Using GPUs at the CHPC

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Overview

- SLURM scheduler basics.
- GPU types.
- SLURM and GPUs.
- Finding (free) GPUs.
- Submitting job with GPUs
  - Open OnDemand
  - Interactive job on terminal
  - SLURM job script
- Monitoring GPU jobs

SLURM basics

- All GPUs are on compute nodes - must run a job to get them
  - Typically GPU partition has "gpu" in its name, e.g. notchpeak-gpu
- Recall basic SLURM commands:
  - `sbatch` - submit a scripted job
  - `salloc` - submit an interactive job
  - `squeue` - see the queued/running jobs (`squeue --me`)
  - `scancel` - cancel a job
  - `sinfo` - list partitions
- Convenience CHPC commands
  - `mychpc batch` - list accounts/partitions available to user
  - `mysqueue` - list user accounts/partitions and jobs on them
  - `mysinfo` - list user accounts/partitions and state of their nodes

GPU types

- CHPC has GPUs from many different generations
  - Their performance and capabilities vary widely
  - https://www.chpc.utah.edu/documentation/guides/gpus-accelerators.php#gpu_types
- (Nvidia) GPU classification:
  - Generation (code name - Maxwell, Pascal, Volta, Turing, Ampere, Hopper)
  - Compute Capability (5.2, 6.0, 6.1, 7.0, 7.5, 8.0, 8.6, 8.9, 9.0) https://developer.nvidia.com/cuda-gpus#compute
  - Theoretical compute throughput (single, double precision, tensor) https://en.wikipedia.org/wiki/Nvidia_Tesla https://en.wikipedia.org/wiki/Quadro https://en.wikipedia.org/wiki/GeForce https://en.wikipedia.org/wiki/GeForce_40_series
  - Amount of memory (~10-80 GB)

Data center GPUs

- Example: A40, A100, H100, H200
  - Data center GPUs, high double precision performance, large memory
  - Expensive (H100 ~$20000 w/ edu discount), hard to get
  - Good for simulations that need high numerical precision (engineering), or high memory (AI)

Model	Micro-architecture	Launch	Core	Core clock (MHz)	Shaders			Memory					Processing power (GFLOPS)[a]			CUDA compute capability[b]	TDP (W)
					CUDA cores (total)	Base clock (MHz)	Max boost clock (MHz)[c]	Bus type	Bus width (bit)	Size (GB)	Clock (MT/s)	Bandwidth (GB/s)	Half precision Tensor Core FP32 Accumulate	Single precision (MAD or FMA)	Double precision (FMA)		
A40 GPU accelerator (PCIe card)[43]		October 5, 2020	1× GA102	—	10,752	1,305	1,740	GDDR6	384	48	7,248	695.8	149,680	37,420	1,168	8.6	300
A100 GPU accelerator (PCIe card)[44][45]		May 14, 2020[46]	1× GA100-883AA-A1	—	6,912	765	1410	HBM2	5,120	40 or 80	1,215	1,555	312,000	19,500	9,700	8.0	250
H100 GPU accelerator (PCIe card)[47]	Hopper	March 22, 2022[48]	1× GH100[49]	—	14,592	1,065	1,755 CUDA 1620 TC	HBM2E	5120	80	1,000	2,039	756,449	51,200	25,600	9.0	350
H100 GPU accelerator (SXM card)				—	16,896	1,065	1,980 CUDA 1,830 TC	HBM3	5,120	80	1,500	3,352	989,430	66,900	33,500	9.0	700

Consumer GPUS

- Example: RTX3090
  - Consumer grade graphics cards, recent don't fit to compute servers
  - Very low double precision performance, good single and tensor performance
  - More affordable (a few thousand $)
  - Good for lower precision numerical calculations, AI with small to medium size models

Model	Launch	Launch MSRP (USD)	Code name(s)[b]	Transistors (billion)	Die size (mm²)	Core config[c]	SM count[d]	L2 cache (MB)	Clock speeds[e]		Fillrate[f][g]		Memory				Processing power (TFLOPS)[h]				TDP (watts)
									Core (MHz)	Memory (GT/s)[i]	Pixel (Gpx/s)	Texture (Gtex/s)	Size (GB)	Band-width (GB/s)	Type	Bus width (bit)	Half (boost)	Single (boost)	Double (boost)	Tensor compute [sparse]	
GeForce RTX 3090 Ti[40][65]	Mar 29, 2022	$1,999	GA102-350	28.3	628.4	10752 336:112:84:336	84	6	1560 (1860)	10.5	174.7 (208.3)	524.1 (625)	24	1008	GDDR6X	384	33.55 (39.99)	33.55 (39.99)	0.524 (0.625)	160[66] [320]	450
GeForce RTX 3090[40][63]	Sep 24, 2020	$1,499	GA102-250[64] GA102-300	28.3	628.4	10496 328:112:82:328	82	6	1395 (1695)	9.75	156.2 (189.8)	457.6 (556)	24	936	GDDR6X	384	29.28 (35.58)	29.28 (35.58)	0.458 (0.556)	142[34] [284]	350

Professional GPUs

- Example: RTX6000, A6000
  - Mid size models (graphical workstations), more memory and a bit pricier than the gaming graphics cards
  - Very low double precision performance, good single and tensor performance
  - Good for lower precision numerical calculations, AI with small to medium size models

Quadro GPU	Launch	Core	Core clock	Memory clock	Memory size (GB)	Memory type	Memory bandwidth	CUDA cores	Tensor cores	RT cores	Half precision	Single precision	Double precision	CUDA Compute Capability
Units			MHz	MHz	GB		GiB/s				TFLOPS	TFLOPS	GFLOPS	
RTX 6000 Ada Generation[202]	2022-12-03	AD102-870	915–2505	2500	48	384-bit GDDR6	960	18176	568	142	91.06[203]	91.06	1423	8.9
RTX A6000[185][186]	2020-10-05	GA102-875	1410–1800	2000	48 (96 with NVLink 3.0)	384-bit GDDR6	768	10752	336	84	38.709[187]	38.709	1209.677	8.6

SLURM and GPUs

- GPUs have to be requested explicitly
  - #SBATCH --gres=gpu:*type*:*count*
- GPU type is also a *feature*

```
$ si -p notchpeak-gpu
PARTITION      NODES NODES(A/I/O/T) S:C:T    FREE_MEM       MEMORY     TIMELIMIT   AVAIL_FEATURES                      NODELIST
notchpeak-gpu  3     3/0/0/3        2:16:2   77298-136143   188000     3-00:00:00  chpc,skl,tesla,v100,c32,m192,cx4    notch[001-003]
notchpeak-gpu  1     1/0/0/1        2:16:2   25778          188000     3-00:00:00  chpc,skl,geforce,2080ti,tesla,p40,c3 notch004
notchpeak-gpu  1     1/0/0/1        2:32:2   146805         508000     3-00:00:00  chpc,rom,geforce,3090,a100,c64,m512, notch293
```

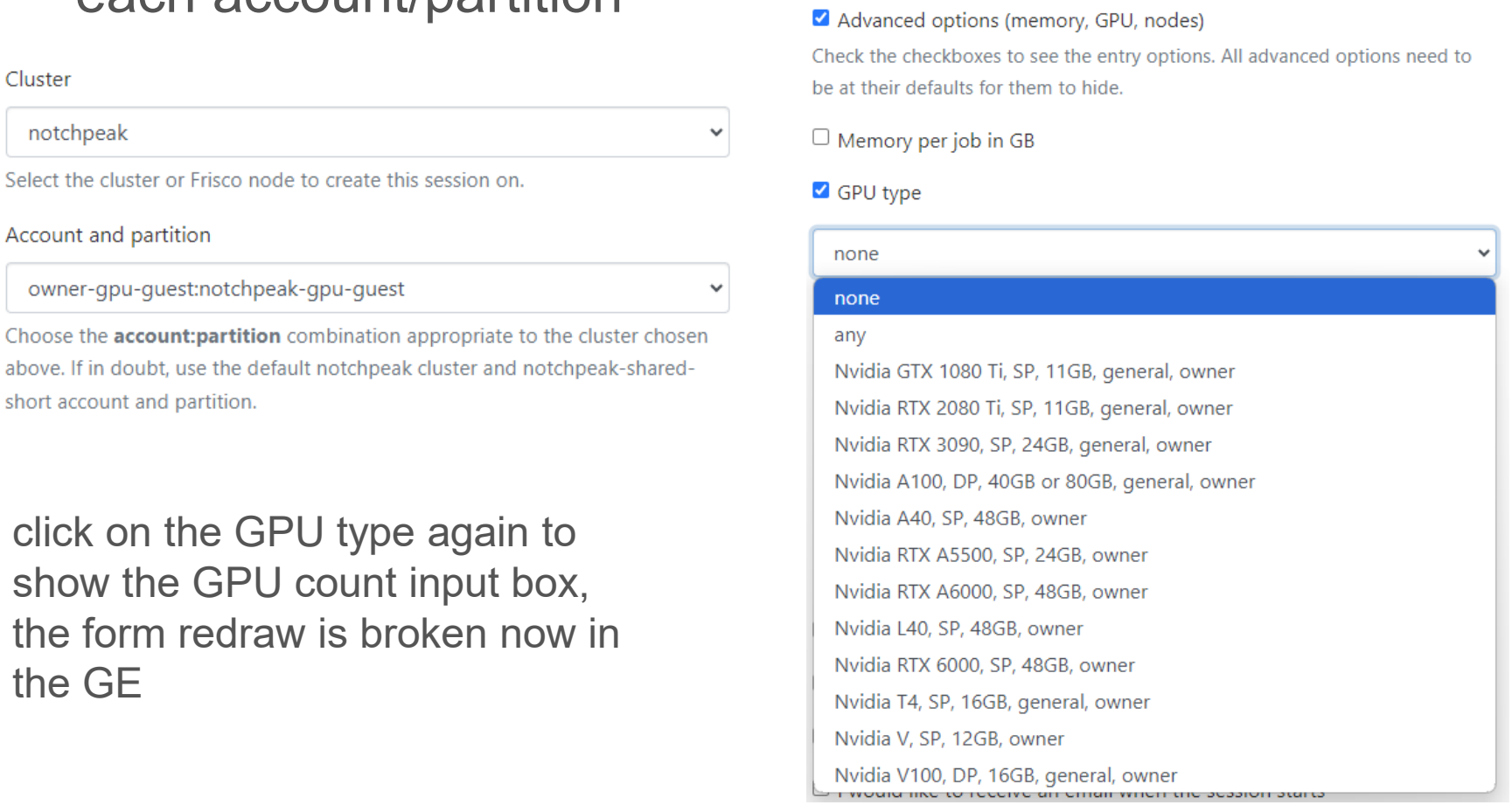
  - no feature/gres for GPU memory (yet)
  - #SBATCH --gres=gpu:v100:1
- Further details on GPU nodes

```
$ sinfo -N -h -p notchpeak-gpu --Format='nodehost,gres:50'
notch001            gpu:v100:3(S:0-1)
notch293            gpu:3090:4(S:0),gpu:a100:4(S:1)

$ sinfo -N -h -p notchpeak-gpu --Format='nodehost,gresused:50'
notch001            gpu:v100:2(IDX:0,2)
notch293            gpu:3090:4(IDX:0-3),gpu:a100:4(IDX:4-7)
```

OOD and GPUs

- Open OnDemand web portal auto-fills available GPUs for each account/partition



click on the GPU type again to show the GPU count input box, the form redraw is broken now in the GE

Find free GPUs

- Special command - `freegpus`

```
$ freegpus -p notchpeak-gpu
GPUS_FREE: notchpeak-gpu
v100 (x5)
2080ti (x6)
3090 (x5)
```

  - x# is the number of free GPUs in the partition
  - #SBATCH --gres=gpu:v100:1 should get the job started right away
  - unless other jobs using GPU(s) on that node use all other resources (CPUs, memory)

- OnDemand's Node Status App
  - empty circle - free GPU,
    full circle - occupied GPU

  - click on the node to open page with more details
    - GPU type, recent jobs, metrics

Find free GPUs

- The owner nodes have much more free GPUs than general nodes

```
$ freegpus -p notchpeak-gpu-guest
GPUS_FREE: notchpeak-gpu-guest
1080ti (x5)
2080ti (x26)
3090 (x8)
a40 (x6)
a5500 (x4)
t4 (x1)
titanv (x4)
a6000 (x18)
a100 (x2)
l40 (x5)
rtx6000 (x9)
```

- BUT the job can be preempted - use the owner usage page to correlate the node with free GPUs to the owner partition and to its recent usage https://www.chpc.utah.edu/usage/constraints/

Owner GPUs

- Notchpeak owner usage
  https://portal.chpc.utah.edu/slurm/guest-feature-availability/notchpeak/

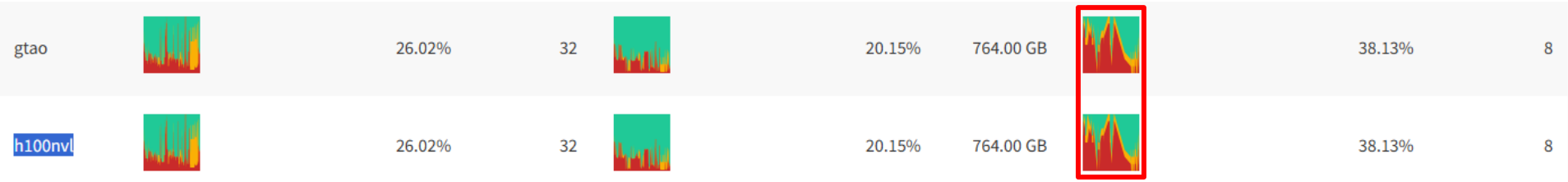
  - find the `leffler` feature's recent usage - 100% used by guest (yellow)
- List of nodes w/ GPUs

```
$ si |grep leffler
...
leffler-gpu-np       1     0/1/0/1        2:28:2   976232          1020000
14-00:00:00 leffler,icl,c56,m1024,a100,cx6       notch348
$ freegpus -p notchpeak-gpu-guest -v |grep notch348
notch348             gpu:a100:1(S:0)          gpu:a100:0(IDX:N/A)
```

  - GPU is free
- Submit interactive job

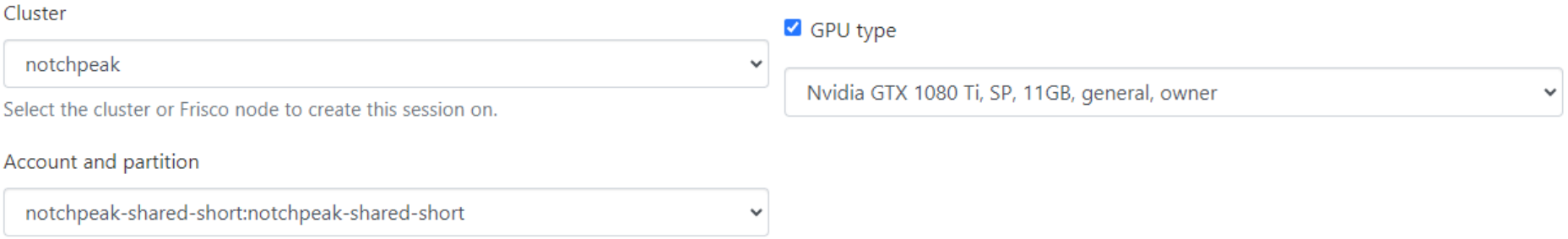
```
$ salloc -N 1 -n 1 -p notchpeak-gpu-guest -A owner-gpu-guest -C leffler --gres=gpu:a100:1 -t
1:00:00
```

  - Should start in a few minutes
  - If no GPUs have zero owner usage - look for those with smaller owner usage

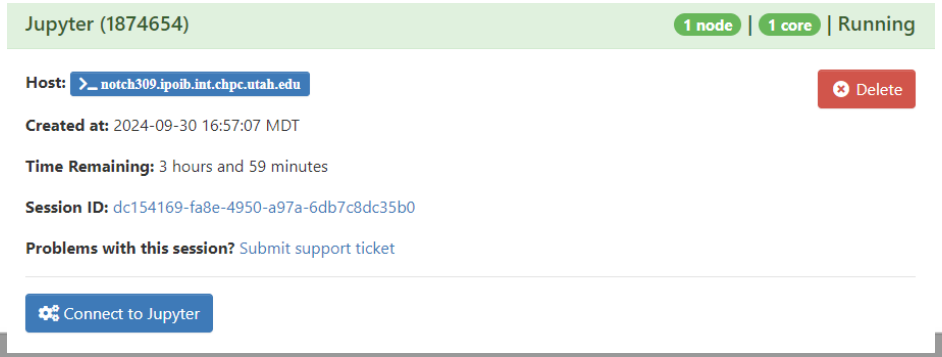


OnDemand job

- Select the Interactive App
- Pick cluster, Account/partition, Advanced options - GPU type and count



- Submit job by clicking Launch
- Wait till job starts, then click on the Connect to ...



Terminal job

- Interactive

```
salloc -N 1 -n 4 -A notchpeak-shared-short -p notchpeak-shared-short --gres=gpu:t4:1 -t 1:00:00
```

- SLURM job script

```
#SBATCH -N 1
#SBATCH -n 4
#SBATCH -A notchpeak-shared-short
#SBATCH -p notchpeak-shared-short
#SBATCH --gres=gpu:t4:1
#SBATCH -t 1:00:00
```

- CPU memory
  - many GPU programs require substantial CPU (host) memory
  - default is 2GB per CPU - often not enough
  - you'll see "OOM" and/or "killed" messages in output if that's the case
  - ask for more CPUs, or, even better, specify CPU memory:

```
#SBATCH --mem=32G
```

Checking jobs

- Check job state

```
$ squeue --me
JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
1894063 notchpeak interact u0101881  R       0:06      1 notch308
$ scontrol show job 1894063
...
 NumNodes=1 NumCPUs=4 NumTasks=4 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
 ReqTRES=cpu=4,mem=16000M,node=1,billing=4,gres/gpu=1
 AllocTRES=cpu=4,mem=16000M,node=1,billing=4,gres/gpu=1
...
 TresPerNode=gres/gpu:t4:1
```

Checking jobs

- Check GPU status (inside job)

```
$ nvidia-smi
Wed Oct  2 09:55:03 2024
+-----------------------------------------------------------------------------------------+
| NVIDIA-SMI 550.54.14              Driver Version: 550.54.14      CUDA Version: 12.4     |
|-----------------------------------------+------------------------+----------------------+
| GPU  Name                 Persistence-M | Bus-Id          Disp.A | Volatile Uncorr. ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |           Memory-Usage | GPU-Util  Compute M. |
|                                         |                        |               MIG M. |
|=========================================+========================+======================|
|   0  Tesla V100-PCIE-16GB           On  |   00000000:3B:00.0 Off |                  Off |
| N/A   33C    P0             36W /  250W |     607MiB /  16384MiB |     11%      Default |
|                                         |                        |                  N/A |
+-----------------------------------------+------------------------+----------------------+

+-----------------------------------------------------------------------------------------+
| Processes:                                                                              |
|  GPU   GI   CI        PID   Type   Process name                              GPU Memory |
|        ID   ID                                                               Usage      |
|=========================================================================================|
|    0   N/A  N/A   2269935      C   /usr/bin/python                                604MiB |
+-----------------------------------------------------------------------------------------+
```

Checking jobs

- Check GPU parameters (inside job)

```
$ ml nvhpc
$ nvaccelinfo
CUDA Driver Version:            12040
NVRM version:                   NVIDIA UNIX x86_64 Kernel Module  550.54.14  Thu Feb 22 01:44:30
UTC 2024

Device Number:                  0
Device Name:                    Tesla V100-PCIE-16GB
Device Revision Number:         7.0
Global Memory Size:             16928342016
Number of Multiprocessors:      80
Concurrent Copy and Execution:  Yes
Total Constant Memory:          65536
Total Shared Memory per Block:  49152
Registers per Block:            65536
Warp Size:                      32
Maximum Threads per Block:      1024
Maximum Block Dimensions:       1024, 1024, 64
Maximum Grid Dimensions:        2147483647 x 65535 x 65535
...
Clock Rate:                     1380 MHz
...
Default Target:                 cc70
```

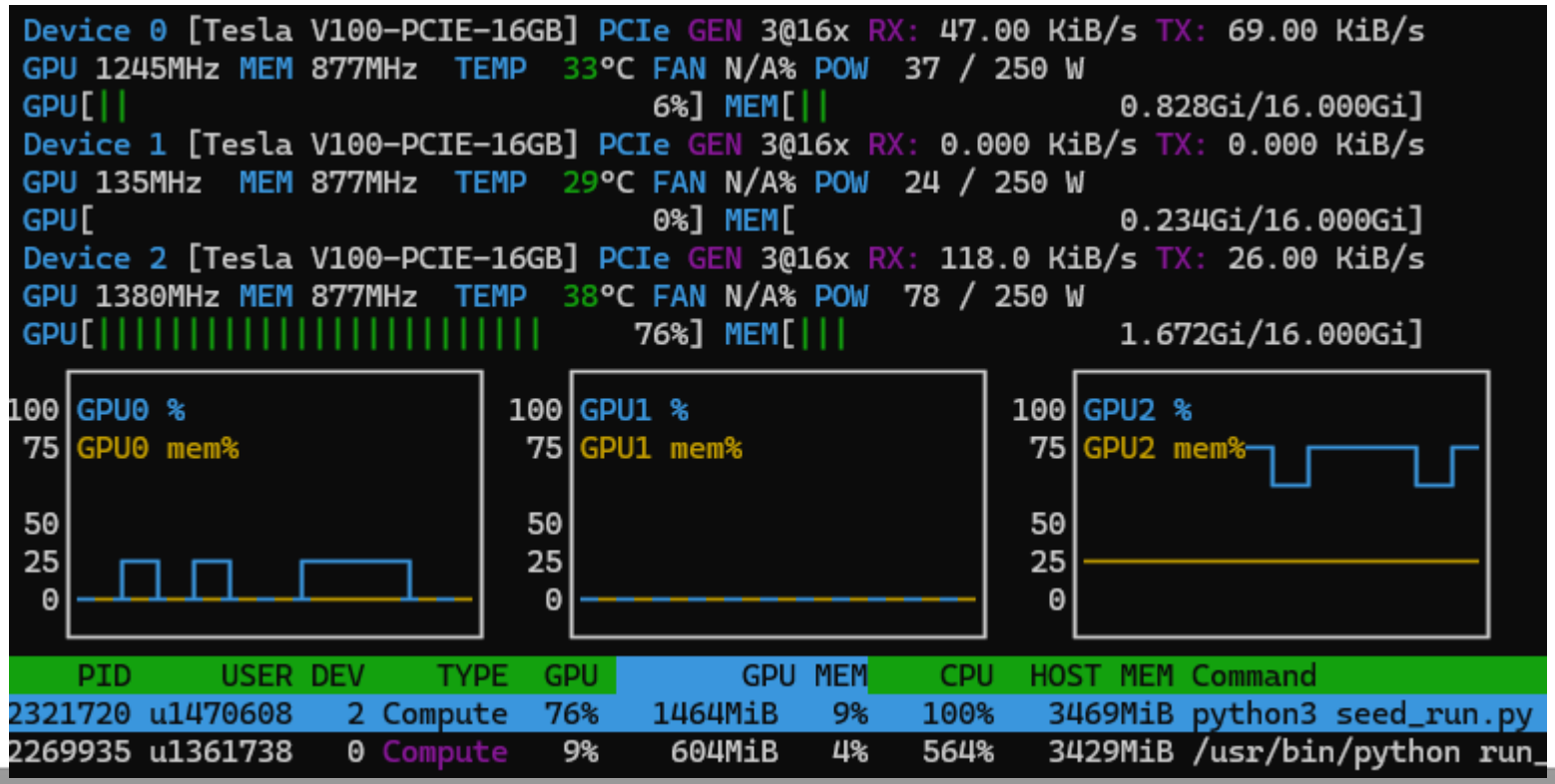
Checking jobs

- Check GPU utilization
  - ssh to the node with the job, run nvtop

```
$ ssh notch001
$ ml nvtop
$ nvtop
```

In Open OnDemand:

Host: >_ notch308.ipoib.int.chpc.utah.edu



Checking jobs

- Check CPU and host memory utilization
  - ssh to the node with the job, run top or htop

```
$ ssh notch001
$ top
```

In Open OnDemand:

Host: >_ notch308.ipoib.int.chpc.utah.edu

```
top - 12:58:18 up 26 days,  1:58,  2 users,  load average: 7.82, 8.14, 8.01
Tasks: 821 total,   3 running, 818 sleeping,   0 stopped,   0 zombie
%Cpu(s): 10.6 us,  0.1 sy,  0.0 ni, 89.2 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
MiB Mem : 191904.0 total, 105313.6 free,  44884.0 used,  41706.4 buff/cache
MiB Swap:  49152.0 total,  49027.3 free,    124.7 used. 144894.7 avail Mem

    PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND
2269935 u1361738  20   0   13.1g   3.5g 414344 S 481.5   1.9  15297:35 pt_main_thread
2321720 u1470608  20   0   11.7g   3.7g 244284 R 101.3   2.0   1034:37 python3
2336952 u1415428  20   0   36.4g  35.0g  87672 R  99.7  18.7  45:06.45 rsession
   9609 root      20   0       0      0      0 S   2.6   0.0 689:08.08 nv_queue
2338236 u0101881  20   0  276076   5712   4076 R   0.7   0.0   0:00.07 top
      1 root      20   0  240180  11744   8032 S   0.0   0.0   0:39.55 systemd
      2 root      20   0       0      0      0 S   0.0   0.0   0:04.29 kthreadd
      3 root       0 -20       0      0      0 I   0.0   0.0   0:00.00 rcu_gp
```

- Job information on Portal
  - e.g. https://portal.chpc.utah.edu/slurm/jobs/notchpeak-6495469/

Checking jobs

- Check if program recognizes GPU
  - Tensorflow

```
$ ml apptainer
$ apptainer pull docker://tensorflow/tensorflow:latest-gpu
$ apptainer exec --nv tensorflow_latest-gpu.sif python -c "from
tensorflow.python.client import device_lib;
print(device_lib.list_local_devices())"
...
incarnation: 6542723605025785350
xla_global_id: -1
, name: "/device:GPU:0"
device_type: "GPU"
memory_limit: 14433386496
locality {
  bus_id: 1
  links {
  }
}
incarnation: 11460771345138423495
physical_device_desc: "device: 0, name: Tesla T4, pci bus id: 0000:3b:00.0, compute
capability: 7.5"
xla_global_id: 416903419
]
```

Checking jobs

- Check if program recognizes GPU
  - PyTorch

```
$ ml apptainer
$ apptainer pull docker://pytorch/pytorch:2.4.1-cuda12.1-cudnn9-devel
$ apptainer exec --nv pytorch_2.4.1-cuda12.1-cudnn9-devel.sif python -c
"import torch;print(torch.cuda.device_count())"
1
$ apptainer shell --nv pytorch_2.4.1-cuda12.1-cudnn9-devel.sif
Apptainer> python
Python 3.11.9 | packaged by conda-forge | (main, Apr 19 2024, 18:36:13) [GCC
12.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import torch
>>> torch.cuda.device_count()
1
>>> device_name = torch.cuda.get_device_name(0)
>>> print("Device name:", device_name)
Device name: Tesla T4
```

Multi-GPU jobs

- Single node
  - ML/AI frameworks should pick up multiple GPUs within a node and use them
  - Other programs may need MPI to run one process per one GPU
    - Consult the program's documentation for how to run
- Multi node
  - Not used much at the CHPC, we don't have too many GPU nodes
  - ML/AI frameworks need a way to communicate - e.g. Horovod library - uses MPI or Nvidia's NCCL - contact us if you have a need for this
  - Other programs - should work if they are built with MPI and CUDA, using CUDA aware MPI
    - e.g GROMACS on 2 nodes with 2 GPUs each

```
ml gcc/11.2.0-gpu  openmpi/5.0.3-gpu gromacs/2024.2-gpu
mpirun -np 4 gmx_mpi mdrun -gpu_id 01
```

  - Upcoming state funded HPE cluster will have efficient multi-node capability

Summary

- Be aware of many different GPU types.
- Use `freegpus` to find what GPUs are free
- Use SLURM's `--gres=gpu` to request a GPU
- Ask for fair amount of host memory (SLURM `--mem`)
- Consider using owner GPUs for quick turnaround
- Monitor job's GPU usage with `nvidia-smi` and `nvtop`
- Watch job's output for information about GPU discovery and utilization