Submit Slurm Batch job on PACE ICE

Steps:

1. Create job script.
2. Create slurm script
3. Upload your files
4. SSH into PACE, submit slurm script to queue
5. Wait
6. Get results
7. (Optional) Using interactive sessions

1. You have some file that does a job you want on the cluster. Let's call it test.py.

2. Make a Slurm script. This is an example of a slurm script named **SlurmPythonExample.sbatch**. In the cluster, it should be added to same folder as the job you want to put in queue.

```
============
#!/bin/bash
#SBATCH -JSlurmPythonExample                    # Job name
#SBATCH -N1 --ntasks-per-node=4                 # Number of nodes and cores per node required
#SBATCH --mem-per-cpu=1G                         # Memory per core
#SBATCH -t15                                    # Duration of the job (Ex: 15 mins)
#SBATCH -oReport-%j.out                         # Combined output and error messages file
#SBATCH --mail-type=BEGIN,END,FAIL              # Mail preferences
#SBATCH --mail-user=gburdell3@gatech.edu        # E-mail address for notifications
cd $SLURM_SUBMIT_DIR                            # Change to working directory
module load anaconda3              # Load module dependencies
srun python test.py                # Example Process
==============
```

The above is a Slurm script that does not request GPU. The below requests GPU. Note the different options.

```
==============
#!/bin/bash
#SBATCH -JHGX_H100_Example              # Job name
#SBATCH -N1 --ntasks-per-node=1          # Number of nodes and cores per node required
#SBATCH --gres=gpu:H100:1                # GPU type (H100) and number of GPUs
#SBATCH --mem-per-gpu=224GB              # Memory per CPU core, 8 CPUs/GPU
#SBATCH -t1:00:00                        # Duration of the job (Ex: 1 hour)
#SBATCH -oReport-%j.out
#SBATCH --mail-type=BEGIN,END,FAIL       # Mail preferences
#SBATCH --mail-user=gburdell3@gatech.edu # E-mail address for notifications
cd ~/nvcc_example
module load gcc
module load cuda
nvcc hello_cuda.cu -o hello_cuda
srun ./hello_cuda
==============
```

3. Now you have your beautiful scripts. Add them to the cluster.

Make a directory on the cluster to hold this file:

ssh [your_gatech_name]@login-ice.pace.gatech.edu mkdir -p yourusername/yourdirectory

Copy your local file(s) to the cluster

scp -r test.py SlurmPythonExample.sbatch [your_gatech_name]@login-ice.pace.gatech.edu:yourusername/yourdirectory

==========

***Beware. Before scp * ing all your local files to PACE, know what files are in the directory you are in. ***

==========

4. SSH to PACE

ssh [your_gatech_name]@login-ice.pace.gatech.edu

Cd your way to your directory where you uploaded the files. Submit the sbatch file to pace with "sbatch SlurmPythonExample.sbatch"

5. Wait patiently. You can check the status of your job with the "squeue" command.

6. After you see that the job is finished, the results will in the directory of the slurm job (or wherever you instructed it to output results).

7. Let's say you don't want to submit an sbatch job, you want to run an interactive GPU session. You can do this in the command line or via an .sh script.

Command line:

salloc --gres=gpu:H100:1 --ntasks-per-node=1

This is for starting a Slurm interactive session with an H100 GPU node, allocating for 1 node with an Nvidia H100 Tensor Core GPU.

It will send a response such as:

salloc: Pending job allocation 1234
salloc: job 1234 queued and waiting for resources

You will then wait until the request is available to you.

salloc: job 1234 has been allocated resources
salloc: Granted job allocation 1234
salloc: Waiting for resource configuration
salloc: Nodes compute-node are ready for job

Begin Slurm Prolog: Feb-29-2024 21:35:52
Job ID: 1234
User ID: gburdell3
Account:
Job name: interactive
Partition: coe-gpu

[gburdell3@compute-node ~]$

One other way to do it is to create a .sh script to handle this for you.

./pace_interactive.sh
[wait till the node is acquired]

Example code for pace_interactive.sh
“””
#!/bin/sh
salloc --gres=gpu:H100:1 --ntasks-per-node=1
exit 0
“””

==========
This was written with help from the official PACE documentation: PACE - External - Using Slurm on ICE (service-now.com)