MICCoM Workshop

Argonne National Lab, Building 240, Room 1501, Oct 13-14, 2022

LCRC account setup

1. Get an LCRC account https://www.lcrc.anl.gov/for-users/getting-started/getting-an-account/
2. Join the budget **`MICCoM-train`**
3. Register your SSH Key https://www.lcrc.anl.gov/for-users/getting-started/ssh/

Computational resources

BEBOP / CPU / 64 cores per node (Intel KNL)
SWING / GPU / 128 cores per node + 8 NVIDIA A100

https://www.lcrc.anl.gov/systems/resources/bebop/
https://www.lcrc.anl.gov/systems/resources/swing/

Reservations

Day 1 – Oct 13, 2022

Computer	Time	Name of reservation	Nodes
Bebop	10:15am – 12:15pm	`miccom_day1_am`	75
Bebop	1:15pm – 5:15pm	`miccom_day1_pm`	75
Swing	12:00pm – 6pm	`miccom_1`	3

Day 2 – Oct 14, 2022

Computer	Time	Name of reservation	Nodes
Bebop	10:15am – 12:15pm	`miccom_day2_am`	75
Bebop	1:15pm – 5:15pm	`miccom_day2_pm`	75
Swing	12:00pm – 6pm	`miccom_2`	3

Connect & submit jobs to BEBOP

Open the terminal and execute this command

```
ssh <username>@bebop.lcrc.anl.gov
```

To interact with the job scheduler, create a file called `bebop.job`

```
#!/bin/bash

#SBATCH --job-name=test
#SBATCH --account=MICCOM-TRAIN
##SBATCH --reservation=<reservation>
#SBATCH --partition=knlall
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=64
#SBATCH --cpus-per-task=1
#SBATCH --time=00:10:00

source /lcrc/project/MICCoM-train/load_bebop_env.sh

srun -N 1 -n 64 -c 1 wstat.x -i wstat.in > wstat.out
```

Then submit the job

```
sbatch bebop.job
```

To check the status of your jobs

```
squeue -u $USER
```

Connect & submit jobs to SWING

Open the terminal and execute this command

```
ssh <username>@swing.lcrc.anl.gov
```

To interact with the job scheduler, create a file called `swing.job`

```
#!/bin/bash

#SBATCH --job-name=test
#SBATCH --account=MICCOM-TRAIN
##SBATCH --reservation=<reservation>
#SBATCH --nodes=1
#SBATCH --gres=gpu:1
#SBATCH --time=00:10:00

module load nvhpc/21.9-4pt64om
module load west/5.2.0

export OMP_NUM_THREADS=1

mpirun -n 1 wstat.x -i wstat.in > wstat.out
```

Then submit the job

```
sbatch swing.job
```

To check the status of your jobs

```
squeue -u $USER
```

Use Jupyter Notebooks at LCRC

You will need to open two terminals: Terminal 1 and Terminal 2.

On Terminal 1: connect to Bebop

```
ssh <username>@bebop.lcrc.anl.gov
```

Set up the environment

```
source /lcrc/project/MICCoM-train/load_bebop_env.sh
```

Request one compute node (the following command should be typed in one line)

```
srun --pty -A MICCOM-TRAIN --reservation <reservation> -p
knlall -N 1 -t 01:30:00 /bin/bash
```

Launch Jupyter notebook

```
miccom_start_jupyter
```

Each person gets a different node and port number printed to screen

```
Your compute node is :  knld-0019
Your port number is  :  27055
Starting Jupyter notebook ...
```

Wait a few seconds and you will receive the following output

```
To access the notebook, open this file in a browser:
    file:///gpfs/fs1/home/yuw/.local/...
Or copy and paste one of these URLs:
    http://localhost:27055/?token=f86350...
or http://127.0.0.1:27055/?token=f86350...
```

Done. Do not do anything else to Terminal 1 until the hands-on session is completed. Keep the terminal open.

On Terminal 2: connect again to Bebop, make sure that the port number (in blue) matches what the Terminal 1 printed to screen

```
ssh -L 27055:localhost:27055 <username>@bebop.lcrc.anl.gov
```

Connect to the node that you have reserved in Terminal 1, i.e., make sure that the port number (in blue) and the name of the node (in green) match what Terminal 1 printed to screen

```
ssh -L 27055:localhost:27055 knld-0019
```

Set up the environment

```
source /lcrc/project/MICCoM-train/load_bebop_env.sh
```

Done. Do not do anything else to Terminal 2 until the hands-on session is completed. Keep the terminal open.

On your laptop: open a browser (e.g., Firefox, Chrome) and visit the **link** (in purple) that Terminal 1 printed to screen

You are good to go!