Parallel Computing Notes
Topic: Using XSEDE

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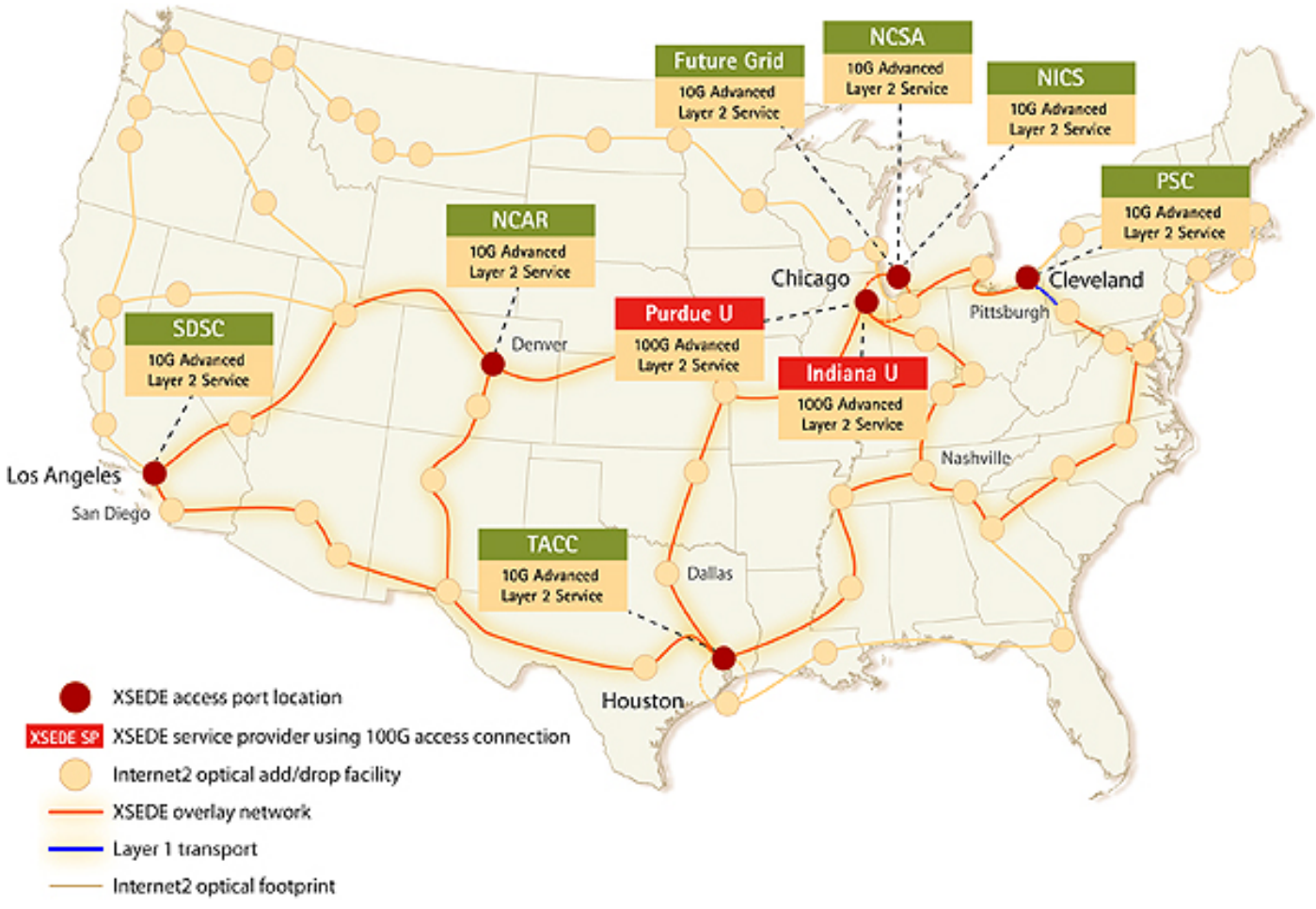

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xsede

Essential Software and Management Tools Needed to Build a Powerful, Flexible, and Highly Available Supercomputer.

HPC Programming Tools

Performance Monitoring	HPCC	Perfctr	IOR	PAPI/IPM	netperf
Development Tools	Cray® Compiler Environment (CCE)	Intel® Cluster Studio	PGI (PGI CDK)	GNU	
Application Libraries	Cray® LibSci, LibSci_ACC	MVAPICH2	OpenMPI	Intel® MPI- (Cluster Studio)	

Middleware Applications and Management

Resource Management / Job Scheduling	SLURM	Grid Engine	MOAB	Altair PBS Pro	IBM Platform LSF	Torque/Maui
File System	NFS	Local FS (ext3, ext4, XFS)	PanFS	Lustre		
Provisioning	Cray® Advanced Cluster Engine (ACE) management software					
Cluster Monitoring	Cray ACE (iSCB and OpenIPMI)					
Remote Power Mgmt	Cray ACE					
Remote Console Mgmt	Cray ACE					

Operating Systems

Operating System	Linux (Red Hat, CentOS, SUSE)

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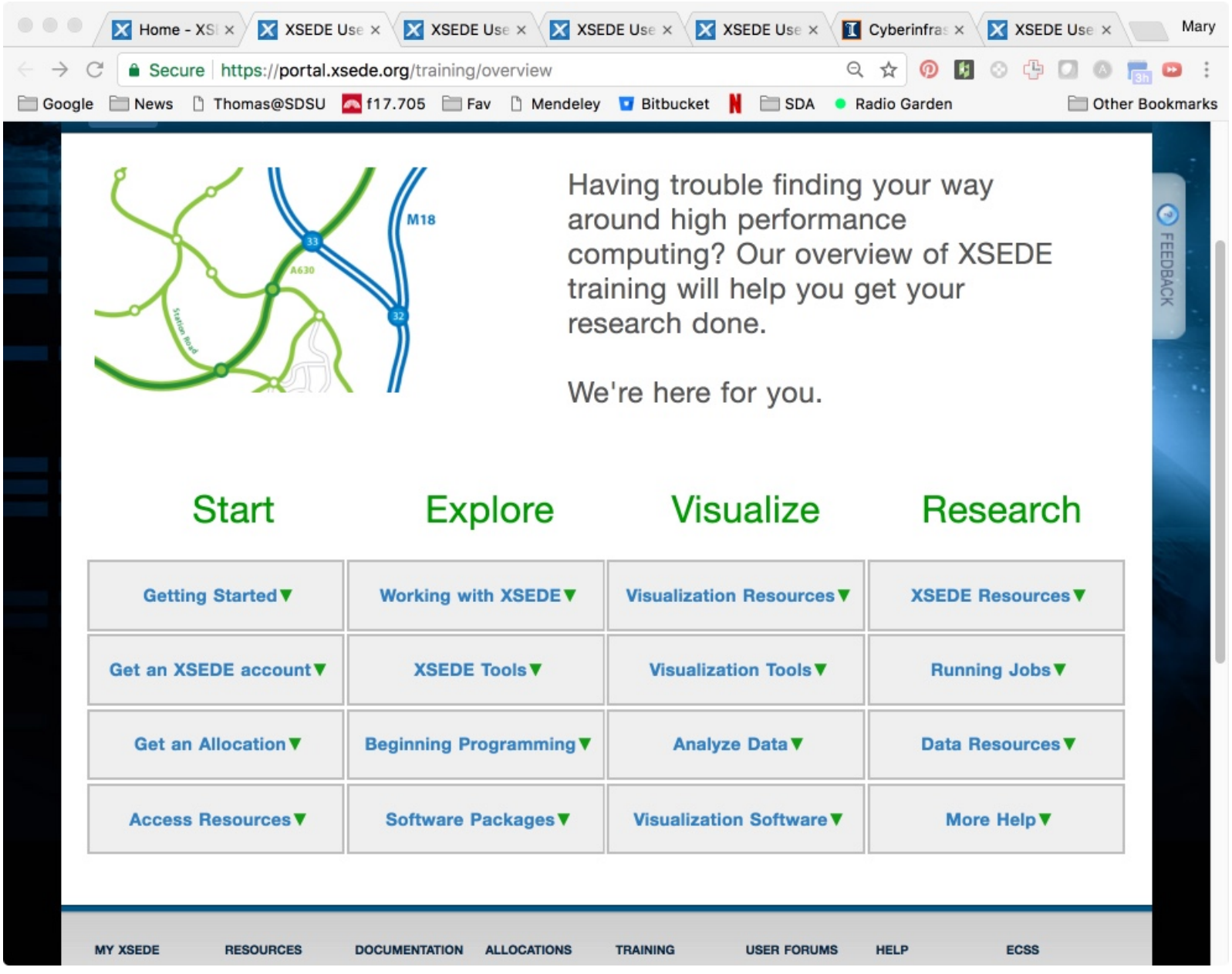
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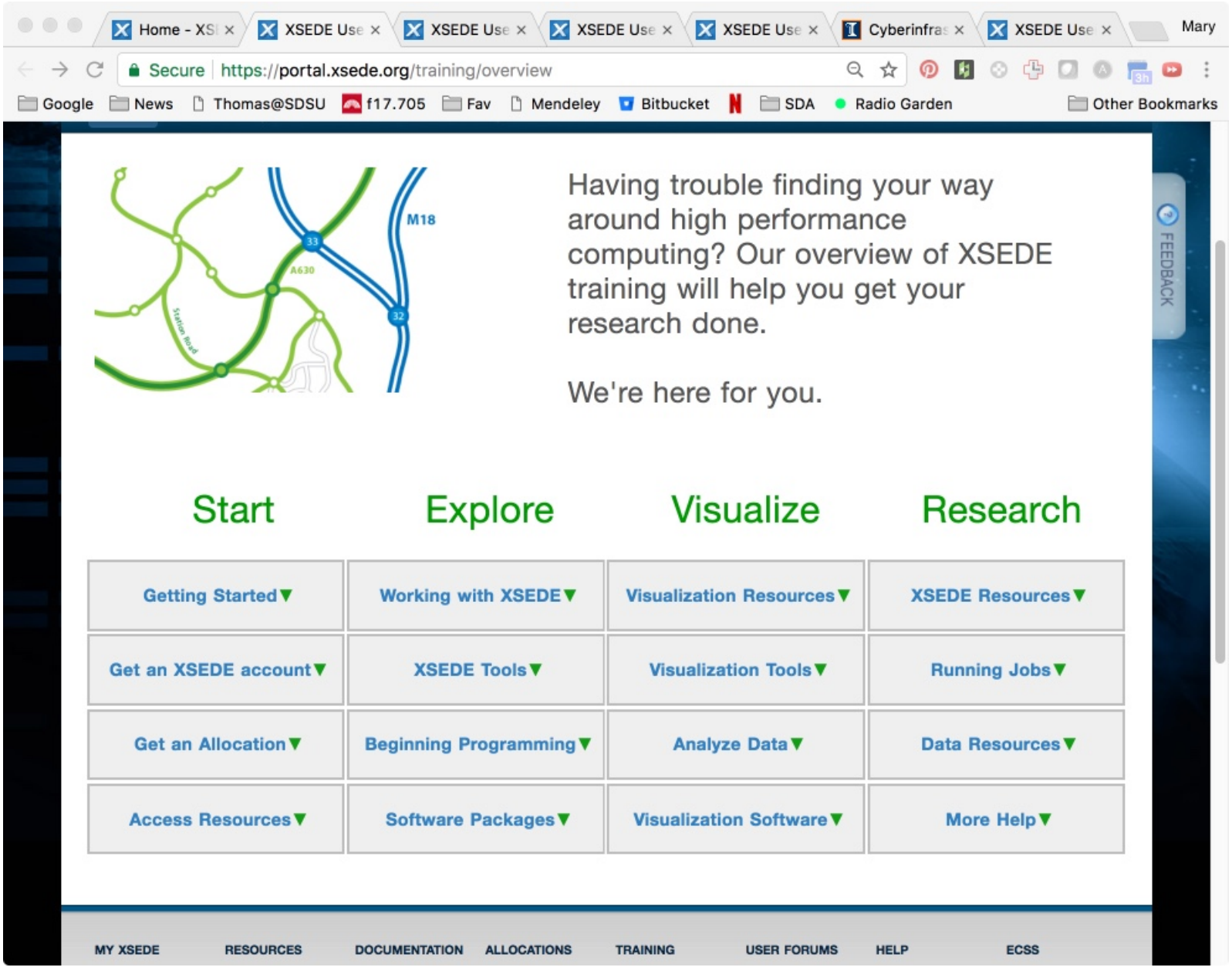
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Getting Access

- Get an account on the portal
- Get your own allocation or get added to someone elses' allocation
- Logon to resource
  - using portal interface
  - using SSH, but need user ID and password
  - use SSO: single sign-on

Single Sign On (SSO) Hub

- `https://portal.xsede.org/web/xup/single-sign-on-hub`
- Two-step authentication.
- (1) Use XSEDE User Portal (XUP) username and password (easy)
  - `login.xsede.org`, is a single point-of-entry to the XSEDE cyberinfrastructure.
  - SSH login: *localhost$ssh – l XUPusernamelogin.xsede.org*
- (2) Use `Duo` service for additional authentication (hard to set up, but then easy to use)
  - Multi-Factor Authentication with Duo: `https://portal.xsede.org/mfa`
  - To setup:
    1. Install Duo app smartphone or other device
    2. Enroll XSEDE Portal account in Duo
    3. Pair Duo-enabled device with XUP account
- Once authenticated, use `gsissh` to any XSEDE compute resource where you have an account without the need for a resource-specific username and password.

SSO Hub Example Work Session

```
1   [my-local-workstation:~ DrJanePhD]$ ssh JaneXUPUser@login.xsede.org
2   Please login to this system using your XSEDE username and password:
3   password:
4   Duo two-factor login for janexupuser
5
6   Enter a passcode or select one of the following options:
7
8   1. Duo Push to XXX-XXX-9999
9   2. Phone call to XXX-XXX-9999
10
11  Passcode or option (1-2): 1
12  Success. Logging you in...
13  Last login: Thu Apr 20 12:55:35 2017 from 70.114.204.80
14
15  #  Welcome to the XSEDE Single Sign-On (SSO) Hub!
```

X.509 credential Info

```
[JaneXUPuser@ssohub ~]$ grid-proxy-info
subject  : /C=US/O=National Center for Supercomputing Applications/CN=[JaneXUPuser
issuer   : /C=US/O=National Center for Supercomputing Applications/
                                OU=Certificate Authorities/CN=MyProxy CA 2013
identity : /C=US/O=National Center for Supercomputing Applications/CN=[JaneXUPuser
type     : end entity credential
strength : 2048 bits
path     : /tmp/x509up_u7121
timeleft : 11:58:3
```

Display Available Hosts

```
1  [JaneXUPuser@ssohub ~]$ xsede-gsissh-hosts
2  bridges
3  comet
4  gordon
5  mason
6  maverick
7  osg
8  stampede
9  supermic
10 wrangler-iu
11 wrangler-tacc
12 xstream
```

Connect to Pittsburgh Supercomputing Center bridges Machine

```
1   [JaneXUPuser@ssohub ~]$ gsissh bridges
2   Last login: Mon Feb 20 14:11:23 2017 from ssohub.iu.xsede.org
3   ...
4   You have connected to br006.pvt.bridges.psc.edu
5   ...
6   ... do science ...
7   ...
8   [janeuser@br006 ~]$ exit
9   logout
10  Connection to bridges.psc.edu closed.
```

Connect to comet.sdsc.edu

```
1   [JaneXUPuser@ssohub ~]$ gsissh bridges
2   [mthomas@gidget:~] ssh thomasm@login.xsede.org
3   Please login to this system using your XSEDE username and password:
4   password:
5   Duo two-factor login for thomasm
6
7   Enter a passcode or select one of the following options:
8
9    1. Duo Push to XXX-XXX-7391
10   2. Phone call to XXX-XXX-7391
11
12  Passcode or option (1-2): 817528
13  Success. Logging you in...
14  Last login: Thu Jun 29 19:40:25 2017 from 146.244.200.93
```

Connect to comet.sdsc.edu

```
[thomasm@ssohub ~]$ gsissh comet
Last login: Thu Jul  6 09:25:04 2017 from rrcs-69-75-224-179.west.biz.rr.com
Rocks 6.2 (SideWinder)
Profile built 16:44 08-Feb-2016
Kickstarted 17:18 08-Feb-2016

                       WELCOME TO
        ------------------  --  ---------------
         ------/ ----/ -- \/  |/  / ----/-  --/
           --/ /   / / / / /|-/ / --/   / /
            / /---/ /-/ / /  / / /---  / /
            \----/\----/-/  /-/-----/ /-/

********************************************************************************

[1] Example Scripts: /share/apps/examples

[2] Filesystems:

     (a) Lustre scratch filesystem : /oasis/scratch/comet/$USER/temp_project
         (Preferred: Scalable large block I/O)
     (b) Compute/GPU node local SSD storage: /scratch/$USER/$SLURM_JOBID
         (Meta-data intensive jobs, high IOPs)
     (c) Lustre projects filesystem: /oasis/projects/nsf
     (d) /home/$USER : Only for source files, libraries, binaries.
         *Do not* use for I/O intensive jobs.

[3] Comet User Guide: http://www.sdsc.edu/support/user_guides/comet.html
********************************************************************************
```

You need to do all work in the $WORK directory

```
[mthomas@comet-ln2 hello]$ cd $WORK
[mthomas@comet-ln2 temp_project]$ pwd
/oasis/scratch/comet/mthomas/temp_project
[mthomas@comet-ln2 temp_project]$
[mthomas@comet-ln2 temp_project]$ ls
total 138
drwxr-xr-x  4 mthomas use300 33280 Jun 26 11:13 .
drwxr-xr-x  3 root    root   33280 Apr 11  2015 ..
drwxr-xr-x  5 mthomas use300 33280 Jul  6 15:22 gccom.git
drwxr-xr-x 42 mthomas use300 41472 Jun 22 21:11 pardev
[mthomas@comet-ln2 temp_project]$ cd pardev/
[mthomas@comet-ln2 pardev]$ ls
total 1411
drwxr-xr-x 42 mthomas use300 41472 Jun 22 21:11 .
drwxr-xr-x  4 mthomas use300 33280 Jun 26 11:13 ..
 drwxr-xr-x  5 mthomas use300 33280 Jun 22 21:10 comms
-rw-r--r--  1 mthomas use300    12 Jun 22 21:10 contributors.txt
drwxr-xr-x  4 mthomas use300 33280 Jun 22 21:10 create-matrix-data
drwxr-xr-x  2 mthomas use300 33280 Jun 22 21:10 critblock
drwxr-xr-x 11 mthomas use300 33280 Jun 22 21:10 cuda
drwxr-xr-x  3 mthomas use300 33280 Jun 22 21:10 gnudbg
drwxr-xr-x  4 mthomas use300 33280 Jun 22 21:10 gropp
drwxr-xr-x  2 mthomas use300 33280 Jun 22 21:10 halo
 drwxr-xr-x  2 mthomas use300 33280 Jun 22 21:12 hello
```

Compile and run a simple hello world:

```
1  [mthomas@comet-ln2 hello]$ mpicc -o hello-cpuid hello-cpuid.c
2  [mthomas@comet-ln2 hello]$ mpirun -np 4 ./hello-cpuid.c
3  [proxy:0:0@comet-ln2.sdsc.edu] HYDU_create_process (utils/launch/launch.
4  execvp error on file ./hello-cpuid.c (Permission denied)
5  [proxy:0:0@comet-ln2.sdsc.edu] HYDU_create_process (utils/launch/launch.
6  execvp error on file ./hello-cpuid.c (Permission denied)
7  [proxy:0:0@comet-ln2.sdsc.edu] HYDU_create_process (utils/launch/launch.
8  execvp error on file ./hello-cpuid.c (Permission denied)
9  [proxy:0:0@comet-ln2.sdsc.edu] HYDU_create_process (utils/launch/launch.
10 execvp error on file ./hello-cpuid.c (Permission denied)
```

What went wrong????

Environment Modules package

- Provides for dynamic modification of shell environment.
- Module commands set, change, or delete environment variables
- Let user choose different versions software, combinations of related codes.
- Example, Intel module and mvapich2_ib module are loaded; user compiles with mpif90, the generated code is compiled with Intel Fortran 90 compiler and linked with mvapich2_ib MPI libraries.

Command	Description
module list	List the modules that are currently loaded
module avail	List the modules that are available
module display <module_name>	Show the environment variables used by <module name> and how they are affected
module unload <module name>	Remove <module name> from the environment
module load <module name>	Load <module name> into the environment
module swap <module one> <module two>	Replace <module one> with <module two> in the environment

Using Modules If you repeatedly keep loading in the same set of modules, build a script to startup your preferred environment

[

```
1  mthomas@comet-ln2 hello]$ cat ~/loadcomp705env.sh
2  module purge
3  module load gnu
4  module load openmpi_ib
5  module load netcdf/4.3.2
6  [mthomas@comet-ln2 hello]$
7  [mthomas@comet-ln2 hello]$ source ~/loadcomp705env.sh
8  [mthomas@comet-ln2 hello]$ module list
9  Currently Loaded Modulefiles:
10   1) gnu/4.9.2              2) openmpi_ib/1.8.4
   3) hdf5/1.8.14            4) netcdf/4.3.2
```

Compile and run as usual:

```
1  [mthomas@comet-ln2 hello]$
2  [mthomas@comet-ln2 hello]$
3  [mthomas@comet-ln2 hello]$ mpicc -o hello-cpuid hello-cpuid.c
4  [mthomas@comet-ln2 hello]$ mpirun -np 4 ./hello-cpuid
5  hello, world from node: comet-ln2.sdsc.edu, core: 13
6  hello, world from node: comet-ln2.sdsc.edu, core: 0
7  hello, world from node: comet-ln2.sdsc.edu, core: 12
8  hello, world from node: comet-ln2.sdsc.edu, core: 1
9  [mthomas@comet-ln2 hello]$
```

Running Jobs on Regular Compute Nodes

Comet uses the Simple Linux Utility for Resource Management (SLURM) batch environment

Queue Name	Max Walltime	Max Nodes	Comments
compute	48 hrs	72	Used for access to regular compute nodes
gpu	48 hrs	8	Used for access to the GPU nodes
gpu-shared	48 hrs	1	Used for shared access to a partial GPU node
shared	48 hrs	1	Single-node jobs using fewer than 24 cores
large-shared	48 hrs	1	Single-node jobs using large memory up to 1.45 TB
debug	30 mins	2	Used for access to debug nodes

Requesting interactive resources using srun

You can request an interactive session using the *srun* command.
The following example will request one node, all 24 cores, in the debug partition for 30 minutes

```
1
2   srun --partition=debug --pty --nodes=1 --ntasks-per-node=24
3               -t 00:30:00 --wait=0 --export=ALL /bin/bash
```

Submitting Jobs Using sbatch

Jobs can be submitted to the sbatch partitions using the *sbatch* command as follows:

```
1  [mthomas@comet-ln2 hello]$ cat slrmbat.hello-cpuid
2  #!/bin/bash
3  #SBATCH --job-name="hello-cpuid"
4  #SBATCH --output="hello-cpuid.%j.%N.out"
5  #SBATCH --partition=compute
6  #SBATCH --nodes=2
7  #SBATCH --ntasks-per-node=24
8  #SBATCH --export=ALL
9  #SBATCH -t 01:30:00
10
11 #This job runs with 2 nodes, with
12 24 cores per node for a total of 48 cores.
13 #ibrun in verbose mode will give binding detail
14
15 ibrun -v ./hello-cpuid
16
17 [mthomas@comet-ln2 hello]$
18 [mthomas@comet-ln2 hello]$ sbatch slrmbat.hello-cpuid
19 Submitted batch job 11881782
20 [mthomas@comet-ln2 hello]$ squeue -u mthomas
21              JOBID PARTITION     NAME     USER ST       TIME
   NODES NODELIST(REASON)
22           11881782   compute hello-cp  mthomas PD
```

XXX

```
[mthomas@comet-ln2 hello]$ ls
total 280
drwxr-xr-x  4 mthomas use300  33280 Oct 16 15:47 .
drwxr-xr-x 42 mthomas use300  41472 Jun 22 21:11 ..
-rw-r--r--  1 mthomas use300    823 Oct 16 14:40 batch.COMET
-rw-r--r--  1 mthomas use300    263 Jun 22 21:10 hello.c
-rwxr-xr-x  1 mthomas use300 101872 Oct 16 15:17 hello-cpuid
-rw-r--r--  1 mthomas use300   2261 Oct 16 15:47 hello-cpuid.11881037.co
```

XXX

```
1
2   output here
```

XXX

```
1
2   output here
```