Using Hoffman2 Cluster

Qiyang Hu

UCLA Institute for Digital Research & Education

May 8th, 2013
Hoffman2: largest and most powerful cluster in UC

**Total:** > 1100 machine
  ~ 11,000 cores
  > 300 GPUs
  ~ 102 Tflops

**Storage:** > 1.5 Petabytes

**CPU:** 8, 12, 16 cores,
2.2 ~ 3.0 GHz

**Memory:** 1G, 4G, 8G /core

**OS:** CentOS Linux 6.4
We have 1,200+ users, 175+ research groups

Research Virtual Shared Cluster
~ 11,000 cores and increasing!

Open to ALL campus users in shared base for <24 hour jobs
Contributed researchers can use their own cores to run longer-hour jobs
Before accessing Hoffman2 cluster

Hoffman2’s official site:
https://idre.ucla.edu/hoffman2

Need to have a log-in ID first
- via Grid Identity Manager: gim.ats.ucla.edu
- open to all current student, staff and faculty member with a valid UCLA log-on ID.
Two modes to use hoffman2

1. Web-service mode:
   - UCLA Grid Portal: grid.ucla.edu
   - Easiest way for windows users
   - Slow, function-limited, deprecating

2. Command-line mode:
   - by logging into login nodes
   - efficient, more control
   - might need some basic unix knowledge + SGE commands
Two modes to use hoffman2

1. **Web-service mode:**
   - UCLA Grid Portal: grid.ucla.edu
   - Easiest way for windows users
   - Slow, function-limited, deprecating

2. **Command-line mode:**
   - by logging into login nodes
   - efficient, more control
   - might need some basic unix knowledge + SGE commands
Outline

1. via Command Line
   - Log in and access files
   - Prepare for the submission
   - Simple batch submission

2. Special topics
   - A few more words about job running
   - Computing in interactive-scheduler mode
   - R Jobs and Matlab Jobs

3. Summary
Outline

1. via Command Line
   - Log in and access files
   - Prepare for the submission
   - Simple batch submission

2. Special topics
   - A few more words about job running
   - Computing in interactive-scheduler mode
   - R Jobs and Matlab Jobs

3. Summary
Outline

1 via Command Line
   - Log in and access files
   - Prepare for the submission
   - Simple batch submission

2 Special topics
   - A few more words about job running
   - Computing in interactive-scheduler mode
   - R Jobs and Matlab Jobs

3 Summary
For Unix, Linux or Mac users

Using `ssh` command:

- `ssh login-id@hoffman2.idre.ucla.edu`
- “Yes” for fingerprint for the first time:
- One of the physical login nodes will be randomly assigned
  - `login1 ~ login4`

Working with interactive GUI applications:

- Activate X11 forwarding:
  - `ssh login-id@hoffman2.idre.ucla.edu -X`

Check Hoffman2 Login Node Fingerprints:

http://fuji.ats.ucla.edu/for-transfer/hoffman2-cluster/access/login_node.htm#fingerprint
For Windows users

- **Getting ssh software:** PuTTY, Xshell, Cygwin, Tunnelier, ...

**Or just using web browser!**

- Chrome Web Store → Secure Shell
- Firefox Add-ons → FireSSH

- **Working with interactive GUI application:**
  - get an X server: PuTTY + Xming, Cygwin + Cygwin+X

- **using NX client (not recommended for Mac user):**
  1. download and install NX client (NoMachine Player for Mac Lion)
  2. get the key from /etc/nxserver/client.id_dsa.key
  3. configure login info and input key

**Do not** run computation on login node!
Additional commands from login nodes

- Change your password by command:
  `passwd`

- Configure your shell (command-line interpreter/scripts):
  - Check your shell: `echo $SHELL`

- Text editor:
  - `vim`, `emacs`, `gedit`...

**Tip: to keep ssh session alive:**

1. `vi ~/.ssh/config`
   - Add: `ServerAliveInterval 5`

2. `vi ~/.bashrc`
   - Add: `export TMOUT=36000`
Home directory: `cd $HOME`
- 20 GB quota for general campus user
- backed up for 30 days

Temporary use:
- on each node: `cd $TMPDIR`
  - 100 GB, keep only during the job’s run
- `cd $SCRATCH`
  - 2 TB limit, keep for 7 days

Remember to check your quota in your home directory

1. ATS scripts: `get_pan_quotas $USER`
2. Linux command: `cd $HOME; du -sh`
Major storage architecture change in June

- absolute home path will change
- distinguish home and sponsored directories
- bash profiles need to be copied into new home
Transferring files

- from Linux/Mac terminal:
  - Use `dtn2` to transfer!
  - `ssh dtn2
    scp [-r] source:path/file target:local_path`

- from Windows/Mac/Linux GUI:
  - Drag & drop FTP software
    (e.g. Cyberduck, Macfusion, FileZilla, etc.)

For bigger files, use our high-speed GlobusOnline service!

http://www.ucgrid.org/go/go.html
UCLA GlobusOnline guidelines

- Multipoint, multi-stream data transfer
  - fault-tolerant
  - fire-and-forget for server-to-server transfer,
  - 5x faster than `scp`

- 4 quick steps to use Web UI:
  1. have your UCLA grid account ready
  2. create a globus online account at Argonne National Lab
  3. install and run GlobusConnect (if to your desktop)
  4. sign in the globusonline.org and go!

- Command-line interface with restricted SSH

- Caveats:
  - may not be appropriate for file transfers to/from a laptop
  - need Cygwin on Windows XP
Don’t forget Modules

- Modules is for setting environmental variables
  - $PATH
  - $LD_LIBRARY_PATH
  - other additional env variables.

- Common commands:
  - current: module list
  - available: module available
  - load: module load matlab
  - unload: module unload matlab
  - show: module show matlab
Outline

1. via Command Line
   - Log in and access files
   - Prepare for the submission
   - Simple batch submission

2. Special topics
   - A few more words about job running
   - Computing in interactive-scheduler mode
   - R Jobs and Matlab Jobs

3. Summary
Taking advantage of Clusters

Many
Single
Core
Programs

Cluster

Result

One Parallel Program

Cluster

Result

Qiyang Hu Using Hoffman2 Cluster
Before submission, you need to know:

1. the type of your job
   - serial or multithreaded or distributed?

2. the group you belong to

3. the name of your executable or input file
   - Your own code:
     - Compile → Link → Executable
   - Precompiled program (FSL, etc):
     - Check the name of the executable
   - Application:
     - Matlab: m file
     - R: R file
     - LAMMPS, etc: input files
Job types on Hoffman2

- **Serial job:** single thread, single core
- **Shared memory job:** multi-threaded, single node
- **MPI Parallel job:** distributed, multiple node
- **Hybrid job:** MPI and OpenMP
- **Array job:** serial or multi-thread
  same executable, different input
For code programmer:

- Intel compiler: 11.1(default), 12.0, 12.1, 13.0
- GCC: 4.4(default), 4.3, 4.7
- Python: 2.4, 2.6(default), 2.7, 3.1
- Java: 1.6.0_23
- matlab: 7.7, 7.11, 7.14(default)
- R: 2.9, 2.12.0, 2.12.1, 2.12.2(default), 2.13.2, 2.15

To check the software, libs installed on the cluster:

- module av
- ls /u/local/apps/
- ask us!
Which group you are in

Different groups, different policies

1. Research group:
   - up to 14 days
   - can use their own group’s core

2. Others:
   - up to 24 hours
   - 4 GB memory/core
   - up to a certain number of cores/user at a moment

Use `mygroup` command to check!
- See "highp" for your own group’s resource
- "queues": rules to jobs for requested resources.
Outline

1. via Command Line
   - Log in and access files
   - Prepare for the submission
   - Simple batch submission

2. Special topics
   - A few more words about job running
   - Computing in interactive-scheduler mode
   - R Jobs and Matlab Jobs

3. Summary
Of cores, nodes and tasks

In Hoffman2, we will always have: **N tasks ⇔ N cores**
Using ATS queue scripts for 5 types of jobs

- **Serial Jobs**
  - job.q

- **Serial Array Jobs**
  - jobarray.q

- **Multi-threaded Jobs**
  - openmp.q

- **Distributed Jobs**
  - mpi.q for MPI
  - mpishm.q for OpenMP with MPI

- **Application Jobs**
  - application.q
A quick transcript to submit a job

1. have the executable or control file ready
2. type `scriptName.q` and answer prompted questions:
   - type `b` to build cmd file
   - input executable or control file name
   - input how much memory, how long time
   - for parallel job: how many cpus
   - ...
   - type `y` to submit
3. type `myjobs` to check the job status

Tip

- Can submit cmd file later by `qsub`
Example: running Serial C++ program

1. Log into hoffman2: `ssh hoffman2.idre...`
2. Write C++ code: `vi testSerial.cpp`
3. Compile and link:
   ```
g++ -o target testSerial.cpp
   ```
4. Submit & build jobs: just type `job.q`
   - Type `b` to build
   - Enter program name: `target`
   - Enter memory request: `1024 MB for default`
   - Enter time limit: `24 hours for default`
   - Use your own group’s cores: `y` for default
   - Enter arguments: if needed
   - Enter to submit
Example: running MPI C++ program

(1) Log into hoffman2: `ssh -l ...`

(2) Write C++ code w/ MPI2 API: `vi testMPI.cpp`

(3) Compile and link: `Makefile → make` or `mpiCC -o[-c] target testMPI.c`

(4) Submit & build jobs in hoffman2: `mpi.q`

- Type `b` to build
- Enter program name: `target`
- Enter memory request: `1024 MB for default`
- Enter time limit: `24 for default`
- Use your own group’s cores: `y` for default
- Enter task numbers: `8` for our example
- Enter arguments: if needed
- Enter to submit
Example: running Matlab using queue scripts

(1) Log into login node: `ssh -l ...`
(2) Write `.m` file: `vi test.m`
(3) Submit & build jobs in hoffman2: `matlab.q`

- Type `b` to build
- Enter control file name: `test`
- Enter a message option: `bea` for default
- Enter memory request: `1024 MB` for default
- Enter time limit: `24` for default
- Use your own group’s cores: `y` for default
- Enter arguments: if needed
- Enter to submit
Most-commonly-used SGE commands

- To submit a job:
  \[ \texttt{qsub myjob.cmd} \]

- To determine the status of a job:
  \[ \texttt{myjobs (ATS scripts)} \]

- To cancel a job:
  \[ \texttt{qdel [-f] jobNum} \]

For more information

Use \texttt{man} command, for example: \texttt{man qsub}
Outline

1 via Command Line
   - Log in and access files
   - Prepare for the submission
   - Simple batch submission

2 Special topics
   - A few more words about job running
   - Computing in interactive-scheduler mode
   - R Jobs and Matlab Jobs

3 Summary
Outline

1. via Command Line
   - Log in and access files
   - Prepare for the submission
   - Simple batch submission

2. Special topics
   - A few more words about job running
   - Computing in interactive-scheduler mode
   - R Jobs and Matlab Jobs

3. Summary
### Summary

**A few more words about job running**

Computing in interactive-scheduler mode

**R Jobs and Matlab Jobs**

<table>
<thead>
<tr>
<th>Group</th>
<th>Job time</th>
<th>Max slots/usr</th>
<th>Guaranteed start time</th>
<th>Job type</th>
<th>SGE –1 option</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contribute</td>
<td>0 ~ 14 days</td>
<td>as purchased</td>
<td>&lt; 24 hrs</td>
<td>any</td>
<td>highp</td>
</tr>
<tr>
<td></td>
<td>0 ~ 24 hrs</td>
<td>unlimited</td>
<td>none</td>
<td>any</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>may change</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>General</td>
<td>0 ~ 24 hrs</td>
<td>400</td>
<td>none</td>
<td>any</td>
<td></td>
</tr>
<tr>
<td>Campus</td>
<td>0 ~ 2 hours</td>
<td>600</td>
<td>none</td>
<td>serial, shm, jobarray</td>
<td>express</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>usually &lt; 5 min</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Interactive</td>
<td>0 ~ 24 hrs</td>
<td>8</td>
<td>immediately</td>
<td>any</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>if available</td>
<td></td>
<td>i</td>
</tr>
</tbody>
</table>

Qiyang Hu

Using Hoffman2 Cluster
More SGE commands

- To changes the attributes of submitted but pending jobs:
  qalter

- To hold a queued job to prevent it running:
  qhold [jobid:taskid]

- To release a held job:
  qrls

- To display node information:
  qhost [-j]
More words on checkpoints

- Job’s running time on Hoffman2 is limited
  - for campus group: as short as 24 hours.

- Application-level solution: *(recommended)*
  - Save your data periodically in a restart file.
  - Resubmit and restart from where it left off.

- System-level solution:
  - Cluster has BLCR kernal library installed.
  - Serial & shared-mem jobs OK.
  - MPI job in test.
Outline

1. via Command Line
   - Log in and access files
   - Prepare for the submission
   - Simple batch submission

2. Special topics
   - A few more words about job running
   - Computing in interactive-scheduler mode
   - R Jobs and Matlab Jobs

3. Summary
Two steps in interactive-scheduler mode

1. Obtain an interactive session
   - interactive session = reservation of resources.
   - Reservation should correspond to your job requirements.
   - Can request nodes up to 24 hours.
   - Using SGE command: `qrsh`

2. Submit/run your job upon

   **Do not** use login node to run your program!
   Just use "`qrsh -l i`" to do test-running.
Using qrsh to request resources

- 1 options:

commonly used parameters:

- `i` (or `interactive`): Request use the int-session nodes
- `time` (or `h_rt`): Wall-clock time limit (default = 2 hrs)
- `mem` (or `h_data`): Request memory size per core
  - Max 1 GB/core for campus user

parameters separated by commas without any space.

Example: request a single core for 2 hours

```
qrsh -l i,mem=1G,time=2:00:00
qrsh -l i,h_data=1024M,h_rt=2:00:00
```
Using `qrsh` to request multiple cores

- **-pe option**
  - OpenMP: `-pe shared 8`
  - MPI: `-pe dc* 22`
  - Hybrid: `-pe 4threads* 20`

- To reserve an entire node:
  - `-l exclusive=True`

**Examples: request an entire node for 4 hour**

- `qrsh -l i,mem=1G,time=4:00:00,exclusive=True`
Better understanding for PEs on Hoffman2

- PE for OpenMP: shared
- PE for MPI: dc*
- PE for hybrid or double memory request: 2threads*
- PE for hybrid or high memory w/ whole node reservation: 8threads*
After request, we can submit/run jobs:

- **Serial, shared-mem, most app job:**
  - same as in a local machine.

- **MPI job:** extra work needed

---

**Example: MPI job (**test**) with 12 cores, 1GB/CPU, for 2 hours**

1. Request CPUs from any nodes:
   
   \[ qrsh \ -l \ i,mem=1G,time=2:00:00 \ -pe \ dc\ast\ 12 \ -now \ n \]

2. Obtain SGE environment variables:
   
   \[ source \ /u/local/bin/set_qrsh_env.sh \]

3. Launch MPI job in OpenMPI:
   
   \[ mpiexec \ -n \ $NSLOTS \ ./test \]
Outline

1. via Command Line
   - Log in and access files
   - Prepare for the submission
   - Simple batch submission

2. Special topics
   - A few more words about job running
   - Computing in interactive-scheduler mode
   - R Jobs and Matlab Jobs

3. Summary
R as a typical CLI application

- Run R interactively:
  - If running R serially: `qrsh -l i`
  - If running R parallelly: `qrsh -l i,exclusive`
  - `module load R`
  - `R`

- Run R in batch:
  - `R.q`

- About R in parallel:
  - multithreading (R 2.14): `multicore`
  - distributed (MPI) (R 2.12): `snow(Rmpi) or npRmpi`
  - both need to modify `cmd` file.

Further info to check

- [https://idre.ucla.edu/hoffman2/software/r](https://idre.ucla.edu/hoffman2/software/r)
- specific library docs
If you want to run a Matlab application:

- Multithreading is default from v7.11
  - take either one slot or one whole node.

- We only have limited number of licenses.
  - 6 for general, 4 for compiler
  - 2 for statistical toolbox, ...

- 2 ways to run matlab jobs
  1. in matlab GUI, via interactive session
  2. in batch, via matlab.q or matexe.q

Special note on newly installed Matlab 7.14

- Parallel toolbox: temporarily not working.
- Singlethread by compiler: temporarily not working.
Matlab GUI

1. **enable X11-forwarding when login:**
   - `ssh hoffman2.idre.ucla.edu -X -l ...`

2. **request an interactive session:**
   - `qrsh -l i,exclusive=True,time=4:00:00`

3. **load matlab module:**
   - `module load matlab`

4. **run matlab:**
   - `matlab`

---

To start matlab with single-thread mode

`matlab`
Mablab batch mode

- `matlab.q` will do 2 steps:
  1. compiling your `m` script to an executable
  2. run the executable as a general job

- Can do 2 steps separately:
  1. `run matmcc.q`
  2. `run matexe.q`

- Parallel Compute Toolbox will need extra work.
  1. export configuration file
  2. add extra code and modify your `m` file

Tip: sometimes hybriding does a better job!

- `qrsh + mcc` do the compilation.
- `matexe.q` do the job submission.
Outline

1. via Command Line
   - Log in and access files
   - Prepare for the submission
   - Simple batch submission

2. Special topics
   - A few more words about job running
   - Computing in interactive-scheduler mode
   - R Jobs and Matlab Jobs

3. Summary
Short answers for survey questions

- How to interactively run my application?
  Ans: use NX client + qrsh

- How to submit my job which will run in batch mode?
  Ans: use ATS queue scripts (job.q, mpi.q, etc)

- How to do HUGE data transferring?
  Ans: use GlobusOnline.

- How to let my job wait less?
  Ans: request short time and less mem.

- How to make my job running faster?
  Ans: request the whole node if possible.

- How to submit a bunch of jobs simultaneously?
  Ans: use job array or qsub -hold_jid [JobName].

- How to use my group’s contributed cores?
  Ans: use highp.

- How to run jobs with longer times (>24 hours)?
  Ans: add checkpoints.
IDRE is helping you!

- Hosting: resources
  - clusters (Hoffman2, UC C²)
  - storages (high performance, archival)
  - web services (RIM, Grid, GlobusOnline)
- Participating: research projects
- Consulting: supports, code clinics, helps
- Tutoring: classes, virtual summer school

Contact HPC consultant

hpc@ucla.edu
Backup slides
UCLA GlobusOnline guidelines

- Data transfer with fault-tolerant, fire-and-forget, 5x faster than `scp`

- 4 quick steps to use Web UI:
  1. have your UCLA grid account ready
  2. create a globus online account at Argonne National Lab
  3. install and run Globus Connect software
  4. sign in the globusonline.org and go!

- Command-line interface with restricted SSH is available for client-side scripting.

- Caveats:
  - may not be appropriate for file transfers to/from a laptop
  - need Cygwin on Windows XP
Running array jobs with `jobarray.queue`

- **Job array**: same executable, different input (variables/files)
- **Each core/task** → specific input file.
- **Input files**:
  - names must include a sequence number.
  - save in the same directory.
- Your code must identify the ID of tasks in Hoffman2.
  - For compiled code:
    - use `getenv("SGE_TASK_ID")` function
  - For script program:
    - use the `$SGE_TASK_ID` environment variable
- Run `jobarray.q` and submit
Example: writing C++ program for array jobs

**testArray.cpp**

```cpp
#include <iostream>
#include <fstream>
#include <sstream>
#include <string>

using namespace std;

int main( int argc, char* argv[] ){
    stringstream testID;
    testID << getenv( "SGE_TASK_ID" );

    string infileName="in";
    string outfileName="out";
    infileName += testID.str()+".dat";
    outfileName += testID.str()+".dat";

    ifstream infile( infileName.c_str() );
    ofstream outfile( outfileName.c_str() );

    int i, j;
    infile >> i >> j ;
    outfile << "i = " << i << endl;
    outfile << "j = " << j << endl;
    return 0;
}
```

Qiyang Hu  Using Hoffman2 Cluster
Advanced job array submission

- More controls on job ids and task ids.
- 3 switches:
  - `hold_jid`: to specify dependency on a job_id
  - `hold_jid_ad`: to specify dependencies between tasks of different array jobs
  - `tc`: to define max number of concurrent jobs in the job array
- example:
  
  Qsub -N job1 -t 1:25 script1.cmd
  Qsub -hold_jid job1 -N job2 -t 26:50 script1.cmd
  Qsub -hold_jid job2 -N job3 -t 51:52 script1.cmd
Running high-memory jobs

Serial:
- No need to combine the options of `-pe` and `-l`!
- Example: Serial job require 3GB memory →

  #!$ -l mem=3G

MPI (e.g. 3 mpi procs, 8GB per proc):
- use `mpi.q` to allocate 3 core, 8G/core
- `h_data` or `mem`: still per core