GPU programming using CUDA

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HPC 2^{nd} Intermediate Training Event, 21^{st} June 2022

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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:

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- Memory coalescing on GPUs
- Shared memory
- What is a warp and should you care

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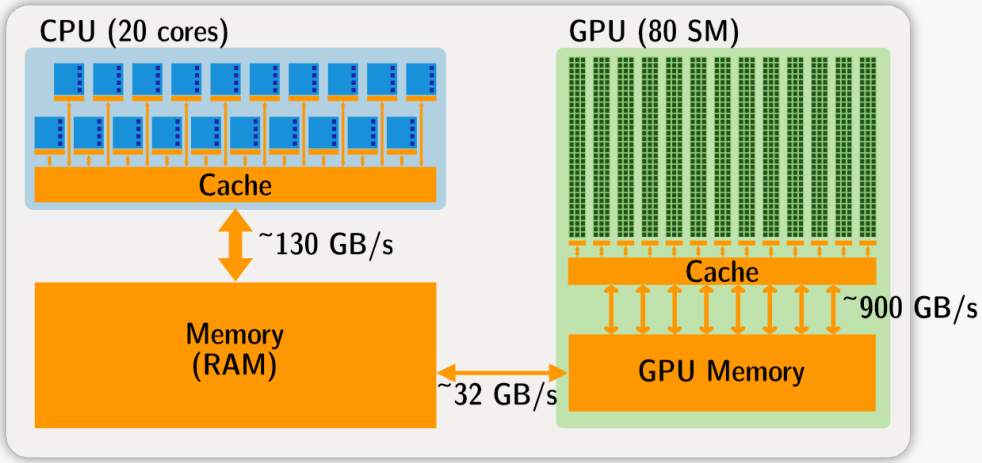
Repo with slides and exercises:

https://github.com/CaSToRC-CyI/NCC-Intermediate-Training-2022

under `Day1/.`

GPU architecture

At a very high level:



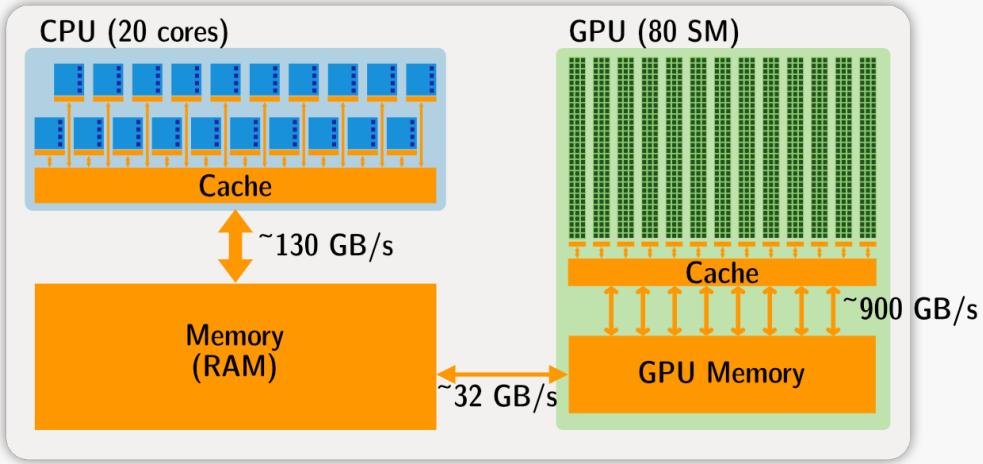
CPU

- 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

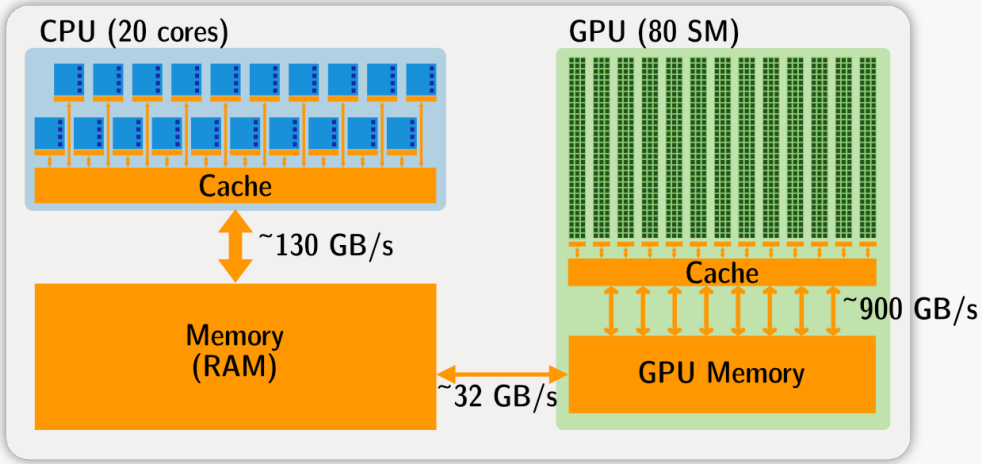


Some numbers from the GPU partition of our Cyclone cluster

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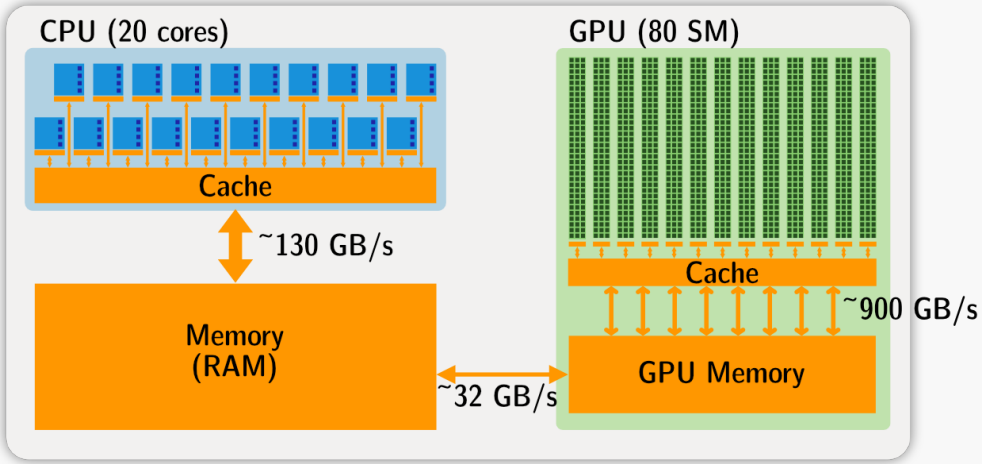
We will come back to these numbers during the hands-on

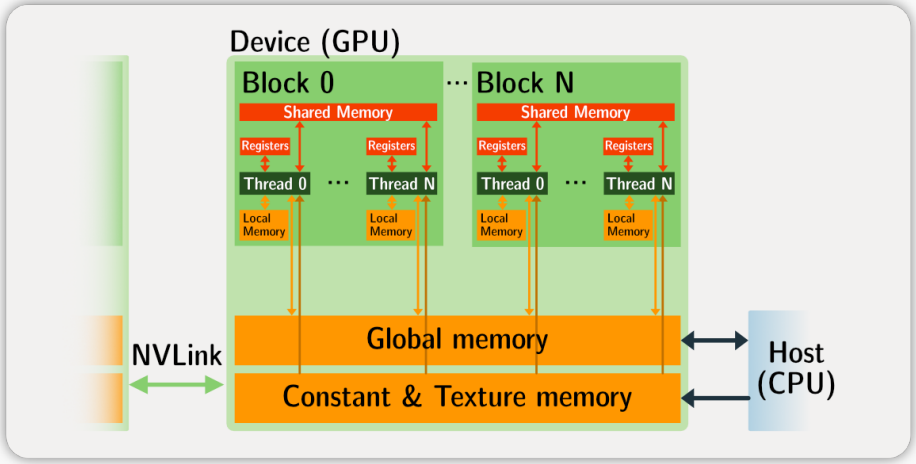
GPU programming model



"Offload" model of programming

- CPU starts program (runs `main()`)
- CPU copies data to GPU memory (over e.g. PCIe, ~32 GB/s)
- CPU dispatches "kernels" for execution on GPU
  - Kernels read/write to GPU memory (~900 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, ~32 GB/s)

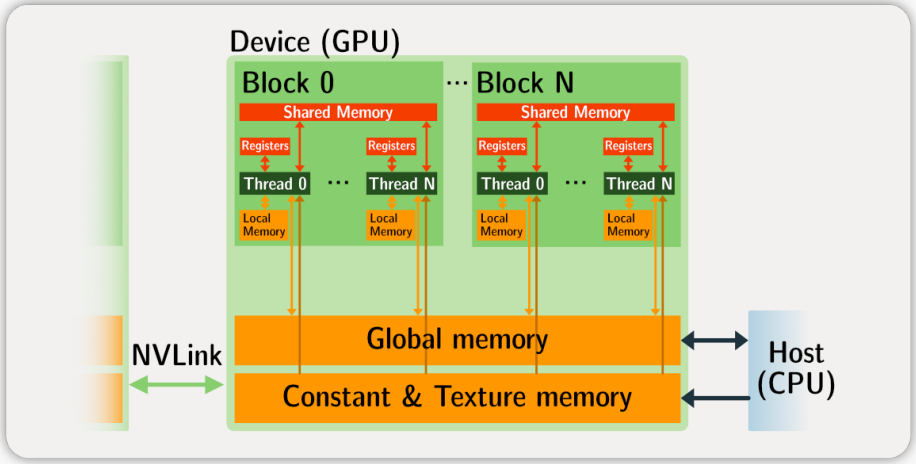
GPU programming model



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

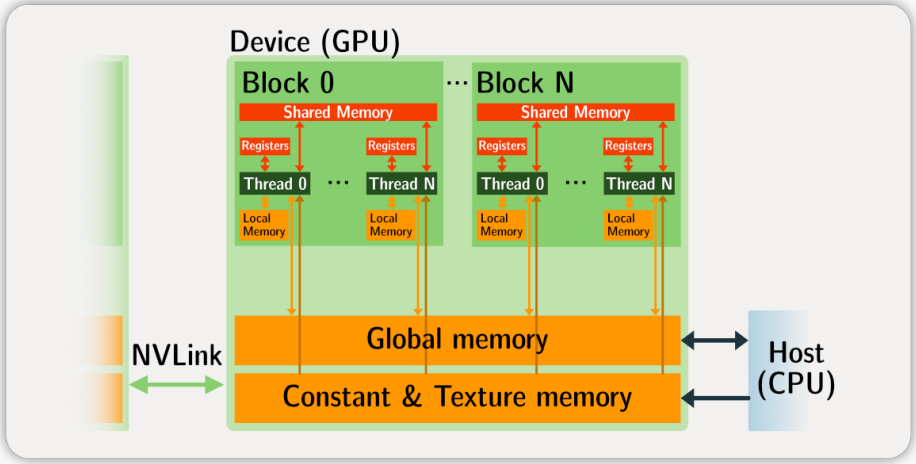
GPU programming model



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<<<nblck, nthr>>>(n, a, x);
  ```

- `nthr`: number of threads per block; can be scalar or a `dim3` type
- `nblck`: 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) */
  ```

CUDA programming basics

Call a CUDA kernel

- Call from host. Example:

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```

Thread coordinates within kernel

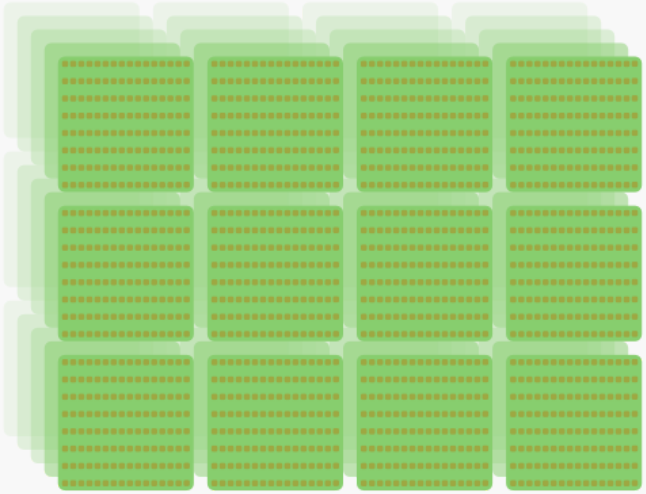
Example:

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

CUDA programming basics

Threads, blocks, grids

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



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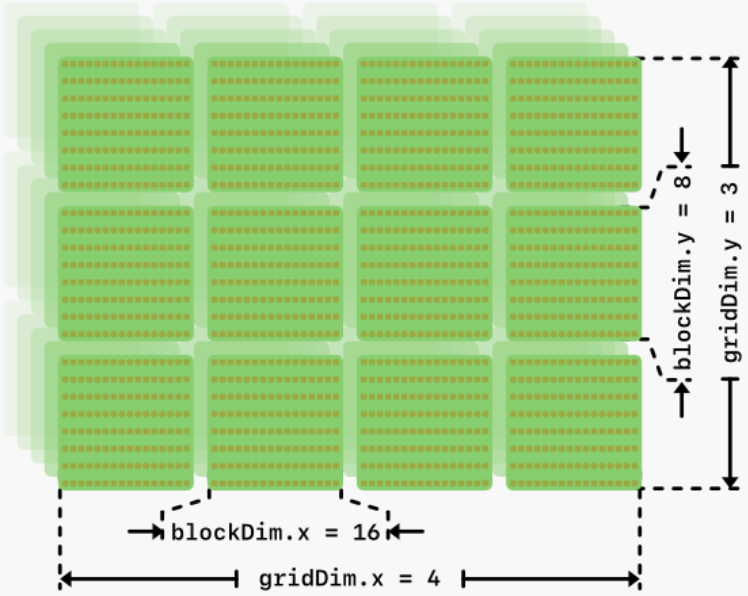

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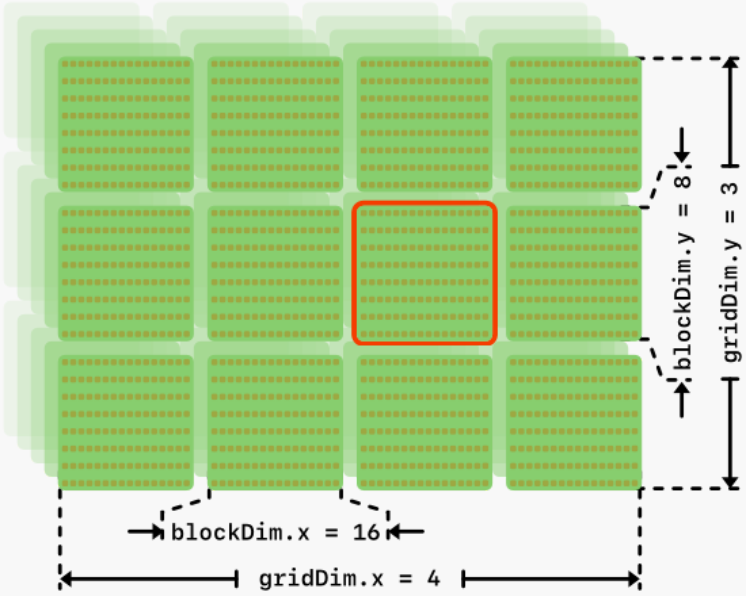

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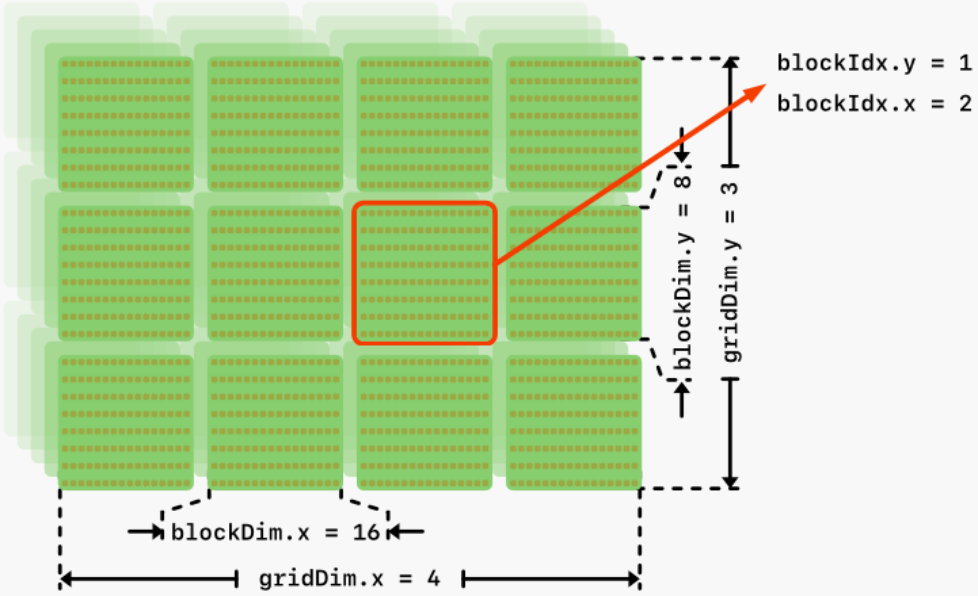

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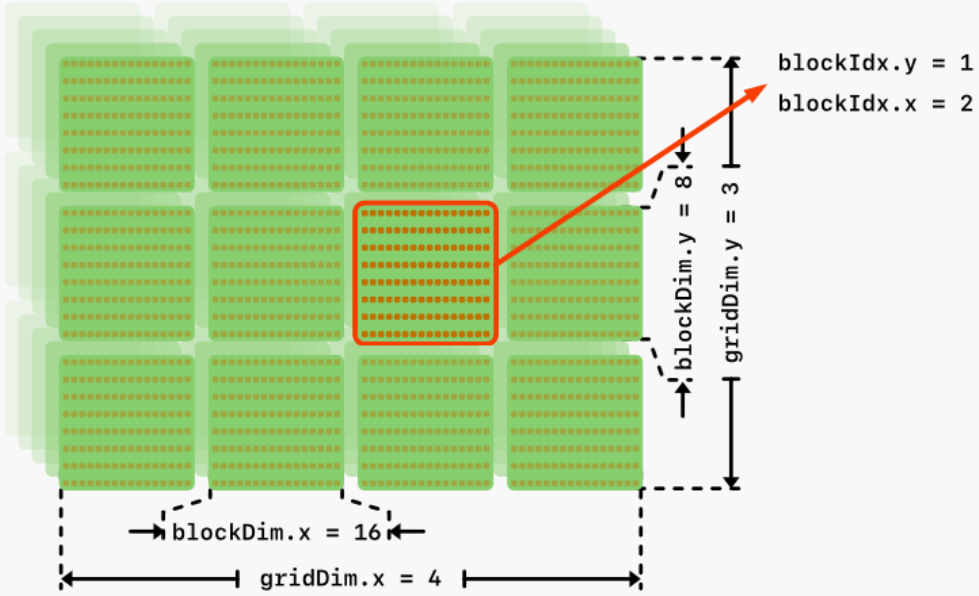

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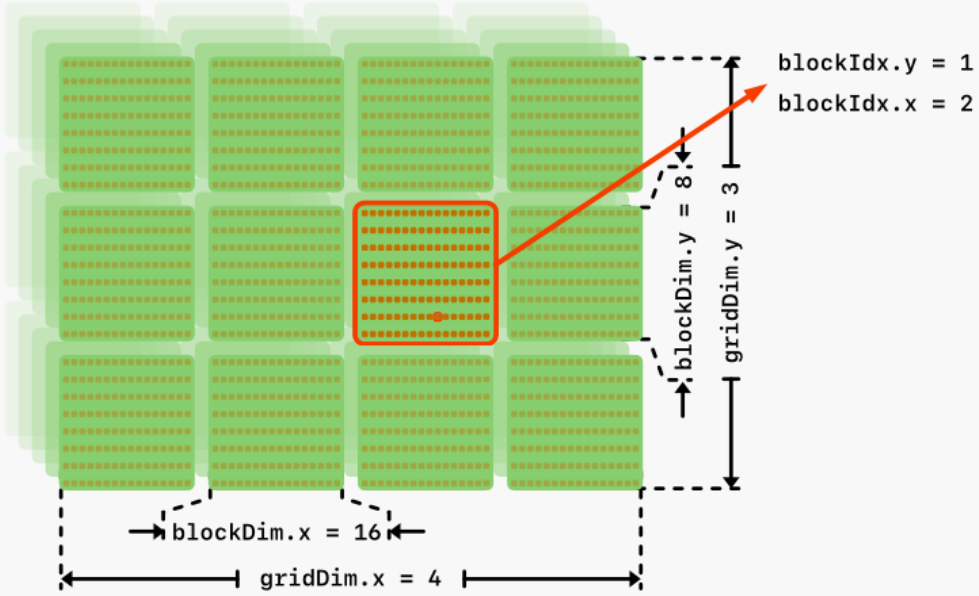

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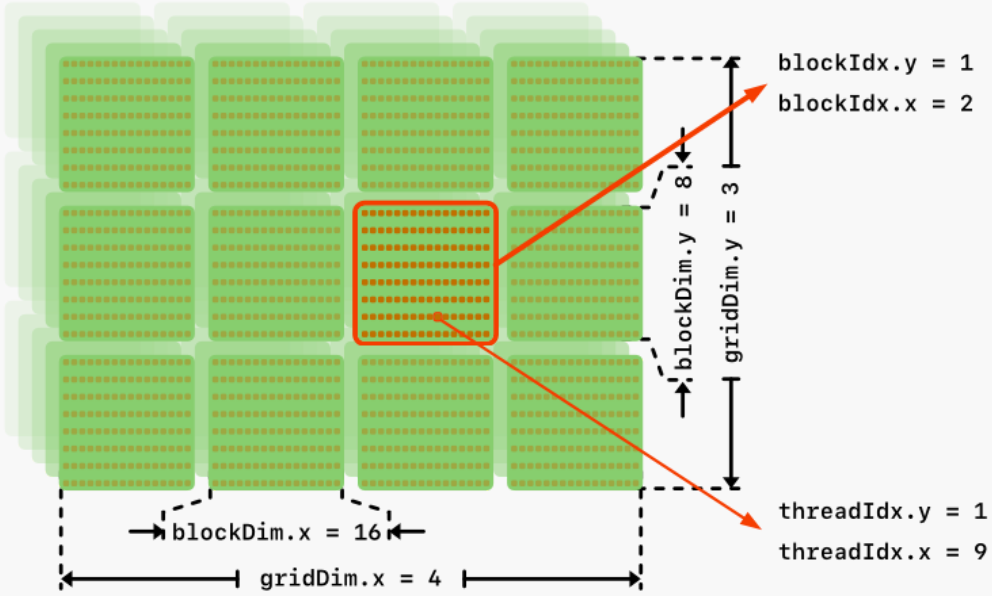

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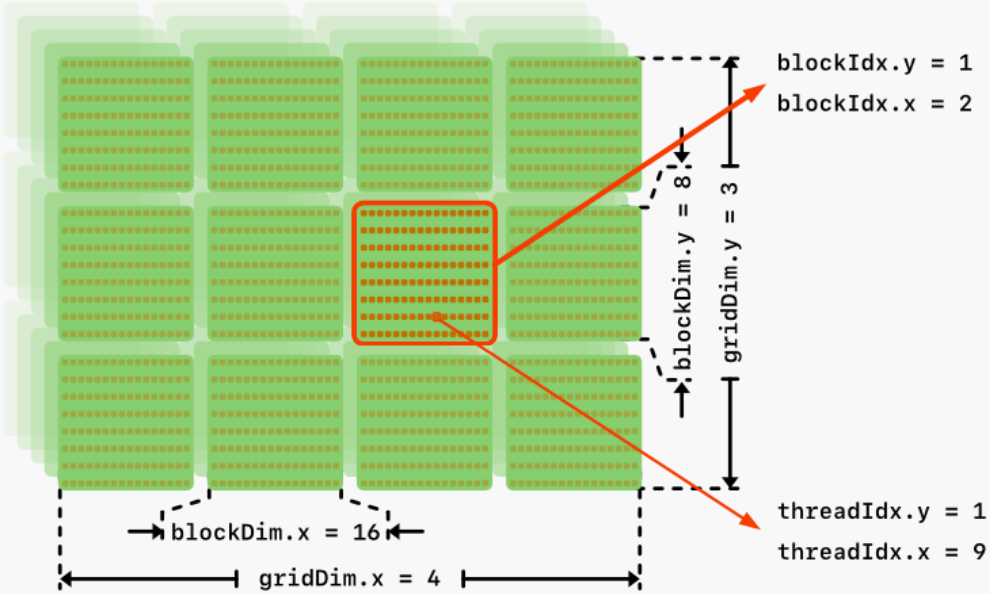

Variables available within kernel

- `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: `/onyx/data/edu16/day1/`

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

$$y_i \leftarrow a \cdot x_i + y_i, \;\; i = 0, \ldots, n-1$$

  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 timing for part `A` and for `B`
  - 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:

```
[userfront01 ~]$ cp -r /onyx/data/edu16/day1/ex01 .
[userfront01 ~]$ cd ex01/
[userfront01 ex01]$ ls -1
axpy.cu
```

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axpy.cu
```

- Compile with `nvcc` including OpenMP:

```
[userfront01 ex01]$ module load gompic
[userfront01 ex01]$ nvcc -O3 -Xcompiler -fopenmp -o axpy axpy.cu
```

- `-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.:

```
[userfront01 ex01] export OMP_PROC_BIND="close"
[userfront01 ex01] export OMP_PLACES="cores"
[userfront01 ex01] export OMP_NUM_THREADS=20
[userfront01 ex01] srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./axpy $((1024*1024*64))
 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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- Copy first exercise from this training's shared space:

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 Diff = 0.000000e+00
```

- 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 `ualloc()` that allocates memory on the GPU and checks whether an error occured
- 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@front01 ex01]$ nvcc -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@front01 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./axpy $((1024*1024*64))
 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@front01 ex01]$ nvcc -O3 -Xcompiler -fopenmp -o axpy axpy.cu
[user@front01 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./axpy $((1024*1024*64))
 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:

```
[user@front01 ex01]$ nvcc -O3 -Xcompiler -fopenmp -o axpy axpy.cu
[user@front01 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./axpy $((1024*1024*64))
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 Diff = 1.021564e-15
```

- This performance is of course extremely poor;

CUDA Example

- Compile and run again:

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[user@front01 ex01]$ nvcc -O3 -Xcompiler -fopenmp -o axpy axpy.cu
[user@front01 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./axpy $((1024*1024*64))
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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:

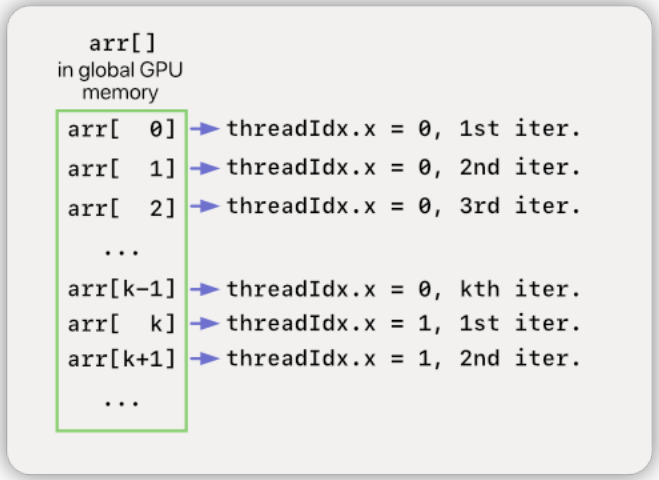
```
[user@front01 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./axpy $((1024*1024*64))
 CPU: nthr =    8   t0 = 0.0064 sec   P =   2.628 Gflop/s   B =  15.765 GB/s
 GPU:               t0 = 0.1316 sec   P =   0.127 Gflop/s   B =   0.765 GB/s
 Diff = 1.022961e-15
```

- 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



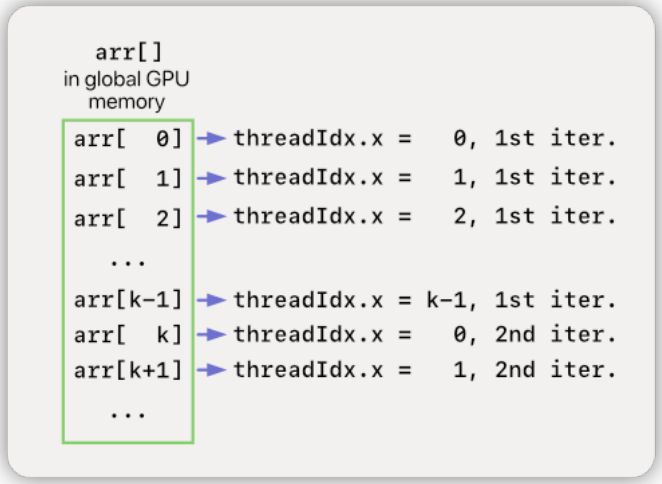
This represents the order by which elements are accessed currently

- 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



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@front01 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./axpy $((1024*1024*64))
 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@front01 ex01]$ srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./axpy $((1024*1024*64))
 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

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 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:

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

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- 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

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

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

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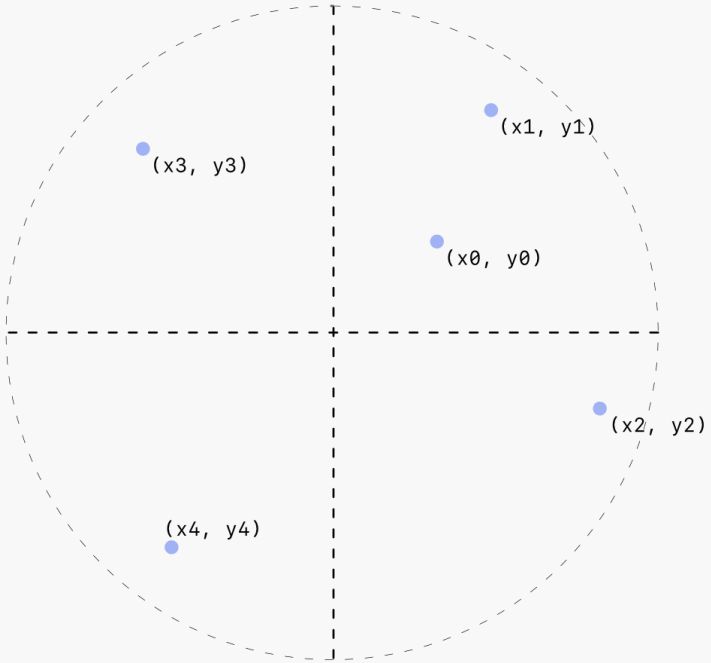

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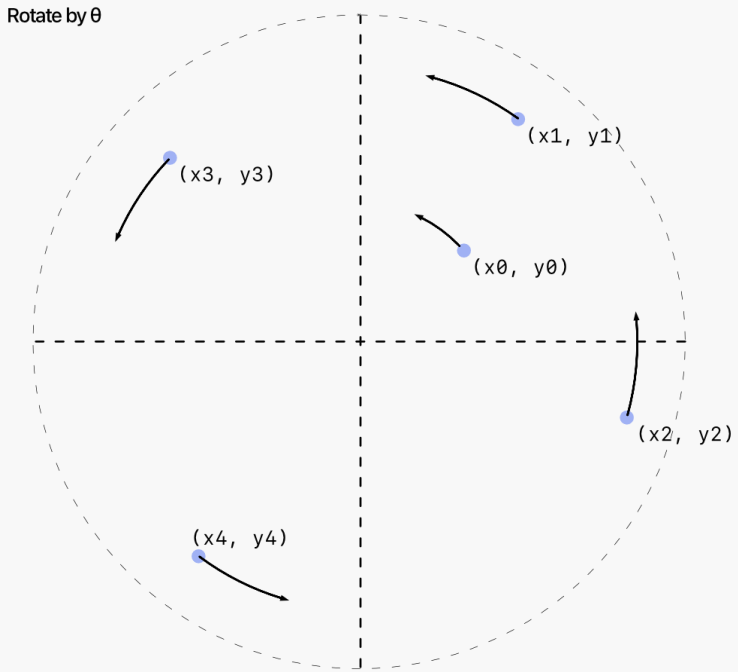

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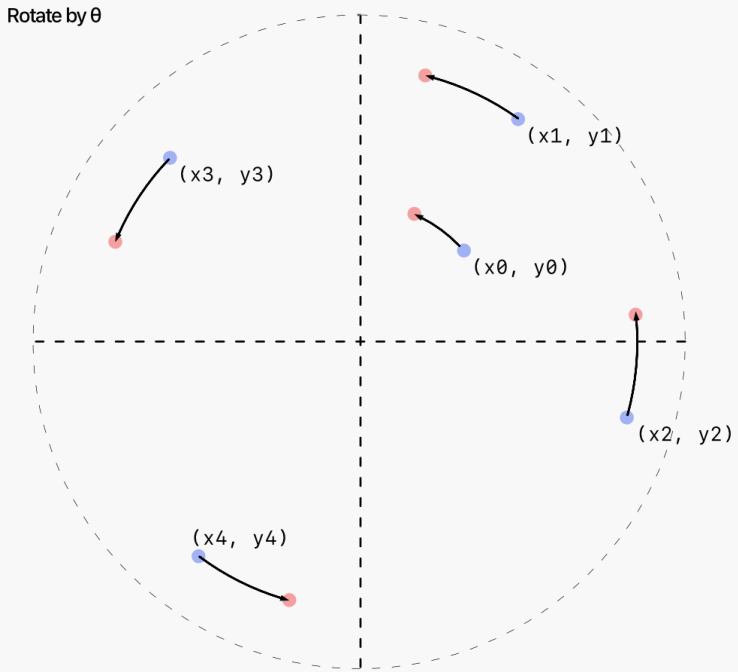

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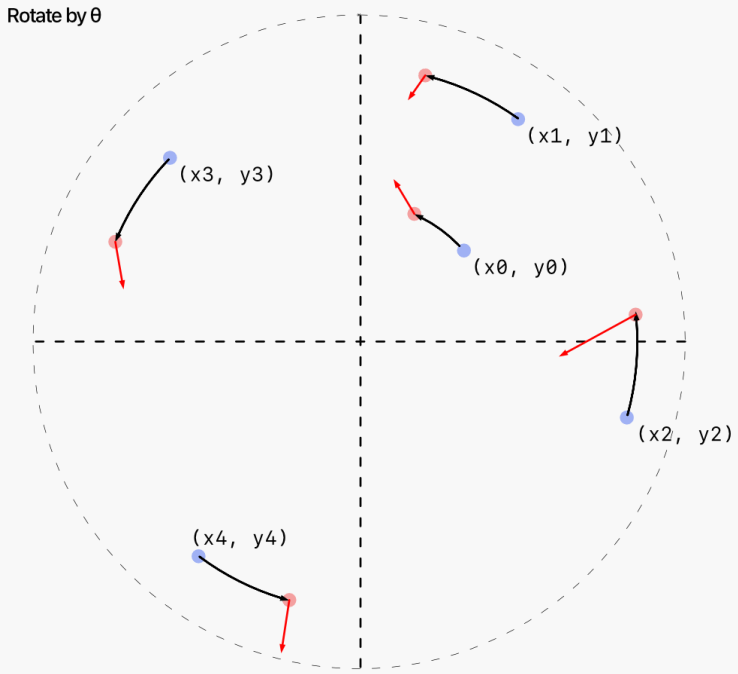

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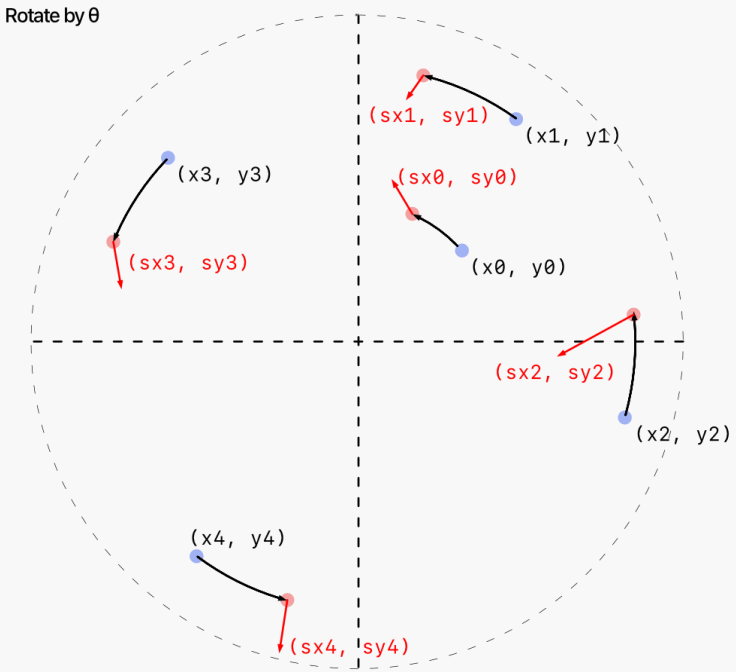

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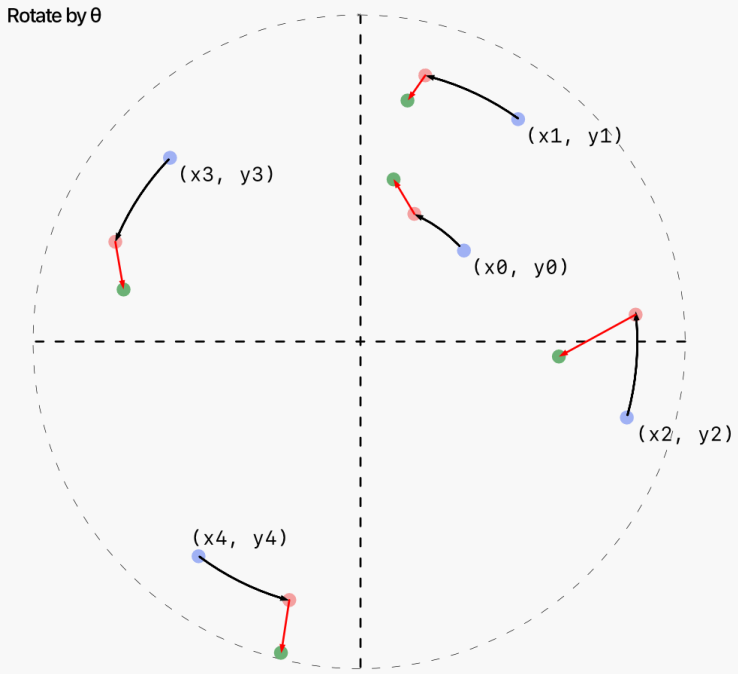

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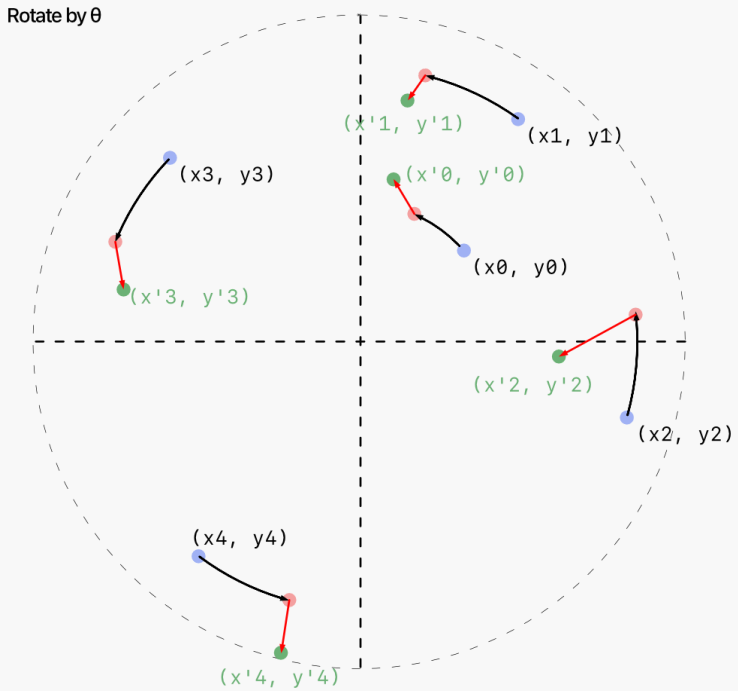

Coordinate transformation using CUDA

TODO, for a first version

- Implement a CUDA version for the second call
- Each GPU thread operating on one point (i)

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Example:

```
[userfront01 ex02] export OMP_PROC_BIND="close"
[userfront01 ex02] export OMP_PLACES="cores"
[userfront01 ex02] export OMP_NUM_THREADS=20
[userfront01 ex02] srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./rot 32 $((1024*1024*128))
 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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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 edu16 --gres=gpu:1 ./rot $th $((1024*1024*128))
> 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*

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- In other words, have:
  - even threads computing the `x` coordinate part of `v[:]`
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- 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[]`:

```
__shared__ float rr[MAX_THR];
```

Coordinate transformation using CUDA

Optimizations

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

```
__shared__ float rr[MAX_THR];
```

- We need a shared array for `r[]`, because different threads will need to access the same elements. In particular, whether odd or even, each thread needs to access both `x` and `y` components of `x[]`
- By reading `r[]` into `rr[]` once, we avoid each thread having to read elements of `r[]` twice from global memory, which is slow

Coordinate transformation using CUDA

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

```
int idx = iblk*nthr + ithr;
rr[ithr] = r[idx];
```

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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__shared__ float rr[MAX_THR];
```

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

```
int idx = iblk*nthr + ithr;
rr[ithr] = r[idx];
```

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:

```
float rs = s[idx] + ct*rr[ithr];
```

Coordinate transformation using CUDA

Optimizations

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

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

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

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

Optimizations

- We are missing:

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

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Coordinate transformation using CUDA

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- We are missing:

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

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- Consider the following:

```
int sw = 1 - 2*(ithr & 1);
```

Coordinate transformation using CUDA

Optimizations

- We are missing:

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

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

- Consider the following:

```
int sw = 1 - 2*(ithr & 1);
```

- `&` is a bitwise "and" operation, meaning `ithr & 1` will evaluate to:
- `0` if `ithr` is even
- `1` if `ithr` is odd

Coordinate transformation using CUDA

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int sw = 1 - 2*(ithr & 1);
```

- `&` is a bitwise "and" operation, meaning `ithr & 1` will evaluate to:
- `0` if `ithr` is even
- `1` if `ithr` is odd

`sw = 1 - 2*(ithr & 1)` therefore yields:

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

Coordinate transformation using CUDA

Optimizations

- 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

Optimizations

- We are missing:

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

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

- Consider:

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

Coordinate transformation using CUDA

Optimizations

- We are missing:

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

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

- Consider:

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

- Then read back into `out[]`:

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

Coordinate transformation using CUDA

Optimizations

- Compile and run, scanning the number of GPU threads (filtering only the GPU line):

```
[user@font01 ex02]$ for((th=4; th<=1024; th*=2))
> do
> srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./rot $th $((1024*1024*128))
> done 2>&1|grep GPU
 GPU: nthr =    4   t0 = 0.1060 sec   P =  10.127 Gflop/s   B =  30.382 GB/s
 GPU: nthr =    8   t0 = 0.0513 sec   P =  20.913 Gflop/s   B =  62.738 GB/s
 GPU: nthr =   16   t0 = 0.0260 sec   P =  41.291 Gflop/s   B = 123.874 GB/s
 GPU: nthr =   32   t0 = 0.0134 sec   P =  80.130 Gflop/s   B = 240.389 GB/s
 GPU: nthr =   64   t0 = 0.0069 sec   P = 155.592 Gflop/s   B = 466.775 GB/s
 GPU: nthr =  128   t0 = 0.0041 sec   P = 258.738 Gflop/s   B = 776.215 GB/s
 GPU: nthr =  256   t0 = 0.0041 sec   P = 260.806 Gflop/s   B = 782.418 GB/s
 GPU: nthr =  512   t0 = 0.0041 sec   P = 259.933 Gflop/s   B = 779.799 GB/s
 GPU: nthr = 1024   t0 = 0.0042 sec   P = 257.069 Gflop/s   B = 771.208 GB/s
```

Coordinate transformation using CUDA

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- Compile and run, scanning the number of GPU threads (filtering only the GPU line):

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```

- Maximum performance saturates with 128 - 1024 threads at ~780 GB/s, or 87% of peak bandwidth

Matrix-vector multiplication

We will look into another example, the matrix vector multiplication

$$y = Ax$$

where y, x are vectors (1-dimensional) and A is a matrix (2-dimensional)

- In the general case A is not square
- $A_{M \times N}, x_N, y_M$

Matrix-vector multiplication

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```
for(int i=0; i<m; i++) {
  y[i] = 0;
  for(int j=0; j<n; j++) {
    y[i] = y[i] + A[i][j] * x[j];
  }
}
```

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  }
}
```

```
for(int i=0; i<m; i++) {
  y[i] = 0;
  for(int j=0; j<n; j++) {
    y[i] += A[i*n + j] * x[j];
  }
}
```

Matrix-vector multiplication

Take `/onyx/data/edu16/day1/ex03/.` for the CPU code:

```
[user@front01 ~]$ cp -r /onyx/data/edu16/day1/ex03 .
[user@front01 ~]$ cd ex03/.
[user@front01 ex03]$ nvcc -O3 -Xcompiler -fopenmp -o matvec matvec.cu
[user@front01 ex03]$ export OMP_PLACES="cores"
[user@front01 ex03]$ export OMP_PROC_BIND="close"
[user@front01 ex03]$ export OMP_NUM_THREADS=20
[user@front01 ex03]$ srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./matvec 4096 8192
 CPU: nthr =   20   t0 = 0.0029 sec   P =  23.253 Gflop/s   B =  46.523 GB/s
 CPU: nthr =   20   t0 = 0.0022 sec   P =  30.341 Gflop/s   B =  60.705 GB/s
```

Matrix-vector multiplication

Our task is to modify the second call of the `Ax()` function to run on the GPU.

Matrix-vector multiplication

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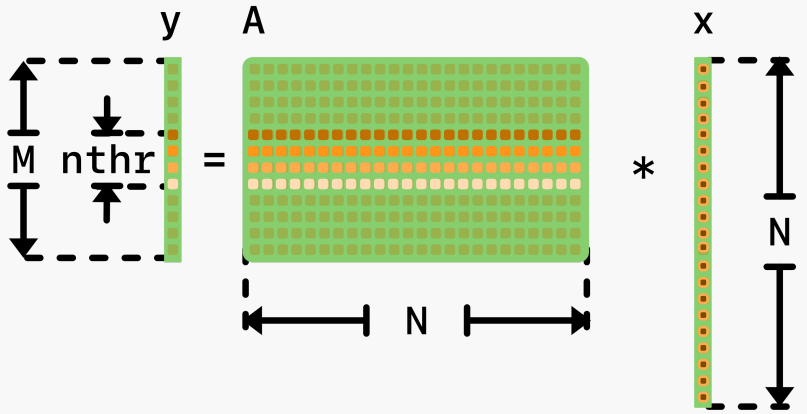

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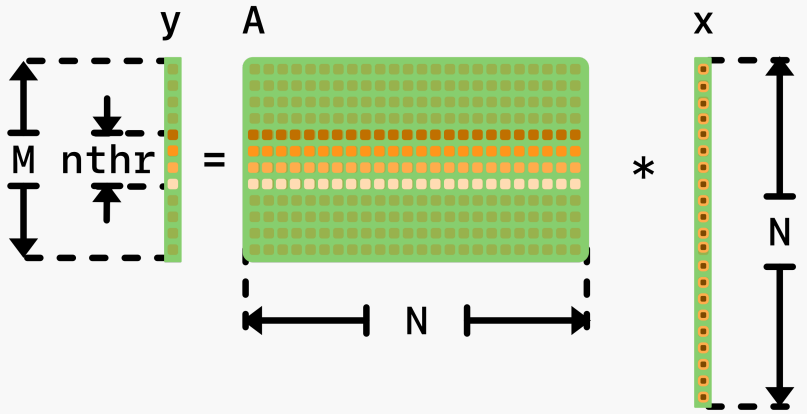

Straight-forward approach to begin with:

- Each block is responsible for one element of `y[]`
  - Each thread must read all elements of the corresponding row of `A[]`
  - Each thread must read all elements of `x[]`

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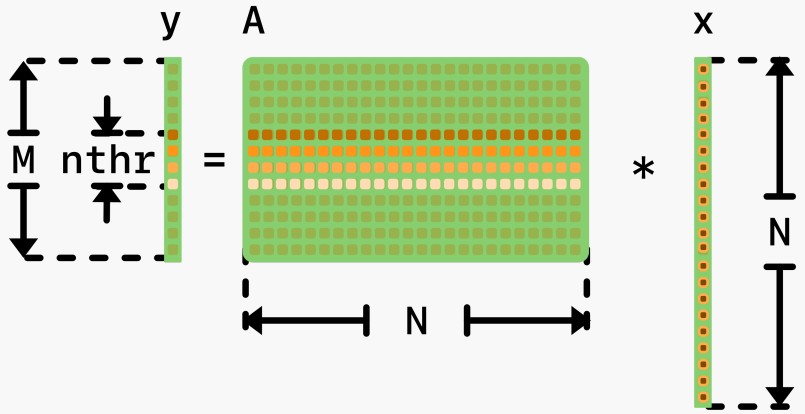


Straight-forward approach to begin with:

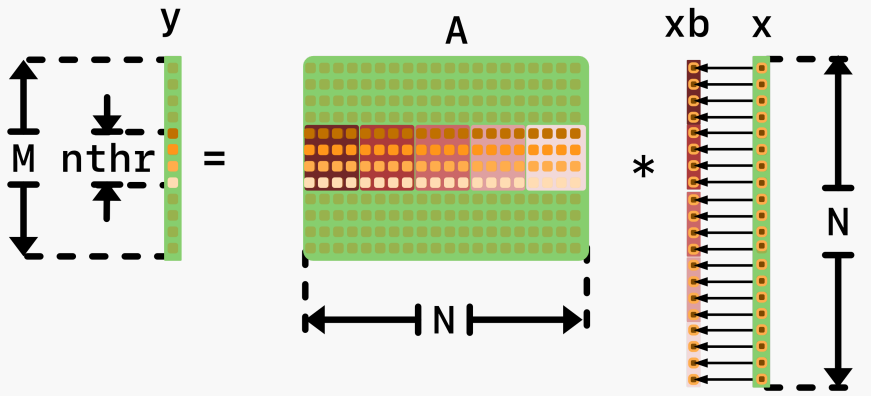
- Each block is responsible for one element of `y[]`
  - Each thread must read all elements of the corresponding row of `A[]`
  - Each thread must read all elements of `x[]`

E.g., using 256 GPU threads:

```
[user@front01 ex03]$ srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./matvec 4096 8192
 CPU: nthr =   20   t0 = 0.0028 sec   P =  23.771 Gflop/s   B =  47.560 GB/s
 GPU: nthr =  256   t0 = 0.0018 sec   P =  36.513 Gflop/s   B =  73.052 GB/s
 Diff = 2.603650e-15
```

Matrix-vector multiplication

Now use a *shared array* to share the elements of `x[]`. Name the shared array `xb[]`:



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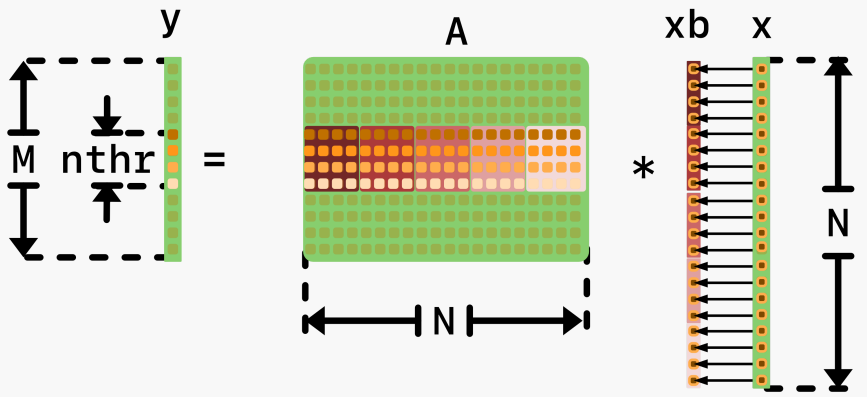

Notice that the shared array is of the size of the number of threads (`blockDim.x`) and therefore smaller than `x[]`

- Within each block, use all threads to read in the elements of `xb[]`
- This requires splitting the matrix-vector multiplication of the block into steps

Matrix-vector multiplication

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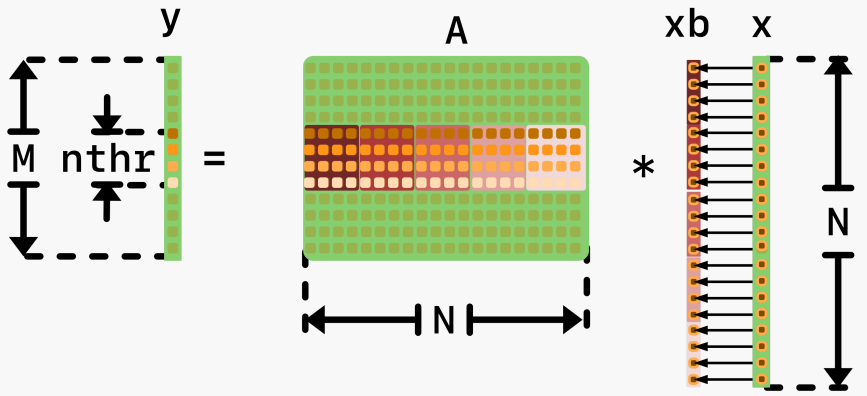

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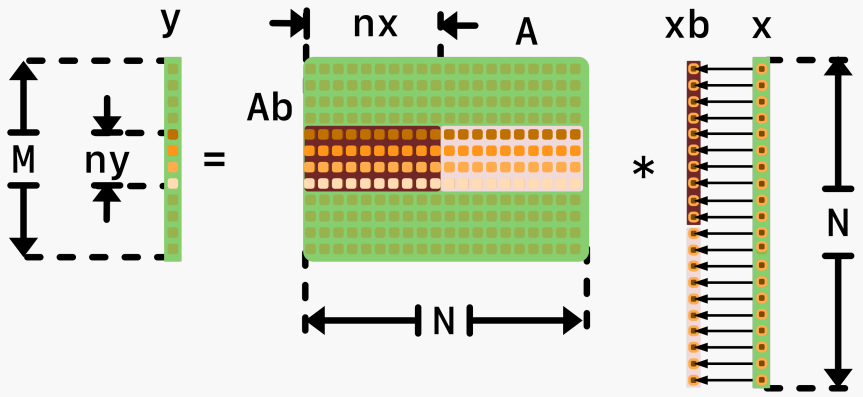
- Within each block, use all threads to read in the elements of `xb[]`
- This requires splitting the matrix-vector multiplication of the block into steps

Using 256 GPU threads:

```
[user@front01 ex03]$ srun -n 1 --cpus-per-task=20 -p gpu --gres=gpu:1 -A edu16 ./matvec 4096 8192
 CPU: nthr =   20   t0 = 0.0031 sec   P =  21.982 Gflop/s   B =  43.979 GB/s
 GPU: nthr =  256   t0 = 0.0018 sec   P =  36.550 Gflop/s   B =  73.128 GB/s
 Diff = 2.603650e-15
```

Matrix-vector multiplication

Now use a *shared array* for both `A[]` and `x[]`. Name them `Ab[]` and `xb[]`:



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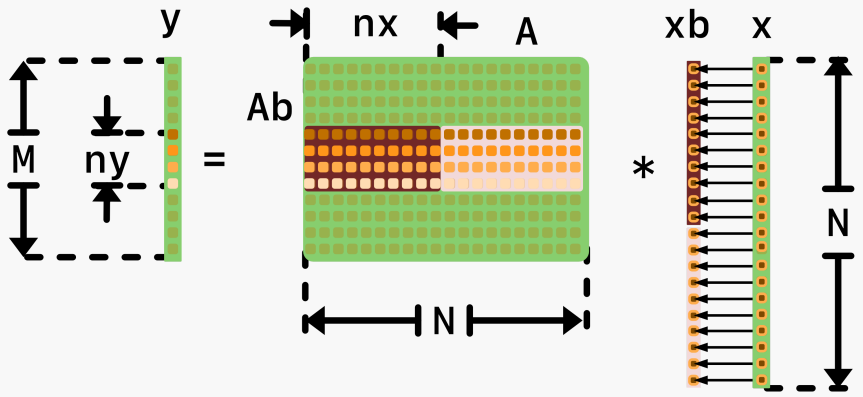

Use a 2-dimensional thread block

- All threads are used to fill in `Ab[]`
- Only some threads fill in `xb[]`
- Only some threads carry out the computation for `y[]`

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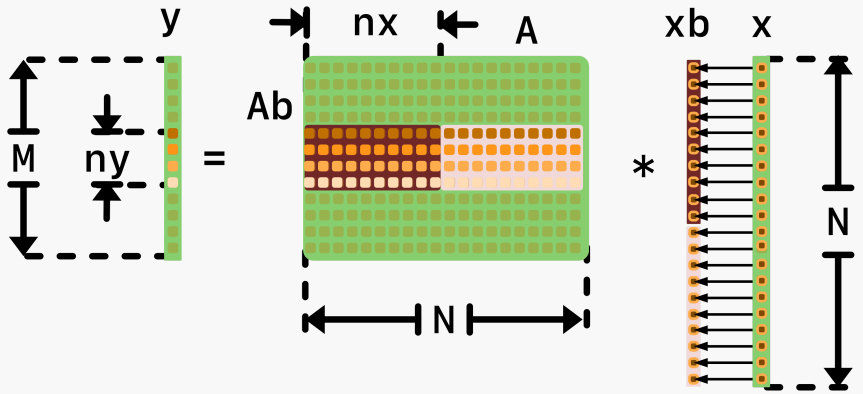

Use a 2-dimensional thread block

- All threads are used to fill in `Ab[]`
- Only some threads fill in `xb[]`
- Only some threads carry out the computation for `y[]`

Using thread-blocks of, e.g. 16$\8:

```
[user@front01 ex03]$ srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./matvec 4096 8192
 CPU: nthr =   20        t0 = 0.0028 sec   P =  23.713 Gflop/s   B =  47.444 GB/s
 GPU: nthr = ( 16,  8)   t0 = 0.0007 sec   P =  97.396 Gflop/s   B = 194.864 GB/s
 Diff = 2.603650e-15
```

Matrix-vector multiplication

Now let's see what we get when using CUDA's implementation of the same kernel

- The matrix-vector multiplication is implemented as part of CUDA's BLAS implementation

```
#include <cublas_v2.h>
```

- The function to use is `cublasSgemv()` -- see: https://docs.nvidia.com/cuda/cublas/index.html#cublas-lt-t-gt-gemv

Matrix-vector multiplication

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- This function is general and computes: $y = \alpha Ax + \beta y$, where α and β are scalars
- In our case, we need: $\alpha = 1$ and $\beta = 0$.

Matrix-vector multiplication

Call the CUBLAS function via:

```
cublasSgemv(handle, CUBLAS_OP_T, n, m, &alpha, d_A, n, d_x, 1, &beta, d_y, 1);
```

Matrix-vector multiplication

Call the CUBLAS function via:

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cublasSgemv(handle, CUBLAS_OP_T, n, m, &alpha, d_A, n, d_x, 1, &beta, d_y, 1);
```

- `CUBLAS_OP_T` means transpose `A`, because CUBLAS expects matrices with the row index running fastest

Matrix-vector multiplication

Call the CUBLAS function via:

```
cublasSgemv(handle, CUBLAS_OP_T, n, m, &alpha, d_A, n, d_x, 1, &beta, d_y, 1);
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- `CUBLAS_OP_T` means transpose `A`, because CUBLAS expects matrices with the row index running fastest
- `handle` is just the CUBLAS context:

```
  cublasHandle_t handle;
  cublasCreate(&handle);
```

- Add `-lcublas` to the compile command

Matrix-vector multiplication

Call the CUBLAS function via:

```
cublasSgemv(handle, CUBLAS_OP_T, n, m, &alpha, d_A, n, d_x, 1, &beta, d_y, 1);
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- `handle` is just the CUBLAS context:

```
  cublasHandle_t handle;
  cublasCreate(&handle);
```

- Add `-lcublas` to the compile command

Now CUBLAS chooses the number of threads for us:

```
[user@front01 ex03]$ srun -n 1 --cpus-per-task=20 -p gpu -A edu16 --gres=gpu:1 ./matvec 4096 8192
 CPU: nthr =   20   t0 = 0.0030 sec   P =  22.302 Gflop/s   B =  44.621 GB/s
 GPU:               t0 = 0.0013 sec   P =  50.344 Gflop/s   B = 100.725 GB/s
 Diff = 1.370746e-12
```