SMUHPC

Added by Fox, David, last edited by Reynolds, Daniel on Jan 28, 2013

SMU HPC

Status:

SMUHPC is normal.

CHANGE:

To use condor you must source /grid/condor/condor.sh(csh) .

Example:

```
[user@smuhpc]$ source /grid/condor/condor.sh

[user@smuhpc]$ condor_q
```

Hardware:

Machine	Purpose	Vendor	Model	Processor	RAM	RAM Speed	SHMMAX	Disk
smuhpc.smu.edu	Interactive Login/Condor Submit	Dell	M610	2x Intel E5540 Xeon 2.53 GHz 8M Cache 5.86 GT/s	48G	1066 MHz	64G	250G
smuhpc2.smu.edu	Interactive Login/Condor Submit	Dell	M610	2x Intel E5540 Xeon 2.53 GHz 8M Cache 5.86 GT/s	48G	1066 MHz	64G	250G
smuhpc3.smu.edu	Interactive Login	Dell	M610	2x Intel E5540 Xeon 2.53 GHz 8M Cache 5.86 GT/s	48G	1066 MHz	64G	500G
smuhpc4.smu.edu	Interactive Login/Condor Submit	Dell	R710	2x Intel E5540 Xeon 2.53 GHz 8M Cache 5.86 GT/s	48G	1066 MHz	65G	500G
highmem1	High Memory Jobs	Dell	R710	2x Intel X5550 Xeon, 2.66 GHz 8M Cache 6.40 GT/s	144G	800 MHz	64G	3TB
highmem2	High Memory Jobs	Dell	R710	2x Intel X5550 Xeon, 2.66 GHz 8M Cache 6.40 GT/s	144G	800 MHz	64G	3TB
diskarraynfs	NFS Storage Node	Dell	R710					500G
diskarray1	NFS Storage Node	Dell	R710	2x Intel E5540 Xeon 2.53 GHz 8M Cache 5.86 GT/s	24G	1066 MHz	64G	40TB
diskarray	Lustre MDS	Dell	R710	2x Intel E5540 Xeon 2.53 GHz 8M Cache 5.86 GT/s	24G	1066 MHz	64G	4TB
diskarray2-6,2b-6b	Lustre Storage Node	Dell	R710	2x Intel E5540 Xeon 2.53 GHz 8M Cache 5.86 GT/s	24G	1066 MHz	64G	40TB
wnode1-27	Batch Worker Nodes	Dell	M610	2x Intel E5540 Xeon 2.53 GHz 8M Cache 5.86 GT/s	48G	1066 MHz	64G	250G
cnode1-80	Batch Worker Nodes	Dell	C6100	2x Intel E5540 Xeon 2.53 GHz 8M Cache 5.86 GT/s	48G	1066 MHz	64G	500G
cwnode1-56	Batch Worker Nodes	Dell	C6100		72G			500G
inode1-16	Parallel Worker Node	Dell	M610	2x Intel E5570 Xeon	48G	1333MHz		500G
iwnode1-32	Parallel Worker Node	Dell	C6100	2x Intel X5660 Xeon 2.8 GHz 12M Cache	72G	1333MHZ	64G	500G
gpu1	GPU Compute Node	Dell/NVIDIA	Precision	2x Intel E5520 Xeon 2.26 GHz 8M Cache 5.86 GT/s 2x NVIDIA GTX 295	6G			300G
gpu2	GPU Compute Node	Dell/NVIDIA	R720	2x Intel E5-2660 Xeon 2.20 GHz 20MB Cache 2x NVIDIA Tesla 2090	128G		64G	500G

There are currently 14TB available for use on the cluster via NFS.

Lustre is online. There are 320TB usable in Lustre.

The machine gpu1 has 960 NVIDIA GPU cores with 3584 MB of RAM on the GPU cards.

OS: Scientific Linux 5.5 64 bit.

Software:

Package	Version	Machines	Location	Usage	Comments	Config
abinit	6.0.2	All machines	/grid/software/abinit-6.0.2			FC=/us CXX=/u prefix=/
Atlas Releases		All machines	/opt/atlas			
ATLASLocalRootBase		All machines	/grid/software/ATLASLocalRootBase	source /grid/software/ATLASLocalRootBase/setup.sh(csh)		
clhep	2.0.4.5	All machines	/grid/software/clhep-2.0.4.5			
clhep	2.0.4.7	All machines	/grid/software/clhep-2.0.4.7			
clhep	2.1.2.3	All machines	/grid/software/clhep-2.1.2.3			
DQ2Clients		All machines	/grid/software/DQ2Clients	source /grid/software/wlcg-client(-64)/setup.sh(csh) source /grid/software/DQ2Clients/setup.sh(csh)	I have installed the 32 bit	

				voms-proxy-init --voms atlas	(/grid/software/wlcg-client) and 64 bit (/grid/wlcg-client-64) versions. If you see and ELF version error try the other version.	
errorhandler	1.1.1	All machines	/grid/software/errorhandler-1.1.1	export PYTHONPATH=/grid/software/errorhandler-1.1.1/lib/python2.6/site-packages/:$PYTHONPATH		
fftw	3.2.2	All machines	/grid/software/fftw			./config
g95 - 32bit default integer	0.92	All machines	/grid/software/g95	source /grid/software/g95/setup.sh(csh)		
g95 - 64bit default integer	0.92	All machines	/grid/software/g95-64	source /grid/software/g95-64/setup.sh(csh)		
gdb		smuhpc highmem1 highmem2				
geant4	4.9.3	All machines	/grid/software/geant4.9.3			
geant4	4.9.4 p02	All machines	/grid/software/geant4.9.4.p02			
geant4	4.9.5.p01	All machines	/grid/software/geant4.9.5.p01			cmake DGEAN DCMAK /home/r
GNU Compilers		All machines				
GNU Compilers	4.5.1	All machines	/grid/software/gcc-4.5.1	source /grid/software/gcc-4.5.1/setup.sh(csh)		
gsl	1.9	All machines	/grid/software/gsl-1.9			
gsl	1.15	All machines	/grid/software/gsl-1.15			
gnuplot		highmem1 highmem2				
hdf5	1.8.3	All machines	/grid/software/hdf5-1.8.3			FC=gfo CC=/gri prefix=/ szlib=/g
ImageMagick		highmem1 highmem2				
ipython	0.12.1	All machines	/grid/software/ipython-0.12.1	source /grid/software/ipython-0.12.1/setup.sh(csh)		
libctl	3.1	All machines	/grid/software/libctl-3.1			
Matlab	2009a	highmem1 highmem2	/usr/local/Matlab2009a			
Matlab	2011b	All machines	/grid/software/MATLAB/2011b			
matplotlib	1.1.0	All machines	/grid/software/matplotlib-1.1.0			
meep	1.1.1	All machines	/grid/software/meep-1.1.1			./config MPICX MPILIB hdf5=/g
mpich2	1.1.1	All machines	/grid/software/mpich2	source /grid/software/mpich2/setup.sh(csh)		./config sharedli
mpich2 - compiled with PGI compilers	1.3.2	All machines	/grid/software/mpich2-1.3.2	source /grid/software/mpich2-1.3.2/setup.sh	Thanks to Kurt Stein for compiling this.	
mvapich		All machines			This is the OS distributed mvapich.	
mvapich2 init script		smuhpc	/grid/software/mvapich2	source /grid/software/mvapich2/mpivars.sh(csh)	There is a bug in the mpivars.sh script from the RPM. Please use this mpivars.sh(csh) script.	
mvapich2 with PGI Compilers		smuhpc4		source /grid/software/pgi-10.5/setup.sh(csh) source /grid/software/mvapich2/mpivars.sh(csh) Use the commad line option -config=pgi.	This is the OS distributed mvapich2 that will use PGI to compile	

				Example: mpif77 hello.f -config=pgi	your code.	
mvapich2 for use with Condor on inode1-16	1.6	smuhpc4	/grid/software/mvapich2-1.6		This is a version of mvapich2 compiled with the GNU compilers specifically to be used on the nodes **inode1-16**.	
mvapich2 with PGI Compilers for use with Condor on inode1-16	1.6	smuhpc4	/grid/software/mvapich2-1.6-PGI	source /grid/software/mvapich2-1.6-PGI/setup.sh	Thanks to Kurt Stein for compiling this. This is a version of mvapich2 compiled with the PGI compilers specifically to be used on the nodes **inode1-16**.	./config FC=pgf
mvapich2 for use with Condor on iwnode1-32	1.6	smuhpc,smuhpc2,smuhpc3	/grid/software/mvapich2-1.6-QL	source /grid/software/mvapich2-1.6-QL/setup.sh(csh)	This is a version of mvapich2 compiled with the GNU compilers specifically to be used on nodes **iwnode1-32**.	./config prefix=/
mvapich2 with PGI Compilers for use with Condor on iwnode1-32	1.6	smuhpc,smuhpc2,smuhpc3	/grid/software/mvapich2-1.6-QL-PGI	/grid/software/mvapich2-1.6-QL-PGI/setup.sh(csh)	This is a version of mvapich2 compiled with the PGI compilers specifically to be used on nodes **iwnode1-32**.	./config prefix=/ CC=pgc
NAG Fortran Compiler	5.2	All machines	/grid/software/NAG-5.2	source /grid/software/NAG-5.2/setup.sh(csh)		
NAG Libraries		All machines	/grid/software/NAGlibs			
numpy	1.6.1	All machines	/grid/software/numpy-1.6.1	export PYTHONPATH=/grid/software/numpy-1.6.1/lib/python2.6/site-packages/:$PYTHONPATH		
PGI Compilers	10.5	All machines	/grid/software/pgi-10.5	source /grid/software/pgi-10.5/setup.sh(csh)	There are 5 seats in this license.	
Paraview	3.14.1	All machines	/grid/software/ParaView-3.14.1-Linux-64bit			
pyproj	1.9.0	All machines	/grid/software/pyproj-1.9.0	export PYTHONPATH=/grid/software/pyproj-1.9.0/lib/python2.6/site-packages/:$PYTHONPATH		
pypy	1.8	All machines	/grid/software/pypy-1.8			
Python	2.6.5	All machines	/grid/software/python-2.6.5	source /grid/software/python-2.6.5/setup.sh(csh)		
R	2.10.0	All machines	/grid/software/R-2.10.0	source /grid/software/R-2.10.0/setup.sh(csh)		
radsrc	1.5	All machines	/grid/software/radsrc_v1.5	source /grid/software/radsrv_v1.5/setup.sh(csh)		
rivet	1.4.0	All machines	/grid/software/rivet	source /grid/software/ATLASLocalRootBase/setup.sh(csh) localSetupGcc source /grid/software/genser/setup.sh(csh) source /grid/software/rivet/rivetenv.sh(csh)		
root	5.14	All machines	/grid/software/root514	source /grid/software/root514/setup.sh(csh)		
root	5.20	All machines	/grid/software/root520	source /grid/software/root520/setup.sh(csh)		
root	5.26	All machines	/grid/software/root526	source /grid/software/root526/setup.sh(csh)	roofit xml fftw3	./config fftw3-in libdir=/g
root	5.28	All machines	/grid/software/root528	source /grid/software/root528/setup.sh(csh)		./config
root	5.30	All machines	/grid/software/root530	source /grid/software/root530/setup.sh(csh)		
scikits-image	0.5	All machines	/grid/software/scikits-image-0.5	export PYTHONPATH=/grid/software/scikits_image-0.5/lib/python2.6/site-packages/:$PYTHONPATH		
scipy	0.10.1	All machines	/grid/software/scipy-0.10.1			export 1.6.1/lib

setuptools	0.6c11	All machines	/grid/software/setuptools-o.6c11	export PYTHONPATH=/grid/software/setuptools-0.6c11/lib/python2.6/site-packages/:$PYTHONPATH		
svn	1.6.2	All machines	/grid/software/subversion-1.6.2	source /grid/software/subversion-1.6.2/setup.sh(csh)	svn 1.4.2 is installed on all machines, if svn 1.6.2 is needed you must source the setup script. If you do not source the setup script you will be using svn 1.4.2.	
swig	2.0.1	All machines	/grid/software/swig-2.0.1			
xlrd	0.7.7	All machines	/grid/software/xlrd-0.7.7	export PYTHONPATH=/grid/software/xlrd-0.7.7/lib/python2.6/site-packages:$PYTHONPATH		
xlutils	1.5.2	All machines	/grid/software/xlutils-1.5.2	export PYTHONPATH=/grid/software/xlutils-1.5.2/lib/python2.6/site-packages/:$PYTHONPATH		
xlwt	0.7.4	All machines	/grid/software/xlwt-0.7.4	export PYTHONPATH=/grid/software/xlwt-0.7.4/lib/python2.6/site-packages:$PYTHONPATH		

Accounts:

Please email ahkumar@smu.edu with account requests.

Login instructions:

To log into the cluster ssh to smuhpc.smu.edu or smuhpc2.smu.edu.

To log into the High Memory nodes ssh to smuhpc.smu.edu or smuhpc2.smu.edu then from there ssh to highmem1 or highmem2.

To log into the GPU computing node ssh to smuhpc.smu.edu or smuhpc2.smu.edu then from there ssh to gpu1 or gpu2.

Condor:

Condor is the batch system used by the compute cluster. For a tutorial please see the link below.

condor.pdf

Condor will run single core jobs, whole machine jobs and parallel jobs.

To use condor you now must source /grid/condor/condor.sh(csh).

Condor Notification Options:

If you would like to get an email when your job completes then put the following line in your condor submit file.

```
notify_user = email@smu.edu
```

Condor Whole Machine Jobs:

Condor can now run Whole Machine Jobs. You can now reserve an entire node for jobs. This is useful for job timing or for multicore processes. An example submit file is below.

```
Universe     = Vanilla
Executable   = myjob.job
Log          = myjob.log
Output       = myjob.out
Error        = myjob.error
Requirements =  CAN_RUN_WHOLE_MACHINE
+RequiresWholeMachine = True
Queue
```

Condor can also allow you to select the type of node that you want to run your job on. On our cluster the only way this can be useful is selecting one of the nodes with 12 cores and 72G of RAM. Simply add the line below to your submit file before the Queue line and your job will run on a 12 core node.

```
requirements = regexp("cwnode", Machine)
```

Condor Parallel Jobs:

Condor can now run parallel jobs on the infiniband connected nodes of the cluster. Parallel jobs must be submitted from smuhpc4.smu.edu only.

There are two seperate infiniband fabrics. You must decide at compile time which fabric you intend to use.

The two fabrics include a 16 8 core node fabric and a 32 12 core node fabric.

To use the **16 node fabric** you must compile your code on smuhpc4 with the mvapich2 libraries in /grid/software/mvapich2-1.6 or /grid/software/mvapich2-1.6-PGI.   Parllel jobs must be submitted to condor from smuhpc4.

To use the 16 node fabric your condor submit file must contain the line:

requirements = regexp("inode", Machine)

The key in the line above is inode. The 16 nodes are named inode1 to inode16.

An example submit file for the 16 node fabric is below.

```
Universe    = parallel
Executable  = myjob.job
Log         = myjob.log.$(NODE)
Output      = myjob.out.$(NODE)
Error       = myjob.error.$(NODE)
machine_count = 2
+WantParallelSchedulingGroups = TRUE
requirements = regexp("inode", Machine)
Queue
```

The variable $(NODE) is the node in the parallel group. Node 0 is the master and nodes 1- are children.

To use the **32 node fabric** you must compile your code on smuhpc, smuhpc2 or smuhpc3 with the mvapich2 libraries in /grid/software/mvapich2-1.6-QL or /grid/software/mvapich2-1.6-QL-PGI.   Parllel jobs must be submitted to condor from smuhpc4.

To use the 32 node fabric your condor submit file must contain the line:

requirements = regexp("iwnode", Machine)

The key in the line above is iwnode. The 32 nodes are named iwnode1 to iwnode32.

An example submit file for the 32 node fabric is below.

```
Universe    = parallel
Executable  = myjob.job
Log         = myjob.log.$(NODE)
Output      = myjob.out.$(NODE)
Error       = myjob.error.$(NODE)
machine_count = 2
+WantParallelSchedulingGroups = TRUE
requirements = regexp("iwnode", Machine)
Queue
```

The variable $(NODE) is the node in the parallel group. Node 0 is the master and nodes 1- are children.

Open MPI jobs:

Open MPI jobs must be submitted from smuhpc4.smu.edu only. Example submit file for an OpenMPI job:

```
universe = parallel
executable = openmpiscript
getenv=true
arguments = actual_mpi_job arg1 arg2 arg3
output = myjob.out.$(NODE)
error  = myjob.error.$(NODE)
log    = myjob.log
notification = never
machine_count = 8
+WantParallelSchedulingGroups = TRUE
```

```
requirements = regexp("inode", Machine)
queue
```

The script openmpiscript can be copied to your directory from /grid/condor/scripts. You MUST source /grid/condor/condor.sh(csh) before you can run the openmpiscript.

MVAPICH2 jobs:

MVAPICH2 jobs must be submitted from smuhpc4.smu.edu only. Example submit file for an MVAPICH job:

```
universe = parallel
executable = mvapich2script
getenv=true
arguments = actual_mpi_job arg1 arg2 arg3
output = myjob.out.$(NODE)
error  = myjob.error.$(NODE)
log    = myjob.log
machine_count = 8
+WantParallelSchedulingGroups = TRUE
requirements = regexp("inode", Machine)
queue
```

The script mvapich2script can be copied to your directory from /grid/condor/scripts. You MUST source /grid/condor/condor.sh(csh) before you can run the mvapich2script.

mvapich2script is for the 16 node cluster compiled with the GNU compilers.

mvapich2PGIscript is for the 16 node cluster compiled with the PGI compilers.

mvapich2QLscript is for the 32 node cluster compiled with the GNU compilers.

mvapich2QLPGIscript is for the 32 node cluster compiled with the PGI compilers.

Condor SSH to Job:

With Whole Machine Jobs in Condor you can SSH to your job. This will allow you to debug your job on the node that it is running on while it is running. Below are the steps necessary to ssh to your job.

```
source /grid/condor/condor.sh
condor_ssh_to_job [job#]
```

Your job number is the job number listed when you run condor_submit. You can also get the number by running condor_q -global | grep [userid].

Like   Liang, Zhihua likes this.   Labels None

3 Child Pages

- ATLAS Data
- Lustre
- MPI

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