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
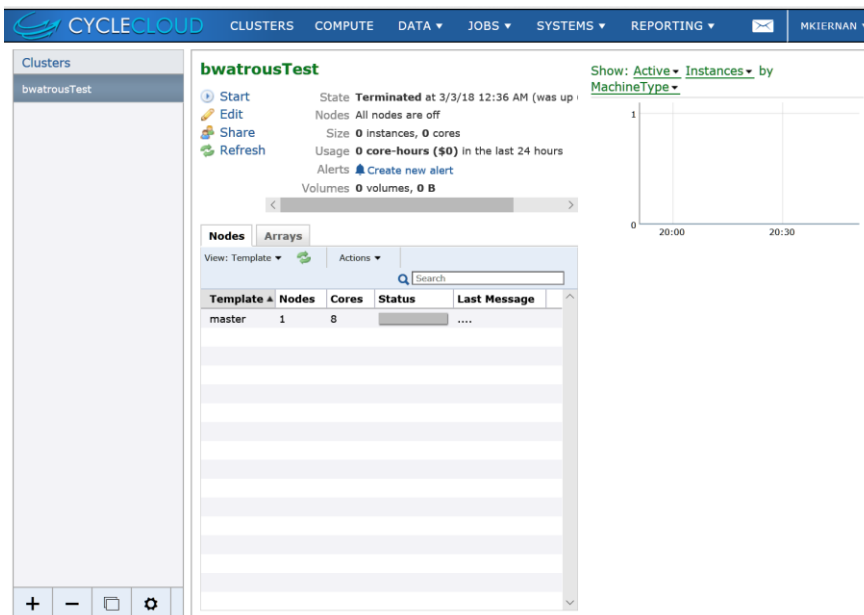
Step 2: Create Your NAMD GridEngine Cluster

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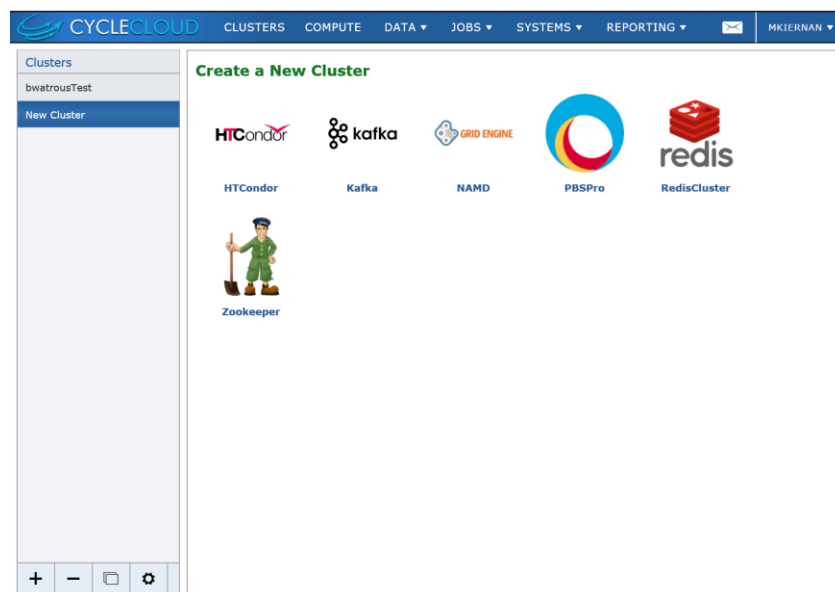
2. Click on the "NAMD" GridEngine cluster
   - This should bring up the Cluster Creation Form

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"

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:
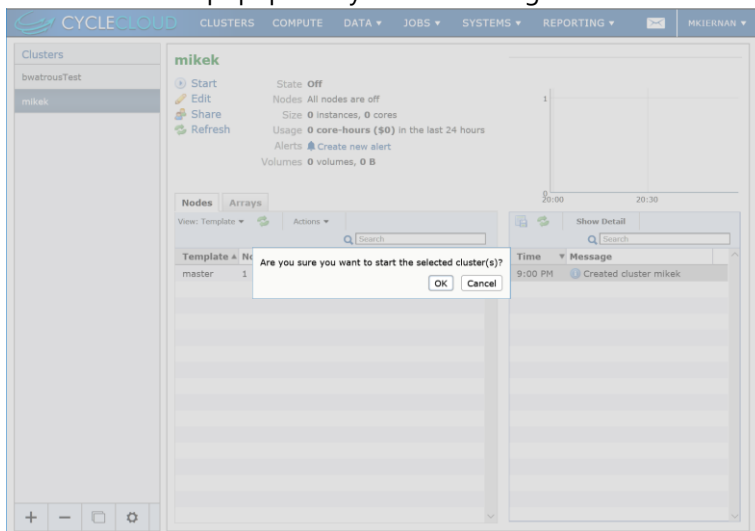
The master node starts to deploy – this process will take around 5-10 minutes;
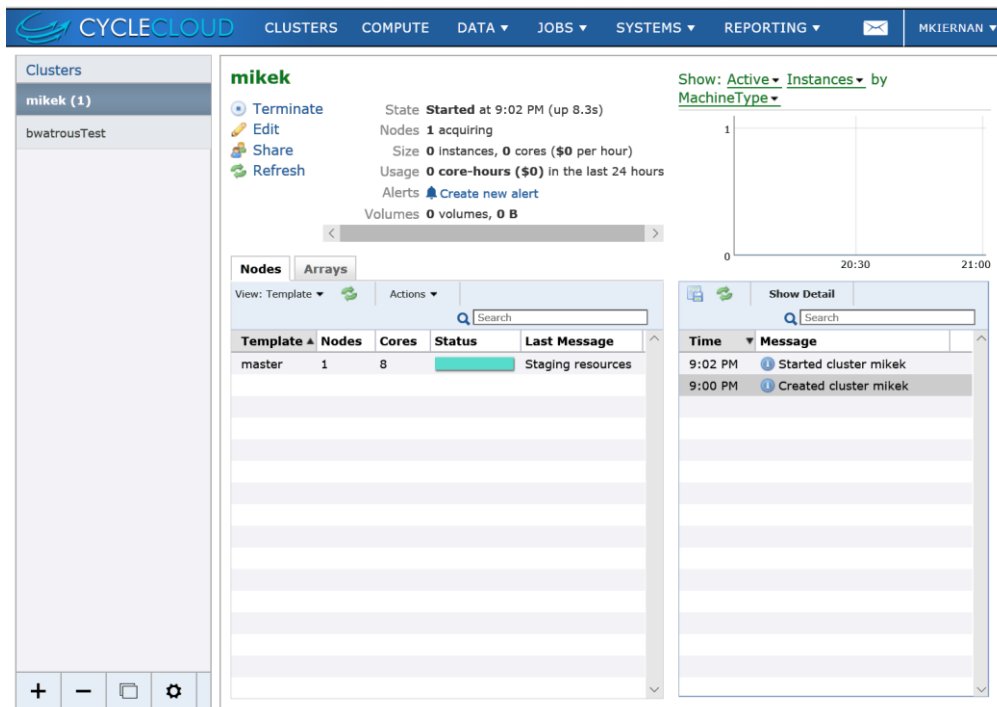
Step 3: Login to Your GridEngine Cluster and Submit a Job

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.

2. This will show you 2 options for sshing in to the Master node
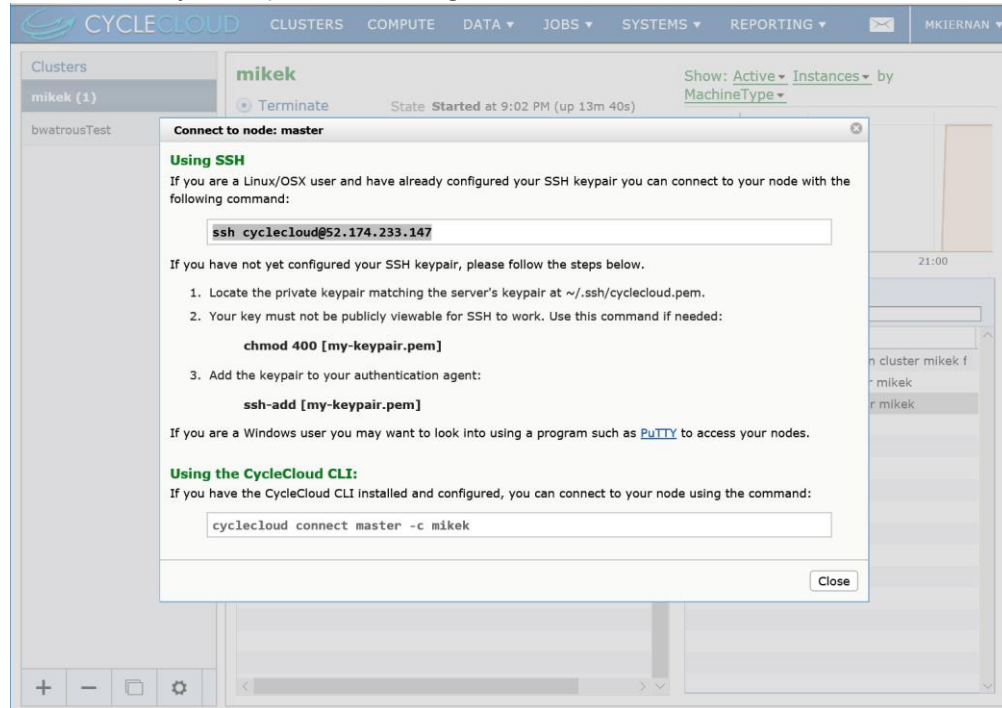
3. Copy the line with the IP Address
4. Log in to the QMaster

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
```

5. Look at the content of the job script

```
$ cat namd.sh
```

6. Submit 3 variants

```
$ qsub namd.sh
```

```
$ qsub namd.sh apoa1
```

```
$ qsub namd.sh f1atpase
```

```
$ watch qstat -f
```

7. Feel free to try modifying the job script and submit your own variants
8. Now return to the GUI and look at the Cluster page
9. 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.
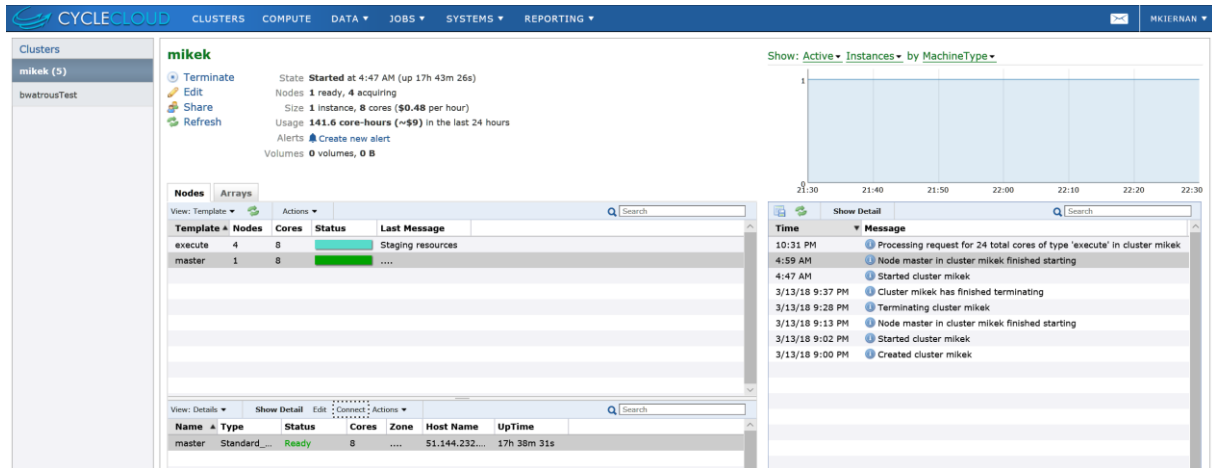
After a few minutes all execute nodes should be green:
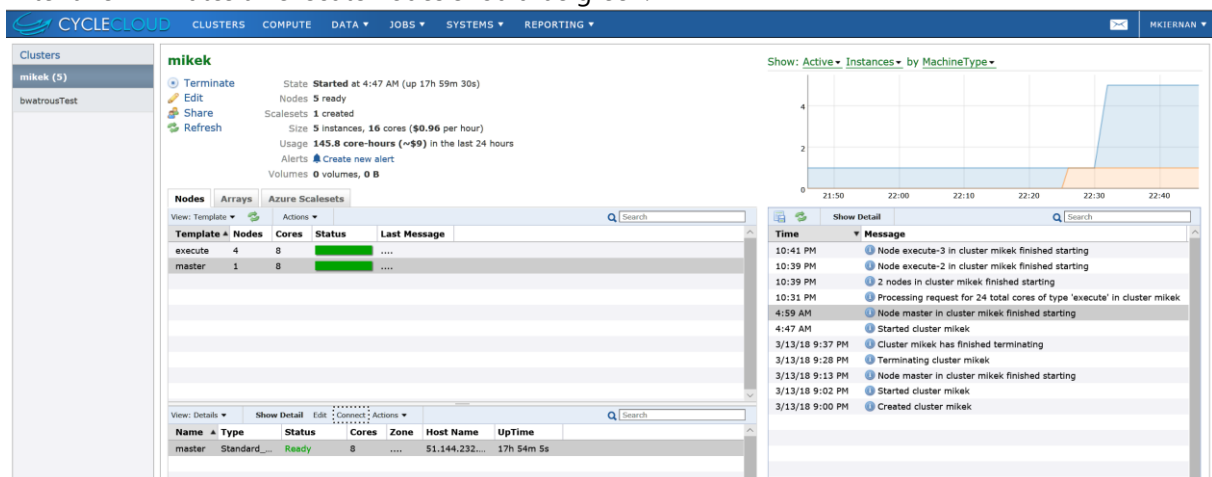
10. Look in the Event Log and you should see the Autoscaler's core requests
11. Next, select the "execute" node row in the Nodes table
12. The table should spit to show each exec node individually
13. Select one of nodes in the bottom pane, and double-click or click "Show Detail"
14. In the Node Details pop-up, look at the statistics collected
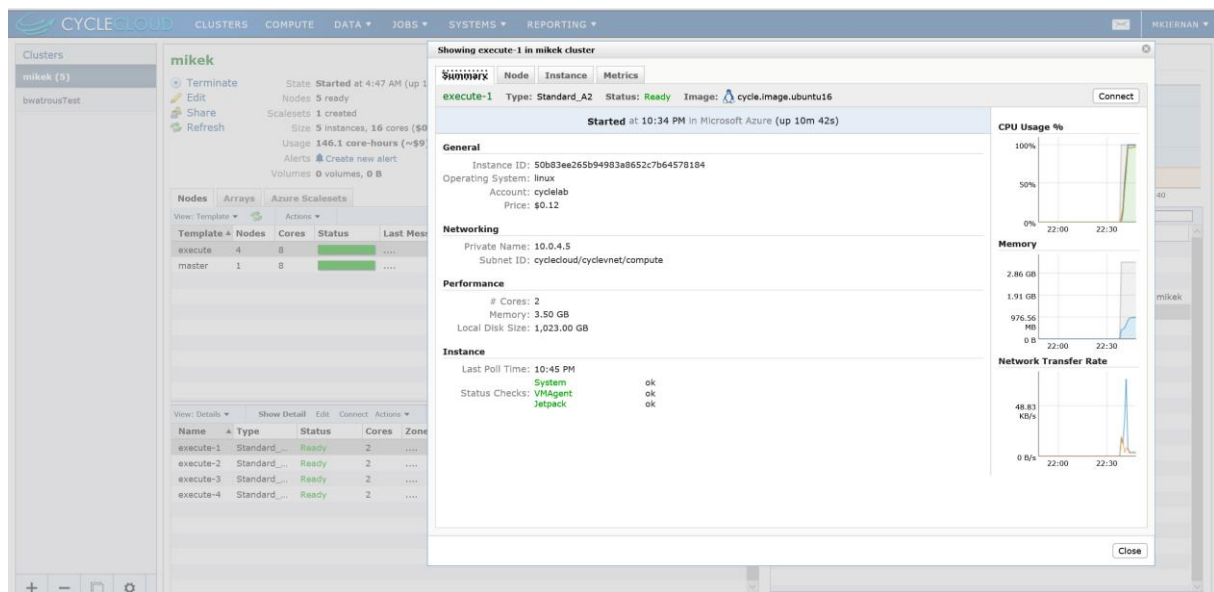
15. You can follow the Node Orchestration workflow on the Node tab in the "PhaseMap"
16. Once the VM has been acquired, the Instance tab will appear with data collected from Azure
17. Once the Node converges, you will see CPU / Memory / Network graphs populate on the Summary Tab and the Metrics tab will 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
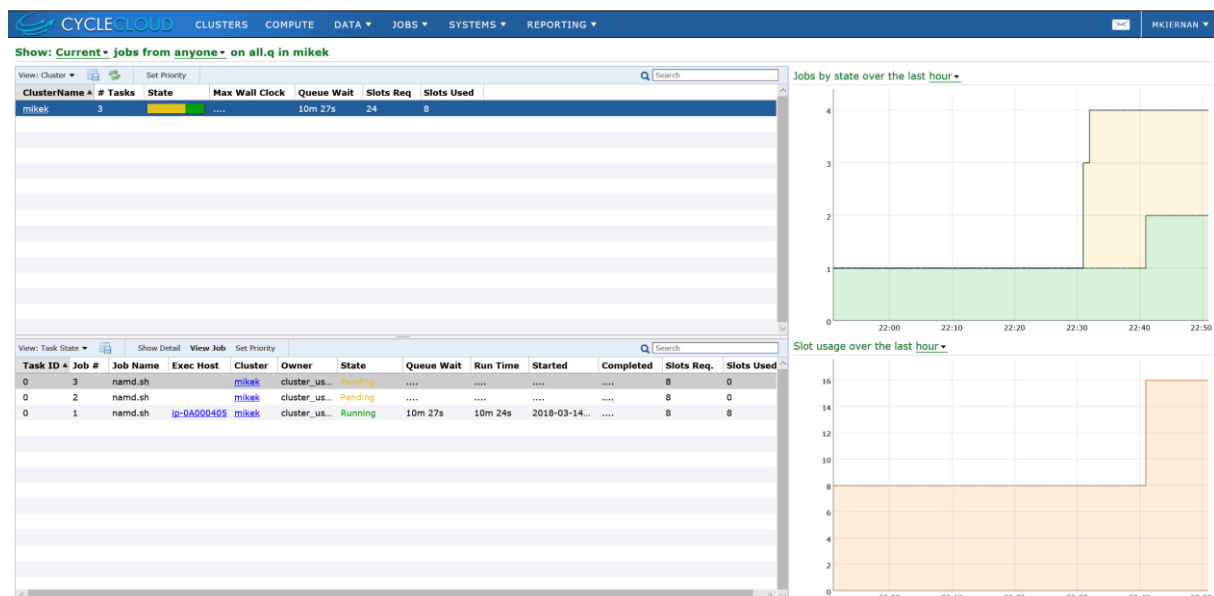
20. If you check back to the qstat -f output on your clusters, you should see the MPI jobs occupying all 8 slots.
21. You can watch the job execute by tailing the "namd.sh.o*" logs

```
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
```
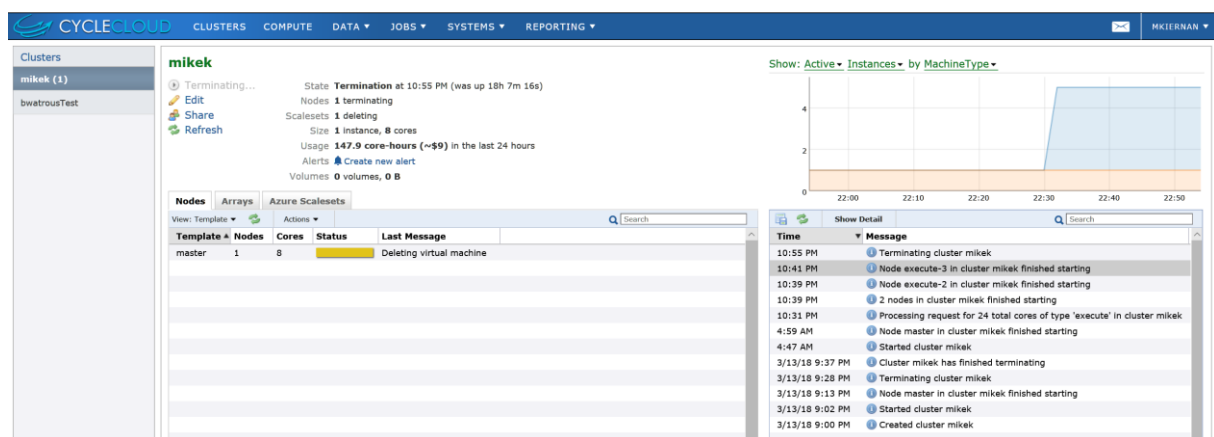
Step 4: Terminate & Delete Your GridEngine Cluster

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