

GPU programming using CUDA

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Data analytics in the era of large-scale machine learning

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Computation-based Science and Technology Research Center,

The Cyprus Institute

Outline

Lecture part

- Review of GPU architecture
- Review of GPU programming and CUDA
- Some details of our training system, "Cyclone"

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Hands-on - Practical examples on GPUs

Covering:

- GPU performance vs CPU performance
- Memory coalescing on GPUs
- Shared memory
- What is a warp and should you care

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- Some familiarity with programming in C or C++
- Familiarity with some common tasks in C, e.g. array allocation, pointers, etc.
- Can edit text files on a remote server, e.g. text-based (emacs or vim) or [VS Code Remote](#)
- Hopefully this will be useful to capture high-level GPU features that affect performance

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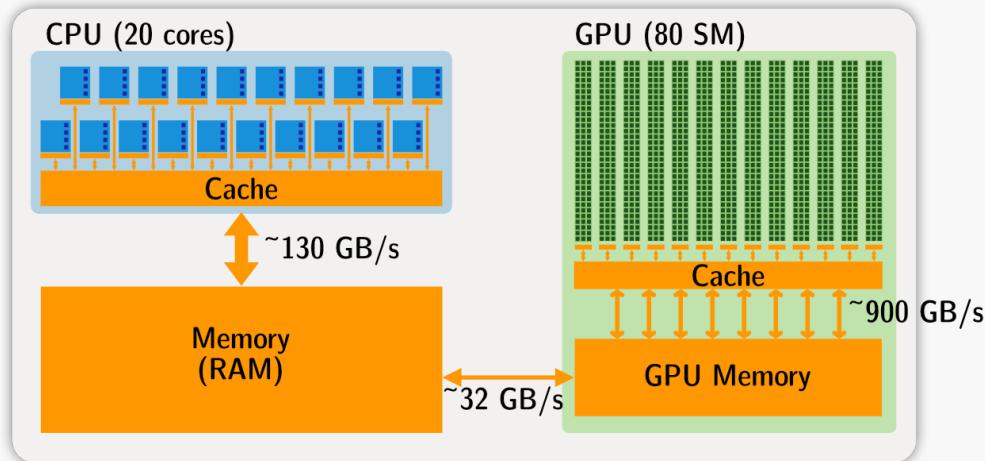
Repo with slides (PDF) and exercises and URL for direct access to slides:

github.com/g-koutsou/NCC-training-202305

<https://sds402.online/training>

GPU architecture

At a very high level:



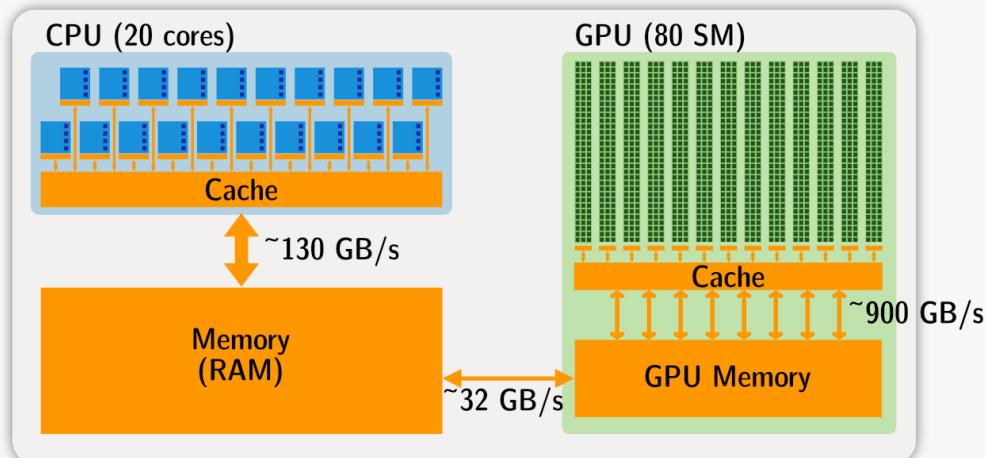
CPU

- Few heavy cores
- Large memory
- Moderate BW to memory
- Optimized for serial execution

GPU

- Many light "cores"
- Smaller memory
- High BW to memory
- Optimized for parallel execution

GPU programming model

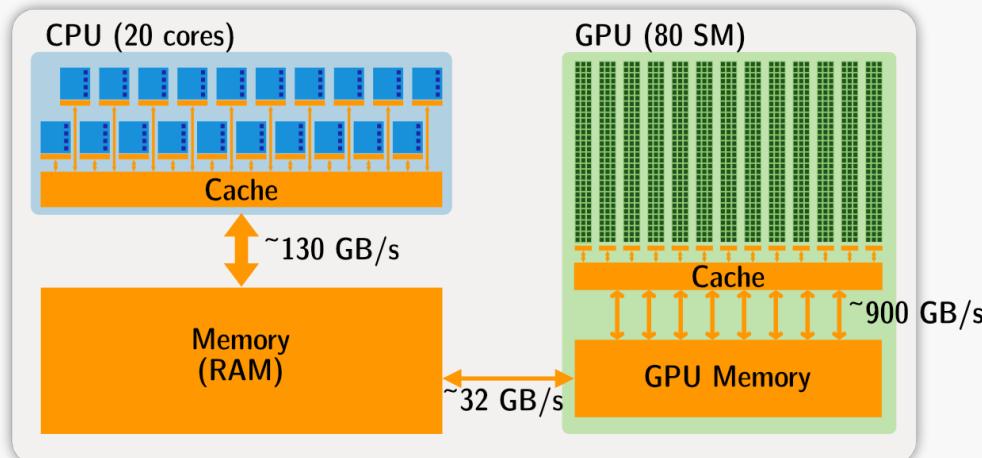


Some numbers from the GPU partition of our Cyclone cluster

NVIDIA V100 Volta GPUs

- 80 Streaming Multiprocessors (SM) per GPU
- 64 "cores" per SM
- GPU memory: 32 GBytes
- Memory bandwidth: 900~GB/s
- Peak performance: 7.8 Tflop/s (double precision)

GPU programming model



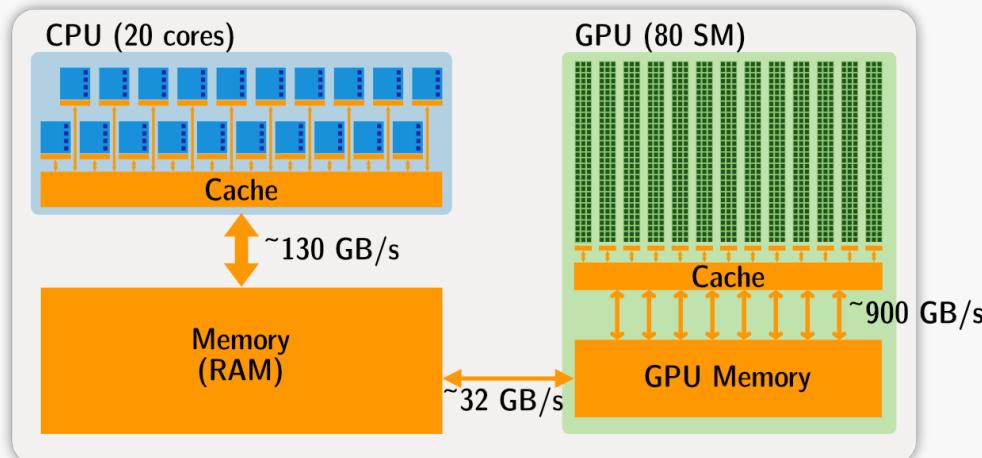
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We will come back to these numbers during the hands-on

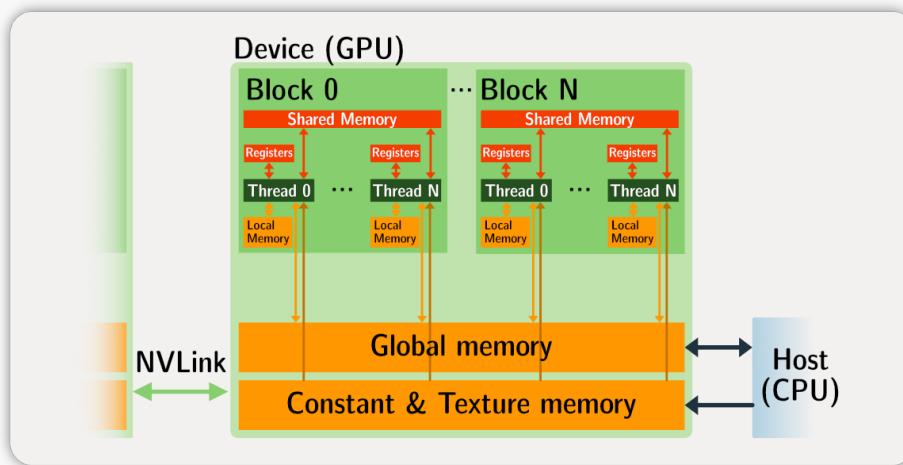
GPU programming model



"Offload" model of programming

- CPU starts program (runs `main()`)
- CPU copies data to GPU memory (over e.g. PCIe, $\sim 32 \text{ GB/s}$)
- CPU dispatches "kernels" for execution on GPU
 - Kernels read/write to GPU memory ($\sim 900 \text{ GB/s}$)
 - Kernels run on GPU threads (thousands) which share *fast* memory [$O(10)$ times faster compared to GPU memory]
- Kernel completes; CPU copies data back from GPU (over e.g. PCIe, $\sim 32 \text{ GB/s}$)

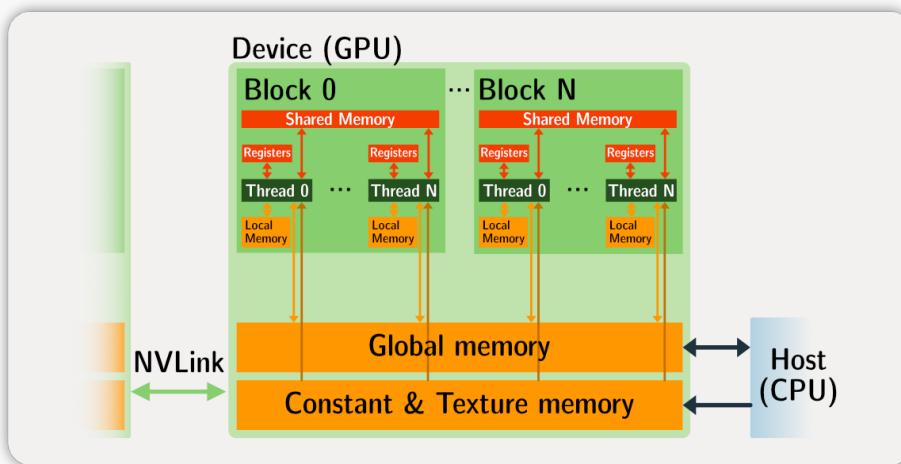
GPU programming model



GPU memory model (NVIDIA model)

- GPU threads: *slow* access to global, constant, and texture memory
- Each thread has *registers* (fast) and *local memory* (slow)
- Threads are grouped into *blocks*; Threads within the same block: *shared memory* (fast)
- Shared memory is limited. E.g. 96 KB per block for V100

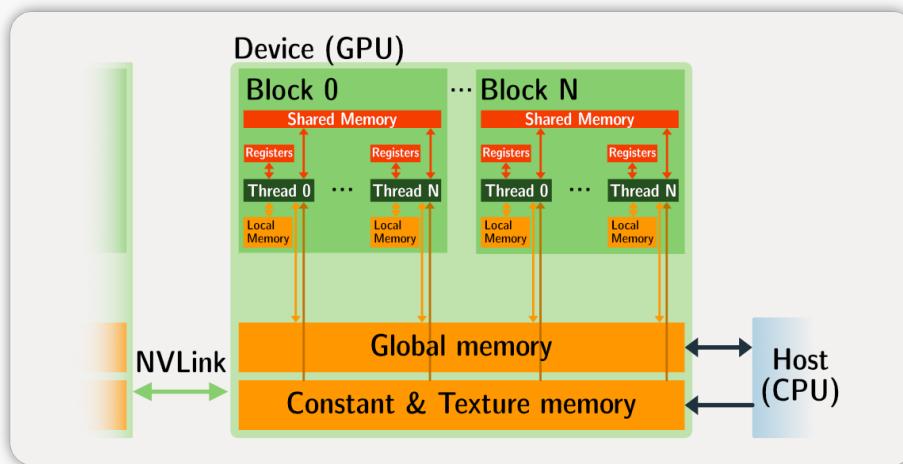
GPU programming model



GPU memory model (NVIDIA model); some numbers for context

- Threads per block: 1024 (max)
- Register memory (per block): 64 KB
- Shared memory (per block): 96 KB
- Also, max. 255 registers per thread

GPU programming model



GPU memory model (NVIDIA model)

- Assumptions about execution order
 - Threads within the same block can be assumed to run concurrently
 - No assumption about the order by which blocks are executed

CUDA programming model

NVIDIA programming framework for NVIDIA GPUs

- Compute Unified Device Architecture
- C-like programming language for writing *CUDA Kernels*
 - Includes C/C++ and Fortran variants
 - Compiler for C/C++: `nvcc`
- Functions for transferring data to/from GPUs, starting kernels, etc.
- Some higher-level functionality also available (linear algebra, random number generations, etc.)
- Concepts generalizable to other accelerator programming frameworks (OpenCL, OpenACC, HiP, etc.)

CUDA programming basics

Nomenclature

- "Host" is the CPU
- "Device" is the GPU

Allocate memory on GPU

```
err = cudaMalloc(&d_ptr, size);
```

- Call from *host* (CPU)
- Allocate `size` bytes of memory on GPU and store the starting address in `d_ptr`
- `d_ptr` is a variable that holds an address to GPU memory i.e. a "device pointer"
- If `err != cudaSuccess` then something went wrong

Free GPU memory

```
cudaFree(d_ptr);
```

CUDA programming basics

Nomenclature

- "Host" is the CPU
- "Device" is the GPU

Copy data to GPU

```
cudaMemcpy(d_ptr, ptr, size, cudaMemcpyHostToDevice);
```

- Call from *host* (CPU)
- Copy data on host pointed to by `ptr` to device at address pointed to by `d_ptr`
- Device memory should have been allocated using `cudaMalloc()` to obtain `d_ptr`

Copy data from GPU

```
cudaMemcpy(ptr, d_ptr, size, cudaMemcpyDeviceToHost);
```

- Call from *host* (CPU)
- Copy data on device pointed to by `d_ptr` to host at address pointed to by `ptr`
- Host memory should have been allocated using e.g. `malloc()` to obtain `ptr`

CUDA programming basics

Declare a CUDA kernel

Example:

```
__global__ void
func(int n, double a, double *x)
{
    ...
    return;
}
```

Call a CUDA kernel

- Call from host. Example:

```
func<<<nblk, nthr>>>(n, a, x);
```

- `nthr`: number of threads per block; can be scalar or a `dim3` type
- `nblk`: number of blocks; can be scalar or a `dim3` type
- Example of `dim3` type:

```
dim3 nthr(1024, 8, 8); /* No. of threads in (x, y, z) */
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CUDA programming basics

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Thread coordinates within kernel

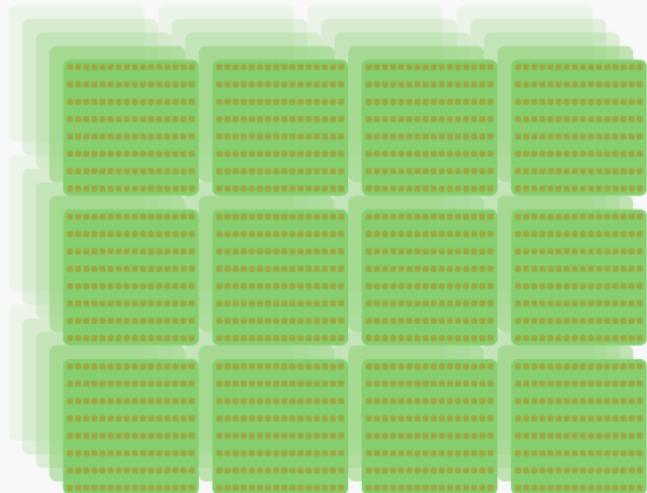
Example:

```
__global__ void
func(int n, double a, double *x)
{
    int idx = threadIdx.x + blockIdx.x*blockDim.x;
    ...
    return;
}
```

CUDA programming basics

Threads, blocks, grids

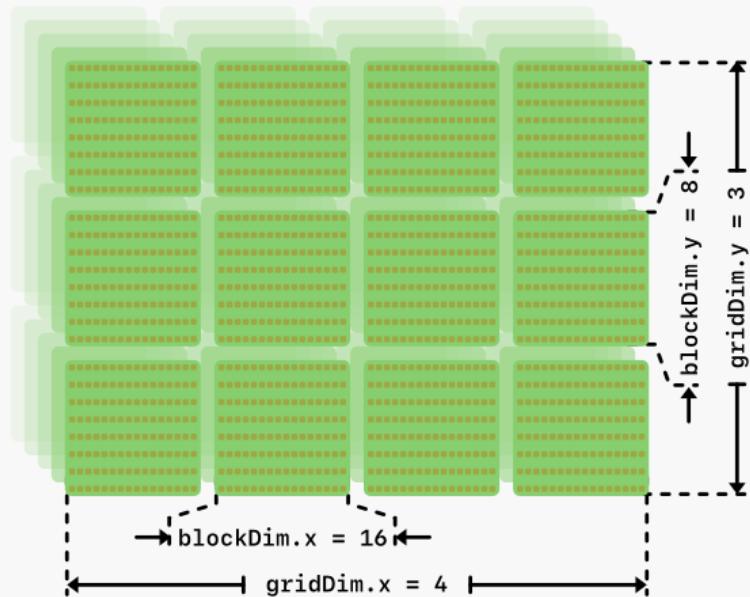
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dim3 blcks( 4, 3, bz);
dim3 thrds(16, 8, tz);
func<<<blcks, thrds>>>( ... );
```



CUDA programming basics

Threads, blocks, grids

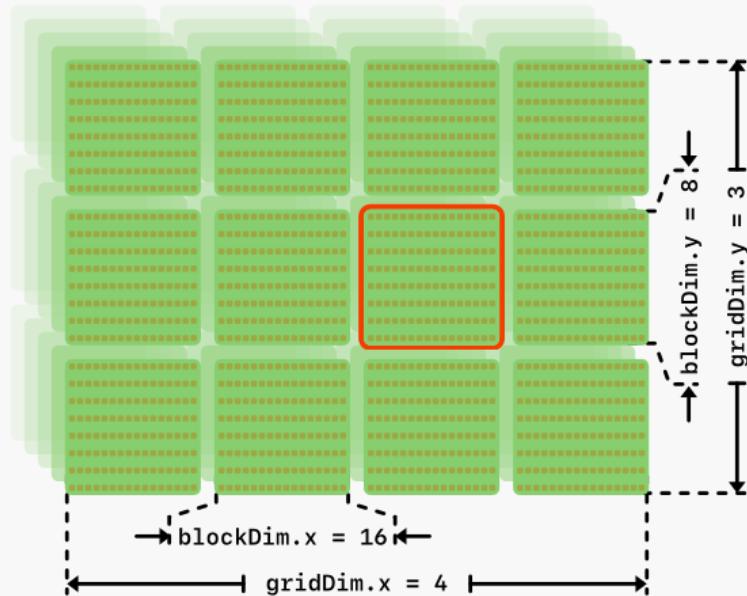
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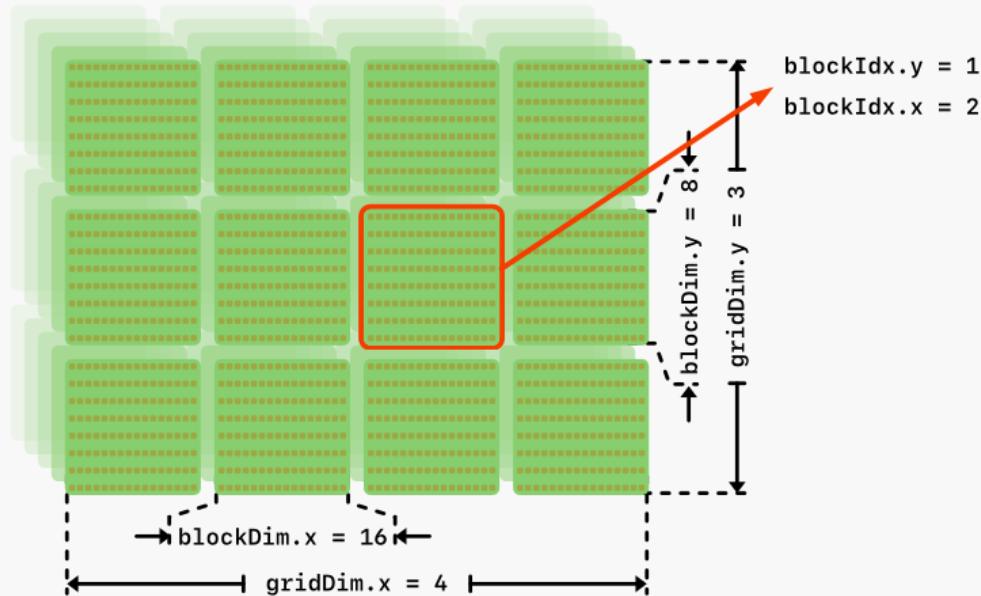
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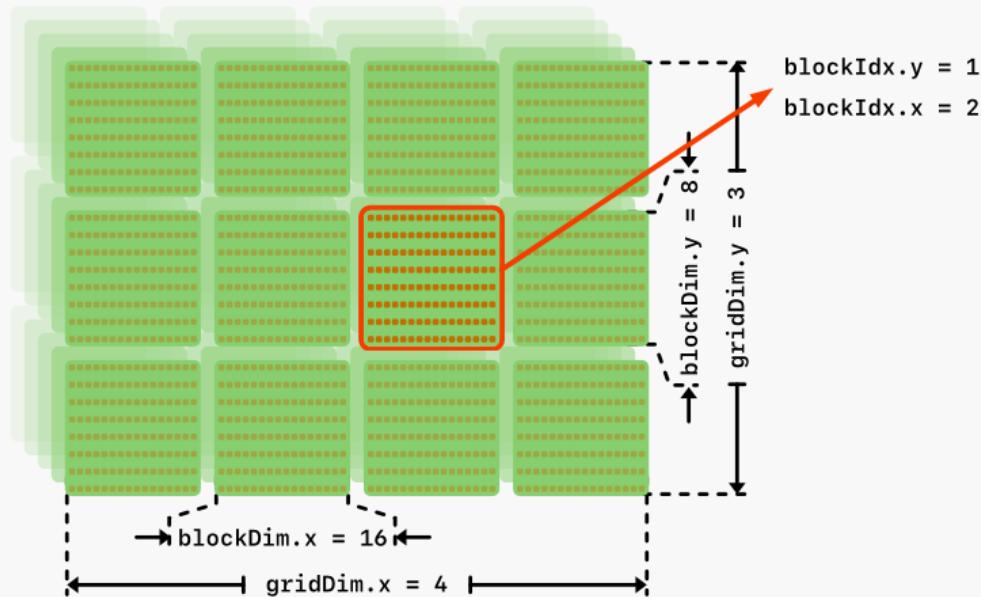
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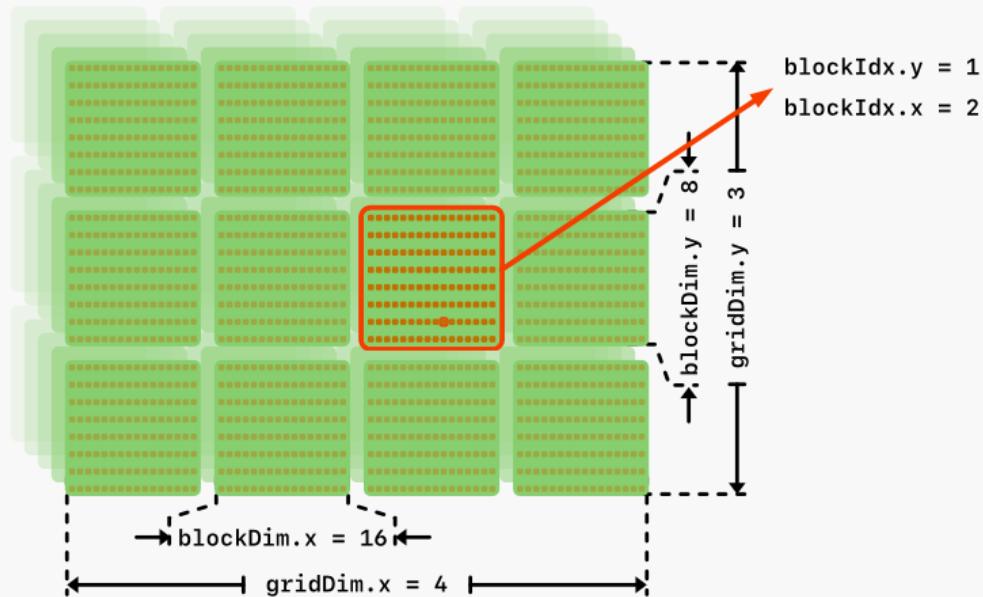
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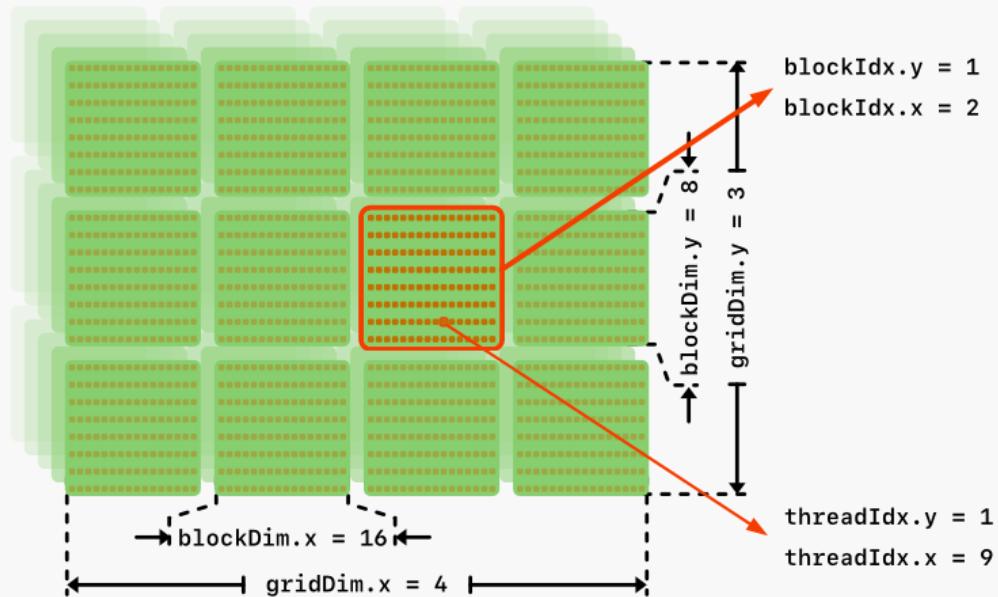
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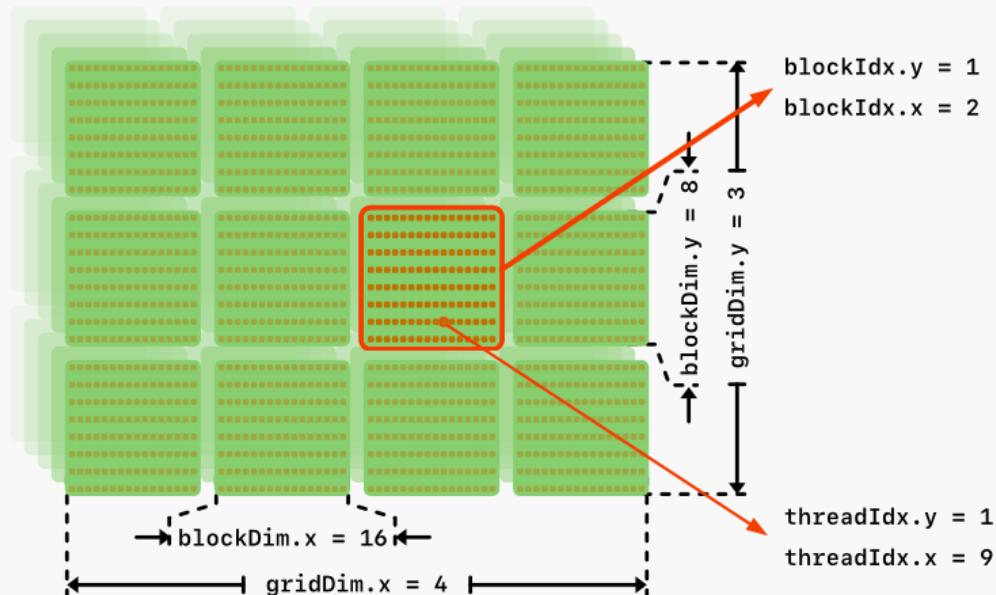
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func<<<blcks, thrds>>>( ... );
```



Variables available within kernel

- `threadIdx.{x,y,z}`
- `blockIdx.{x,y,z}`
- `blockDim.{x,y,z}`
- `gridDim.{x,y,z}`

CUDA, by example

Warp-up: port a simple code to GPU and investigate performance

Sources: /nvme/scratch/da23/gpus/

- ex01/axpy.cu implements a so-called "axpy" operation (a-times-x-plus-y):

$$y_i \leftarrow a \cdot x_i + y_i, \quad i = 0, \dots, n - 1$$

with a scalar and y and x vectors of length n .

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This will cover:

- Allocation of memory on the GPU;
- Transferring memory to/from GPU;
- Invoking kernels;
- Placement of threads and memory access

CUDA Example

File: ex01/axpy.cu

- Contains the C program we will begin with: `axpy.cu`
- Even though the file extension is `.cu`, the program contains no CUDA. Only OpenMP
- Allocates four arrays: `x0[n]`, `x1[n]`, `y0[n]`, and `y1[n]`, with `n` read from the command line
- `x0` and `y0` are initialized to random numbers
- `x1` and `y1` are initialized to `x0` and `y0` respectively
- The program:
 - performs `y0[:] = a*x0[:] + y0[:]` in the first part marked with `A:`
 - performs `y1[:] = a*x1[:] + y1[:]` in the second part marked with `B:`
 - reports the timing for part `A` and for `B`
 - reports the difference between `y0` and `y1`

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 - reports the difference between `y0` and `y1`

Take some time to inspect `axpy.cu` before we compile and run

CUDA Example

- Copy first exercise from this training's shared space:

```
[user@front02 ~]$ cp -r /nvme/scratch/da23/gpus/ex01 .
[user@front02 ~]$ cd ex01/
[user@front02 ex01]$ ls -1
axpy.cu
```

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- Compile with `nvcc` including OpenMP:

```
[user@front02 ex01]$ module load gompi
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[user@front02 ex01]$ nvcc -O3 -arch sm_70 -Xcompiler -fopenmp -o axpy axpy.cu
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- `-Xcompiler -fopenmp`: tells `nvcc` to pass `-fopenmp` to the underlying C compiler (here `gcc`)

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- Run on the CPUs of a GPU node
- Use `srun` to run interactively, e.g.:

```
[user@front02 ex01]$ export OMP_PROC_BIND="close"
[user@front02 ex01]$ export OMP_PLACES="cores"
[user@front02 ex01]$ export OMP_NUM_THREADS=20
[user@front02 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A da23 --gres=gpu:1 --reservation=data-analytics ./axpy
CPU: nthr = 20 t0 = 0.0089 sec P = 15.024 Gflop/s B = 90.142 GB/s
CPU: nthr = 20 t0 = 0.0086 sec P = 15.667 Gflop/s B = 94.000 GB/s
Diff = 0.000000e+00
```

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```

- Compare ~90 GB/s achieved vs ~130 GB/s peak memory bandwidth

CUDA Example

Use a GPU to replace part B of the calculation

- Edits outside of `main()`:
 1. Add the `cuda_runtime.h` header file
 2. Add the GPU `axpy` kernel, naming it `gpu_axpy()`
 3. Add a function similar to `malloc()` that allocates memory on the GPU and checks whether an error occurred
- Edits within `main()`:
 1. Allocate arrays on GPU
 2. Copy `x1[:]` and `y1[:]` to GPU
 3. Call `gpu_axpy()`
 4. Copy `y1[:]` from GPU

CUDA Example

Edits outside of `main()` 1/3

- Add the `cuda_runtime.h` header file on line 5:

```
#include <cuda_runtime.h>
```

CUDA Example

Edits outside of `main()` 2/3

- Add the GPU `axpy` kernel, naming it `gpu_axpy()`, after the CPU `axpy`, around line 64:

```
/***
 * Do y <- a*x + y on the GPU
 ***/
__global__ void
gpu_axpy(int n, float a, float *x, float *y)
{
    for(int i=0; i<n; i++)
        y[i] = a*x[i] + y[i];

    return;
}
```

CUDA Example

Edits outside of `main()` 3/3

- At around line 30 add a function similar to `ualloc()` that allocates memory on the GPU and checks whether an error occurred

```
/***
 * Allocate memory on GPU; print error if not successful
 ***/
void *
gpu_alloc(size_t size)
{
    void *ptr;
    cudaError_t err = cudaMalloc(&ptr, size);
    if(err != cudaSuccess) {
        fprintf(stderr, "cudaMalloc() returned %d; quitting...\n", err);
        exit(-2);
    }
    return ptr;
}
```

CUDA Example

Edits within `main()` 1/4

- Allocate arrays on GPU, within B part. Free arrays before closing B part:

```
/*
 * B: Run axpy(), return to y1, report performance
 */
{
    /* Allocate GPU memory */
    float *d_x = (float *)gpu_alloc(n*sizeof(float));
    float *d_y = (float *)gpu_alloc(n*sizeof(float));
    ...
    cudaFree(d_x);
    cudaFree(d_y);
}
```

CUDA Example

Edits within `main()` 2/4

- Copy `x1[:]` and `y1[:]` to GPU

```
cudaMemcpy(d_x, x1, sizeof(float)*n, cudaMemcpyHostToDevice);
cudaMemcpy(d_y, y1, sizeof(float)*n, cudaMemcpyHostToDevice);
```

CUDA Example

Edits within `main()` 3/4

- Call `gpu_axpy()`. For the moment use 1 thread and 1 block. Replace `axpy(n, a, x, y)` of part B with:

```
double t0 = stop_watch(0);
gpu_axpy<<<1, 1>>>(n, a, d_x, d_y);
t0 = stop_watch(t0);
```

Note we need to pass the *device pointers* since it is these pointers that point to the memory allocated on the GPU

CUDA Example

Edits within `main()` 4/4

- Copy `y1[:]` from GPU:

```
/* Copy y1 back from GPU */
cudaMemcpy(y1, d_y, sizeof(float)*n, cudaMemcpyDeviceToHost);
```

- Also change:

```
printf(" CPU: nthr = %4d    ...);
```

to:

```
printf(" GPU:           ...);
```

and remove OpenMP parallel region.

CUDA Example

Compile and run

- Compile as before:

```
[user@front02 ex01]$ nvcc -arch sm_70 -O3 -Xcompiler -fopenmp -o axpy axpy.cu
```

- Run as before (I'm assuming `OMP_BIND`, `OMP_PLACES`, and `OMP_NUM_THREADS` were set before):

```
[user@front02 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A da23 --gres=gpu:1 --reservation=data-analytics .  
CPU: nthr = 20 t0 = 0.0089 sec P = 15.035 Gflop/s B = 90.212 GB/s  
GPU: t0 = 0.0000 sec P = 3198.579 Gflop/s B = 19191.476 GB/s  
Diff = 1.021564e-15
```

This performance is infeasible. What's going on?

CUDA Example

Edits within `main()` 3/4

- The problem is here:

```
double t0 = stop_watch(0);
gpu_axpy<<<1, 1>>>(n, a, d_x, d_y);
t0 = stop_watch(t0);
```

- CUDA kernels return **immediately**; the kernel is still being executed on the device when `stop_watch(t0)` is called. We are **not** timing the kernel execution time, but the time it takes to dispatch the kernel to the GPU.
- Correct this by adding `cudaDeviceSynchronize();` after the CUDA kernel, which blocks until all running CUDA kernels are complete:

```
double t0 = stop_watch(0);
gpu_axpy<<<1, 1>>>(n, a, d_x, d_y);
cudaDeviceSynchronize();
t0 = stop_watch(t0);
```

CUDA Example

- Compile and run again:

```
[user@front02 ex01]$ nvcc -arch sm_70 -O3 -Xcompiler -fopenmp -o axpy axpy.cu
[user@front02 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A da23 --gres=gpu:1 --reservation=data-analytics ..
CPU: nthr = 20 t0 = 0.0088 sec P = 15.199 Gflop/s B = 91.193 GB/s
GPU: t0 = 3.9670 sec P = 0.034 Gflop/s B = 0.203 GB/s
Diff = 1.021564e-15
```

CUDA Example

- Compile and run again:

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[user@front02 ex01]$ nvcc -arch sm_70 -O3 -Xcompiler -fopenmp -o axpy axpy.cu
[user@front02 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A da23 --gres=gpu:1 --reservation=data-analytics .,
CPU: nthr = 20 t0 = 0.0088 sec P = 15.199 Gflop/s B = 91.193 GB/s
GPU: t0 = 3.9670 sec P = 0.034 Gflop/s B = 0.203 GB/s
Diff = 1.021564e-15
```

- This performance is of course extremely poor;

CUDA Example

- Compile and run again:

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GPU: t0 = 3.9670 sec P = 0.034 Gflop/s B = 0.203 GB/s
Diff = 1.021564e-15
```

- This performance is of course extremely poor;
- We're using only one GPU thread in the kernel

CUDA Example

Use more threads

- In this step, we will use 512 GPU threads. First, change the call to the GPU kernel:

```
double t0 = stop_watch(0);
gpu_axpy<<<1, 512>>>(n, a, d_x, d_y);
cudaDeviceSynchronize();
t0 = stop_watch(t0);
```

CUDA Example

Use more threads

- In this step, we will use 512 GPU threads. First, change the call to the GPU kernel:

```
double t0 = stop_watch(0);
gpu_axpy<<<1, 512>>>(n, a, d_x, d_y);
cudaDeviceSynchronize();
t0 = stop_watch(t0);
```

- Then we need to change the kernel. We need in each GPU thread to calculate which elements it will operate on:

```
/**
 * Do y <- a*x + y on the GPU
 */
__global__ void
gpu_axpy(int n, float a, float *x, float *y)
{
    int ithr = threadIdx.x;
    int nthr = blockDim.x;
    int lt = n/nthr;
    for(int i=ithr*lt; i<(ithr+1)*lt; i++)
        y[i] = a*x[i] + y[i];
    return;
}
```

- With the above, each thread operated on $n/nthr$ contiguous elements

CUDA Example

- Compile and run again:

```
[user@front02 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A da23 --gres=gpu:1 --reservation=data-analytics .,
CPU: nthr =     8    t0 = 0.0064 sec    P =   2.628 Gflop/s    B =  15.765 GB/s
GPU:                 t0 = 0.1316 sec    P =   0.127 Gflop/s    B =   0.765 GB/s
Diff = 1.022961e-15
```

- Better than before, but still very poor performance. Can we do better?

CUDA Example

Optimized GPU memory access

Always keep in mind that on GPUs, it is more optimal if contiguous threads access contiguous memory locations

```
arr[]  
in global GPU  
memory  
  
arr[ 0] → threadIdx.x = 0, 1st iter.  
arr[ 1] → threadIdx.x = 0, 2nd iter.  
arr[ 2] → threadIdx.x = 0, 3rd iter.  
...  
arr[k-1] → threadIdx.x = 0, kth iter.  
arr[ k] → threadIdx.x = 1, 1st iter.  
arr[k+1] → threadIdx.x = 1, 2nd iter.  
...  
...
```

This represents the order by which elements are accessed currently

- The same thread accesses continuous elements
- Very common approach on CPUs
- On GPUs, this results in so-called *bank conflicts*
- *Suboptimal!*

CUDA Example

Optimized GPU memory access

Always keep in mind that on GPUs, it is more optimal if contiguous threads access contiguous memory locations

```
arr[]  
in global GPU  
memory  
  
arr[ 0] -> threadIdx.x = 0, 1st iter.  
arr[ 1] -> threadIdx.x = 1, 1st iter.  
arr[ 2] -> threadIdx.x = 2, 1st iter.  
...  
arr[k-1] -> threadIdx.x = k-1, 1st iter.  
arr[ k] -> threadIdx.x = 0, 2nd iter.  
arr[k+1] -> threadIdx.x = 1, 2nd iter.  
...
```

This represents an optimal data access pattern

- Different threads accesses continuous elements
- Each thread is served by a different memory bank

CUDA Example

Optimized GPU memory access

Always keep in mind that on GPUs, it is more optimal if contiguous threads access contiguous memory locations

In our example:

```
/***
 * Do y <- a*x + y on the GPU
 ***/
__global__ void
gpu_axpy(int n, float a, float *x, float *y)
{
    int ithr = threadIdx.x;
    int nthr = blockDim.x;
    for(int i=0; i<n; i+=nthr)
        y[i+ithr] = a*x[i+ithr] + y[i+ithr];
    return;
}
```

- Compile and run:

```
[user@front02 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A da23 --gres=gpu:1 --reservation=data-analytics
CPU: nthr = 20 t0 = 0.0097 sec P = 13.788 Gflop/s B = 82.730 GB/s
GPU:          t0 = 0.0665 sec P = 2.018 Gflop/s B = 12.111 GB/s
Diff = 1.021564e-15
```

CUDA Example

Blocks and threads

Now let's use blocks. Let's use as many blocks and threads as we can

- Upper limit of 1024 threads
- Upper limit of $2^{31} - 1$ blocks

```
double t0 = stop_watch(0);
int nthr = 1024;
gpu_axpy<<<n/nthr, nthr>>>(n, a, d_x, d_y);
cudaDeviceSynchronize();
t0 = stop_watch(t0);
```

```
/**
 * Do y <- a*x + y on the GPU
 */
__global__ void
gpu_axpy(int n, float a, float *x, float *y)
{
    int ithr = threadIdx.x;
    int nthr = blockDim.x;
    int iblk = blockIdx.x;
    int idx = ithr + iblk*nthr;
    y[idx] = a*x[idx] + y[idx];
    return;
}
```

CUDA Example

Blocks and threads

- Compile and run:

```
[user@front02 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A da23 --gres=gpu:1 --reservation=data-analytics .  
CPU: nthr = 20    t0 = 0.0088 sec    P = 15.188 Gflop/s    B = 91.129 GB/s  
GPU:           t0 = 0.0011 sec    P = 119.930 Gflop/s    B = 719.578 GB/s  
Diff = 1.021564e-15
```

- ~720 GB/s is ~80% of peak bandwidth (which is 900 GB/s)

CUDA Example

Blocks and threads

- Compile and run:

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[user@front02 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A da23 --gres=gpu:1 --reservation=data-analytics .  
CPU: nthr = 20    t0 = 0.0088 sec    P = 15.188 Gflop/s    B = 91.129 GB/s  
GPU:           t0 = 0.0011 sec    P = 119.930 Gflop/s    B = 719.578 GB/s  
Diff = 1.021564e-15
```

- ~720 GB/s is ~80% of peak bandwidth (which is 900 GB/s)
- Try varying the number of threads per block. E.g. with 512 threads I got ~730 GB/s.

CUDA, another example

Exercise: rotate and shift an array of (x, y) coordinates

- `ex02/rot.cu` calls, as before, the same kernel twice
- Operation is $\vec{v}_i = U\vec{r}_i + \vec{s}_i$
- Where:

$$U = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$$

CUDA, another example

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- `ex02/rot.cu` calls, as before, the same kernel twice
- Operation is $\vec{v}_i = U\vec{r}_i + \vec{s}_i$
- Where:

$$U = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$$

- Equivalently:

$$v_{i,x} = \cos(\theta)r_{i,x} - \sin(\theta)r_{i,y} + s_{i,x}$$

$$v_{i,y} = \sin(\theta)r_{i,x} + \cos(\theta)r_{i,y} + s_{i,y}$$

Coordinate transformation using CUDA

- $\vec{v}_i = U\vec{r}_i + \vec{s}_i \Rightarrow$

$$v_{i,x} = \cos(\theta)r_{i,x} - \sin(\theta)r_{i,y} + s_{i,x}$$

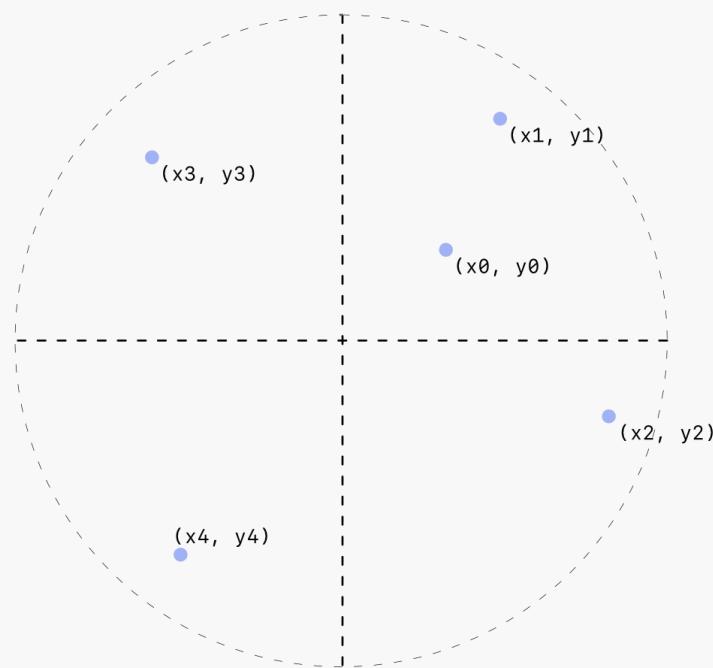
$$v_{i,y} = \sin(\theta)r_{i,x} + \cos(\theta)r_{i,y} + s_{i,y}$$

Coordinate transformation using CUDA

- $\vec{v}_i = U\vec{r}_i + \vec{s}_i \Rightarrow$

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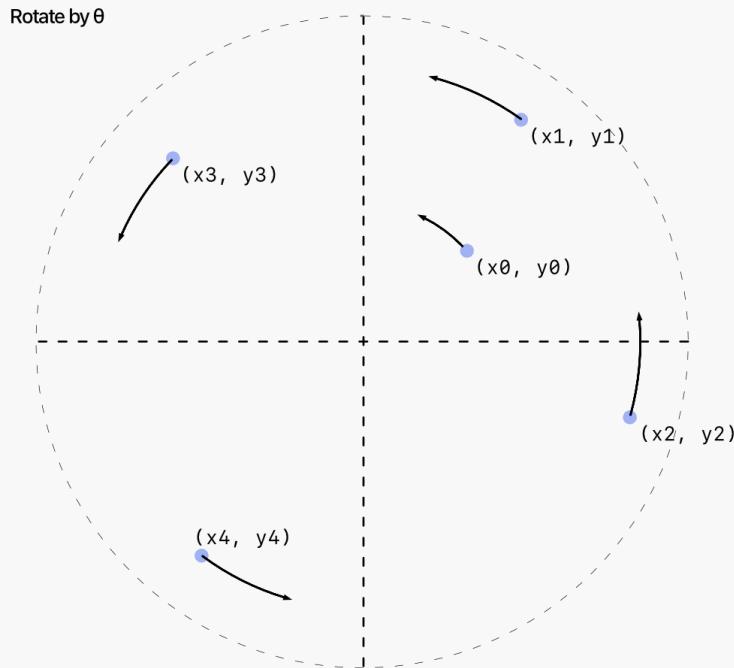


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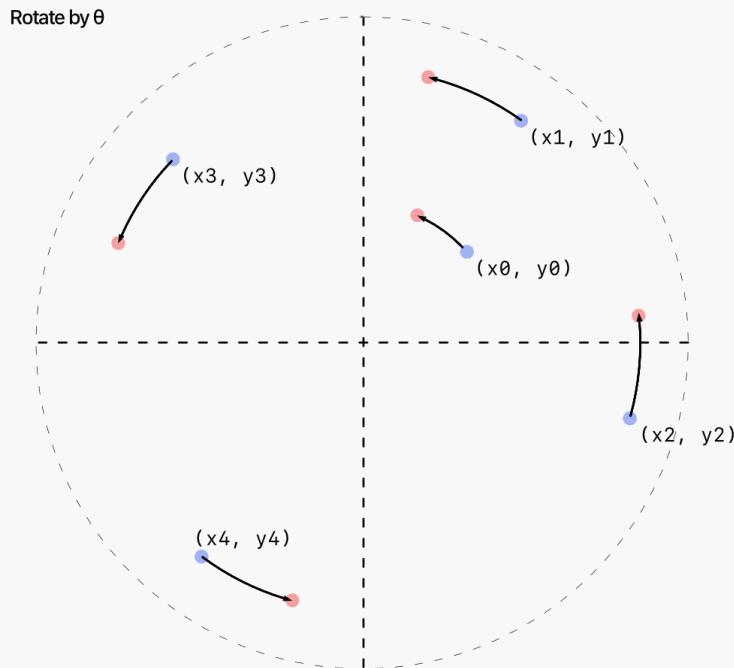


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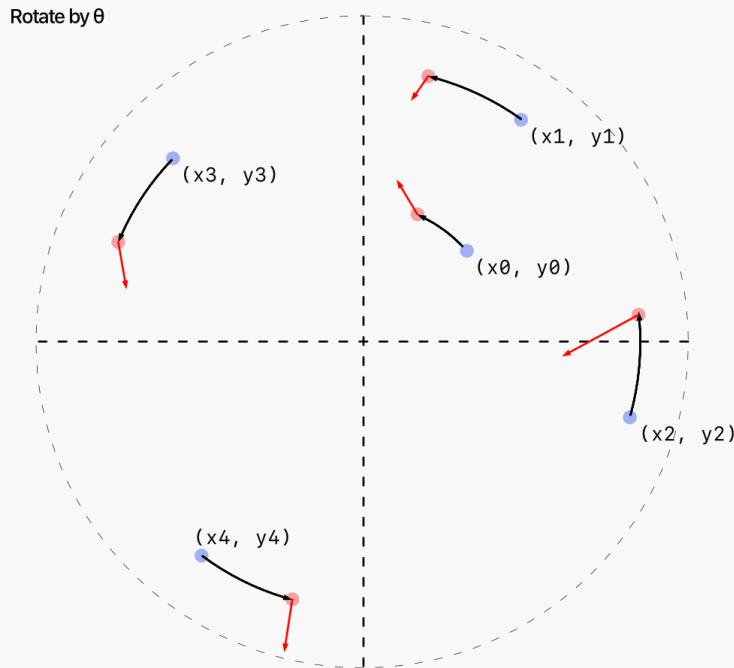


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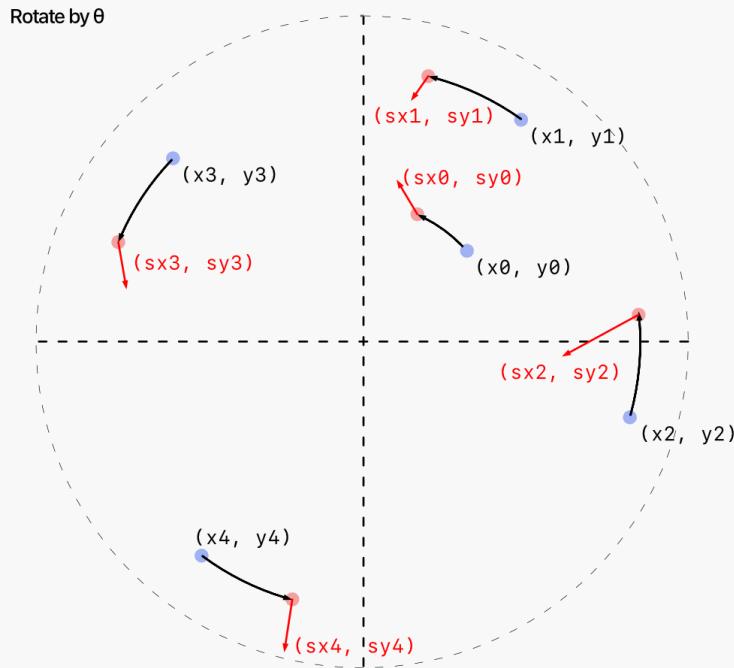


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- $\vec{v}_i = U\vec{r}_i + \vec{s}_i \Rightarrow$

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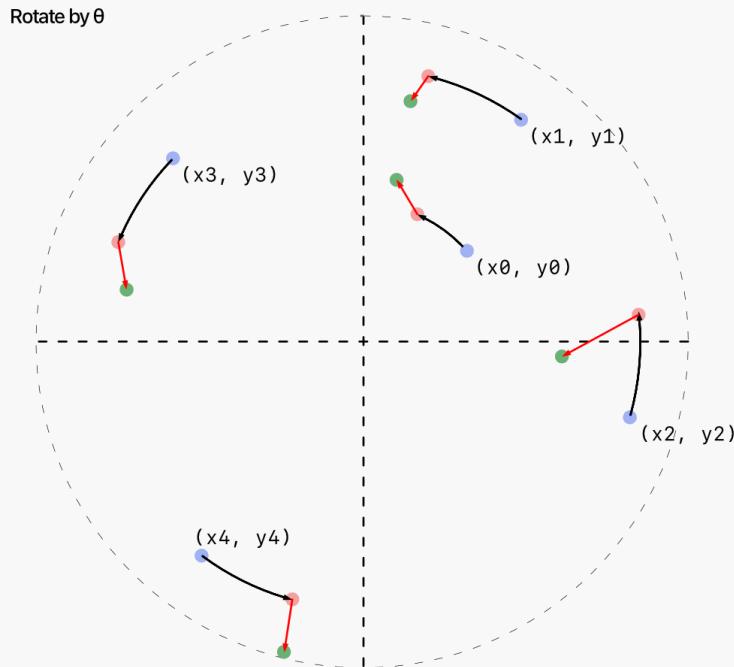


Coordinate transformation using CUDA

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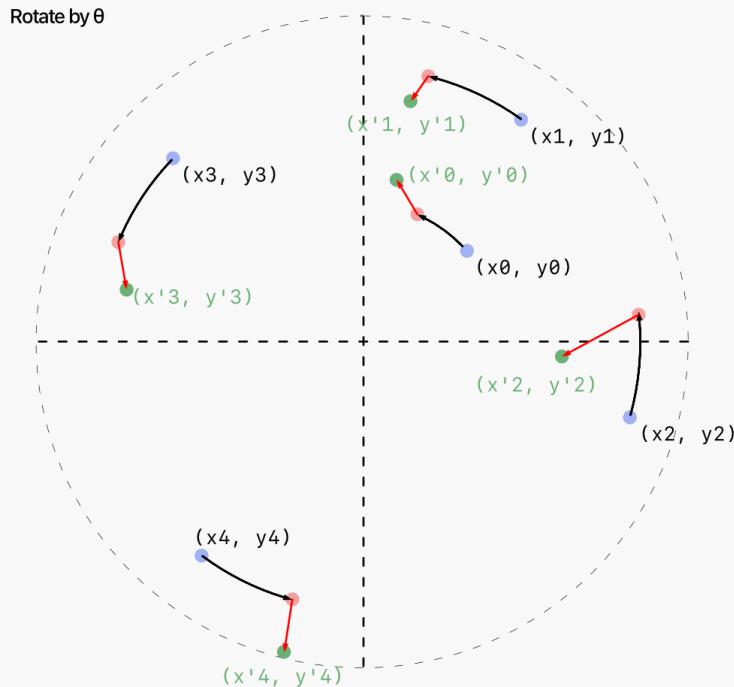


Coordinate transformation using CUDA

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Coordinate transformation using CUDA

TODO, for a first version

- Implement a CUDA version for the second call
- Each GPU thread operating on one point (i)
- Pass number of GPU threads to use as command line argument, i.e. using `argv []`

Coordinate transformation using CUDA

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- Implement a CUDA version for the second call
- Each GPU thread operating on one point (i)
- Pass number of GPU threads to use as command line argument, i.e. using `argv []`

Example:

```
[user@front02 ex02] export OMP_PROC_BIND="close"
[user@front02 ex02] export OMP_PLACES="cores"
[user@front02 ex02] export OMP_NUM_THREADS=20
[user@front02 ex02] srun -n 1 --cpus-per-task=20 -p gpu -A da23 --gres=gpu:1 --reservation=data-analytics ./ex02
CPU: nthr = 20 t0 = 0.0610 sec P = 17.608 Gflop/s B = 52.823 GB/s
GPU: nthr = 32 t0 = 0.0069 sec P = 155.683 Gflop/s B = 467.049 GB/s
Diff = 1.115821e-15
```

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Diff = 1.115821e-15
```

```
/*
 * Do r <- U*r on the GPU using CUDA
 */
__global__ void
gpu_rotate(int n, coords *r_out, float theta, coords *r_in, coorsd *s)
{
    float ct = cos(theta);
    float st = sin(theta);

    int ithr = threadIdx.x;
    int nthr = blockDim.x;
    int iblk = blockIdx.x;
    int idx = (ithr + iblk*nthr);

    r_out[idx].x = ct*r_in[idx].x - st*r_in[idx].y + s[idx].x;
    r_out[idx].y = st*r_in[idx].x + ct*r_in[idx].y + s[idx].y;

    return;
}
```

Coordinate transformation using CUDA

The optimal number of threads is not necessarily the maximum

- If we allow the number of threads to be a command line argument, we can easily scan for it

```
[user@font01 ex02]$ for((th=4; th<=1024; th*=2))
> do
> srun -n 1 --cpus-per-task=20 -p gpu -A da23 --gres=gpu:1 --reservation=data-analytics ./rot $th $((1024*1024))
> done 2>&1|grep GPU
GPU: nthr =    4    t0 = 0.0514 sec    P =  20.902 Gflop/s    B =  62.707 GB/s
GPU: nthr =    8    t0 = 0.0266 sec    P =  40.389 Gflop/s    B = 121.168 GB/s
GPU: nthr =   16    t0 = 0.0134 sec    P =  80.393 Gflop/s    B = 241.178 GB/s
GPU: nthr =   32    t0 = 0.0067 sec    P = 159.498 Gflop/s    B = 478.495 GB/s
GPU: nthr =   64    t0 = 0.0049 sec    P = 220.171 Gflop/s    B = 660.513 GB/s
GPU: nthr =  128    t0 = 0.0049 sec    P = 217.839 Gflop/s    B = 653.516 GB/s
GPU: nthr =  256    t0 = 0.0049 sec    P = 219.217 Gflop/s    B = 657.652 GB/s
GPU: nthr =  512    t0 = 0.0048 sec    P = 222.818 Gflop/s    B = 668.454 GB/s
GPU: nthr = 1024    t0 = 0.0048 sec    P = 221.852 Gflop/s    B = 665.557 GB/s
```

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```

- Tops at ~670 GBytes/s or ~75%. Can we do better?

Coordinate transformation using CUDA

Optimizations

- Note the loading of elements of `r[]` from global memory \Rightarrow two continuous component per thread
- Optimization opportunity: use one thread per *component*

Coordinate transformation using CUDA

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Coordinate transformation using CUDA

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- Optimization opportunity: use one thread per *component*
 - \Rightarrow Instead of each thread operating on one point, consider each thread operating on a single component of the coordinate
- In other words, have:
 - even threads computing the `x` coordinate part of `v[:]`
 - odd threads computing the `y` coordinate of `v[:]`

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- Shared memory is declared with the `shared` attribute, i.e.:

```
__shared__ float arr[SIZE];
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__shared__ float arr[SIZE];
```

- Note that here `SIZE` **must** be known at **compile time**
- Alternatively, we can have dynamic allocation of shared memory (relatively recent CUDA feature)

Coordinate transformation using CUDA

Optimizations

- Below is how we would like to organize this calculation:

```
i2=2*i
(x coord. of elem. i + 0) thread = 0; v[i2+0] = r[i2+0]*ct - r[i2+1]*st + s[i2+0]
(y coord. of elem. i + 0) thread = 1; v[i2+1] = r[i2+1]*ct + r[i2+0]*st + s[i2+1]
(x coord. of elem. i + 1) thread = 2; v[i2+2] = r[i2+2]*ct - r[i2+3]*st + s[i2+2]
(y coord. of elem. i + 1) thread = 3; v[i2+3] = r[i2+3]*ct + r[i2+2]*st + s[i2+3]
(x coord. of elem. i + 2) thread = 4; v[i2+4] = r[i2+4]*ct - r[i2+5]*st + s[i2+4]
(y coord. of elem. i + 2) thread = 5; v[i2+5] = r[i2+5]*ct + r[i2+4]*st + s[i2+5]
(x coord. of elem. i + 3) thread = 6; v[i2+6] = r[i2+6]*ct - r[i2+7]*st + s[i2+6]
(y coord. of elem. i + 3) thread = 7; v[i2+7] = r[i2+7]*ct + r[i2+6]*st + s[i2+7]
...
...
```

- Notice that odd threads and even threads carry out different operations
- But on a GPU, it is important for performance to have all threads in a kernel execute the **same** operations
- In other words, try to avoid as much as possible constructs like:

```
if(ithr % 2 == 0){ ... };
```

Coordinate transformation using CUDA

Optimizations

- First define a macro at the beginning of the file:

```
#define MAX_THR 1024
```

- Then, when invoking the kernel, change the call to use twice the number of blocks:

```
gpu_rotate<<<2*n/n_gpu_thr, n_gpu_thr>>>(n, d_v, theta, d_r, d_s);
```

Coordinate transformation using CUDA

Optimizations

- In the kernel, declare a shared array, to be used to store the elements of `r[]`:

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```

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- By reading `r[]` into `rr[]` once, we avoid each thread having to read elements of `r[]` twice from global memory, which is slow

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- Read the elements of `r[]` corresponding to this block into `rr[]`:

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int idx = iblk*nthr + ithr;
rr[ithr] = r[idx];
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This way, the loading is done parallel: each thread reads in one component of `r[]`

Coordinate transformation using CUDA

Optimizations

- Now insert the following, which only achieves the operation partially:

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float rs = s[idx] + ct*rr[ithr];
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- The operation is still incomplete; what we have achieved with the above is:

$$v_x \leftarrow \cos(\theta)r_x + s_x$$

$$v_y \leftarrow \cos(\theta)r_y + s_y$$

Coordinate transformation using CUDA

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we are missing:

$$v_x \leftarrow v_x - \sin(\theta)r_y$$

$$v_y \leftarrow v_y + \sin(\theta)r_x$$

Coordinate transformation using CUDA

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- Consider the following:

```
int sw = 1 - 2*(ithr & 1);
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Coordinate transformation using CUDA

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- `&` is a bitwise "and" operation, meaning `ithr & 1` will evaluate to:
 - 0 if `ithr` is even
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 - `0` if `ithr` is even
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`sw = 1 - 2*(ithr & 1)` therefore yields:

```
ithr = 0, 1, 2, 3, ...
sw   = 1, -1, 1, -1, ...
```

Coordinate transformation using CUDA

Optimizations

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$$v_x \leftarrow v_x - \sin(\theta)r_y$$

$$v_y \leftarrow v_y + \sin(\theta)r_x$$

- Consider:

```
rs = rs - sw*st*rr[ithr+sw];
```

Coordinate transformation using CUDA

Optimizations

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$$v_x \leftarrow v_x - \sin(\theta)r_y$$

$$v_y \leftarrow v_y + \sin(\theta)r_x$$

- Consider:

```
rs = rs - sw*st*rr[iTHR+sw];
```

- Then read back into `out[]`:

```
out[idx] = rs;
```

