Volta Cluster User Guide

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⚠️ WARNING ⚠️

READ ALL SECTIONS OF THIS GUIDE CAREFULLY

MOST SUPPORT REQUESTS & QUESTIONS FROM USERS ARE ALREADY ANSWERED WITHIN THIS GUIDE

Contents

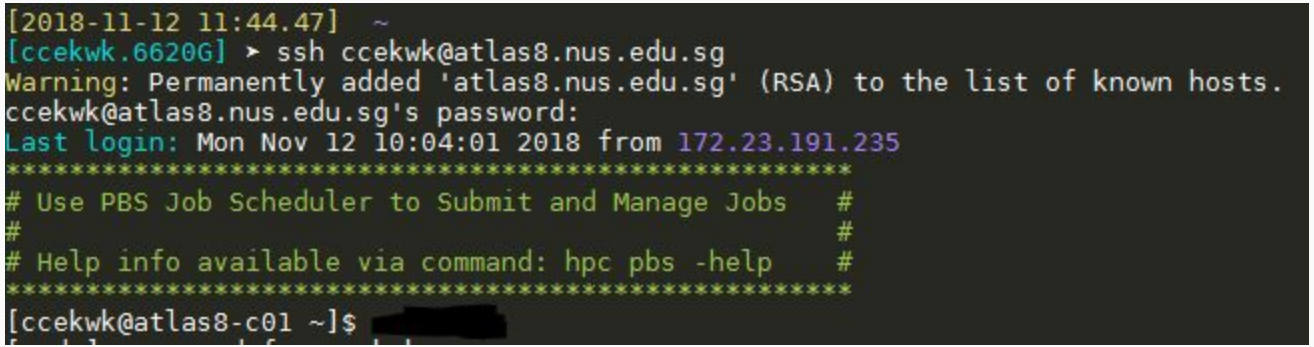
Access

Access

- Login via ssh to NUS HPC login nodes
  - atlas9
  - atlas8-c01.nus.edu.sg
- If you are connecting from outside NUS network, please connect to Web VPN first
  - http://webvpn.nus.edu.sg

Access

OS	Access Method	Command
Linux	ssh from terminal	`ssh nusnet_id@atlas8-c01.nus.edu.sg`
MacOS	ssh from terminal	`ssh username@hostname`
Windows	ssh using mobaxterm or putty or terminal	`ssh username@hostname`


[2018-11-12 11:44.47] ~
[ccekwk.6620G] ➤ ssh ccekwk@atlas8.nus.edu.sg
Warning: Permanently added 'atlas8.nus.edu.sg' (RSA) to the list of known hosts.
ccekwk@atlas8.nus.edu.sg's password:
Last login: Mon Nov 12 10:04:01 2018 from 172.23.191.235
Use PBS Job Scheduler to Submit and Manage Jobs
# #
Help info available via command: hpc pbs -help
[ccekwk@atlas8-c01 ~]$

File Transfer

1. Mobaxterm built-in sftp client
2. Filezilla client
3. Linux/Mac OS/Windows Terminal Tools
    a. scp
    b. rsync
    c. sftp

Resources

Resources: Hardware

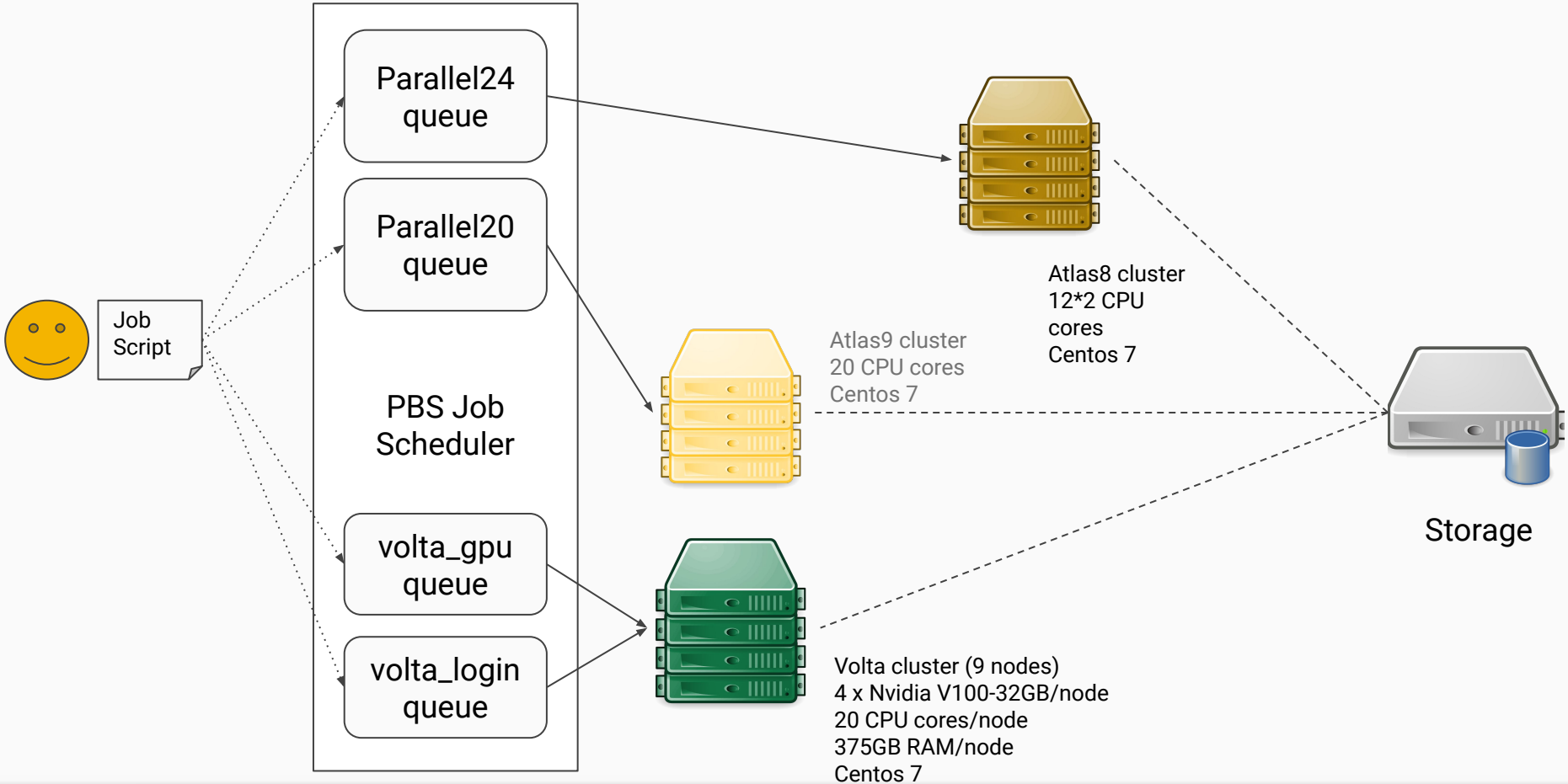
- Standard CPU HPC Clusters
  - Atlas 8 - parallel24 queue
  - Atlas 9 - parallel20 queue
- GPU Clusters
  - 9 nodes x 4 Nvidia Tesla V100-32GB

No internet access on Volta Servers

Resources: Storage

Directories	Feature	Disk Quota	Backup	Description
`/home/svu/$USERID`	Global	20 GB	Snapshot	Home Directory. U:drive on your PC.
`/hpctmp/$USERID`	Local on All Atlas/Volta cluster	500 GB	No	Working Directory. Files older than 60 days are purged automatically
`/scratch/$USERID`	Local to each **Volta** node only	5 TB	No	For quick read/write access to datasets. Create a folder with your NUSNET ID. Routinely purged.
`/scratch2/$USERID`	Available on Atlas 9 and Volta Cluster	1 TB	No	For quick read/write access to datasets. Create a folder with your NUSNET ID. Files older than 60 days are purged automatically

Note: Type “hpc s” to check your disk quota for your home directory


Parallel24 queue
Parallel20 queue
PBS Job Scheduler
volta_gpu queue
volta_login queue
Job Script
Atlas8 cluster
12*2 CPU cores
Centos 7
Atlas9 cluster
20 CPU cores
Centos 7
Storage
Volta cluster (9 nodes)
4 x Nvidia V100-32GB/node
20 CPU cores/node
375GB RAM/node
Centos 7

Resources: Containers

IMPORTANT

Each Deep Learning framework has its own singularity container:

e.g.: For Pytorch 1.4, use
`pytorch_1.4_ffmpeg_cuda10.0-cudnn7-devel-ubuntu18.04-py36.simg`

Containers are located in: **/app1/common/singularity-img/3.0.0/**

Please take a look in the above folder to find the container with the Deep Learning Library you need

All scripts must be executed within a container.

- For Ubuntu containers with CUDA and Python see the following folder:
  `/app1/common/singularity-img/3.0.0/CUDA`

Resources: Containers

1. Contact us only if you have any customised container requests.
2. If you build your own container, **contact us** so we can check if it has the required and compatible CUDA libraries the GPUs

Resources: Containers (Singularity)

- **Simple:** with all components packaged in a single file, including the definitions, configurations, metadata, and security keys.
- **Fast**: with native support for GPU.
- Possible to **Build your own Singularity Container** and upload for use on NUS HPC
  - https://www.sylabs.io/docs/

Building Your Own Container

If you build your own container, please

1. ensure that you install cuda drivers/libraries
2. you do not have to install GPU drivers (this is provided by host system)
3. verify that it can use GPUs
    a. use interactive queue:
    b. `singularity exec your_container.simg nvidia-smi`

IMPORTANT TO READ

Running a Container (Volta Nodes)

```
$ singularity exec $image bash
```

Substitute **$image** with full path to container image file

E.g.:

```
$ singularity exec /app1/common/singularity-img/3.0.0/tensorflow_1.12_nvcr_19.01-py3.simg bash
```

Put the commands in a **job script**. It is required.
This slide applies only to VOLTA nodes.

DO NOT RUN THE ABOVE IN ATLAS NODES

Jobs

Types of Jobs

1. Short, Interactive Jobs
    a. For debugging
    b. For checking if your code works
2. Batch Jobs
    a. For running working code for long periods of time.

Short or Interactive Jobs

Short Interactive Jobs

Run short interactive jobs meant for **debugging** your code on GPU.

```
qsub -I -l select=1:mem=50GB:ncpus=10:ngpus=1 -l walltime=02:00:00 -q volta_login
```

- `-I` : Interactive
- Mem: Max 96GB, Min 50GB
- ncpus: 6 to 20
- ngpus: 1 to 2 (Choose less, wait less)
- `-q` : volta_login queue

1. Default Walltime: 1 hour
2. Max Walltime: 4 hours

Short Interactive Jobs

- Once the interactive job is launched, you will be brought into **volta01**.
- In Volta01, you can launch a container of your choice to debug your deep learning python script.

```
qsub -I -l select=1:mem=50GB:ncpus=10:ngpus=1 -l walltime=02:00:00 -q volta_login

singularity exec -e $image bash
```

- You can replace `$image` with the container image of your choice, e.g.:
  `/app1/common/singularity-img/3.0.0/tensorflow_1.12_nvcr_19.01-py3.simg`

```
[ccekwk@atlas9-c01 horovod]$ qsub -I -l select=1:ncpus=5:ngpus=1 -l walltime=0:05:00 -q volta_login
qsub: waiting for job 789846.venus01 to start
qsub: job 789846.venus01 ready

[ccekwk@volta01 ~]$ uname -a
Linux volta01 3.10.0-862.el7.x86_64 #1 SMP Fri Apr 20 16:44:24 UTC 2018 x86_64 x86_64 x86_64 GNU/Linux
[ccekwk@volta01 ~]$ cat /etc/centos-release
CentOS Linux release 7.5.1804 (Core)
[ccekwk@volta01 ~]$
```

```
[ccekwk@volta01 ~]$ singularity exec /app1/common/singularity-img/3.0.0/tensorflow_1.12_nvcr_19.01-py3.simg bash
ccekwk@volta01:~$ uname -i
x86_64
ccekwk@volta01:~$ cat /etc/lsb-release
DISTRIB_ID=Ubuntu
DISTRIB_RELEASE=16.04
DISTRIB_CODENAME=xenial
DISTRIB_DESCRIPTION="Ubuntu 16.04.5 LTS"
```

Interactive Jupyter Notebook

- You can run a Jupyter Notebook instance for a short amount of time (up to 4 hours) using the **volta_login** interactive queue
- The Jupyter Notebook instance will run inside a container of your choice.

Interactive Jupyter Notebook

- Login to Atlas9 or Atlas8 and set your Jupyter password (ONLY DO ONCE)
- In Atlas9 run the following commands:

```
bash
module load singularity
singularity exec $image jupyter notebook --generate-config
singularity exec $image jupyter notebook password
```

- You can replace `$image` with the container image of your choice, e.g.:
  `/app1/common/singularity-img/3.0.0/tensorflow_1.12_nvcr_19.01-py3.simg`
- Set your password as prompted

Interactive Jupyter Notebook

- Launch an Interactive Job from Atlas9
- Change walltime and other resources as required

```
qsub -I -l select=1:mem=50GB:ncpus=5:ngpus=1 -q volta_login -l walltime=0:10:00
```

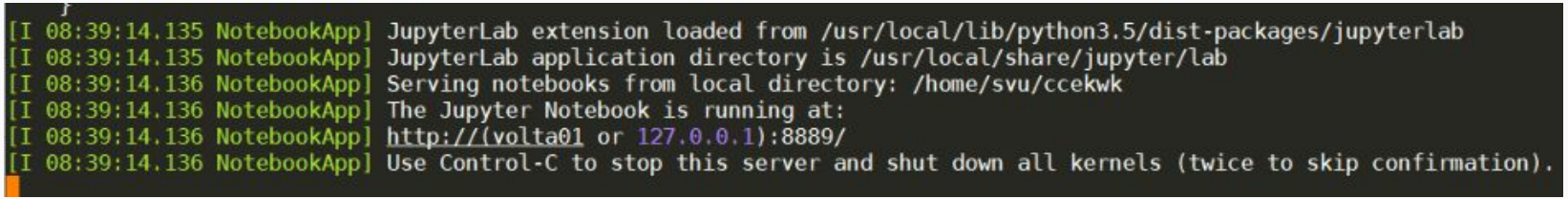
```
[ccekwk@atlas9-c01 ~]$ qsub -I -l select=1:mem=10GB:ncpus=5:ngpus=1 -q volta_login -l walltime=0:10:00
qsub: waiting for job 797088.venus01 to start
qsub: job 797088.venus01 ready

[ccekwk@volta01 ~]$
```

Interactive Jupyter Notebook

- In Volta1 node, launch jupyter notebook in a container of your choosing
- Execute the following command in 1 line

```
singularity exec -e $image jupyter notebook --no-browser --port=8889 --ip=0.0.0.0
```

- You can replace `$image` with the container image of your choice, e.g.:
  `/app1/common/singularity-img/3.0.0/tensorflow_1.12_nvcr_19.01-py3.simg`

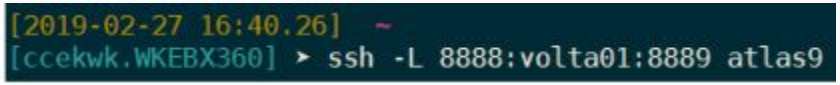


Interactive Jupyter Notebook

- On your personal computer in a new Mobaxterm tab run the following command

Entry Port | Target Host | Exit Port | You | Tunnel Host

```
ssh -L 8888:volta01:8889 nusnet_id@atlas9
```



- Open your browser and browse to http://localhost:8888

Your Computer | Entry Port

Interactive Jupyter Notebook

- When launching jupyter notebook, if you receive an error that says port 8889 is already in use, choose another port

e.g.

- `singularity exec -e $image jupyter notebook --no-browser --port=8181 --ip=0.0.0.0`
- `ssh -L 8888:volta01:8181 nusnet_id@atlas9`

Batch Jobs

Batch Jobs

- Up to 2 GPUs per job
  - Please request only what you need.
  - ENSURE THAT YOUR CODE IS MODEL OR DATA PARALLEL
  - Using >1 GPU has to be **explicitly programmed** in your code.
  - Choose LESS, wait LESS
- Most applications use only 1 GPU by default
  - Requesting >1 GPUs does not make it faster. The other GPUs will not be utilised at all.
- Most applications will not scale well with > 1 GPUs
- 1 GPU is most likely more than enough as the V100-32GB has large memory capacity

Queue Resources

Max RAM = 241gb
Max No. of CPU cores = 20
Max No. of GPUs = 2
Max Walltime = 72:00:00
Minimum No. of CPU cores = 5
Minimum No. of GPU = 1
Default Walltime = 04:00:00
Request CPU Core in increments of 1

Sample Job Script

For Batch Jobs

Note:

1. **Do not copy and paste** the job script in the next slide directly into your text editor.
2. Please **type it out manually** to avoid hidden characters.
3. Ensure that the jobscript **conforms to BASH syntax.**

Batch Job Script for volta_gpu

DO NOT COPY AND PASTE

Green is user configurable
Black is fixed

```
#!/bin/bash
#PBS -P project_name
#PBS -j oe
#PBS -N tensorflow
#PBS -q volta_gpu
#PBS -l select=1:ncpus=10:mem=80gb:ngpus=1
#PBS -l walltime=24:00:00

cd $PBS_O_WORKDIR;
np=$(cat ${PBS_NODEFILE} | wc -l);

image="/app1/common/singularity-img/3.0.0/tensorflow_1.12_nvcr_19.01-py3.simg"

singularity exec -e $image bash << EOF > stdout.$PBS_JOBID 2> stderr.$PBS_JOBID

python cifar10_resnet.py

# you can put more commands here
# echo “Hello World”

EOF
```

Wrong:

```
image = “/path/to/container/”
```

Correct

```
image=”/path/to/container”
```

Multi-GPU Scaling

Using Multiple GPUs

1. Ensure that your code allows for Multi-GPU training
   a. DataParallel on Pytorch
   b. Distributed training with Keras
   c. Custom training loops (distributed) with Tensorflow
   d. Horovod for Tensorflow/Keras/Pytorch
2. Then request for 2 GPUs
   a. `#PBS -l select=1:ncpus=10:mem=80gb:ngpus=2`
   b. Do NOT request for 2 GPUs if your code does not meet the conditions in Step 1.

Scaling for Multi GPU with Horovod

For better scaling when utilising multiple gpus, use Horovod.
Distributed training framework for TensorFlow, Keras, PyTorch, and MXNet.

To use Horovod, you need to set the following in your job script.

```
#PBS -l select=1:ncpus=10:mem=100gb:ngpus=2


NCCL_DEBUG=INFO ; export NCCL_DEBUG
mpirun -np 2 -x NCCL_DEBUG python keras_mnist_advanced.py
```

Use mpirun to execute python

Horovod Job Script for volta_gpu

DO NOT COPY AND PASTE

Green is user configurable
Black is fixed

```
#!/bin/bash
#PBS -P volta_pilot
#PBS -j oe
#PBS -N tensorflow
#PBS -q volta_gpu
#PBS -l select=1:ncpus=20:mem=100gb:ngpus=2
#PBS -l walltime=24:00:00

cd $PBS_O_WORKDIR;
np=$(cat ${PBS_NODEFILE} | wc -l);

image="/app1/common/singularity-img/3.0.0/tensorflow_1.12_nvcr_19.01-py3.simg"

singularity exec -e $image bash << EOF > stdout.$PBS_JOBID 2> stderr.$PBS_JOBID

NCCL_DEBUG=INFO ; export NCCL_DEBUG
mpirun -np 2 -x NCCL_DEBUG python keras_mnist_advanced.py

EOF
```

Multi-Node Multi-GPU Scaling

- Not supported/allowed in NUS HPC Volta Cluster
- Use NSCC DGX-1 Cluster
  - 8 x V100-16GB, 6 Nodes

Python Packages

Installing Python Packages: Specify Custom Path **(Recommended)**

On **Atlas8 or Atlas7** **(NO NEED TO LAUNCH JOB)**:

```
module load singularity

singularity exec -e /app1/common/singularity-img/3.0.0/[yourcontainer.simg] bash
```

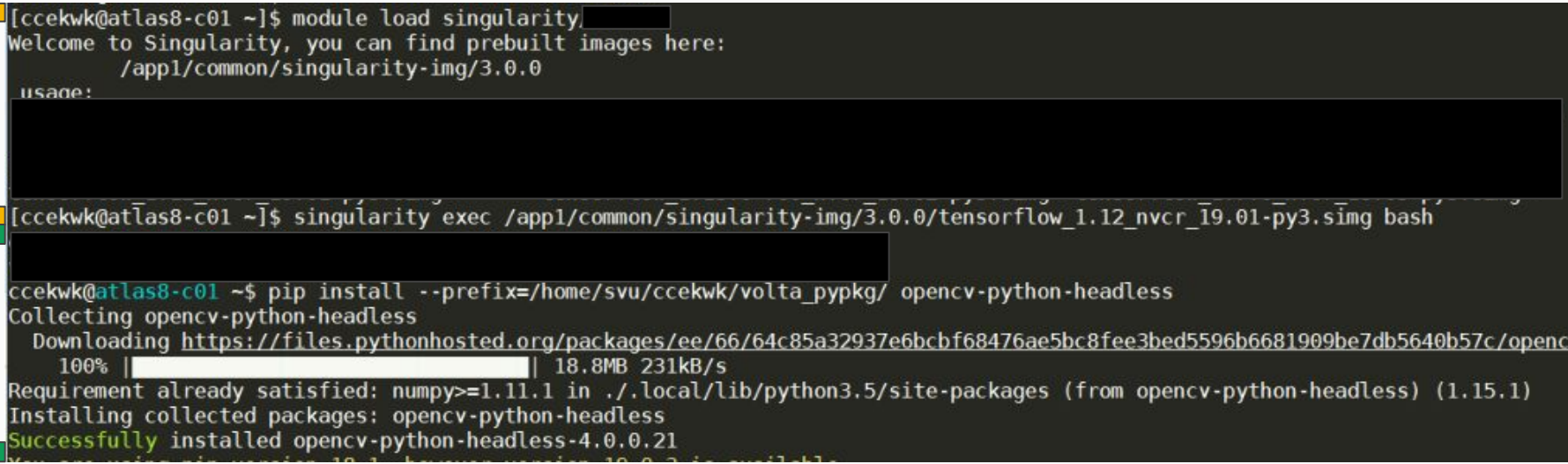
Executing the above commands will bring you into the container.
In Container:

```
pip install --prefix=/home/svu/[nusnet_id]/volta_pypkg/ package_name
```

Note: volta_pypkg is an example directory. You can name it anything you want when you create it.
Replace [nusnet_id] with YOUR NUSNET ID.

In Host

In Container



Installing Python Packages: Default User Package Path (Not Recommended)

On **Atlas8 (NO NEED TO LAUNCH JOB)**:

```
$ module load singularity

$ singularity exec /app1/common/singularity-img/3.0.0/[cont.simg] bash
```

In Container:

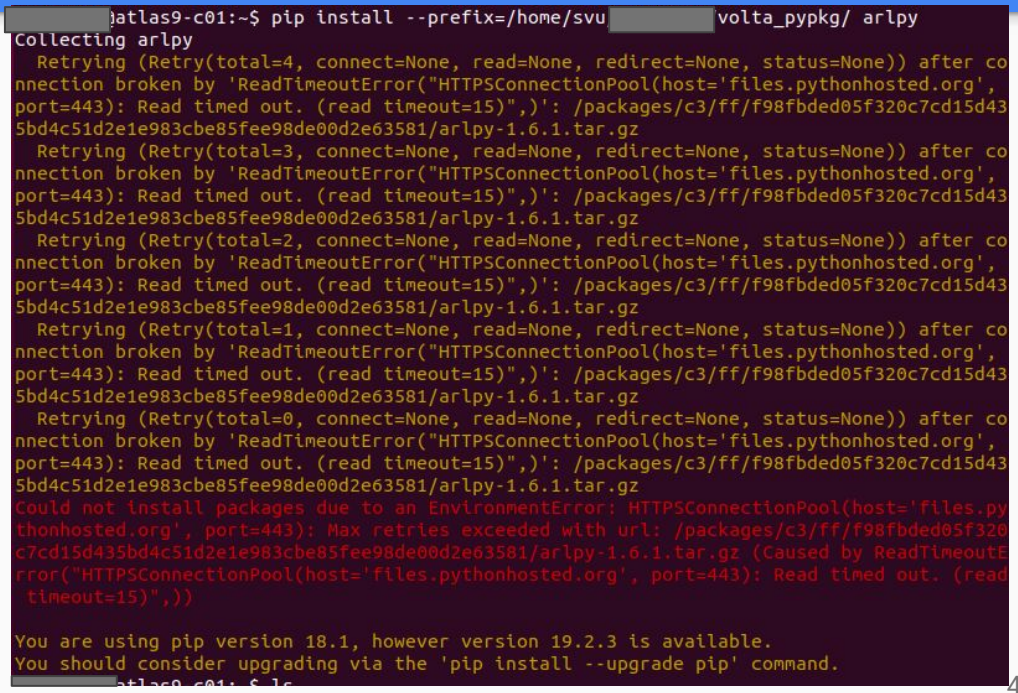
```
$ pip install --user package_name
```

Python in the container will automatically locate packages installed with this method

Pip Install Errors 1

If you encounter this error, it means you're using **ATLAS 9** and not **ATLAS 8 or 7.**

Use ATLAS 8 or 7 ONLY



Pip Install Errors 2

```
You are using pip version 18.1, however version 19.2.3 is available.
You should consider upgrading via the 'pip install --upgrade pip' command.
```

This is **not** an **error.**

Do not attempt to upgrade pip.

Using User-installed Python Packages: Custom Path (Recommended)

In job script add the following:

If you used Tensorflow 1.x container:

```
export PYTHONPATH=$PYTHONPATH:/home/svu/[nusnet_id]/volta_pypkg/lib/python3.5/site-packages
```

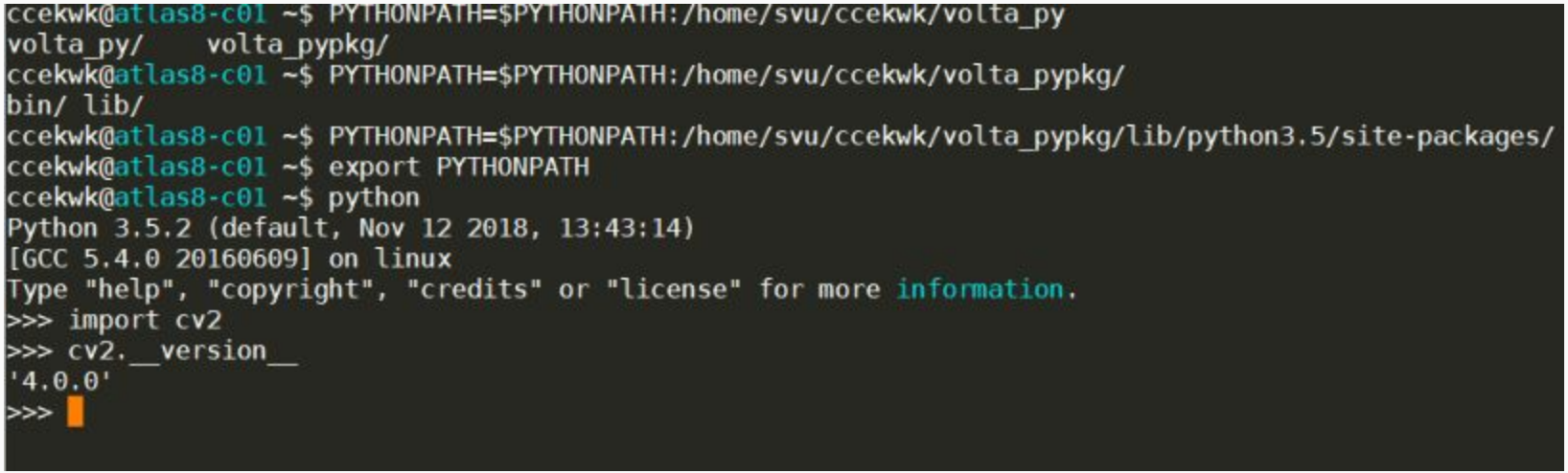
If you used Tensorflow 1.x container:

```
export PYTHONPATH=$PYTHONPATH:/home/svu/[nusnet_id]/volta_pypkg/lib/python3.8/site-packages
```

If you used Pytorch container:

```
export PYTHONPATH=$PYTHONPATH:/home/svu/[nusnet_id]/volta_pypkg/lib/python3.6/site-packages
```

If you named volta_pypkg something else, please remember to change it
Replace [nusnet_id] with YOUR NUSNET ID


ccekwk@atlas8-c01 ~$ PYTHONPATH=$PYTHONPATH:/home/svu/ccekwk/volta_py
volta_py/ volta_pypkg/
ccekwk@atlas8-c01 ~$ PYTHONPATH=$PYTHONPATH:/home/svu/ccekwk/volta_pypkg/
bin/ lib/
ccekwk@atlas8-c01 ~$ PYTHONPATH=$PYTHONPATH:/home/svu/ccekwk/volta_pypkg/lib/python3.5/site-packages/
ccekwk@atlas8-c01 ~$ export PYTHONPATH
ccekwk@atlas8-c01 ~$ python
Python 3.5.2 (default, Nov 12 2018, 13:43:14)
[GCC 5.4.0 20160609] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import cv2
>>> cv2.__version__
'4.0.0'
>>>

Batch Job Script for volta_gpu with Custom Python Lib Path

Green is user configurable
Black is fixed

```
#!/bin/bash
#PBS -P volta_pilot
#PBS -j oe
#PBS -N tensorflow
#PBS -q volta_gpu
#PBS -l select=1:ncpus=5:mem=50gb:ngpus=1
#PBS -l walltime=24:00:00

cd $PBS_O_WORKDIR;
np=$(cat ${PBS_NODEFILE} | wc -l);

image="/app1/common/singularity-img/3.0.0/tensorflow_1.12_nvcr_19.01-py3.simg"

singularity exec -e $image bash << EOF > stdout.$PBS_JOBID 2> stderr.$PBS_JOBID

PYTHONPATH=$PYTHONPATH:/home/svu/[nusnet_id]/volta_pypkg/lib/python3.5/site-packages
export PYTHONPATH

python cifar10_resnet.py
EOF
```

Internet Access

Internet Access from within Containers

If for some reason you need to access the internet from within a container, do the following:

1. Login to Atlas8 and run the following commands
2. module load singularity
3. singularity exec $container_path bash

Replace $container_path with container of your choice.

e.g.: `singularity exec /app1/common/singularity-img/3.0.0/CUDA/cuda_10.0-cudnn7-devel-ubuntu16.04-py3.simg bash`

PBS Job Scheduler

Submitting a Job

Steps

You have to run:

1. Prepare your python script in your working directory
2. Create a PBS job script and save it in your working directory
    a. Example job scripts are in the following 2 slides
3. Submit PBS job script to PBS Job Scheduler

Server will run:

1. Job is in PBS Job Scheduler queue
2. Job Scheduler waits for server resources to be available
3. If available, Job Scheduler runs your script on remote gpu server

Submitting a Job

Save your job script (previous slides for examples) in a text file (e.g. train.pbs) then run the following commands

```
shell$ qsub train.pbs
675674.venus01


shell$ qstat -xfn

venus01:
                                                                  Req'd  Req'd   Elap
Job ID          Username Queue    Jobname    SessID NDS TSK Memory Time  S Time
--------------- -------- -------- ---------- ------ --- --- ------ ----- - -----
669468.venus01  ccekwk   volta    cifar_noco    --    1   1   20gb 24:00 F   --
    --
674404.venus01  ccekwk   volta    cifar_noco    --    1   1   20gb 24:00 F   --
   TestVM/0
675674.venus01  ccekwk   volta    cifar_noco    --    1   1   20gb 24:00 Q   --
    --
```

Statuses: Q(ueue), F(inish), R(unning), E(nding), H(old)

```
[ccekwk@atlas8-c01 classification]$ qsub train.pbs
697978.venus01
[ccekwk@atlas8-c01 classification]$ qstat -xfn

venus01:
                                                                  Req'd  Req'd   Elap
Job ID          Username Queue    Jobname    SessID NDS TSK Memory Time  S Time
--------------- -------- -------- ---------- ------ --- --- ------ ----- - -----
695126.venus01  ccekwk   azgpu    cifar_noco    --    1   4   40gb 24:00 F   --
    --
697978.venus01  ccekwk   azgpu    cifar_noco    --    1   4   40gb 24:00 R   --
   TestVM/0*4
[ccekwk@atlas8-c01 classification]$
```

Statuses: Q(ueue), F(inish), R(unning), E(nding), H(old)

Job Chaining and Dependencies

Execute jobs in sequence

- `qsub -W depend=afterok:<Job-ID> <JOB SCRIPT>`
  - `qsub -W depend=afterany:836578.venus01 volta_benchmark.pbs`
- Job script <QSUB SCRIPT> will be submitted after the Job, <Job-ID> is successfully completed. Useful options to "depend=..." are:
  - **afterok**:<Job-ID> Job is scheduled if the Job <Job-ID> exits without errors or is successfully completed.
  - **afternotok**:<Job-ID> Job is scheduled if the Job <Job-ID> exited with errors.
  - **afterany**:<Job-ID> Job is scheduled if the Job <Job-ID> exits with or without errors

```
ccekwk@atlas9-c01 /hpctmp/ccekwk/tf_benchmarks/container$ qsub volta_benchmark.pbs
836578.venus01
ccekwk@atlas9-c01 /hpctmp/ccekwk/tf_benchmarks/container$ vim volta_benchmark.pbs
ccekwk@atlas9-c01 /hpctmp/ccekwk/tf_benchmarks/container$ qsub -W depend=afterany:836578.venus01 volta_benchmark
.pbs
836582.venus01
ccekwk@atlas9-c01 /hpctmp/ccekwk/tf_benchmarks/container$ qstat -fns1

venus01:
                                                            Req'd  Req'd   Elap
Job ID          Username Queue    Jobname    SessID NDS TSK Memory Time  S Time
--------------- -------- -------- ---------- ------ --- --- ------ ----- - -----
836578.venus01  ccekwk   volta_lo gpu_tf_ben 392016   1  20   80gb 04:00 R 00:01 volta01/0*20
   Job run at Thu Apr 18 at 09:00 on (volta01:ncpus=20:mem=83886080kb:ngpu...
836582.venus01  ccekwk   volta_lo gpu_tf_ben     --    1  20   80gb 04:00 H   --    --
```

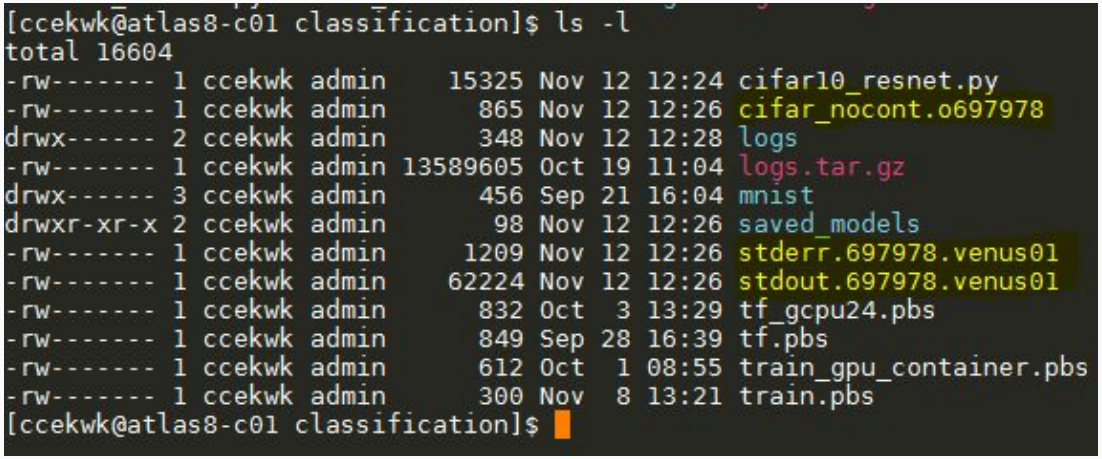
Useful PBS Commands

Action	Command
Job submission	`qsub my_job_script.txt`
Job deletion	`qdel my_job_id`
Job listing (Simple)	`qstat`
Job listing (Detailed)	`qstat -ans1`
Queue listing	`qstat -q`
Completed Job listing	`qstat -H`
Completed and Current Job listing	`qstat -x`
Full info of a job	`qstat -f job_id`

Checking Jobs

Log Files

- Output (stdout)
  - `stdout.$PBS_JOBID`
- Error (stderr)
  - `stderr.$PBS_JOBID`
- Job Summary
  - `job_name.o$PBS_JOBID`



Status of Queues

```
[ccekwk@atlas9-c01 atlas9_test]$ qstat -q

server: venus01

Queue            Memory CPU Time Walltime Node   Run   Que   Lm  State
---------------- ------ -------- -------- ---- ----- ----- ----  -----
login              --      --    720:00:0  --      0     0   --    E R
Q3500              --      --       --     --     35     0   --    E R
Q3800              --      --    720:00:0  --      0     0   --    E R
C2100              --      --    720:00:0  --      1     0   --    E R
Q3300              --      --       --     --      0     0   --    D S
Q3400              --      --       --     --      0     0   --    D R
Q3700              --      --       --     --      0     0   --    E R
Q3600              --      --       --     --      0     0   --    D R
normal             --      --    720:00:0  --      0     0   --    D R
Q3200              --      --       --     --      2     0   --    E R
iworkq             --      --    48:00:00  --      3    12   --    E R
dmloginv4          --      --    24:00:00  --      0     0   --    D R
dmlogina7          --      --    24:00:00  --      0     0   --    E R
benchmark2         --      --    720:00:0  --      0     0   --    E R
dmlogina8          --      --    24:00:00  --      3     0   --    E R
dmlogint2          --      --    24:00:00  --      0     0   --    E R
benchmark          --      --    720:00:0  --      0     0   --    E R
dmlogingold        --      --    24:00:00  --      0     0   --    E R
dmlogina6          --      --    24:00:00  --      2     0   --    E R
dmlogina5          --      --    24:00:00  --      0     1   --    E R
Q3100              --      --       --     --      5     0   --    E R
parallel24         --      --    360:00:0  --     47    58   --    E R
parallel_test      --      --    01:00:00  --      0     0   --    E R
azgpu              --      --    48:00:00  --      0     0   --    E R
openmp             --      --    720:00:0  --     10    14   --    E R
short              --      --    24:00:00  --      1     0   --    E R
serial             --      --    720:00:0  --     83    80   --    E R
gpu                --      --    720:00:0  --      0     0   --    E R
parallel8          --      --    720:00:0  --     37     2   --    E R
parallel12         --      --    720:00:0  --    208   134   --    E R
parallel20         --      --    720:00:0  --     33    11   --    E R
volta_gpu        375gb     --    48:00:00  --      3     0   --    E R
volta_login       96gb     --    04:00:00  --      0     0   --    E R
                                                ----- -----
                                                  473   312
```

See statuses of Queue:

- Max Memory
- Max Walltime
- Number of running jobs
- Number of queued jobs

Run `qstat -q` command on login node.

View Queue Configuration

```
[ccekwk@atlas9-c01 atlas9_test]$ qstat -Qf volta_login
Queue: volta_login
    queue_type = Execution
    total_jobs = 0
    state_count = Transit:0 Queued:0 Held:0 Waiting:0 Running:0 Exiting:0 Begun
        :0
    from_route_only = False
    resources_max.mem = 96gb
    resources_max.ncpus = 20
    resources_max.ngpus = 2
    resources_max.walltime = 04:00:00
    resources_min.ncpus = 1
    resources_min.ngpus = 1
    resources_default.walltime = 01:00:00
    default_chunk.model = volta
    default_chunk.ncpus = 1
    default_chunk.ngpus = 1
    resources_available.model = volta
    resources_assigned.mem = 0gb
    resources_assigned.mpiprocs = 0
    resources_assigned.ncpus = 0
    resources_assigned.nodect = 0
    node_group_key = cluster
    enabled = True
    started = True
```

To see individual queue configuration and resource limits use the following command:

`qstat -Qf queue_name`

Status of Nodes

```
[ccekwk@atlas9-c01 atlas9_test]$ gstat

============================================
  TIME: Tue Mar  5 11:30:01 SGT 2019
============================================

======== Status of Parallel Queues ========
         Queue :    Running :    Waiting
    parallel20 :         33 :         11
    parallel24 :         47 :         58
    parallel12 :        196 :         39
     parallel8 :         36 :          3
--------------------------------------------

=== Status of Serial/Openmp/App Queues ====
         Queue :    Running :    Waiting
           gpu :          0 :          0
        openmp :         10 :         28
        serial :         83 :        160
         short :          1 :          0
     volta_gpu :          3 :          0
--------------------------------------------

============== Status of all compute nodes ==================
  Cluster :  Total  Busy  Partial-Free Free   Off   Down  Oth
   atlas5 :     63    52       2         1     3     3     2
   atlas6 :     96    89       1         3     0     0     3
   atlas7 :    152    95       4        40     0     1    11
   atlas8 :     64    52       1        10     0     0     1
   atlas9 :     23    14       9         0     0     0     0
     gold :     15     1       0        12     0     0     2
   tiger2 :     96    57       4        33     0     0     2
    volta :      5     0       2         3     0     0     0
------------------------------------------------------------
```

To view status of nodes use the following command

`gstat`

Tips and Tricks

Recommendations

- **Max** walltime: 72 hours
- **Default** walltime: 24 hours
- Implement weights/model checkpointing
  - Save your model weights after every training epoch
- Save weights to `/hpctmp/nusnet_id/` directory
  - **Backup** your important weights from /hpctmp often to your own computer
- Use **volta_login (interactive mode)** to **test** your python **scripts** before submitting to volta_gpu

Speed Ups (Data Access)

Copy **large datasets** or **datasets with a lot of small files** to **/scratch/nusnet_id** on Volta nodes (SSD drives local on each Volta node)

Make directory in /scratch: This creates a directory if it doesn't exist.

```
mkdir -p /scratch/`whoami`
```

Sync dataset folder to /scratch using rsync: Synchronises dataset in hpctmp to/scratch folder

```
rsync -hav /hpctmp/nusnet_id/example/dataset_folder /scratch/nusnet_id/
```

`dataset_folder` will appear in `/scratch/nusnet_id/dataset_folder`

Please put the above commands in your **job script** .
Remember to set the correct dataset path in your python script

Batch Job Script for volta_gpu with Speed Ups (Data Access)

```
#!/bin/bash
#PBS -P volta_pilot
#PBS -j oe
#PBS -N tensorflow
#PBS -q volta_gpu
#PBS -l select=1:ncpus=5:mem=50gb:ngpus=1
#PBS -l walltime=24:00:00

cd $PBS_O_WORKDIR;
np=$(cat ${PBS_NODEFILE} | wc -l);
mkdir -p /scratch/nusnet_id
rsync -hav /hpctmp/nusnet_id/example/dataset_folder /scratch/nusnet_id/

image="/app1/common/singularity-img/3.0.0/tensorflow_1.12_nvcr_19.01-py3.simg"

singularity exec $image bash << EOF > stdout.$PBS_JOBID 2> stderr.$PBS_JOBID
PYTHONPATH=$PYTHONPATH:/home/svu/[nusnet_id]/volta_pypkg/lib/python3.5/site-packages
export PYTHONPATH

python cifar10_resnet.py
EOF
```

Green is user configurable
Black is fixed

Speed Ups (Image Processing)

If you are using any image processing that utilises PIL/Pillow,

- install an optimised version called Pillow-SIMD
  - pip uninstall pillow
  - pip install pillow-simd
- More info here https://github.com/uploadcare/pillow-simd

Tips on How to Game the Queue

1. Request less or reasonable amount of resources (or request just enough).
    a. Less: e.g. NCPUS or MEM
        i. Each node only has a maximum of 40 NCPUS and 300GB of RAM shared with 4 GPUs
        ii. if User A requests for 20 NCPUs, 100GB RAM and 1 GPU. User B requests for 20 NCPUs, 100 GB RAM and 1 GPU, the remaining 2 GPU will not be able to be allocated to other users.
    b. Reasonable NCPUs or MEM
        i. 5 to 10, 15 NCPUs is good. Don't request weird numbers like 11, 13, 16, 17, etc
        ii. 50~80, 90GB of MEM is good. If you need more than 100 GB, you might not be doing Deep Learning efficiently.
2. Load your data in batches, do not load 200GB worth into RAM at the same time.
    a. It doesn't make sense to load 200GB into RAM at the same time as the GPU only has 32GB of memory.

Debugging

Visit: Python_Debugging_Guide.pptx

FAQ/Common Problems

Visit: Volta_Cluster_FAQ.pptx

Acknowledgement of Usage of NUS HPC Resources

Our primary mission is to provide the best of class, high-performance computing resources to support your computational research needs free of charge. To continuously improve the service, anticipate future demands, and keep track of our HPC facility's impact on the NUS research community in general, we request you to cite the REC team in your published research works.

Below is an example of a citation that may work for you:

"We would like to acknowledge that computational work involved in this research work is partially / fully supported by NUS IT's Research Computing group"

We would appreciate if you could send us a copy of your publication as well.

Additional Support

nTouch

https://ntouch.nus.edu.sg/ux/myitapp/#/catalog/home

Project/Research Collaboration or Long Term Engagement or Support

Email

dataengineering@nus.edu.sg

nTouch Support Request Template

1. Login node used:
2. Container used:
3. What are you trying to do:
4. Description of error:
5. Screenshots or copy paste log:
6. Copy and paste the following line:
    a. “I have read the entire Volta Guide and have not found a solution to my problem in the guide.”
7. Attach Job Script (if applicable)

Not Supported:
Conda with Containers

Installing Miniconda with your Container

Installing miniconda in a plain container

(/app1/common/singularity-img/3.0.0/CUDA/cuda_10.0-cudnn7-devel-ubuntu16.04.simg)

On Atlas 8:

```
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
module load singularity
singularity exec /app1/common/singularity-img/3.0.0/CUDA/cuda_10.0-cudnn7-devel-ubuntu16.04.simg bash
bash Miniconda3-latest-Linux-x86_64.sh
```

#Take note of installation directory target. Change /my/install/directory accordingly

```
eval "$(/my/install/directory/miniconda3/bin/conda shell.bash hook)"
```

run the above command every time before you use conda in a new session.
You are now ready to run anaconda

Creating Environment and Installing Packages

Assuming you've followed the previous slide and still on the same session:

```
# Create your environment
conda create -n my_environment_name python=3.6

# Activate your environment
conda activate my_environment_name

# Install a package
conda install tensorflow-gpu
```

Using Conda on Volta

On Volta, in a new session

```
# Load conda
eval "$(/my/install/directory/miniconda3/bin/conda shell.bash hook)"

# Activate your environment
conda activate my_environment_name
```