

Exercise 4: Deploy NAMD GridEngine Cluster with CycleCloud

Duration: 30 minutes

In this exercise, we will use CycleCloud to deploy an "Auto Scaling" HPC Cluster running the SGE scheduler and NAMD application. We will submit some tests jobs, observe what happens, and then terminate and destroy the cluster.

Step 1: Login to the CycleCloud GUI

1. Find your **desk number**

Your CycleCloud Username will be "demouser\${DESK_NUMBER}"

Your CycleCloud Password will be "demouser\${DESK_NUMBER};"

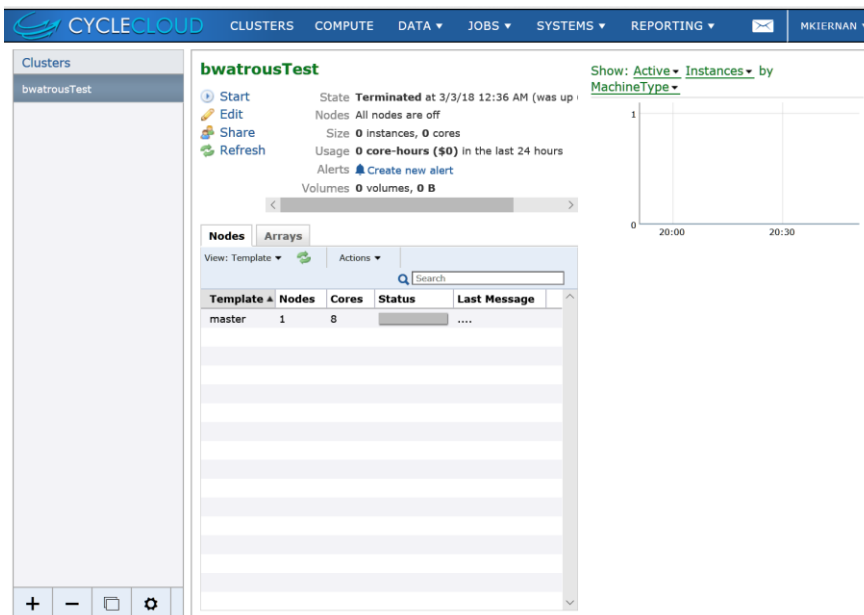
Example: demouser1 : demouser1;

2. Log in to the CycleCloud GUI at:

<https://cycleserverzlyprb.westeurope.cloudapp.azure.com/>

3. When your browser warns about an invalid certificate, accept and continue.
4. When prompted for Username and Password, enter the demouser creds for your desk

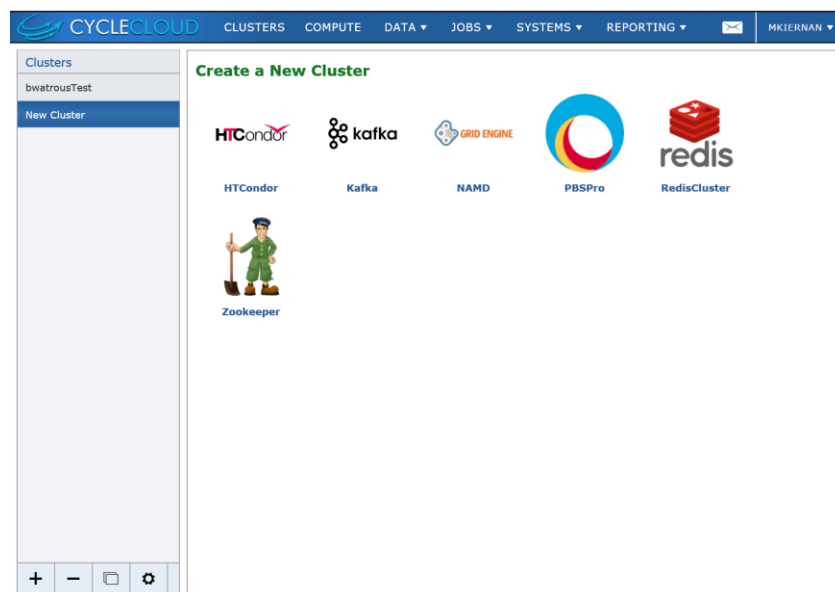
5. You should now see the CycleCloud Cluster Creation page and an empty cluster list frame on the left



Step 2: Create Your NAMD GridEngine Cluster

Now we're all going to create a simple NAMD cluster and run some test jobs

1. Click the "+" icon in the bottom left. This brings up the "Create a New Cluster" view.



2. Click on the "NAMD" GridEngine cluster
 - This should bring up the Cluster Creation Form

CYCLECLOUD CLUSTERS COMPUTE DATA JOBS SYSTEMS REPORTING MKIERNAN

New NAMD Cluster

General Settings

Cluster Software

Compute Backend

Cloud Service Provider Configuration

Configure the Cloud Provider account options.

Cloud Provider: Azure

Credentials: cyclelab (default)

Region: West Europe

Subnet ID: cyclecloud: cyclevnet-compute

Base OS: cycle.image.ubuntu16

Previous Next Save Cancel

3. In the "Cluster Name" field:

- Enter a unique Name for your cluster - We recommend using your initials plus a name that you will recognize
- The other drop-downs are locked down to specific parameter settings because we're operating in a very limited demo subscription.

4. If you want, click "Next" to see the other options, but since there's nothing else we need to modify for the demo, when you're ready, click "Save"

CYCLECLOUD CLUSTERS COMPUTE DATA JOBS SYSTEMS REPORTING MKIERNAN

mikek

Start Edit Share Refresh

State: Off

Nodes: All nodes are off

Size: 0 instances, 0 cores

Usage: 0 core-hours (\$0) in the last 24 hours

Alerts: Create new alert

Volumes: 0 volumes, 0 B

Nodes Arrays

View: Template Actions

Template	Nodes	Cores	Status	Last Message
master	1	8	

Show: Active Instances by MachineType

Show Detail

Time	Message
9:00 PM	Created cluster mikek

You have just created a cluster, but notice that it is in the Terminated/Off state

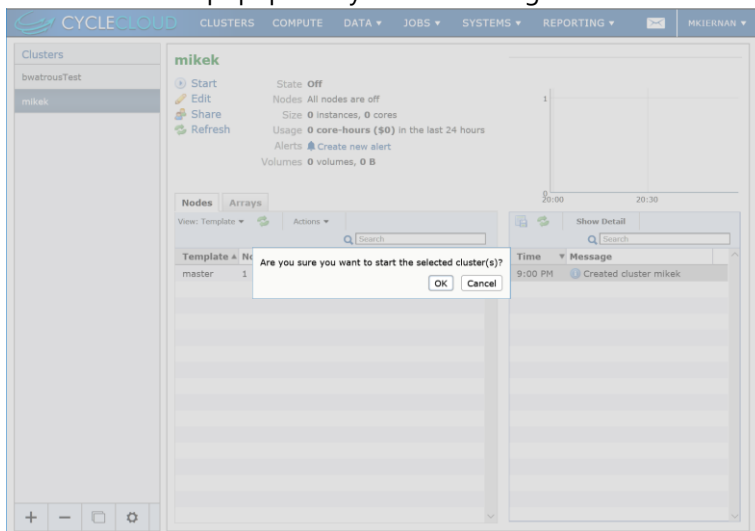
Nothing is running, and the billing is currently \$0 per hour

Step 2: Start Your NAMD GridEngine Cluster

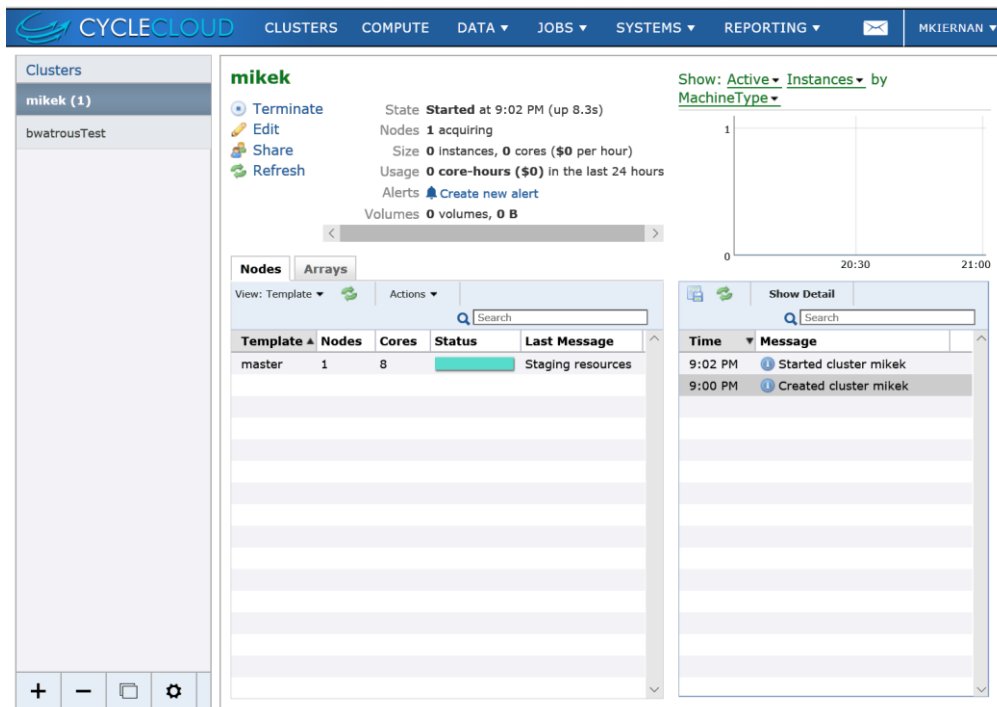
1. Now click the "Start" button at the top of the Cluster page

- This will "start" the cluster by launching the Master node only.
- Compute nodes will be automatically added ("Auto-scaled") when you submit a job in the next step.

Click "ok" in the popup "Are you sure" dialogue:



The master node starts to deploy – this process will take around 5-10 minutes;



Step 3: Login to Your GridEngine Cluster and Submit a Job

When the master node has finished deploying & installing, the status bar will turn green:

1. Get the Public IP address of the "master" node by selecting the Master node in the upper table, which splits the view, and then in the lower table that appears, you can click "Connect" on the menu above the table.

The screenshot displays the CYCLECLOUD web interface. The top navigation bar includes links for CLUSTERS, COMPUTE, DATA, JOBS, SYSTEMS, and REPORTING, along with a user profile for MKIERNAN. On the left sidebar, the 'Clusters' section is active, showing a list with 'mikek (1)' and 'bwatrousTest'. The main content area is titled 'mikek' and shows the cluster's state as 'Started at 9:02 PM (up 14m 40s)'. It lists 1 ready node, 8 cores, and a usage of 1.8 core-hours. A 'Connect' button is highlighted in the 'Nodes' table. The 'Nodes' table has columns for Template, Nodes, Cores, Status, and Last Message. The 'Show Detail' panel on the right shows a timeline of events: 'Created cluster mikek' at 9:00 PM, 'Started cluster mikek' at 9:02 PM, and 'Node master in cluster mikek f' at 9:13 PM. The 'Host Name' column in the 'Nodes' table shows the IP address 52.174.233...

Clusters

- mikek (1)
- bwatrousTest

mikek

State: **Started** at 9:02 PM (up 14m 40s)

Nodes: **1** ready

Size: **1** instance, **8** cores (\$0.48 per hour)

Usage: **1.8** core-hours (\$0) in the last 24 hours

Alerts: [Create new alert](#)

Volumes: **0** volumes, **0** B

Nodes | Arrays

View: Template | Actions

Template	Nodes	Cores	Status	Last Message
master	1	8	Ready	...

View: Details | Show Detail | Edit | **Connect** | Actions

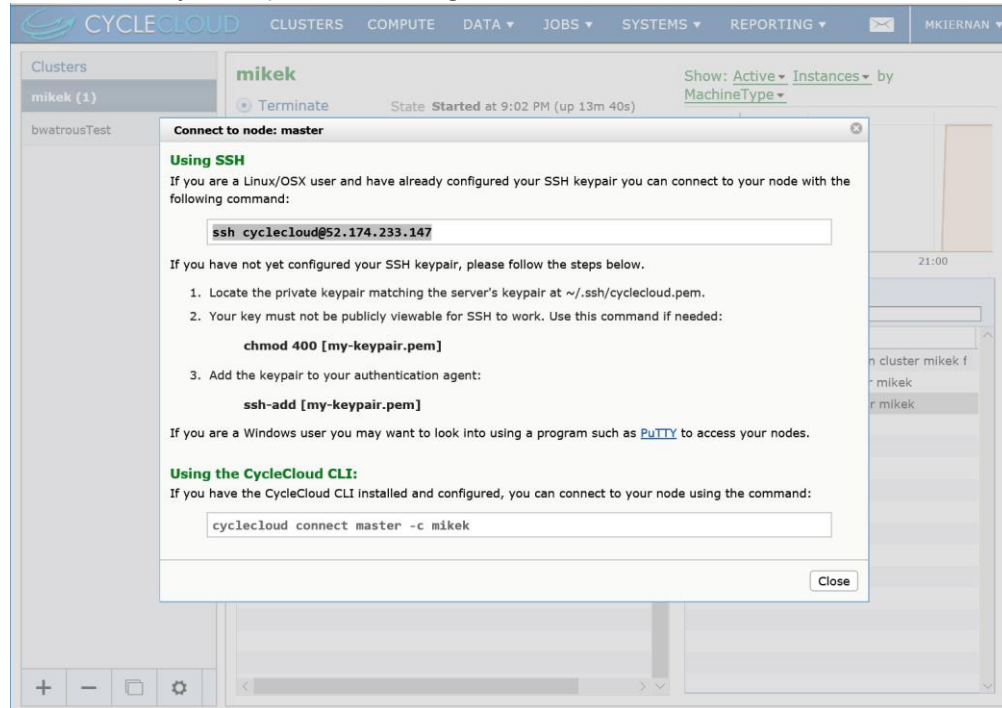
Name	Type	Status	Cores	Zone	Host Name
master	Standa...	Ready	8	...	52.174.233...

Show Detail

Time | Message

- 9:13 PM: Node master in cluster mikek f
- 9:02 PM: Started cluster mikek
- 9:00 PM: Created cluster mikek

2. This will show you 2 options for sshing in to the Master node



3. Copy the line with the IP Address
4. Log in to the QMaster

Grab the ssh private key here:

https://cyclestorage.blob.core.windows.net/keys/clusteruser.sc_frontiers.pem

```
$ wget https://cyclestorage.blob.core.windows.net/keys/clusteruser.sc_frontiers.pem
```

Set the permissions and login using the private key:

```
$ chmod 700 clusteruser.sc_frontiers.pem
```

```
$ ssh -i clusteruser.sc_frontiers.pem cluster_user@13.95.22.183
```

```
cluster_user@ip-0A000404: ~
Welcome to Ubuntu 16.04.3 LTS (GNU/Linux 4.13.0-1011-azure x86_64)

* Documentation:  https://help.ubuntu.com
* Management:    https://landscape.canonical.com
* Support:       https://ubuntu.com/advantage

Get cloud support with Ubuntu Advantage Cloud Guest:
http://www.ubuntu.com/business/services/cloud

20 packages can be updated.
3 updates are security updates.

The programs included with the Ubuntu system are free software;
the exact distribution terms for each program are described in the
individual files in /usr/share/doc/*/copyright.

Ubuntu comes with ABSOLUTELY NO WARRANTY, to the extent permitted by
applicable law.

 _ _ | _ | _ | _ | _ | _ | _ | _ | _ | _ | _ | _ | _ | _ | _ |
Cluster: mikek
Version: 6.8.0
Run List: recipe[cyclecloud], role[sge_master_role], recipe[cluster_init]
cluster_user@ip-0A000404:~$ ls
namd.sh
cluster_user@ip-0A000404:~$ cat namd.sh
#!/bin/bash
#
#$ -pe mpi 8
#
INPUTS=/shared/scratch/namd-inputs

case "$1" in
    apo1)
        TARGET=apo1/apo1.namd
        ;;
    flatpase)
        TARGET=flatpase/flatpase.namd
        ;;
    *)
        echo "Usage: $0 {apo1|flatpase}"
        exit 1
    esac
```

5. Look at the content of the job script

```
$ cat namd.sh
```

6. Submit 3 variants

```
$ qsub namd.sh
```

```
$ qsub namd.sh apo1
```

```
$ qsub namd.sh flatpase
```

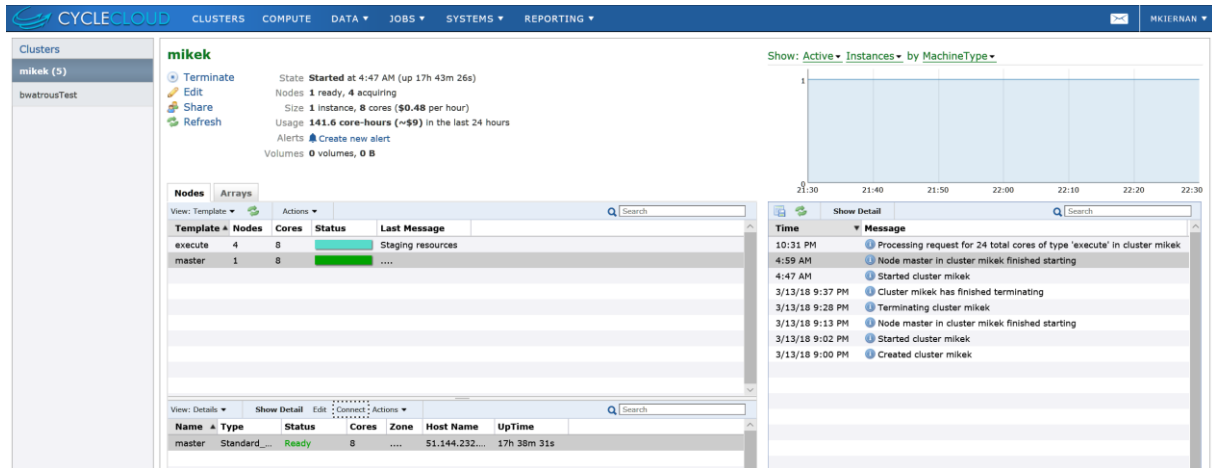
```
$ watch qstat -f
```

```
cluster_user@ip-0A000404: ~
Every 2.0s: qstat -f
Wed Mar 14 21:31:17 2018

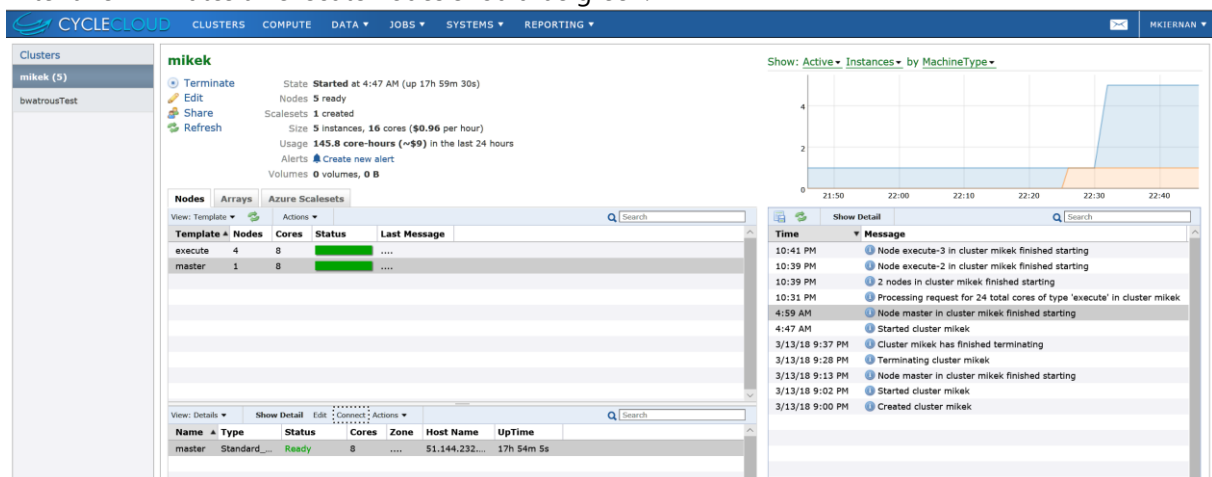
-----
queue      name      qtype resv/used/tot. load_avg arch      states
-----
all.q@ip-0A000404      BIP    0/0/8      0.07    linux-x64

#####
- PENDING JOBS - PENDING JOBS - PENDING JOBS - PENDING JOBS - PENDING JOBS
#####
   1 0.56000 namd.sh      cluster_user qw    03/14/2018 21:30:31    8
   2 0.55500 namd.sh      cluster_user qw    03/14/2018 21:30:35    8
   3 0.55333 namd.sh      cluster_user qw    03/14/2018 21:30:42    8
```

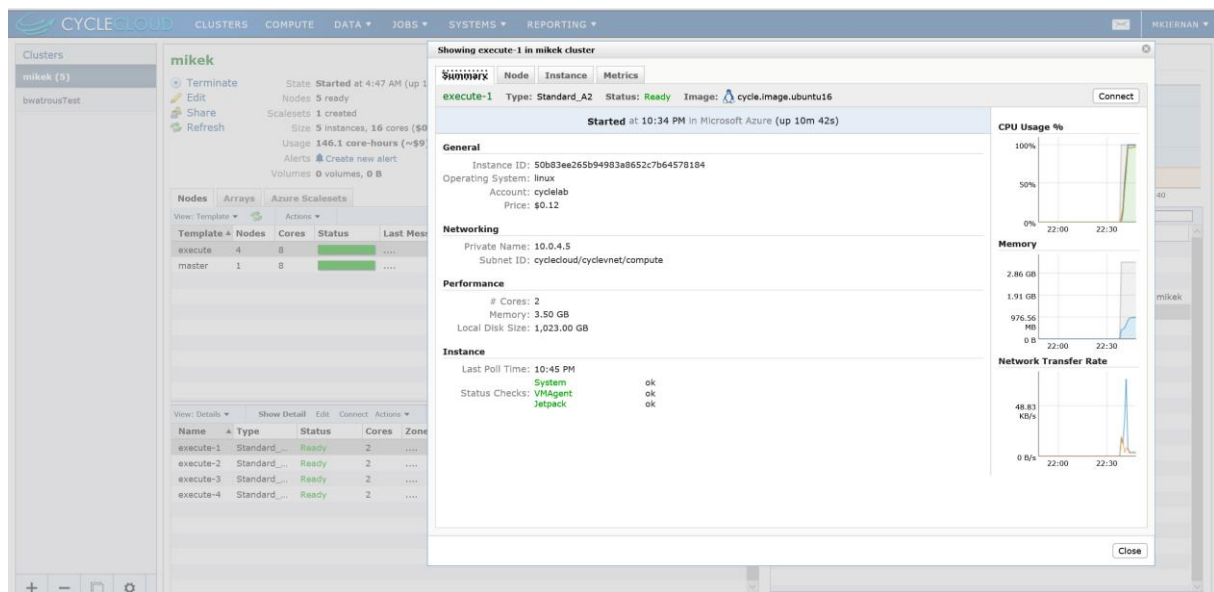
- Feel free to try modifying the job script and submit your own variants
- Now return to the GUI and look at the Cluster page
- Shortly you should see CycleCloud begin to spin up a node (or set of nodes) – this is the “auto scale” functionality spinning up the cores needed to run the jobs you just submitted.



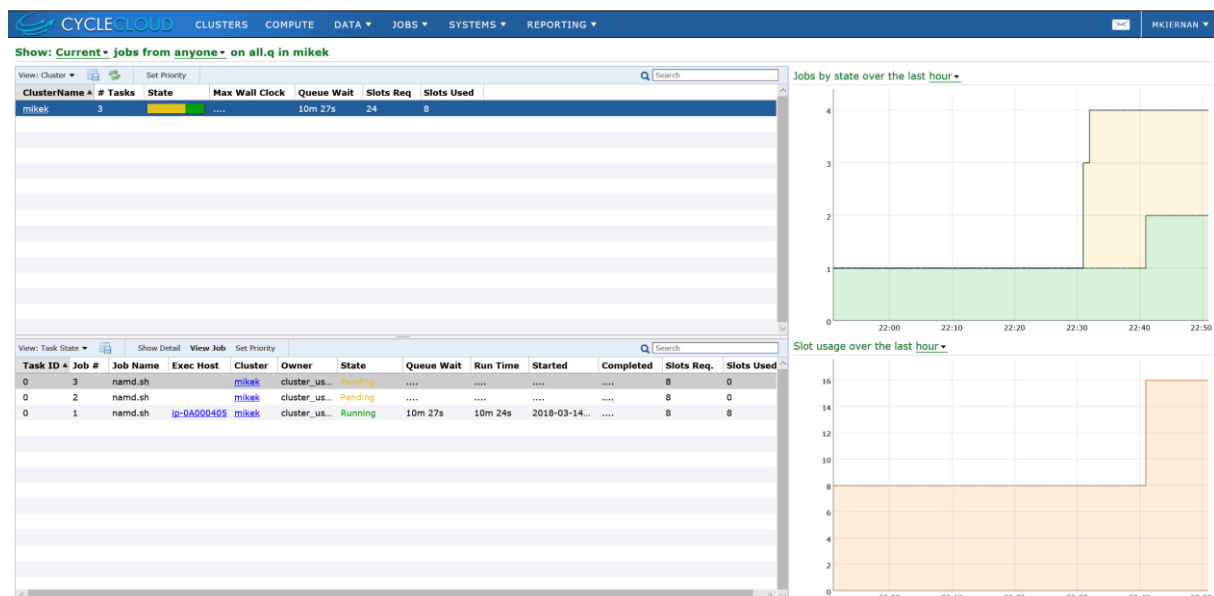
After a few minutes all execute nodes should be green:



- Look in the Event Log and you should see the Autoscaler's core requests
- Next, select the "execute" node row in the Nodes table
- The table should spit to show each exec node individually
- Select one of nodes in the bottom pane, and double-click or click "Show Detail"
- In the Node Details pop-up, look at the statistics collected



15. You can follow the Node Orchestration workflow on the Node tab in the "PhaseMap"
16. Once the VM has been acquired, the Instance tab will appear with data collected from Azure
17. Once the Node converges, you will see CPU / Memory / Network graphs populate on the Summary Tab and the Metrics tab will appear with a snapshot of Node performance data
18. If you select the Compute menu item, you'll see a summary of current cluster usage
19. If you select the Jobs -> Overview menu item, you'll see the current job queues for all clusters



20. If you check back to the qstat -f output on your clusters, you should see the MPI jobs occupying all 8 slots.
21. You can watch the job execute by tailing the "namd.sh.o*" logs

```
cluster_user@ip-0A000404:~$ ls
namd.sh namd.sh.e1 namd.sh.o1 namd.sh.pe1 namd.sh.po1
cluster_user@ip-0A000404:~$ tail -f namd.sh.o1
ENERGY: 279 21984.3649 19593.9432 5677.5176 184.5187 -335888.5802 22096.4199
0.0000 0.0000 43975.0881 -222376.7278 159.9693 -266351.8159 -222065.2022
159.9693 -4044.3213 -2682.8389 921491.4634 -4044.3213 -2682.8389

ENERGY: 279 21984.3649 19593.9432 5677.5176 184.5187 -335888.5802 22096.4198
0.0000 0.0000 43975.0882 -222376.7278 159.9693 -266351.8160 -222065.2023
159.9693 -4044.3213 -2682.8390 921491.4634 -4044.3213 -2682.8390

ENERGY: 267 19648.0904 20691.2680 5707.0583 187.8501 -334831.4855 21930.8372
0.0000 0.0000 44220.2167 -222446.1647 160.8610 -266666.3815 -222055.6586
160.8610 -2435.4235 -2662.6784 921491.4634 -2435.4235 -2662.6784

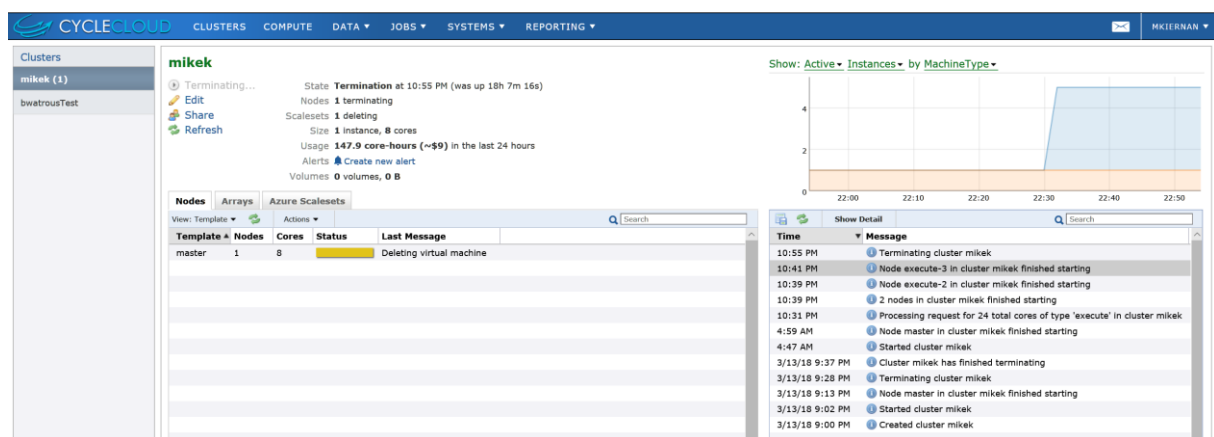
ENERGY: 276 19401.8504 19594.7508 5701.2547 182.4904 -333292.1284 21971.0408
0.0000 0.0000 44028.5272 -222412.2142 160.1637 -266440.7414 -222072.9397
160.1637 -1580.1303 -2417.6043 921491.4634 -1580.1303 -2417.6043

ENERGY: 268 19962.9161 20375.7517 5700.1930 187.9286 -335513.7451 21959.1257
0.0000 0.0000 44823.5377 -222504.2923 163.0557 -267327.8300 -222075.9874
163.0557 -2903.2126 -2658.6181 921491.4634 -2903.2126 -2658.6181
```

Step 4: Terminate & Delete Your GridEngine Cluster

Finally, let's terminate the cluster to stop billing now that the workload is complete (no need to wait for the job to finish unless you want to). Click on "Clusters" to return to the cluster view from the job view.

1. Click the "Terminate" button at the top of the Clusters page for your cluster.



2. Once the CycleCloud has finished terminating the cluster and cleaning up its resources, you may delete the cluster by clicking the "-" button on the bottom of the Cluster List frame
 - Deleting the cluster removes any persistent resources such as data volumes that are retained for the lifetime of the cluster