

# Martinos Center Compute Clusters

---

## Intro

- What are the compute clusters
- How to gain access
- Housekeeping

## Usage

- Log In
- Submitting Jobs
- Queues
- Request CPUs/vmem
- Email Status
- I/O
- Interactive
- Dependencies
  - Daisy Chain
  - Wrapper Script
  - In Progress

## Job Status

- Running Jobs
  - Show Job Status
  - See Standard Output
- Completed Jobs
- Failed Jobs
- Delete Jobs

# Martinos Center Compute Clusters

---

Intro - What are the compute clusters?

## launchpad

At Needham Data Center

127 nodes

~115 “normal” nodes

Two 64 bit Intel Xeon quad cores

56 GB RAM

~12 GPU nodes

Available exclusively for GPU jobs

## tensor

In CNY “cold room”

107 nodes

89 “normal” nodes

Dual cores with 4GB RAM

18 “big” nodes

Dual cores with 8GB RAM each

I will only talk about launchpad today. We recommend you primarily use launchpad. Use tensor if launchpad is full, if launchpad resources are overkill, or if the data for your jobs are local and are slowed by the I/O problem.

# Martinos Center Compute Clusters

---

Intro - How to gain access

Email: [clusteradm \[at\] nmr.mgh.harvard.edu](mailto:clusteradm@nmr.mgh.harvard.edu)  
Let us know who/what/why/how you need access.

# Martinos Center Compute Clusters

---

## Intro - Housekeeping

### Questions?:

- Any specific questions (extend the walltime of your jobs etc.) can be sent to us: clusteradm [at] nmr.mgh.harvard.edu
- General questions can be sent to the group for advice and help: batch-users [at] nmr.mgh.harvard.edu

### Limits:

- We prefer each user to only use 100 job slots during normal usage.
- Evenings/weekends you may use up to 200 slots of CPU/vmem
- While there is a queue, we request you only use 50 CPU/vmem slots

Do not run another directly on launchpad. Submit your jobs. Any programs found running on the master node will be deleted, no exceptions.

### Matlab:

- There are only 60 Matlab licenses for the entire center. For this reason, we recommend any Matlab code submitted for execution should be “compiled” ahead of time. Please see the URL to the article on how to do it.

When the program is compiled, it doesn't use a matlab license and they are no longer under a matlab restriction.

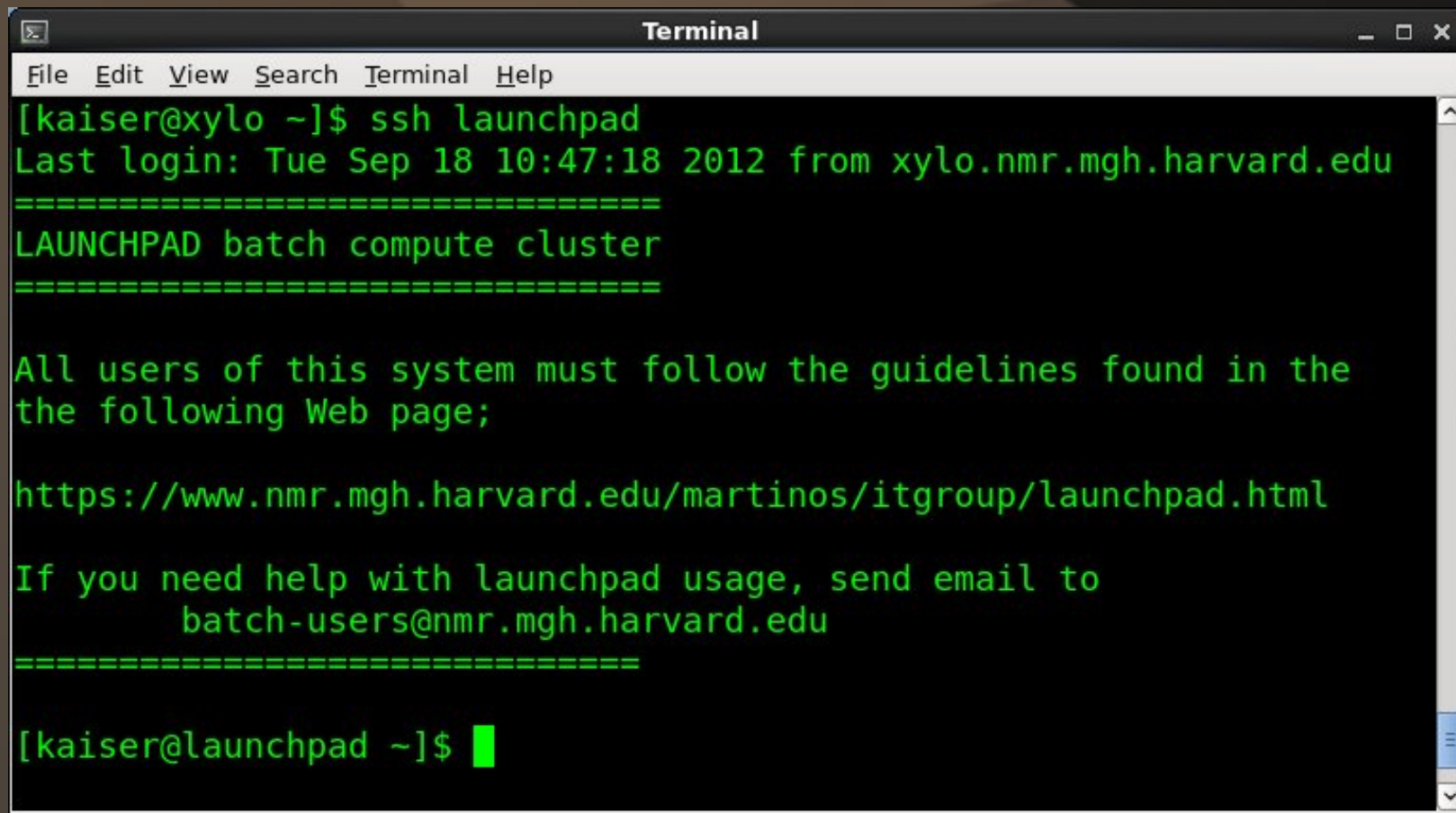
Courtesy of coutu:

<http://nmr.mgh.harvard.edu/martinos/itgroup/deploytool.html>

# Martinos Center Compute Clusters

---

Usage - Log In



```
Terminal
File Edit View Search Terminal Help
[kaiser@xylo ~]$ ssh launchpad
Last login: Tue Sep 18 10:47:18 2012 from xylo.nmr.mgh.harvard.edu
=====
LAUNCHPAD batch compute cluster
=====

All users of this system must follow the guidelines found in the
the following Web page;

https://www.nmr.mgh.harvard.edu/martinos/itgroup/launchpad.html

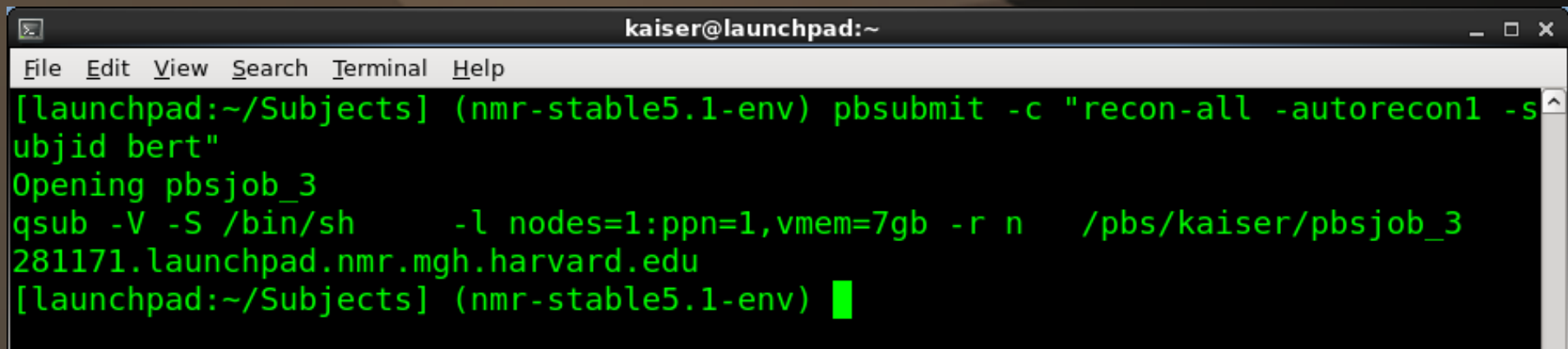
If you need help with launchpad usage, send email to
    batch-users@nmr.mgh.harvard.edu
=====

[kaiser@launchpad ~]$ █
```

# Martinos Center Compute Clusters

---

## Usage – Submitting Jobs



```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) pbsubmit -c "recon-all -autorecon1 -s  
ubjid bert"  
Opening pbsjob_3  
qsub -V -S /bin/sh -l nodes=1:ppn=1,vmem=7gb -r n /pbs/kaiser/pbsjob_3  
281171.launchpad.nmr.mgh.harvard.edu  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

pbsubmit is a wrapper script that:

- formats the command that is executed (/pbs/kaiser/pbsjob\_3)
- automatically selects the default settings (unless overridden)
  - Select the number of nodes (nodes=1)
  - Select the number of CPUs (ppn=1)
  - Select the amount of virtual memory (vmem=7gb)
- submits the job using the qsub command

pbsjob\_3

is the Job Number

281171.launchpad.nmr.mgh.harvard.edu

is the Job ID

# Martinos Center Compute Clusters

## Usage - Queues

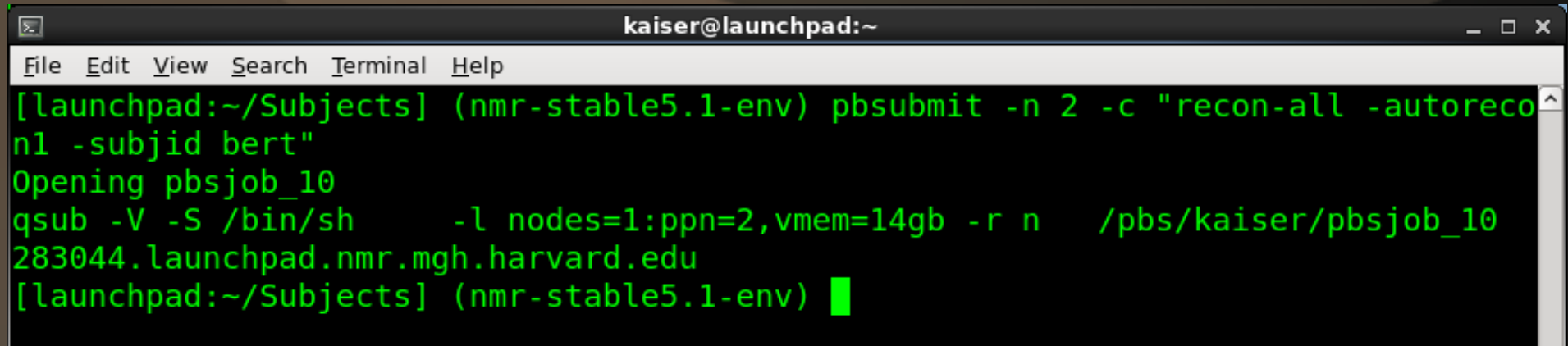
Queue	Priority	Max CPU/User	Description
default	10100	150	Walltime of 96 hours
p20	10200	Unlimited	
p30	10300	Unlimited	
GPU	90	Unlimited	GPU nodes
extended	8000	50	Walltime of 196 hours
matlab	10100	20	Limit of 60 matlab licenses for the Center
max10	10100	10	
max20	10100	20	
max50	10100	50	
max75	10100	75	
max100	10100	100	
max200	8000	200	

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) pbsubmit -q max100 -c "recon-all -aut  
orecon1 -subjid bert"  
Opening pbsjob_4  
qsub -V -S /bin/sh -q max100 -l nodes=1:ppn=1,vmem=7gb -r n /pbs/kaiser/pbs  
job_4  
281184.launchpad.nmr.mgh.harvard.edu  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

# Martinos Center Compute Clusters

---

## Usage - Request CPUs/vmem



```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) pbsubmit -n 2 -c "recon-all -autoreco  
n1 -subjid bert"  
Opening pbsjob_10  
qsub -V -S /bin/sh -l nodes=1:ppn=2,vmem=14gb -r n /pbs/kaiser/pbsjob_10  
283044.launchpad.nmr.mgh.harvard.edu  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

Only request more CPUs or Virtual Memory if you need them.

### CPUs

- You should only request extra CPUs if the program you are running is multi-threaded.
- If you aren't sure if the program is multi-threaded, it probably isn't.

### Virtual Memory

- Only request as much as you need.
- If you aren't sure how much you'll need, run a single test case. Start with the default of 7GB of vmem. If it fails due to a lack of memory, request 14GB. Then 21GB etc...

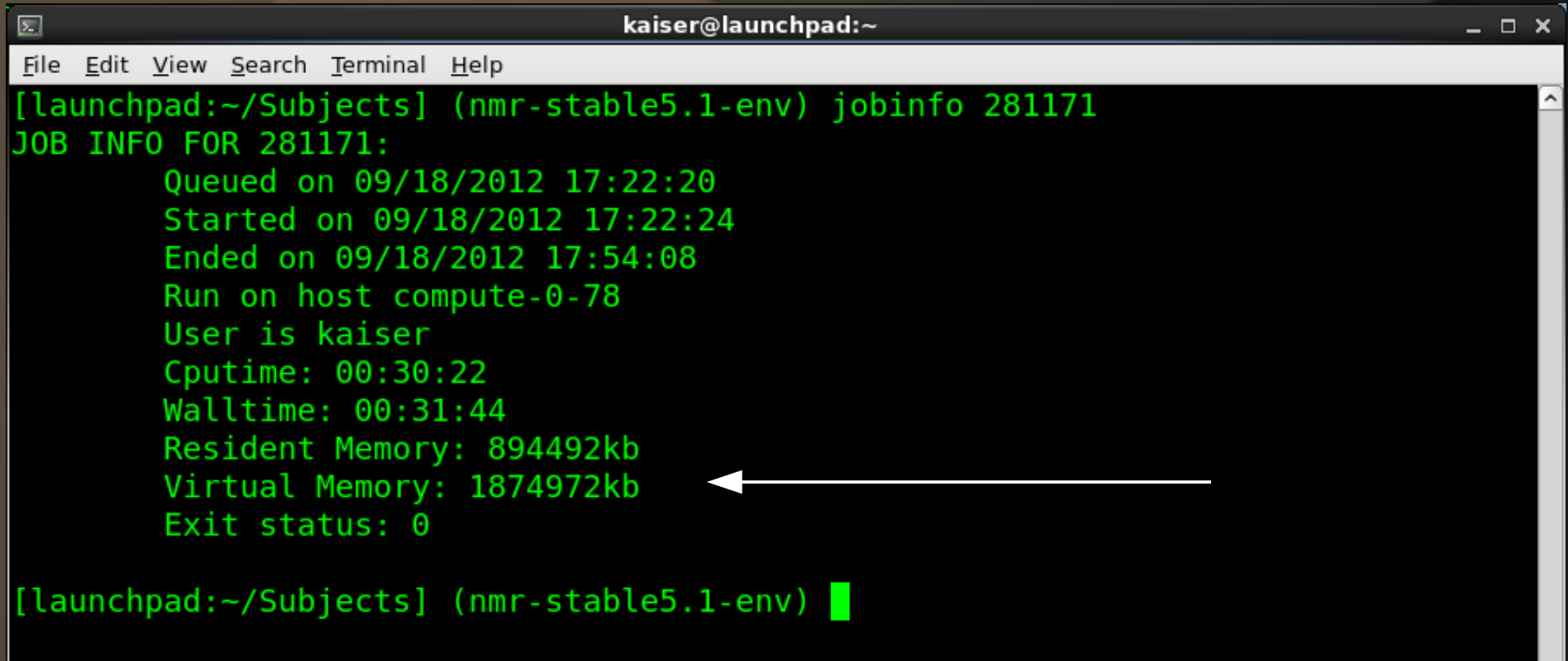
So, how much virtual memory did the job use?



# Martinos Center Compute Clusters

---

Usage – Request CPUs/vmem

A terminal window titled 'kaiser@launchpad:~' with a menu bar (File, Edit, View, Search, Terminal, Help). The terminal output shows job information for job 281171. A white arrow points to the 'Virtual Memory' line.

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) jobinfo 281171  
JOB INFO FOR 281171:  
  Queued on 09/18/2012 17:22:20  
  Started on 09/18/2012 17:22:24  
  Ended on 09/18/2012 17:54:08  
  Run on host compute-0-78  
  User is kaiser  
  Cputime: 00:30:22  
  Walltime: 00:31:44  
  Resident Memory: 894492kb  
  Virtual Memory: 1874972kb  
  Exit status: 0  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

Only used 1.9GB of virtual memory. Safely under the default request of 7GB. No need to ask for more.

Limits – keep in mind that we prefer each user to only use 100 job slots during the day.  
A job that requests 1 CPU and 14GB of vmem counts as two slots worth of resources.  
Submit the jobs to the max50 queue ('-q max50') to self-regulate.

# Martinos Center Compute Clusters

## Usage - Email Status

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) pbsubmit -m kaiser -c "recon-all -aut  
orecon1 -subjid bert"  
Opening pbsjob_5  
qsub -V -S /bin/sh -m abe -M kaiser -l nodes=1:ppn=1,vmem=7gb -r n /pbs/kai  
ser/pbsjob_5  
282509.launchpad.nmr.mgh.harvard.edu  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

Start Execution:

```
pine  
File Edit View Search Terminal Help  
ALPINE 2.02(1266) MESSAGE TEXT INBOX Message 2,  
Date: Wed, 19 Sep 2012 13:09:30 -0400  
From: adm <adm@nmr.mgh.harvard.edu>  
To: kaiser@nmr.mgh.harvard.edu  
Subject: PBS JOB 282509.launchpad.nmr.mgh.harvard.edu  
  
PBS Job Id: 282509.launchpad.nmr.mgh.harvard.edu  
Job Name: pbsjob_5  
Exec host: compute-0-64/4  
Begun execution
```

Finish Execution:

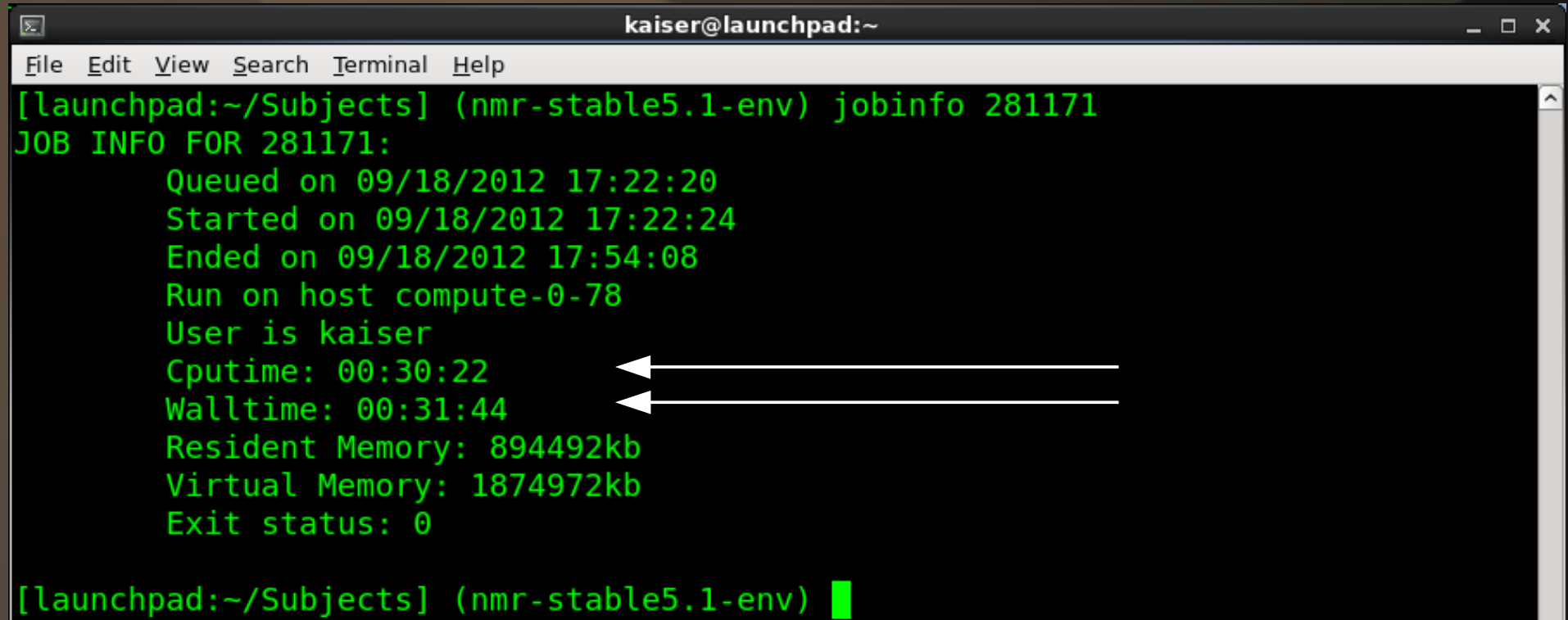
```
pine  
File Edit View Search Terminal Help  
ALPINE 2.02(1266) MESSAGE TEXT INBOX Message 2,  
Date: Wed, 19 Sep 2012 13:18:06 -0400  
From: adm <adm@nmr.mgh.harvard.edu>  
To: kaiser@nmr.mgh.harvard.edu  
Subject: PBS JOB 282509.launchpad.nmr.mgh.harvard.edu  
  
PBS Job Id: 282509.launchpad.nmr.mgh.harvard.edu  
Job Name: pbsjob_5  
Exec host: compute-0-64/4  
Execution terminated  
Exit_status=0  
resources_used.cput=00:07:33  
resources_used.mem=984016kb  
resources_used.vmem=1964488kb  
resources_used.walltime=00:08:36
```

Sends email to user (replace 'kaiser' with your username) on job start and finish

- To receive email only if job completes with an error, append '-e' to command line
- To receive email only upon job completion (error or no error), append '-f' to command line

# Martinos Center Compute Clusters

## Usage - I/O



```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) jobinfo 281171  
JOB INFO FOR 281171:  
    Queued on 09/18/2012 17:22:20  
    Started on 09/18/2012 17:22:24  
    Ended on 09/18/2012 17:54:08  
    Run on host compute-0-78  
    User is kaiser  
    Cputime: 00:30:22  
    Walltime: 00:31:44  
    Resident Memory: 894492kb  
    Virtual Memory: 1874972kb  
    Exit status: 0  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

Compare CPUtime and Walltime. If Walltime is larger than CPUtime, time was wasted in I/O.

This job was run using data from my local machine. Over one minute was wasted transferring data back and forth between launchpad (in Needham) to my computer at Martinos.

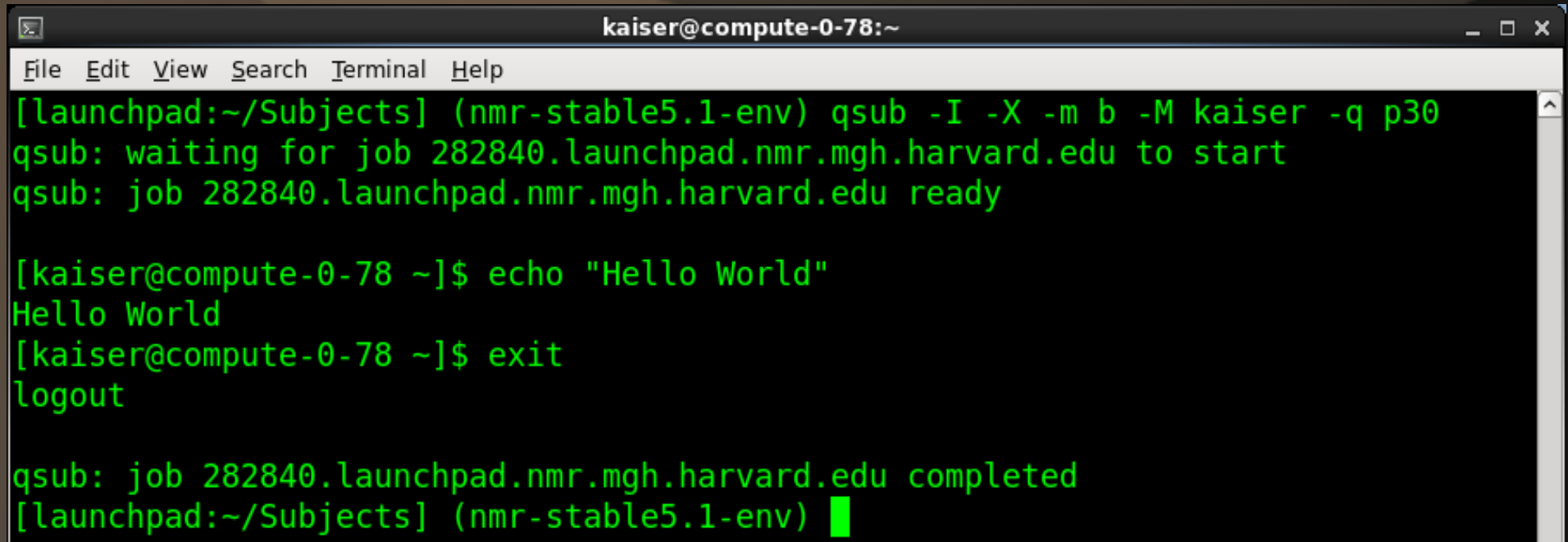
Tips:

- Copy/move local data to /cluster/ directories before running jobs.
- Have scripts/programs write temp data to /cluster/scratch/
- Instead of launchpad, use tensor which lives in CNY.
- Space out submission of jobs so they don't all have large I/O needs at the same time.

# Martinos Center Compute Clusters

---

## Usage – Interactive Jobs

A terminal window titled 'kaiser@compute-0-78:~' with a menu bar (File, Edit, View, Search, Terminal, Help). The terminal shows the following sequence of commands and outputs:

```
[launchpad:~/Subjects] (nmr-stable5.1-env) qsub -I -X -m b -M kaiser -q p30
qsub: waiting for job 282840.launchpad.nmr.mgh.harvard.edu to start
qsub: job 282840.launchpad.nmr.mgh.harvard.edu ready

[kaiser@compute-0-78 ~]$ echo "Hello World"
Hello World
[kaiser@compute-0-78 ~]$ exit
logout

qsub: job 282840.launchpad.nmr.mgh.harvard.edu completed
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

Use the `qsub` command to start an interactive job using the high priority `p30` queue. You will receive an email when the job begins execution. **Replace 'kaiser' with your username!** Actively wait until the job is slated for execution. Don't immediately leave for lunch.

1. As soon as a slot becomes available, the job is assigned a Job ID and you are ssh'ed to the node where your job will execute.
2. Run your commands...
3. When completed, exit out of the node. Your job will not be completed until you exit.

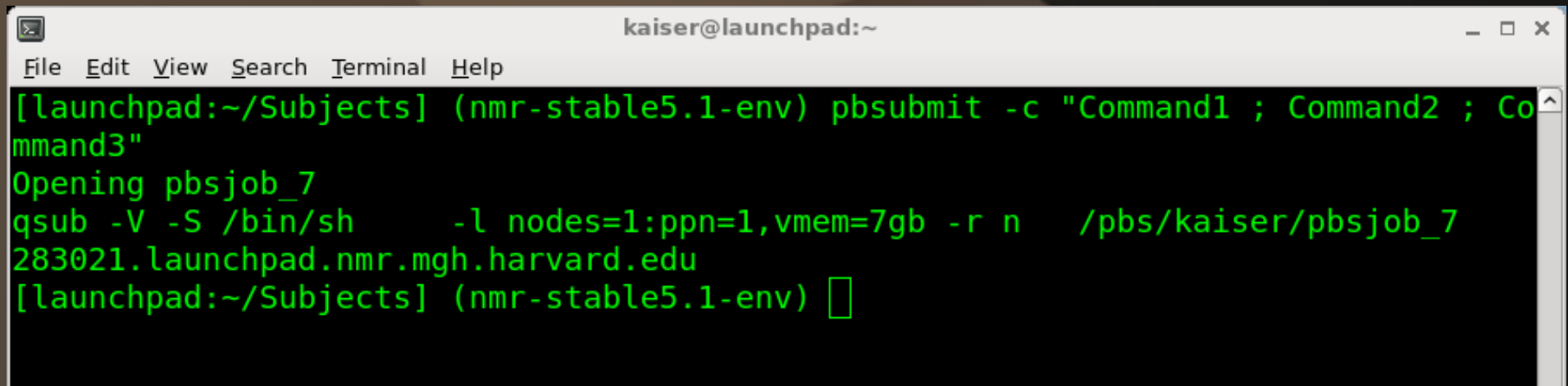
Please attend to an interactive session. As soon as the job begins and you are ssh'ed into the node, you take up a job slot. Exit out of the node as soon as your commands are done. You will continue to take up a job slot until you exit out of the node.

# Martinos Center Compute Clusters

---

Usage – Dependencies – Daisy Chain

If you have a series of commands that you want to execute in a row (one after another). The easiest way to do it is to daisy chain the commands together on the command line:

A terminal window titled 'kaiser@launchpad:~' with a menu bar (File, Edit, View, Search, Terminal, Help). The terminal shows a green prompt '[launchpad:~/Subjects] (nmr-stable5.1-env)'. The user enters the command 'pbsubmit -c "Command1 ; Command2 ; Command3"'. The terminal output shows 'Opening pbsjob\_7', 'qsub -V -S /bin/sh -l nodes=1:ppn=1,vmem=7gb -r n /pbs/kaiser/pbsjob\_7', and '283021.launchpad.nmr.mgh.harvard.edu'. The prompt returns to '[launchpad:~/Subjects] (nmr-stable5.1-env)'.

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) pbsubmit -c "Command1 ; Command2 ; Command3"  
Opening pbsjob_7  
qsub -V -S /bin/sh -l nodes=1:ppn=1,vmem=7gb -r n /pbs/kaiser/pbsjob_7  
283021.launchpad.nmr.mgh.harvard.edu  
[launchpad:~/Subjects] (nmr-stable5.1-env) □
```

The commands are separated on the command line by a colon (;).

Each command will run even if one before it failed.

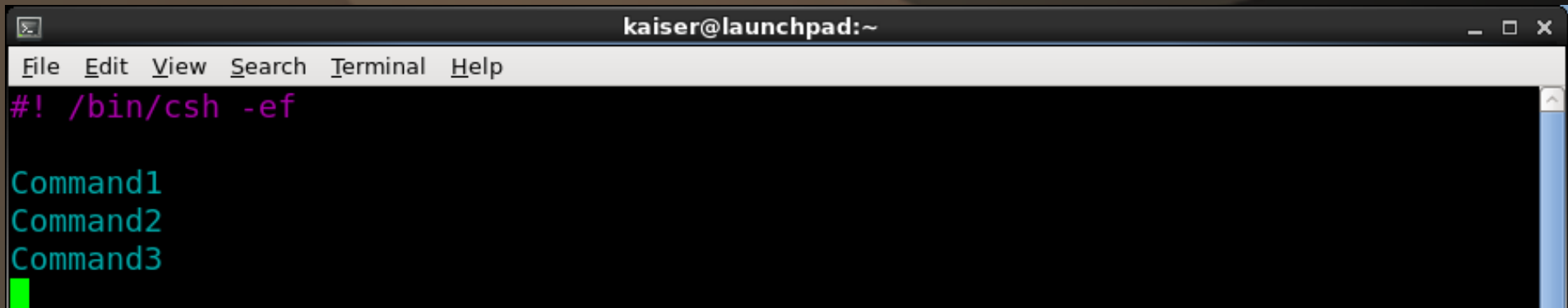
Replace Command1, Command2, Command3 with the specific commands you want to run

# Martinos Center Compute Clusters

---

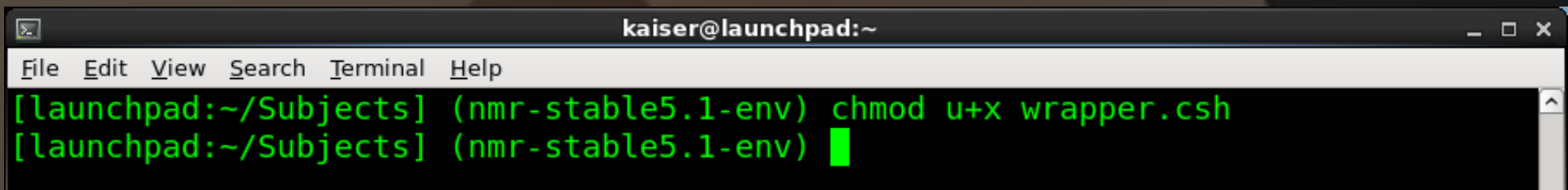
## Usage – Dependencies – Wrapper Script

A more elegant way to do it is to write a wrapper script. Use a text editor to create a file called wrapper.csh with these contents:



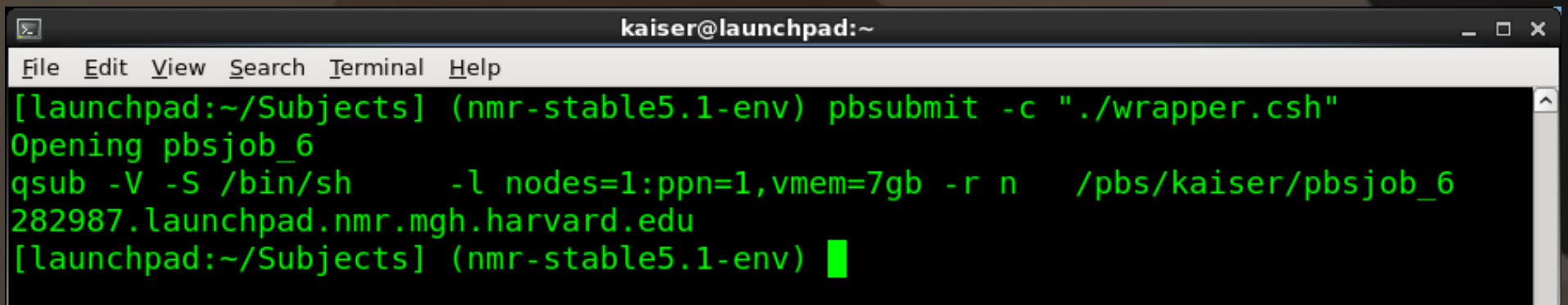
```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
#!/bin/csh -ef  
  
Command1  
Command2  
Command3  
█
```

The -e flag above, instructs the script to exit if any of the individual commands exit with an error. Make the script executable:



```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) chmod u+x wrapper.csh  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

Submit the script for execution:



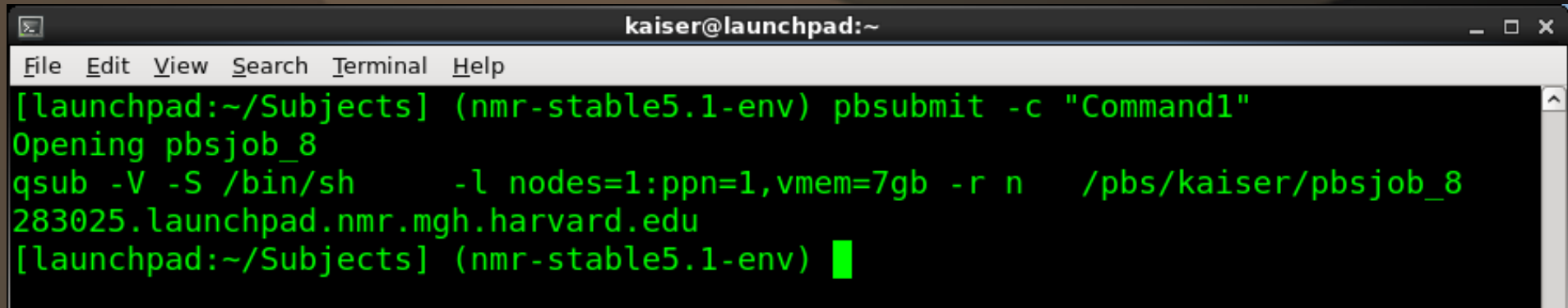
```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) pbsubmit -c "./wrapper.csh"  
Opening pbsjob_6  
qsub -V -S /bin/sh -l nodes=1:ppn=1,vmem=7gb -r n /pbs/kaiser/pbsjob_6  
282987.launchpad.nmr.mgh.harvard.edu  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

# Martinos Center Compute Clusters

---

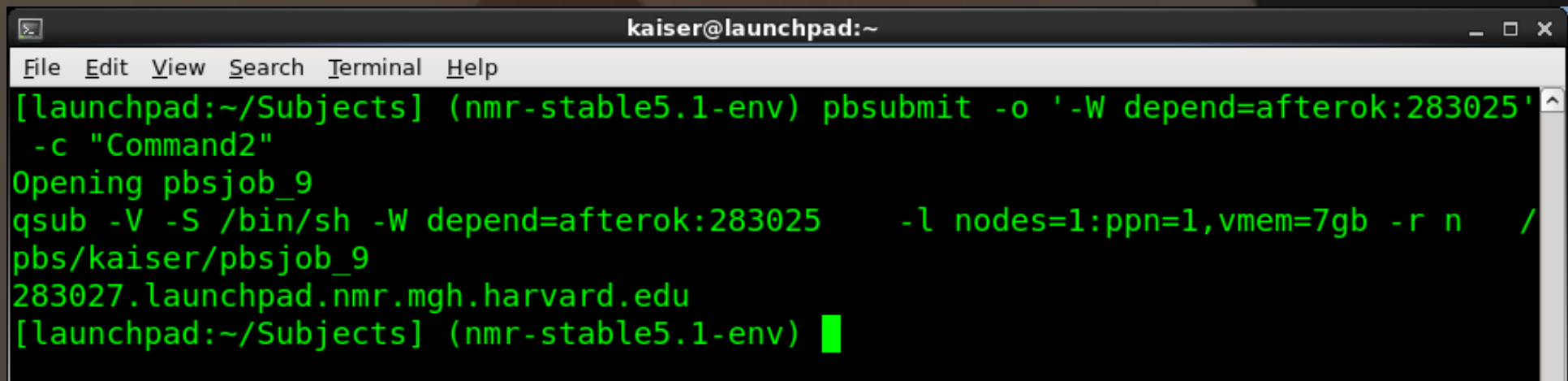
Usage – Dependencies – In Progress

If you already have a job running....



```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) pbsubmit -c "Command1"  
Opening pbsjob_8  
qsub -V -S /bin/sh -l nodes=1:ppn=1,vmem=7gb -r n /pbs/kaiser/pbsjob_8  
283025.launchpad.nmr.mgh.harvard.edu  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

And you want to start another job that will run immediately after the first job completes without error:



```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) pbsubmit -o '-W depend=afterok:283025'  
-c "Command2"  
Opening pbsjob_9  
qsub -V -S /bin/sh -W depend=afterok:283025 -l nodes=1:ppn=1,vmem=7gb -r n /  
pbs/kaiser/pbsjob_9  
283027.launchpad.nmr.mgh.harvard.edu  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

This second job will be held until the first one completes without error. If the first job exits with an error, the second job will not run.

# Martinos Center Compute Clusters

## Job Status - Running Jobs – Show Job Status

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) qstat  
283568.launchpad      pbsjob_201      krienens       02:57:33 R default  
283569.launchpad      pbsjob_252      khoa           02:46:16 R default  
283604.launchpad      pbsjob_34       spaeth         01:47:00 R default  
283605.launchpad      pbsjob_35       spaeth         01:45:58 R default  
283617.launchpad      ...0_real011.txt slbowen        00:34:47 R default  
283672.launchpad      pbsjob_2        kbickart       00:27:59 R max10  
283673.launchpad      pbsjob_3        kbickart       00:20:10 R max10  
283675.launchpad      pbsjob_4        kbickart       00:20:22 R max10  
283676.launchpad      pbsjob_5        kbickart       00:20:26 R max10  
283677.launchpad      pbsjob_6        kbickart       00:18:20 R max10  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

Job ID	-	Job Name	-	User	-	CPUtime	-	State	-	Queue
--------	---	----------	---	------	---	---------	---	-------	---	-------

[R]unning  
[Q]ueued

Additional options:  
To see just your jobs:  
qstat -u <username>  
qstat | grep <username>

To get all your running and queued jobs:  
qstat | grep <username> | grep -w R  
qstat | grep <username> | grep -w W

Another Job Status command is 'showq':  
To see just your jobs:  
showq -u <username>  
showq | grep <username>

To get all your running and queued jobs:  
showq -r -u <username>  
showq -i -u <username>



# Martinos Center Compute Clusters

---

Job Status - Running Jobs – See Standard Output

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) pbsubmit -c "sleep 60;echo 'Hello World';sleep 60"  
Opening pbsjob_12  
qsub -V -S /bin/sh -l nodes=1:ppn=1,vmem=7gb -r n /pbs/kaiser/pbsjob_12  
283802.launchpad.nmr.mgh.harvard.edu  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

Job is running:

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) qstat | grep kaiser  
283802.launchpad pbsjob_12 kaiser 00:00:00 R default  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

Check on the standard output of the job:

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) jobinfo -o 283802  
Hello World  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

To see the standard error of an actively running job; 'jobinfo -e <Job ID>'

# Martinos Center Compute Clusters

---

## Job Status - Completed Jobs

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) jobinfo 283802  
JOB INFO FOR 283802:  
    Queued on 09/20/2012 11:03:00  
    Started on 09/20/2012 11:03:03  
    Ended on 09/20/2012 11:05:03  
    Run on host compute-0-115  
    User is kaiser  
    Cputime: 00:00:00  
    Walltime: 00:02:00  
    Resident Memory: 3540kb  
    Virtual Memory: 321552kb  
    Exit status: 0  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

Check the Exit Status of the job. Zero means it successfully completed.

The job script, standard output, standard error and the exit status are all saved as separate text files in your pbs directory:

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) ls /pbs/kaiser/pbsjob_12*  
/pbs/kaiser/pbsjob_12          /pbs/kaiser/pbsjob_12.o283802  
/pbs/kaiser/pbsjob_12.e283802 /pbs/kaiser/pbsjob_12.status  
/pbs/kaiser/pbsjob_12.env  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

# Martinos Center Compute Clusters

---

## Job Status - Failed Jobs

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) pbsubmit -c "BadCommand"  
Opening pbsjob_13  
qsub -V -S /bin/sh -l nodes=1:ppn=1,vmem=7gb -r n /pbs/kaiser/pbsjob_13  
283853.launchpad.nmr.mgh.harvard.edu  
[launchpad:~/Subjects] (nmr-stable5.1-env) jobinfo 283853  
JOB INFO FOR 283853:  
    Queued on 09/20/2012 11:34:11  
    Started on 09/20/2012 11:34:14  
    Ended on 09/20/2012 11:34:14  
    Run on host compute-0-48  
    User is kaiser  
    Cputime: 00:00:00  
    Walltime: 00:00:00  
    Resident Memory: 0kb  
    Virtual Memory: 0kb  
    Exit status: 127  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

Ack! My job finished with an Exit Status of 127.

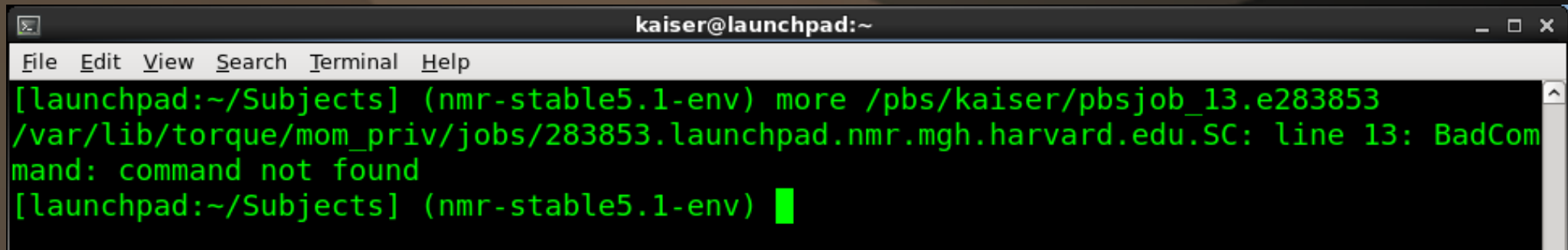
How do I troubleshoot???

# Martinos Center Compute Clusters

---

## Job Status - Failed Jobs

Check the standard error and standard output files for any hints:



```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) more /pbs/kaiser/pbsjob_13.e283853  
/var/lib/torque/mom_priv/jobs/283853.launchpad.nmr.mgh.harvard.edu.SC: line 13: BadCom  
mand: command not found  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

## Other Possible Hints:

### Resource Related

- Check vmem is under the requested amount (default: 7GB)

- Check walltime is under the requested amount (default: 96 hours)

### Command Related

- Check standard error and standard output files!!

- If the program is home-made, was it compiled for the launchpad architecture?

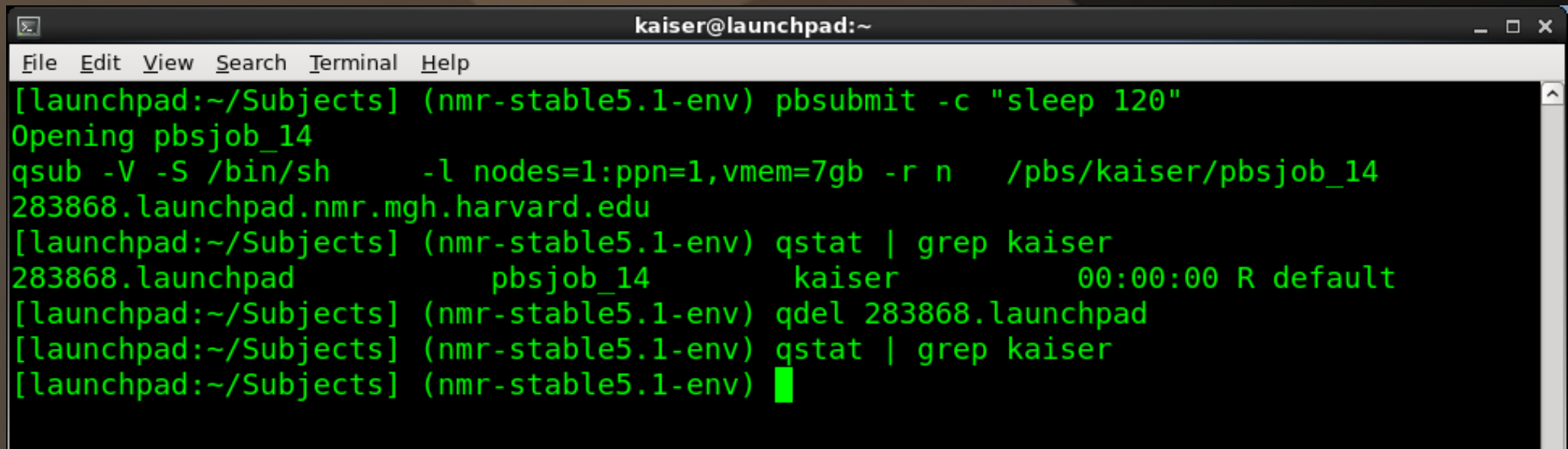
- Test-run the command locally. If it breaks, the problem is probably not with the cluster.

# Martinos Center Compute Clusters

---

## Job Status - Delete Jobs

You submit a job, realize there is a mistake and want to delete it:

A terminal window titled 'kaiser@launchpad:~' with a menu bar (File, Edit, View, Search, Terminal, Help). The terminal shows a sequence of commands and their outputs. The user submits a job with 'pbsubmit -c "sleep 120"', which opens 'pbsjob\_14'. The user then checks the job status with 'qstat | grep kaiser', showing the job is running. Finally, the user deletes the job with 'qdel 283868.launchpad', and a subsequent 'qstat | grep kaiser' command shows no results.

```
kaiser@launchpad:~  
File Edit View Search Terminal Help  
[launchpad:~/Subjects] (nmr-stable5.1-env) pbsubmit -c "sleep 120"  
Opening pbsjob_14  
qsub -V -S /bin/sh -l nodes=1:ppn=1,vmem=7gb -r n /pbs/kaiser/pbsjob_14  
283868.launchpad.nmr.mgh.harvard.edu  
[launchpad:~/Subjects] (nmr-stable5.1-env) qstat | grep kaiser  
283868.launchpad pbsjob_14 kaiser 00:00:00 R default  
[launchpad:~/Subjects] (nmr-stable5.1-env) qdel 283868.launchpad  
[launchpad:~/Subjects] (nmr-stable5.1-env) qstat | grep kaiser  
[launchpad:~/Subjects] (nmr-stable5.1-env) █
```

# Martinos Center Compute Clusters

---

Adios