Special hardware available (GPUs) & how to use it

March 12, 2025

TOP500 List November 2024

Rank	Nation	Machine	Performance	Accelerators
1.		El Capitan	1742 PFLOPs/s	AMD MI300A
2.		Frontier	1353 PFLOPs/s	AMD MI250X
3.		Aurora	1012 PFLOPs/s	INTEL DatCntGPUMax1550
4.		Eagle	561 PFLOPs/s	NVIDIA H100
5.		HPC6	478 PFLOPs/s	AMD MI250X
6.		Fugaku	442 PFLOPs/s	
7.		Alps	435 PFLOPs/s	NVIDIA GH200
8.		Lumi	380 PFLOPs/s	AMD MI250X
9.		Leonardo	241 PFLOPs/s	NVIDIA A100
10.		Tuolumne	208 PFLOPs/s	AMD MI300A

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GPUs @ VSC

Partition	Model	#Cores	Clock Freq (GHz)	Memory (GB)	Bandwidth (GB/s)	TDP (W)	FP32/FP64 (GFLOPs/s)
zen2_0256_a40x2	45 x 2 x A40	5376/336	1.74	48	696	300	37000/578
zen3_0512_a100x2	60 x 2 x A100	6912/432	1.40	40	1600	400	20000/10000
gpu_rtx2080ti[†]	19 x 1 x rtx2080ti	4352/544	1.45	11	616	255	13400/400

[†] private nodes, available only at idle times

Getting Started with GPUs, Interactive Sessions

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4. cuda−zen sh n3071−003:~$ spack unload
   cuda−zen sh n3071−003:~$ spack load cuda@11.8.0%gcc@9.5.0/ananl33
   cuda−zen sh n3071−003:~$ cd ~/examples/09_special_hardware/matrixMul
   cuda−zen sh n3071−003:~/examples/special_hardware/matrixMul$ nvcc -arch=native ./matrixMul.cu
   cuda−zen sh n3071−003:~/examples/special_hardware/matrixMul$ ./a.out
   cuda−zen sh n3071−003:~/examples/special_hardware/matrixMul$ cd
   cuda−zen sh n3071−003:~$ cd ~/examples/09_special_hardware/matrixMulCUBLAS
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6. cuda−zen sh n3071−003:~$ deviceQuery (... from the SDK now to be self-compiled)

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SLURM Submission to GPU Nodes

```
#!/bin/bash
#
# usage: sbatch ./gpu_test.scrpt
#
#SBATCH -J a100
#SBATCH -N 1
#SBATCH -p zen3_0512_a100x2
#SBATCH --qos=zen3_0512_a100x2
#SBATCH --gres=gpu:2

spack unload
spack load cuda@11.8.0%gcc@9.5.0/ananl33

nvidia-smi
```

Exercise/Example/Problem

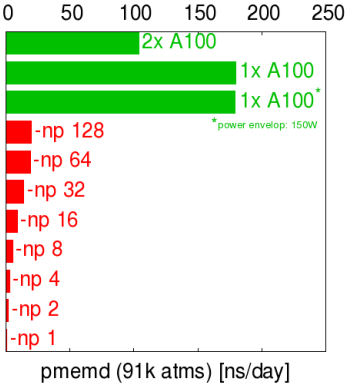
Using interactive mode or batch submission, figure out whether we have ECC enabled on GPUs of type A100 ?

Hint: *nvidia-smi -i 0 -q* will query all settings on the first device, ie number 0

GPUs are Power-Efficient

Example: AMBER-22

Performance:



Power Efficiency: