A NERSC Primer for DES Data Analysis and Simulations or: How to meet your next DES publication deadline ...

DES Large Chicagoland Meeting, December 9, 2014

National Energy Research Scientific Computing Center

NOVEL ALGORITHMS HELP ILLUMINATE DARK ENERGY

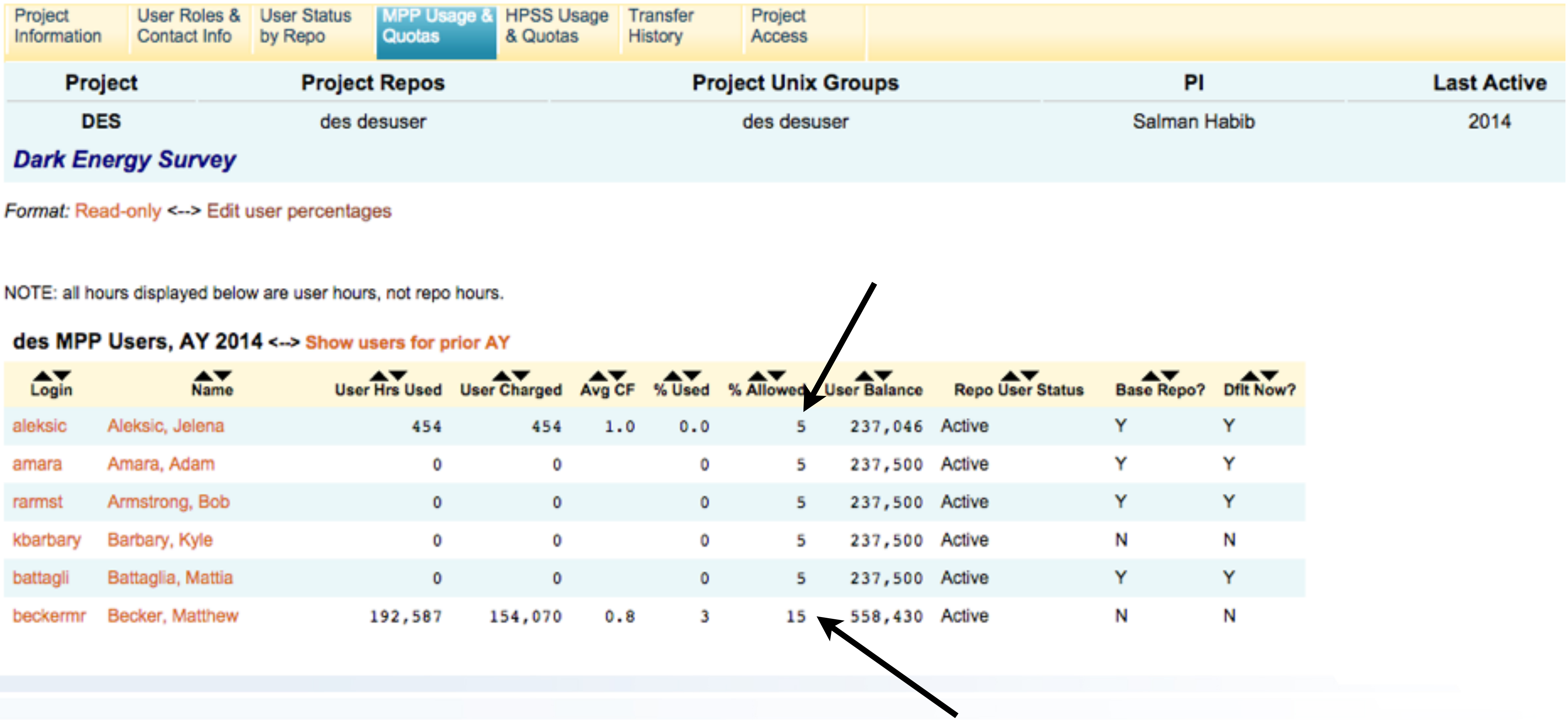
Using NERSC supercomputers, Berkeley researchers developed novel computational tools to help the Dark Energy Survey identify and monitor Type 1a supernovae.

Introduction

- **First question: Should I run at NERSC?**
  - If you run DES analysis tasks regularly, yes!
  - NERSC supports jobs of all sizes, from serial jobs to very large parallel jobs
  - If you have a large number of small jobs to run, you can bundle them up easily and run them as one large job (examples will follow)
  - Queuing times for jobs might seem annoying at first, but with some thought can be kept reasonably short (more on that to follow)
- **Second question: How do I get started?**
  - If you haven’t done so yet, send an email to habib@anl.gov and you will be added to the DES allocation at NERSC
  - Lots of information on NERSC webpages: https://www.nersc.gov/users/getting-started/

DES Allocation at NERSC

- **DES has this year an allocation of 4.5M core hours, requested more for next year**
  - With your account you will get by default (controlled by Salman) 5% of time of that
  - If you need more, you can ask once you have used up your allocation
  - Salman (PI of DES allocation) can monitor usage
  - You therefore cannot “by mistake” use up all the DES allocation :)



Project	Project Repos	Project Unix Groups	PI	Last Active
DES	des desuser	des desuser	Salman Habib	2014

Dark Energy Survey

Format: Read-only <--> Edit user percentages

NOTE: all hours displayed below are user hours, not repo hours.

des MPP Users, AY 2014 <--> Show users for prior AY

Login	Name	User Hrs Used	User Charged	Avg CF	% Used	% Allowed	User Balance	Repo User Status	Base Repo?	Dflt Now?
aleksic	Aleksic, Jelena	454	454	1.0	0.0	5	237,046	Active	Y	Y
amara	Amara, Adam	0	0		0	5	237,500	Active	Y	Y
rarmst	Armstrong, Bob	0	0		0	5	237,500	Active	Y	Y
kbarbary	Barbary, Kyle	0	0		0	5	237,500	Active	N	N
battagli	Battaglia, Mattia	0	0		0	5	237,500	Active	Y	Y
beckermr	Becker, Matthew	192,587	154,070	0.8	3	15	558,430	Active	N	N

Getting Started, File systems

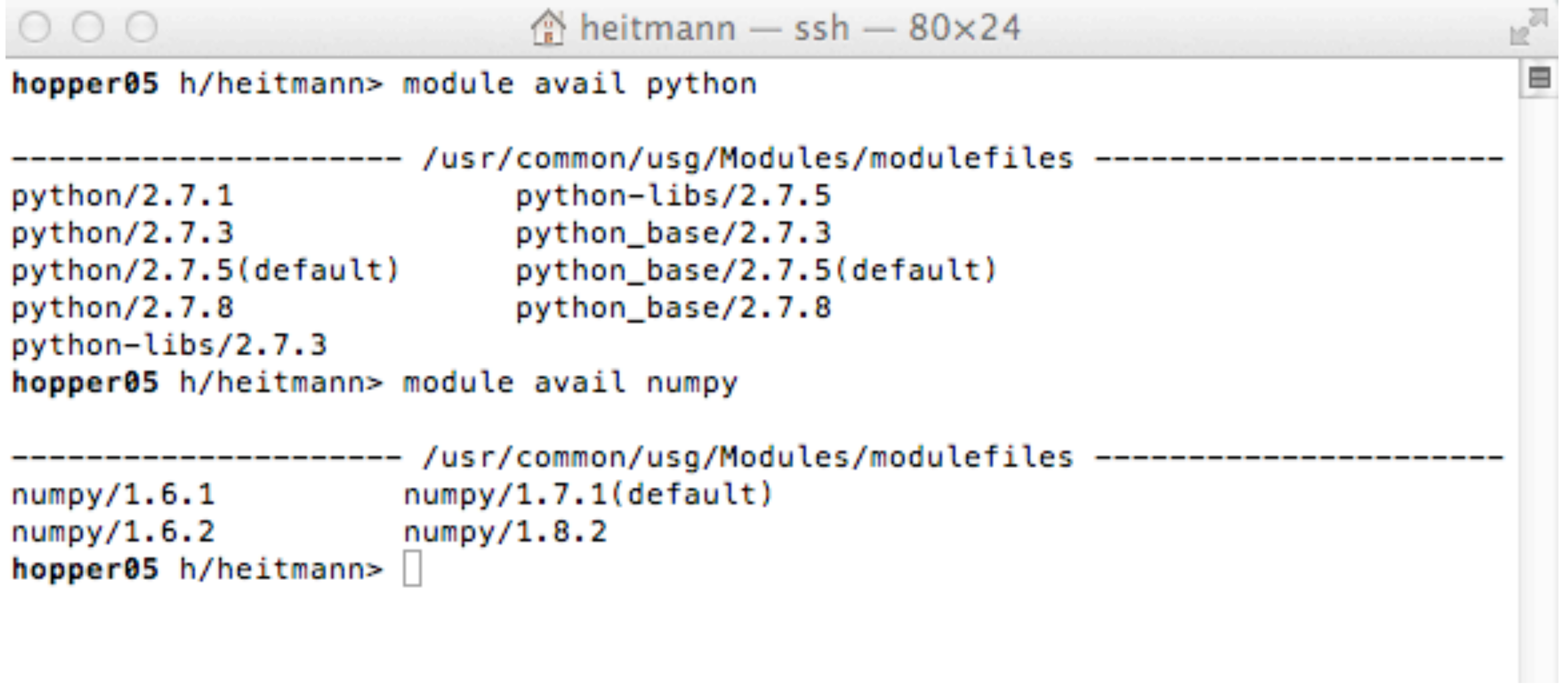
https://www.nersc.gov/users/data-and-file-systems/

- **Two major machines: Hopper and Edison (Carver will retire next year), all machines share common file systems**
- **File systems:**
  - Your home directory: 40GB, backed up, good place to store your source codes, not a good place to run analysis or store data
  - Project space for DES: /project/projectdirs/des, accessible for everybody in the group, 40TB shared amongst all DES users, holds currently some DES data in /project/projectdirs/des/wl/desdata/DES, not backed up but will also not be deleted. DES can purchase more storage if needed
  - Scratch space: /scratch/scratchdirs/yourname (automatically added), 20TB, not backed up and will be purged after some time if the data is not touched, good for short-term use
  - HPSS: tape, to get there, type hsi, leads you to your tape partition, almost indefinite amount of space, not backed up but not purged, htar allows you to package small files and put them on tape

Finding Software of Interest

https://www.nersc.gov/users/software/

- NERSC uses modules to help you:
  - module avail: shows you all the software packages available
  - module list: shows you what is loaded by default in your user environment
  - module load xxx (where xxx can be idl, python, any number of compilers, gsl, mathematica....) will load software package xxx which you can then use
  - module avail xxx lets you search for a specific software package

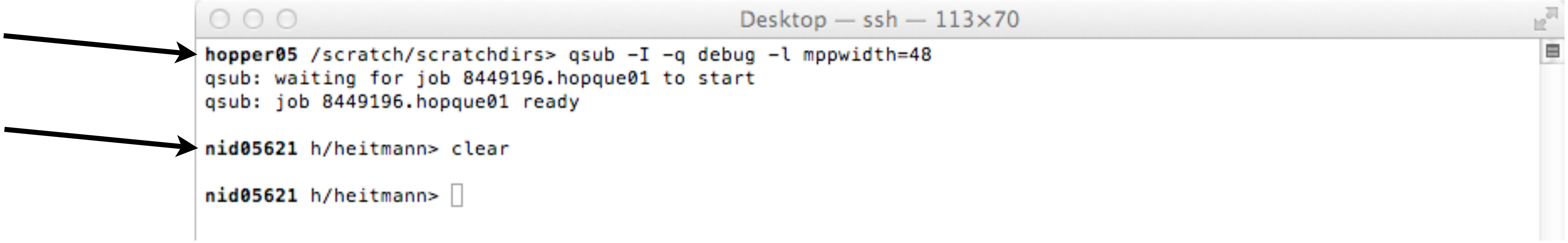


```
hopper05 h/heitmann> module avail python

--------------------- /usr/common/usg/Modules/modulefiles ----------------------
python/2.7.1              python-libs/2.7.5
python/2.7.3              python_base/2.7.3
python/2.7.5(default)     python_base/2.7.5(default)
python/2.7.8              python_base/2.7.8
python-libs/2.7.3
hopper05 h/heitmann> module avail numpy

--------------------- /usr/common/usg/Modules/modulefiles ----------------------
numpy/1.6.1          numpy/1.7.1(default)
numpy/1.6.2          numpy/1.8.2
hopper05 h/heitmann> 
```

Queues and Job Submission

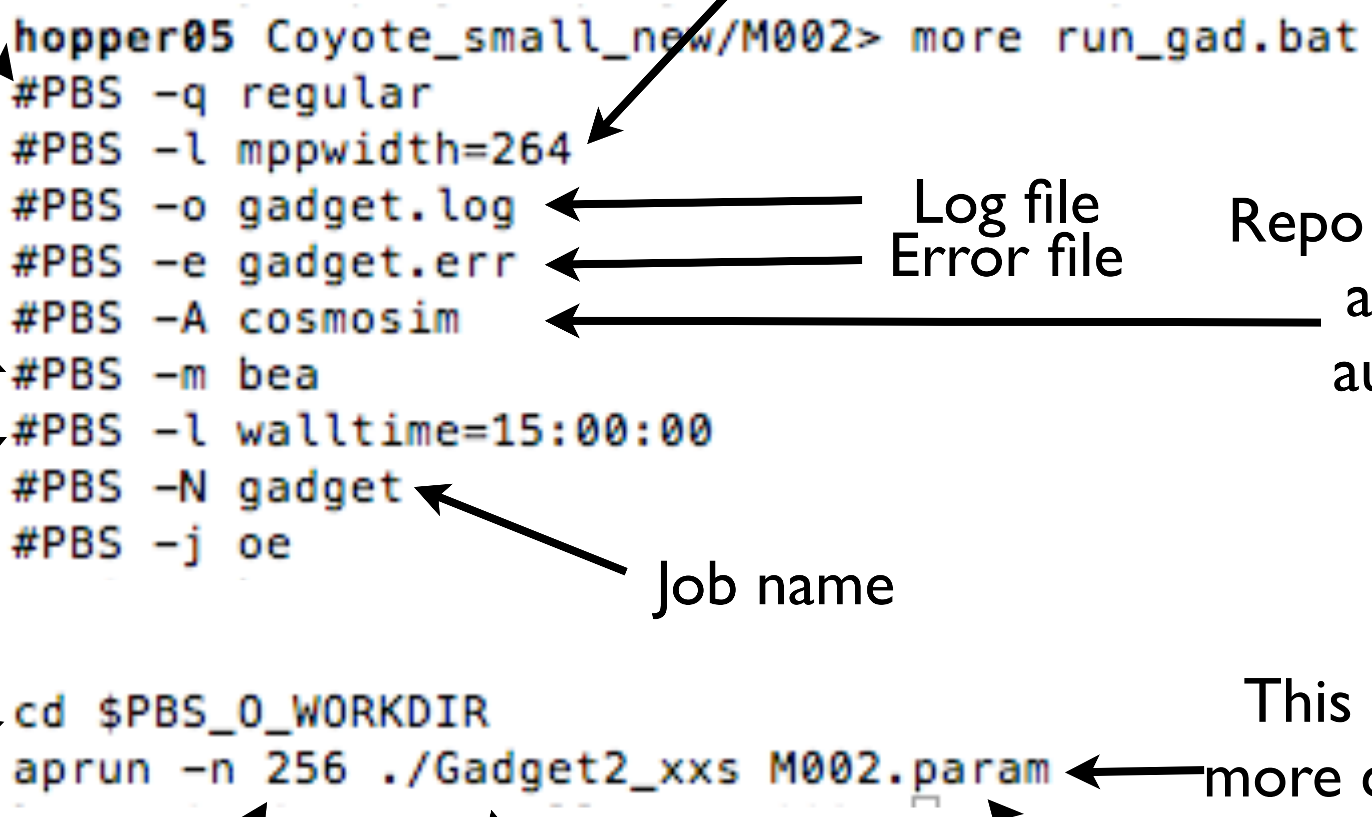
https://www.nersc.gov/users/queues/

- **When you log into Hopper or Edison, you will be on a front-end node, here you can compile your code**
- **DO NOT run your jobs on the front-end, this would slow down everybody else**
- **Instead, login in via an interactive queue or submit jobs to the back-end nodes**
  - Interactive job: qsub -I -q debug -l mppwidth=48
  - On hopper, this gets you 48 cores (or 2 nodes) for 30 minutes
  - To run your job: aprun -n 48 ./a.out
  - Or: submit a job via qsub run.sh (example for submission script next)



```
hopper05 /scratch/scratchdirs> qsub -I -q debug -l mppwidth=48
qsub: waiting for job 8449196.hopque01 to start
qsub: job 8449196.hopque01 ready

nid05621 h/heitmann> clear

nid05621 h/heitmann> 
```

Example Submission Script



```
hopper05 Coyote_small_new/M002> more run_gad.bat
#PBS -q regular
#PBS -l mppwidth=264
#PBS -o gadget.log
#PBS -e gadget.err
#PBS -A cosmosim
#PBS -m bea
#PBS -l walltime=15:00:00
#PBS -N gadget
#PBS -j oe

cd $PBS_O_WORKDIR
aprun -n 256 ./Gadget2_xxs M002.param
```

Queue, depends on number of cores and length of the job, system will pick correct one automatically

Number of cores, divisible by 24 (number of cores per node)

Log file

Error file

Repo used for run, if you are only in DES, automatically set

Sends you an email when job begins/ ends/aborts

Guess for run time

Job name

Puts you into your work directory (without it, job will try running in your home directory)

This line can be more complicated, e.g. include threads

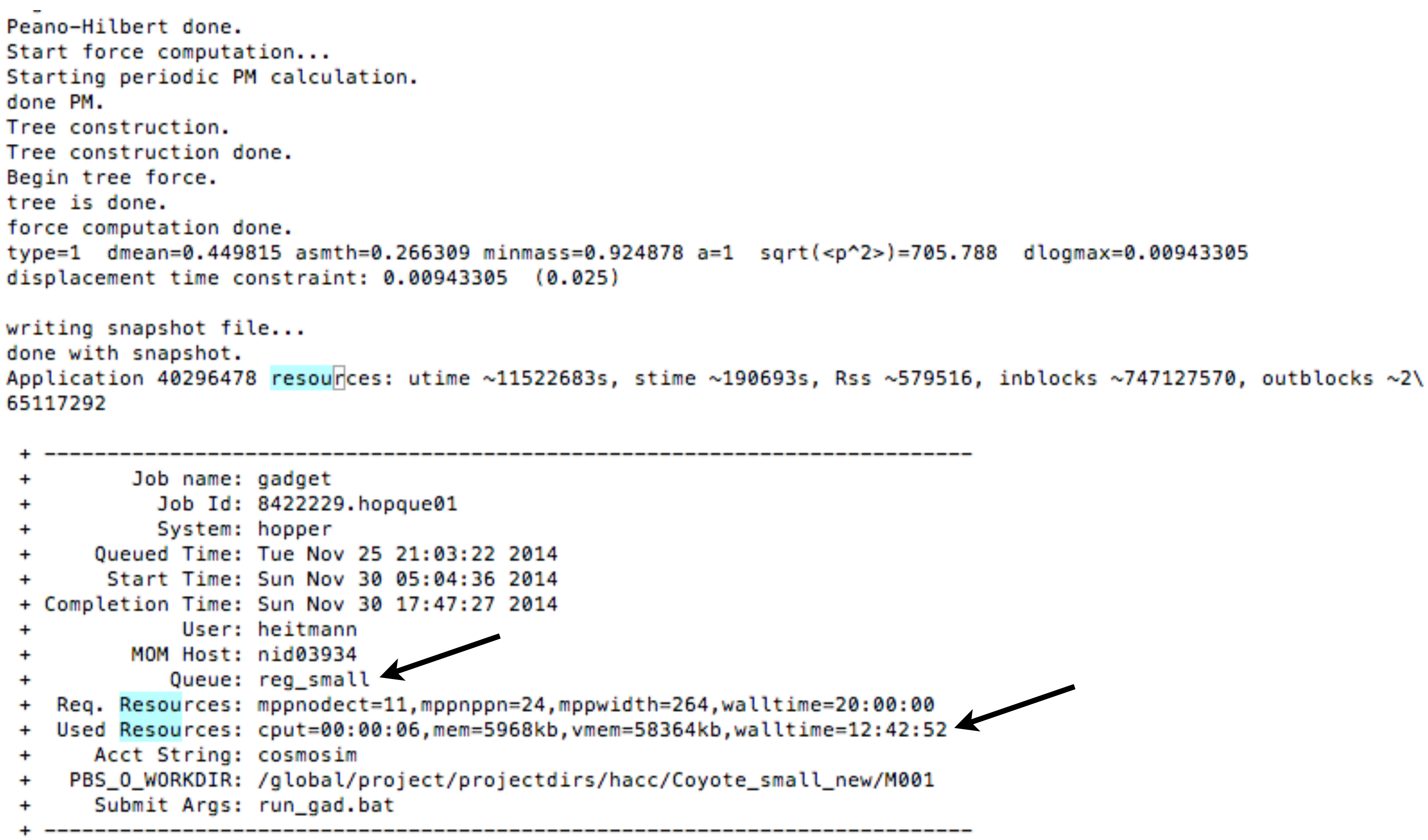
Number of cores

Executable

Input

https://www.nersc.gov/users/computational-systems/hopper/running-jobs/example-batch-scripts/

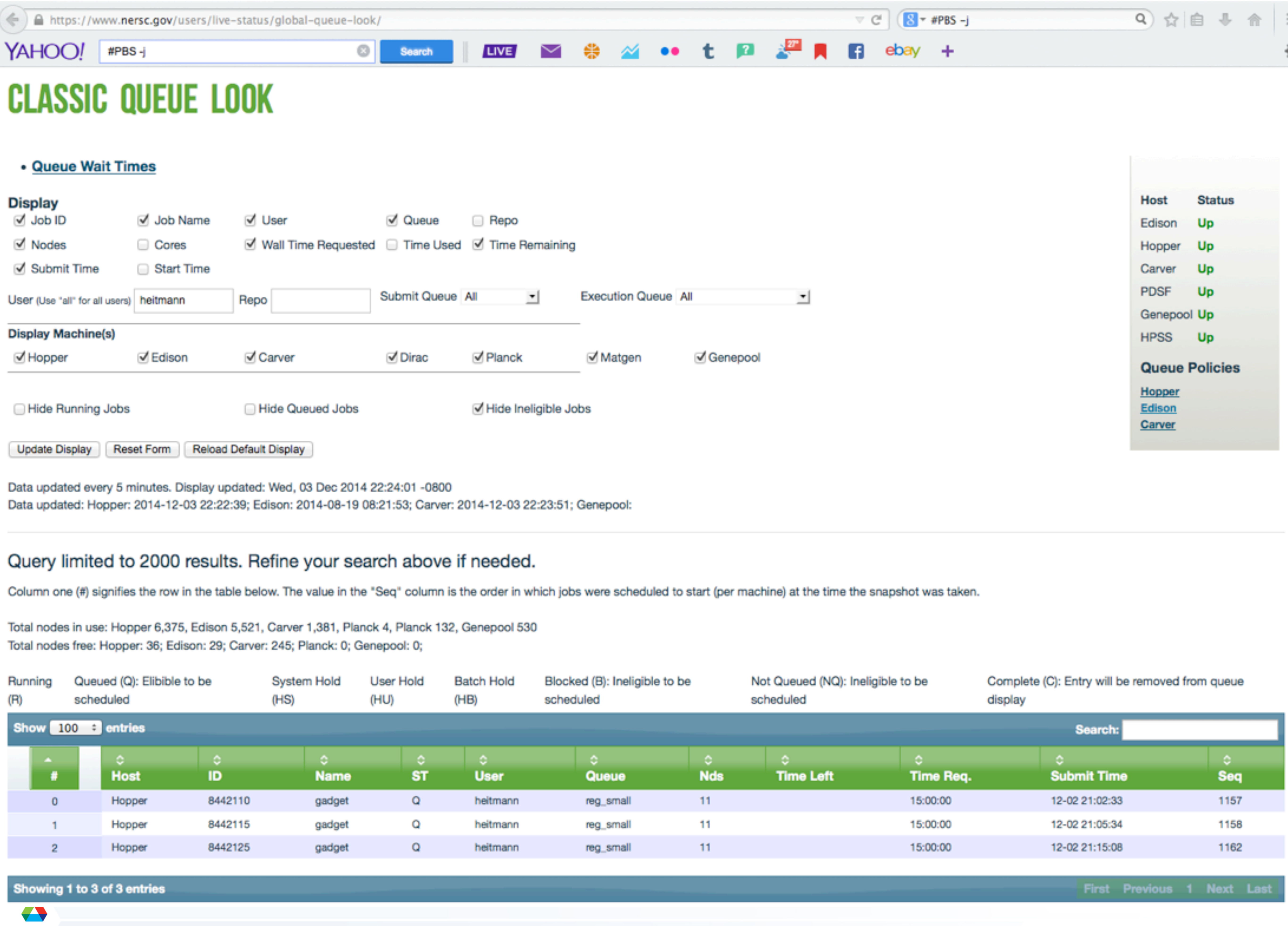
End of a Log file



```
Peano-Hilbert done.
Start force computation...
Starting periodic PM calculation.
done PM.
Tree construction.
Tree construction done.
Begin tree force.
tree is done.
force computation done.
type=1  dmean=0.449815 asmth=0.266309 minmass=0.924878 a=1  sqrt(<p^2>)=705.788  dlogmax=0.00943305
displacement time constraint: 0.00943305  (0.025)

writing snapshot file...
done with snapshot.
Application 40296478 resources: utime ~11522683s, stime ~190693s, Rss ~579516, inblocks ~747127570, outblocks ~2\
65117292

 + --------------------------------------------------------------------------
 +        Job name: gadget
 +          Job Id: 8422229.hopque01
 +          System: hopper
 +     Queued Time: Tue Nov 25 21:03:22 2014
 +      Start Time: Sun Nov 30 05:04:36 2014
 + Completion Time: Sun Nov 30 17:47:27 2014
 +            User: heitmann
 +        MOM Host: nid03934
 +           Queue: reg_small
 +  Req. Resources: mppnodect=11,mppnppn=24,mppwidth=264,walltime=20:00:00
 +  Used Resources: cput=00:00:06,mem=5968kb,vmem=58364kb,walltime=12:42:52
 +     Acct String: cosmosim
 +   PBS_O_WORKDIR: /global/project/projectdirs/hacc/Coyote_small_new/M001
 +     Submit Args: run_gad.bat
 + --------------------------------------------------------------------------
```

Other useful commands

- qdel job-id: delete your job
- qstat -f job-id: status of the job
- qhold job-id: puts job in the queue on hold (in case you want to change something but still have to think, you don’t have to delete the job and loose your position in the queue)
- qalter -t: allows you to change the time for which you have submitted the job while the job is waiting in the queue
- showq: shows all the jobs (qstat by itself works too)
- showq | grep heitmann: shows my jobs
- showstate: shows which jobs are running on which racks, if nodes are down etc.



CLASSIC QUEUE LOOK

- Queue Wait Times

Display

☑ Job ID ☑ Job Name ☑ User ☑ Queue □ Repo
☑ Nodes □ Cores ☑ Wall Time Requested □ Time Used ☑ Time Remaining
☑ Submit Time □ Start Time

User (Use "all" for all users): heitmann
Repo:
Submit Queue: All
Execution Queue: All

Display Machine(s)

☑ Hopper ☑ Edison ☑ Carver ☑ Dirac ☑ Planck ☑ Matgen ☑ Genepool

□ Hide Running Jobs □ Hide Queued Jobs ☑ Hide Ineligible Jobs

Update Display | Reset Form | Reload Default Display

Host	**Status**
Edison	Up
Hopper	Up
Carver	Up
PDSF	Up
Genepool	Up
HPSS	Up

Queue Policies

Hopper
Edison
Carver

Data updated every 5 minutes. Display updated: Wed, 03 Dec 2014 22:24:01 -0800
Data updated: Hopper: 2014-12-03 22:22:39; Edison: 2014-08-19 08:21:53; Carver: 2014-12-03 22:23:51; Genepool:

Query limited to 2000 results. Refine your search above if needed.

Column one (#) signifies the row in the table below. The value in the "Seq" column is the order in which jobs were scheduled to start (per machine) at the time the snapshot was taken.

Total nodes in use: Hopper 6,375, Edison 5,521, Carver 1,381, Planck 4, Planck 132, Genepool 530
Total nodes free: Hopper: 36; Edison: 29; Carver: 245; Planck: 0; Genepool: 0;

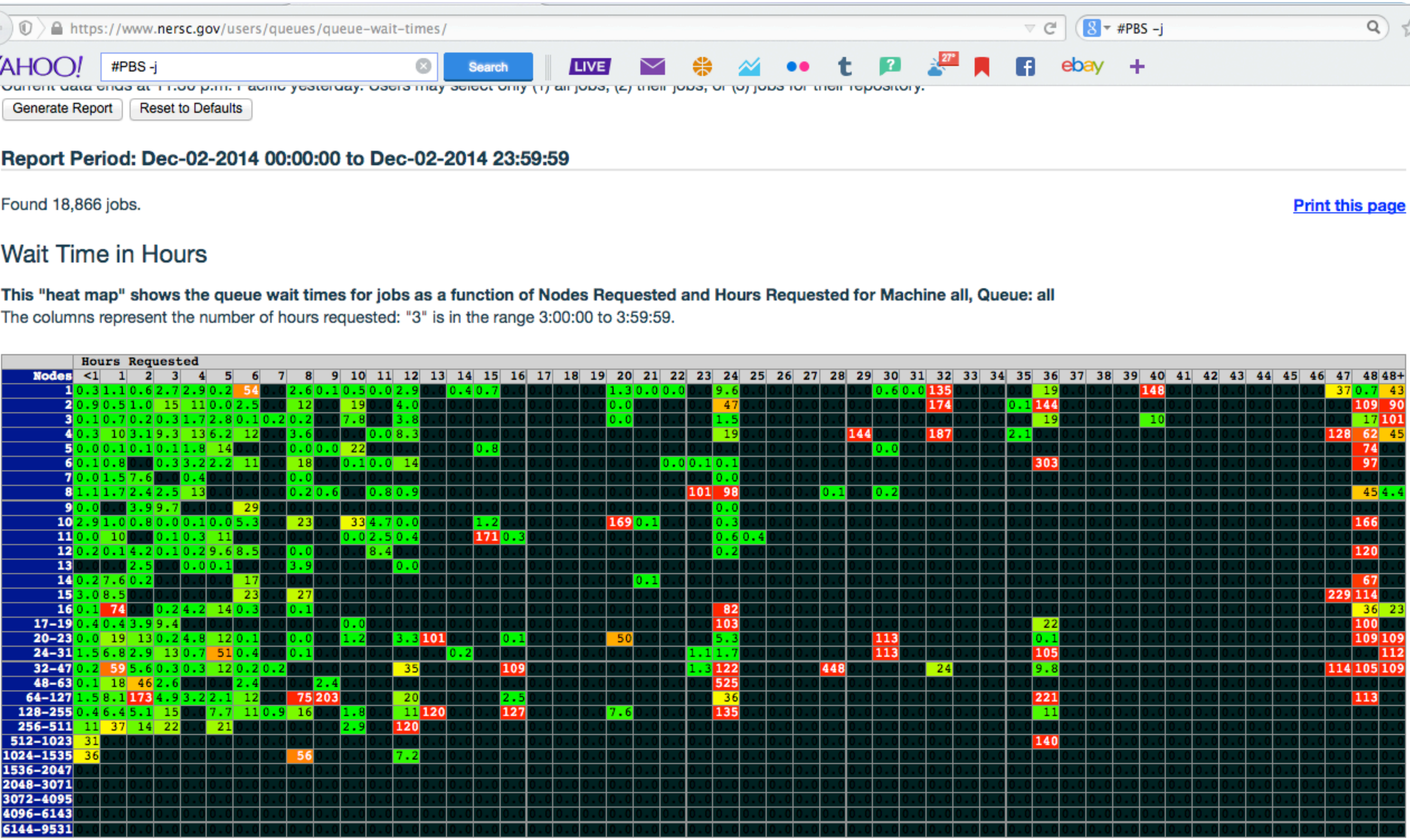
Running (R)	Queued (Q): Elibible to be scheduled	System Hold (HS)	User Hold (HU)	Batch Hold (HB)	Blocked (B): Ineligible to be scheduled	Not Queued (NQ): Ineligible to be scheduled	Complete (C): Entry will be removed from queue display

Show 100 entries Search:

#	Host	ID	Name	ST	User	Queue	Nds	Time Left	Time Req.	Submit Time	Seq
0	Hopper	8442110	gadget	Q	heitmann	reg_small	11		15:00:00	12-02 21:02:33	1157
1	Hopper	8442115	gadget	Q	heitmann	reg_small	11		15:00:00	12-02 21:05:34	1158
2	Hopper	8442125	gadget	Q	heitmann	reg_small	11		15:00:00	12-02 21:15:08	1162

Showing 1 to 3 of 3 entries

First Previous 1 Next Last



Current data ends at 11:59 p.m. Pacific yesterday. Users may select only (1) all jobs, (2) their jobs, or (3) jobs for their repository.

Generate Report | Reset to Defaults

Report Period: Dec-02-2014 00:00:00 to Dec-02-2014 23:59:59

Found 18,866 jobs.

Print this page

Wait Time in Hours

This "heat map" shows the queue wait times for jobs as a function of Nodes Requested and Hours Requested for Machine all, Queue: all

The columns represent the number of hours requested: "3" is in the range 3:00:00 to 3:59:59.

	Hours Requested																																																	
Nodes	<1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	48+
1	0.3	1.1	0.6	2.7	2.9	0.2	54	0.0	2.6	0.1	0.5	0.0	2.9	0.0	0.4	0.7	0.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	9.6	0.0	0.0	0.0	0.0	0.0	0.6	0.0	135	0.0	0.0	0.0	19	0.0	0.0	0.0	148	0.0	0.0	0.0	0.0	0.0	0.0	37	0.7	43
2	0.9	0.5	1.0	15	11	0.0	2.5	0.0	12	0.0	19	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	47	0.0	0.0	0.0	0.0	0.0	0.0	0.0	174	0.0	0.0	0.1	144	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	109	90
3	0.1	0.7	0.2	0.3	1.7	2.8	0.1	0.2	0.2	0.0	7.8	0.0	3.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	19	0.0	0.0	0.0	10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17	101
4	0.3	10	3.1	9.3	13	6.2	12	0.0	3.6	0.0	0.0	0.0	8.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	19	0.0	0.0	0.0	0.0	144	0.0	0.0	187	0.0	0.0	2.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	128	62	45
5	0.0	0.1	0.1	0.1	1.8	14	0.0	0.0	0.0	0.0	22	0.0	0.0	0.0	0.0	0.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	74	0.0
6	0.1	0.8	0.0	0.3	3.2	2.2	11	0.0	18	0.0	0.1	0.0	14	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	303	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	97	0.0
7	0.0	1.5	7.6	0.0	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	1.1	1.7	2.4	2.5	13	0.0	0.0	0.0	0.2	0.6	0.0	0.8	0.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	101	98	0.0	0.0	0.0	0.1	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	45	4.4
9	0.0	0.0	3.9	9.7	0.0	0.0	29	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10	2.9	1.0	0.8	0.0	0.1	0.0	5.3	0.0	23	0.0	33	4.7	0.0	0.0	0.0	1.2	0.0	0.0	0.0	0.0	169	0.1	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	166	0.0
11	0.0	10	0.0	0.1	0.3	11	0.0	0.0	0.0	0.0	0.0	2.5	0.4	0.0	0.0	171	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.6	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12	0.2	0.1	4.2	0.1	0.2	9.6	8.5	0.0	0.0	0.0	0.0	8.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	120	0.0
13	0.0	0.0	2.5	0.0	0.0	0.1	0.0	0.0	3.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14	0.2	7.6	0.2	0.0	0.0	0.0	17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	67	0.0
15	3.0	8.5	0.0	0.0	0.0	0.0	23	0.0	27	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	229	114	0.0
16	0.1	74	0.0	0.2	4.2	14	0.3	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	82	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	36	23
17-19	0.4	0.4	3.9	9.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	103	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	22	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100	0.0
20-23	0.0	19	13	0.2	4.8	12	0.1	0.0	0.0	0.0	1.2	0.0	3.3	101	0.0	0.0	0.1	0.0	0.0	0.0	50	0.0	0.0	0.0	5.3	0.0	0.0	0.0	0.0	0.0	113	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	109	109
24-31	1.5	6.8	2.9	13	0.7	51	0.4	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.1	1.7	0.0	0.0	0.0	0.0	0.0	113	0.0	0.0	0.0	0.0	0.0	105	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	112
32-47	0.2	59	5.6	0.3	0.3	12	0.2	0.2	0.0	0.0	0.0	0.0	35	0.0	0.0	0.0	109	0.0	0.0	0.0	0.0	0.0	0.0	1.3	122	0.0	0.0	0.0	448	0.0	0.0	0.0	24	0.0	0.0	0.0	9.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	114	105	109
48-63	0.1	18	46	2.6	0.0	0.0	2.4	0.0	0.0	2.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	525	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
64-127	1.5	8.1	173	4.9	3.2	2.1	12	0.0	75	203	0.0	0.0	20	0.0	0.0	0.0	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	36	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	221	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	113	0.0
128-255	0.4	6.4	5.1	15	0.0	7.7	11	0.9	16	0.0	1.8	0.0	11	120	0.0	0.0	127	0.0	0.0	0.0	7.6	0.0	0.0	0.0	135	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
256-511	11	37	14	22	0.0	21	0.0	0.0	0.0	0.0	2.9	0.0	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
512-1023	31	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	140	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1024-1535	36	0.0	0.0	0.0	0.0	0.0	0.0	0.0	56	0.0	0.0	0.0	7.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1536-2047	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2048-3071	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3072-4095	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4096-6143	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6144-9531	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Submission of Multiple Jobs

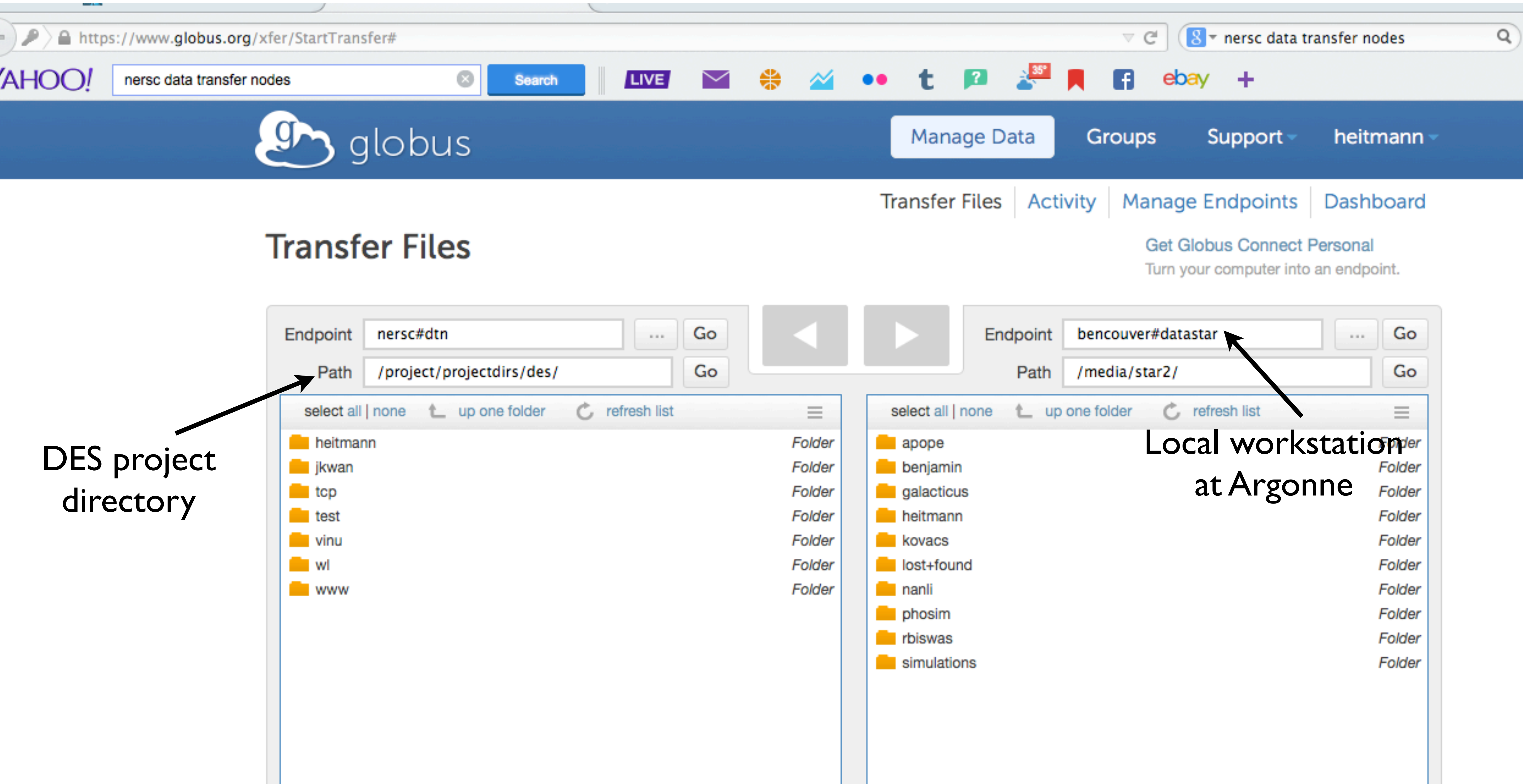
https://www.nersc.gov/users/computational-systems/hopper/running-jobs/example-batch-scripts/

- **Several options:**
  - TaskFarmer: software that helps to launch a number t of independent small jobs on n cores. Within the submission script use tf -t 100 -n 2 ./task.sh instead of aprun -n 2 ./a.out, example for task.sh on NERSC webpage (small script)
  - CCM (Cluster Compatable Mode), include module load ccm in submission script and ccmrun ./runtask.sh where runtask.sh holds a list of jobs (example on NERSC webpage)
  - Python: mpi4py, again explained on NERSC webpage
  - Using MPI code to bundle up calls

Vinu's DEMO

Moving Large Data Sets to and from NERSC

- Data transfer nodes dedicated to data transfer: dtn01.nersc.gov … dtn04.nersc.gov
- If possible use Globus Online for data transfers



https://www.globus.org/xfer/StartTransfer#

nersc data transfer nodes

Transfer Files

Get Globus Connect Personal

Turn your computer into an endpoint.

Endpoint: nersc#dtn

Path: /project/projectdirs/des/

heitmann	Folder
jkwan	Folder
tcp	Folder
test	Folder
vinu	Folder
wl	Folder
www	Folder

Endpoint: bencouver#datastar

Path: /media/star2/

apope	Folder
benjamin	Folder
galacticus	Folder
heitmann	Folder
kovacs	Folder
lost+found	Folder
nanli	Folder
phosim	Folder
rbiswas	Folder
simulations	Folder

DES project directory

Local workstation at Argonne

Useful Links

- Getting started: http://www.nersc.gov/users/getting-started/
- Queues: http://www.nersc.gov/users/queues/
- Python tools: http://www.nersc.gov/users/software/development-tools/python-tools/
- Serial jobs: https://www.nersc.gov/users/computational-systems/edison/running-jobs/serial-queue/
- Example batch scripts: https://www.nersc.gov/users/computational-systems/hopper/running-jobs/example-batch-scripts/ (including examples to package up several jobs into one
- How to use modules to manage your software environment: https://www.nersc.gov/users/software/nersc-user-environment/modules/
- Links to the different supercomputers: https://www.nersc.gov/users/computational-systems/

Installing Software without Root

https://theodorekisner.com/software/hpcports/

- HPCPorts is a tool to manage software (I have not used it myself)
- For DES NERSC, a specific module has been created, to load it, follow instructions below (again, I have not used these so can't comment on them much)

```
source /global/project/projectdirs/des/wl/setup/setup.sh

source /project/projectdirs/cmb/modules/carver/hpcports.sh

module load python

module load des-nersc
```