Introduction to GPU Programming

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Outline II

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Motivation

Theoretical GFLOP/s: GPU vs. CPU

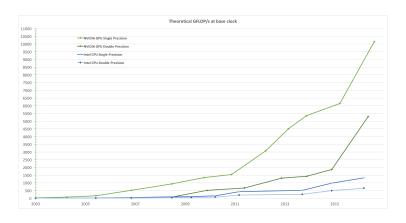
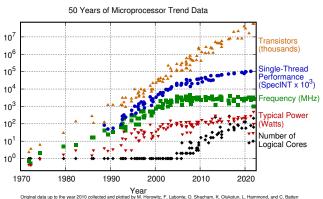


Figure: Theoretical GFLOP/s: GPUs vs. CPUs.^a

 $^{{\}it a} https://docs.nvidia.com/cuda/archive/9.1/pdf/CUDA_C_Programming_Guide.pdf$

CPU processor trend (last 50 years)



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten New plot and data collected for 2010-2021 by K. Rupp

 After the year 2000, freq./power for a single CPU core reaches a max. (Heat dissipation!).

Energy efficiency per job: GPU vs. CPU

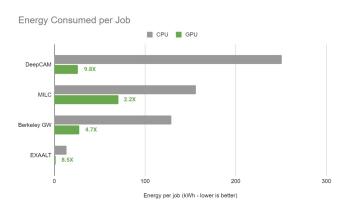


Figure: Energy efficiency per job (NERSC).^a

^ahttps://blogs.nvidia.com/blog/gpu-energy-efficiency-nersc/ (05/21/2023)

Hardware

Streaming Multiprocessor (SM)

- GPU device connected to the CPU by a PCIe bus.
- each GPU device contains an array (x) of Streaming Multiprocessors (SM).
- each SM has:
 - a Single-Instruction Multiple-Thread (SIMT) Architecture.
 - contains y regular cores and [z tensor cores].
- scalable: newer generations: increase of x, y and [z], e.g.:
 - NVIDIA A100-PCIE-40GB (notch293)
 - global memory: 40 GB.
 - 108 SMs, 64 Cores/SM, 4 Tensor Cores/SM.
 - GPU Max. Clock Rate: 1.41 GHz.
 - NVIDIA H100 SXM5 NVL (grn008)
 - global memory: 93 GB.
 - 132 SMs, 128 Cores/SM, 4 Tensor Cores/SM.
 - GPU Max. Clock Rate: 1.78 GHz.



NVIDIA GH100 SM



Figure: GH100 SM

NVIDIA GH100 Full Device



Figure: NVIDIA GH100 Full Device (144 SMs).

GPU Threads - Warps

- Each SM:
 - generates, schedules, executes threads in batches of 32 threads.
 - WARP: a batch of 32 threads
- each thread in a WARP executes the same instructions but runs its own "path".
- if threads within a WARP diverge, the threads become inactive/disabled.

Software

GPGPU & CUDA

- GPU (Graphic Processing Unit): orginally developed for graphical applications.
- GP-GPU: General-Purpose GPU, i.e.
 the use of GPUs beyond graphical applications.
 CAVEAT: problem to be reformulated in terms of the graphics API.
- 2007: NVIDIA introduces the CUDA¹ framework (Compute Unified Device Architecture)
 - CUDA API: extension of the C language.
 - handles the GPU thread level parallelism.
 - deals with moving data between CPU and GPU.
 - also support for C++, Fortran and Python.

- CUDA Driver
- CUDA Toolkit (nvcc,nvprof, ..., libraries, header files).

¹The CUDA Toolkit consists of 2 parts:

Structure of a GPU computation

- Allocate memory space on the GPU device.
- 2 Transfer the data from the CPU to the GPU device.
- Perform the calculation on the GPU device.
 - kernel: function executed on the GPU.
 - To enhance performance: keep data as long as possible on the GPU device.
- Transfer the result back from the GPU device to the CPU.
- Deallocate memory space on the GPU device.

Note: source code & makefile available in ./src

Alloc. & free of global memory on the GPU

- cudaError_t
 CUDA Error types.
- cudaError_t cudaMalloc(void **devPtr, size_t size)
 Allocates memory on the device.
- cudaError_t cudaFree(void *devPtr)
 Frees memory on the device.

```
double *M.d, *N.d, *P.d; // Pointers (device)
int const SZ=16;
int const SZ=SZ*SZ;

// Allocate M on device (M.d)
if(cudaMalloc(&M.d, sizeof(double)*SZ2) != cudaSuccess)
{
    printf(" ERROR: alloc vector M on DEVICE \n");
    return 1;
}

// Deallocate matrix M.d
if(cudaFree(M.d) != cudaSuccess)
{
    printf(" ERROR: unable to deallocate M.d (DEVICE)\n");
    return 1;
}
```

Listing 1: Alloc/Free extract

Copy data between host (CPU) and device (GPU)

Copy data bewteen host (CPU) and device (CPU)

- Direction (kind):
 - cudaMemcpyHostToHost
 - cudaMemcpyHostToDevice
 - cudaMemcpyDeviceToHost
 - cudaMemcpyDeviceToDevice

Listing 2: cudaMemcpy extract

CUDA Kernel

- CUDA kernel: alias for a function which may run on a GPU device.
- Kernel declaration syntax:

```
funcspec void kernelName(args){ body }
where:
```

- funcspec: function type qualifier, i.e.
 __global___,__host___,__device__
- kernelName: name of the kernel/CUDA function.
- args: argument list of the kernel/CUDA function.
- body: body of the kernel/CUDA function (your code).
- Kernel call syntax:

kernelName<<<gridSize,blockSize>>>(args)

where:

- gridSize: size of the grid of thread blocks.
- blockSize: size of a thread block.



Function type qualifiers

Qualifier	Called from	Executed on
global	host	device
host	host	host
device	device	device

Table: Function type qualifiers

Note:

 You can have to different versions of a function i.e.: one with __host__ & one with __device__

Grids, Blocks and Threads

We have a hierarchical (software) implementation.

- uint3,dim3:
 - CUDA defined structures of unsigned integer x,y,z
 - dim3: based on uint3 but unspecified components are initialized to 1.
- Grid: each Grid consists of Blocks
 - dim3 gridDim: dimensions of the Grid.
 - uint3 blockIdx: block index within the Grid.
- Block: each Block consists of Threads
 - dim3 blockDim: dimensions of the Block
 - uint3 threadIdx: thread index within the block.

Preliminary notion: matrix storage as a 1D vector

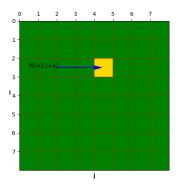


Figure: P: 8x8 Matrix (d = 8)

• P[i,j] is stored as 1D vector: P[i*d+j] where $i,j \in [0,8)$.

Matrix Multiplication P = M N

Matrix multiplication: P = M N where $M, N \in \mathbb{R}^{d \times d}$

•
$$P[i,j] = \sum_{k=0}^{d-1} M[i,k] N[k,j]$$

- M[i, k] is stored as: M[i * d + k]
- N[k,j] is stored as: N[k*d+j]
- Therefore,

$$P[i*d+j] = \sum_{k=0}^{d-1} M[i*d+k] N[k*d+j]$$
 (1)

Matrix Mul.: kernel (v. 1)

- Each Thread (threaldx) is represented as a 2D object, i.e. (threadIdx.x, threadIdx.y) (cfr. a point in plane geometry)
- Each Thread calculates only 1 element of P.

Implementation of Eq. (1) using 1 Block of Threads.

Listing 3: Kernel (v. 1)

Invoking kernel (v. 1)

Invoking 1 Block of Threads

```
int main(void)
{
   int const SZ=16;
   // ...
   // Invoke Kernel to generate P=MxN
   dim3 dimBlock(SZ,SZ,1);
   dim3 dimGrid(1,1,1);
   MatrixMulKernel1<<<<di>dimBlock>>>(M_d,N_d,P_d,SZ);
   //..
}
```

Listing 4: Invoking kernel (v. 1)

Mat. Mul (v.2): Grid of 2D Blocks

- int tx = blockIdx.x*blockDim.x + threadIdx.x;
- int ty = blockIdx.y*blockDim.y + threadIdx.y;

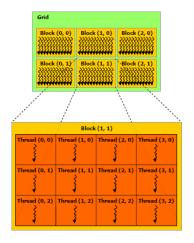


Figure: 2D-Grid of 2D-Blocks of Threads

Matrix Mul.: visualization (v. 2)

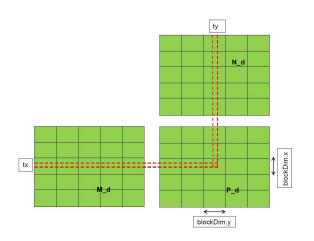


Figure: Matrix Mul. (2D Grid)

Matrix Mul.: kernel (v. 2)

Listing 5: Kernel (v. 2)

Invoking kernel (v. 2)

• Invoking a grid of blocks of threads

```
int main(void)
{
   int const SZ=500;

   // ..
   int const THREADX=16;
   int const THREADY=16;
   int const THREADY=16;
   dim3 dimBlock(THREADX, THREADY, 1);
   int numBlocksX=(SZ%THREADX==0 ? SZ/THREADX : SZ/THREADX +1);
   int numBlocksY=(SZ%THREADY==0 ? SZ/THREADY : SZ/THREADY +1);
   dim3 dimGrid(numBlocksX, numBlocksY, 1);

MatrixMulKernel2<<<dimGrid, dimBlock>>>(M_d, N_d, P_d, SZ);
   //..
}
```

Listing 6: Invoking kernel (v. 2)

Types of GPU memory

- global memory: (largest, slowest and often the bottleneck).
- constant memory: cached, read-only
 - __constant__: constant memory space specifier
- registers: fast, on-chip memory (exclusive to each thread).
- shared memory: allocated per thread block & low latency
 - __shared__: shared memory space specifier
 - __syncthreads(): barrier function which forces all threads in a block to wait until all threads have arrived before proceeding. (block level synchronization).

Matrix Mul.: use of shared memory (v. 3)

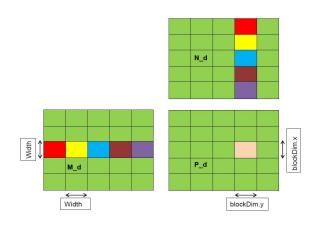


Figure: Matrix Mul.: use of shared memory

Matrix Mul.: kernel (v. 3) - use of shared memory

```
#include <mul.h>
#define WIDTH 16
__global__ void MatrixMulKernel3(double *M_d, double *N_d, double *P_d, int const SZ)
    int tx = blockldx.x * blockDim.x + threadIdx.x;
    int tv = blockldx.v * blockDim.v + threadIdx.v:
    __shared__ double M_s[WIDTH][WIDTH];
    __shared__ double N_s[WIDTH][WIDTH];
    double Pval = 0.0:
    int nslices=(SZ%WIDTH==0)?(SZ/WIDTH):(SZ/WIDTH+1);
    for(int islice=0: islice < nslices: islice++)
        M_s[threadIdx.x][threadIdx.y]=M_d[tx*SZ + islice*WIDTH + threadIdx.y];
        N_s[threadIdx.x][threadIdx.v] = N_d[islice*WIDTH*SZ + threadIdx.x*SZ + tv]:
        __syncthreads();
        for (int k=0: k<WIDTH: k++)
             Pval += M_s[threadIdx.x][k]* N_s[k][threadIdx.y];
        __syncthreads();
    if(tx < SZ \&\& ty < SZ)
       P_d[tx*SZ+ty] = Pval;
    return:
```

Listing 7: Kernel (v. 3)

Building/Compiling CUDA applications

General scheme:

- Source code for CUDA applications:
 - C/C++ host code with extensions to deal with the device(s).
 - Other programming languages are allowed e.g. Fortran
- Primo: separate device functions from host code.
- Device code: preprocessing, compilation with the NVIDIA compiler (nvcc).
- Host code: preprocessed, compiled with a host (C/C++) compiler
 e.g. (gcc, g++, icc, icpc, ...)
- Compiled device functions are embedded as fatbinary images in the host object file.
- Linking stage: adding CUDA runtime libraries to the host object file to create an executable.

Further concepts

- .cu : Suffix for CUDA source file (host code (C,C++) & device code).
- .cuf: Suffix for CUDA source file (host code (Fortan) & device code).
- .ptx: Suffix for Parallel Thread Execution (PTX) files. An intermediate representation (similar to assembly for a virtual GPU architecture²
- .cubin: Suffix for the CUDA device binary file pertaining to a real GPU architecture³
- fatbin: Multiple PTX [& cubin] files are merged into a fatbin file.

²Virtual architectures bear the "compute_" prefix e.g. "compute_70".

³Real (physical) architectures bear the "sm_" prefix e.g. "sm_70".

Compilation trajectory (cont.)

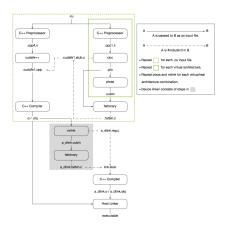


Figure: Compilation trajectory

In praxi,

We will now address the following questions:

- What are the recent CUDA architectures
- How to find the compute capability (CC) of a device
- How to build an executable for a particular device.
- How to build an executable for multiple architectures

Recent CUDA Architectures/Generations

- NVIDA GPU: xy x:generation (major) y: minor
- new generation: major improvement in functionality/chip
- binary compatibility is **NOT** garantueed among generations.

Architecture/	Year	compute_	sm_
Generation		(virtual)	(real)
Maxwell	2014	50, 52, 53	50, 52, 53
Pascal	2016	60, 61, 62	60, 61, 62
Volta	2017	70, 72	70, 72
Turing	2018	75	75
Ampere	2020	80, 86, 87	80, 86, 87
Ada Lovelace	2022	89	89
Hopper	2022	90, 90a	90, 90a

Table: Some of the recent CUDA architectures (10/08/2024)

Retrieval of the Compute Compability (CC)

You can:

- write some basic C/C++ code ⁴. relying on the following CUDA APIs:
 - cudaGetDeviceCount(int *tot):
 returns the number of devices on the localhost.
 - cudaGetDeviceProperties(cudaDeviceProp *p, int idev): returns information about the compute-device idev.
- use existing tools, e.g. nvaccelinfo (part of NVIDIA HPC SDK)
- O Note:

The nvidia-smi executable displays the architecture but not the CC of the device(s): nvidia-smi -q

The name of the corresponding executable is devinfo or the corresponding executable is devinfo.

⁴Already available in src/devicequery.

Retrieval of CC through some simple CUDA APIs

```
[u0253283@notch001:~]$ devinfo
Node: notch001
#Devices detected: 3
 Device: 0
    Device Name : Tesla V100-PCIE-16GB
    ECC Enabled
    Compute Capability
    Compute Mode
    #SM on device
    Device Clock Rate (GHz) : 1.3800E+00
    Peak Memory clock frequency (GHz): 8.7700E-01
   L2 Cache Size (bytes)
                                   : 6291456
    Warp Size in Threads
                                   : 32
   Max. #Blocks/SM
                                   : 32
   Max. Size of each dim. of a Grid : (2147483647,65535,65535)
   Max. Size of each dim. of a Block: (1024,1024,64)
   Max. #Threads/Block
                                  : 2048
   Max. Resident Threads/SM
    Global Mem. available on device (bytes) : 16928342016
    Constant Mem. available on device (bytes): 65536
   #32-bit Registers available per SM
   #32-bit Registers available per Block
                                           : 65536
    Shared Mem. available per Block (bytes) : 49152
    Shared Mem. available per SM (bytes) : 98304
 Device: 1
   Device Name : Tesla V100-PCIE-16GB
   ECC Enabled
   Compute Capability : 70
```

Figure: devinfo based on a few CUDA APIs

Retrieval of CC using nvaccelinfo

```
[u0253283@notch001:~]$ module load nvhpc
[u0253283@notch001:-ls nvaccelinfo
CUDA Driver Version:
NVRM version:
                               NVIDIA UNIX x86 64 Kernel Module 550.54.14 Thu Feb 22 01:44:30 UTC 2024
Device Number:
Device Name:
                               Tesla V100-PCIE-16GB
Device Revision Number:
                               7.0
Global Memory Size:
                               16928342016
Number of Multiprocessors:
Concurrent Copy and Execution: Yes
Total Constant Memory:
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
Maximum Memory Pitch:
Texture Alignment:
                               512B
Clock Rate:
                               1380 MHz
Execution Timeout:
                               No
Integrated Device:
                               No
Can Map Host Memory:
Compute Mode:
                               default
Concurrent Kernels:
                               Yes
ECC Enabled:
                               No
Memory Clock Rate:
                               877 MHz
Memory Bus Width:
                               4896 bits
L2 Cache Size:
                               6291456 bytes
Max Threads Per SMP:
                               2848
Async Engines:
Unified Addressing:
                               Yes
Managed Memory:
                               Yes
Concurrent Managed Memory:
                               Yes
Preemption Supported:
                               Yes
Cooperative Launch:
  Multi-Device:
Default Target:
Device Number:
Device Name:
                               Tesla V100-PCIE-16GB
```

Figure: Use of nvaccelinfo to retrieve compute_

Use of nvidia-smi

```
[u0253283@notch001:~]$ nvidia-smi -q --id=0
=======NVSMT_LOG=========
Timestamp
                                           : Thu Oct 10 15:27:58 2024
Driver Version
                                           . 550 54 14
CUDA Version
                                          : 12.4
                                          : 3
Attached GPIIs
GPII 000000000:38:00.0
    Product Name
                                           : Tesla V100-PCTF-16GB
   Product Brand
                                           : Tesla
   Product Architecture
                                           : Volta
   Display Mode
                                           : Enabled
   Display Active
                                          : Disabled
    Persistence Mode
                                          : Enabled
   Addressing Mode
                                          : N/A
    MTG Mode
        Current
                                           : N/A
        Pendina
                                          : N/A
   Accounting Mode
                                          : Disabled
   Accounting Mode Buffer Size
                                           : 4000
    Driver Model
        Current
                                           : N/A
                                           : N/A
        Pending
    Serial Number
                                           : 0323617020275
                                           : GPU-f6724368-1832-e33f-3525-16b8b86a9e85
    GPU UUID
```

Figure: nvidia-smi

Compiling your code for a particular device/devices

- Compilation goes in 2 steps:
 - PTX representation: generic assembly instructions for a virtual (compute_ prefix) GPU architecture. The resulting .ptx file is human readable (text file).
 - Binary generation: generation of an object file for the real (sm_ prefix) GPU architecture (based on the PTX file).
- -arch/-code flags
 - --gpu-architecture|-arch <arch>: specifies the name of 1 virtual GPU architecture for which the code needs to be compiled.
 e.g.-arch=compute_50
 - --gpu-code|-code <arch>: specifies the name(s) of the real GPU architecture(s) for which the binary needs to be compiled.
 e. g. -code=sm_52

Compiling your code (cont.)

- Therefore, choose 1 virtual architecture and the accompanying real architectures
 - e.g. -arch=compute_50 -code=sm_50,sm_51,sm_52
 - PTX file generated for the compute_50 (virtual) arch.
 - fatbinary object created for the (real) arch. sm_50,sm_51,sm_52
- --generate-code|-gencode arch=<arch>,code=<code> ...
 - Generalization of the previous construct:
 - --gpu-architecture=<arch> --gpu-code=<code>.
 - allows the creation of binaries for different architectures.
 - example:

```
# Compiler flags simultaneously targeting # Maxwell & Pascal architectures
-gencode arch=compute_50,code=sm_50 \
-gencode arch=compute_52,code=sm_52 \
-gencode arch=compute_53,code=sm_60 \
-gencode arch=compute_61,code=sm_61 \
-gencode arch=compute_62,code=sm_62
```

Profiling & debugging

CUDA SDK comes with:

- its own profiler: nvprof.
- its own debugger: nvsight

Profiling mul3 using nvprof

```
[u0253283@notch001:3]$ nvprof ./mul3
==2424062== NVPROF is profiling process 2424062, command: ./mul3
Calling Kernel ...
Kernel Call Finished ...
Frob. Norm(P-P h):
                      0.0000000000
==2424062== Profiling application: ./mul3
==2424062== Profiling result:
           Type Time(%)
                              Time
                                                   Ava
                                                             Min
                                                                      Max
                                                                           Name
GPU activities:
                  59.70% 1.1707ms
                                              1.1707ms 1.1707ms 1.1707ms
                                                                           MatrixMulKernel3(double*, double*, double*, int)
                  32.02% 627.87us
                                              313.93us 307.13us
                                                                 320.73us
                                                                            [CUDA memcpy HtoD]
                   8.28% 162.33us
                                              162.33us 162.33us
                                                                 162.33us
                                                                            [CUDA memcpy DtoH]
                                             46.151ms 109.78us 138.23ms
                                                                           cudaMalloc
     API calls:
                  95.82% 138.45ms
                   2.88% 4.1668ms
                                             1.3889ms 494.15us 3.1420ms
                                                                           cudaMemcpv
                   0.82% 1.1901ms
                                             1.1901ms 1.1901ms 1.1901ms
                                                                           cudaLaunchKernel
                                             131.81us
                                                        94.455us 202.38us
                   0.27% 395.44us
                                                                           cudaFree
                                                           291ns
                                                                 103.89us
                                                                           cuDeviceGetAttribute
                         250.22us
                                             2.1940us
                                              16.428us 16.428us
                   0.01%
                         16.428us
                                                                 16.428us
                                                                           cuDeviceGetPCIBusId
                   0.01% 12.713us
                                              12.713us
                                                       12.713us
                                                                 12.713us cuDeviceGetName
                   0.00% 1.5660us
                                                 522ns
                                                           321ns
                                                                     905ns cuDeviceGetCount
                   0.00% 1.2730us
                                                 636ns
                                                           338ns
                                                                     935ns cuDeviceGet
                                                           613ns
                                                                     613ns cuModuleGetLoadingMode
                   0.00%
                   0.00%
                             556ns
                                                 556ns
                                                           556ns
                                                                     556ns cuDeviceTotalMem
                   0.00%
                             547ns
                                                                     547ns cudaGetLastError
                                                 547ns
                                                           547ns
                   0.00%
                             337ns
                                                 337ns
                                                           337ns
                                                                     337ns cuDeviceGetUuid
```

Figure: Profiling mul3 on notch001

Important CUDA libraries

In order to increase the performance of your code we recommend to use highly-optimized libraries. Among them, we have:

- cuBLAS: Basic Linear Algebra Subroutines on NVIDIA GPUs.
- MAGMA: Matrix Algebra on GPU and Multi-core Architectures.
- cuRAND: Random Number Generation library.
- cuFFT: CUDA Fast Fourier Transform library.
- NCCL: NVIDIA Collective Communications Library.
- cuDNN: CUDA Deep Neural Network library.
- cuTENSOR: GPU-accelerated Tensor Linear Algebra.
- DALI: Library for decoding & augmenting images (DL applications).
- . . .

Alternatives to CUDA

- Similar to CUDA
 - ROCM (AMD)
- OpenACC (use of directives (cfr. OpenMP)
 - GCC: supports OpenACC for NVIDIA & AMD GPUs.
 - NVIDIA HPC SDK (formerly PGI)
 - Sourcery Codebench (AMD GPU)
- Higher-level abstractions
 - Kokkos (prog. model for parallel algorithms for many-core chips)

Links

- CUDA Toolkit Documentation
- CUDA C++ Programming Guide Release 12.6 (10/01/24)
- CUDA C++ Best Practices Guide, Release 12.6 (09/24/24)
- NVIDIA CUDA Compiler Driver NVCC, Release 12.6 (09/24/24)
- PTX & ISA Release 8.5 (09/24/24)

Use of GPUs at the CHPC

GPU devices on lp/kp/np/grn

GPU device type	compute capability
NVIDIA GeForce GTX TITAN X	5.2
Tesla P100-PCIE-16GB	6.0
Tesla P40	6.1
NVIDIA GeForce GTX 1080 Ti	6.1
NVIDIA Titan V	7.0
NVIDIA Tesla V100-PCIE-16GB	7.0
Tesla T4	7.5
NVIDIA GeForce RTX 2080 Ti	7.5
NVIDIA A100-PCIe-40GB	8.0
NVIDIA A100-SXM4-80GB	8.0
NVIDIA A800 40GB Active	8.0

Table: GPU devices on lp/kp/np/grn (10/01/2024)

GPU devices on lp/kp/np/grn (cont.)

GPU device type	compute capability
NVIDIA GeForce RTX 3090	8.6
NVIDIA A40	8.6
NVIDIA RTX A5500	8.6
NVIDIA RTX A6000	8.6
NVIDIA RTX 6000 Ada Generation	8.9
NVIDIA L40	8.9
NVIDIA L40S	8.9
NVIDIA H100 NVL/Deep Dive	9.0

Table: GPU devices on lp/kp/np/grn (10/01/2024)

GPU devices on redwood

GPU device type	compute capability
NVIDIA GeForce GTX 1080 Ti	6.1
NVIDIA A100-SXM4-40GB	8.0
NVIDIA A100 80GB PCIe	8.0
NVIDIA A30	8.0
NVIDIA A40	8.6
NVIDIA RTX 6000 Ada Generation	8.9
NVIDIA H100 NVL/Deep Dive	9.0

Table: GPU devices on redwood (10/01/2024)

Accessing GPUs at CHPC

• Using GPUs at the CHPC (Presentation by Martin Čuma)

Questions

Questions?

Thank you! Any questions?