

# Lab 1: A Gentle Introduction to CUDA

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Accessing the CUDA Servers

How do we measure/reason about Performance?

GPUs: Short Motivation, Desing & Challenges

Basic CUDA Programming

# Get CUDA Up and Running

Option 1: Personal computer

- <https://developer.nvidia.com/cuda-downloads>
- Don't do this now!

# Get CUDA Up and Running on the Official Servers

The information is provided on the Course github

<https://github.com/diku-dk/pmph-e2024-pub?tab=readme-ov-file#gpu--multicore-machines>

All but a few of you, that have registered late, should already have the accounts set up.

## Importantly:

- You need to be connected to VPN, if you are confused please see <https://github.com/diku-dk/howto/blob/main/vpn.md>,
- You need to successfully ssh to our servers hendrixfut01fl or hendrixfut03fl (see github, previous to that you will need to update your ssh config with a paragraph).

- Once you are there you need to execute:

```
$ module load cuda;  
$ module load futhark;
```

You should probably place the later two in your `$HOME/.bash.profile` or `$HOME/.bashrc` so you do not have to execute them every time.

- You are ready to go if `nvcc` is found, i.e., try `$ nvcc`

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# What Is Performance? How to Measure it?

## (1) What is performance?

Performance measures the degree to which hardware resources are utilized.

## (2) How do we measure performance?

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- ▶ If program has low arithmetic intensity  $\implies$  **memory bandwidth/throughput**:

$$\frac{\text{total number of bytes accessed}}{\text{Running time } (\mu s) \cdot 10^3} \quad (\text{GB/sec})$$

- ▶ If program has high arithmetic intensity  $\implies$  **computational performance**:

$$\frac{\text{total number of float operations}}{\text{Running time } (\mu s) \cdot 10^3} \quad (\text{GFlop/sec})$$

- ▶ If in between  $\implies$  roofline model.

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2.2 How to reason about the degree of hardware utilization?

- ▶ compute the percentage achieved by your implementation relative to the peak memory bandwidth or peak flops performance of the hardware.
- ▶ if these are not listed, compare your performance with the best-known implementation of your algorithm for a certain hardware type, e.g., Cublas for MMM.



# Comparing Performance Across Different Implementations

- ...

2.3 How to compare performance across datasets & different implementations?

# Comparing Performance Across Different Implementations

■ ...

## 2.3 How to compare performance across datasets & different implementations?

- ▶ Use the total number of bytes (or float ops) of the “golden sequential” implem!
- ▶ If top hardware performance not listed, sometimes it is useful to compare with simpler algorithms that have the same characteristics and are known to have near-optimal performance.

```
// Inclusive Prefix Sum:  
// Input:  A = {a0, ..., an-1}  
// Result: X = {a0, a0 + a1, ...,  $\sum_{i=0}^{n-1} a_i$ }  
float acc = 0;  
for(int i=0; i<n; i++) {  
    acc = acc + A[i];  
    X[i] = acc;  
}
```

```
// Malloc  
// Input:  A = {a0, ..., an-1}  
// Result: X = {a0, ..., an-1}  
  
for(int i=0; i<n; i++) {  
    X[i] = A[i];  
}
```

- **Prefix sum** is challenging to implement efficiently for GPU;
- **Malloc** is trivial and has the same access pattern:  $n$  reads +  $n$  writes.
- If your prefix scan reaches 80% of malloc's parallel performance  $\implies$  happy!

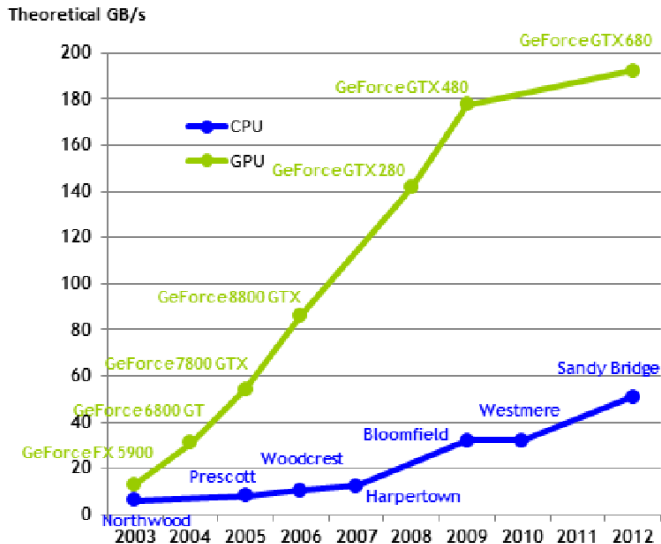
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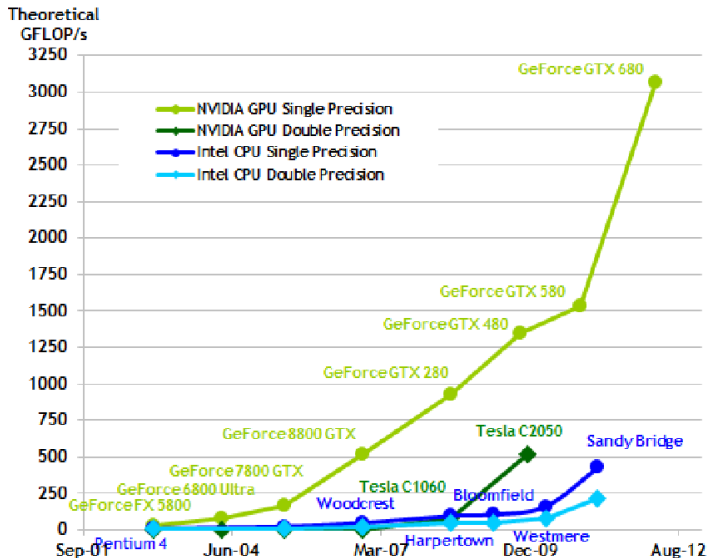
**GPUs: Short Motivation, Desing & Challenges**

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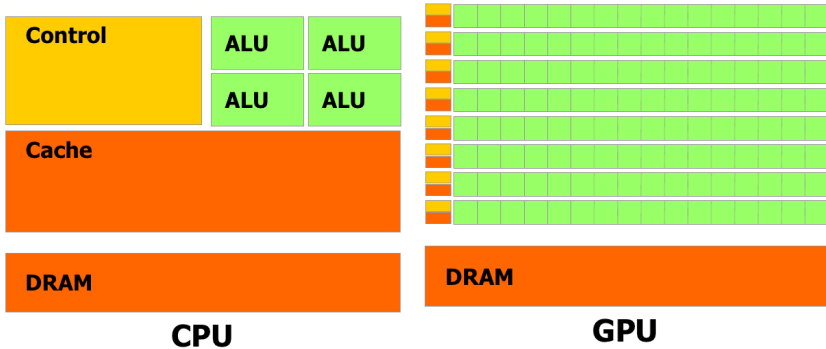
# Peak Memory Performance: GPU vs CPU



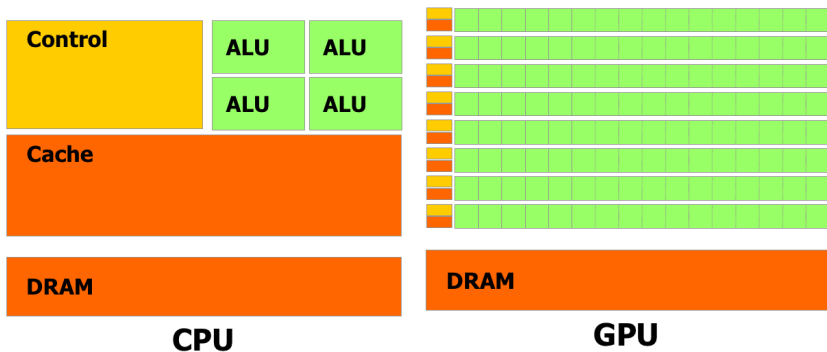
# Peak Computational Performance: GPU vs CPU



# Key Ideas in GPU Design

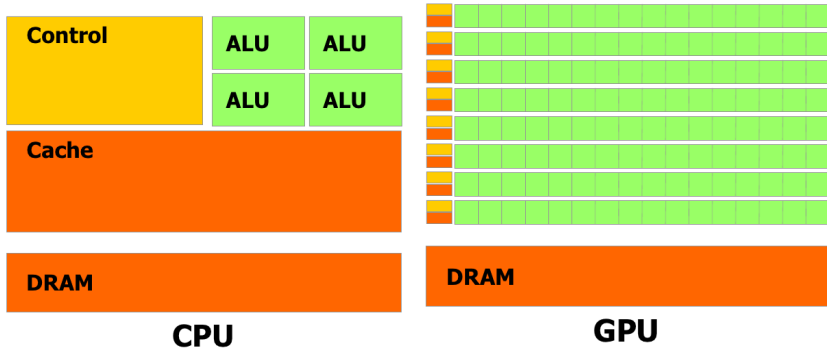


# Key Ideas in GPU Design



- 1 Remove the hardware components that help a single instruction stream run fast,
- 2 SIMD: amortizes the management of an instruction stream across many ALUs,
- 3 Aggressively use hardware(-supported) multi-threading to hide latency.

# Key Ideas in GPU Design

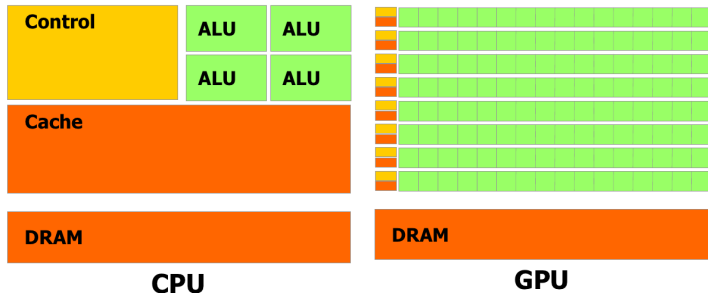


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- 2 SIMD: amortizes the management of an instruction stream across many ALUs,
- 3 Aggressively use hardware(-supported) multi-threading to hide latency.

**Spatial locality to global memory means “coalesced accesses”:** threads executing in lock step a load/store SIMD instruction access consecutive memory locations!



# CPUs compared to CPUs



- GPUs have *thousands* of simple cores and taking full advantage of their compute power requires *tens/hundred of thousands* of threads.
- GPU threads are very *restricted* in what they can do: no stack, no allocation, limited control flow, etc.
- Potential *very high performance* and *lower power usage* compared to CPUs, but programming them is *hard*.

Accessing the CUDA Servers

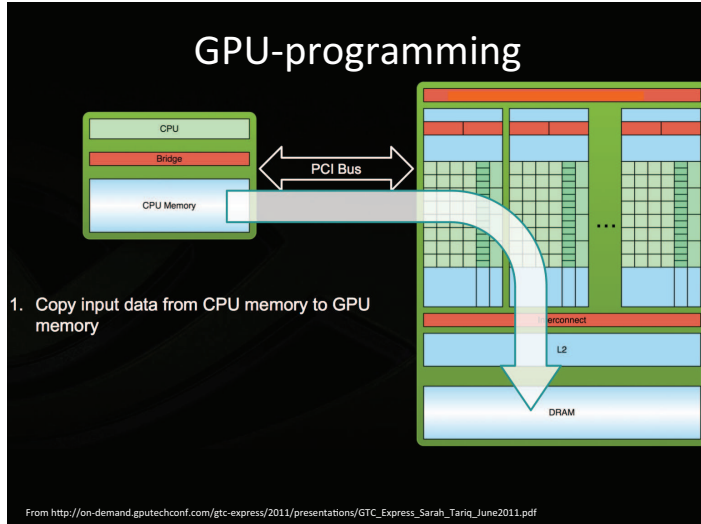
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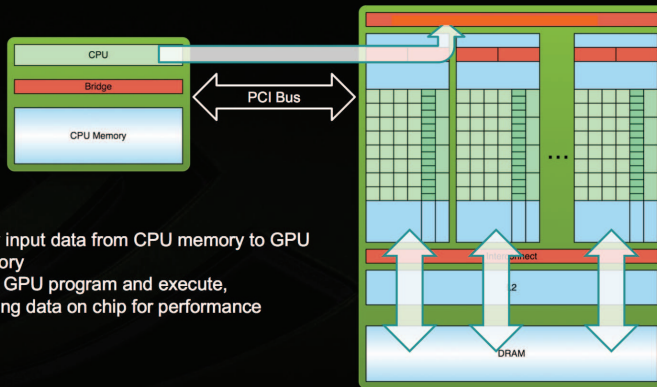
# Basic GPU Programming

The device (GPU) and host (CPU) have different memory spaces!



# Basic GPU Programming

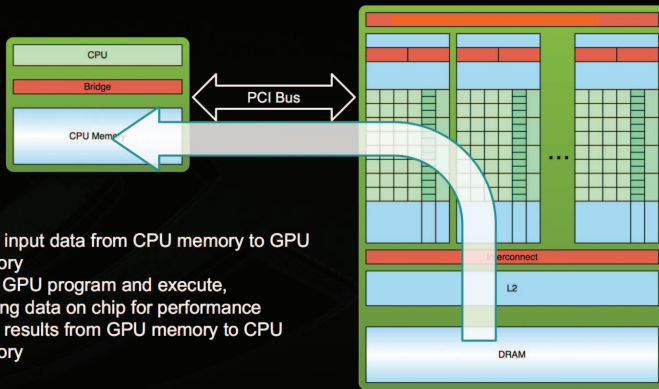
## GPU-programming



1. Copy input data from CPU memory to GPU memory
2. Load GPU program and execute, caching data on chip for performance

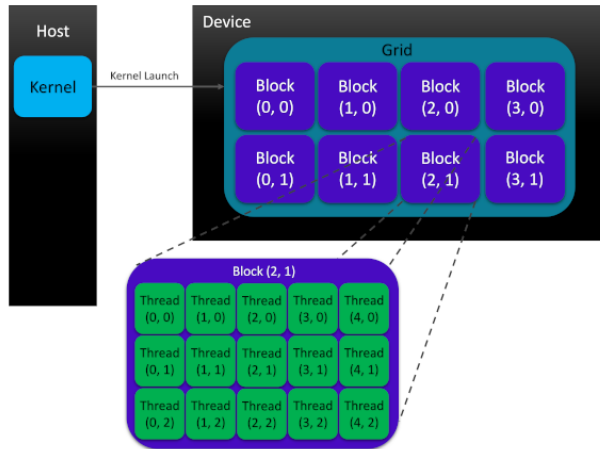
# Basic GPGPU programming

## GPU-programming



# Cuda: Grid-Block Structure of Threads

Credit: pictures taken from <http://education.molssi.org/gpu.programming.beginner/03-cuda->

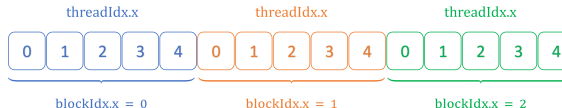


Blocks and Grids have at most three dimensions—denoted  $x, y, z$ , with  $x$  innermost and  $z$  outermost. Their sizes are specified at kernel launch. Inside the **kernel** you may use:

- `blockDim.x`: block size in dim  $x$
- `blockIdx.x`: current block index (in  $x$ )
- `threadIdx.x`: local index of the current thread inside its block (in dim  $x$ )
- `gridDim.x` number of blocks on dim  $x$
- Ditto for dimensions  $y$  and  $z$ .

**The global thread index in dim  $q \in \{x, y, z\}$ :**

**$\text{threadIdx.q} + \text{blockIdx.q} \cdot \text{blockDim.q}$**



# Multiply with 2 Each Element of an Array in CUDA

## Golden Sequential:

```
// Y and X are arrays of length N
for(int i=0; i<N; i++) {
    Y[i] = 2.0 * X[i];
}
```

How do we do this in CUDA?

- We provide a very naive version in this folder  
<https://github.com/diku-dk/pmph-e2024-pub/tree/main/HelperCode/Lab-1-Cuda>  
Please be advised that it works correctly only for arrays of  $\leq 1024$  elements.
- Then we will provide instruction/code in the slides so that you can type in a generally-correct solution.

First let's examine the available code. The actual code is a bit larger than the one on the slides since it also performs runtime measurement and validation.

# A Simple CUDA Program

```
#include <stdlib.h>
#include <stdio.h>
#include <string.h>
#include <math.h>
#include <cuda_runtime.h>

// CUDA kernel:
__global__ void mul2Kernel(float* X, float *Y) {
    const unsigned int gid = threadIdx.x; // threadIdx.x is the local id inside a
                                           // CUDA block; Ok since we only have 1 block.
    Y[gid] = 2 * X[gid]; // computes and updates the result array
}

int main(int argc, char** argv) {
    unsigned int N = atoi(argv[1]);
    unsigned int mem_size = N*sizeof(float);

    // allocate host memory
    float* h_in = (float*) malloc(mem_size);
    float* h_out = (float*) malloc(mem_size);

    // initialize the memory
    for(unsigned int i=0; i<N; ++i) { h_in[i] = (float)i; }
```



## A Simple CUDA Program (continuation)

```
float *d_in , *d_out;
cudaMalloc((void**)&d_in , mem_size);           // allocate device memory
cudaMalloc((void**)&d_out , mem_size);

cudaMemcpy(d_in , h_in , mem_size , cudaMemcpyHostToDevice); // copy host input to device

for(int r = 0; r < GPU_RUNS; r++) {
    mul2Kernel<<< 1, N>>>(d_in , d_out);        // execute the kernel
}
cudaDeviceSynchronize();
// ^ Needed only for measuring runtime (see longer comment in actual code)
// Please note that the execution of multiple kernels in Cuda runs correctly
// without such explicit synchronizations (which are expensive).

gpuAssert( cudaPeekAtLastError() );              // check for errors

cudaMemcpy(h_out , d_out , mem_size , cudaMemcpyDeviceToHost); //copy device result to host

free(h_in);   free(h_out);   cudaFree(d_in);   cudaFree(d_out); // clean-up memory
}
```

## Save, Compile, Run

```
$ nvcc -O3 -o trivial trivial.cu
```

```
$ ./trivial
```

Or even better, use and adjust the Makefile.

## Trouble Ahead

This week assignment: *Write a CUDA program that maps the function  $(x/(x-2.3))^3$  to the array  $[0, 1, \dots, \text{some-big-number}]$  ...*

This shouldn't be a problem with our program (adapt the kernel)

- GPU logical threads organized in a grid of blocks, in which the grid and the block can have up to three dimensions.
- However CUDA does **not** accept a block of size 32757
  - ▶ a *CUDA warp* is formed by 32 threads that execute SIMD.
  - ▶ a *CUDA block* may contain up to 1024 threads (included); ideally the block size is a multiple of 32, but not necessarily.
  - ▶ Synchronization/communication is possible inside a CUDA block by means of barriers & scratchpad memory (shared memory).
  - ▶ Barrier synchronization is not possible across threads in different CUDA blocks, i.e., only by finishing the kernel!

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  - ▶ Barrier synchronization is not possible across threads in different CUDA blocks, i.e., only by finishing the kernel!
- Finally if the size of the computation does not matches exactly a multiple of block size, then you need to spawn extra threads, hence you need to add an `if` inside the kernel code, to make the extra threads iddle!

# GPGPU in More Detail

- A set of Streaming Multiprocessors (SMs)

From deviceQuery:

(15) Multiprocessors, (192) CUDA Cores/MP: 2880 CUDA Cores

- Each SM executes 1 'thread block' at a time.
- Each block has access to
  - Global memory (function arguments)

From deviceQuery:

Total amount of global memory: 3072 MBytes

- Shared memory (`__shared__ int array[512]`)

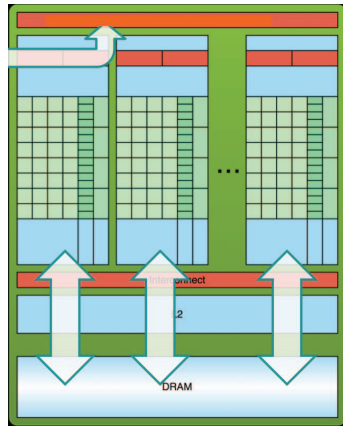
From deviceQuery:

Total amount of shared memory per block: 49152 bytes

- Local memory (local variables)

From deviceQuery:

Total number of registers available per block: 65536



# Step 1 in Fixing Our CUDA Program

## Golden Sequential:

```
// Y and X are arrays of length N  
for(int i=0; i<N; i++) {  
    Y[i] = 2.0 * X[i];  
}
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# Step 1 in Fixing Our CUDA Program

## Golden Sequential:

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}
```

In order to handle values of  $N$  greater than the CUDA-block size (1024), we need to modify the host code to orchestrate the kernel into a grid of multiple blocks:

- We use a 1D grid and a 1D block,
- We chose a “good block size”, for example 128, 256,
- we compute how many blocks our parallel dimension requires; this is “the grid”,
- we update the kernel call with the new grid/block and also pass  $N$  as parameter!

## Calling the kernel from host/CPU-executed code:

```
unsigned int B = 256; // chose a suitable block size in dimension x
unsigned int numblocks = (N + B - 1) / B; // number of blocks in dimension x
dim3 block(B,1,1), grid(numblocks,1,1); // total number of threads (numblocks*B) may overshoot N!
mul2Kernel<<<grid, block>>>(d_in, d_out, N); // pass N as parameter as well;
                                           // d_in and d_out are in device memory
```

## Step 2 in Fixing Our CUDA Program

### Golden Sequential:

```
// Y and X are arrays of length N  
for(int i=0; i<N; i++) {  
    Y[i] = 2.0 * X[i];  
}
```



## Step 2 in Fixing Our CUDA Program

### Golden Sequential:

```
// Y and X are arrays of length N
for(int i=0; i<N; i++) {
    Y[i] = 2.0 * X[i];
}
```

### We modify the CUDA Kernel:

- 1 to contain as extra/third parameter the array length  $N$
- 2 to compute correctly the global thread id  
(now that we have multiple CUDA blocks, we cannot use `threadIdx.x`)
- 3 to perform the write to global memory *if and only if* the global id is within the array bounds.

```
--global-- void mul2Kernel(float* X, float* Y, int N) {
    // compute global thread id in dimension x
    const unsigned int gid = blockIdx.x * blockDim.x + threadIdx.x;
    if(gid < N) { // don't access out of bounds
        Y[gid] = 2.0 * X[gid];
    }
}
```

# How fast does it go?

The program already contains built-in validation and measuring of performance in terms of runtime and more importantly of Gflops/sec. Once it validates, run your program for a big  $N$ , e.g., 200 millions; what performance do you obtain?

The peak bandwidth of our A100 GPU is about 1.55 TBytes/sec. What do you get?

How is performance affected if you change the line of your kernel

```
Y[gid] = 2.0 * X[gid];
```

to

```
Y[threadIdx.x*gridDim.x + blockIdx.x] = 2.0 * X[gid];
```

**The reason is that good spatial locality for global memory is achieved when a warp of consecutive threads access in their SIMD load/store instruction contiguous memory locations. This is dubbed “coalesced access”. The latter access pattern is uncoalesced, hence performance should suffer.**