HPC basics and introduction to Xanadu cluster

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Computational Biology Core

UCONN
UNIVERSITY OF CONNECTICUT
A non textbook introduction...
Development of models begins at small scale.

Working on your laptop is convenient, simple.

Actual analysis, however is slow.

“Scaling up” typically means a small server or fast multi-core desktop.

Speed exists, but for very large models, not significant.

Single machines don’t scale up forever.
For the larger problems/models, a different approach is required
High-performance computing (HPC)

High-Performance computing involves mainly distinct computer processors working together on the same problem/calculation.

Large problem/calculations are divided into smaller parts and distributed among the many computers.

HPC is a cluster of quasi-independent computers which are coordinated by a central scheduler.
Typical HPC cluster

SGE: Sun Grid Engine
PBS: Portable Batch System
SLURM: Simple Linux Utility for Resource Management

/\$HOME
/data_storage
HPC architecture: Xanadu (Queue/Partition info)

Queue/Partition | Nodes
--- | ---
xeon/general | xanadu01-11
amd/general | shangrila01-19, xanadu20-28
himem1-5 | xanadu29-31
gpu /xeon/ general | xanadu01

cpu: 4
RAM: 8GB
cpu: 32 – 48
RAM: 128 – 512 GB
Performance comes at a price: **Complexity**

- Applications must be written specifically to take advantage of distributed computing
- Debugging becomes more of a challenge

*Applications must be written specifically to take advantage of distributed computing.*

- Explicitly split your problem into smaller “chunks”
- “Message passing” between processes
Parallel Computing on a Large Number of Servers is More Efficient than using Specialized Systems
Accessing Xanadu
Get an account

https://bioinformatics.uconn.edu/contact-us/  or  google search : CBC UCONN
Connecting to Xanadu...
Xanadu

- Login Node
  - CPU: 4
  - RAM: 8 GB

Queue/Partition | Nodes
--- | ---
xeon/general | xanadu01-11
amd/general | shangrila01-19 xanadu20-28
himem1-5 | xanadu29-31
gpu /xeon/general | xanadu01

xanadu-submit-ext.cam.uchc.edu
xanadu-submit-int.cam.uchc.edu
Putty: https://www.chiark.greenend.org.uk/~sgtatham/putty/latest.html or google search “putty”

Open Putty it will open window1.
1. Provide host name e.g. username@xanadu-submit-ext.cam.uchc.edu
2. Expand SSH tab and select X11 (shown in window2)
3. Enable X11 forwarding by selecting it. (window2)
4. Scroll up the left panel and select Session.(window1)
5. Name your session e.g. BBC_cluster and click save tab to save.
6. Your session name should appear in saved sessions. Double click on your session name to connect to server with SSH session.
Login: On the submit-int node (Storrs and Outside Health Centre)

Use VPN (Open Pulse secure)

1. Open Pulse secure
2. Add new connection
3. Set Server URL to : vpn.uchc.edu/cam
4. Save
5. Connect and login with CAM ID and Passwd
Connecting to Xanadu

xanadu-submit-int Node: ssh <user_name>@xanadu-submit-int.cam.uchc.edu
Xanadu-submit-ext Node: ssh <user_name>@xanadu-submit-ext.cam.uchc.edu
Login: (using terminal on mac)

Logged on ext-submit node:

```bash
$ ssh vsingh@xanadu-submit-ext.cam.uchc.edu
vsingh@xanadu-submit-ext.cam.uchc.edu's password: _
```

```bash
$ ssh vsingh@xanadu-submit-ext.cam.uchc.edu
vsingh@xanadu-submit-ext.cam.uchc.edu's password: _
Last failed login: Thu Jun 1 17:04:42 EDT 2017 from d80h208.public.uconn.edu on ssh:notty
There were 3 failed login attempts since the last successful login.
Last login: Thu Jun 1 09:11:14 2017 from 137.99.88.208
xanadu-submit-ext - $ _
```
ssh username@xanadu-submit-ext.cam.uchc.edu

Queue/Partition      Nodes
xeon/general         xanadu01-11
amd/general           shangrila01-19 xanadu20-28
himem1-5              xanadu29-31
gpu /xeon/            xanadu01
general

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- cpu: 2
- RAM: 8GB
- cpu: 32 – 48
- RAM: 128 – 512 GB
ssh username@xanadu-submit-ext.cam.uchc.edu

```
srun --pty bash
sbatch myscript.sh
```

**Queue/Partition** | **Nodes**
--- | ---
xeon/general | xanadu01-11
amd/general | shangrila01-19
himem1-5 | xanadu29-31
gpu /xeon/ general | xanadu01
Common Linux commands

- `pwd` : Present Working directory
- `cd destination` : Change directory to destination
- `cd` : Change directory to $HOME
- `ls` : List contents of directory
- `cp source/file destination/file` : Copy file from source in destination folder
- `mv source/file destination/file` : Move file from source to destination folder
- `mv name name2` : Rename file from name to name2
- `touch filename` : Create an empty file with name filename
- `mkdir directory` : Make directory
- `rm file` : delete file
- `rm -r directory` : delete file with its content
- `~` : Home directory
- `cat` : Read contents of file
- `less` : Contents of file, scroll, q to quit it
- `head -10 file` : first 10 lines of file
- `tail -10 file` : Bottom 10 lines of file

Resources: [http://linuxcommand.org/writing_shell_scripts.php](http://linuxcommand.org/writing_shell_scripts.php)
• NANO
• VIM
• EMACS

Classical learning curves for some common editors

Text Editors

Notepad

nano

Visual Studio

vim

emacs
Demo Nano and VIM
Software/tool/packages on cluster

Environment Modules:
The Environment Modules package provides for the dynamic modification of a user's environment via module files.

module avail : List modules that are available
module load modulefile : Loads the module to user environment
module list : List modules that are loaded
module unload modulefile : Unloads module from user environment
module display modulefile : Displays information on module
swap [modulefile1] modulefile2 : Switch loaded modulefile1 with modulefile2.
Demo module
## Xanadu Resources

### Partitions

```
xanadu-submit-ext ~ $ sinfo
PARTITION AVAIL TIMELIMIT NODES STATE NODELIST
general* up infinite 4 mix xanadu-[20-22,25]
general* up infinite 13 idle xanadu-[01-11,23-24]
xeon up infinite 11 idle xanadu-[01-11]
amd up infinite 4 mix xanadu-[20-22,25]
amd up infinite 2 idle xanadu-[23-24]
himem up infinite 4 idle xanadu-[30-33]
xanadu-submit-ext ~ $
```

```
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xanadu-submit-ext ~ $ sinfo -N -l -p general
Thu Jun 1 22:41:40 2017

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<tr>
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```
### Partition: himem

```bash
xanadu-submit-ext ~ $ sinfo -N -l -p himem
Thu Jun 1 22:42:13 2017

<table>
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<tr>
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<th>NODES</th>
<th>PARTITION</th>
<th>STATE</th>
<th>CPUS</th>
<th>S:C:T</th>
<th>MEMORY</th>
<th>TMP_DISK</th>
<th>WEIGHT</th>
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```
## Summary of the nodes in the Xanadu cluster

<table>
<thead>
<tr>
<th>NODELIST</th>
<th>PARTITION</th>
<th>PROCESSOR TYPE</th>
<th>CPUS</th>
<th>MEMORY</th>
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</table>
Interactive session
ssh `username@xanadu-submit-ext.cam.uchc.edu`

**Queue/Partition**  **Nodes**

- **xeon/general**  xanadu01-11
- **amd/general**  shangrila01-19  xanadu20-28
- **himem1-5**  xanadu29-31
- **gpu /xeon/ general**  xanadu01

**Start of an interactive session**

```bash
tsxanadu-submit-ext
sxanadu-submit-int
```

```bash
ssh username@xanadu-submit-ext.cam.uchc.edu
do stuff
srun --pty bash
```

This command starts an interactive session.
Xanadu

Queue/Partition  Nodes

text content
Queue/Partition  |  Nodes
--- | ---
xeon/general  |  xanadu01-11
amd/general  |  shangrila01-19, xanadu20-28
himem1-5  |  xanadu29-31
gpu /xeon/ general  |  xanadu01
Interactive session

srun --pty bash

screen -S screen_name : Start screen session
srun --pty bash : Start interactive session
hostname : Confirm interactive session
........ : Run code /commands (wget/ftp/others)
Ctrl + A + D : Detach an active screen

screen -r NNNN : Attach a detached screen
screen -ls : List all screens
screen -X -S NNNN quit : Kill or quit a screen session
Composing a script for cluster

Script:
1. Resource request
   • number of CPUs,
   • computing expected duration,
   • amounts of RAM or disk space, etc
2. Job commands
   • describe **tasks** that must be done, software which must be run
Resource request:

#!/bin/bash

#SBATCH --j myscript  Is the name of your job
#SBATCH --n 1  Request number of tasks
#SBATCH --N 1  This line requests that the cores are all on node.
Only change this to >1 if you know your code uses a message passing protocol like MPI. SLURM makes no assumptions on this parameter -- if you request more than one core (-n > 1) and your forget this parameter, your job may be scheduled across nodes; and unless your job is MPI (multinode) aware, your job will run slowly, as it is oversubscribed on the master node and wasting resources on the other(s).

#SBATCH --c 1  Request number of cores for your job
#SBATCH --p general  This line specifies the SLURM partition (in this instance it will be the general partition) under which the script will be run

#SBATCH --mail-user=first.last@uconn.edu  Email which the notification should be sent to
#SBATCH --mail-type=END  Mailing options to indicate the state of the job. In this instance it will send a notification at the end
#SBATCH -o myscript-%j.out  Specifies the file to which the standard output will be appended
#SBATCH -e myscript-%j.err  Specifies the file to which standard error will be appended
more on Resource request:

```
#!/bin/bash
#SBATCH --time=10-01:00:00 # days-hh:mm:ss
#SBATCH --job-name=masurca_KG
#SBATCH --mail-user=user@uconn.edu
#SBATCH --mail-type=ALL
#SBATCH --comment=dataset_with_jump_libraries
#SBATCH -N 1
#SBATCH -n 1
#SBATCH -c 8
#SBATCH --mem-per-cpu=10240 # 10GB
or #SBATCH --mem=100G
#SBATCH -o filterGTF-%j.output
#SBATCH -e filterGTF-%j.error
```
**Job commands:**

They are regular linux/module commands

```bash
#SBATCH --job-name=myscript
#SBATCH --n 1
#SBATCH --N 1
#SBATCH --c 1
#SBATCH --partition=general
#SBATCH --mail-type=END
#SBATCH --mail-user=first.last@uconn.edu
#SBATCH -o myscript-%j.out
#SBATCH -e myscript-%j.err

echo "Hello World"
```

Save the script as `myscript.sh`
Submit the script:

```
$ sbatch myscript.sh
```

Monitor Job:

```
$ squeue
```
squeue -j jobIDNUMBER

$ clear$ squeue -j 301013

<table>
<thead>
<tr>
<th>JOBID</th>
<th>PARTITION</th>
<th>NAME</th>
<th>USER</th>
<th>ST</th>
<th>TIME</th>
<th>NODES</th>
<th>NODELIST(REASON)</th>
</tr>
</thead>
<tbody>
<tr>
<td>301013</td>
<td>amd</td>
<td>ProtMasN</td>
<td>vsingh</td>
<td>R</td>
<td>21:49:06</td>
<td>1 xanadu-24</td>
<td></td>
</tr>
</tbody>
</table>

**JOB STATE CODES**

Jobs typically pass through several states in the course of their execution. The typical states are PENDING, RUNNING, SUSPENDED, COMPLETING, and COMPLETED. An explanation of each state follows.

- **CA** CANCELLED: Job was explicitly cancelled by the user or system administrator. The job may or may not have been initiated.
- **CD** COMPLETED: Job has terminated all processes on all nodes with an exit code of zero.
- **CF** CONFIGURING: Job has been allocated resources, become ready for use (e.g. booting).
- **CG** COMPLETING: Job is awaiting resource allocation.
- **F** FAILED: Job terminated with non-zero exit code or other failure condition.
- **NF** NODE_FAIL: Job terminated due to failure of one or more allocated nodes.
- **PD** PENDING: Job is awaiting resource allocation.
- **PR** PREEMPTED: Job terminated due to preemption.
- **R** RUNNING: Job currently has an allocation.
- **ST** STOPPED: Job has an allocation, but execution has been stopped with SIGSTOP signal.
  CPUs have been retained by this job.
- **S** SUSPENDED: Job has an allocation, but execution has been suspended and CPUs have been released for other jobs.
- **TO** TIMEOUT: Job terminated upon reaching its time limit.
$squeue -u vsingh

<table>
<thead>
<tr>
<th>JOBID</th>
<th>PARTITION</th>
<th>NAME</th>
<th>USER</th>
<th>ST</th>
<th>TIME</th>
<th>NODES</th>
<th>NODELIST(REASON)</th>
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</thead>
<tbody>
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<td>himem</td>
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<td>vsingh</td>
<td>PD</td>
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<td>(Priority)</td>
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<tr>
<td>301089</td>
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<td>ProtMasW</td>
<td>vsingh</td>
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<td>1</td>
<td>(Priority)</td>
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</table>

$squeue -u vsingh -t PENDING

$ squeue -u vsingh -t PENDING

<table>
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<th>PARTITION</th>
<th>NAME</th>
<th>USER</th>
<th>ST</th>
<th>TIME</th>
<th>NODES</th>
<th>NODELIST(REASON)</th>
</tr>
</thead>
<tbody>
<tr>
<td>301086</td>
<td>himem</td>
<td>ProtMasN</td>
<td>vsingh</td>
<td>PD</td>
<td>0:00</td>
<td>1</td>
<td>(Priority)</td>
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<tr>
<td>301089</td>
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<td>vsingh</td>
<td>PD</td>
<td>0:00</td>
<td>1</td>
<td>(Priority)</td>
</tr>
</tbody>
</table>

$squeue -u userID -t RUNNING
scontrol show jobid <jobid>

$ scontrol show jobid 301086

JobId=301086 JobName=ProtMasNoSOAP
UserId=vsingh(183147) GroupId=domain users(10000) MCS_label=N/A
Priority=5262 Nice=0 Account=pi-wegrzyn QOS=general
JobState=PENDING Reason=Priority Dependency=(null)
Requeue=1 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
RunTime=00:00:00 TimeLimit=UNLIMITED TimeMin=N/A SubmitTime=2017-06-28T15:50:23
Deadline=N/A
PreemptTime=None SuspendTime=None SecsPreSuspend=0
Partition=himem AllocNode:Sid=xanadu-submit-ext:32674
ReqNodeList=(null) ExcNodeList=(null)
NumNodes=1-1 NumCPUs=30 NumTasks=30 CPUs/Task=1 ReqB:S:C:T=0:0:*:*: *
TRES=cpu=30,mem=512000,node=1 Socks/Node=* NtasksPerN:B:S:C=0:0:*:1 CoreSpec=* 
MinCPUsNode=1 MinMemoryNode=500G MinTmpDiskNode=0 Features=(null) Gres=(null)
Reservation=(null) OverSubscribe=OK Contiguous=0 Licenses=(null) Network=(null)
Command=/home/CAM/vsingh/protea_repens/scripts/assemble_protea_config_noSOAPassembly.sh WorkDir=/home/CAM/vsingh/protea_repens/scripts
StdErr=/home/CAM/vsingh/protea_repens/LogFiles/ProtMasNoSOAP-301086.error
StdIn=/dev/null StdOut=/home/CAM/vsingh/protea_repens/LogFiles/ProtMasNoSOAP-301086.output Power=

scontrol show jobid –dd <jobid>
Script submission and other commands

sbatch myscript.sh : Sumit script for execution
squeue : Status of Jobs currently running on cluster (all users)
squeue -j jobIDNUMBER : Status of job with jobIDNumber
squeue -u UserID : Status of all the jobs submitted by user
scancel jobID_number : Delete job with jobID_number
scancel <jobid> <index> : Delete an array job
scancel -u UserID : Delete all the jobs of a user
#!/bin/bash
#SBATCH --mail-user=user@uconn.edu
#SBATCH --mail-type=ALL
#SBATCH --ntasks=1
#SBATCH --mem=1G
#SBATCH --array=1-1002%100
#SBATCH --output=fastqc_%A_%a.out
hostname

cd /NGSseq/data
module load fastqc/0.11.5

echo "SLURM_JOBID: " $SLURM_JOBID
echo "SLURM_ARRAY_TASK_ID: " $SLURM_ARRAY_TASK_ID
echo "SLURM_ARRAY_JOB_ID: " $SLURM_ARRAY_JOB_ID

arrayfile=`ls | awk -v line=$SLURM_ARRAY_TASK_ID '{if (NR == line) print $0}'`

fastqc $arrayfile

This line will create 1002 jobs, but it instructs slurm to limit the total number of simultaneously running jobs to 100. This avoids swamping the queue, and shares bursting level with others in the group.

This will create 1002 files to catch stdin, stdout and stderr for each respective job in the array. If the array job ID is 23678, we will fine 1002 files starting with fastqc_23678_1.out … fastqc_23678_1002.out

Start: Slurm job ID and increase with each array job
Slurm job ID
Array job ID : 1-1002

This will list all the files from the directory (/NGSseq/data) and then pick up one file at a time and then run it through fastqc application.
### Some important Informations:

<table>
<thead>
<tr>
<th>Xanadu</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>User Space</td>
<td>/home/CAM/username or</td>
</tr>
<tr>
<td></td>
<td>/home/FCAM/username</td>
</tr>
<tr>
<td></td>
<td>(default)</td>
</tr>
<tr>
<td>Lab/Group Space</td>
<td>/UCHC/LABS/</td>
</tr>
<tr>
<td></td>
<td>(Request)</td>
</tr>
<tr>
<td>Archiving data</td>
<td>/linuxshare/userfolder</td>
</tr>
<tr>
<td></td>
<td>(Request)</td>
</tr>
<tr>
<td>Collaborative projects</td>
<td>/linuxshare/projects</td>
</tr>
<tr>
<td></td>
<td>(Request)</td>
</tr>
</tbody>
</table>

/scratch: Please do not use this directory as long term storage the disk gets cleaned up regularly.
Data Transfer to/from Xanandu
(wget/ftp/sftp/scp)

DON’T : Do not initiate transfer on Submit nodes

DO : Start an interactive session
    : Use `scp` for small size files
    : For large size files use Globous

Tutorial: https://bioinformatics.uconn.edu/resources-and-events/tutorials/

Section: Data transfer
Reporting Issues or submitting requests

https://bioinformatics.uconn.edu/contact-us/

https://bioinformatics.uconn.edu/contact-us/technical-issues/

Email: cbcsupport@uconn.edu
Cluster Etiquette

Do not run code on the head node.
Do not ssh directly into a node.

Do not submit a large number of jobs without testing.
Do not Hog Resources.

Do monitor your jobs periodically
Monitor your disk usage:
Do not fill up the whole disk with unnecessary output files from your runs.
TOP: Process Status

'D' = uninterruptible sleep
'R' = running
'S' = sleeping
'T' = traced or stopped
'Z' = zombie
Thank you