GPU HPC Cluster

The University of Texas
Rio Grande Valley

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Backup storage node Login node

GPU node with 8x A100-80GB PCle 4.0 and 12x NVLink

2x Intel Xeon Gold 6330 (28 cores, 2.0GHz)

256GB DDR4 memory

2x 960GB SSD

OS mirrored with linux mdadm

12x 12TB SAS HDD

RAID-6 with cache protection

120TB usable (/home)

2x 10GbE SFP+

Campus network

Bonded for redundancy

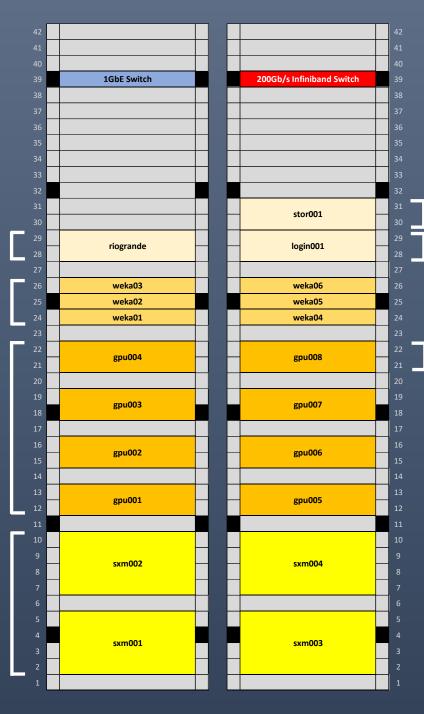
200Gb/s Infiniband

Head node

WekaFS file servers

GPU nodes with 8x A100-80GB PCIe 4.0

GPU nodes with 8x A100-80GB SXM4 (600GB/s NVSwitch)



Same as head node

Backup storage node

Login node

Same as head node minus storage

GPU node with 8x A100-80GB PCIe 4.0 and 12x NVLink

Head node

WekaFS file servers

GPU nodes with 8x A100-80GB PCIe 4.0

2x Intel Xeon Gold 6330 (28 cores, 2.0GHz)

2x Intel Xeon Gold 6330 (28 cores, 2.0GHz)

1TB DDR4 memory

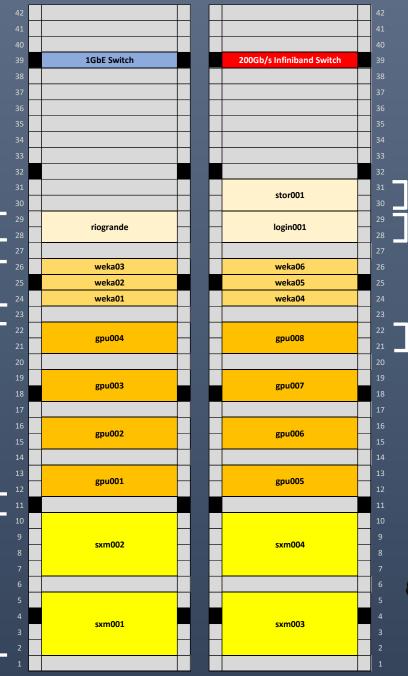
1TB DDR4 memory

3.84TB NVMe SSD 200Gb/s Infiniband

3.84TB NVMe SSD

200Gb/s Infiniband

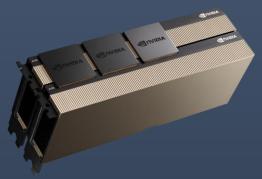
GPU nodes with 8x A100-80GB SXM4 (600GB/s NVSwitch)



Backup storage node Login node

GPU node with 8x A100-80GB PCIe 4.0 and 12x NVLink

NVLink bridges connect pairs of GPUs



Parallel file system

/weka/scratch

92TB usable

4M Read IOPS

630K Write IOPS

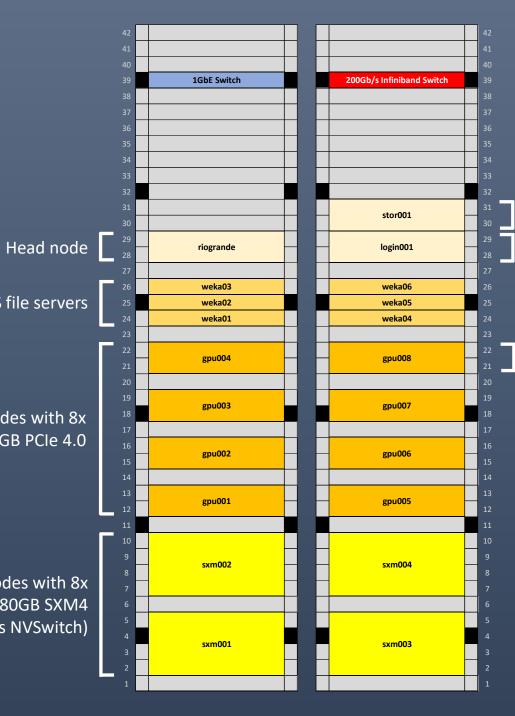
67GB/s Read BW

33GB/s Write BW

WekaFS file servers

GPU nodes with 8x A100-80GB PCIe 4.0

GPU nodes with 8x A100-80GB SXM4 (600GB/s NVSwitch)

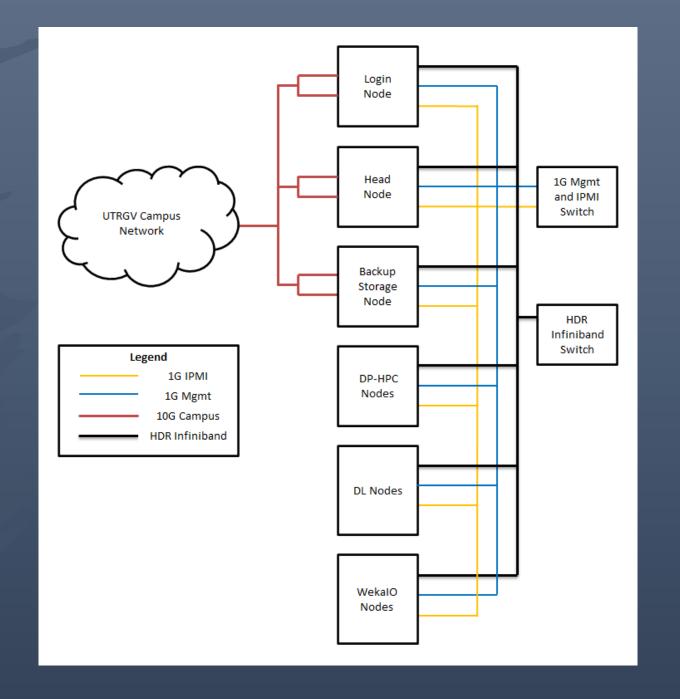


Backup storage node Login node

GPU node with 8x A100-80GB PCIe 4.0 and 12x NVLink

Networks

- In-band management
 - 1GbE
 - Linux CLI, ssh, SLURM, ...
- Out-of-band management (IPMI)
 - 1GbE
 - Remote power on/off, system event log, ...
- HPC communication fabric
 - 200Gb/s Infiniband
 - MPI and data transfer



Cluster Software

Rocky Linux 8.6

Atipa Phoenix Cluster Management 2.2

Mellanox OFED 5.6

Environment Modules 4.5.2

SLURM 21.08.8

gcc-toolset-11 (gcc 11.2.1)

OpenMPI 4.1.3

Intel OneAPI 2022.1.2

ganglia 3.7.2

CUDA 11.6

cuDNN 8

pytorch 1.10.2

tensorflow 2.6.2

caffe2

Data Storage: /home

Head Node (riogrande)

- 12x 12TB SAS HDD
- RAID-6 (10+2)
- 120TB usable
 - /home
 - NFS export to all nodes
 - Synced to stor001 every night

Backup Storage Node (stor001)

- 12x 12TB SAS HDD
- RAID-6 (10+2)
- 120TB usable
 - /backup
 - /etc/cron.daily/backupUserDirs

```
[root@stor001 ~]# ls -l /backup/
total 0
drwxr-xr-x 3 root root 19 Jun 15 2020 home
[root@stor001 ~]# ls -l /backup/home/
total 4
drwx----- 31 atipa atipa 4096 Jul 25 09:56 atipa
```

Power On Sequence

1. Switches

Come on as soon as power is plugged in

2. Head node (riogrande)

Power button

3. WekaFS nodes (weka01...06)

```
# ipmipower –u ADMIN2 –p UTRGV@6002900 –h weka0[1-6]-ipmi --on (note the double "-" before "on")
```

- 4. Start Weka file system (Tuesday afternoon training session)
- 5. Login and backup storage nodes (login001, stor001)

```
# ipmipower –u ADMIN2 –p UTRGV@6002900 –h login001-ipmi --on
# ipmipower –u ADMIN2 –p UTRGV@6002900 –h stor001-ipmi --on
```

6. GPU nodes (gpu001...008, sxm001...004)

```
# ipmipower –u ADMIN2 –p UTRGV@6002900 –h gpu00[1-8]-ipmi --on
# ipmipower –u ADMIN2 –p UTRGV@6002900 –h sxm00[1-4]-ipmi --on
```

Since the head node is powered on before the Weka nodes, WekaFS needs to be mounted manually on riogrande after the file system is started:

mount /weka/scratch

Last login: Wed Jul 27 07:42:29 2022 from 172.20.168.15

	os	DRIVE STATU	S	
Raid Array	Active	Working	Failed	State
/dev/md0	2	2	0	clean
/dev/md2	2	2	0	active
/dev/md4	2	2	0	clean
/dev/md6	2	2	0	clean

		Size	
239	RAID6	109.135 TB	Optimal

HARD DISK STATUS

Drive	Size		State
0	10.913	TB	Online
1	10.913	TB	Online
2	10.913	TB	Online
3	10.913	TB	Online
4	10.913	TB	Online
5	10.913	TB	Online
6	10.913	TB	Online
7	10.913	TB	Online
8	10.913	TB	Online
9	10.913	TB	Online
10	10.913	TB	Online
11	10.913	TB	Online

HOME DIRECTORY USAC

SIZE	USED	AVAILABLE
110T	803G	109T

Logging into the Head Node

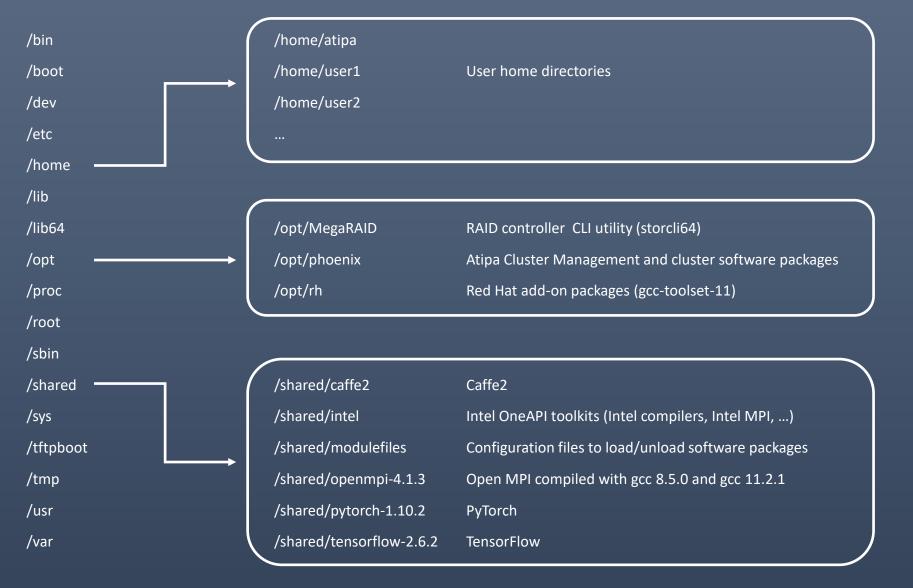
ssh root@riogrande

Storage summary:

- checkSoftwareRAID (linux mdadm RAID-1)
- checkRAID (RAID controller RAID-6)

Note: regular users should log into login001 to compile codes and launch jobs

Directory Structure



WARNING: /opt/phoenix/sbin contains scripts used to initialize the cluster nodes. Running these scripts from the Linux command line can break the cluster.

/shared is exported via NFS to all nodes

Use /shared to install 3rd party software that needs to be available on all nodes

Software packages with a "configure" script often have a "--prefix" option to specify the installation directory

Checking Hardware Health: clusterQC

```
[root@riogrande ~] # clusterQC
         Property
                            | Actual Value
                                              | Expected Value
                                                                  Result
Class
bios
          date
                             10/28/2021
                                                10/28/2021
                                                                  >>> Good
bios
          revision
                             F09
                                                F09
                                                                  >>> Good
                             1040852
                                                1040852
                                                                  >>> Good
part
          boot
                             818667972
                                                818667972
part
          root
                                                                  >>> Good
                             67009572
                                                67009572
                                                                  >>> Good
part
          var
                             33504276
                                                33504276
                                                                  >>> Good
part
          tmp
                             117181521920
          home
                                               117181521920
                                                                  >>> Good
part
cpu
                             56
                                               56
                                                                  >>> Good
          cores
                             Intel(R) Xeon(R) Gold 6330 CPU @ 2.00GHz| Intel(R) Xeon(R) Gold 6330 CPU @ 2.00GHz| >>> Good
          version
cpu
                             263724788
                                                263724788
          memtotal
                                                                  >>> Good
mem
          swaptotal
                                                33554424
mem
                             33554424
                                                                  >>> Good
          number
hdd
                                                                  >>> Good
nfs
                             [/opt/phoenix-2.2.0, /shared, /home] | [/opt/phoenix-2.2.0, /shared, /home] | >>> Good
          exports
ib
                                                                  >>> Good
          firmware version |
                             20.33.1048
                                                20.33.1048
ib
                             200
                                                200
                                                                  >>> Good
          rate
ib
                             Active
                                                Active
          state
                                                                  >>> Good
ib
          physical state
                             LinkUp
                                               LinkUp
                                                                  >>> Good
ipmi
          firmware
                             13.03
                                               13.03
                                                                  >>> Good
          CPU0
                                                                  >>> Good
                             OK
                                                OK
sensors
          CPU1
                             OK
                                                OK
                                                                  >>> Good
sensors
          INLET
                             OK
                                                OK
                                                                  >>> Good
sensors
         FAN1A
                             OK
                                                OK
                                                                  >>> Good
sensors
sensors
         FAN2A
                             OK
                                                OK
                                                                  >>> Good
          FAN3A
                             OK
                                                OK
                                                                  >>> Good
sensors
                                               OK
sensors | FAN4A
                             OK
                                                                  >>> Good
                             4.18.0-372.9.1.el8.x86 64| 4.18.0-372.9.1.el8.x86 64| >>> Good
kernel
          version
Done!
[root@riogrande ~] # clusterQC | grep -i bad
[root@riogrande ~]#
```

Creating User Accounts: cuseradd

cuseradd <username>

Create a new Linux user account on the head node, generate ssh keys, and propagate the user account info to all other nodes

```
[root@riogrande ~] # cuseradd bart

The username given is available.
Creating new user: bart

setting password...

New password:
Retype new password:
Changing password for user bart.
passwd: all authentication tokens updated successfully.
generating ssh key...
```

Executing Commands on all Nodes

fornodes

fornodes <command>

Execute <command> in parallel on all nodes in /opt/phoenix/etc/phoenix/phoenix.nodes (default: sxm001...004, gpu001...008)

Example: fornodes uptime

fornodes -s <command>

Execute <command> sequentially on all nodes in /opt/phoenix/etc/phoenix/phoenix.nodes

Example: fornodes –s uptime

fornodes -b <basename> -i <range> <command>

Execute <command> on range of nodes with base name

Example: fornodes –b gpu –i 1-4 uptime

fornodes –b sxm –i 1-4 "clusterQC | grep –i bad"

Copying a File to all Nodes

acp

Copy <file> in parallel to all nodes in /opt/phoenix/etc/phoenix/phoenix.nodes (default: sxm001...004, gpu001...008)

Example: acp /tmp/test.txt /tmp/

Copy <file1>, <file2>, ... in parallel to all nodes in /opt/phoenix/etc/phoenix/phoenix.nodes (default: sxm001...004, gpu001...008)

Example: acp "/tmp/test.txt /tmp/test2.txt" /tmp/

Copy <file> to range of nodes with base name

Example: acp -b gpu -i 1-4 /tmp/test.txt /tmp/

WARNING: Be careful copying configuration files to all nodes, e.g. copying /etc/fstab to all nodes will render nodes unbootable!

Syncing Configuration Files to all Nodes

syncConfig syncPasswds

syncConfig

Copy files in /opt/phoenix/etc/phoenix/syncFiles.xml from head to all nodes in /opt/phoenix/etc/phoenix/phoenix.nodes (default: sxm001...004, gpu001...008)

Example: syncConfig

Should only be necessary if files are added to syncFiles.xml or files in are syncFiles.xml edited

syncPasswds

Copy /etc/passwd, /etc/group, /etc/shadow from head to all nodes in /opt/phoenix/etc/phoenix/phoenix.nodes (default: sxm001...004, gpu001...008)

Example: *syncPasswds*

Should only be necessary if a user account was created without *cuseradd*

Options:

-n: Copy to specific node, e.g. syncConfig –n gpu004

-b, -i: Copy to range of nodes with base name

Checking OS Disk Health in Head, Login, Storage Nodes

2x 960GB SSD mirrored with Linux software RAID cat /proc/mdstat

checkSoftwareRAID

[root@riogrande ~] # checkSoftwareRAID					
	OS DRIVE STATUS				
Raid Array	Active	Working	Failed	State	
/dev/md0	2	2	0	clean	
/dev/md2	2	2	0	clean	
/dev/md4	2	2	0	clean	
/dev/md6	2	2	0	clean	

Checking RAID Disk Health in Head/Storage Nodes

12x 12TB HDD hardware RAID-6 *checkRAID*

[root@ri	ogrande ~]# che	ckRAID			
	RAID STATUS				
		TYPE Size RAID6 109.135 TB			
		HARD DISK STATUS			
		Size State			
	0 1	10.913 TB Onlin 10.913 TB Onlin			
	2	10.913 TB Onlin			
	3	10.913 TB Onlin			
	4	10.913 TB Onlin	е		
	5	10.913 TB Onlin	е		
	6	10.913 TB Onlin			
	7	10.913 TB Onlin			
	8	10.913 TB Onlin			
	9	10.913 TB Onlin			
	10	10.913 TB Onlin			
	11	10.913 TB Onlin	е		
		HOME DIRECTORY USAGE			
		AVAILABLE PERCE	NT USED		
	110T 793G	109T 1%			

/opt/MegaRAID/storcli/storcli64 /c0 show all

Checking the Infiniband Subnet Manager

```
[root@riogrande ~] # systemctl status opensmd
 opensmd.service - LSB: Activates/Deactivates InfiniBand Subnet Manager
  Loaded: loaded (/etc/r.d/init.d/opensmd; generated)
  Active (active (running) since Wed 2022-07-27 11:52:27 CDT; 1 day 7h ago
    Docs: man-systemd-sysv-generator(8)
  Process: 3154 ExecStart=/etc/rc.d/init.d/opensmd start (code=exited, status=0/SUCCESS)
 Main PID: 3216 (opensm)
   Tasks: 184 (limit: 1648042)
  Memory: 76.3M
  CGroup: /system.slice/opensmd.service
           |-3216 /usr/sbin/opensm --daemon
           `-3219 osm crashd
Jul 27 11:52:26 riogrande systemd[1]: Starting LSB: Activates/Deactivates InfiniBand Subnet Manager...
Jul 27 11:52:26 riogrande OpenSM[3216]: /var/log/opensm.log log file opened
Jul 27 11:52:26 riogrande OpenSM[3216]: OpenSM 5.11.0.MLNX20220418.fd3d650
Jul 27 11:52:26 riogrande OpenSM[3216]: Entering DISCOVERING state
Jul 27 11:52:26 riogrande OpenSM[3216]: SM port is down
Jul 27 11:52:27 riogrande opensmd[3154]: Starting IB Subnet Manager.[ OK ]
Jul 27 11:52:27 riogrande systemd[1]: Started LSB: Activates/Deactivates InfiniBand Subnet Manager.
Jul 27 11:52:36 riogrande OpenSM[3216]: SM port is up
Jul 27 11:52:36 riogrande OpenSM[3216]: Entering MASTER state
[root@riogrange ] # sminfo
```

sminfo: sm lid 1 m quid 0xe8ebd3030008483e, activity count 37974 priority 14 state 3 SMINFO MASTER

The Infiniband fabric needs at least one instance of opensmd (subnet manager) to be running on the cluster

Master SM: riogrande

Standby SM: stor001

systemctl status opensmd

sminfo

Checking Infiniband Host Card Status

ibstat

Check port rate on all GPU nodes:

fornodes "ibstat | grep Rate"

Checking the Infiniband Fabric

ibdiagnet

Sweep the fabric and collect information from all Infiniband devices (switches and host cards)

Example: *ibdiagnet*

ibdiagnet --get_cable_info

iblinkinfo

Report info on all links in the fabric

Example: iblinkinfo

NVIDIA System Management Interface

nvidia-smi nvidia-smi –q nvidia-smi –q –i 0 (GPU 0)

[root@gpu001 ~]# nvidia-smi Thu Jul 28 19:50:32 2022				
NVIDIA-SMI 510.4	7.03 Driver	Version: 510.47.03	CUDA Version: 11.6	
GPU Name Fan Temp Perf 			Volatile Uncorr. ECC GPU-Util Compute M. MIG M.	
	80G On 43W / 300W	00000000:1B:00.0 Off 0MiB / 81920MiB		
	80G On 42W / 300W	000000000:1C:00.0 Off 0MiB / 81920MiB		
2 NVIDIA A100 N/A 36C P0 	80G On 44W / 300W	00000000:4F:00.0 Off 0MiB / 81920MiB		
3 NVIDIA A100 N/A 36C P0	80G On 43W / 300W	00000000:50:00.0 Off 0MiB / 81920MiB		
4 NVIDIA A100 N/A 36C P0	80G On 42W / 300W	00000000:9C:00.0 Off 0MiB / 81920MiB		
5 NVIDIA A100 N/A 36C P0	80G On 45W / 300W	00000000:9D:00.0 Off 0MiB / 81920MiB		
6 NVIDIA A100 N/A 36C P0	80G On 43W / 300W	000000000:CE:00.0 Off 0MiB / 81920MiB		
	80G On 42W / 300W	00000000:CF:00.0 Off 0MiB / 81920MiB		
+				
GPU GI CI ID ID	PID Typ	oe Process name	GPU Memory Usage 	
No running proc	esses found			

Reprovisioning a Node

reinstall

reinstall –f

Force reinstall without prompting for confimation

Example:

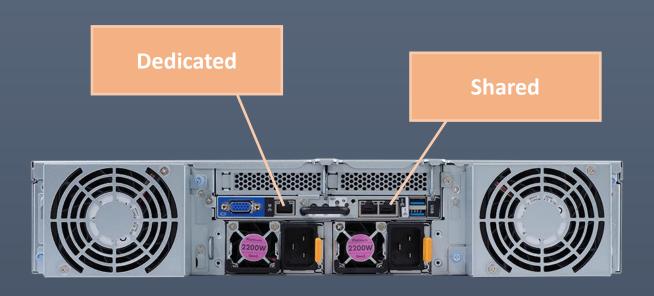
[root@gpu001 ~]# reinstall

Reinstalling the operating system will cause all local data on the node to be lost.

Are you sure you want to continue?

The *reinstall* command wipes out the OS disk, reboots the node, and loads the installation image over the network (PXE Boot)

Intelligent Platform Management Interface (IPMI)



- Standardized hardware management interface
- Dedicated hardware chip on motherboard
 - Baseboard Management Controller (BMC)
 - Always powered on even when system is off
 - Shared or dedicated NIC
- Most commonly use to
 - Remotely power server on/off
 - Remotely check server hardware

Displaying IPMI Sensor Information

parseSensors ipmi-sensors ipmitool sdr

In-Band (run locally on each host)

parseSensors

Display summary of main temperature and fan sensors

```
[root@riogrande ~] # parseSensors
CPU0 Temp 44.00 C 'OK'
CPU1 Temp 45.00 C 'OK'
INLET Temp 27.00 C 'OK'
FAN1A Speed 8700.00 RPM 'OK'
FAN2A Speed 8700.00 RPM 'OK'
FAN3A Speed 8700.00 RPM 'OK'
FAN4A Speed 8700.00 RPM 'OK'
```

ipmi-sensors

ipmitool sdr

Display full IPMI sensor information

Out-of-Band (run from the head node)

ipmitool –U <user> –P <passwd> –H <host> sdr

Example:

ipmitool -U ADMIN2 -P UTRGV@6002900 -H gpu001-ipmi }dr

Displaying IPMI Event Log Information

ipmitool sel clear

In-Band (run locally on each host)

ipmitool sel list

Display the IPMI event log

```
[root@stor001 ~]# ipmitool sel list
    1 | 07/31/2022 | 13:47:17 | Event Logging Disabled #0xel | Log area reset/cleared | Asserted
    2 | 07/31/2022 | 13:47:25 | Power Unit #0xff | Power off/down | Asserted
    3 | 07/31/2022 | 13:48:29 | System Event | OEM System boot event | Asserted
    4 | 07/31/2022 | 13:48:35 | System Event | OEM System boot event | Asserted
    5 | 07/31/2022 | 13:49:59 | OS Boot #0x22 | boot completed - device not specified | Asserted
```

ipmitool sel clear

Clear the IPMI event log

Out-of-Band (run from the head node)

ipmitool –U <user> –P <passwd> –H <host> sel list

Example:

ipmitool -U ADMIN2 -P UTRGV@6002900 -H gpu001-ipmi sel list

Remotely Powering Servers On/Off

ipmipower

Out-of-Band (run from the head node)

```
ipmipower -u < user > -p < passwd > -h < host > --on
Power on the host
```

```
ipmipower –u <user> –p <passwd> –h <host> --off
Power off the host
```

```
[root@riogrande ~]# ipmipower -u ADMIN2 -p UTRGV@6002900 -h gpu001-ipmi -s gpu001-ipmi: off
[root@riogrande ~]# ipmipower -u ADMIN2 -p UTRGV@6002900 -h gpu001-ipmi --on gpu001-ipmi: ok
[root@riogrande ~]# ipmipower -u ADMIN2 -p UTRGV@6002900 -h gpu001-ipmi -s gpu001-ipmi: on
```

Other Useful IPMI Commands

ipmitool bmc reset cold ipmitool

In-Band (run locally on each host)

ipmitool bmc reset cold

Reboot the Baseboard Management Controller (IPMI will be unresponsive for ~2min)

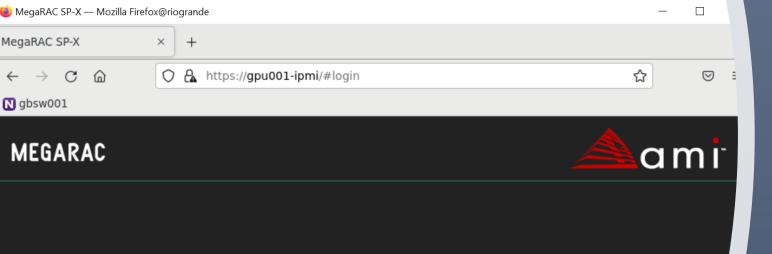
ipmitool lan print

Display BMC network information

```
[root@riogrande ~] # ipmitool lan print
                        : Set Complete
Set in Progress
Auth Type Support
                         : NONE MD2 MD5 PASSWORD OEM
Auth Type Enable
                         : Callback : MD5
                         : User
                                    : MD5
                         : Operator : MD5
                         : Admin
                                    : MD5
                         : Static Address
IP Address Source
IP Address
                         : 192.168.122.1
Subnet Mask
                         : 255.255.255.0
MAC Address
                         : d8:5e:d3:68:25:44
```

Out-of-Band (run from the head node)

ipmitool –U <user> –P <passwd> –H <host> bmc reset cold

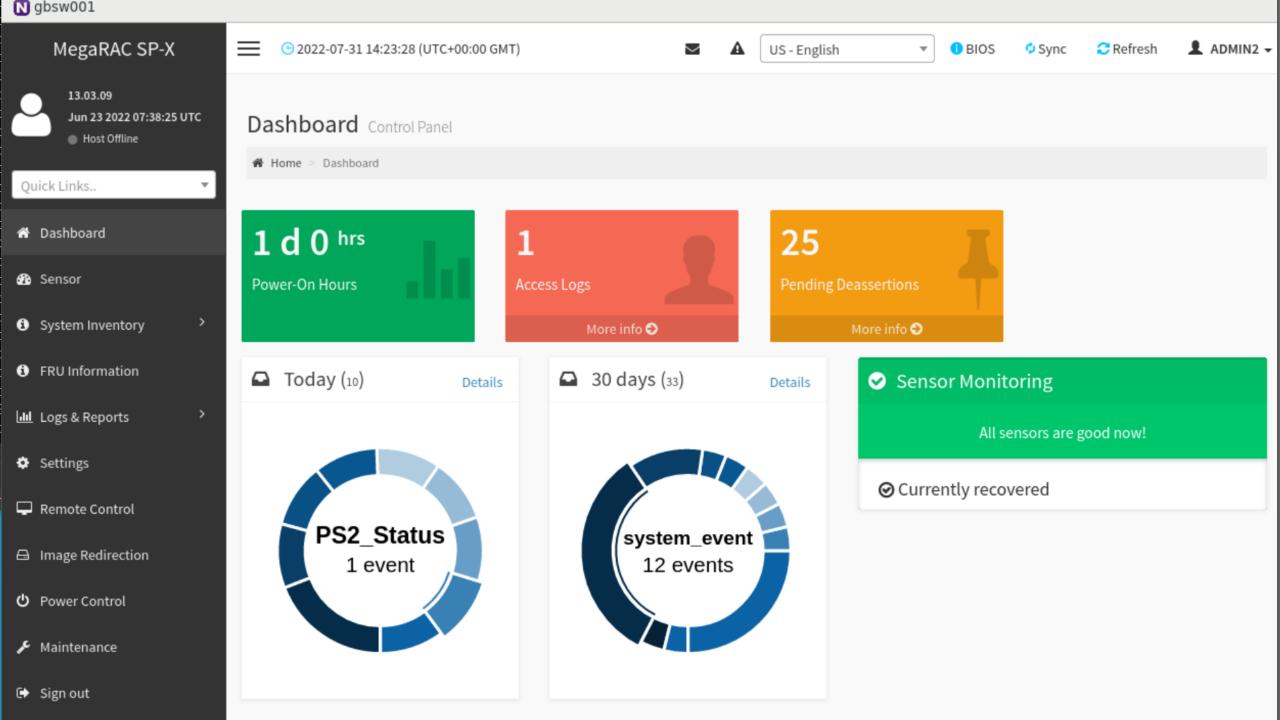


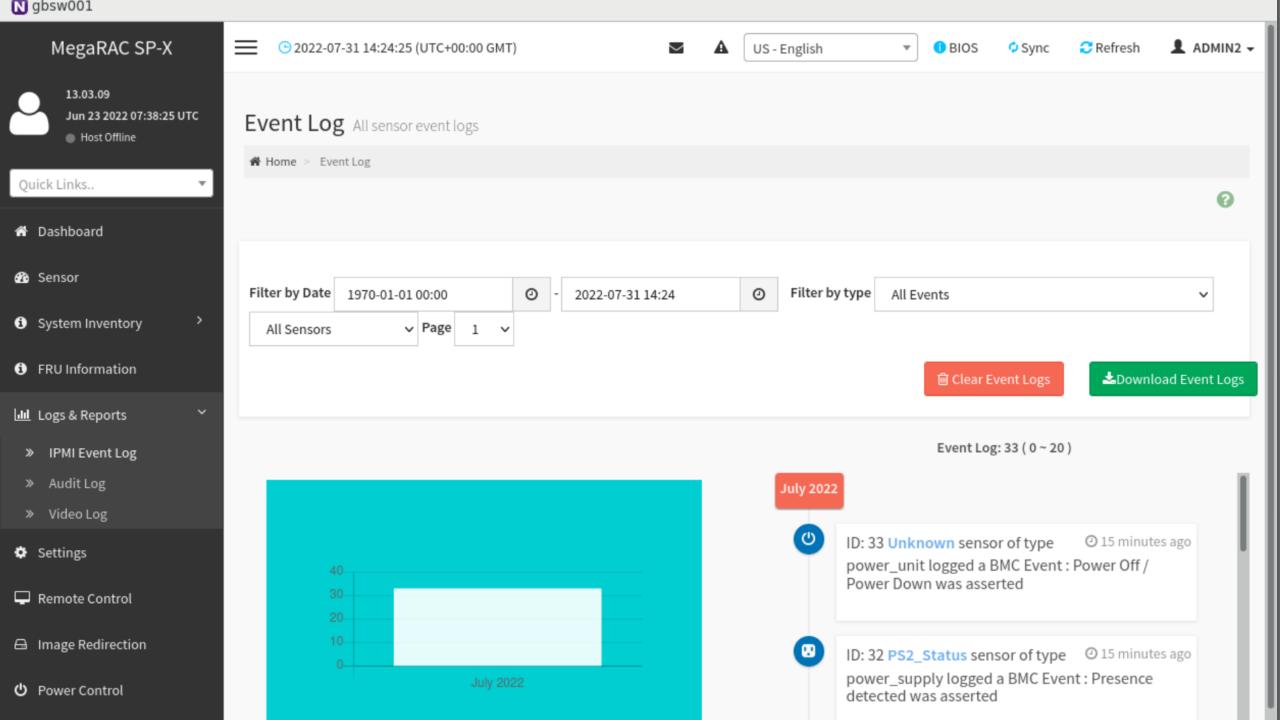
Username Password US - English Remember Username Sign me in I forgot my password

IPMI WebGUI

Launch firefox on the head node:

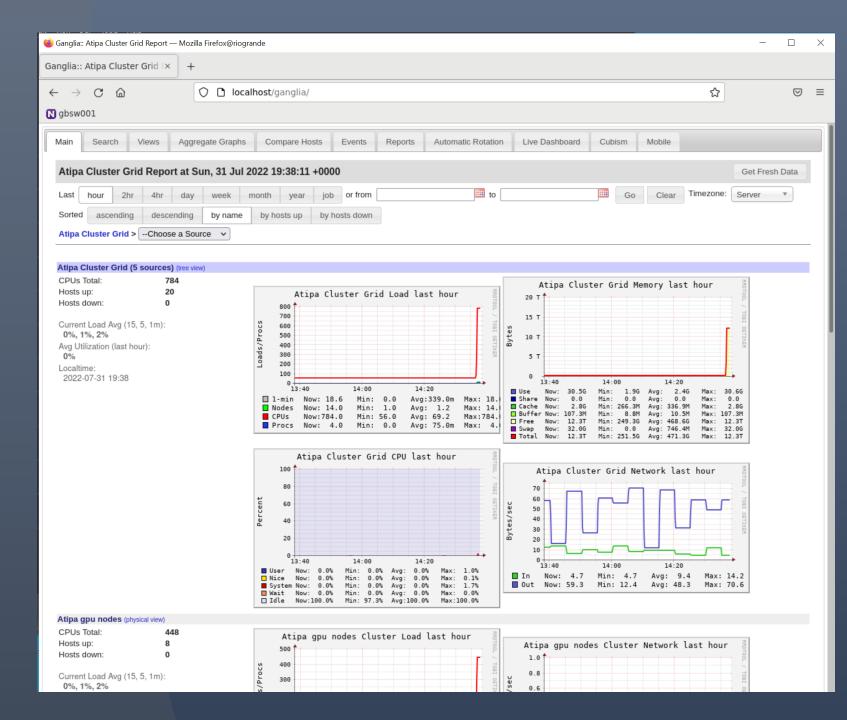
https://<host>-ipmi/





Ganglia: Cluster Health WebGUI

http://localhost/ganglia



Ganglia: Cluster Health WebGUI

http://localhost/ganglia



Installing 3rd Party Software

/shared is accessible by all compute nodes and does not conflict with stock OS packages

Example:

```
[root@riogrande ~]# gcc -v
gcc version 11.2.1
[root@riogrande ~]# cd /opt/phoenix/install/contrib/src
[root@riogrande ~]# wget https://download.open-mpi.org/release/open-mpi/v4.1/openmpi-4.1.3.tar.gz
[root@riogrande src]# tar xvfz openmpi-4.1.3.tar.gz
[root@riogrande src]# cd openmpi-4.1.3
[root@riogrande openmpi-4.1.3]# ./configure --prefix=/shared/openmpi-4.1.3/gcc-11.2.1 --enable-mpirun-prefix-by-default --
enable-static --without-verbs --with-ucx --with-knem=/opt/knem-1.1.4.90mlnx1 --with-cuda CC=gcc CXX=g++ FC=gfortran
[root@riogrande openmpi-4.1.3]# make -j 32 all
[root@riogrande openmpi-4.1.3]# make install
[root@riogrande openmpi-4.1.3]# cp config.log /shared/openmpi-4.1.3/gcc-11.2.1/
```

```
[root@riogrande ~] # module avail
                                         /shared/modulefiles
qcc/11.2.1 openmpi/4.1.3/qcc/8.5.0 openmpi/4.1.3/qcc/11.2.1
                                 -- /shared/intel/oneapi/modulefiles ------
advisor/2022.0.0
                        debugger/2021.5.0
                                                init openc1/2022.0.2
                                                                              mk132/2022.0.2
                                                init opencl/latest
advisor/latest
                        debugger/latest
                                                                              mk132/latest
                        dev-utilities/2021.5.2
cc1/2021.5.1
                                                inspector/2022.0.0
                                                                              mpi/2021.5.1
ccl/latest
                        dev-utilities/latest
                                                inspector/latest
                                                                              mpi/latest
                                                intel ipp ia32/2021.5.2
clck/2021.5.0
                        dnnl-cpu-gomp/latest
                                                                              oclfpga/2022.0.2
                                                intel ipp ia32/latest
                        dnnl-cpu-iomp/latest
                                                                              oclfpga/latest
clck/latest
compiler-rt/2022.0.2
                        dnnl-cpu-tbb/latest
                                                intel ipp intel64/2021.5.2
                                                                              tbb/2021.5.1
                                                intel ipp intel64/latest
compiler-rt/latest
                        dnn1/latest
                                                                              tbb/latest
compiler-rt32/2022.0.2
                                                intel ippcp ia32/2021.5.1
                       dpct/2022.0.0
                                                                              tbb32/2021.5.1
compiler-rt32/latest
                                                intel ippcp ia32/latest
                        dpct/latest
                                                                              tbb32/latest
compiler/2022.0.2
                        dp1/2021.6.0
                                                intel ippcp intel64/2021.5.1
                                                                              vp1/2022.0.0
compiler/latest
                        dpl/latest
                                                intel ippcp intel64/latest
                                                                              vpl/latest
compiler32/2022.0.2
                        icc/2022.0.2
                                                itac/2021.5.0
                                                                              vtune/2022.0.0
compiler32/latest
                                                itac/latest
                        icc/latest
                                                                              vtune/latest
da1/2021.5.3
                        icc32/2022.0.2
                                                mk1/2022.0.2
dal/latest
                        icc32/latest
                                                mkl/latest
```

Environment Modules

- Add/remove locations of binaries (\$PATH) and libraries (\$LD_LIBRARY_PATH) to the user environment by loading/unloading modules
- Module definitions are located in /shared/modulefiles
- Add preferred default modules to \$HOME/.bash_profile

Loading and Unloading Modules

```
[root@riogrande ~] # module list
Currently Loaded Modulefiles:
1) qcc/11.2.1
[root@riogrande ~] # which mpirun
/usr/bin/which: no mpirun in (/opt/rh/qcc-toolset-11/root/usr/bin:/usr/share/Modules/bin:/usr/local/sb
in:/usr/local/bin:/usr/sbin:/usr/bin:/usr/local/cuda/bin:/opt/phoenix-2.2.0/sbin:/opt/phoenix-2.2.0/bi
n:/root/bin)
[root@riogrande ~] # module load openmpi/4.1.3/gcc/11.2.1
[root@riogrande ~]# module list
Currently Loaded Modulefiles:
1) gcc/11.2.1 2) openmpi/4.1.3/gcc/11.2.1
[root@riogrande ~]# which mpirun
/shared/openmpi-4.1.3/gcc-11.2.1/bin/mpirun
[root@riogrande ~]# module purge
[root@riogrande ~] # module list
No Modulefiles Currently Loaded.
```

module list

Display currently loaded modules

module load <module>

Load <module>

module unload <module>

Unload <module>

module purge

Unload all currently loaded modules

Installing RPM Packages

Rocky Linux packages

yum install <package>
Example: yum install ipmitool

• 3rd Party RPM packages

Download to /opt/phoenix/install/contrib/RPMS/

Update repo setupRepos –u –r contrib yum

Clear cache yum clean all

Install yum install <package>

Do not run setupRepos on the Rocky Linux repositories (BaseOS and AppStream)!

 When installing RPMs on the GPU nodes, they should also be added to the node provisioning system (contact us)

Installing Deep Learning Frameworks

Step 1: Install in \$HOME as a non-privileged user

Step 2: If multiple users need the same framework, repeat the installation as root in /shared

Use python "virtual environments"

Each virtual environment has its own Python binary (which matches the version of the binary that was used to create this environment) and can have its own independent set of installed Python packages in its site directories.

https://docs.python.org/3/library/venv.html

Example: Installing TensorFlow

```
[root@riogrande ~]# cd /shared
[root@riogrande shared]# mkdir tensorflow-2.6.2
[root@riogrande shared]# cd tensorflow-2.6.2
[root@riogrande tensorflow-2.6.2]# python3 -m venv tf_env
[root@riogrande tensorflow-2.6.2]# source tf env/bin/activate
(tf_env) [root@riogrande tensorflow-2.6.2]# pip install --upgrade pip
(tf env) [root@riogrande tensorflow-2.6.2]# pip install --upgrade tensorflow-gpu
                                                                                 Install TensorFlow
(tf_env) [root@riogrande tensorflow-2.6.2]# pip show tensorflow-gpu
Name: tensorflow-qpu
Version: 2.6.2
(tf_env) [root@riogrande tensorflow-2.6.2]# python -c 'import tensorflow as tf; print(tf. version )'
2.6.2
(tf env) [root@riogrande tensorflow-2.6.2]# deactivate
[root@riogrande tensorflow-2.6.2]#
```

Create virtual environment tf env Activate virtual environment Update Python Package Manager



SLURM

Open-source, highly scalable resource managemer and job scheduler

https://slurm.schedmd.com/tutorials.html

https://lists.schedmd.com/cgibin/mailman/listinfo/slurm-users

SLURM Services

slurmctld

Runs on head node (riogrande)

Controller accepts jobs from users and allocates resources to jobs

systemctl status slurmctld.service

slurmd

Runs on compute nodes and login node Monitors tasks, accepts work from slurmctld, starts/stops tasks

systemctl status slurmd.service

Log files: /var/log/slurm

SLURM Configuration File

/etc/slurm/slurm.conf

Needs to be the same on ALL nodes
Restart service to activate any changes

systemctl restart slurmctld.service systemctl restart slurmd.service OR fornodes "systemctl restart slurmd, service" login001 is only used to submit jobs

for WekaFS

2 cores reserved

cat /etc/slurm/slurm.conf

...

NodeName=gpu00[1-8] CPUs=56 RealMemory=1024000 Sockets=4 CoresPerSocket=14 ThreadsPerCore=1 Gres=gpu:8 State=UNKNOWN CpuSpecList=0,1 NodeName=sxm00[1-4] CPUs=56 RealMemory=1024000 Sockets=4 CoresPerSocket=14 ThreadsPerCore=1 Gres=gpu:8 State=UNKNOWN CpuSpecList=0,1 NodeName=login001 CPUs=56 RealMemory=257000 Sockets=4 CoresPerSocket=14 ThreadsPerCore=1 CpuSpecList=0,1

PartitionName=gpuq Nodes=gpu00[1-8] Default=YES MaxTime=INFINITE State=UP PartitionName=gpunvq Nodes=gpu008 Default=NO MaxTime=INFINITE State=UP PartitionName=sxmq Nodes=sxm00[1-4] Default=NO MaxTime=INFINITE State=UP

3 job queues

SLURM Administrator Commands I

sinfo

View partition and node information

```
[root@riogrande ~] # sinfo
PARTITION AVAIL TIMELIMIT NODES STATE NODELIST
gpuq* up infinite 8 idle gpu[001-008]
gpunvq up infinite 1 idle gpu008
sxmq up infinite 4 idle sxm[001-004]
```

scontrol update nodename=<nodename> state=draining reason="..."

Change node state to draining

```
[root@riogrande ~] # scontrol update nodename=gpu00[2-3] state=drain reason="Memory error"
[root@riogrande ~] # sinfo
PARTITION AVAIL TIMELIMIT NODES STATE NODELIST
            up infinite
                                  drain gpu[002-003]
gpuq*
            up infinite
                                   idle gpu[001,004-008]
qpuq*
            up infinite
                                   idle gpu008
gpunvq
            up infinite
                                   idle sxm[001-004]
sxmq
[root@riogrande ~] # sinfo -R
REASON
                    USER
                              TIMESTAMP
                                                  NODELIST
                              2022-08-01T15:53:20 gpu[002-003]
Memory error
                    root
```

scontrol update nodename=<nodename> state=resume

Change node state to resume

SLURM Administrator Commands II

scontrol show node <NodeName>

Change node state to draining

```
[root@riogrande ~] # scontrol show node gpu001
NodeName=gpu001 Arch=x86 64 CoresPerSocket=14
  CPUAlloc=0 CPUTot=56 CPULoad=0.00
  AvailableFeatures=(null)
  ActiveFeatures=(null)
  Gres=qpu:8
  NodeAddr=gpu001 NodeHostName=gpu001 Version=21.08.8
  OS=Linux 4.18.0-372.9.1.el8.x86 64 #1 SMP Tue May 10 14:48:47 UTC 2022
  RealMemory=1024000 AllocMem=0 FreeMem=1029050 Sockets=4 Boards=1
  CoreSpecCount=2 CPUSpecList=0-1
  State=IDLE ThreadsPerCore=1 TmpDisk=0 Weight=1 Owner=N/A MCS label=N/A
  Partitions=qpuq
  BootTime=2022-08-10T09:04:23 SlurmdStartTime=2022-08-10T09:07:09
  LastBusyTime=2022-08-10T09:07:09
  CfgTRES=cpu=56, mem=1000G, billing=56
  AllocTRES=
  CapWatts=n/a
  CurrentWatts=0 AveWatts=0
  ExtSensorsJoules=n/s ExtSensorsWatts=0 ExtSensorsTemp=n/s
```

SLURM User Commands

sbatch <ScriptName>

Submit a batch script to Slurm

squeue

Display job info

scancel <JobID>

Cancel job

scontrol show job <JobID>

Display detailed job state

```
[atipa@riogrande mpihello]$ squeue
            JOBID PARTITION
                                                              NODES NODELIST (REASON)
                                 NAME
                                          USER ST
                        gpuq mpihello
                18
                                         atipa PD
                                                        0:00
                                                                   4 (Resources)
                        gpug mpihello
                                         atipa PD
                                                                  4 (Priority)
                                                        0:00
                        gpuq mpihello
                                         atipa PD
                                                        0:00
                                                                   4 (Priority)
                        gpuq mpihello
                                                        0:00
                21
                                         atipa PD
                                                                  4 (Priority)
                        gpug mpihello
                                         atipa PD
                                                                  4 (Priority)
                                                        0:00
                        gpuq mpihello
                                         atipa PD
                                                                   4 (Priority)
                23
                                                        0:00
                        gpuq mpihello
                                         atipa R
                                                        0:09
                                                                  4 gpu[001-004]
                        gpug mpihello
                                         atipa R
                                                        0:05
                                                                  4 qpu[005-008]
[atipa@riogrande mpihello]$ scontrol show job 18
JobId=18 JobName=mpihello
  UserId=atipa(1000) GroupId=atipa(1000) MCS label=N/A
  Priority=4294901755 Nice=0 Account=(null) QOS=(null)
  JobState=PENDING Reason=Resources Dependency=(null)
  Requeue=1 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
  RunTime=00:00:00 TimeLimit=00:10:00 TimeMin=N/A
  SubmitTime=2022-08-04T07:42:05 EliqibleTime=2022-08-04T07:42:05
  AccrueTime=2022-08-04T07:42:05
  StartTime=Unknown EndTime=Unknown Deadline=N/A
  SuspendTime=None SecsPreSuspend=0 LastSchedEval=2022-08-04T07:42:10 Scheduler=Main
  Partition=gpug AllocNode:Sid=riogrande:496548
  ReqNodeList=(null) ExcNodeList=(null)
  NodeList=(null)
  NumNodes=4-4 NumCPUs=216 NumTasks=216 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
  TRES=cpu=216, mem=21600M, node=4, billing=216
  Socks/Node=* NtasksPerN:B:S:C=54:0:*:* CoreSpec=*
  MinCPUsNode=54 MinMemoryCPU=100M MinTmpDiskNode=0
  Features=(null) DelayBoot=00:00:00
  OverSubscribe=OK Contiguous=O Licenses=(null) Network=(null)
  Command=/home/atipa/mpihello/slurm submit gpuq-openmpi.sh
  WorkDir=/home/atipa/mpihello
  StdErr=/home/atipa/mpihello/mpihello.out.18
  StdIn=/dev/null
  StdOut=/home/atipa/mpihello/mpihello.out.18
   Power=
```

Submitting a job to SLURM I

```
[atipa@riogrande ~] cd /home/atipa/mpihello
[atipa@riogrande mpihello]$ cat slurm submit gpuq-openmpi.sh
#!/bin/bash
#SBATCH --job-name=mpihello
#SBATCH --output=mpihello.out.%j
                                               JobID
#SBTACH --error=mpihello.err.%j
#SBATCH -N 4 --ntasks-per-node=54
                                               4 Nodes, 54 Cores per Node
#SBATCH --time=10:00
                                               Run-time limit, hours:minutes:seconds
#SBATCH -p gpuq
                                               Job queue/partition (A100 PCIe nodes)
module purge
module load openmpi/4.1.3/gcc/8.5.0
module list
                                               Job commands
mpirun mpihello
```

Submitting a job to SLURM I



Submitting a job to SLURM II

```
[atipa@riogrande ~] cd /home/atipa/mpihello
[atipa@riogrande mpihello]$ cat slurm submit gpuq-keras.sh
#!/bin/bash
#SBATCH --job-name=keras resnet cifar
#SBATCH --output=keras_resnet_cifar.out.%j
#SBTACH --error=keras resnet cifar.err.%j
#SBATCH -N 1 --ntasks-per-node=1
                                               1 Node, 1 Core
#SBATCH --gres=gpu:4
                                                4 GPUs
#SBATCH -p gpuq
                                                Job queue/partition (A100 PCIe nodes)
#SBATCH --time=1:00:00
                                                Run-time limit, hours:minutes:seconds
```

(Note: keras is not part of TensorFlow)

echo "CUDA_VISIBLE_DEVICES: \$CUDA_VISIBLE_DEVICES"

source /shared/tensorflow-2.6.2/tf_env/bin/activate cd /home/atipa/keras-examples/TensorFlow2-tutorial/01-basic-image-classification python3 ./resnet_cifar.py deactivate

── Job commands

Submitting a job to SLURM II

```
[atipa@riogrande mpihello]$ sbatch slurm submit gpuq-keras.sh
Submitted batch job 25
[atipa@riogrande mpihello]$ squeue
             JOBID PARTITION
                                NAME
                                         USER ST
                                                        TIME NODES NODELIST (REASON)
                        gpuq keras re
                                        atipa R
                                                        0:02
                                                                 1 qpu001
[atipa@riogrande mpihello]$ scontrol show job 25
JobId=25 JobName=keras resnet cifar
  UserId=atipa(1000) GroupId=atipa(1000) MCS label=N/A
  Priority=4294901748 Nice=0 Account=(null) QOS=(null)
  JobState=RUNNING Reason=None Dependency=(null)
  Requeue=1 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
  RunTime=00:01:20 TimeLimit=01:00:00 TimeMin=N/A
  SubmitTime=2022-08-10T12:04:08 EligibleTime=2022-08-10T12:04:08
  AccrueTime=2022-08-10T12:04:08
  StartTime=2022-08-10T12:04:08 EndTime=2022-08-10T13:04:08 Deadline=N/A
  SuspendTime=None SecsPreSuspend=0 LastSchedEval=2022-08-10T12:04:08 Scheduler=Main
  Partition=gpuq AllocNode:Sid=riogrande:1816784
  ReqNodeList=(null) ExcNodeList=(null)
  NodeList=gpu001
  BatchHost=gpu001
  NumNodes=1 NumCPUs=1 NumTasks=1 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
  TRES=cpu=1, node=1, billing=1
  Socks/Node=* NtasksPerN:B:S:C=1:0:*:* CoreSpec=*
  MinCPUsNode=1 MinMemoryNode=0 MinTmpDiskNode=0
  Features=(null) DelayBoot=00:00:00
  OverSubscribe=OK Contiguous=O Licenses=(null) Network=(null)
  Command=/home/atipa/mpihello/slurm submit gpuq-keras.sh
  WorkDir=/home/atipa/mpihello
  StdErr=/home/atipa/mpihello/keras resnet cifar.out.25
  StdIn=/dev/null
  StdOut=/home/atipa/mpihello/keras resnet cifar.out.25
  Power=
  TresPerNode=gres:gpu:4
```

[atipa@gpu001 ~]\$ nvidia-smi Wed Aug 10 12:04:20 2022										
+										
	GPU Fan	Name Temp	Perf	Persistence-M Pwr:Usage/Cap		Disp.A Memory-Usage				
	0 N/A	NVIDIA 41C	A100 P0	80G On 69W / 300W		0:1B:00.0 Off iB / 81920MiB		0 Default Disabled		
1	1 N/A	NVIDIA 39C	A100 P0	80G On 63W / 300W		0:1C:00.0 Off iB / 81920MiB		0 Default Disabled		
1	2 N/A	NVIDIA 40C	A100 P0	80G On 67W / 300W		0:4F:00.0 Off iB / 81920MiB		0 Default Disabled		
1	3 N/A	NVIDIA 40C	A100 P0	80G On 66W / 300W		0:50:00.0 Off iB / 81920MiB		0 Default Disabled		
1	4 N/A	NVIDIA 40C	A100 P0	80G On 42W / 300W		0:9C:00.0 Off iB / 81920MiB		0 Default Disabled		
1	5 N/A	NVIDIA 38C	A100 P0			0:9D:00.0 Off iB / 81920MiB		0 Default Disabled		
1	6 N/A	NVIDIA 41C	A100 P0	80G On 44W / 300W		0:CE:00.0 Off iB / 81920MiB		0 Default Disabled		
 N 	7 N/A	NVIDIA 39C	A100 P0	80G On 43W / 300W		0:CF:00.0 Off iB / 81920MiB		0 Default Disabled		
+										
I	Proce GPU	esses: GI ID	CI	PID Ty	pe Proce	ess name		 GPU Memory Usage		
	0 1 2 3	N/A N/A	N/A N/A N/A N/A	25218 25218 25218 25218	C pytho C pytho C pytho C pytho	on3 on3		79531MiB 79531MiB 79531MiB 79531MiB		

Best Practices I

- Check storage status daily (riogrande, stor001, login001)
 - OS disks: checkSoftwareRAID or "cat /proc/mdstat"
 - /home and /backup: checkRAID or "/opt/MegaRAID/storcli/storcli64 /c0 show"
- Install 3rd party software in /shared when possible
 - Include version numbers in the directory structure
- Install new applications as an unprivileged user first
- Be careful adding external yum repositories (e.g. epel) to the cluster
 - Download RPMs locally instead
- If it's not broken, don't fix it (updates can wreak havoc)
 - Kernel updates will require Infiniband driver updates
 - Infiniband driver updates require WekaFS updates
 - •

Best Practices II

- Document all changes
- Backup configuration files before making changes

```
Create a time-stamped backup of a file: backupFile <file>
Example:
[root@riogrande ~]# Is -I /etc/slurm/slurm.conf*
-rw-r--r-- 1 root root 3515 Jul 27 12:14 /etc/slurm/slurm.conf
-rw-r--r-- 1 root root 3062 May 11 11:40 /etc/slurm/slurm.conf.example
[root@riogrande ~]# backupFile /etc/slurm/slurm.conf
File /etc/slurm/slurm.conf was backed up to /etc/slurm/slurm.conf.07282022-15:41:13
[root@riogrande ~]# Is -I /etc/slurm/slurm.conf*
-rw-r--r-- 1 root root 3515 Jul 27 12:14 /etc/slurm/slurm.conf
-rw-r--r-- 1 root root 3515 Jul 27 12:14 /etc/slurm/slurm.conf.07282022-15:41:13
-rw-r--r-- 1 root root 3062 May 11 11:40 /etc/slurm/slurm.conf.example
```

• If possible, reboot after changes

atípa technologies

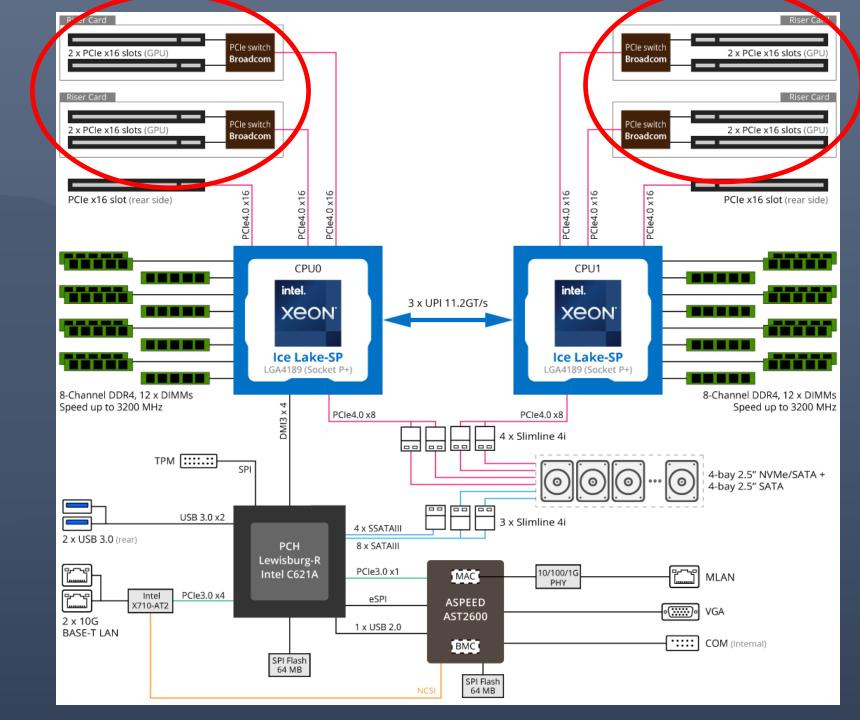
Thank you!

• Support: support@atipa.com

• Sales Order: 6002900

GPU Topology

nvidia-smi topo -m



GPU Topology

nvidia-smi topo -m

root@c	mu001 ^	√l# nvidi	a-smi top	00 - m			_				_	_
10000	GPU0	GPU1	GPU2	GPU3	GPU4	GPU5	GPU6	GPU7	mlx5 0	CPU Aff	inity	NUMA Affinity
PU0	X	PIX	SYS	SYS	SYS	SYS	SYS	SYS	SYS	0-6	0	1
PU1	PIX	X	SYS	SYS	SYS	SYS	SYS	SYS	SYS	0-6	0	
PU2	SYS	SYS	X	PIX	SYS	SYS	SYS	SYS	NODE	7-13	1	
PU3	SYS	SYS	PIX	X	SYS	SYS	SYS	SYS	NODE	7-13	1	
PU4	SYS	SYS	SYS	SYS	X	PIX	SYS	SYS	SYS	14-20	2	
PU5	SYS	SYS	SYS	SYS	PIX	X	SYS	SYS	SYS	14-20	2	
PU6	SYS SYS	SYS	SYS	SYS	SYS	SYS	X	PIX	SYS	21-27	3 3	
PU7 1x5 0	SYS	SYS SYS	SYS NODE	SYS NODE	SYS SYS	SYS SYS	PIX SYS	X SYS	SYS X	21-27	3	
	515	515	NODE	NODE	515	515	515	515	21			
egend:												
X	= Self											
SYS									tween NUM			
											ges wit	hin a NUMA node
PHB									ically th			
PXB								traversi	ng the PC	le Host	Bridge)
PIX NV#			aversing aversing									
					u set or	# NATTI	.KS					
LOOLEG	GPU0	GPU1	a-smi top GPU2	GPU3	GPU4	GPU5	GPU6	GPU7	mlx5 0	CPU Aff	inity	NUMA Affinity
PU0	X	NV12	SYS	SYS	SYS	SYS	SYS	SYS	SYS	0-6	0	Horar Hilling
PU1	NV12	X	SYS	513	SYS	SYS	SYS	SYS	SYS	0-6	0	
PU2	STS	- 515	X	NV12	SYS	SYS	SYS	SYS	NODE	7-13	1	
PU3	SYS	SYS	NV12	Х	SYS	SYS	SYS	SYS	NODE	7-13	1	
PU4	SYS	SYS	Syc	STS	X	NV12	SYS	SYS	SYS	14-20	2	
PU5	SYS	SYS	SYS	SYS	NV12	X	SYS	SYS	SYS	14-20	2	
PU6	SYS	SYS	SYS	SYS	515	518	X	NV12	SYS	21-27	3	
PU7	SYS SYS	SYS	SYS	SYS	SYS	SYS	NV12	X	SYS	21-27	3	
1x5_0	515	SYS	NODE	NODE	SYS	SYS	Syp	218	X			
egend:												
X	= Self											()
									tween NUM			
PHB									n РС1е но ically th		jes witi	nin a NUMA node
PXB									ng the PC		Bridge	
PIX			aversing					CIAVELDI	ing the re	Te nost	Dirage,	
NV#			aversing									
root.@s			a-smi top									
	GPU	GPU1	GPU2	GPU3	GPU4	GPU5	GPU6	GPU7	mlx5 0	CPU Aff	inity	NUMA Affinity
PU0	Х	NV12	NV12	NV12	NV12	NV12	NV12	NV12	NODE	0-6	0	
PV1	NV12	X	NV12	NV12	NV12	NV12	NV12	NV12	NODE	0-6	0	
PU2	NV12	NV12	X	NV12	NV12	NV12	NV12	NV12	PAB	0-6	0	
PU3	NV12	NV12	NV12	X	NV12	NV12	NV12	NV12	PXI	0-6	0	
PU4	NV12	NV12	NV12	NV12	X	NV12	NV12	NV12	SY	14-20	2	
PU5	NV12 NV12	NV12 NV12	NV12 NV12	NV12 NV12	NV12 NV12	X	NV12 X	NV12 NV12	SYS SYS	14-20 21-27	2 3	
PU7	NV12	NV12 NV12	NV12 NV12	NV12 NV12	NV12 NV12	NV12 NV12	NV12	NVIZ	SYS	21-27	3	
	NODE		PXB	PXB	SYS	SYS	SYC	SYS	X	21 21	5	
egend:												
v	- Colf											
X	= Self	ction to	aversing	PCTo on	well as	the CMD	interco	nnect hot	tueen NUM	A nodos	(A (C	OPT /IIPT)
SYS = Connection traversing PCIe as well as the SMP interconnect between NUMA nodes (e.g., QPI/UPI) NODE = Connection traversing PCIe as well as the interconnect between PCIe Host Bridges within a NUMA node												
PHB = Connection traversing PCIe as well as a PCIe Host Bridge (typically the CPU)												
									ng the PC		Bridge)	
			aversing						,			
			aversing									

Without NVLink
GPUs communicate
via PCIe (32GB/s)

With NVLink bridges
GPUs in a pair
communicate
"directly" (600GB/s)

With NVSwitch all GPUs communicate "directly" (600GB/s)