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Introduction to modern graphics processing units (GPU) architecture and programming in CUDA

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Why GPUs ?

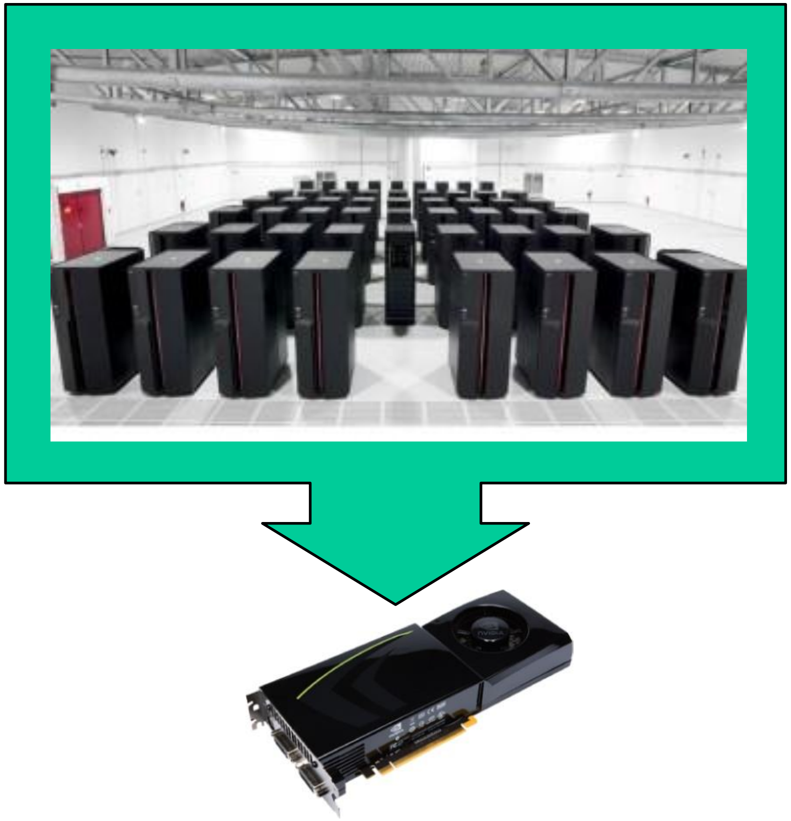
❑ Parallel processing units

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

❑ GPU embedded, low latency, RAM

❑ Various programming environments

❑ Low cost & energy consumption based on their computational power



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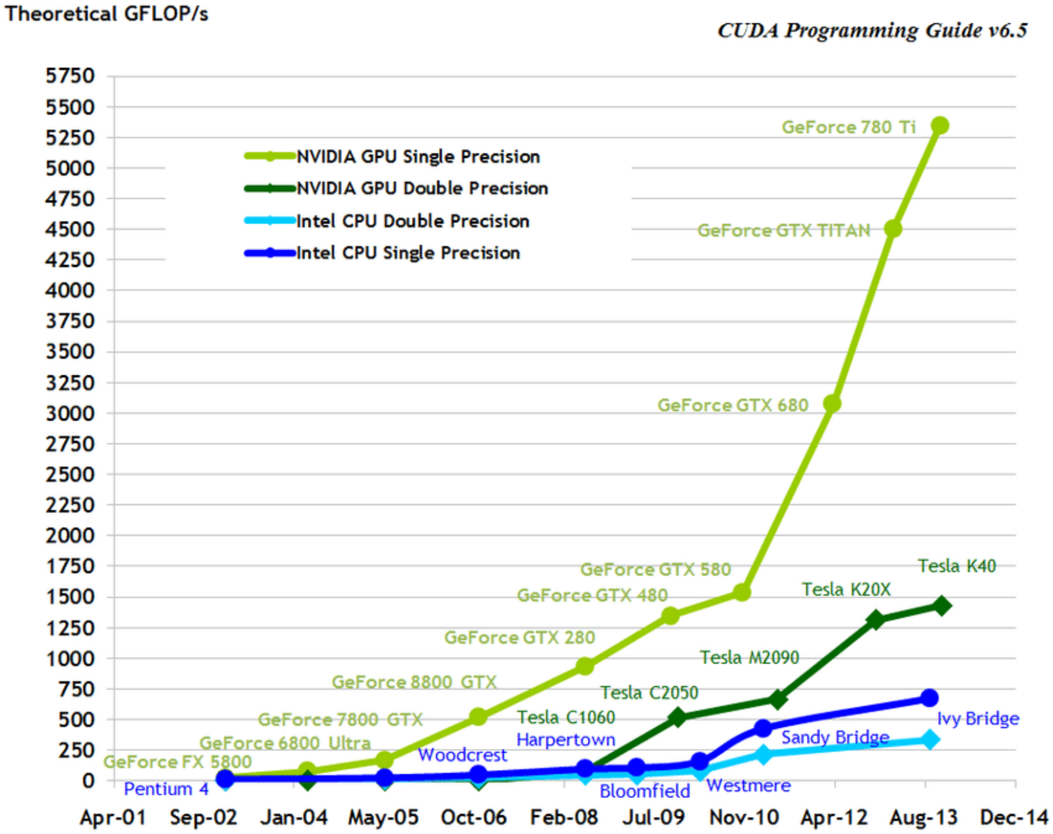

CUDA Programming Guide v6.5

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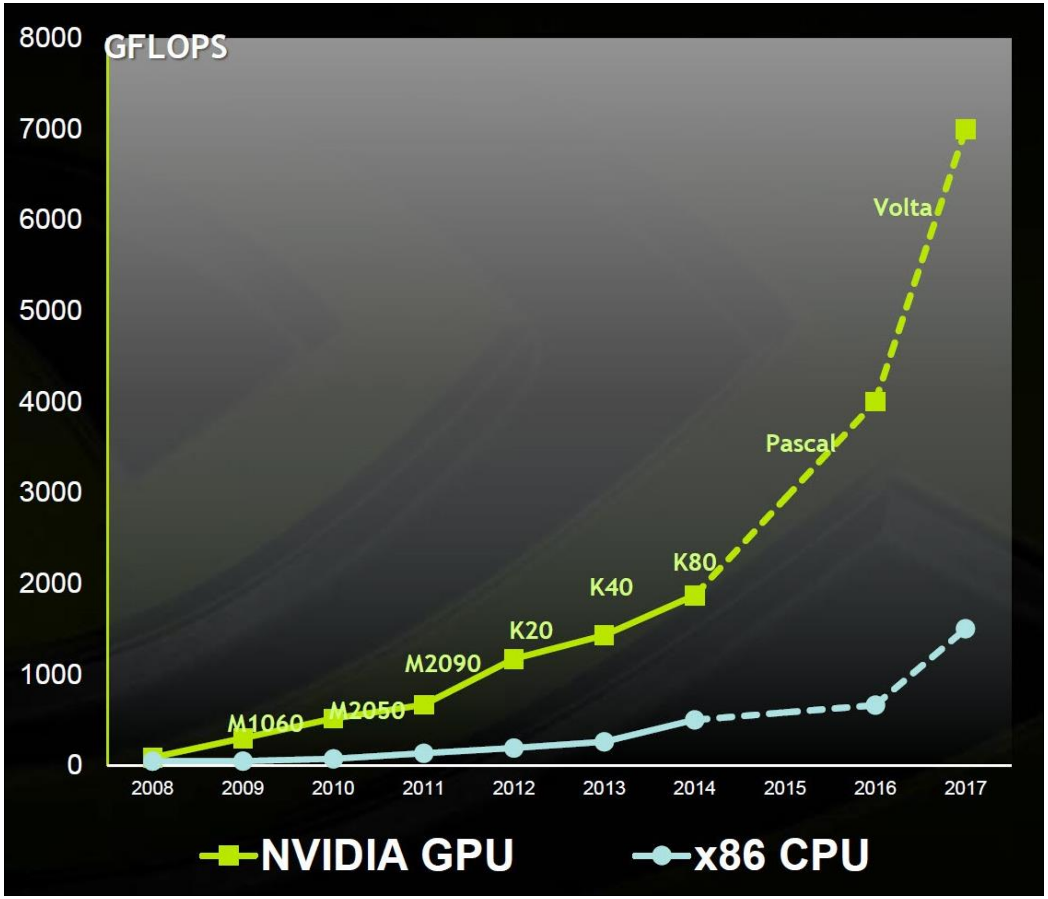

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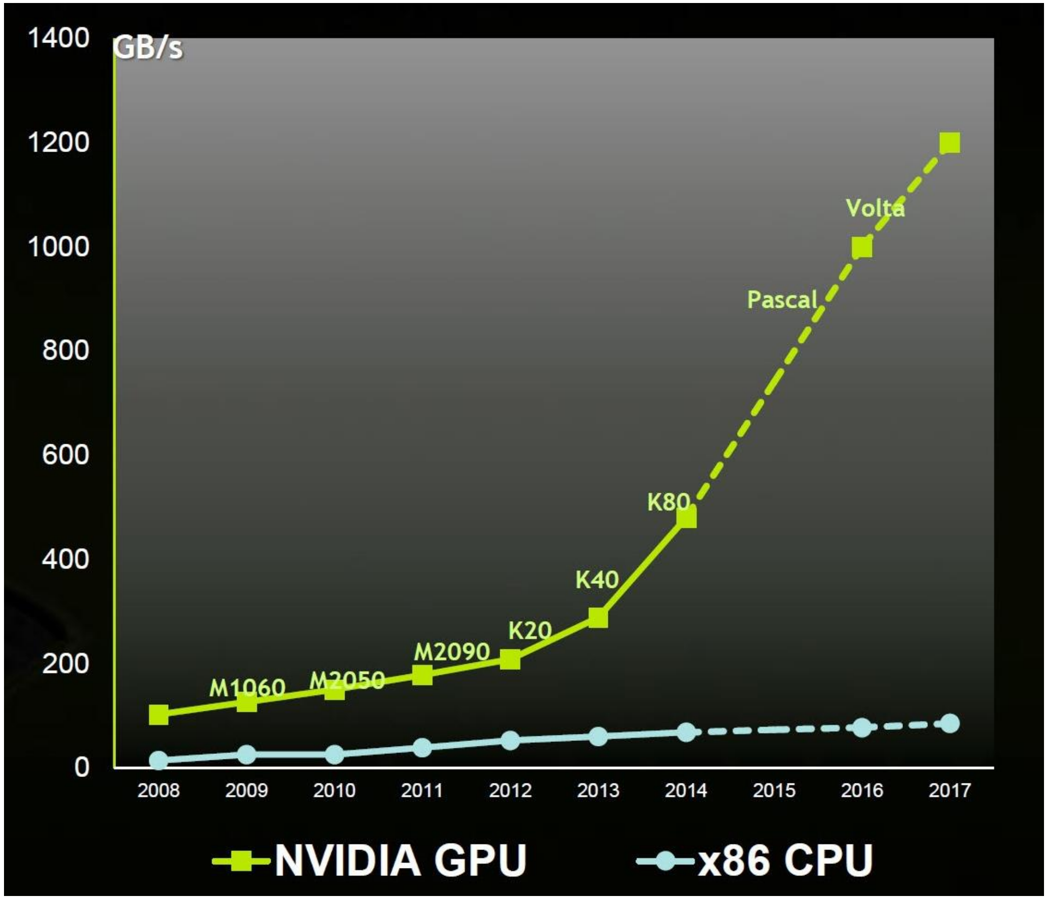

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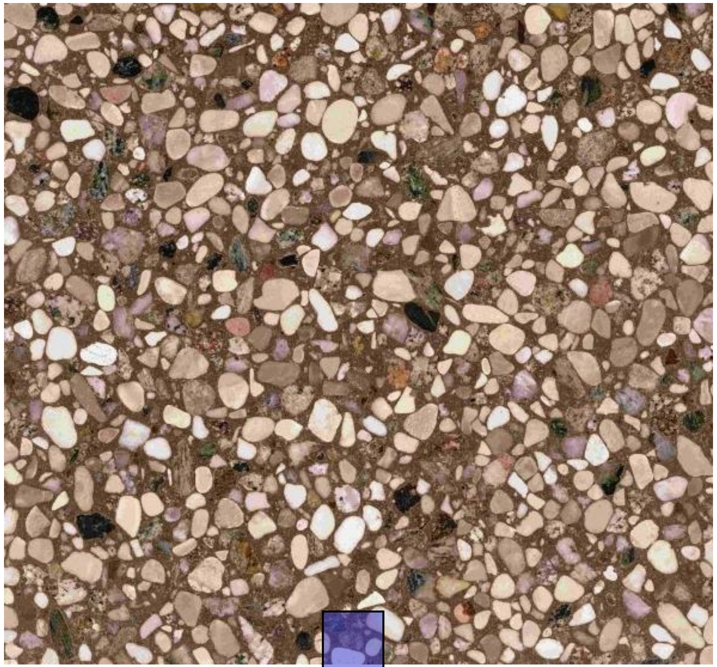
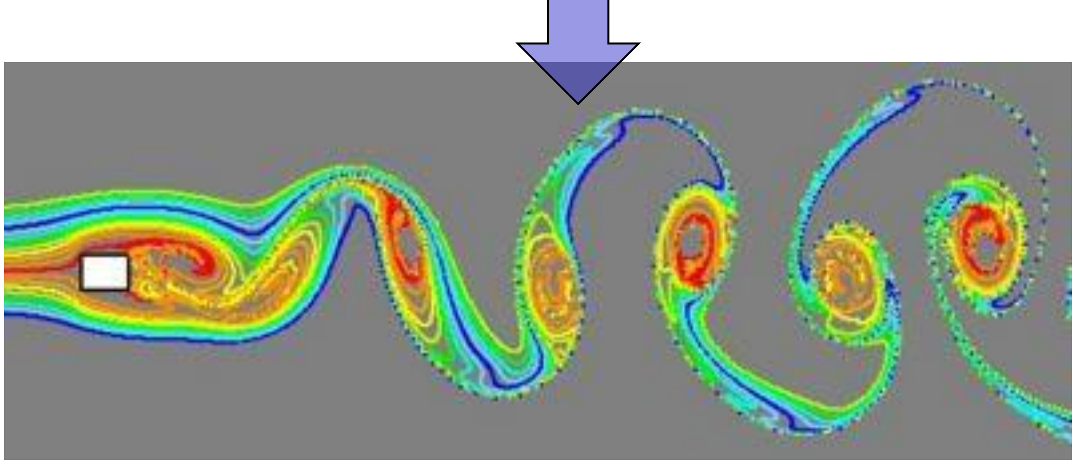


OpenCL: Cross platform implementation
- C++

CUDA: Developed by NVIDIA, specialized for NVIDIA GPUs
- C++
- FORTRAN
- Python



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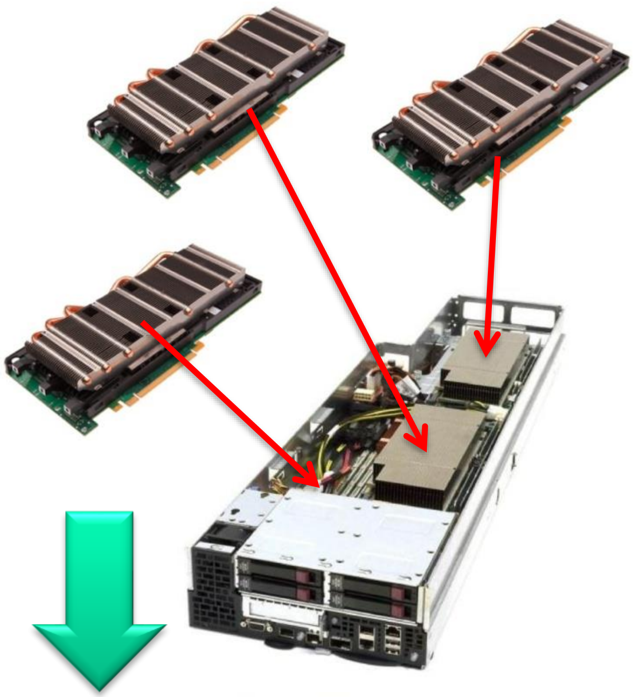

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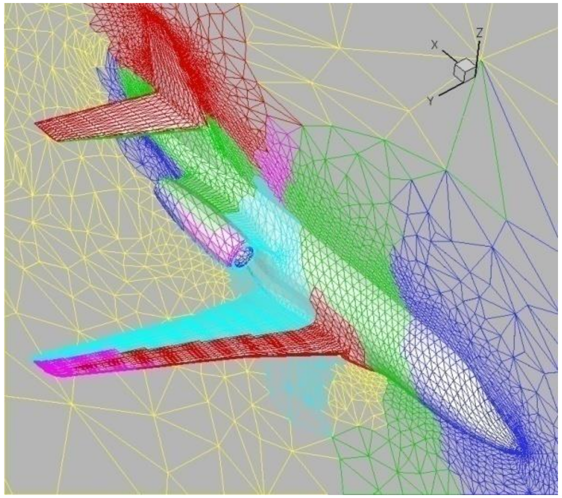
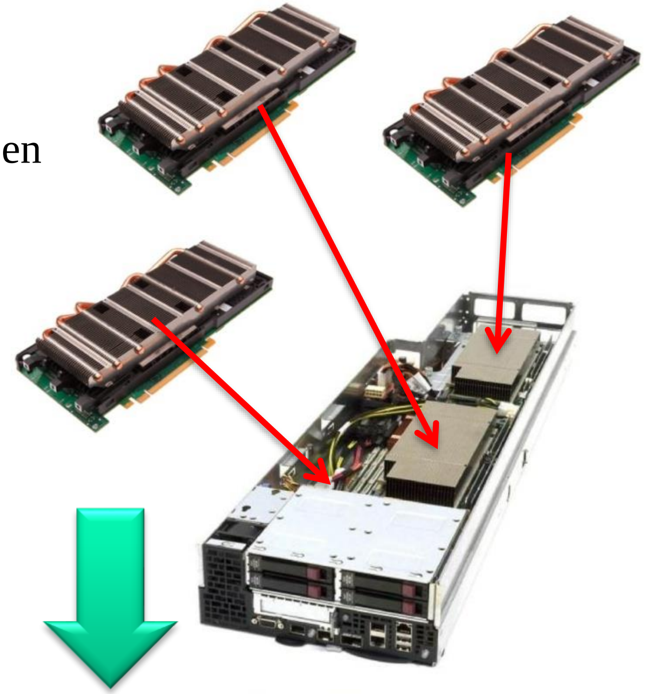


❑ 1 sub-domain per GPU.

❑ MPI → data transactions between GPUs on different computational nodes.

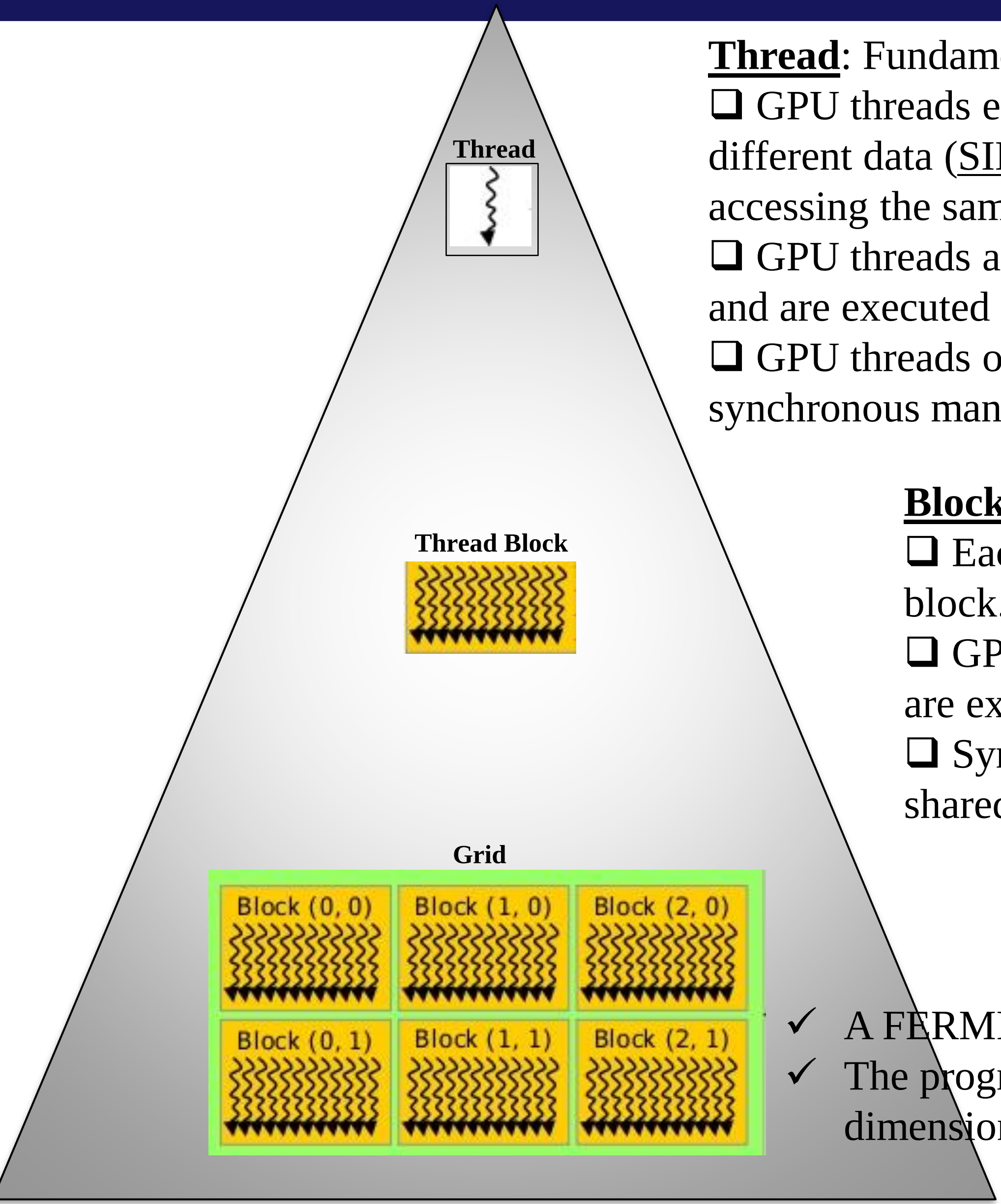
❑ Shared “host” memory → data transactions between GPUs on the same node.



Why GPUs ?

GPUs = Powerful, massively parallel CPU co-processors

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 grouped in 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.

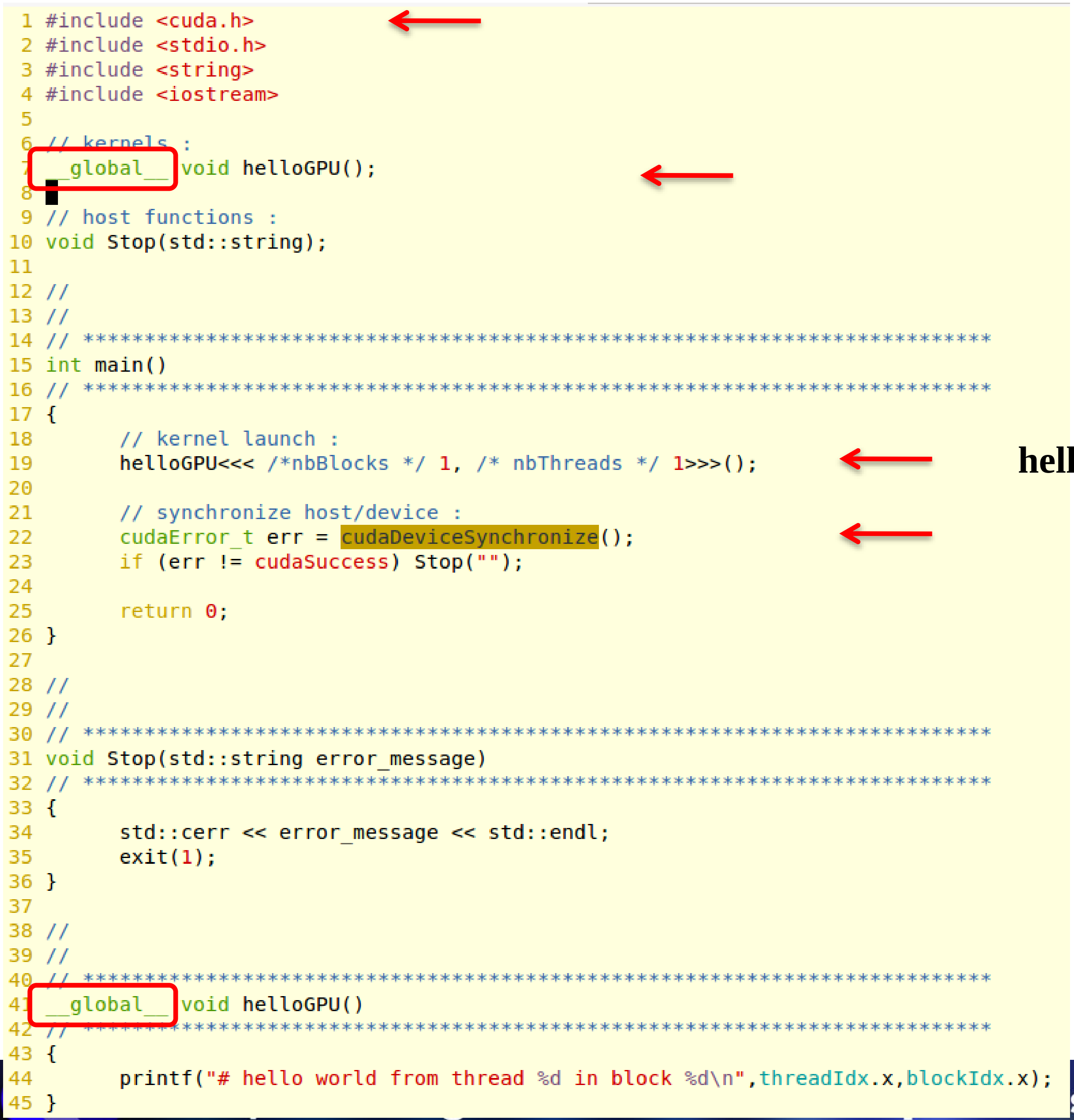
□ Synchronization and fast data transactions through shared memory

Grid: Cluster of thread blocks

✓ A FERMI GPU can execute up to 24,576 threads in parallel

✓ The programmer defines the thread block and grid dimensions

Hello World



```
#include <cuda.h>
#include <stdio.h>
#include <string>
#include <iostream>

// kernels :
__global__ void helloGPU();

// host functions :
void Stop(std::string);

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

        // synchronize host/device :
        cudaError_t err = cudaDeviceSynchronize();
        if (err != cudaSuccess) Stop("");

        return 0;
}

//
//
// **************************************************************************
void Stop(std::string error_message)
// **************************************************************************
{
        std::cerr << error_message << std::endl;
        exit(1);
}

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

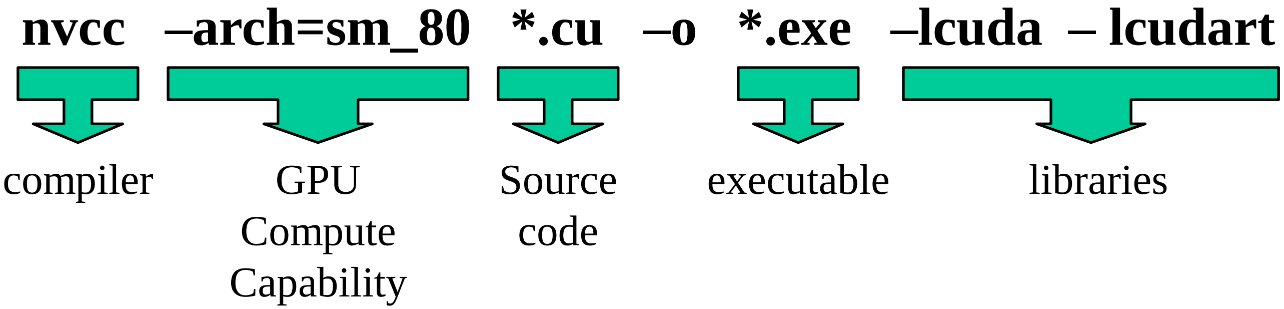
#include <cuda.h>

__global__ void helloGPU();

helloGPU<<<GridDim, BlockDim>>>();

Host-Device Synchronization

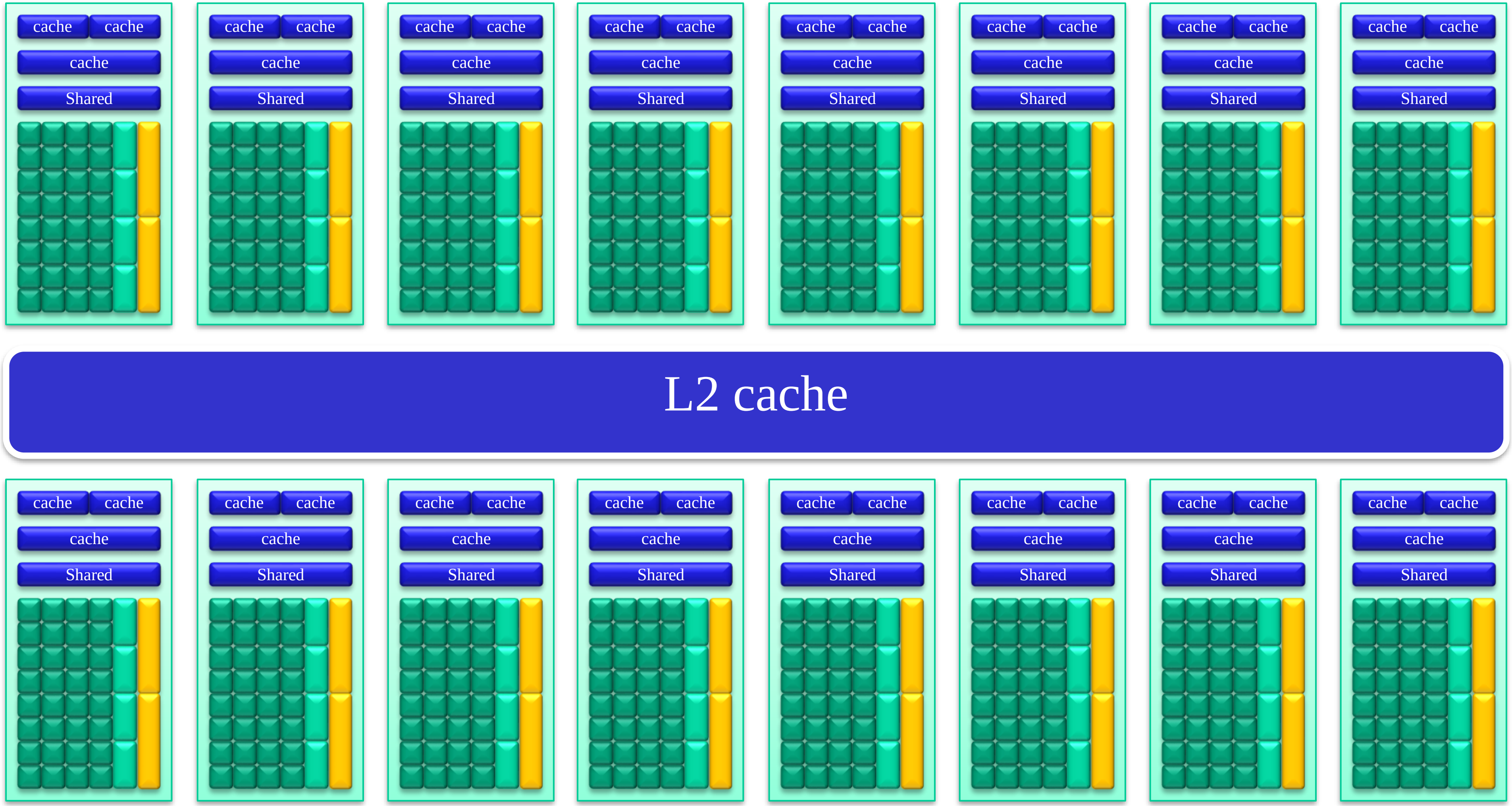
compile



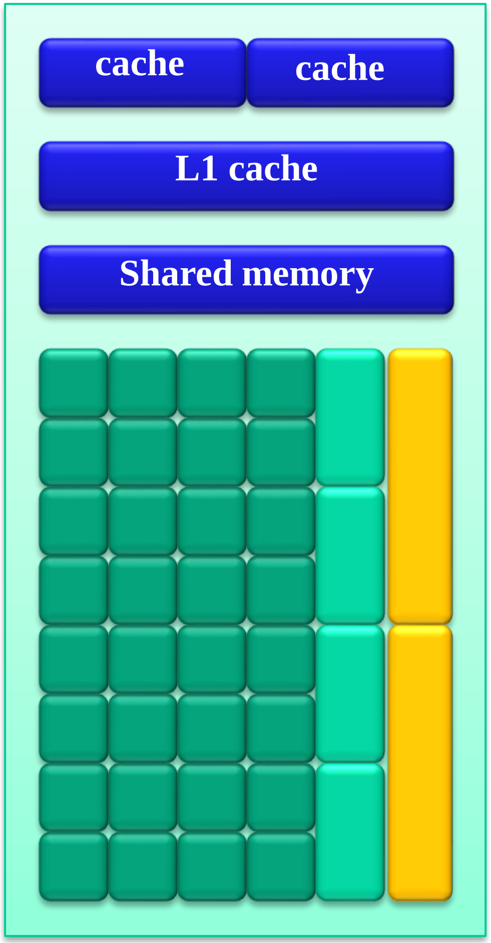
nvcc –arch=sm_80 *.cu –o *.exe –lcuda – lcudart

GPU Architecture

Fermi:16 multiprocessors



GPU Architecture



1 FERMI multiprocessor consists of:

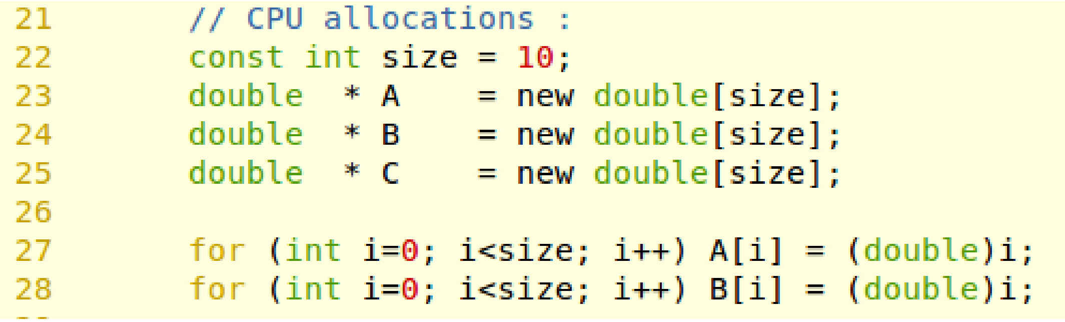
- ❑ 32 (CUDA) cores
- ❑ 4 Special Function Units (SFUs)
- ❑ 2 warp schedulers
- ❑ Shared memory
- ❑ cache memory (L1, constant & texture)
- ❑ 32768 32-bit registers

GPU Architecture

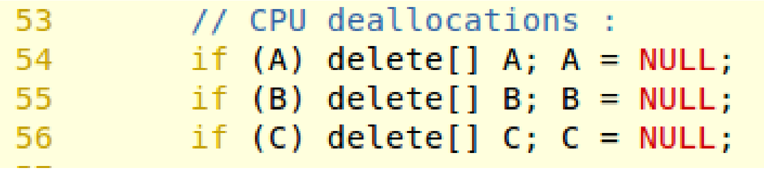
❑ Thread blocks are “split” into the multiprocessors based on kernel’s requirements on registers and shared memory. Then, the warp schedulers of each multiprocessor organize block threads into warps.

❑ The best performing block size is related only with the GPU architecture and kernel requirements not with the application itself.

Vector summation

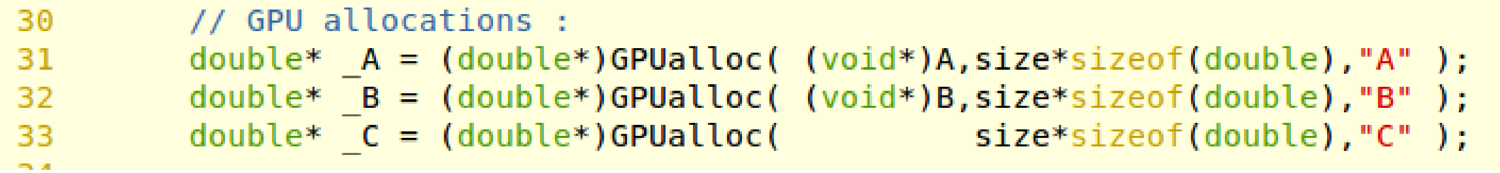


```
        // CPU allocations :
        const int size = 10;
        double  * A     = new double[size];
        double  * B     = new double[size];
        double  * C     = new double[size];

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

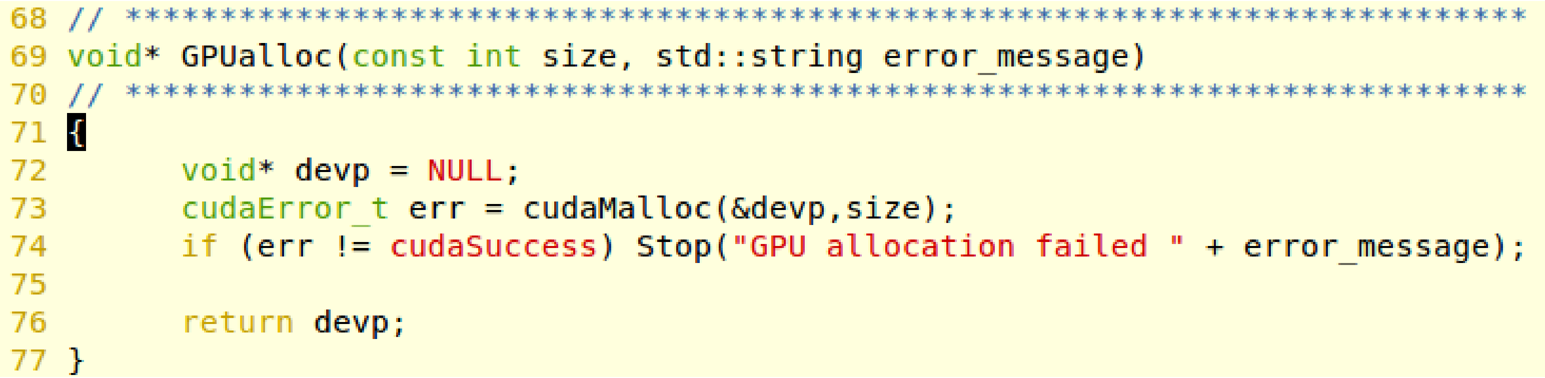


```
        // CPU deallocations :
        if (A) delete[] A; A = NULL;
        if (B) delete[] B; B = NULL;
        if (C) delete[] C; C = NULL;
```

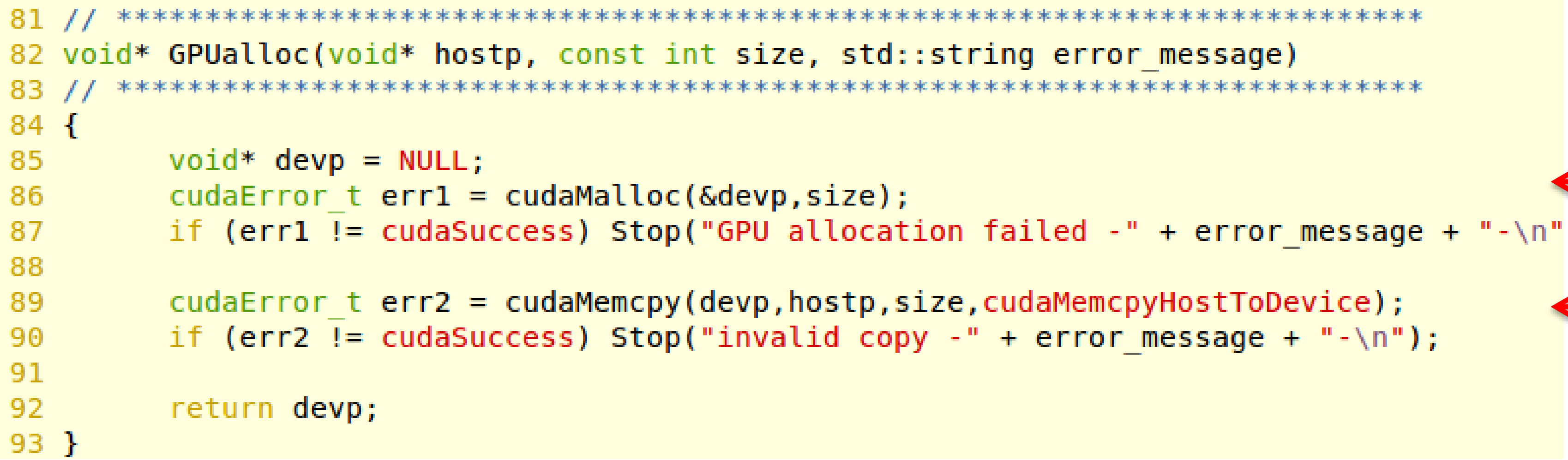
Vector summation



```
      // GPU allocations :
      double* _A = (double*)GPUalloc( (void*)A,size*sizeof(double),"A" );
      double* _B = (double*)GPUalloc( (void*)B,size*sizeof(double),"B" );
      double* _C = (double*)GPUalloc(          size*sizeof(double),"C" );
```

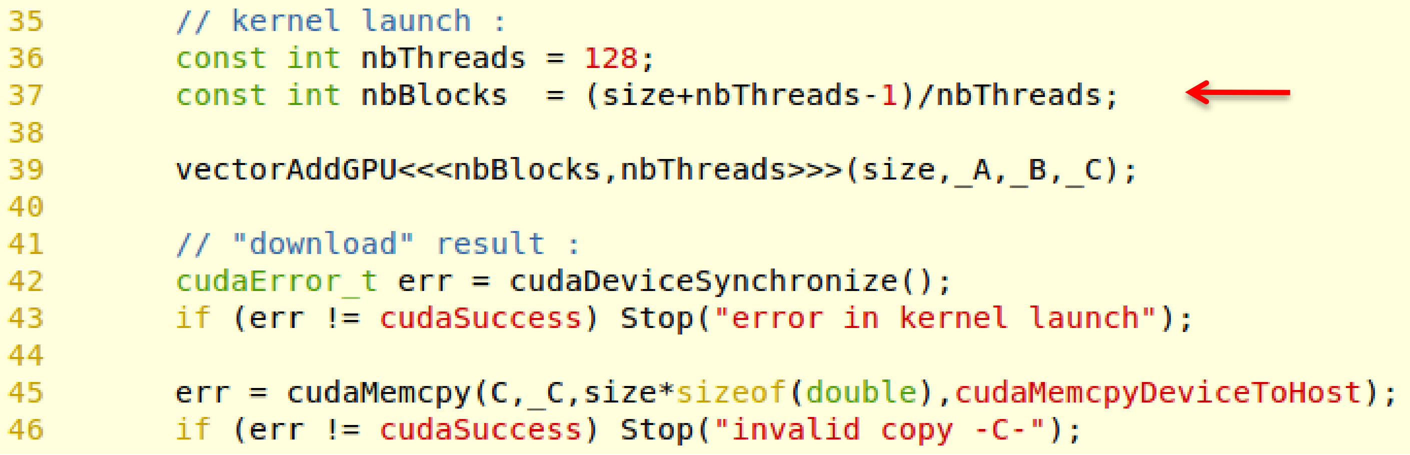


```
// ************************************************************************
void* GPUalloc(const int size, std::string error_message)
// ************************************************************************
{
      void* devp = NULL;
      cudaError_t err = cudaMalloc(&devp,size);
      if (err != cudaSuccess) Stop("GPU allocation failed " + error_message);

      return devp;
}
```

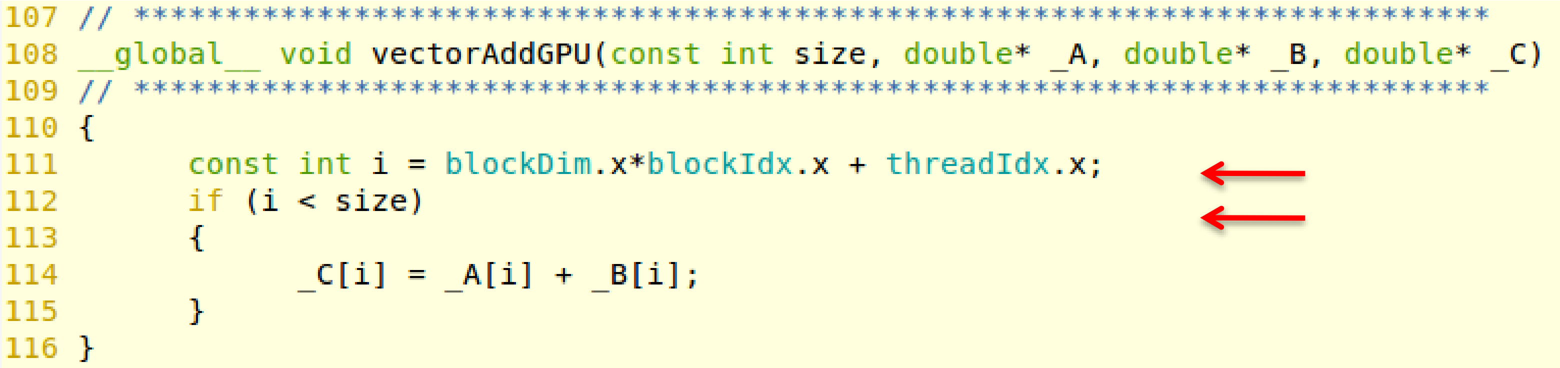


```
// ************************************************************************
void* GPUalloc(void* hostp, const int size, std::string error_message)
// ************************************************************************
{
      void* devp = NULL;
      cudaError_t err1 = cudaMalloc(&devp,size);
      if (err1 != cudaSuccess) Stop("GPU allocation failed -" + error_message + "-\n"

      cudaError_t err2 = cudaMemcpy(devp,hostp,size,cudaMemcpyHostToDevice);
      if (err2 != cudaSuccess) Stop("invalid copy -" + error_message + "-\n");

      return devp;
}
```

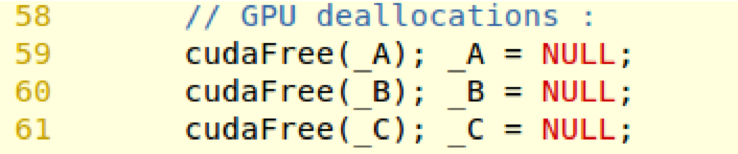
Vector summation



```
        // kernel launch :
        const int nbThreads = 128;
        const int nbBlocks  = (size+nbThreads-1)/nbThreads;

        vectorAddGPU<<<nbBlocks,nbThreads>>>(size,_A,_B,_C);

        // "download" result :
        cudaError_t err = cudaDeviceSynchronize();
        if (err != cudaSuccess) Stop("error in kernel launch");

        err = cudaMemcpy(C,_C,size*sizeof(double),cudaMemcpyDeviceToHost);
        if (err != cudaSuccess) Stop("invalid copy -C-");
```



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



```
        // GPU deallocations :
        cudaFree(_A); _A = NULL;
        cudaFree(_B); _B = NULL;
        cudaFree(_C); _C = NULL;
```

Piece of advice

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

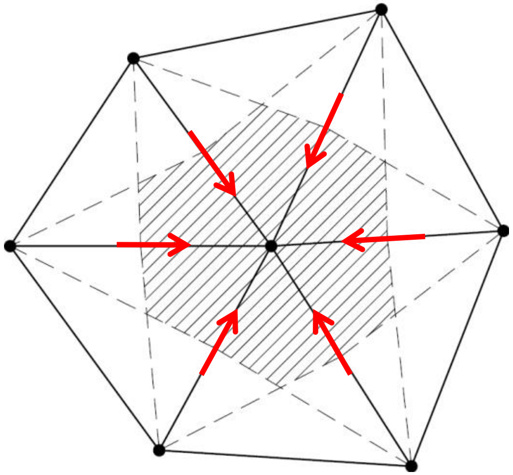
❑ Threads from the same warp should access to the same device memory segment, since access to a 128-byte device memory segment can be performed within a single memory transaction.

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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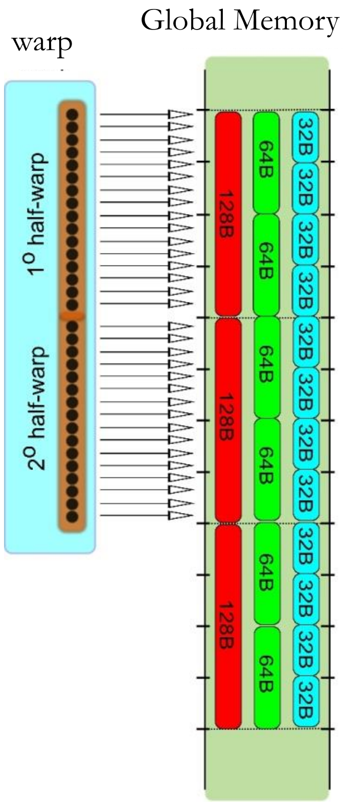

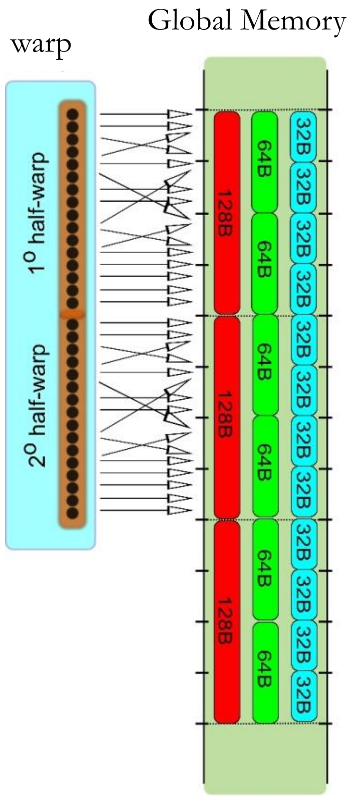

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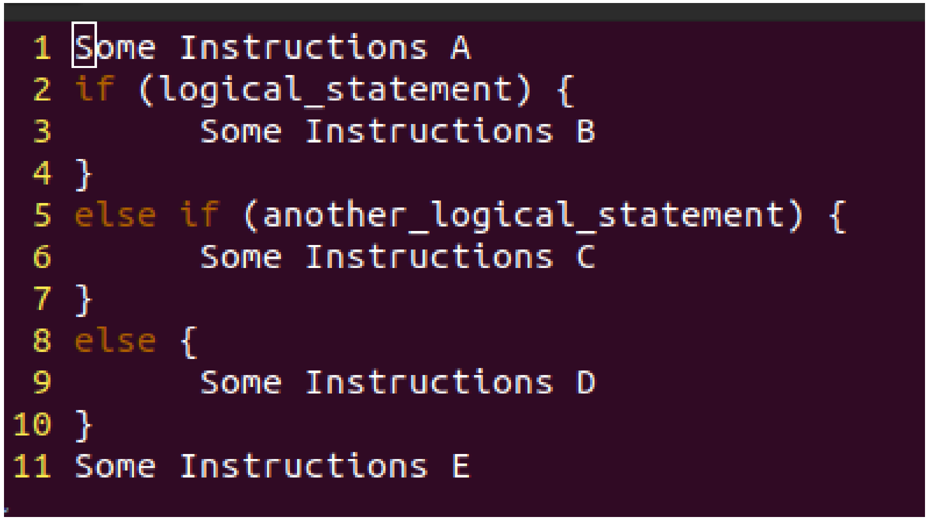

```
Some Instructions A
if (logical_statement) {
        Some Instructions B
}
else if (another_logical_statement) {
        Some Instructions C
}
else {
        Some Instructions D
}
Some Instructions E
```

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$$\overbrace{\underbrace{\frac{\partial \vec{R}}{\partial \vec{U}}}_{\textbf{SPA}} \Delta \vec{U} = \underbrace{-R\left(\vec{U}\right)}_{\textbf{DPA}}}^{\textbf{MPA}}$$

$$\vec{U}^{n+1} = \vec{U}^{n} + \Delta \vec{U}$$

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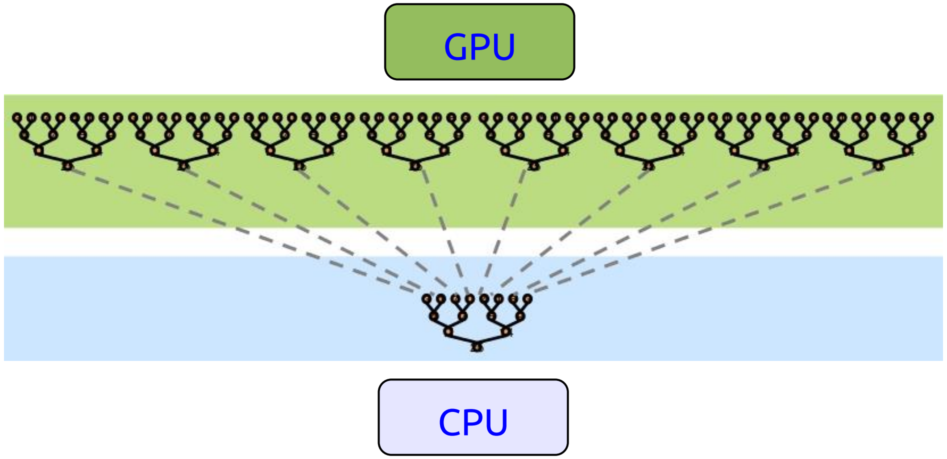
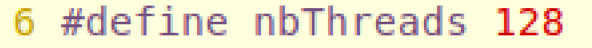
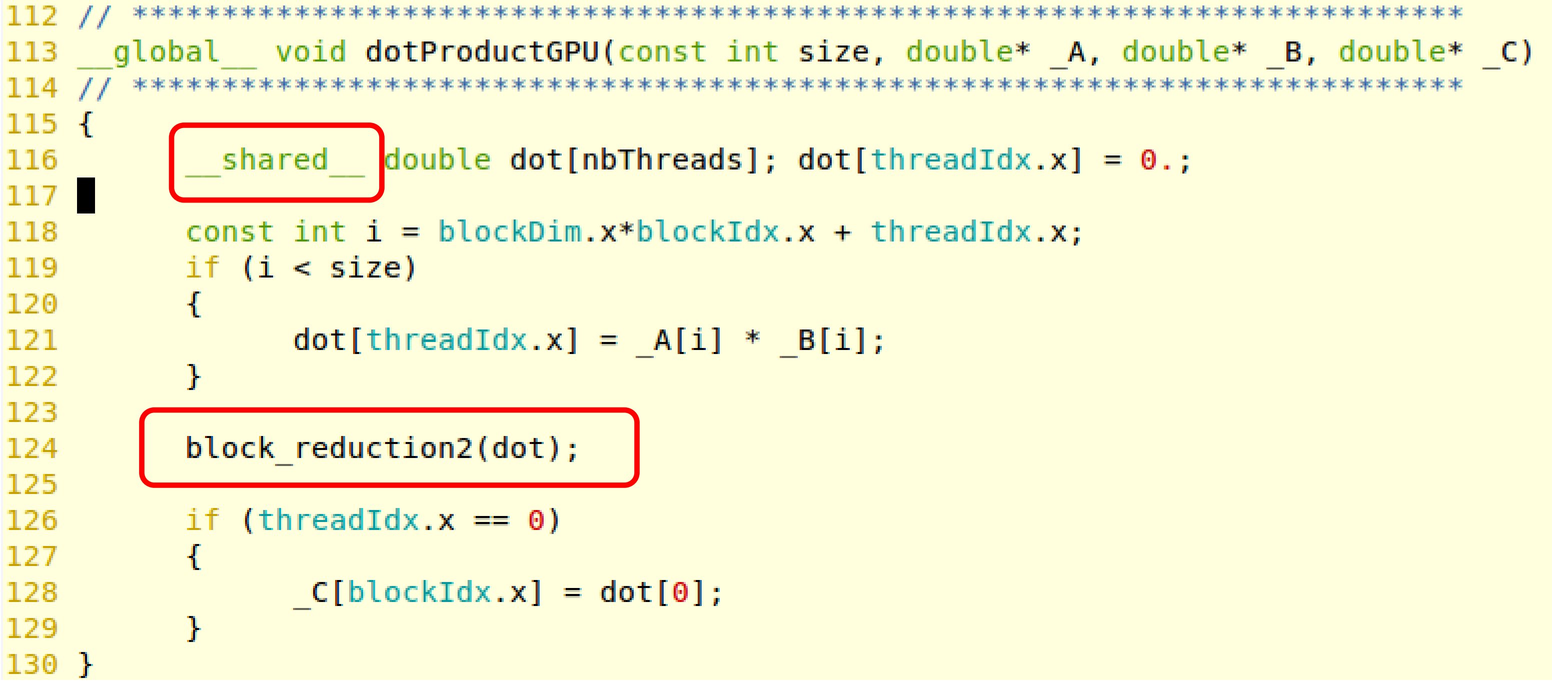


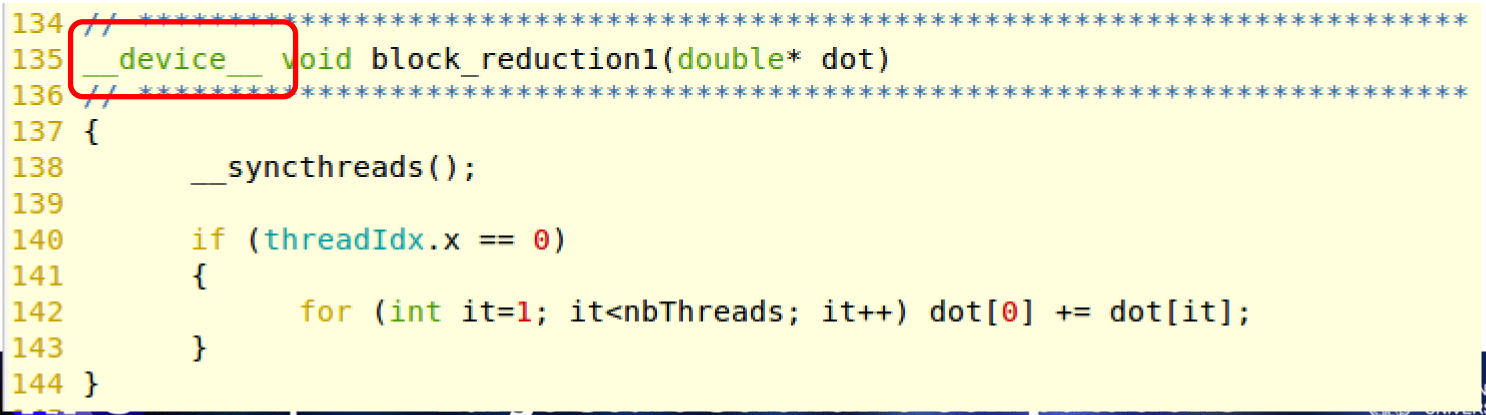
Dot product



```
#define nbThreads 128
```

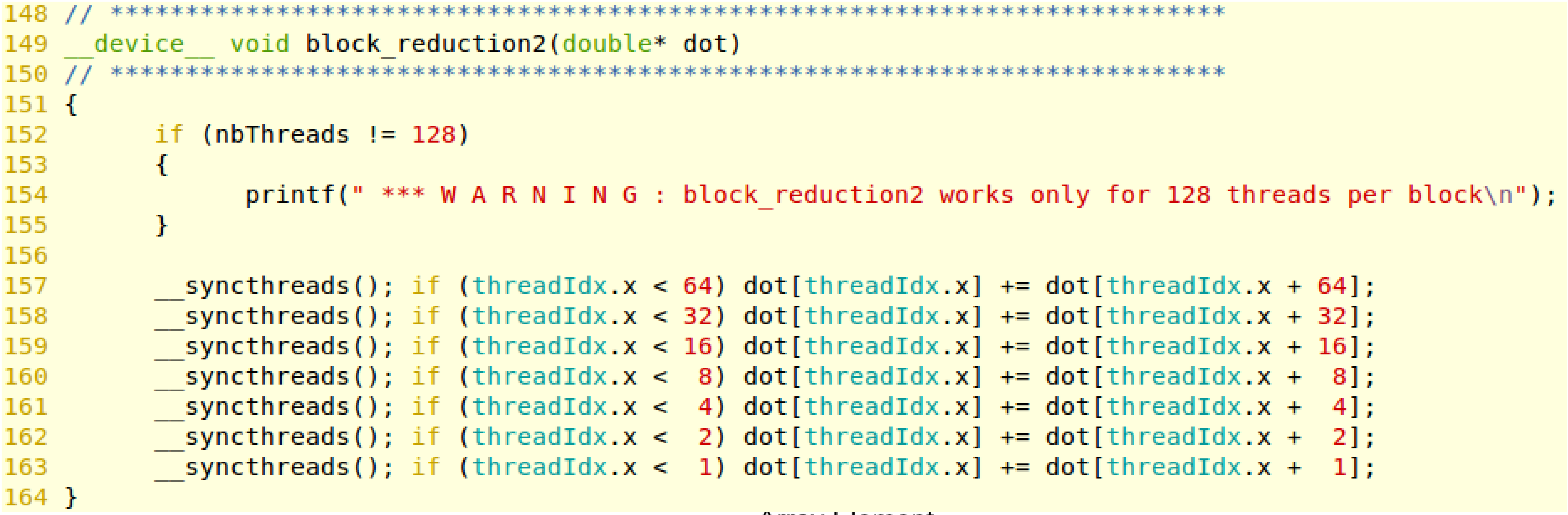


```
// ***************************************************************************
__global__ void dotProductGPU(const int size, double* _A, double* _B, double* _C)
// ***************************************************************************
{
	__shared__ double dot[nbThreads]; dot[threadIdx.x] = 0.;

	const int i = blockDim.x*blockIdx.x + threadIdx.x;
	if (i < size)
	{
		dot[threadIdx.x] = _A[i] * _B[i];
	}

	block_reduction2(dot);

	if (threadIdx.x == 0)
	{
		_C[blockIdx.x] = dot[0];
	}
}
```

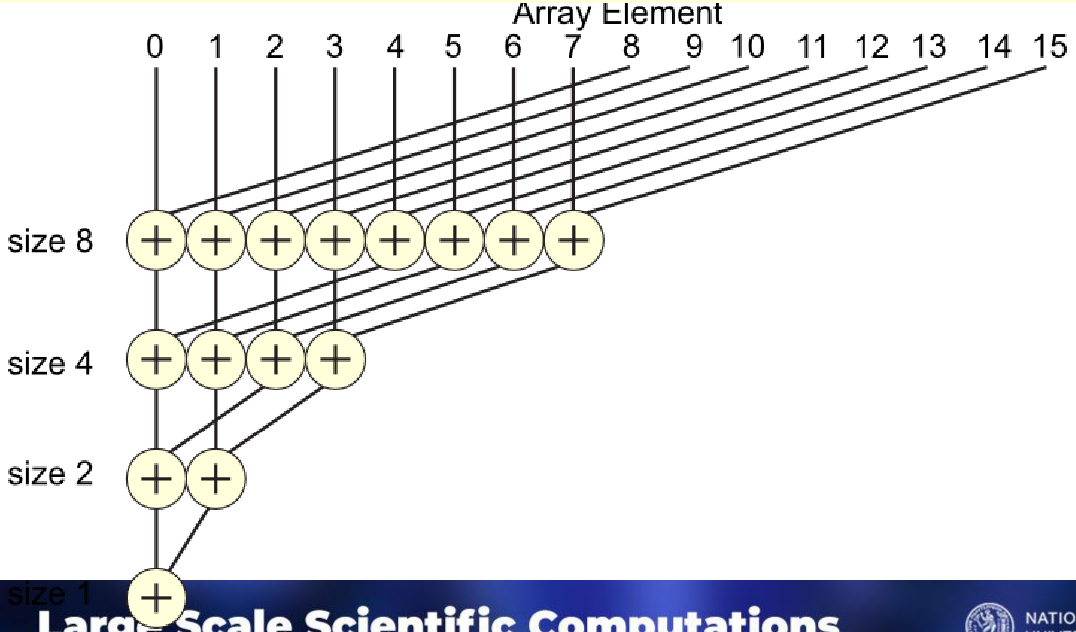


```
// ***************************************************************************
__device__ void block_reduction1(double* dot)
// ***************************************************************************
{
	__syncthreads();

	if (threadIdx.x == 0)
	{
		for (int it=1; it<nbThreads; it++) dot[0] += dot[it];
	}
}
```

Dot product



```
// ***************************************************************************
__device__ void block_reduction2(double* dot)
// ***************************************************************************
{
      if (nbThreads != 128)
      {
            printf(" *** W A R N I N G : block_reduction2 works only for 128 threads per block\n");
      }

      __syncthreads(); if (threadIdx.x < 64) dot[threadIdx.x] += dot[threadIdx.x + 64];
      __syncthreads(); if (threadIdx.x < 32) dot[threadIdx.x] += dot[threadIdx.x + 32];
      __syncthreads(); if (threadIdx.x < 16) dot[threadIdx.x] += dot[threadIdx.x + 16];
      __syncthreads(); if (threadIdx.x <  8) dot[threadIdx.x] += dot[threadIdx.x +  8];
      __syncthreads(); if (threadIdx.x <  4) dot[threadIdx.x] += dot[threadIdx.x +  4];
      __syncthreads(); if (threadIdx.x <  2) dot[threadIdx.x] += dot[threadIdx.x +  2];
      __syncthreads(); if (threadIdx.x <  1) dot[threadIdx.x] += dot[threadIdx.x +  1];
}
```



Summary

- ❑ __global__ : GPU function launched by the host (kernel)
- ❑ __device__ : GPU function launched by the device
- ❑ __host__ : CPU function launched by the host

- ❑ __shared__ : Variable in the shared memory

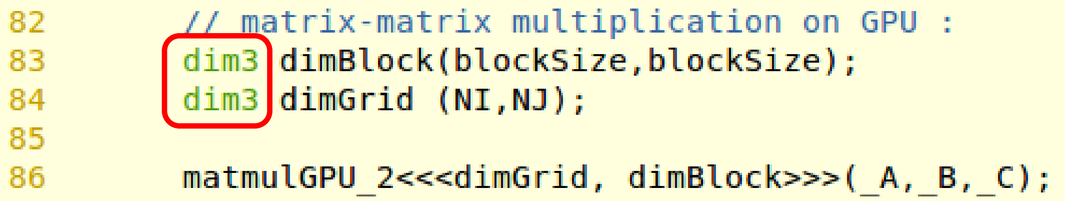
- ❑ __syncthreads() : Block thread synchronization
- ❑ cudaDeviceSynchronize() : CPU-GPU synchronization

- ❑ cudaError_t cudaMalloc(void** ptr, size_t size);

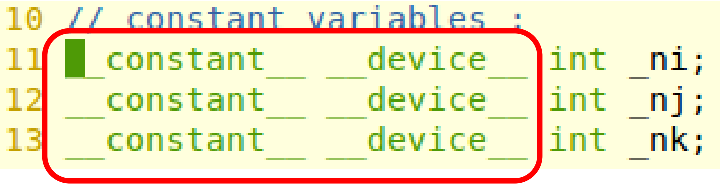
- ❑ cudaError_t cudaFree(void* ptr);

- ❑ cudaError_t cudaMemcpy(void* destination, void* source, size_t size, cudaMemcpyKind kind);

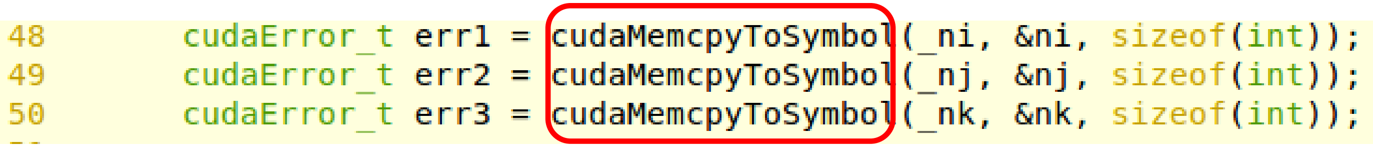
Matrix-matrix multiplication



```
        // matrix-matrix multiplication on GPU :
        dim3 dimBlock(blockSize,blockSize);
        dim3 dimGrid (NI,NJ);

        matmulGPU_2<<<dimGrid, dimBlock>>>(_A,_B,_C);
```

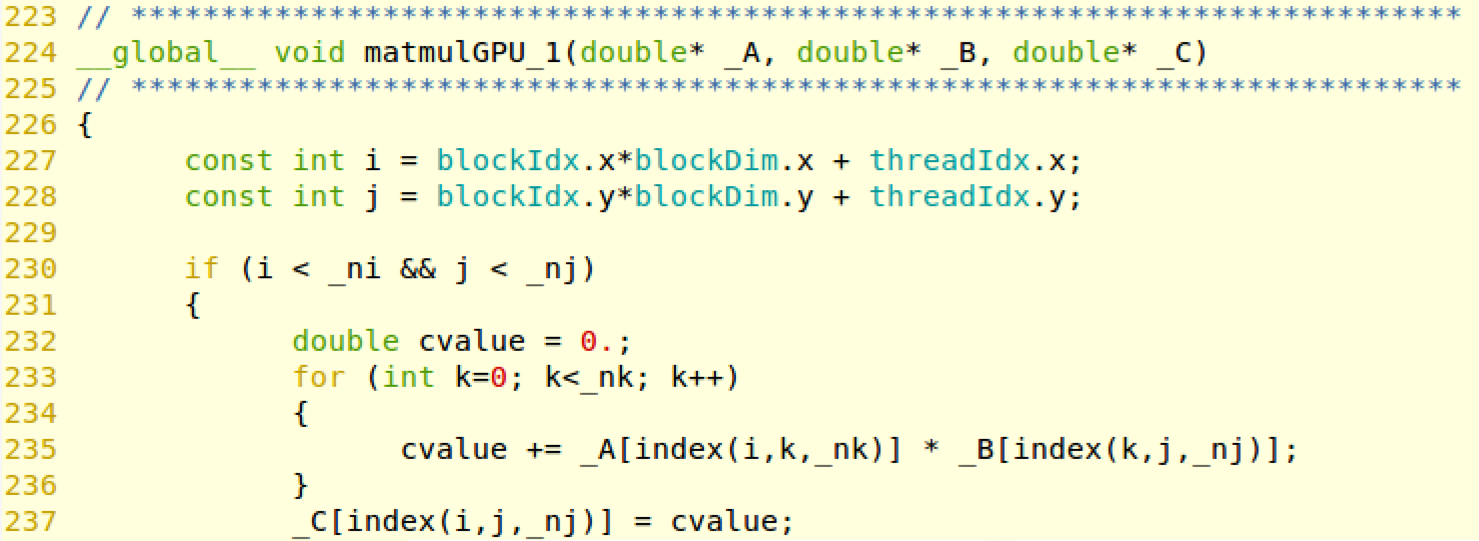


```
// constant variables :
__constant__ __device__ int _ni;
__constant__ __device__ int _nj;
__constant__ __device__ int _nk;
```

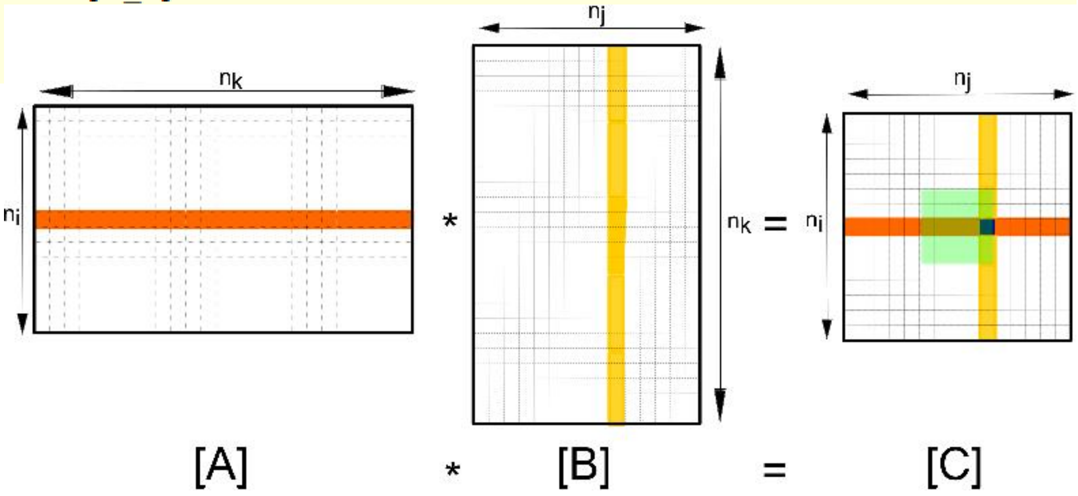


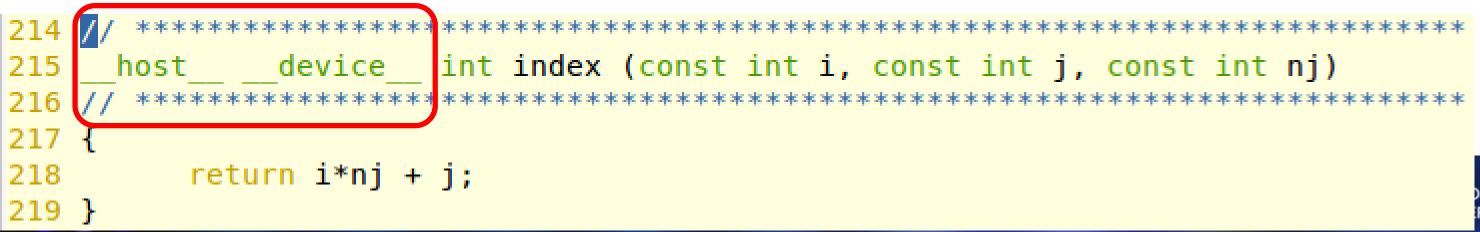
```
        cudaError_t err1 = cudaMemcpyToSymbol(_ni, &ni, sizeof(int));
        cudaError_t err2 = cudaMemcpyToSymbol(_nj, &nj, sizeof(int));
        cudaError_t err3 = cudaMemcpyToSymbol(_nk, &nk, sizeof(int));
```

Matrix-matrix multiplication



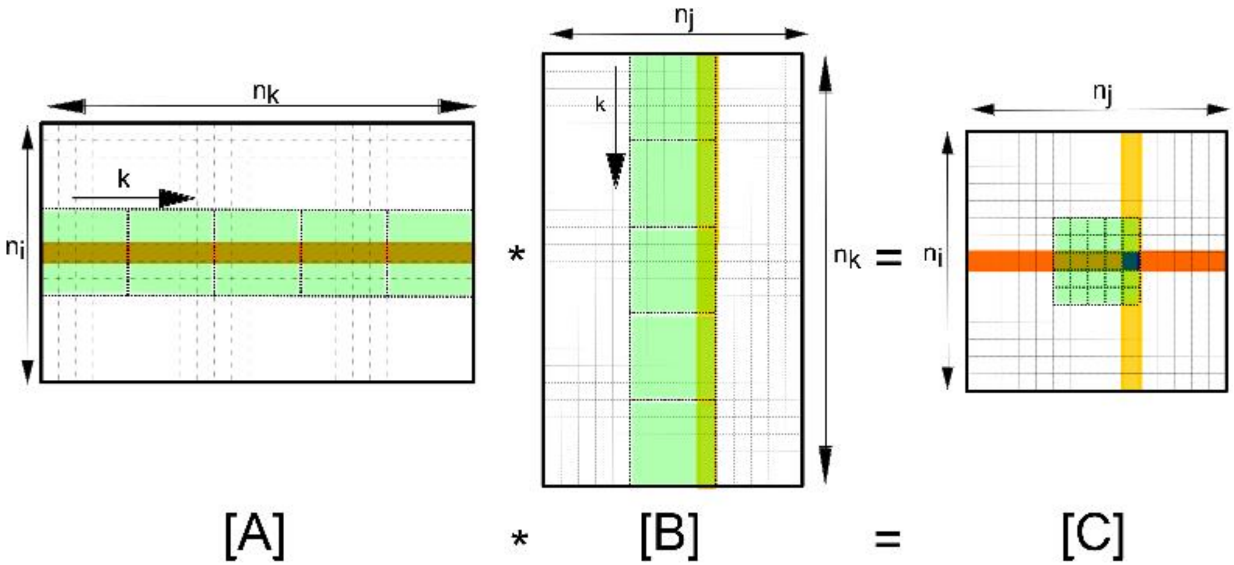
```
// ***************************************************************************
__global__ void matmulGPU_1(double* _A, double* _B, double* _C)
// ***************************************************************************
{
      const int i = blockIdx.x*blockDim.x + threadIdx.x;
      const int j = blockIdx.y*blockDim.y + threadIdx.y;

      if (i < _ni && j < _nj)
      {
            double cvalue = 0.;
            for (int k=0; k<_nk; k++)
            {
                  cvalue += _A[index(i,k,_nk)] * _B[index(k,j,_nj)];
            }
            _C[index(i,j,_nj)] = cvalue;
      }
}
```



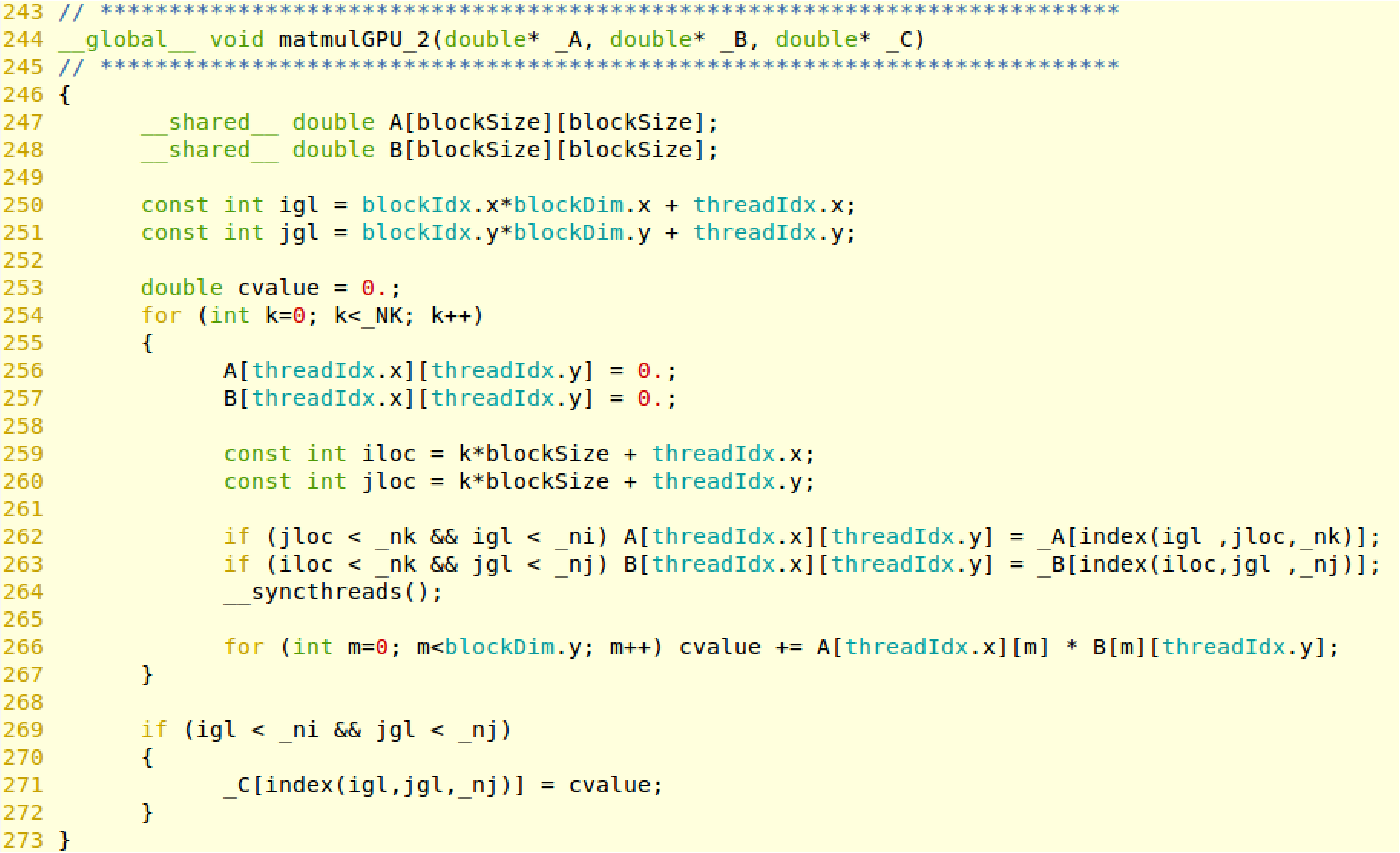


```
// ***************************************************************************
__host__ __device__ int index (const int i, const int j, const int nj)
// ***************************************************************************
{
      return i*nj + j;
}
```

Matrix-matrix multiplication



Matrix-matrix multiplication



```
// *************************************************************************
__global__ void matmulGPU_2(double* _A, double* _B, double* _C)
// *************************************************************************
{
      __shared__ double A[blockSize][blockSize];
      __shared__ double B[blockSize][blockSize];

      const int igl = blockIdx.x*blockDim.x + threadIdx.x;
      const int jgl = blockIdx.y*blockDim.y + threadIdx.y;

      double cvalue = 0.;
      for (int k=0; k<_NK; k++)
      {
            A[threadIdx.x][threadIdx.y] = 0.;
            B[threadIdx.x][threadIdx.y] = 0.;

            const int iloc = k*blockSize + threadIdx.x;
            const int jloc = k*blockSize + threadIdx.y;

            if (jloc < _nk && igl < _ni) A[threadIdx.x][threadIdx.y] = _A[index(igl ,jloc,_nk)];
            if (iloc < _nk && jgl < _nj) B[threadIdx.x][threadIdx.y] = _B[index(iloc,jgl ,_nj)];
            __syncthreads();

            for (int m=0; m<blockDim.y; m++) cvalue += A[threadIdx.x][m] * B[m][threadIdx.y];
      }

      if (igl < _ni && jgl < _nj)
      {
            _C[index(igl,jgl,_nj)] = cvalue;
      }
}
```