Running code on the Wesleyan Cluster

This document is intended as a quick reference guide for running code on the Wesleyan computing cluster. It is not an introduction to high-performance cluster computing (I would not be qualified to write such a document) but it does cover the details of computing power available, and how to get started using it.

1. Cluster Basics

The Wesleyan computing center contains a number of clusters all available through one scheduler. Each cluster consists of a collection of nodes, each with a multiple cores. The number of nodes range from 5 to 32 with the number of cores ranging from one to 32 (with hyperthreading turned on). A separate cluster holds the Home directory, with a total of 10 TB, as well as a scratch directory, with a total of 5 TB. More details on the exact hardware setup is available online[1] along with a list of available software[2] and basic, although slightly out of date, information about connecting to the cluster[3]

The first thing to do is contact Henk Meij to set up an account on the cluster. This will give you access to swallowtail, greentail, petaltail and cottontail (soon the be exclusively cottontail), which are the machines used to access the cluster. Once this is done you can ssh into a machine (I usually use greentail) you will be dumped into your home directory (e.g. */home/kflaherty*). This is where you will house your code and store your results. A simple scp command[4] can be used to copy the code from your personal machine to the cluster.

Listed below are sample codes useful for setting up a program that runs in serial and a program that runs in parallel, followed by some useful command line utilities. The example serial/parallel script include examples of code for specifying various parameters in the job submission program, setting up python and miriad, copying the data over to a local scratch directory, and running the code itself.

2. Scripts

Jobs are submitted to the queue of your choice as scripts containing a series of commands following a basic structure. These shell scripts set up the details of the job (e.g. name of the

[1]https://dokuwiki.wesleyan.edu/doku.php?id=cluster:126

[2]https://dokuwiki.wesleyan.edu/doku.php?id=cluster:73

[3]https://wesfiles.wesleyan.edu/departments/SCIC/Public/Documentation/unix_cluster/JOB_ON_SWALLOWTAIL.pdf

[4]e.g. Starting from your home machine enter: scp myfile.fits kflaherty@greentail:/home/kflaherty/code/

job, number of cores needed), define any system variables (e.g. for running miriad) and call your actual workhorse code. Outlined below are the basic commands used in a script used for a serial job and for a parallel job. Examples of these pieces of code are available in Henk's home directory */home/hmeij/jobs* in the *serial* and *parallel* directories. Note that these scripts do not include checkpointing, discussed below, and should be used as starting points to understand basic scripting and to make sure your code works as expected when ported to the cluster. Full production runs should use the wrappers that include checkpointing to ensure that any mid-run crashes do not severely disrupt your work.

2.1. Basic serial script

Here are some of the commands that go into a basic serial computing script.

$$\#!/bin/bash \tag{1}$$

Set up the bash shell. Any shell scripts called by your code must be setup in bash, not csh or tcsh.

$$\begin{aligned} &\#BSUB\ \ -q\ mw256fd \\ &\#BSUB\ \ -J\ test \\ &\#BSUB\ \ -o\ test.stdout \\ &\#BSUB\ \ -e\ test.stderr \end{aligned} \tag{2}$$

Set up a number of parameters for the *bsub* command. The first line specifies the queue to which the code is sent. The second line gives the name of the job, while the third and fourth line specify names for output files and error output files. These last two files are created once the job is complete and they contain standard outputs from your code, as well as any error messages generated while running the code. The *test.stdout* file will contain basic information on the name of the job, the home directory, the working directory, the job id, a snippet of the code, plus some other information about the run. The *.stderr* file contains error messages produced by your code while it is running.

$$\begin{aligned} &export\ PYTHONHOME = /home/apps/python/2.6.1 \\ &export\ PYTHONPATH = /home/apps/python/2.6.1/site-packages \\ &export\ PATH = \$PYTHONHOME/bin : \$PATH \\ &.\ /home/apps/miriad/MIRRC.sh \\ &export\ PATH = \$MIRBIN : \$PATH \end{aligned} \tag{3}$$

These commands set up environment variables necessary to call supporting programs (don't forget the space after the period in the fourth line above). In this case, I am using a couple of python packages as well as MIRIAD. The first three lines set up the python paths, specifically referencing python 2.6.1. Note that multiple versions of python exist on the cluster, but version 2.6.1 contains numpy, scipy, astropy and emcee which are all used in my own code. The last two lines set up the MIRIAD installation. First it calls the MIRIAD initialization script, which sets up the variable *$MIRBIN*, which is then added to the path. Note that the MIRIAD installation requires a fortran library that is only available on the mw256[fd] queues. So even though we don't need the extra memory space available on this clster, we need to use it to run MIRIAD.

$$cp\ -r\ mydata.vis\ /sanscratch/\$LSB\_JOBID \tag{4}$$

When your job starts, a temporary directory is created within the /sanscratch directory. Data I/O should be done from this directory to avoid over taxing the /home directory. Many people forget to do this, and the I/O on the /home directory slows down. This temporary directory is created using your unique job id number, accessed with the environment variable it $LSB_JOBID. It is also erased as soon as your job is completed. Make sure to copy any data you need out of this directory before the end of your script! In your code use the name 'sanscratch' but if want to look into this directory from the command line (e.g. with an ls command to make sure things got transfered over) you want to use that name 'sanscratch_sharptail'.

$$python\ test.py\ /sanscratch/\$LSB\_JOBID \tag{5}$$

This is the command to call my actual code. In this case, my code is called *test.py* and it takes as input the temporary working directory.

That covers all of the basics of a serial code. This is a shell script, so any shell commands will also work here, but any heavy lifting should probably be left to your code to leave this script as simple as possible.

2.2. Basic Parallel script

Running a parallel code is similar to running a serial code, with some minor additions, which are outlined below.

$$\begin{array}{l} \#BSUB\ -n\ 8 \\ \#BSUB\ -R\ \text{“}span[ptile = 1]'' \\ \#BSUB\ -R\ \text{“}span[hosts = 1]'' \end{array} \tag{6}$$

The first command specifies the number of hosts to send this job to, in this case 8. The next two commands are actually mutually exclusive, but are both included here for illustration. The *ptile=1* command tells the scheduler to one send one job to each node, and to use as many nodes as are specified (for reference the mw256fd queue has 5 nodes with 32 threads per node, so you would be limited to -n 5). The *hosts=1* command tells the scheduler to dump all of the jobs onto one node. The advantage/disadvantage of each depends on the exact nature of your code. Try both options and see which provides the best results.

$$\begin{array}{l} export\ PATH = /share/apps/openmpi/1.2 + intel - 10/bin : \$PATH \\ export\ LD\_LIBRARY\_PATH = /share/apps/openmpi/1.2 + intel - 10/lib : \$LD\_LIBRARY\_PATH \end{array} \tag{7}$$

These commands set up various path variables pointing to the installation of openmpi.

$$./lava.openmpi.wrapper\ python\ mpi\_run\_models.py \tag{8}$$

Calling your code is slightly different here that in the serial case. Here was call a wrapper (*lava.openmpi.wrapper*) that sets various variables (the machine file and number of parallel jobs) for this code. Basically instead of directly calling *mpirun*, as you would on your local machine, use this wrapper. You will need to copy over this wrapper from Hank's directory (/home/hmeij/jobs/parallel/)

Everything else should be run as it was in the serial script. You still need to setup the paths for python and miriad, as well as copy the data to and from the scratch directory.

3. Checkpointing

Recently Henk has set up the cluster to take advantage of checkpointing within the code, based on the Berkeley Laboratory Checkpoint/Restart tool. What this means is that if the cluster crashes, you can restart from the last checkpoint, rather than having to restart from the very beginning. This is very useful if you e.g. are running a week long MCMC chain and the cluster crashes on day four. The details of how this works are complicated, but Henk has hidden most of this within new execution files, having worked closely with me and Jesse Tarnes ('16, within Seth's group) to make sure our code works with checkpointing.

Information on both serial[5] and parallel[6] jobs can be found online. These resources include same wrappers to be used when calling a serial or parallel job, replacing the sample scripts in */home/hmeij/jobs*. Here I will highlight some of the differences in the code, and how to use checkpointing.

[5]https://dokuwiki.wesleyan.edu/doku.php?id=cluster:147

[6]https://dokuwiki.wesleyan.edu/doku.php?id=cluster:148

3.1. Checkpointing scripts

Once you have copied over Henk's scripts, you will notice some small differences from the original sample scripts. The first thing the script does is set the scratch directory as a system variable and move all code from the home directory to this scratch directory.

$$\begin{array}{l} export\ MYSANSCRATCH = /sanscratch/\$LSB\_JOBID \\ cd\ \$MYSANSCRATCH \\ pre\_cmd ='' \ scp\ \ \$HOME/kflaherty/test.py\ .'' \\ post\_cmd ='' \ scp\ \ \$MYSANSCRATCH/result.txt\ \$HOME/kflaherty/\text{“} \end{array} \tag{9}$$

These commands first set up the *$MYSANSCRATCH* system variable, move to the temporary directory and set up commands that will copy over your code at the start of the run, and copy back any results (*result.txt*) of the run. These commands are not executed at this moment, but they are set up to be executed later. Moving everything to the temporary directory, including your code, is important when checkpointing because the BLCR code has to recover everything that was used by the code in order to properly restart it. This includes every file created by the code while it is running. In the example above, I only have the file *test.py* that needs to be copied over at the beginning, but this can be expanded to include any pieces of code, data sets, support files, etc. that are needed.

The next few specify whether this is the start of a new run, or the restart of a run that crashed.

$$\begin{array}{l} mode = start \\ queue = test \\ cmd ='' \ python\ test.py\ /sanscratch/\$LSB\_JOBID'' \\ \\ \#mode = restart \\ \#queue = test \\ \#orgjobid = 250 \end{array} \tag{10}$$

The first three lines are to be used when starting a new run. This sets up the correct queue as well as the command that is used to call the code. If instead you are restarting a prematurely terminated run, then comment out the first three lines and uncomment the next three lines. The variable *orgjobid* refers to the JOBID (found using the *bjobs* command when it was running) and must be adjusted to the proper value.

The final command, which likely occurs earlier in the script, sets the time interval between checkpointing.

$$cpti = 15m \tag{11}$$

This sets will define checkpointing to occur every 15 minutes. For any production run of your code this is overkill, and should only be used if you are testing the checkpointing process. More appropriate values are 12h, 18h or 1d depending on the full length of your run.

3.2. How Checkpointing works

There are detailed descriptions online of how to recover from a crash, and here I will highlight the more important details. The first step is to uncomment the start block of the wrapper. Once this is done, the wrapper can be submitted to the queue like any other script.

$$bsub < blcr\_wrapper \tag{12}$$

This will generate a temporary directory as before, but it will also create a file in the checkpoints directory (*/sanscratch/checkpoints/$JOBID*). This folder will contain the checkpoint updates. As soon as a file titled *chk.PID* shows up, the code has completed its first checkpoint. From here on the code can be resumed from this point after it crashes. The process for restarting is straightforward. Simply comment out the start block, and uncomment the restart block, and resubmit the blcr_wrapper script. The restart does need to submitted to the same queue as the original run, but doesn't need to land on the same node. It will take a few minutes to restart, but should get going soon enough.

4. Useful Commands

In addition to the scripts that set up the code, there are a number of useful command line utilities. Many of these have an associated man page that contains more information on their function as well as various flags that accompany the command.

bsub < my.code (Figure 1) Short for bsubmit, this is the main code used to submit a job to the queue. The file *my.code* contains the commands needed to run your code, as outlined in the previous section.

bqueues (Figure 2) This command lists information on the available queues including the name of the queues, its priority, status, the maximum number of jobs, the number of jobs per host, the number of total jobs on this machine, the number of pending jobs and the number of jobs currently running (and suspended). There are a number of different clusters to which your code can be sent.

If you have a very memory intensive job (as in many GB of memory), then send it to mw256[fd]. If you can run the code on your own machine then hp12 should be good enough. If your code runs on a gpu then mwgpu is the queue for you. The queue hp12 is made up of 32 nodes, each with 12 GB of memory, while mw256[fd] are each made of 5 nodes with 256 GB of memory. The hp12 nodes (n1-n32) can each handle 16 jobs per node, while the mw256fd nodes (n38-n45) can each handle 32 jobs per node, while mw256 (n33-n37) can handle 28 jobs per node (the extra 4 jobs per node are reserved for GPU calculations).

bjobs (Figure 3) This command will list any current jobs that you are running. This shows the unique jobid number, the user that submitted the job, its status, the queue it is assigned to, the host from which the command was sent, the nodes that are executing the command, the name of the job and the time the job was submitted. To view the jobs submitted by all users, use the *-u all* keyword. Call this command with the *-q queue* flag, where *queue* is the specific queue of interest, to see all of the jobs for a specific queue. Specify the *-m node* flag to look at the jobs related to a particular node (e.g. n45).

bkill jobid This command kills a job that you are currently running. Most jobs, even when they fail, will exit on their own, although there are some exceptions.

lsload node (Figure 5) Check the load on a node. Usefully to make sure you aren't overloading the node, which is usually a sign of something wrong

ssh node top -u username -b -n 1 (Figure 6) This is another useful command for checking a load on a particular node. This command calls *top* for that node, with various flags to e.g. only list the programs run by one user. This also contains information on your total memory usage (important to keep track of)

4.1. Misc.

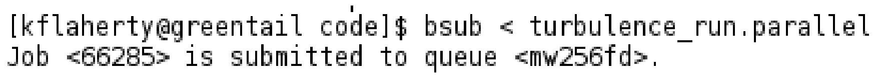
Miriad on the cluster: Miriad runs the same as on our local machines, with one small exception. This has to do with how *uvmodel* handles polarized data and an unpolarized model. On my local machine, if the data has dimensions N_{base}xN_{chan}x3x2, where N_{base} is the number of baselines and N_{chan} is the number of channels and the last dimension splits the data into XX and YY, then when the model is run through *uvmodel* it results in a visibility file with dimensions $2N_{base}$xN_{chan}x3x1. The last dimension has been reduced while the first dimension has been doubled, with the intensity copied into twice as many baseline positions. On the cluster *uvmodel* does not do this. It maintains the original dimensions of the data (N_{base}xN_{chan}x3x2) and copies intensity into the XX,YY positions in the array. This requires slightly different handling of the model visibilities when they are loaded into python. Check out */home/kflaherty/code/single_model.py*, under the compare_vis function.

Also note that miriad is very talkative, and likes to tell you all about things that are going on when it is running. This can become burdensome when hundreds of thousands of models are run since all of this information will be dumped into the *.stderr* and *.stdout* files created at the end of each run (described below). These files could reach hundreds of MB! To avoid keeping this useless information, I usually pipe the command into a file (e.g. *python code.py > test.out*. The file *test.out* will slowly grow with time, which a useful way to test that your code has not crashed. If you place this file in the scratch directory then it will deleted once the code is done running. When checkpointing is used, the file *test.out* may not appear, but the output is instead placed in */.lsbatch/[0-9]*.JOBID.out*. When the job ends, this file becomes the *.out* file.

Crashing without stopping: Most of the time if your code crashes the job will be killed, and error messages will be output to the *.stderr* and *.stdout* files. But I have run into some instances where the code while crash, but the job will not kill itself. This can happen if *emcee* runs into a problem with a particular model and isn't able to proceed any further along its chains. If you have piped your output into *test.out* as described above, then you can see this happen when *test.out* stops growing. At this point you have to kill the job and examine the error file to discern what went wrong.

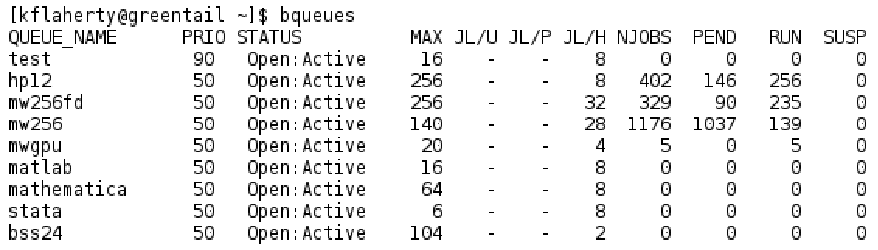
Generic file names: Also, if you output any files (e.g. model images that need to be run through miriad tasks) be careful about giving them generic names. When running a parallel job you could potentially end up with many files with the same name, which is a recipe for disaster. Take advantage of the python utility that generates a unique name to keep parallel processes separate (and clean up after yourself). An example of how to do this is in the */home/kflaherty/code/single_model.py* code within the function *lnlike* (look for the *cleanup* keyword).

Shell type: The cluster uses bsh, which is different than my machine. If you are using a shell script to e.g. call miriad tasks make sure it references the correct shell (taken care of with the first line in the script).



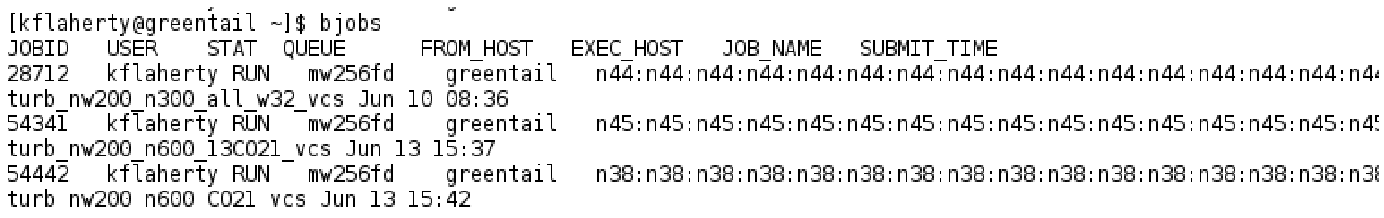
```
[kflaherty@greentail code]$ bsub < turbulence_run.parallel
Job <66285> is submitted to queue <mw256fd>.
```

Fig. 1.— Example of the *bsub* command. A script is submitted to the mw256fd queue and is assigned a job id number.



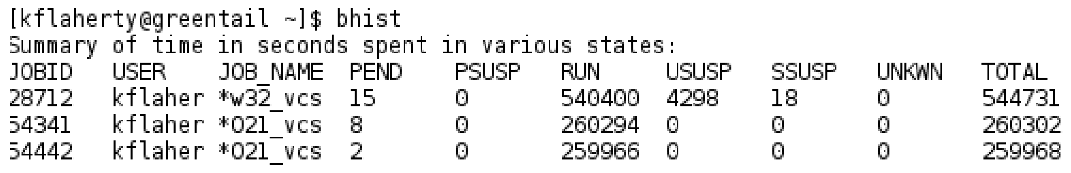
```
[kflaherty@greentail ~]$ bqueues
QUEUE_NAME      PRIO STATUS          MAX JL/U JL/P JL/H NJOBS  PEND   RUN  SUSP
test             90  Open:Active      16    -    -    8     0     0     0     0
hp12             50  Open:Active     256    -    -    8   402   146   256     0
mw256fd          50  Open:Active     256    -    -   32   329    90   235     0
mw256            50  Open:Active     140    -    -   28  1176  1037   139     0
mwgpu            50  Open:Active      20    -    -    4     5     0     5     0
matlab           50  Open:Active      16    -    -    8     0     0     0     0
mathematica      50  Open:Active      64    -    -    8     0     0     0     0
stata            50  Open:Active       6    -    -    8     0     0     0     0
bss24            50  Open:Active     104    -    -    2     0     0     0     0
```

Fig. 2.— Example of the *bqueues* command. This lists all of the available queues, the maximum number of jobs, the allowable jobs per host, the number of submitted jobs, the number of pending jobs, the number of running jobs and the number of suspended jobs. Most of the queues are currently overloaded, although this tends to fluctuate with time.



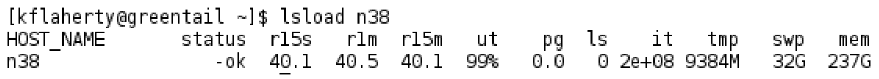
```
[kflaherty@greentail ~]$ bjobs
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
28712   kflaherty RUN   mw256fd    greentail   n44:n44:n44:n44:n44:n44:n44:n44:n44:n44:n44:n44:n44:n44:n44:n4
turb_nw200_n300_all_w32_vcs Jun 10 08:36
54341   kflaherty RUN   mw256fd    greentail   n45:n45:n45:n45:n45:n45:n45:n45:n45:n45:n45:n45:n45:n45:n45:n4
turb_nw200_n600_13CO21_vcs Jun 13 15:37
54442   kflaherty RUN   mw256fd    greentail   n38:n38:n38:n38:n38:n38:n38:n38:n38:n38:n38:n38:n38:n38:n38:n3
turb nw200 n600 CO21 vcs Jun 13 15:42
```

Fig. 3.— Example of a call to *bjobs*. I have submitted three jobs from greentail, all of which are running. Each job is taking up eight cores on different nodes.



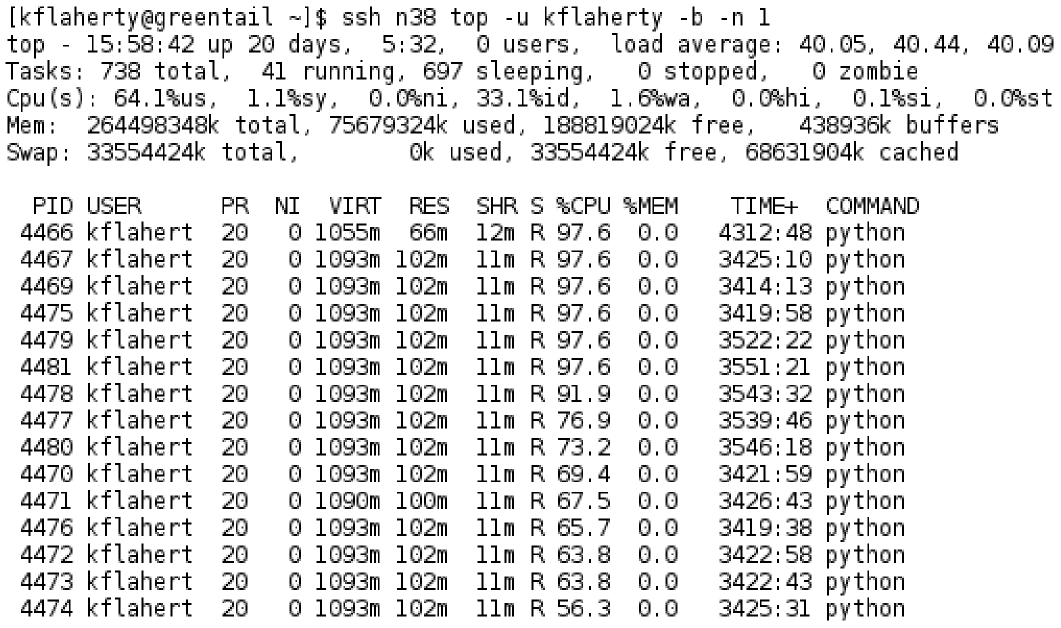
```
[kflaherty@greentail ~]$ bhist
Summary of time in seconds spent in various states:
JOBID   USER    JOB_NAME  PEND    PSUSP   RUN     USUSP   SSUSP   UNKWN   TOTAL
28712   kflaher *w32_vcs  15      0       540400  4298    18      0       544731
54341   kflaher *021_vcs  8       0       260294  0       0       0       260302
54442   kflaher *021_vcs  2       0       259966  0       0       0       259968
```

Fig. 4.— Example of a call to *bhist*. This shows the three jobs currently running, along with the number of seconds they have spent in various states.



```
[kflaherty@greentail ~]$ lsload n38
HOST_NAME       status  r15s   r1m  r15m   ut    pg  ls    it   tmp   swp   mem
n38                -ok  40.1  40.5  40.1  99%   0.0   0 2e+08 9384M   32G  237G
```

Fig. 5.— Example of a call to *lsload*. The values *r15s*, *r1m*, *r15m* shows the core usage averaged over the previous 15 seconds, 1 miute and 15 minutes.



```
[kflaherty@greentail ~]$ ssh n38 top -u kflaherty -b -n 1
top - 15:58:42 up 20 days,  5:32,  0 users,  load average: 40.05, 40.44, 40.09
Tasks: 738 total,  41 running, 697 sleeping,   0 stopped,   0 zombie
Cpu(s): 64.1%us,  1.1%sy,  0.0%ni, 33.1%id,  1.6%wa,  0.0%hi,  0.1%si,  0.0%st
Mem:  264498348k total, 75679324k used, 188819024k free,   438936k buffers
Swap: 33554424k total,        0k used, 33554424k free, 68631904k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
 4466 kflahert  20   0 1055m  66m  12m R 97.6  0.0   4312:48 python
 4467 kflahert  20   0 1093m 102m  11m R 97.6  0.0   3425:10 python
 4469 kflahert  20   0 1093m 102m  11m R 97.6  0.0   3414:13 python
 4475 kflahert  20   0 1093m 102m  11m R 97.6  0.0   3419:58 python
 4479 kflahert  20   0 1093m 102m  11m R 97.6  0.0   3522:22 python
 4481 kflahert  20   0 1093m 102m  11m R 97.6  0.0   3551:21 python
 4478 kflahert  20   0 1093m 102m  11m R 91.9  0.0   3543:32 python
 4477 kflahert  20   0 1093m 102m  11m R 76.9  0.0   3539:46 python
 4480 kflahert  20   0 1093m 102m  11m R 73.2  0.0   3546:18 python
 4470 kflahert  20   0 1093m 102m  11m R 69.4  0.0   3421:59 python
 4471 kflahert  20   0 1090m 100m  11m R 67.5  0.0   3426:43 python
 4476 kflahert  20   0 1093m 102m  11m R 65.7  0.0   3419:38 python
 4472 kflahert  20   0 1093m 102m  11m R 63.8  0.0   3422:58 python
 4473 kflahert  20   0 1093m 102m  11m R 63.8  0.0   3422:43 python
 4474 kflahert  20   0 1093m 102m  11m R 56.3  0.0   3425:31 python
```

Fig. 6.— Example of calling *top* for a particular node. There are lots of python processes running right now.