Special hardware available (GPUs) & how to use it

June 19, 2024

TOP500 List November 2023

Rank	Nation	Machine	Performance	Accelerators
1.		Frontier	1206 PFLOPs/s	AMD MI250X
2.		Aurora	1012 PFLOPs/s	INTEL DatCntGPUMax1550
3.		Eagle	561 PFLOPs/s	NVIDIA H100
4.		Fugaku	442 PFLOPs/s	
5.		Lumi	380 PFLOPs/s	AMD MI250X
6.		Alps	270 PFLOPs/s	NVIDIA GH200
7.		Leonardo	241 PFLOPs/s	NVIDIA A100
8.		MareNostrum5	175 PFLOPs/s	NVIDIA H100
9.		Summit	149 PFLOPs/s	NVIDIA V100
10.		EosNVIDIA DGX SPOD	121 PFLOPs/s	NVIDIA H100

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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

1. VSC-5> salloc -N 1 -p zen3_0512_a100x2 --qos zen3_0512_a100x2 --gres gpu:2

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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
   cuda−zen sh n3071−003:~/examples/special_hardware/matrixMulCUBLAS$ which nvcc
   cuda−zen sh n3071−003:~/examples/special_hardware/matrixMulCUBLAS$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/gpfs/opt/sw/cuda-zen/spack-0.19.0/opt/spack/linux-almalinux8-zen/gcc-9.5.0/cuda-11.8.0-ananl33ltrpp33xetcoltkbbbfuxoeez/lib64
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5. cuda−zen sh n3071−003:~$ nvidia-smi

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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

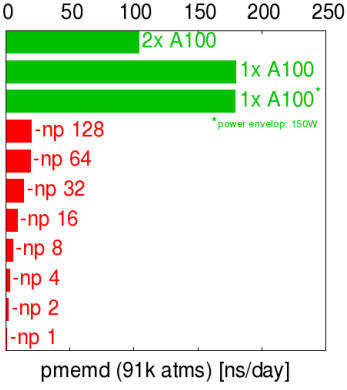
Using interactive mode or batch submission, figure out whether we have ECC enabled on GPUs of type A100 ?

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: