SoC GPU

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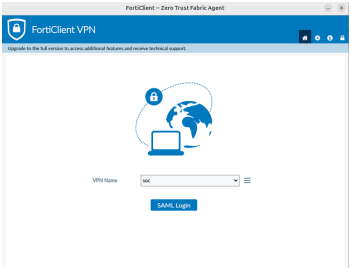
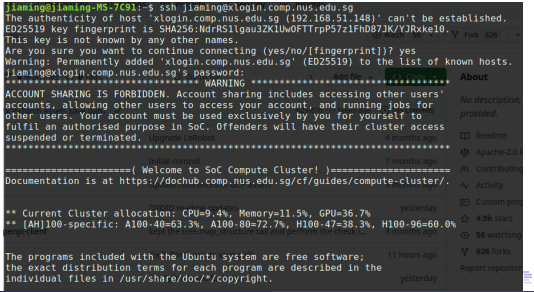
Accessing SoC Compute Cluster

- **Create SoC account**: `https://mysoc.nus.edu.sg/~newacct`
- **Enable service**: `https://mysoc.nus.edu.sg/~myacct/services.cgi`
- **SoC VPN is required if not in SoC network**: `https://dochub.comp.nus.edu.sg/cf/guides/network/vpn/`
- **After account is setup, SSH to login node**:

```
ssh username@xlogin.comp.nus.edu.sg
```





Slurm Basics

- Scheduler: **Slurm** (submit jobs; avoid heavy compute on xlogin)
- Common commands:

```
sinfo              # cluster/partition status
squeue -u $USER    # your jobs in queue
sbatch job.slurm   # submit batch job
salloc             # interactive allocation
scancel <jobid>    # cancel job
sacct              # finished jobs accounting
```

Example Workflow Overview

1. Install/activate your own Conda.
2. Create environment and install dependencies (e.g. PyTorch)
3. Write training script (`train_toy.py`).
4. Write Slurm script (`run_toy.slurm`).
5. Submit job with `sbatch` and monitor.
6. Retrieve logs/results (e.g., `scp`).

Create Environment & Install PyTorch

```
# if conda is not installed, download & run installer (on xlogin)
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
bash Miniconda3-latest-Linux-x86_64.sh

# Initialize shell so ‘conda‘ works
source ~/.bashrc

# Create & activate an environment
conda create -n torch-env python=3.9 -y
conda activate torch-env

# Install PyTorch (CPU by default; GPU if CUDA present)
pip install torch numpy
```

Toy PyTorch Training Script (train_toy.py)

```
import torch
import torch.nn as nn
import torch.optim as optim

# Toy dataset
x = torch.randn(100, 10)
y = torch.randint(0, 2, (100,))

# Simple MLP
model = nn.Sequential(nn.Linear(10, 32), nn.ReLU(), nn.Linear(32, 2))
loss_fn = nn.CrossEntropyLoss()
opt = optim.Adam(model.parameters(), lr=1e-3)

for epoch in range(5):
    opt.zero_grad()
    out = model(x)
    loss = loss_fn(out, y)
    loss.backward()
    opt.step()
    print(f"Epoch {epoch}: loss={loss.item():.4f}")
```

Slurm Batch Script (run_toy.slurm)

```
#!/bin/bash
#SBATCH --job-name=toytrain
#SBATCH --output=toytrain.log
#SBATCH --time=00:05:00
#SBATCH --partition=standard
#SBATCH --gpus=1        # remove or change if GPU not needed

# Ensure conda is available in batch context
source ~/.bashrc
conda activate torch-env

python train_toy.py
```

Submit, Monitor, and Inspect Logs

```
# Submit
sbatch run_toy.slurm

# Monitor your job(s)
squeue -u $USER
sacct --format=JobID,State,Elapsed,MaxRSS,ExitCode

# Inspect training logs
tail -f toytrain.log   # or: cat toytrain.log
```

```
(gnn-env) jiaming@xlogin2:~$ sbatch run_toy.slurm
sbatch: The 'standard' partition is renamed 'normal'.
Submitted batch job 117062
(gnn-env) jiaming@xlogin2:~$ cat toytrain.log
(gnn-env) jiaming@xlogin2:~$ cat toytrain.log
(gnn-env) jiaming@xlogin2:~$ squeue -u $USER
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
(gnn-env) jiaming@xlogin2:~$ cat toytrain.log
Epoch 0, Loss: 0.7209059000015259
Epoch 1, Loss: 0.7180317640304565
Epoch 2, Loss: 0.7152751088142395
Epoch 3, Loss: 0.7126396894454956
Epoch 4, Loss: 0.7101239562034607
(gnn-env) jiaming@xlogin2:~$
```

Retrieve Results to Your Laptop

```
# From your laptop/desktop terminal
scp username@xlogin.comp.nus.edu.sg:~/toytrain.log .

# Copy a directory of results
scp -r username@xlogin.comp.nus.edu.sg:~/results ./results
```

Optional: Interactive Debug Session

```
# Request an interactive allocation
salloc --gpus=1 --time=00:10:00

# Get a shell on the compute node
srun --pty bash

# Inside the node: run the script
source ~/.bashrc && conda activate torch-env
python train_toy.py

# Exit to release resources
exit   # leaves node shell
exit   # ends allocation
```

Tips & Good Practices

- Keep jobs short while testing; extend time after validation.
- Prefer `sbatch` for reproducibility; use `salloc` only for debugging.
- Write outputs to your $HOME/$WORK; clean up temporary files.