commands
https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo2 - How to open an interactive session

1. Type qlogin commands from Login node to open Interactive node:
   - `qlogin_intel`: Start an interactive session on an Intel node
   - `qlogin_amd`: Start an interactive session on an AMD node
   - `qlogin`: start an interactive job on either type of nodes

2. Type `exit` command to quit and back to Login node
Purpose 1: Open interactive node for running interactive tasks of R, Python, Bash scripts, etc.

- qlogin
- qsub: waiting for job 12426.sapelo2 to start
- qsub: job 12426.sapelo2 ready

zhuofei@n204 ~$ module spider R
R: R/3.4.1-foss-2016b-X11-20160819-GACRC
... zhuofei@n204 ~$ ml R/3.4.1-foss-2016b-X11-20160819-GACRC
zhuofei@n204 ~$ R
R version 3.4.1 (2017-06-30) -- "Single Candle"
...
[Previously saved workspace restored]
> a<-1 ; b<-7
> a+b
[1] 8
>
qlogin Commands

Purpose2: Open interactive node for compiling/testing source codes of Fortran, C/C++, Python, etc.

zhuofei@sapelo2-sub1 ~$ qlogin_intel
qsub: waiting for job 20912.sapelo2 to start
qsub: job 20912.sapelo2 ready

zhuofei@n206 ~$ module spider iomkl
--------------------------------------------
iomkl:
--------------------------------------------
Description:
Intel Cluster Toolchain Compiler Edition provides Intel C/C++ and Fortran compilers, Intel MKL & OpenMPI.

Versions:
iomkl/2018a
...
zhuofei@n206 ~$ module load iomkl/2018a
zhuofei@n206 ~$ icc mysource.c -o myexec.x
zhuofei@n206 ~$
**Code Compilation**

[https://wiki.gacrc.uga.edu/wiki/Code_Compilation_on_Sapelo2](https://wiki.gacrc.uga.edu/wiki/Code_Compilation_on_Sapelo2)

- Use `module load` command to load, e.g.:

<table>
<thead>
<tr>
<th>Software Package</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>GCC/7.2.0-2.29</td>
<td>GNU 7.2.0-2.29 compiler suite</td>
</tr>
<tr>
<td>PGI/17.9-GCC-6.3.0-2.28</td>
<td>PGI 17.9 compiler suite</td>
</tr>
<tr>
<td>iccifort/2018.1.163-GCC-6.4.0-2.28</td>
<td>Intel 18.0.1.163 compiler suite</td>
</tr>
<tr>
<td>foss/2016b</td>
<td>GCC 5.4.0, OpenMPI 1.10.3, OpenBLAS 0.2.18, FFTW 3.3.4, ScaLAPACK 2.0.2</td>
</tr>
<tr>
<td>foss/2018a</td>
<td>GCC 6.4.0, OpenMPI 2.1.2, OpenBLAS 0.2.20, FFTW 3.3.7, ScaLAPACK 2.0.2</td>
</tr>
<tr>
<td>gmvolf/2016b</td>
<td>GCC 5.4.0, MVAPICH2 2.2, OpenBLAS 0.2.18, FFTW 3.3.4, ScaLAPACK 2.0.2</td>
</tr>
<tr>
<td>iomkl/2018a</td>
<td>Intel 2018.1.163 compiler suite, OpenMPI 2.1.2, MKL 2018.1.163</td>
</tr>
<tr>
<td>imvmkl/2018a</td>
<td>Intel 2018.1.163 compiler suite, MVAPICH2 2.2, MKL 2018.1.163</td>
</tr>
</tbody>
</table>
Request Sapelo2 User Account

Sapelo2 cluster user account: MyID@sapelo2.gacrc.uga.edu

Note: A valid official UGA MyID is a MUST to create a user account!

1. The UGA PI uses the GACRC online form http://help.gacrc.uga.edu/userAcct.php to request a user account for a group member.

2. Once we received the request, we will verify it with the PI.

3. After verification by the PI, the new user will be required to attend a training session.

4. After the user attended training, we will provision a Sapelo account for the user.

5. A welcome letter is sent to the user once user account is ready.
GACRC Wiki and Support

Main Page: http://wiki.gacrc.uga.edu

Running Jobs: https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo2

Software: https://wiki.gacrc.uga.edu/wiki/Software

Transfer File: https://wiki.gacrc.uga.edu/wiki/Transferring_Files

Linux Command: https://wiki.gacrc.uga.edu/wiki/Command_List

Training: https://wiki.gacrc.uga.edu/wiki/Training

User Account Request: https://wiki.gacrc.uga.edu/wiki/User_Accounts

Support: https://wiki.gacrc.uga.edu/wiki/Getting_Help