



EURO
Greece

HPC Training Series

Introduction to modern graphic processing unit (GPU) architecture
and programming in CUDA

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Why GPUs ?

- ❑ Parallel processing units
- ❑ High floating-point operations rate (double and single precision arithmetic)
- ❑ GPU embedded, low latency, RAM
- ❑ Various programming environments
- ❑ Low cost & energy consumption compared to their computational power

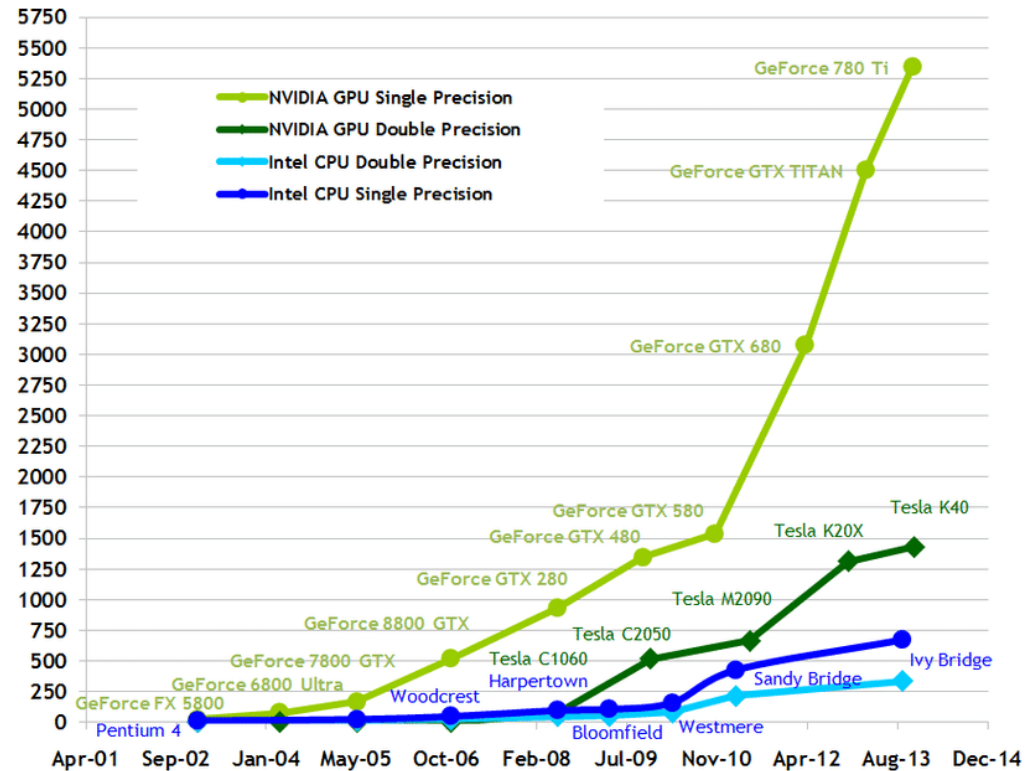


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Theoretical GFLOP/s

CUDA Programming Guide v6.5



Why GPUs ?

- ❑ Parallel processing units
- ❑ High floating-point operations rate
(double and single precision arithmetic)

NVIDIA A100 (Ampere, 2020)

- ✓ 19.5 TFLOPS (single precision)
- ✓ 9.7 TFLOPS (double precision)
- ✓ 156 / 19.5 TFLOPS with Tensor cores

- ❑ GPU embedded, low latency, RAM
- ❑ Various programming environments
- ❑ Low cost & energy consumption
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Why GPUs ?

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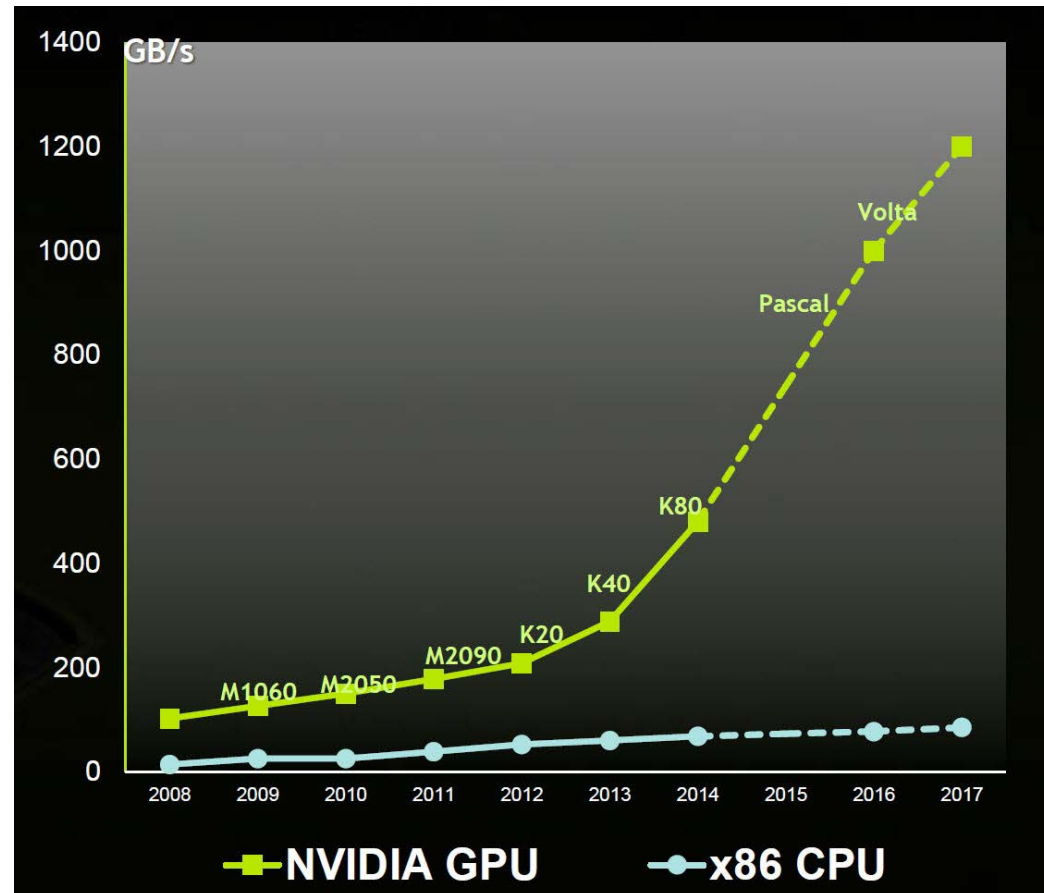
❑ GPU embedded, low latency, RAM

NVIDIA A100 (Ampere, 2020)

- ✓ 40 GB of RAM
- ✓ Peak memory bandwidth: 1.6TB/s

❑ Various programming environments

❑ Low cost & energy consumption compared to their computational power



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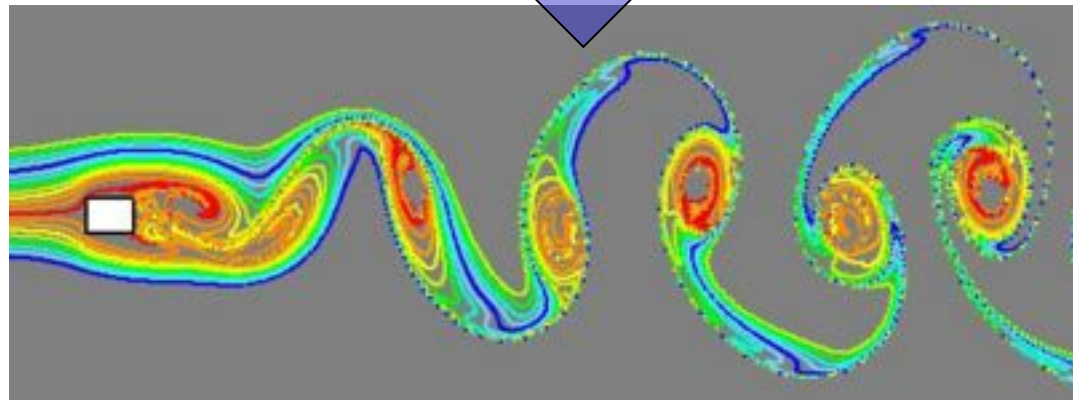
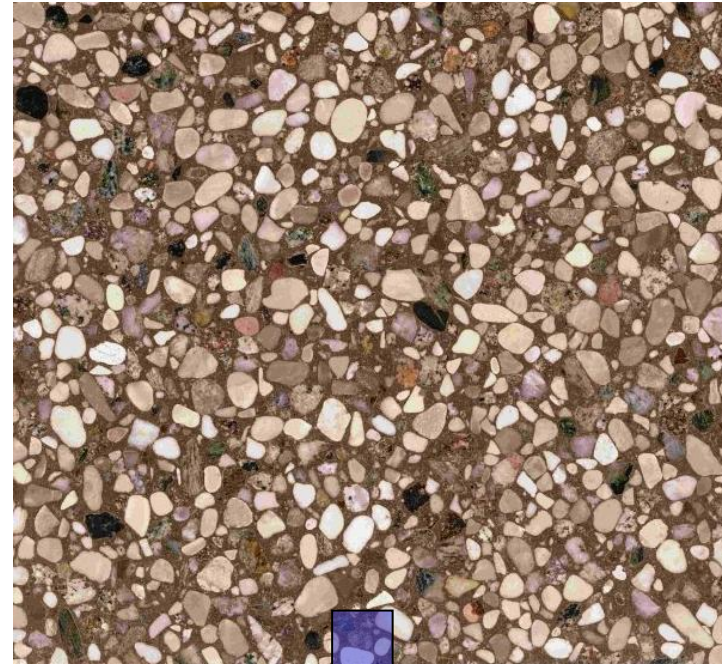
OpenCL: Cross platform implementation

- C++
- Python

CUDA: Developed by NVIDIA, specialized for NVIDIA GPUs

- C++
- FORTRAN
- Python

OpenACC



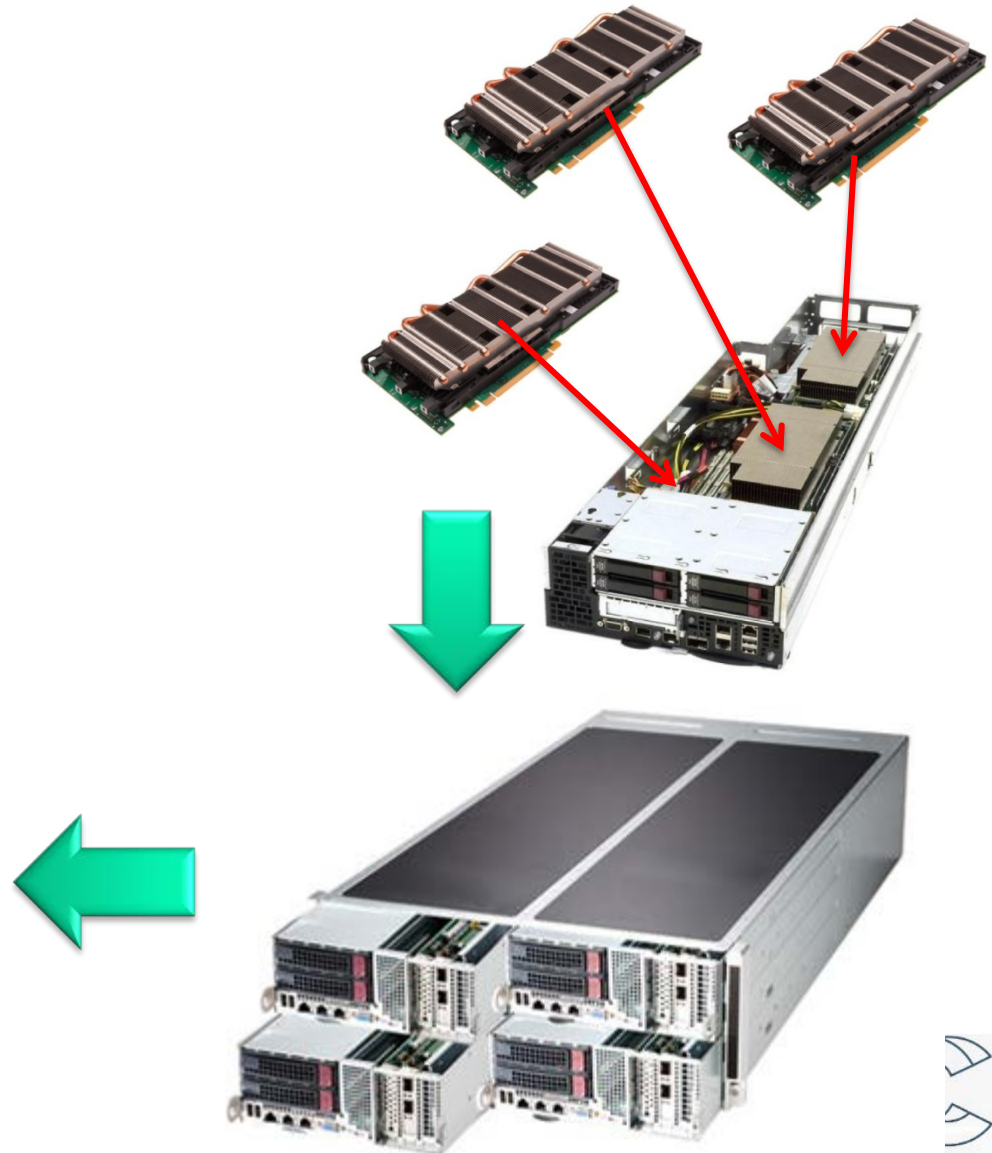
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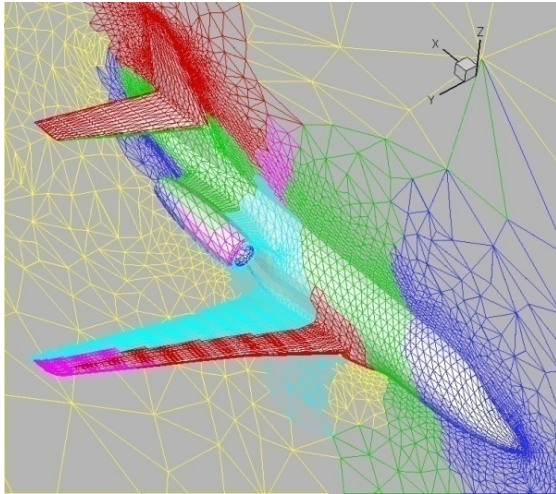


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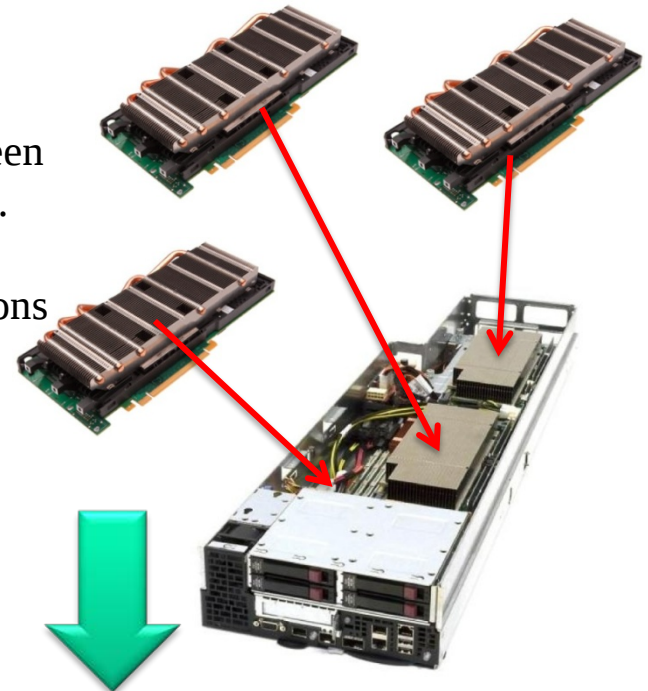
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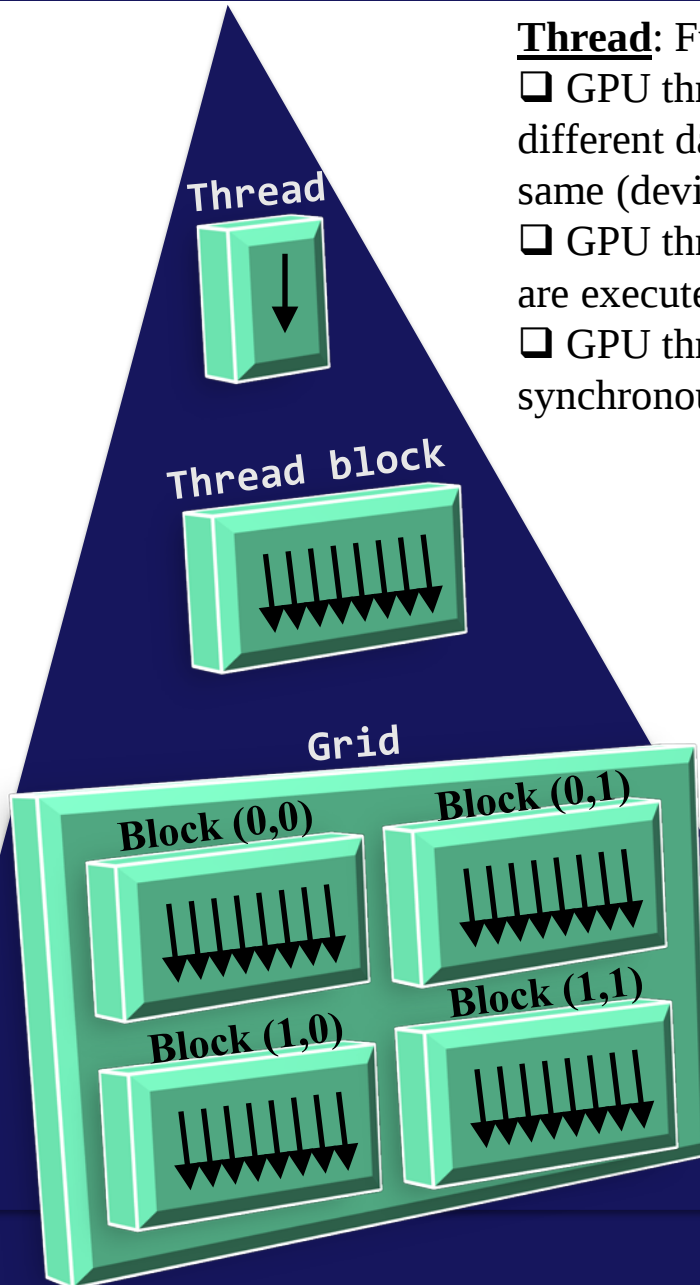
Why GPUs ?



- ❑ 1 sub-domain per GPU.
- ❑ MPI → data transactions between GPUs on different compute nodes.
- ❑ Host memory → data transactions between GPUs on the same node.



GPU Architecture



Thread: Fundamental computational unit

- ❑ GPU threads execute the same fragment of code (**kernel**) using different data (**SIMT**: Single Instruction Multiple Threads) accessing the same (device) memory.
- ❑ GPU threads are organized into **warps** (i.e. group of 32 threads) and are executed at GPU multiprocessors.
- ❑ GPU threads of the same warp are executed in parallel in a synchronous manner.

Block: Cluster of warps

- ❑ Each multiprocessor can execute at least a thread block.
- ❑ GPU block threads, which belong to different warps, are executed in parallel and asynchronous manner.
- ❑ Synchronization and fast data transactions through shared memory

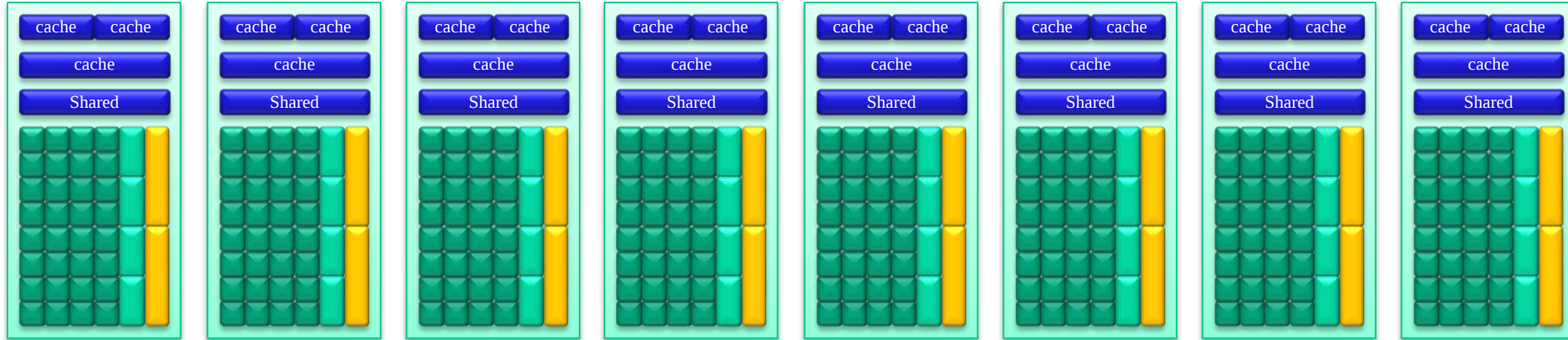
Grid: Cluster of thread blocks

- ✓ A100 can execute up to 221,184 threads in parallel

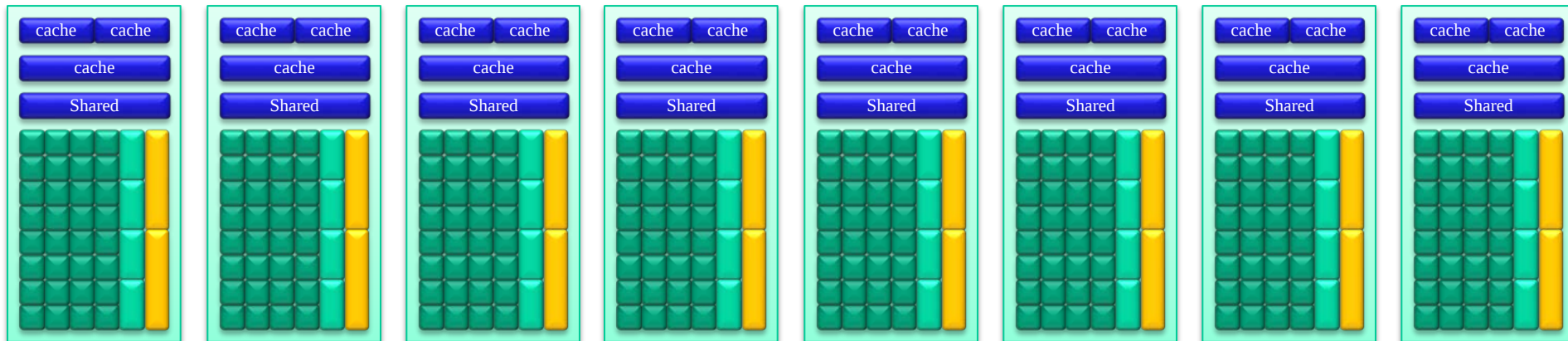


GPU Architecture

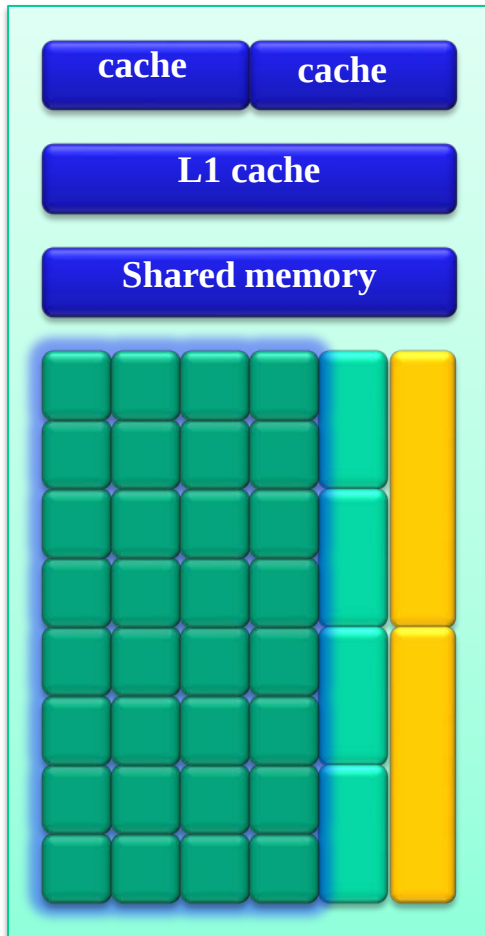
Fermi (2010): 16 streaming multiprocessors (SMs)



L2 cache



GPU Architecture

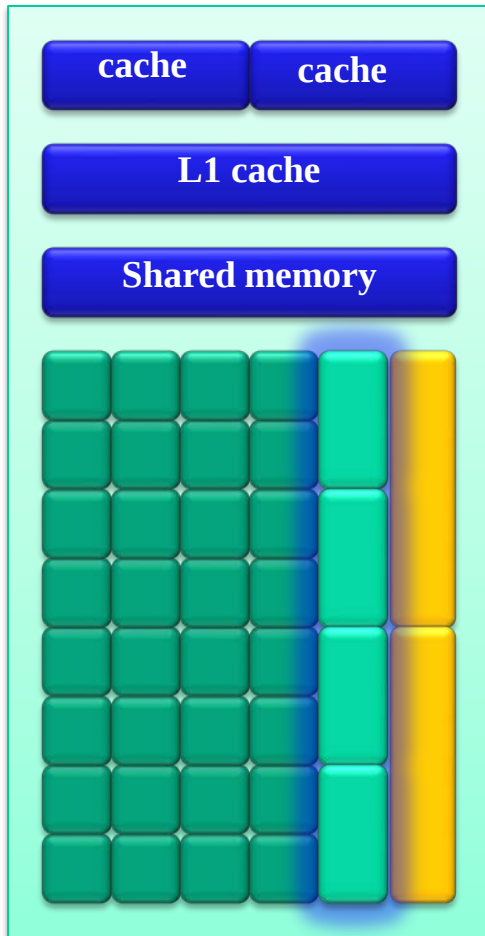


Each Fermi SM consists of:

- ☐ 32 (CUDA) cores
- ☐ 4 Special Function Units (SFUs)
- ☐ 2 warp schedulers
- ☐ Shared memory
- ☐ cache memory (L1, constant & texture)
- ☐ 32768 32-bit registers



GPU Architecture

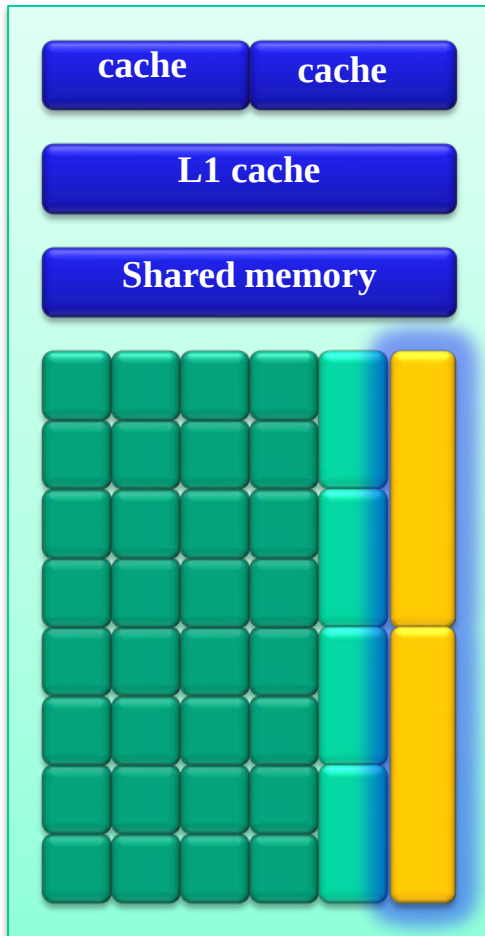


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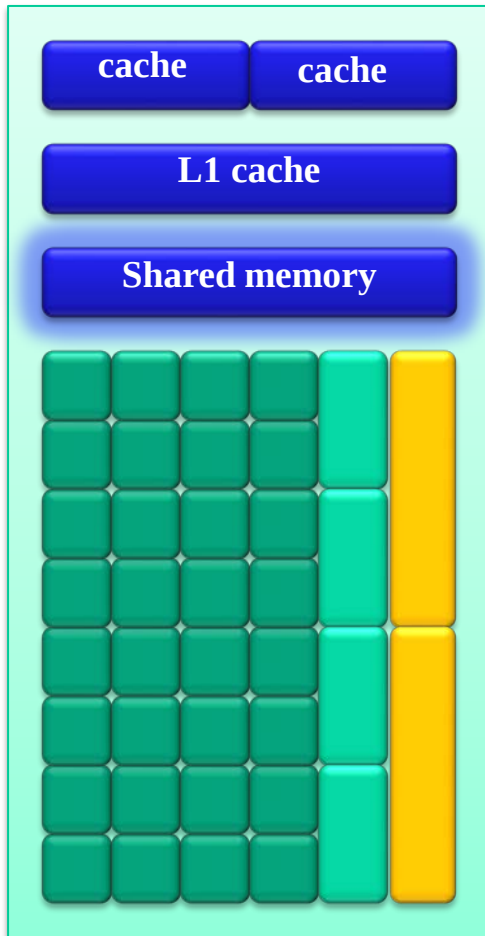
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GPU Architecture

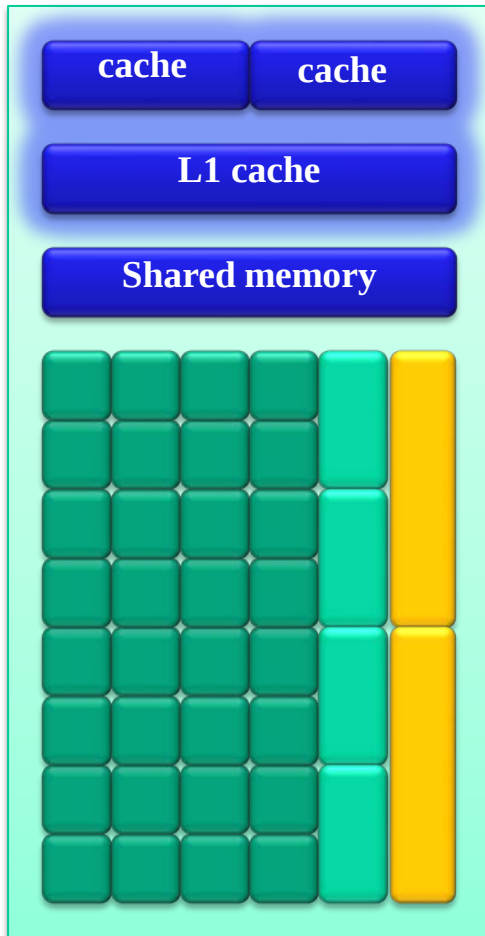


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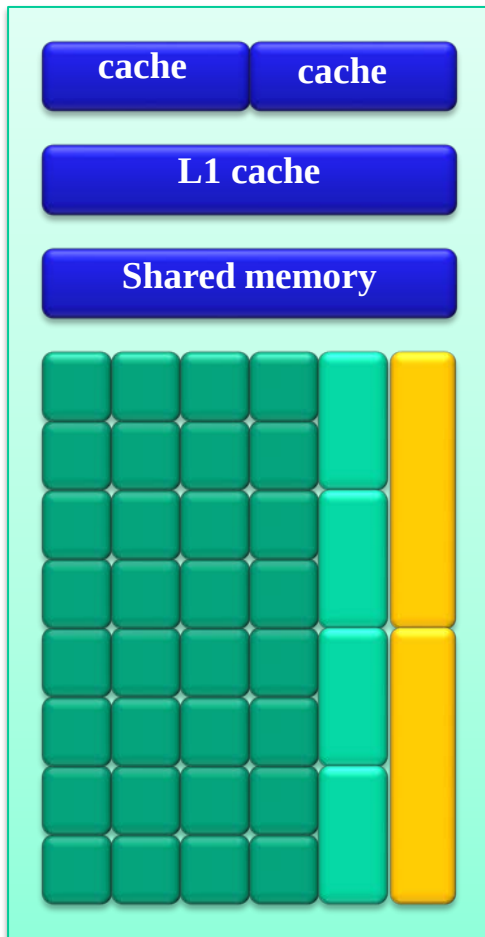
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GPU Architecture



	Fermi (2010)	Ampere (2020)
CUDA cores	32	128
Tensor cores	-	8
Shared memory & L1 cache	64 KB	192 KB
Texture cache	12 KB	12 KB
Constant cache	8 KB	8 KB
Registers	32,768 32-bit	65,536 32-bit
SMs	16	108 (A100)
Max. threads per SM	1,536	2,048
Max threads	24,576	221,184



Hello World: CPU implementation

```
#include <iostream>

int main()
{
    printf("# Hello world from the host\n");
    return 0;
}
```

Hello World: GPU implementation

```
#include <iostream>

__global__ void helloGPU(); // kernel declaration

int main()
{
    // kernel launch:
    helloGPU <<< /*GridSize*/ 1, /*BlockSize*/ 1 >>> ();

    return 0;
}

__global__ void helloGPU()
{
    printf("# Hello world from thread %d in block %d\n",threadIdx.x,blockIdx.x);
}
```

Number of blocks into the grid

Number of threads into the block

Return type: void

**** This code compiles but it prints nothing in the screen

Hello World: GPU implementation

```
#include <iostream>

__global__ void helloGPU(); // kernel declaration

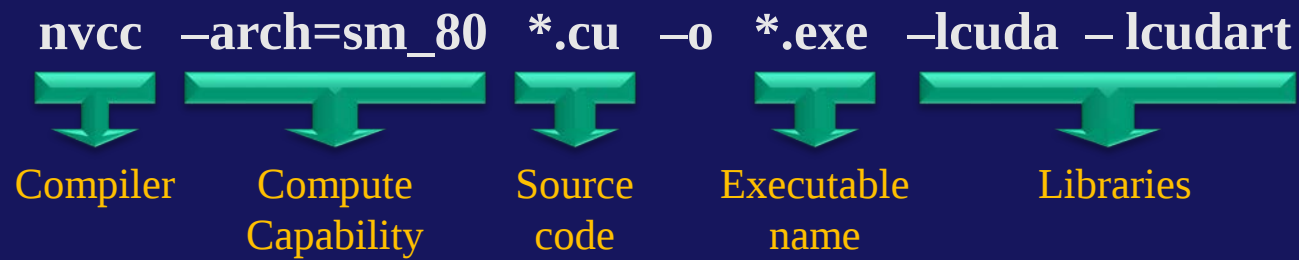
int main()
{
    // kernel launch:
    helloGPU <<< /*GridSize*/ 1, /*BlockSize*/ 1 >>> ();

    // synchronize host & device:
    cudaDeviceSynchronize();

    return 0;
}

__global__ void helloGPU()
{
    printf("# Hello world from thread %d in block %d\n",threadIdx.x,blockIdx.x);
}
```

Host-device synchronization



Vector addition: CPU implementation

```
#include <iostream>
#include <cmath>

int main()
{
    constexpr long size = 10;

    double* A = new double[size];
    double* B = new double[size];
    double* C = new double[size];

    for (auto i=0; i < size; i++) A[i] = (double)i;
    for (auto i=0; i < size; i++) B[i] = (double)i;
    for (auto i=0; i < size; i++) C[i] = NAN;

    for (auto i=0; i < size; i++) {
        C[i] = A[i] + B[i];
    }

    for (auto i=0; i < size; i++) {
        std::cout << A[i] << " + " << B[i] << " = " << C[i] << std::endl;
    }

    if (A != nullptr) delete[] A; A = nullptr;
    if (B != nullptr) delete[] B; B = nullptr;
    if (C != nullptr) delete[] C; C = nullptr;

    return 0;
}
```

Vector addition: GPU implementation (1/6)

```
#include <cuda.h> // include CUDA header
#include <iostream>
#include <cmath>

int main()
{
    // STEP1: Allocate device memory and copy data to GPU
    // STEP2: Launch kernel(s)
    // STEP3: Copy results from device to host memory

    return 0;
}
```

Vector addition: GPU implementation (2/6)

// **STEP1**: Device memory allocations & initialization :

```
double* _A = (double*)device_alloc( (void*)A, size*sizeof(double), "A" );
double* _B = (double*)device_alloc( (void*)B, size*sizeof(double), "B" );
double* _C = (double*)device_alloc(          size*sizeof(double), "C" );
```

```
void* device_alloc(const long size, const std::string& varname)
```

```
{
```

```
    void* devptr = nullptr;
```

```
    cudaError_t err = cudaMalloc(&devptr, size /*SIZE IN BYTES*/);
```

```
    if (err != cudaSuccess) std::cerr << "Invalid allocation of \""+varname+"\"" << std::endl;
```

```
    if (err != cudaSuccess) exit(1);
```

```
    return devptr;
```

```
}
```

Allocate space in device memory

```
void* device_alloc(void* hostptr, const long size, const std::string& varname)
```

```
{
```

```
    void* devptr = device_alloc(size, varname);
```

```
    cudaError_t err = cudaMemcpy(devptr, hostptr, size, cudaMemcpyHostToDevice);
```

```
    if (err != cudaSuccess) std::cerr << "Invalid copy to \""+varname+"\"" << std::endl;
```

```
    if (err != cudaSuccess) exit(1);
```

```
    return devptr;
```

```
}
```

Memory copy



Vector addition: GPU implementation (2/6)

```
// STEP1: Device memory allocations & initialization :
```

```
constexpr long size = 10;
```

```
double* A = new double[size];
```

```
double* B = new double[size];
```

```
double* C = new double[size];
```

```
for (auto i=0; i < size; i++) A[i] = (double)i;
```

```
for (auto i=0; i < size; i++) B[i] = (double)i;
```

```
for (auto i=0; i < size; i++) C[i] = NAN;
```

```
double* _A = (double*)device_alloc( (void*)A, size*sizeof(double), "A" );
```

```
double* _B = (double*)device_alloc( (void*)B, size*sizeof(double), "B" );
```

```
double* _C = (double*)device_alloc( size*sizeof(double), "C" );
```



Vector addition: GPU implementation (3/6)

```
// STEP3: Device memory deallocations :  
if (_A != nullptr) cudaFree(_A); _A = nullptr;  
if (_B != nullptr) cudaFree(_B); _B = nullptr;  
if (_C != nullptr) cudaFree(_C); _C = nullptr;
```

Free device memory



```
if (A != nullptr) delete[] A; A = nullptr;  
if (B != nullptr) delete[] B; B = nullptr;  
if (C != nullptr) delete[] C; C = nullptr;
```

Vector addition: GPU implementation (4/6)

```
// STEP2: Launch kernel:
```

```
const int blockSize = 1024;
const int gridSize  = (size+blockSize-1)/blockSize;
```

Create as many threads as the size of the outputs

```
vectorAddGPU <<< gridSize, blockSize >>> (size, _A, _B, _C);
```

```
cudaDeviceSynchronize();
```

Is host-device synchronization needed here ?

```
cudaError_t err = cudaGetLastError();
```

```
if (err != cudaSuccess) {
```

```
    std::cerr << " Launch failure: " << cudaGetErrorString(err) << std::endl;
```

```
    exit(1);
```

```
}
```

```
// Copy results to host :
```

```
err = cudaMemcpy(C, _C, size*sizeof(double), cudaMemcpyDeviceToHost);
```

```
if (err != cudaSuccess) std::cerr << "Invalid device to host copy" << std::endl;
```

```
if (err != cudaSuccess) exit(1);
```

```
for (int i=0; i < size; i++) {
```

```
    std::cout << A[i] << " + " << B[i] << " = " << C[i] << std::endl;
```

```
}
```

```
__global__ void vectorAddGPU(const long size, double* _A, double* _B, double* _C )
```

```
{
```

```
    const long i = blockIdx.x*blockDim.x + threadIdx.x;
```

```
    if (i < size) {
```

```
        _C[i] = _A[i] + _B[i];
```

```
    }
```

```
}
```

Each thread processes a single element of arrays A, B



Vector addition: GPU implementation (5/6)

```
int main()
{
```

```
    constexpr long size = 10;
```

```
    double* A = (double*)alloc_managed_mem(size*sizeof(double), "A");
```

```
    double* B = (double*)alloc_managed_mem(size*sizeof(double), "B");
```

```
    double* C = (double*)alloc_managed_mem(size*sizeof(double), "C");
```

```
    for (auto i=0; i < size; i++) A[i] = (double)i;
```

```
    for (auto i=0; i < size; i++) B[i] = (double)i;
```

```
    for (auto i=0; i < size; i++) C[i] = NAN;
```

```
    const int blockSize = 1024;
```

```
    const int gridSize = (size+blockSize-1)/blockSize;
```

```
    vectorAddGPU <<< gridSize, blockSize >>> (size,A,B,C);
```

```
    cudaDeviceSynchronize();
```

```
    cudaError_t err = cudaGetLastError();
```

```
    if (err != cudaSuccess) {
```

```
        std::cerr << " Launch failure: " << cudaGetErrorString(err) << std::endl;
        exit(1);
    }
```

```
    for (auto i=0; i < size; i++) {
```

```
        std::cout << A[i] << " + " << B[i] << " = " << C[i] << std::endl;
```

```
    }
```

```
    if (A != nullptr) cudaFree(A); A = nullptr;
```

```
    if (B != nullptr) cudaFree(B); B = nullptr;
```

```
    if (C != nullptr) cudaFree(C); C = nullptr;
```

```
    return 0;
```

```
}
```

Maintaining pointers for both host and device memory makes GPU code too large. Wouldn't it be great to manage both using a single pointer?

Is host-device synchronization needed here ?

Use cudaFree to free memory



Vector addition: GPU implementation (6/6)

```
void* alloc_managed_mem(const long size, const std::string& varname)
{
    void* devptr = nullptr;
    cudaError_t err = cudaMallocManaged(&devptr, size /*SIZE IN BYTES*/);
    if (err != cudaSuccess) std::cerr << "Invalid allocation of \""+varname+"\"" << std::endl;
    if (err != cudaSuccess) exit(1);

    return devptr;
}

// CHECK whether the compute device supports managed memory:
int attr;
cudaDeviceGetAttribute(&attr, cudaDevAttrManagedMemory, 0);
if (attr == 0) std::cerr << "This device does not support managed memory" << std::endl;
if (attr == 0) exit(1);
```

UVA



Piece of advice

- ❑ Avoid threads running in parallel to write at the same memory position (memory conflict).

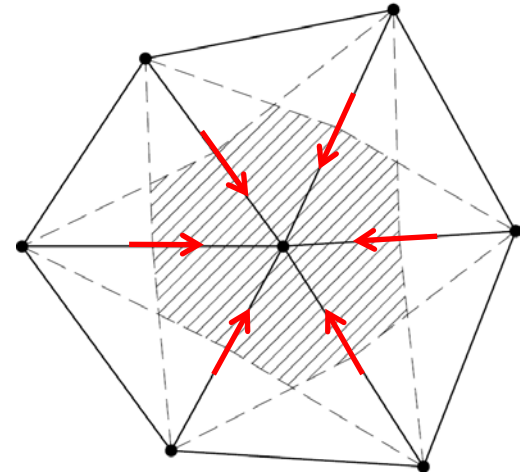
- ❑ Threads from the same warp should access to the same device memory segment, since access to a 128-byte device memory segment can be performed within a single memory transaction.

Use Shared, constant and/or texture memory when possible.

- ❑ Be careful with *if statements* – avoid thread divergence.

- ❑ If it is possible, use single precision instead of double precision arithmetic. In Fermi GPUs, single precision operation rate is 2x higher than the double precision one.

- ❑ Use all the available resources (GPU + CPU).



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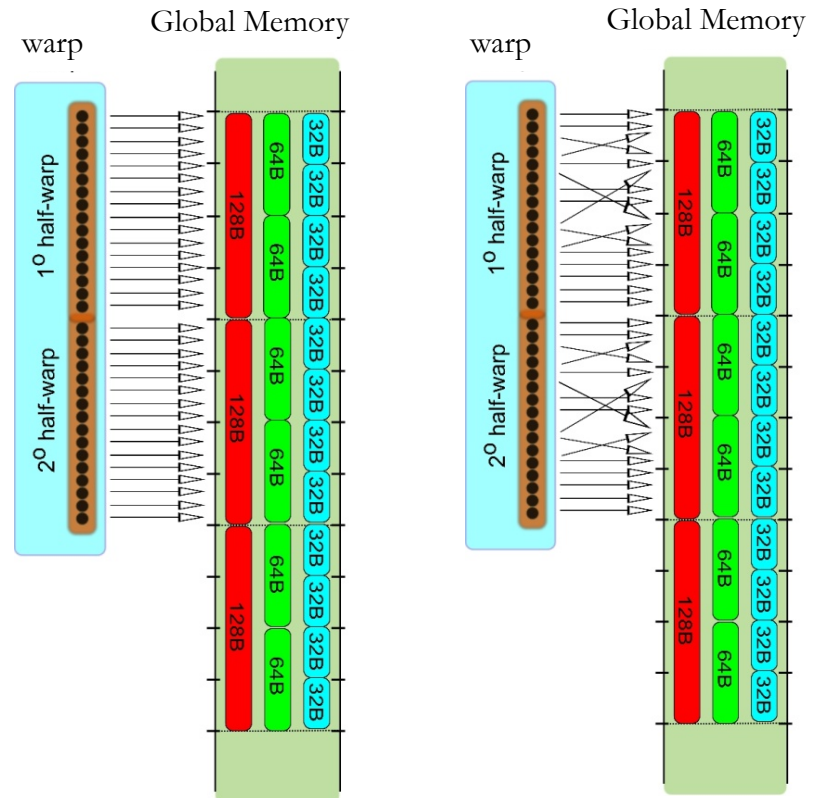
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Coalesced memory access



Piece of advice

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- ❑ Use all the available resources (GPU + CPU).

```
1 Some Instructions A
2 if (logical_statement) {
3     Some Instructions B
4 }
5 else if (another_logical_statement) {
6     Some Instructions C
7 }
8 else {
9     Some Instructions D
10 }
11 Some Instructions E
```



Piece of advice

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$$\underbrace{\underbrace{\frac{\partial \vec{R}}{\partial \vec{U}}}_{\text{SPA}} \Delta \vec{U}}_{\text{MPA}} = \underbrace{-R(\vec{U})}_{\text{DPA}}$$
$$\vec{U}^{n+1} = \vec{U}^n + \Delta \vec{U}$$



Piece of advice

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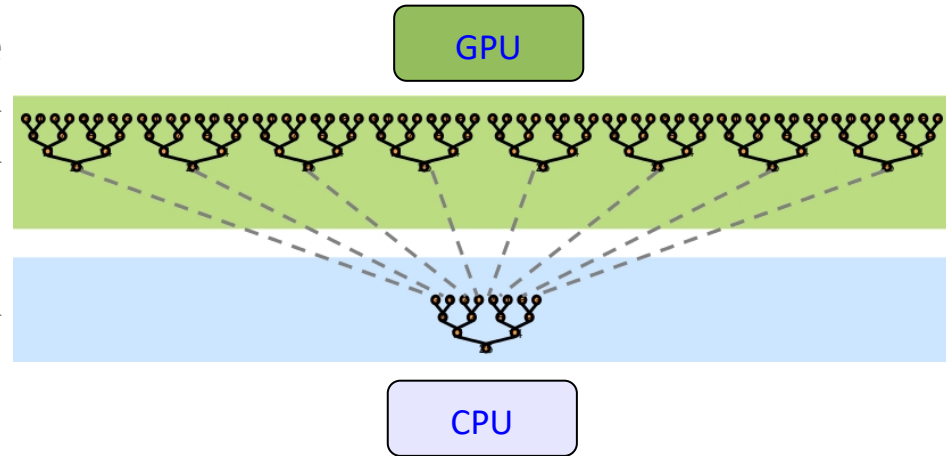
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- ❑ Use all the available resources (GPU + CPU).



Dot product: CPU implementation

```
#include <iostream>

int main()
{
    constexpr long size = 10000;

    // Memory allocations & initialization :
    double* A = new double[size];
    double* B = new double[size];

    for (auto i=0; i < size; i++) A[i] = (double)i;
    for (auto i=0; i < size; i++) B[i] = (double)(size-i);

    // Dot product :
    double C = 0.0;
    for (auto i=0; i < size; i++) {
        C += A[i]*B[i];
    }
    std::cout << "DOT PRODUCT = " << C << std::endl;

    // Memory deallocations :
    if (A != nullptr) delete[] A; A = nullptr;
    if (B != nullptr) delete[] B; B = nullptr;

    return 0;
}
```

Dot product: GPU implementation (1/7)

`_device_ double _C;`

Static variable

```
int main()
{
    constexpr long size = 10000;

    // Memory allocations & initialization :
    double* A = (double*)alloc_managed_mem(size*sizeof(double), "A");
    double* B = (double*)alloc_managed_mem(size*sizeof(double), "B");

    for (auto i=0; i < size; i++) A[i] = (double)i;
    for (auto i=0; i < size; i++) B[i] = (double)(size-i);

    // Compute dot product:
    double C = 0.0;
    cudaMemcpyToSymbol(_C,&C,sizeof(double)); // STEP1: Initializes _C

    constexpr int blockSize = 1024;
    constexpr int gridSize = 1000;
    dotProductGPU <<< gridSize, blockSize >>> (size,A,B); // STEP2: Computes dot product, stored in _C

    cudaMemcpyFromSymbol(&C,_C,sizeof(double)); // STEP3: Copy result from device

    cudaError_t err = cudaGetLastError();
    if (err != cudaSuccess) std::cerr << " Launch failure: " << cudaGetErrorString(err) << std::endl;
    if (err != cudaSuccess) exit(1);

    std::cout << "DOT PRODUCT = " << C << std::endl;

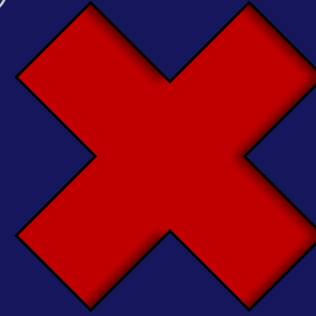
    // Memory deallocations :
    if (A != nullptr) cudaFree(A); A = nullptr;
    if (B != nullptr) cudaFree(B); B = nullptr;

    return 0;
}
```

Dot product: GPU implementation (2/7)

```
__global__ void dotProductGPU(const long size, double* _A, double* _B)
{
    const long i = blockDim.x*blockIdx.x + threadIdx.x;
    if (i < size) {
        _C += _A[i] * _B[i];
    }
}
```

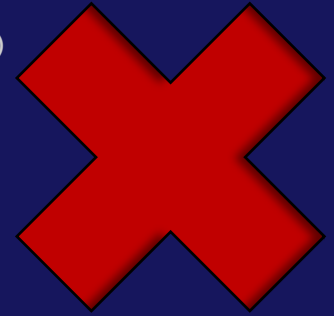
Memory conflict



Dot product: GPU implementation (3/7)

```
__global__ void dotProductGPU(const long size, double* _A, double* _B, double& _C)
{
    const long i = blockDim.x*blockIdx.x + threadIdx.x;
    if (i < size) {
        _C += _A[i] * _B[i];
    }
}
```

Passing arguments by
reference is invalid



Dot product: GPU implementation (4/7)

```
__global__ void dotProductGPU(const long size, double* _A, double* _B)
{
    const long i = blockDim.x*blockIdx.x + threadIdx.x;
    if (i < size) {
        const double partial_sum = _A[i] * _B[i];
        atomicAdd(&_C,partial_sum);
    }
}
```

```
__global__ void dotProductGPU(const long size, double* _A, double* _B)
{
    double partial_sum = 0.0;
    for (long i = blockDim.x*blockIdx.x + threadIdx.x; ; i += blockDim.x)
    {
        if (i < size) {
            partial_sum += _A[i] * _B[i];
        }
        else break;
    }
    atomicAdd(&_C,partial_sum);
}
```

Dot product: GPU implementation (5/7)

```
__global__ void dotProductGPU(const long size, double* _A, double* _B)
{
```

```
    double partial_sum = 0.0;
    for (long i = blockDim.x*blockIdx.x + threadIdx.x; ; i += blockDim.x*blockDim.x)
    {
        if (i < size) {
            partial_sum += _A[i] * _B[i];
        }
        else break;
    }
```

```
    block_reduction(partial_sum);
```

Block-wise reduction

```
    if (threadIdx.x == 0) atomicAdd(&_C, partial_sum);
```

Only the first thread per block performs atomicAdd

```
__device__ void block_reduction(double& partial_sum)
{
```

```
    constexpr int blockSize = 1024;
    if (blockSize != blockDim.x) printf("Invalid block size\n");
```

```
    __shared__ double partial_sums[blockSize];
    partial_sums[threadIdx.x] = partial_sum;
```

Static allocation; the allocation size should be known at compile time

```
    __syncthreads();
```

```
    if (threadIdx.x == 0) {
        for (int iThread=1; iThread < blockDim.x; iThread++) partial_sum += partial_sums[iThread];
    }
```

```
}
```



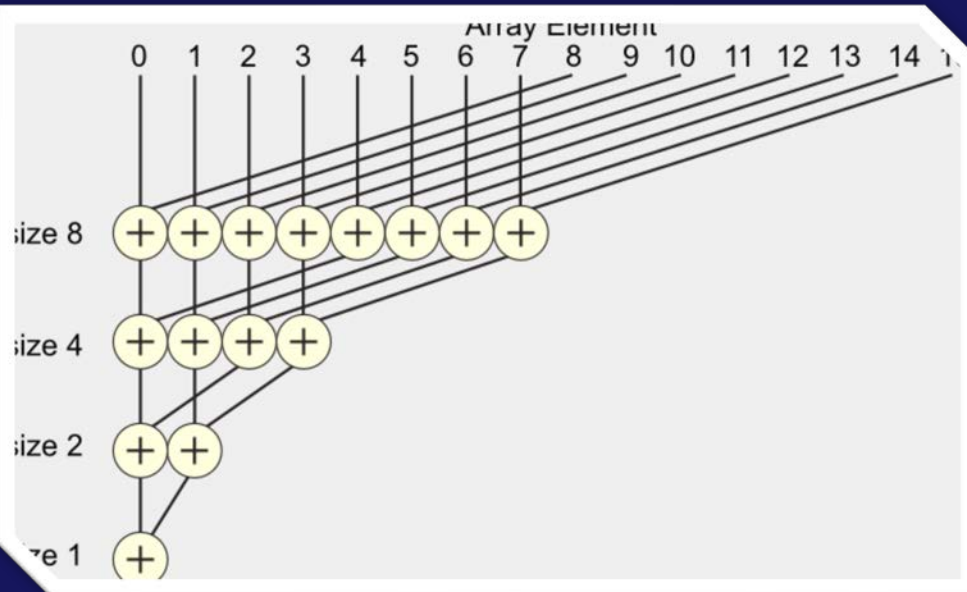
Dot product: GPU implementation (6/7)

```
__device__ void block_reduction(double& partial_sum)
{
    constexpr int blockSize = 1024;
    if (blockSize != blockDim.x) printf("Invalid block size\n");

    __shared__ double partial_sums[blockSize];
    partial_sums[threadIdx.x] = partial_sum;

    for (int stride=blockDim.x/2; stride > 0; stride /= 2) {
        __syncthreads();
        if (threadIdx.x < stride)
            partial_sums[threadIdx.x] += partial_sums[threadIdx.x + stride];
    }

    if (threadIdx.x == 0) {
        partial_sum = partial_sums[0];
    }
}
```



Dot product: GPU implementation (7/7)

```
#define FULL_MASK 0xffffffff
```

```
__device__ void block_reduction(double& partial_sum)
{
    // Warp-wise reduction:
    const int iWarp    = threadIdx.x / warpSize;          // Warp ID within the block
    const int iThread  = threadIdx.x - warpSize*iWarp;    // Thread ID within the warp

    for (int stride=warpSize/2; stride > 0; stride /= 2) {
        partial_sum += __shfl_down_sync(FULL_MASK, partial_sum, stride);
    }

    // Block-wise reduction:
    const int nbWarps = blockDim.x / warpSize;

    __shared__ double partial_sums[32];
    if (iThread == 0) partial_sums[iWarp] = partial_sum;

    for (int stride=nbWarps/2; stride > 0; stride /= 2) {
        __syncthreads();
        if (iThread == 0 && iWarp < stride) partial_sums[iWarp] += partial_sums[iWarp + stride];
    }

    if (threadIdx.x == 0) {
        partial_sum = partial_sums[0];
    }
}
```

Matrix-matrix multiplication

```
class Matrix
{
public:
    Matrix(const int ni, const int nj, const double value = NAN);
    Matrix(const Matrix& matrix);
    ~Matrix();

private:
    int ni_ = 0;
    int nj_ = 0;
    double* values_ = nullptr;

public:
    __host__ void random_init() const;
    __host__ __device__ bool is_valid(const int i, const int j) const;

    __host__ __device__ int ni() const { return ni_; }
    __host__ __device__ int nj() const { return nj_; }

    __host__ __device__ double& operator()(const int i, const int j){ return values_[i*nj_+j]; }
    __host__ __device__ double operator()(const int i, const int j) const { return values_[i*nj_+j]; }
};
```

```
matrixMultGPU <<< gridSize, blockSize >>> (A,B,C);
```

Kernel launch

Matrix-matrix multiplication

```
Matrix::Matrix(const int ni, const int nj, const double value)
```

```
: ni_(ni), nj_(nj)
```

```
{
```

```
    values_ = (double*)alloc_managed_mem(ni*nj*sizeof(double), "Matrix::Elements");
```

```
    for (int index=0; index < ni*nj; index++) values_[index] = value;
```

```
}
```

Allocate managed memory

```
Matrix::Matrix(const Matrix& matrix)
```

```
{
```

```
    ni_ = matrix.ni_;
```

```
    nj_ = matrix.nj_;
```

```
    values_ = matrix.values_;
```

```
}
```

Shallow copy

```
Matrix::~~Matrix()
```

```
{
```

```
    cudaFree(values_);
```

```
}
```

Free memory by
using cudaFree



Matrix-matrix multiplication

```
int main()
{
    constexpr int NI = 150;
    constexpr int NJ = 200;
    constexpr int NK = 120;

    Matrix A(NI,NJ), B(NJ,NK), C(NI,NK,0.0);

    A.random_init();
    B.random_init();

    for (int i=0; i < C.ni(); i++)
    for (int j=0; j < C.nj(); j++)
    {
        for (int k=0; k < A.nj(); k++)
        {
            C(i,j) += A(i,k)*B(k,j);
        }
    }

    return 0;
}
```

Matrix-matrix multiplication

```
int main()
{
    constexpr int NI = 150;
    constexpr int NJ = 200;
    constexpr int NK = 120;

    Matrix A(NI,NJ), B(NJ,NK), C(NI,NK,0.0);

    A.random_init();
    B.random_init();

    dim3 gridSize, blockSize = {32,32};
    gridSize.x = (C.ni()+blockSize.x-1)/blockSize.x;
    gridSize.y = (C.nj()+blockSize.y-1)/blockSize.y;
    matrixMultGPU <<< gridSize, blockSize >>> (A,B,C);

    cudaDeviceSynchronize();
    cudaError_t err = cudaGetLastError();
    if (err != cudaSuccess) {
        std::cerr << " Launch failure: " << cudaGetErrorString(err) << std::endl;
        exit(1);
    }

    return 0;
}
```

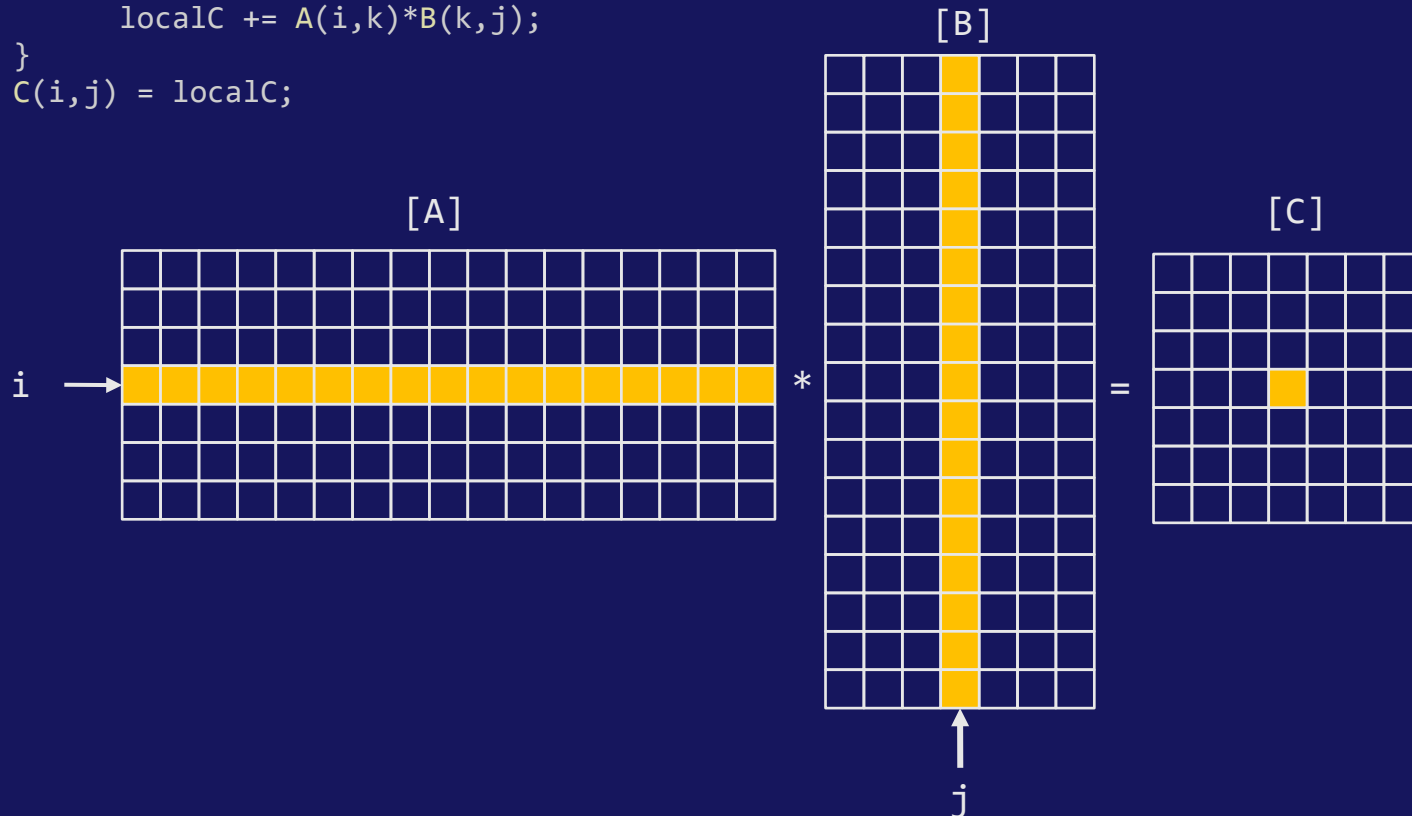
Matrix-matrix multiplication

```
__global__ void matrixMultGPU(Matrix A, Matrix B, Matrix C)
{
    const int i = blockDim.x*blockIdx.x + threadIdx.x;
    const int j = blockDim.y*blockIdx.y + threadIdx.y;

    if (i < C.ni() && j < C.nj())
    {
        double localC = 0.0;
        for (int k=0; k < A.nj(); k++)
        {
            localC += A(i,k)*B(k,j);
        }
        C(i,j) = localC;
    }
}
```



**Low
performance**



Matrix-matrix multiplication

Row-major order: $\text{index} \leftarrow i * M + j$

The diagram illustrates a 2D array structure. It shows a horizontal sequence of cells representing the first two rows of an $[N \times M]$ array. The first row, labeled "1st row", contains cells with coordinates $(0,0)$, $(0,1)$, $(0,2)$, an ellipsis, $(0,M-1)$, and then the second row, labeled "2nd row", starts with $(1,0)$, $(1,1)$, $(1,2)$, an ellipsis, and $(1,M-1)$. The entire sequence is labeled $[N \times M]$ at the top left.

column-major order: $iThread \leftarrow threadIdx.y * blockDim.y + threadIdx.x$

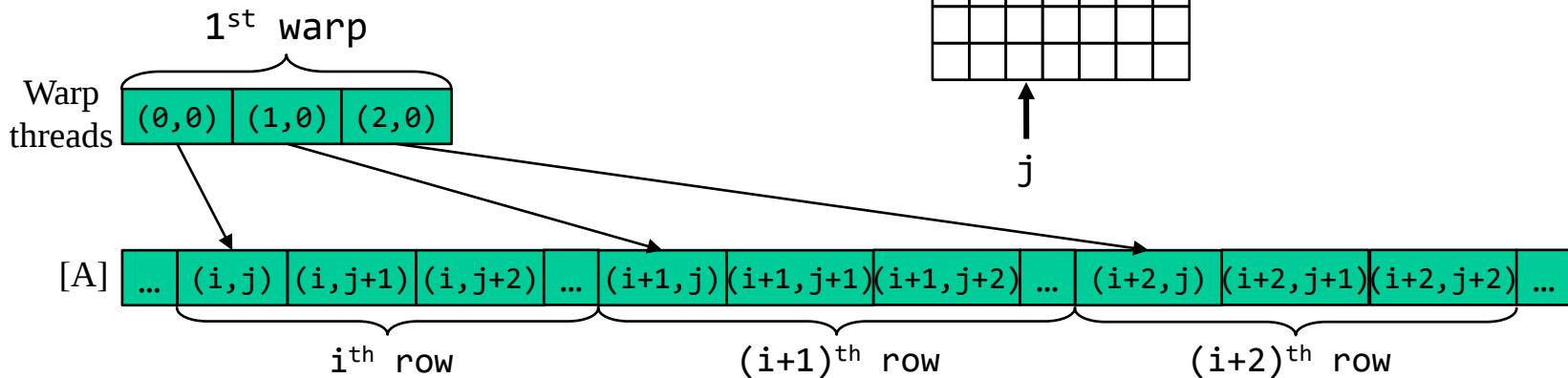
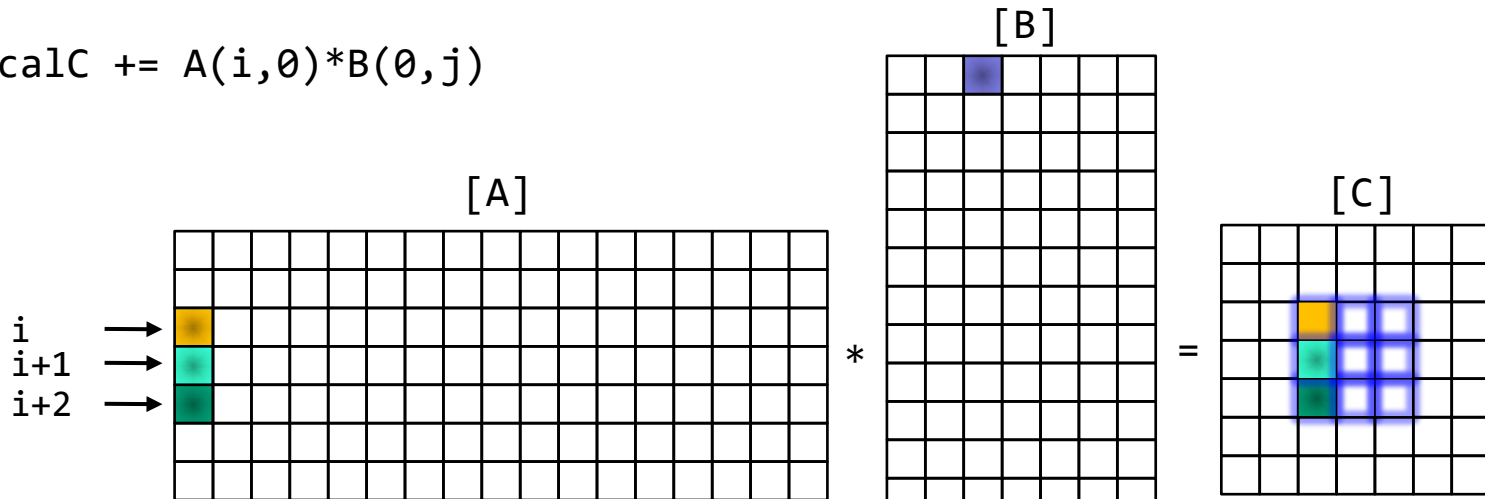
Warp threads

$(0,0)$	$(1,0)$	$(2,0)$	...	$(31,0)$	$(0,1)$	$(1,1)$	$(2,1)$	...	$(31,1)$	...
---------	---------	---------	-----	----------	---------	---------	---------	-----	----------	-----

1st warp 2nd warp

Matrix-matrix multiplication

```
localC += A(i,0)*B(0,j)
```

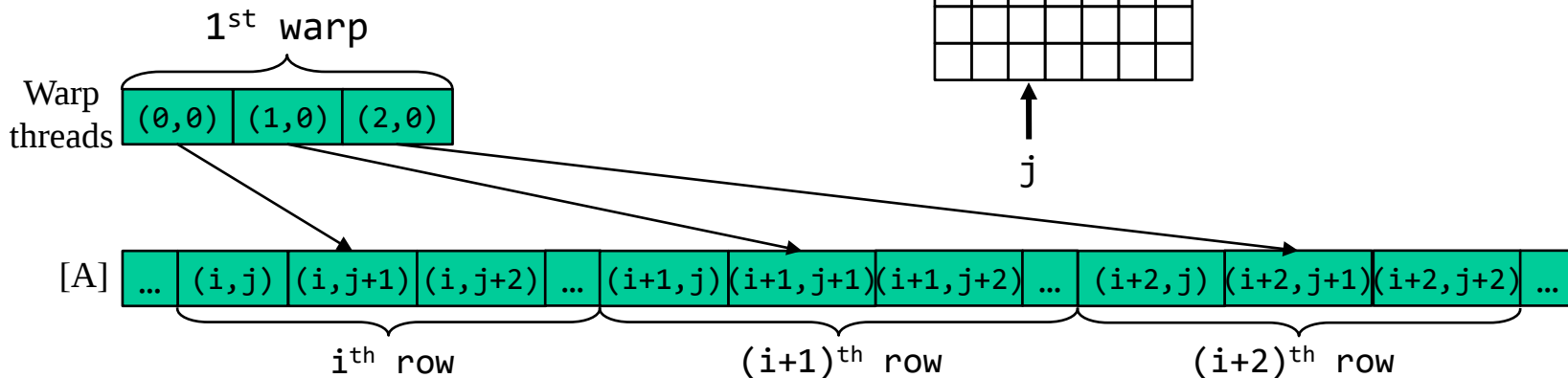
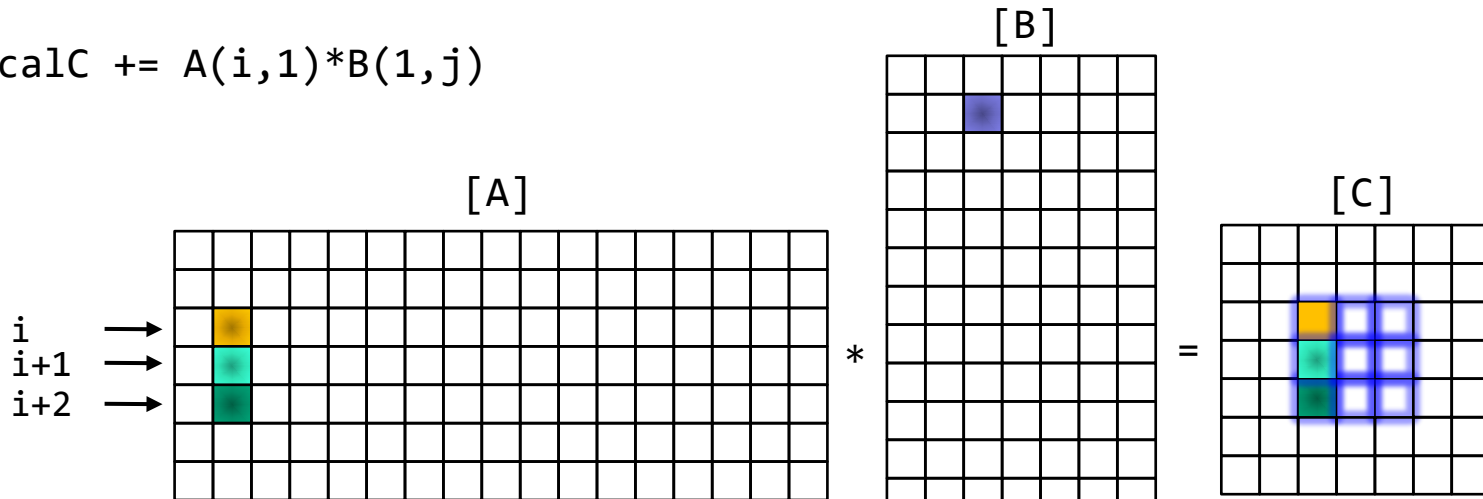


```
i = blockDim.x*blockIdx.x + threadIdx.x;  
j = blockDim.y*blockIdx.y + threadIdx.y;
```



Matrix-matrix multiplication

```
localC += A(i,1)*B(1,j)
```

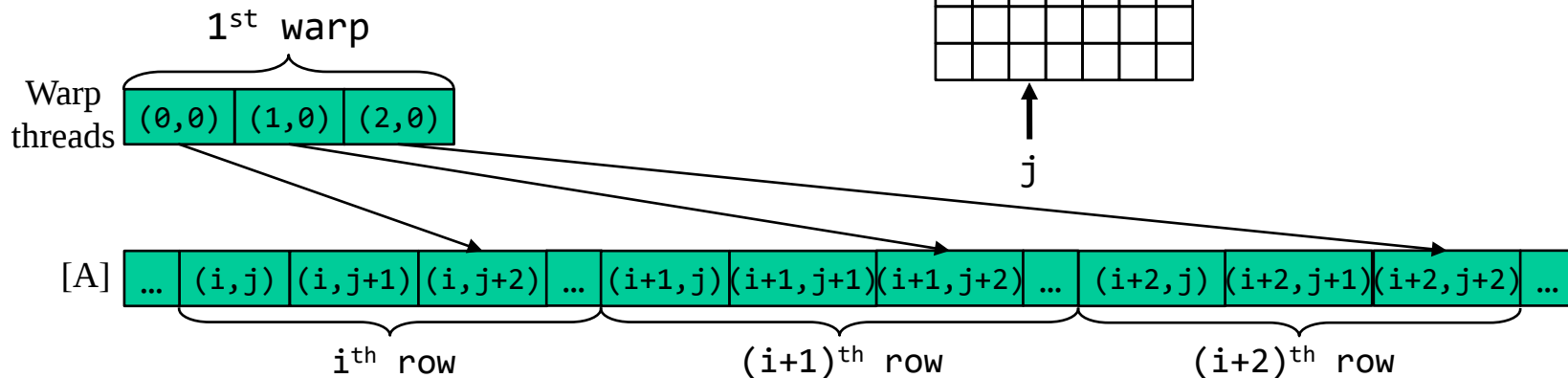
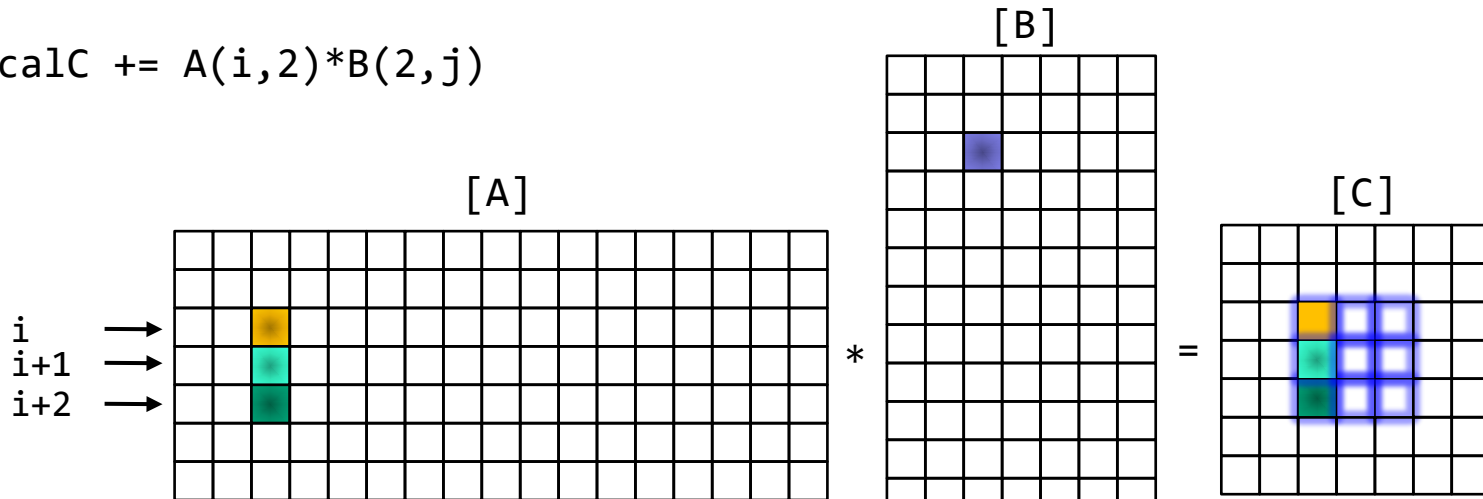


```
i = blockDim.x*blockIdx.x + threadIdx.x;
j = blockDim.y*blockIdx.y + threadIdx.y;
```



Matrix-matrix multiplication

```
localC += A(i,2)*B(2,j)
```



```
i = blockDim.x*blockIdx.x + threadIdx.x;  
j = blockDim.y*blockIdx.y + threadIdx.y;
```



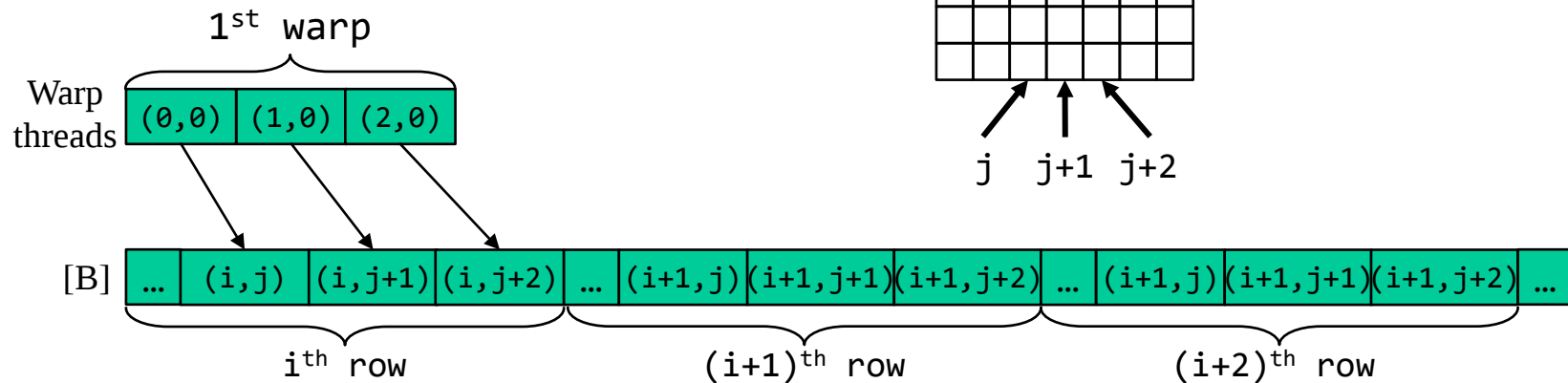
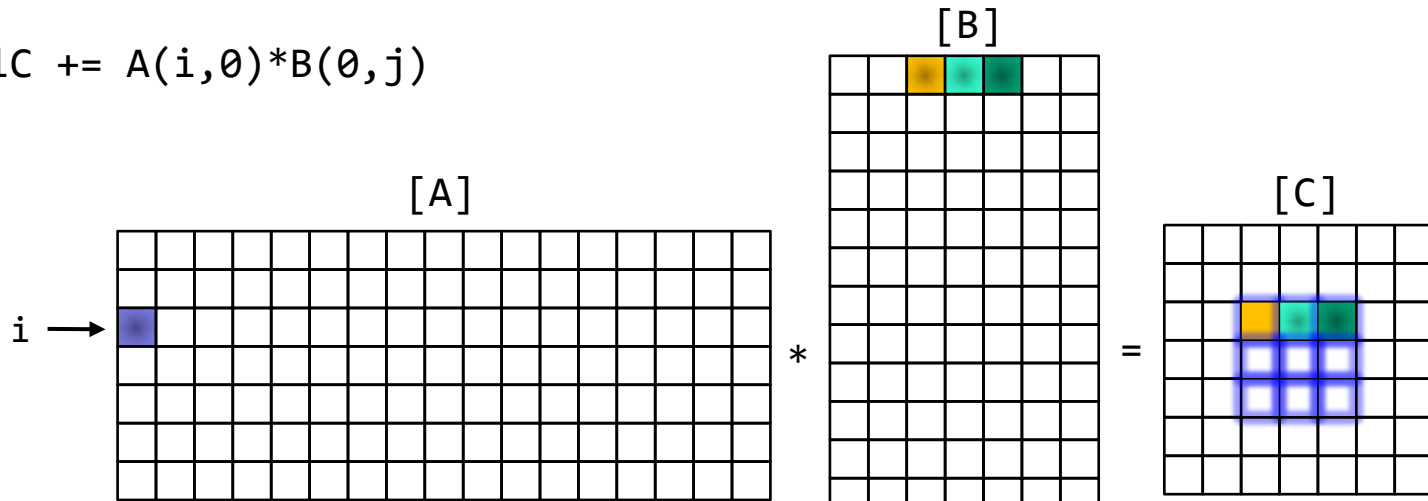
Matrix-matrix multiplication

```
gridSize.x = (C.nj()+blockSize.x-1)/blockSize.x;  
gridSize.y = (C.ni()+blockSize.y-1)/blockSize.y;
```

```
__global__ void matrixMultGPU(Matrix A, Matrix B, Matrix C)  
{  
    const int j = blockDim.x*blockIdx.x + threadIdx.x;  
    const int i = blockDim.y*blockIdx.y + threadIdx.y;  
  
    if (i < C.ni() && j < C.nj())  
    {  
        double localC = 0.0;  
        for (int k=0; k < A.nj(); k++)  
        {  
            localC += A(i,k)*B(k,j);  
        }  
        C(i,j) = localC;  
    }  
}
```

Matrix-matrix multiplication

```
localC += A(i,0)*B(0,j)
```

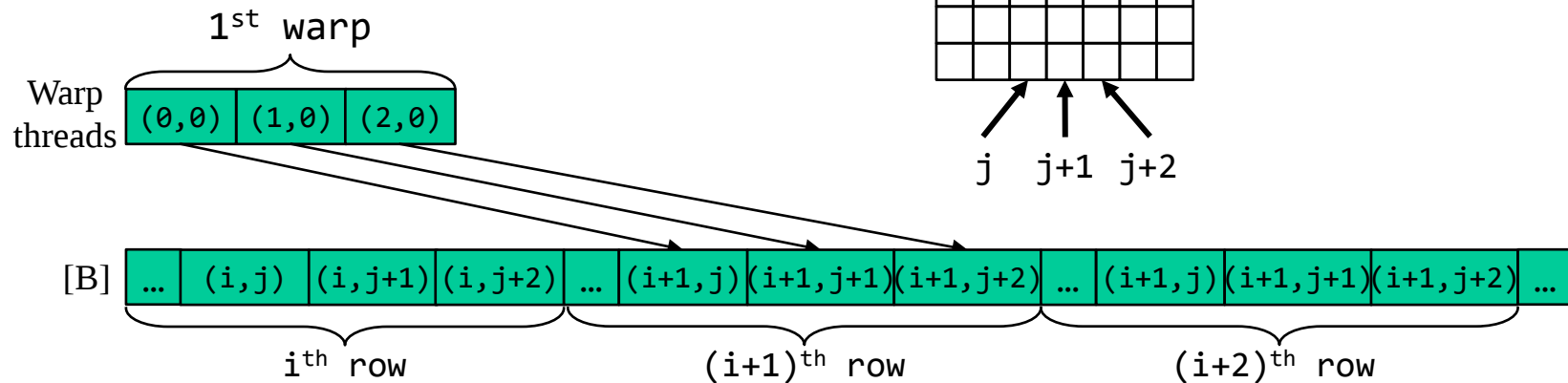
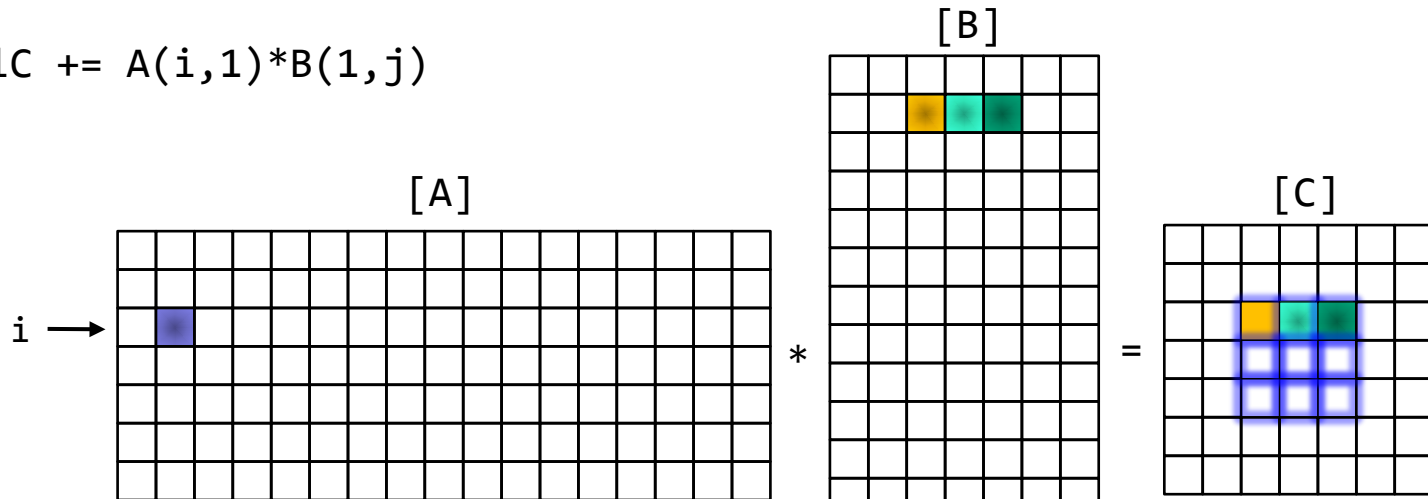


```
j = blockDim.x*blockIdx.x + threadIdx.x;
i = blockDim.y*blockIdx.y + threadIdx.y;
```



Matrix-matrix multiplication

```
localC += A(i,1)*B(1,j)
```

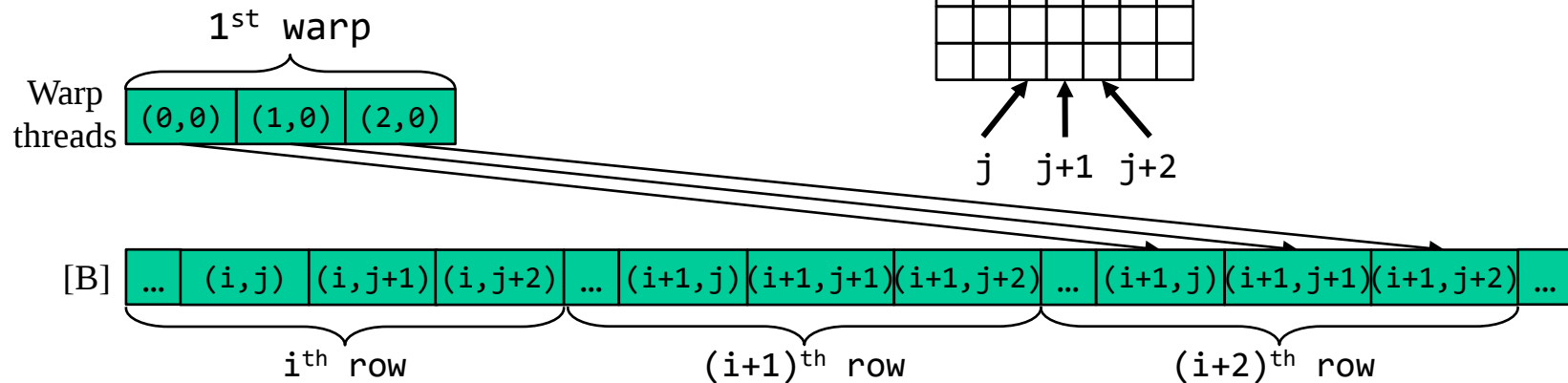
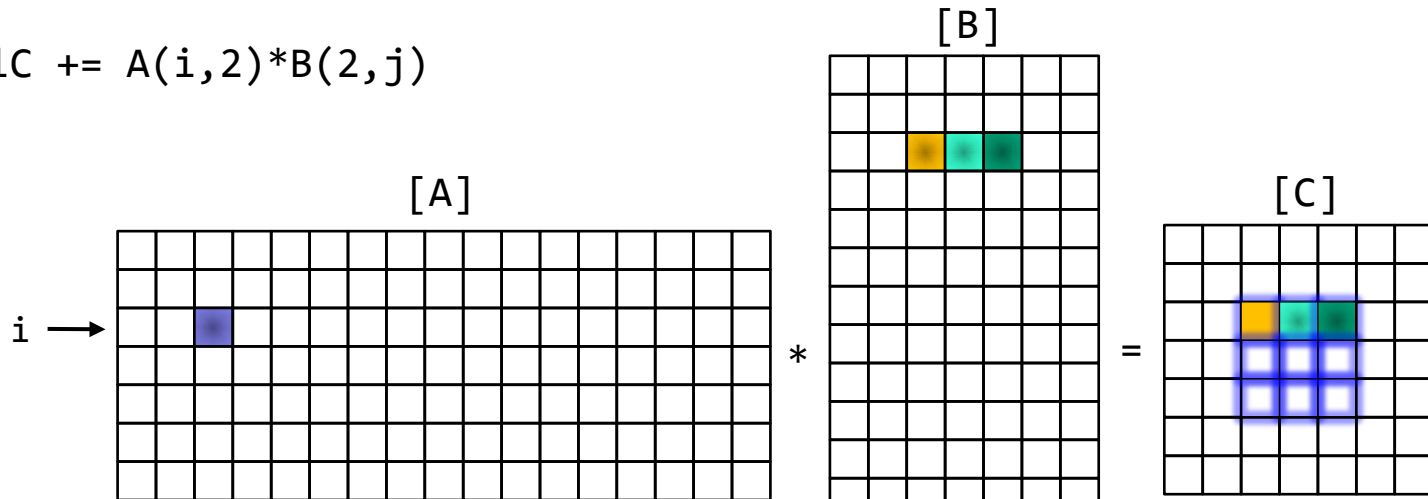


```
j = blockDim.x*blockIdx.x + threadIdx.x;  
i = blockDim.y*blockIdx.y + threadIdx.y;
```



Matrix-matrix multiplication

```
localC += A(i,2)*B(2,j)
```

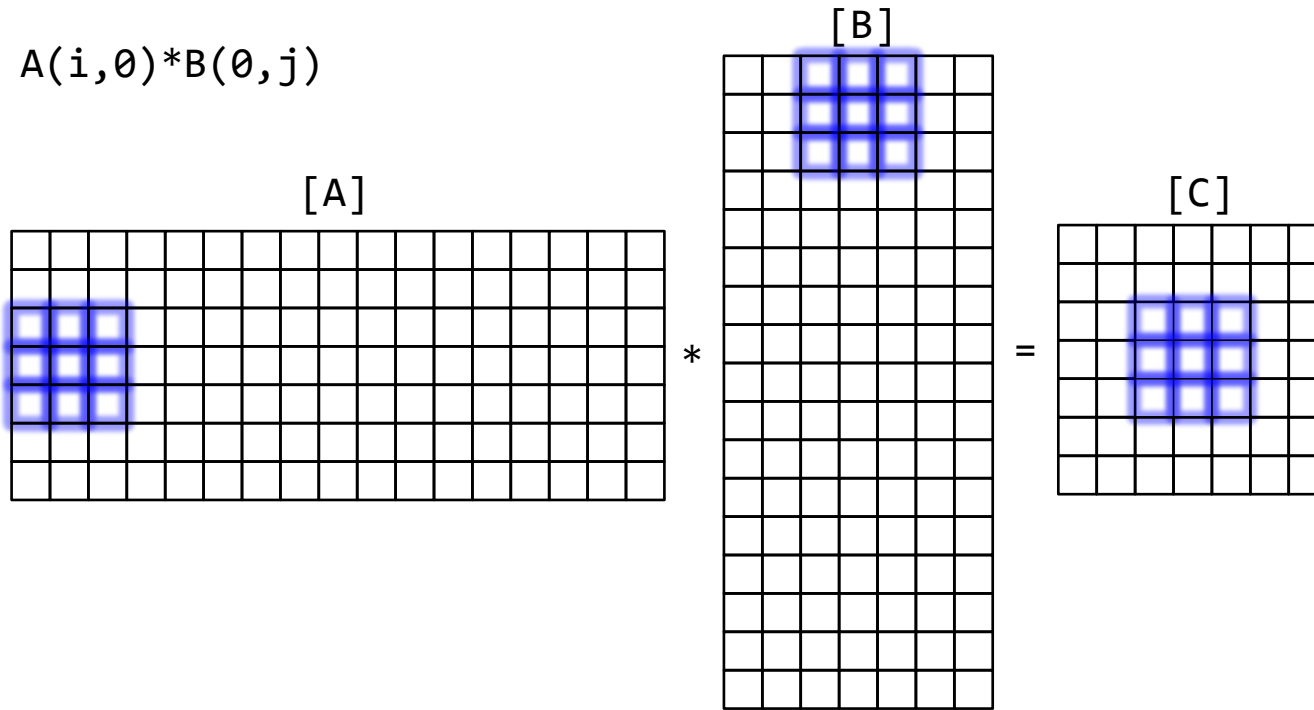


```
j = blockDim.x*blockIdx.x + threadIdx.x;
i = blockDim.y*blockIdx.y + threadIdx.y;
```



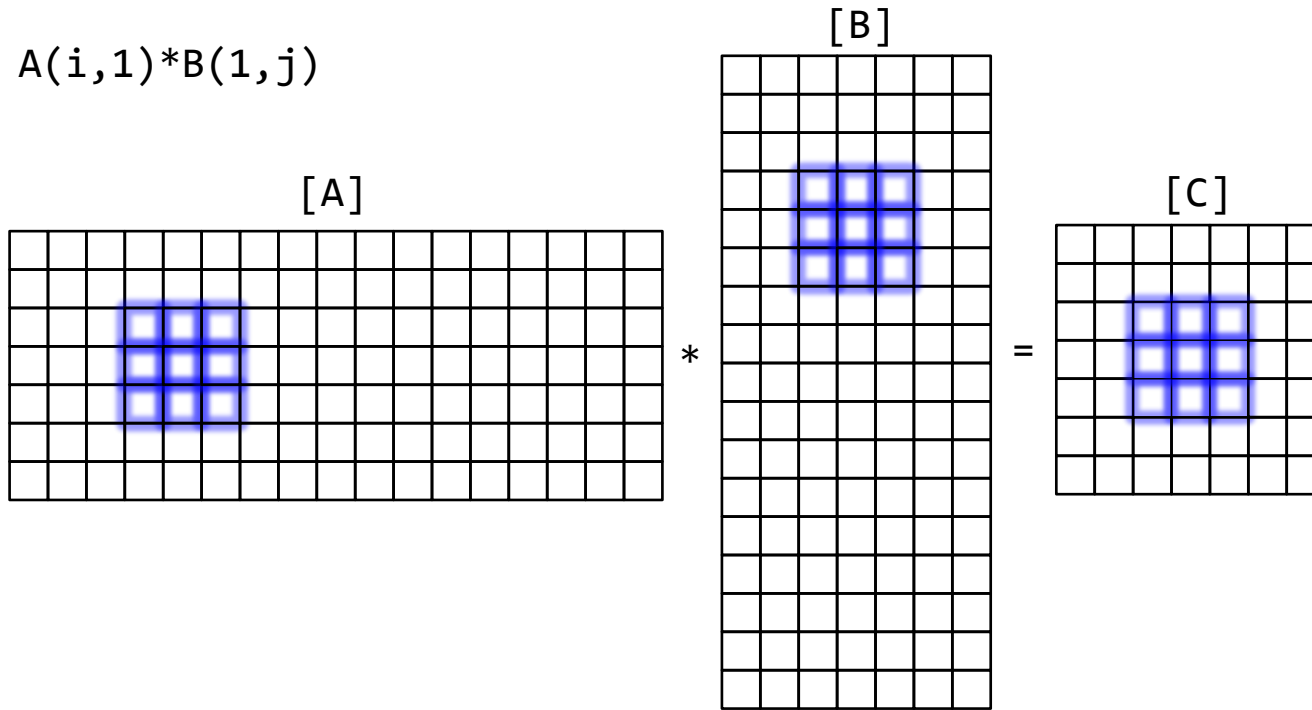
Matrix-matrix multiplication

`localC += A(i,0)*B(0,j)`



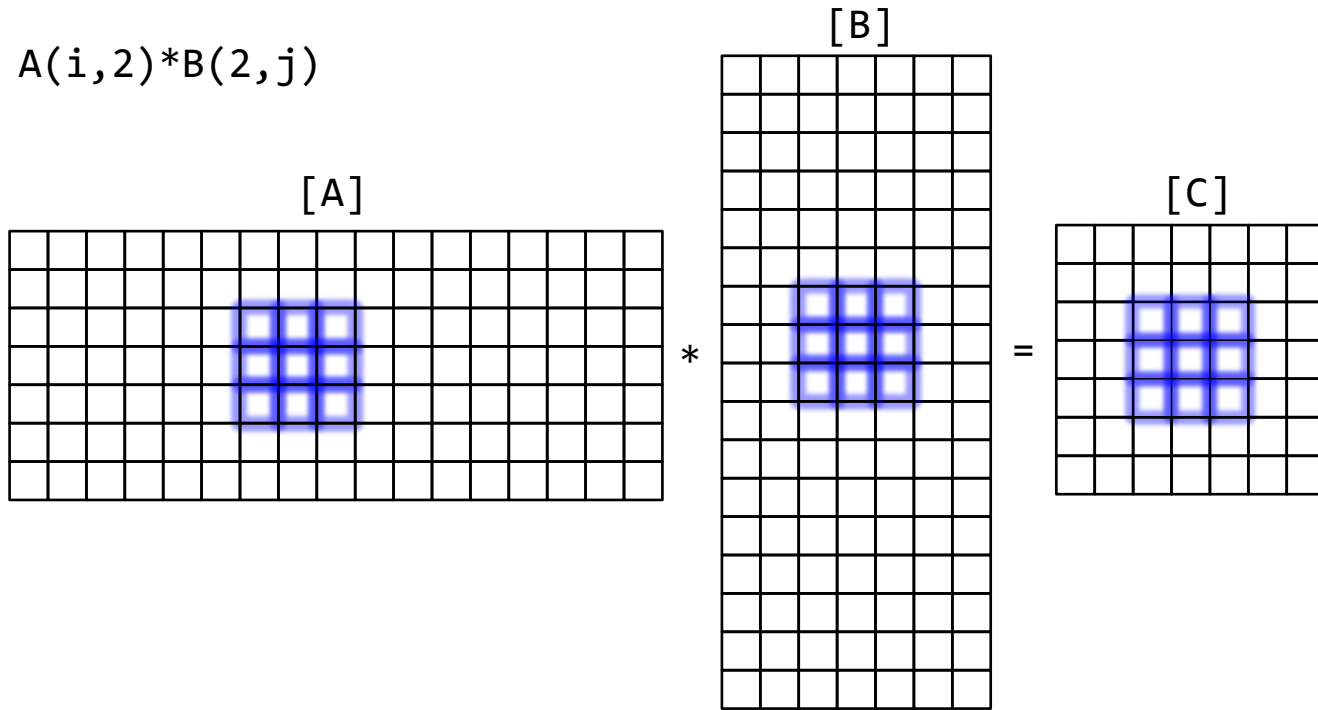
Matrix-matrix multiplication

`localC += A(i,1)*B(1,j)`



Matrix-matrix multiplication

`localC += A(i,2)*B(2,j)`



Matrix-matrix multiplication

```
__global__ void matrixMultGPU(Matrix A, Matrix B, Matrix C)
{
    const int j = blockDim.x*blockIdx.x + threadIdx.x;
    const int i = blockDim.y*blockIdx.y + threadIdx.y;

    constexpr short ts = 32;
    __shared__ double subA[ts][ts], subB[ts][ts];

    const int nbTiles = (A.nj()+ts-1)/ts;

    double localC = 0.0;
    for (int iTile=0; iTile < nbTiles; iTile++)
    {
        subA[threadIdx.y][threadIdx.x] = 0.0;
        subB[threadIdx.y][threadIdx.x] = 0.0;

        const int k = iTile*ts;
        if (A.is_valid(i,k+threadIdx.x) == true) subA[threadIdx.y][threadIdx.x] = A(i,k+threadIdx.x);
        if (B.is_valid(k+threadIdx.y,j) == true) subB[threadIdx.y][threadIdx.x] = B(k+threadIdx.y,j);
        __syncthreads();

        for (int l=0; l<ts; l++) {
            localC += subA[threadIdx.y][l] * subB[l][threadIdx.x];
        }
        __syncthreads();

        if (C.is_valid(i,j)) C(i,j) = localC;
    }
}
```

The barrier ensures that all block threads load submatrices of A and B into shared memory

The barrier ensures that no thread re-writes on shared memory until all threads have updated variable *localC*

*** More optimizations ...

Non-included items

- ❑ Multi-GPUs; same host controlling many GPUs connected to the same CPU via PCIe
- ❑ Pinned memory; enables threads to access host memory
- ❑ Cooperative groups; enable grid-level or even multigrid-level synchronizations
- ❑ Dynamic parallelism; enables kernel launches within kernels
- ❑ CUDA streams & events; enable kernel launches and memory copies to overlap
- ❑ Constant & Texture memory; Utilizes constant and texture caches, texture filtering and access models
- ❑ Tensor cores; cuBLAS & cuDNN libraries, TensorFlow & pyTorch deep-learning frameworks
- ❑ Libraries; cuBLAS, cuSPARCE, cuSOLVER, cuDNN, cuFFT, AMGX
- ❑ ...

