Gaea

From GFDL

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This is a Gaea draft wiki site

This is a temporary place to build the Gaea wiki. This page, and its referenced pages will, as soon as the wiki is ready, be moved to www.ncrc.gov/web_site. Please see Naresh Kosgi or Tara McQueen if you have any questions.

Overview

About Gaea

Gaea is a DOE/ORNL Hosted Cray XE6 system

- 260 TF
  - 1,288 compute nodes, each with 64 GB memory
    - 30,912 AMD Magny-Cours Compute Cores
    - 82.4TB of DDR3 Compute Memory
- Storage
  - 1PB Fast Scratch file System
  - 4PB Staging file system
- Connectivity @ 2x10GB/s to NOAA N-Wave research network

HPC Systems in NOAA

- Gaea
  - www.ncrc.gov (http://www.ncrc.gov)
  - http://wiki.gfdl.noaa.gov/index.php/Gaea_System_Details
- GFDL
- Jet
- Vapor
- Zeus (https://nesccdocs.rdhpcs.noaa.gov/wiki/index.php/Main_Page)

Getting Started

Obtain an Account.

- The account form can be found at: http://www.gfdl.noaa.gov/cms-filesystem-action?file=/administrative/computer_account_request.pdf

Login to Gaea

First time Login

First time login to **gaea** is different from regular login.

- Using your shell type: ssh userid@gaea-rsa.rdhpcs.noaa.gov

- You should now see a message to enter the PASSCODE from the RSA FOB

- Make sure the FOB has at least 3 bars on the left corner of the screen and enter the 6 digits as displayed on the screen and press enter

- A message should appear stating that to continue you must enter a new pin at least 8 alphanumeric characters
- Enter the new pin (8 alphanumeric characters) and press enter.
- Then re-enter the same pin & press enter
- If the pins compare, you should see a message stating that the new pin has been accepted.
- You will now see a message asking to enter the PASSCODE from the FOB again. This time you will need to add your pin to the PASSCODE and Press enter.
  - (ex. if you pin was abcd1234 you would enter "abcd1234xxxxxx" where the x's are randomly generated numbers from the rsa fob)
- At this point the prompt will ask you to create a passphrase. Create a minimum of 3 words pass phrase for your grid certificate. This only occurs if you did not already generate a passphrase.
- Confirm the passphrase. Once confirmed it will take up to 24 hours for the certificate to be processed. Once the certificate is processed, login using the regular login instructions.
- If your certificate is not processed in a timely manner, contact support

Regular Login

Regular Login is much simpler:

- ssh userid@gaea-rsa.rdhpcs.noaa.gov
- Enter your pin and passcode from the RSA FOB
  - (ex. if you pin was abcd1234 you would enter "abcd1234xxxxxx" where x's are the randomly generated numbers from the rsa fob)
- If you have issue with certificate contact contact support

Certificates

When a user first logs into Gaea, they generate a master certificate that expires in 1 year. From that day on, every time a user logs on they renew a proxy certificates which expires in 30 days. Users need to have a valid master and proxy certificate to properly authenticate and connect to Gaea. Going over 30 days without renewing will lead to an expired proxy certificate. The next time a user with an expired proxy certificate logs on, they will need to generate a new proxy certificate. This is where the user generated passphrase is used. Users will be prompted to renew their certificate with their passphrase. Users who cannot remember their passphrase will need to enter it incorrectly until they are prompted to create a new passphrase. Only during this process of making a new passphrase will a user have to go through the certificate signing delay again and generate a new master certificate as noted in the steps of first time login.

Setting up your environment

- How to change your shell

Using modules

The Environment Modules system is a tool to help users manage their Unix or Linux shell environment. It allows groups of related environment-variable settings to be made or removed dynamically.

Modules provides commands to dynamically load, remove and view software.

Module Commands

Some Module Commands and description. For more: http://modules.sourceforge.net/man/module.html

- **module help [module]** - Print the usage of each sub-command. If an argument is given, print the Module-specific help information for the module file(s)
  - ex. module help gcp/1.1

```
Sets up the shell environment for gcp
```

- **module avail** - List of all available modulefiles in the current MODULEPATH.
  - ex: module avail

```
------------------------------------------------------------------------------------------ /opt/cray/ss
portals/2.2.0-1.0301.22039.18.1.ss(default) rca/1.0.0-2.0301.21810.11.20.ss(default)
------------------------------------------------------------------------------ /opt/cray/xt-asyncpe
xtpe-accel-nvidia20  xtpe-barcelona       xtpe-istanbul        xtpe-mc12            xtpe-mc8
------------------------------------------------------------------------------------------ /opt/cray/m
atp/1.0.2(default)                   perftools/5.1.0(default)             portals/2.2.0-1.0300.206
atp/1.1.1                            perftools/5.1.2                      rca/1.0.0-2.0300.20198.8
ga/4.3.3(default)                    pmi/1.0-1.0000.7628.10.2.ss          rca/3.0.20
gdb/7.2(default)                     pmi/1.0-1.0000.7901.22.1.ss(default) stat/1.0.0(default)
iobuf/2.0.1(default)                 pmi/1.0-1.0000.8256.50.1.ss          stat/1.1.3
NOTE: this is not the complete print out of what your shell might print out
```

- **module add module_file** - Load module file(s) into the shell environment
- **module load module_file** - Load module file(s) into the shell environment
  - ex: module load gcp/1.1
- **module list** - List of Loaded modules.
  - ex: module list

```
1) modules/3.2.6                            6) xt-mpt/5.0.1                              11) PrgE
2) xt-sysroot/3.1.29.securitypatch.20100707  7) pmi/1.0-1.0000.7901.22.1.ss              12) eswr
3) xtpe-network-seastar                     8) xt-sysroot/3.1.29                         13) moab
4) pgi/10.6.0                               9) portals/2.2.0-1.0301.22039.18.1.ss        14) torq
5) xt-libsci/10.4.6                        10) xt-asyncpe/4.4                            15) xtpe

note gcp/1.4.3 is now Loaded at no.18
```

- **module rm module_file** - unload the module
- **module unload module_file** - unload the module
    - ex: module unload gcp/1.4.3

```
module list
1) modules/3.2.6.6                              6) xt-mpt/5.0.1                              11) PrgE
2) xt-sysroot/3.1.29.securitypatch.20100707   7) pmi/1.0-1.0000.7901.22.1.ss               12) eswr
3) xtpe-network-seastar                         8) xt-sysroot/3.1.29                         13) moab
4) pgi/10.6.0                                   9) portals/2.2.0-1.0301.22039.18.1.ss        14) torq
5) xt-libsci/10.4.6                            10) xt-asyncpe/4.4                            15) xtpe

note gcp/1.4.3 is not Loaded
```

- **module Switch [available_module] replacement_module** - Switch loaded available_module with replacement_module. If available_module is not specified, then it is assumed to be the currently loaded module with the same root name as replacement_module
- **module swap [available_module] replacement_module** - Switch loaded available_module with replacement_module. If available_module is not specified, then it is assumed to be the currently loaded module with the same root name as replacement_module
    - ex: module load gcp/1.1

```
   module list
Currently Loaded Modulefiles:
1) modules/3.2.6.6                              6) xt-mpt/5.0.1                              11) Prg
2) xt-sysroot/3.1.29.securitypatch.20100707   7) pmi/1.0-1.0000.7901.22.1.ss               12) esw
3) xtpe-network-seastar                         8) xt-sysroot/3.1.29                         13) moa
4) pgi/10.6.0                                   9) portals/2.2.0-1.0301.22039.18.1.ss        14) tor
5) xt-libsci/10.4.6                            10) xt-asyncpe/4.4                            15) xtp

  module swap gcp/1.1 gcp/1.5.0
1) modules/3.2.6.6                              6) xt-mpt/5.0.1                              11) Prg
2) xt-sysroot/3.1.29.securitypatch.20100707   7) pmi/1.0-1.0000.7901.22.1.ss               12) esw
3) xtpe-network-seastar                         8) xt-sysroot/3.1.29                         13) moa
4) pgi/10.6.0                                   9) portals/2.2.0-1.0301.22039.18.1.ss        14) tor
5) xt-libsci/10.4.6                            10) xt-asyncpe/4.4                            15) xtp
Note: the gcp is now version 1.5.0
```

- **module show modulefile** - Display information about one or more modulefiles. The display sub-command will list the full path of the modulefile(s) and all (or most) of the environment changes the modulefile(s) will make if loaded. (It will not display any environment changes found within conditional statements.)
- **module display modulefile** - Display information about one or more modulefiles. The display sub-command will list the full path of the modulefile(s) and all (or most) of the environment changes the modulefile(s) will make if loaded. (It will not display any environment changes found within conditional statements.)
    - ex: module show CmrsEnv

```
-------------------------------------------------------------------
/sw/eslogin/modulefiles/CmrsEnv:
module-whatis    Sets up environment variables for the NCRC CMRS.
setenv           CARCHIVE /lustre/fs/archive/fms
setenv           CSCRATCH /lustre/fs/scratch
setenv           CSTAGE /lustre/ltfs/stage
```

```
setenv           CWORK /lustre/ltfs/scratch
setenv           CHOME /ncrc/home1/Naresh.Kosgi
-----------------------------------------------------------------
```

- **module use [-a]--append] directory** - Prepend one or more directories to the MODULEPATH environment variable. The --append flag will append the directory to MODULEPATH.

WARNING: please DO NOT use the command module purge on Gaea. This will remove all modules currently loaded by default and wipe out the system environment. If you have accidentally used the command purge, you will want to open a new connection to Gaea. This will give you the default environment with the default modules loaded.

Getting help

Create a help desk ticket

- In order to obtain help with any issues regarding Gaea please email a help desk ticket to **oar.rdhpcs.gaea-help@noaa.gov**

Please include the following details in your ticket description:

- Host
- Date/time
- User name/ account name
- description
- stdout, stderr, screen output
    - please include world readable paths to these files if available
- occurrence count (have you retried, does it occur x/y times)

Escalating Critical issues

- If the issue is too critical for a help desk ticket then it can be escalated by contacting:
    - For GFDL
        - Operations:
            - 609-452-6560
        - Frank
            - 609-452-5303
        - Ron Bewtra
            - 609-452-6555
-
    - For NCEP
        - Kate Howard
            - need kate's number

Transferring Data

gcp is the convenient wrapper tool used to transfer data between **gaea** and within different file systems on **gaea**. You can obtain a version of gcp by doing a

```
module load gcp
```

on a login node.

LTFS to FS Transfer

- In order to Transfer data from LTFS to FS file systems use:
  - gcp /lustre/ltfs/scratch/$USER/file /lustre/fs/scratch/$USER/file
  - use on es partition

FS to LTFS Transfer

- In order to Transfer data from FS to LTFS file systems use:
  - gcp /lustre/fs/scratch/$USER/file /lustre/ltfs/scratch/$USER/file
  - use on es partition

Gaea to remote host

- In order to transfer data from gaea to remote host you can use the /usw/user_scripts/es_rdtn_gridftp script
- Grab the script and move it into your home directory:
  - cp /usw/user_scripts/es_rdtn_gridftp /your/local/directory/
- Edit the script to change the relevant #PBS options, especially #PBS -d, #PBS -o, and #PBS -l walltime= options.
- run the script giving it the source directories first followed by the destination directory:
  - ./es_rdtn_gridftp -s dtn-002.remote.location.server.gov /gaea/source/location/ /another/gaea/source/location/ /remote/location/
  - ./es_rdtn_gridftp -s dtn-002.remote.location.server.gov /gaea/source/location/ /remote/location/
  - Note: the first example has two sources and the second has only one source
- Use showq, checkjob, or less on the stdout to monitor the progress of your job.
  - The stdout for your job will usually be in ${HOME}/.es_rdtn_gridftp/
- WARNING: When the source is a directory, the directory level is not copied but its files are copied. In this case please make the directory first:
  - example /home/user/stuff/ /archive/user/
    - What we want is: /archive/user/stuff/(stuff content)
    - What we get is: /archive/user/(stuff content)
    - In this example we would like to copy the folder stuff and all its contents, however stuff folder is not copied, just its contents are.
- You may use the '-r' option to copy from the remote site to Gaea.
  - In this case, the source(s) must exist on the remote site and the destination must be valid on Gaea.
- In no case will /lustre/**fs** be a source or destination: That filesystem is not accessible from the RDTNs.

Running a simple job

This tutorial is about running a basic script on **gaea**. Provided is a skeleton script for **gaea** c1ms to help users who don't have access to or prefer not to use a workflow manager like FRE. As written, the script copies everything in the experiment subdirectory from ltfs to fs, runs the experiment, and then copies the changed and new files from fs to ltfs.

Running the Script

This script assumes that the data and executable are staged to /lustre/ltfs/scratch/$USER/$experiment_subdir. The scripts and data are located at /usw/user_scripts/

- Use gcp to get the skeleton script from /usw/user_scripts/c1ms_skeleton to your local home directory
  - gcp /usw/user_scripts/c1ms_skeleton ~$USER/

- Use gcp to get other files from /usw/user_scripts/ to your ltfs directory
  - gcp -r /usw/user_scripts/ /lustre/ltfs/scratch/$USER/$experiment_subdir

- Open the skeleton script (There are also comments in the script to help you understand what each item does.)
  - vim ~$USER/c1ms_skeleton

- Users MUST modify the paths in the '#PBS -d' and '#PBS -o' lines and the walltime in the '#PBS -l walltime' line. (i.e /lustre/fs/scratch/YourUserid/ for -d and -o, and walltime can be set to 20 min for this tutorial)
  - WARNING do not use environment variables like $USER in setting the directory as it will not be available at run time for the script

- now go to your home directory and submit your job
  - msub c1ms_skeleton

Once the job is submitted

Once the job is submitted there are commands to check on your job.

- use showq -u $USER to view the status of your job
  - HINT - use showq -u $USER -c to see jobs which have completed with exit codes

- use checkjob jobid to check a detailed status of your job
  - example checkjob gaea.123456789

Once the job is Finished

- Once your job is finished you will have a output file in your fs directory and output folder in your ltfs directory.

- In the fs folder you should have a .o output file (ex. c1ms_skeleton.o208178)

- In the ltfs folder you should have a folder with the output files (ex. c1ms_skeleton_208178.c1ms-sys0.ncrc.gov)

System Status

- Gaea System Status can be found at: http://www.ncrc.gov/dashboard/
- Additionally, information can be found using moab commands

FAQ

Gaea-FAQ (http://wiki.gfdl.noaa.gov/index.php/Gaea_FAQ)

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