GPU PROGRAMMING WITH CUDA

Matrix multiplication

April 26, 2022 | Kaveh Haghighi Mood, Jochen Kreutz | JSC

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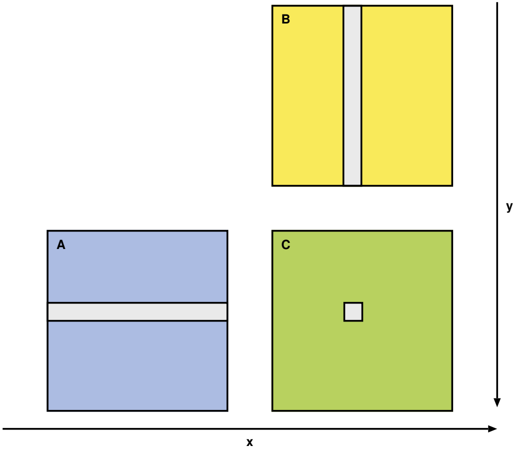
CUDA MATRIX MULTIPLICATION

Distribution of work

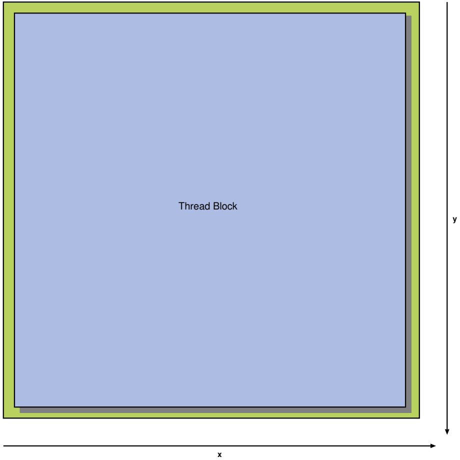


$$C_{row,col} = \sum_{i=1}^{N} A_{row,i} * B_{i,col}$$

- Each thread computes one element of the reuslt matrix C
- n * n threads will be needed (for square matrix C of size n)
- Thread indexing corresponds to 2d indexing of matrices
- Thread (x,y) will compute result element C(x,y) using row y of A and column x of B

CUDA MATRIX MULTIPLICATION

Execution grid layout

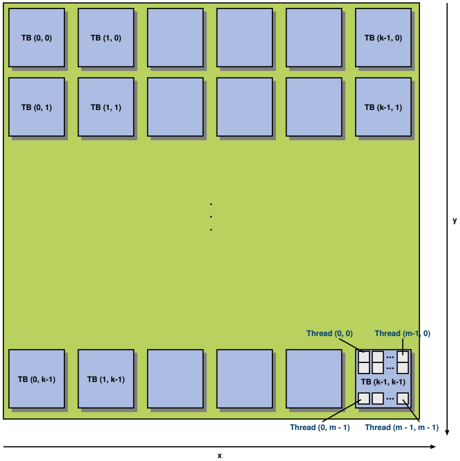


First naive idea:

- use one big thread block to cover all result elements
- Thread blocks are limited in size, thus we need several thread blocks to cover the full matrix C
- In addition, using only one thread block will decrease performance (due to reduced device occupancy)

CUDA MATRIX MULTIPLICATION

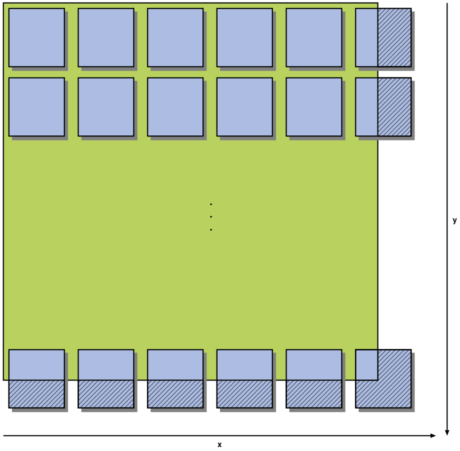
Execution grid layout



- Cover result matrix C of size n x n by using a 2d kernel execution grid with k * k thread blocks (TB)
- Use 2d thread blocks with fixed block size m
- k = n / m (n divisible by m)
- k = n / m + 1 (n not divisible by m)

CUDA MATRIX MULTIPLICATION

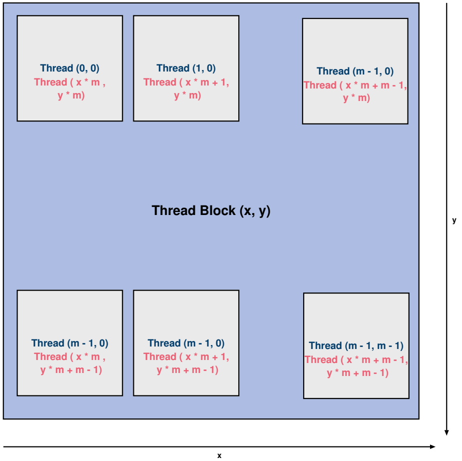
Execution grid layout



- k = n / m + 1 (n not divisible by m)
- All thread blocks have the same size
- Not possible to create ”partial blocks”
- To take care that some threads might not have to do any work (avoid out ouf bound memory access !)

CUDA MATRIX MULTIPLICATION

Execution grid layout



- Threads can be addressed via local index (block internal) and global index (full grid)
- Use available keywords in your kernel for targetting certain threads:
  - `blockIdx.[x, y, z]`
  - `blockDim.[x, y, z]`
  - `threadIdx.[x, y, z]`

CUDA MATRIX MULTIPLICATION

Execution grid layout

dim3 blockDim

```
dim3 blockDim { size_t blockDimX, size_t blockDimY, size_t blockDimZ }
```

On JUWELS Booster (Nvidia A100):

- Max. dim. of a block: `1024 x 1024 x 64`
- Max. number of threads per block: `1024`

Example

```
// Create 3d thread block with 512 threads
dim3 blockDim (16, 16, 2);
```

CUDA MATRIX MULTIPLICATION

Execution grid layout

dim3 gridDim

```
dim3 gridDim { size_t gridDimX, size_t gridDimY, size_t gridDimZ }
```

On JUWELS Booster (Nvidia A100):

- Max. dim. of a grid: `2147483647 x 65535 x 65535`
- Use `cudaGetDeviceProperties()` to get device properties

Example

```
// problem dimension: nx * ny = 1000 * 1000
dim3 blockDim (16, 16) // don't need to write z = 1
int gx = (nx % blockDim.x == 0) ? nx / blockDim.x : nx / blockDim.x + 1
int gy = (ny % blockDim.y == 0) ? ny / blockDim.y : ny / blockDim.y + 1
dim3 gridDim (gx, gy); // don't need to write z = 1
```

CUDA MATRIX MULTIPLICATION

Calling the kernel

Define dimensions of thread blocks

```
dim3 blockDim { size_t blockDimX, size_t blockDimY, size_t blockDimZ }
```

Define dimensions of execution grid

```
dim3 gridDim { size_t gridDimX, size_t gridDimY, size_t gridDimZ }
```

Launch the kernel

```
kernel_name <<< dim3 gridDim, dim3 blockDim >>> ([kernel args])
```

CUDA MATRIX MULTIPLICATION

Cuda kernel

Example

```
__global__ void mm_kernel(float* A, float* B, float* C, int n) {
        int col = blockIdx.x * blockDim.x + threadIdx.x;
        int row = blockIdx.y * blockDim.y + threadIdx.y;
        if (row < n && col < n) {
                for (int i = 0; i < n; ++i) {
                        C[row*n + col] += A[row*n + i] * B[i*n + col];
                }
        }
}
mm_kernel <<< dimGrid, dimBlock >>> (d_a, d_b, d_c, n);
```

EXERCISE

Simple matrix multiplication with Cuda

Location:

.../exercises/tasks/Cuda_MM_simple/Instructions.ipynb

PERFORMANCE CONSIDERATIONS

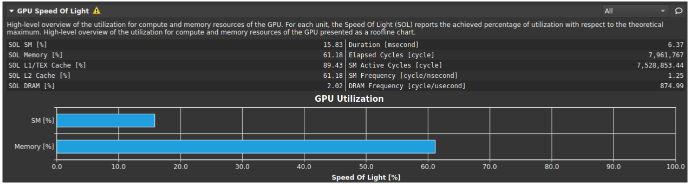
Measured numbers

JUWELS Cluster: 1 x V100 (theoretical peak: 7 TFlops DP)
JUWELS Booster: 1 x A100 (theoretical peak: 9.7 TFlops DP, 19.5 with TC)

matrix size	64	1024	10240	64	1024	10240
	JW Cluster [gflops]			**JW Booster** [gflops]		
with `cvalue`	1.2	319	1146	1.1	286.2	1587.1
direct write	1.02	196	391	0.9	198.3	562.2

PERFORMANCE CONSIDERATIONS

Profiler hints for simple matrix multiplication



- get useful hints from profiler
- helps to identify hotspots and potential performance issues
- get an overview timeline using Nsight Systems
- can analyse kernels individually using Nsight Compute
- indicates very low compute utilization
- `dgemm` kernel is memory-bound (GPU cores spend lots of time waiting for data)

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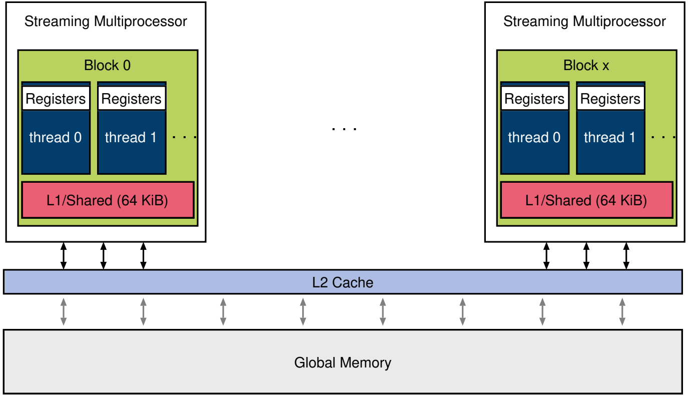
PERFORMANCE CONSIDERATIONS

GPU memory layout (schematics)



- matrix array `C` located in global memory
- `cvalue` located in registers on SM: faster write operations

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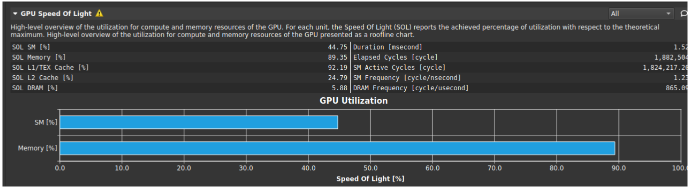
PERFORMANCE CONSIDERATIONS

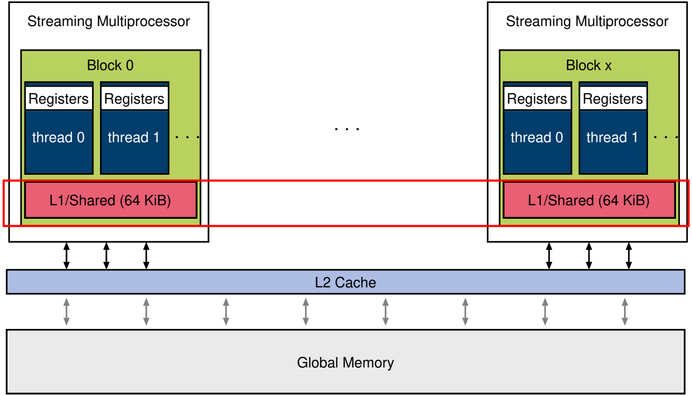
Profiler hints for simple matrix multiplication



- Using `cvalue` reduces the access to the global memory

PERFORMANCE CONSIDERATIONS

GPU memory layout (schematics)



what about using Shared Memory ?!

- matrix array `C` located in global memory
- `cvalue` located in registers on SM: faster write operations

SHARED MEMORY

How to use inside your kernels

Allocate shared memory

```
// allocate vector in shared memory
__shared__ float[size];
// can also define multi-dimensional arrays: BLOCK_SIZE is length (and width) of a thread block here
__shared__ float Msub[BLOCK_SIZE][BLOCK_SIZE];
```

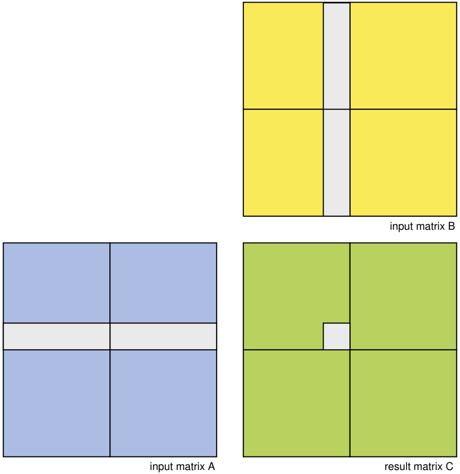
Copy data into shared memory

```
// fetch data from global to shared memory
Msub[threadIdx.y][threadIdx.x] = M[TidY * width + TidX];
```

Remember: only shared between threads within the same thread block !

BLOCK MATRIX MULTIPLICATION

Idea

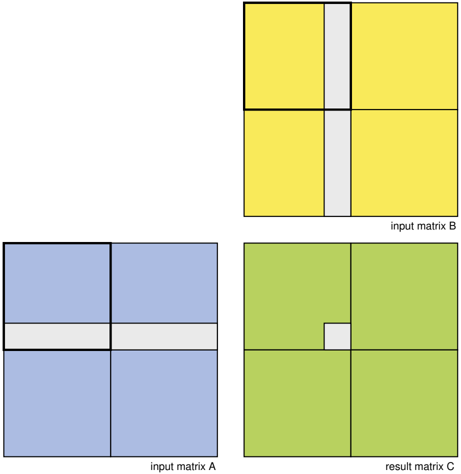


Split computation of result element into parts (assume N is even here)

$$C_{row,col} = \sum_{i=1}^{N} A_{row,i} * B_{i,col}$$

BLOCK MATRIX MULTIPLICATION

Idea



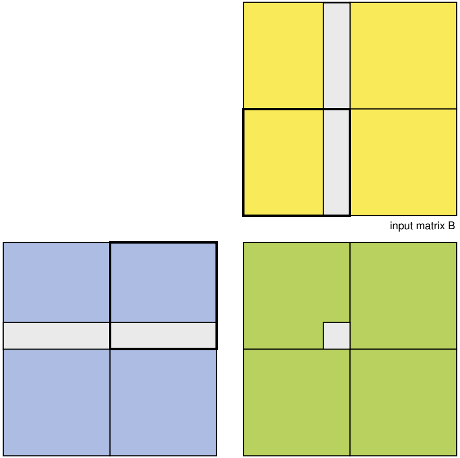
Split computation of result element into parts (assume N is even here)

$$C_{row,col} = \sum_{i=1}^{N} A_{row,i} * B_{i,col}$$

$$= \sum_{i=1}^{\frac{N}{2}} A_{row,i} * B_{i,col}$$

BLOCK MATRIX MULTIPLICATION

Idea



Split computation of result element into parts (assume N is even here)

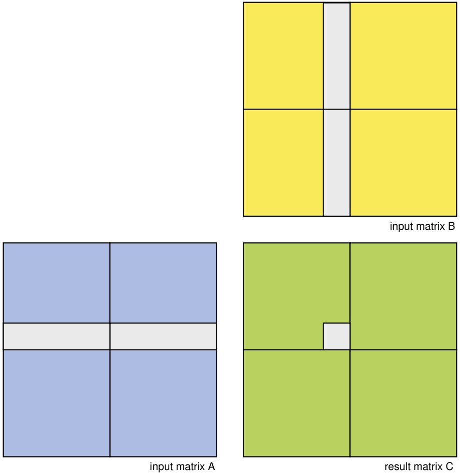
$$C_{row,col} = \sum_{i=1}^{N} A_{row,i} * B_{i,col}$$

$$= \sum_{i=1}^{\frac{N}{2}} A_{row,i} * B_{i,col}$$

$$+ \sum_{i=\frac{N}{2}+1}^{N} A_{row,i} * B_{i,col}$$

BLOCK MATRIX MULTIPLICATION

Idea



$$C_{row,col} = \sum_{i=1}^{\frac{N}{2}} A_{row,i} * B_{i,col} + \sum_{i=\frac{N}{2}+1}^{N} A_{row,i} * B_{i,col}$$

consider all result elements within the same block in C:

$$C_{11} = A_{11} * B_{11} + A_{12} * B_{21}$$

$$C_{12} = A_{11} * B_{12} + A_{12} * B_{22}$$

$$C_{21} = A_{21} * B_{11} + A_{22} * B_{21}$$

$$C_{22} = A_{21} * B_{12} + A_{22} * B_{21}$$

BLOCK MATRIX MULTIPLICATION

Example

$$C = A * B \qquad C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$$

$$A = \begin{pmatrix} \begin{pmatrix} 1 & 2 \\ 4 & 1 \end{pmatrix} & \begin{pmatrix} 3 & 4 \\ 2 & 3 \end{pmatrix} \\ \begin{pmatrix} 3 & 4 \\ 2 & 3 \end{pmatrix} & \begin{pmatrix} 1 & 2 \\ 4 & 1 \end{pmatrix} \end{pmatrix} \qquad B = \begin{pmatrix} \begin{pmatrix} -9 & 11 \\ 1 & -9 \end{pmatrix} & \begin{pmatrix} 1 & 1 \\ 11 & 1 \end{pmatrix} \\ \begin{pmatrix} 1 & 1 \\ 11 & 1 \end{pmatrix} & \begin{pmatrix} -9 & 11 \\ 1 & -9 \end{pmatrix} \end{pmatrix} * \frac{1}{40}$$

$$C_{11} = \begin{pmatrix} 1 & 2 \\ 4 & 1 \end{pmatrix} * \frac{1}{40} \begin{pmatrix} -9 & 11 \\ 1 & -9 \end{pmatrix} + \begin{pmatrix} 3 & 4 \\ 2 & 3 \end{pmatrix} * \frac{1}{40} \begin{pmatrix} 1 & 1 \\ 11 & 1 \end{pmatrix} \tag{1}$$

BLOCK MATRIX MULTIPLICATION

Example

$$C = A * B$$

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$$

$$A = \begin{pmatrix} \begin{pmatrix} 1 & 2 \\ 4 & 1 \end{pmatrix} & \begin{pmatrix} 3 & 4 \\ 2 & 3 \end{pmatrix} \\ \begin{pmatrix} 3 & 4 \\ 2 & 3 \end{pmatrix} & \begin{pmatrix} 1 & 2 \\ 4 & 1 \end{pmatrix} \end{pmatrix}$$

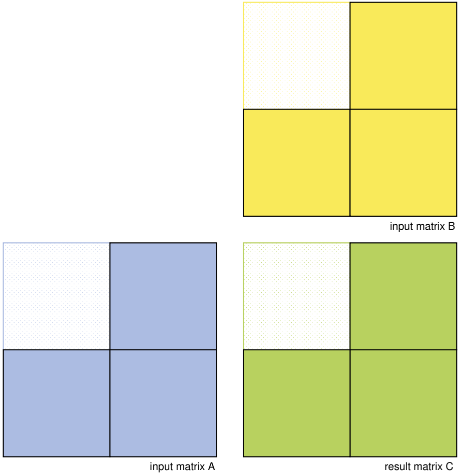
$$B = \begin{pmatrix} \begin{pmatrix} -9 & 11 \\ 1 & -9 \end{pmatrix} & \begin{pmatrix} 1 & 1 \\ 11 & 1 \end{pmatrix} \\ \begin{pmatrix} 1 & 1 \\ 11 & 1 \end{pmatrix} & \begin{pmatrix} -9 & 11 \\ 1 & -9 \end{pmatrix} \end{pmatrix} * \frac{1}{40}$$

$$= \frac{1}{40} * \begin{pmatrix} -7 & -7 \\ -35 & 35 \end{pmatrix} + \frac{1}{40} * \begin{pmatrix} 47 & 7 \\ 35 & 5 \end{pmatrix} = \frac{1}{40} * \begin{pmatrix} 40 & 0 \\ 0 & 40 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

do C_{12}, C_{21} and C_{22} the same way

BLOCK MATRIX MULTIPLICATION

Using shared memory

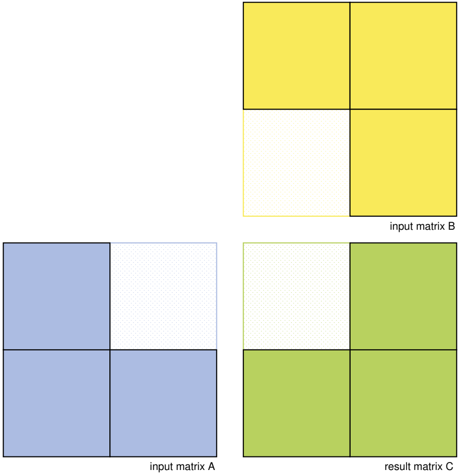


consider all result elements within the same block:

- all threads dealing with those elements will have to access input data from the same blocks of A and B for the first part of the computation

BLOCK MATRIX MULTIPLICATION

Using shared memory

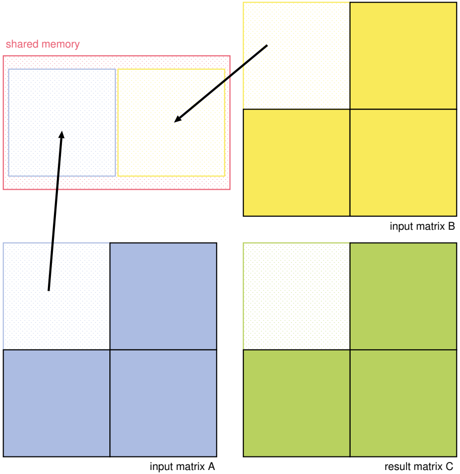


consider all result elements within the same block:

- all threads dealing with those elements will have to access input data from the same blocks of A and B for the first part of the computation
- same counts for the successing compute parts

BLOCK MATRIX MULTIPLICATION

Using shared memory

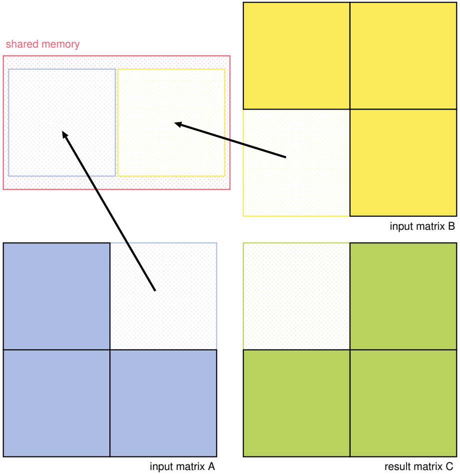


consider all result elements within the same block:

- all threads dealing with those elements will have to access input data from the same blocks of A and B for the first part of the computation
- same counts for the successing compute parts
- hence store a data copy of the input blocks into shared memory
- this prevents repeated reads from the global memory

BLOCK MATRIX MULTIPLICATION

Using shared memory

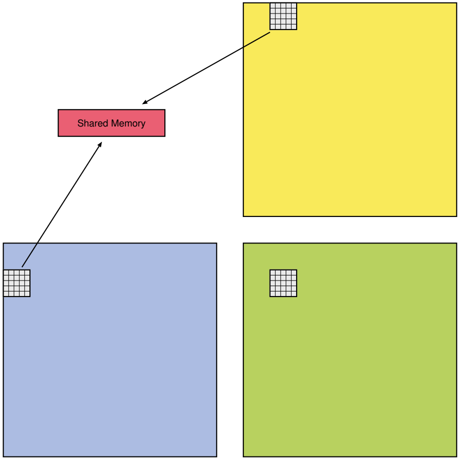


consider all result elements within the same block:

- mapping logical matrix blocks to your Cuda thread blocks ensures that all threads in your result blocks see the same shared memory
- each thread reads 1 element of A and 1 element of B and stores in into the shared memory

BLOCK MATRIX MULTIPLICATION

Workflow

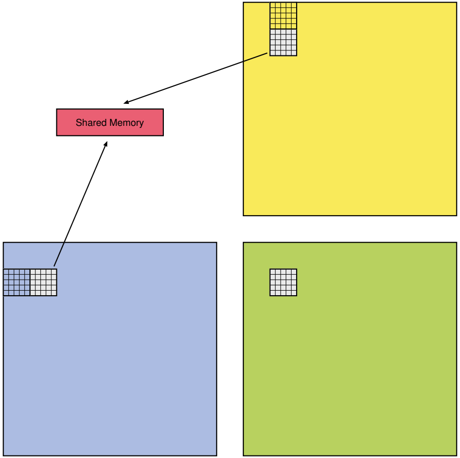


for each result element (thread):

- set result element to zero
- for each pair of blocks
  - copy input data to shared memory (one element from A and B)
  - do partial sum using shared memory
  - add partial sum to result element

BLOCK MATRIX MULTIPLICATION

Workflow



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BLOCK MATRIX MULTIPLICATION

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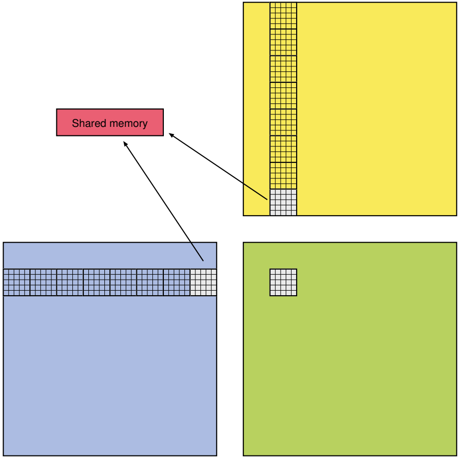

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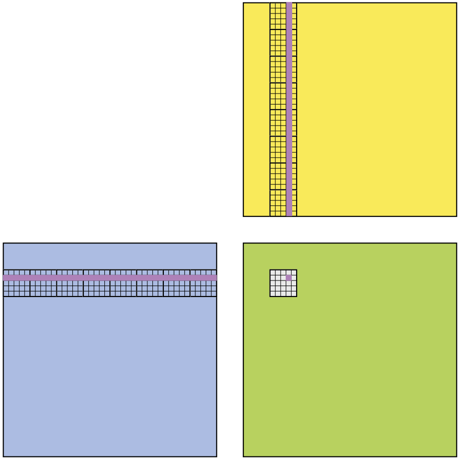
BLOCK MATRIX MULTIPLICATION

Workflow



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  - copy input data to shared memory (one element from A and B)
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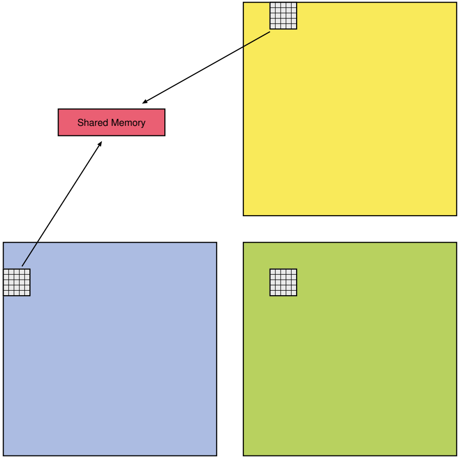
BLOCK MATRIX MULTIPLICATION

Thread synchronization



Thread synchronization

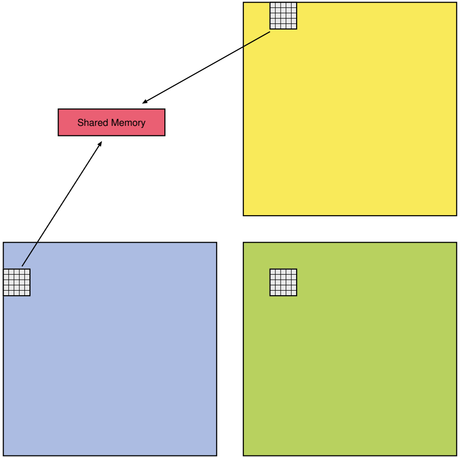
Threads within a thread block might be executed one after the other. Hence, synchronization is needed !

Synchronize threads within a thread block

```
__syncthreads ();
```

BLOCK MATRIX MULTIPLICATION

Thread synchronization

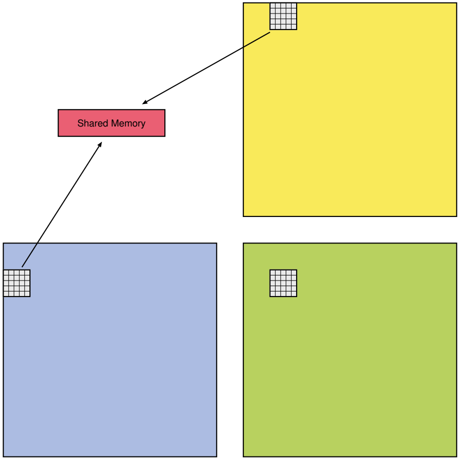


for each result element (thread):

- set result element to zero
- for each pair of blocks
  - copy input data to shared memory (one element from A and B)
  - wait until all threads have copied their data
  - do partial sum
  - wait until all threads finished computation on current data
  - add partial sum to result element

BLOCK MATRIX MULTIPLICATION

Offsets and indexes



idea: use (2d coordinates of) upper left corner of input blocks as reference

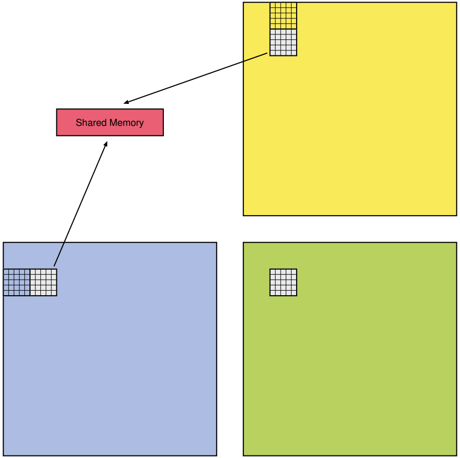
- relative positions inside the input blocks correspond to the local (block internal) thread indexes

starting point:

- row in A (`blockAy`):
  `blockIdx.y * block_size`
- col in B (`blockBx`):
  `blockidx.x * block_size`
- `blockAx` and `blockBy` will be `0` at start

BLOCK MATRIX MULTIPLICATION

Offsets and indexes



idea: use (2d coordinates of) upper left corner of input blocks as reference

moving input blocks:

- A moving to x direction by adding: `block_size`
- B moving to y direction by adding: `n * block_size`

shared memory blocks:

- use local (block internal) thread indexes to select correct row and column

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EXERCISE

Matrix multiplication with Cuda using shared memory

Location:

.../exercises/tasks/Cuda_MM_shared/Instructions.ipynb

EXERCISE

Measured numbers

Results on JUWELS Booster (gflops):

matrix size	1024	4096	8192	16384
Simple	286	1186	1554	1769
Shared memory(16,16)	296	952	1560	1742
Shared memory(32,32)	339	1369	1945	2205

EXERCISE

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Thank you for your attention!