

Programming paradigms for GPU devices



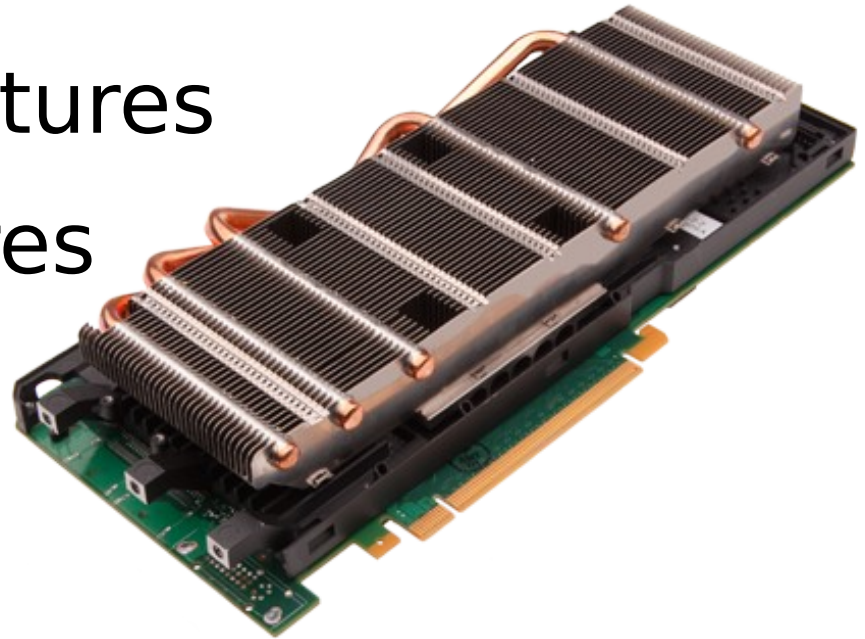
28th Summer School on
Parallel Computing

1-12 July 2019

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- General Purpose GPU Computing
- CPU vs GPU architectures
- HPC GPU architectures
- GPU programming models

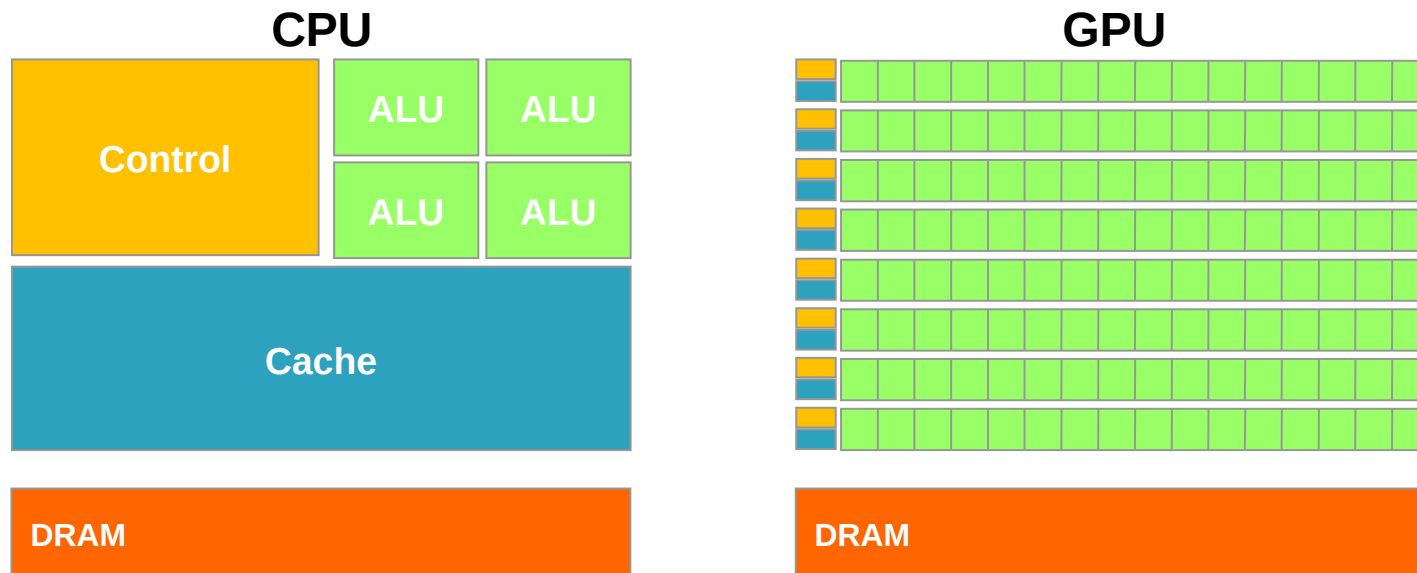


What is a GPU ?

- **Graphics Processor Unit**
 - a device equipped with an highly parallel microprocessor (*many-core*) and a private memory with very high bandwidth
- born in response to the growing demand for high definition 3D rendering graphic applications

CPU vs GPU Architectures

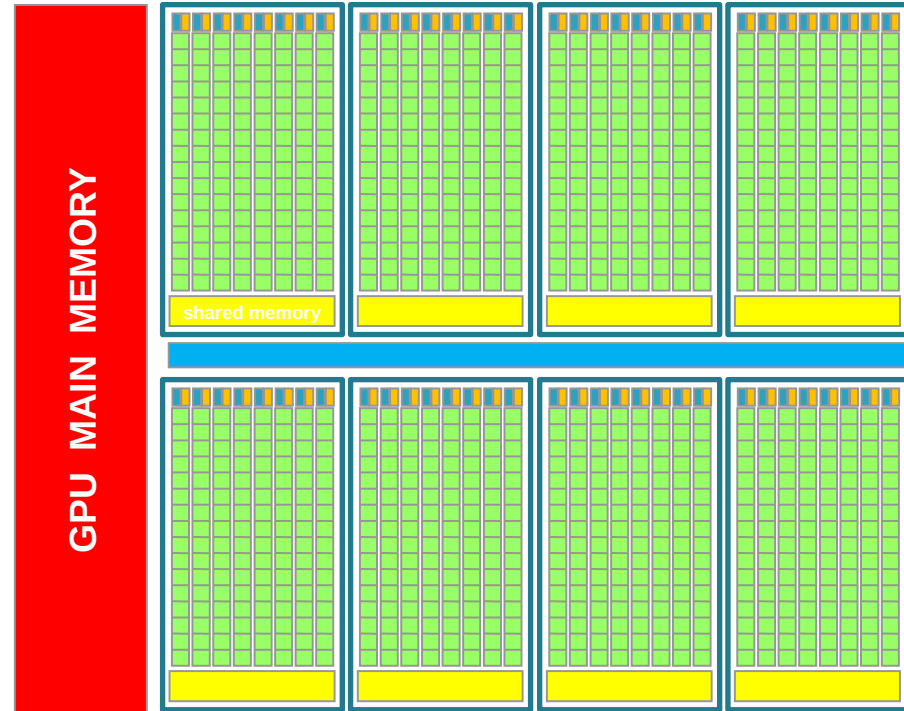
- GPU hardware is specialized for problems which can be classified as *intense data-parallel computations*
 - the same set of operation is executed many times in parallel on different data
 - designed such that more transistors are devoted to data processing rather than data caching and flow control



"The GPU devotes more transistors to Data Processing"
(NVIDIA CUDA Programming Guide)

GPU Architectures

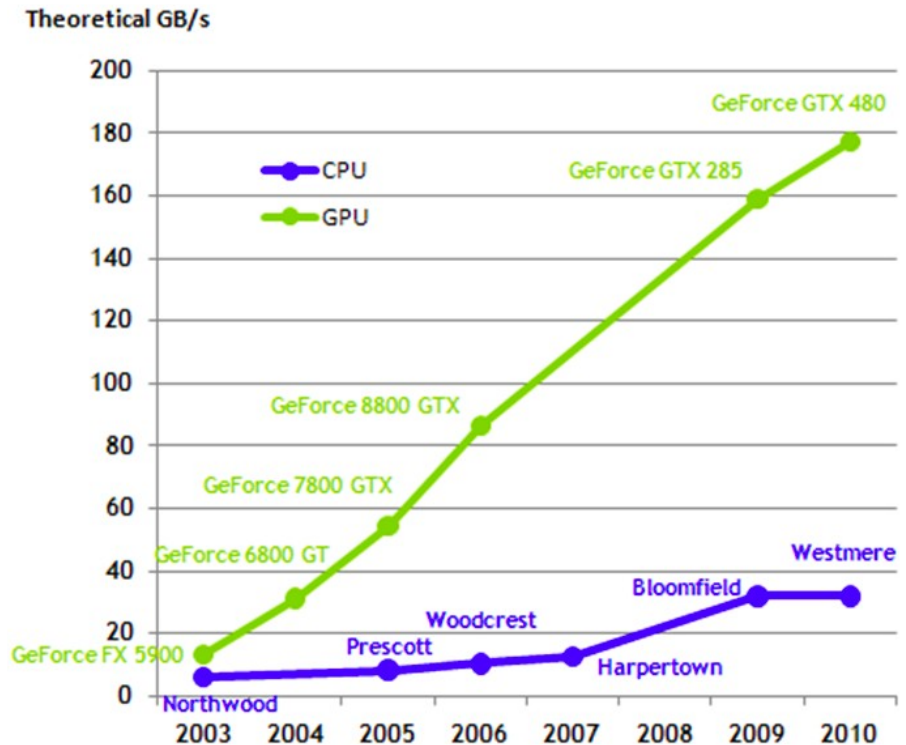
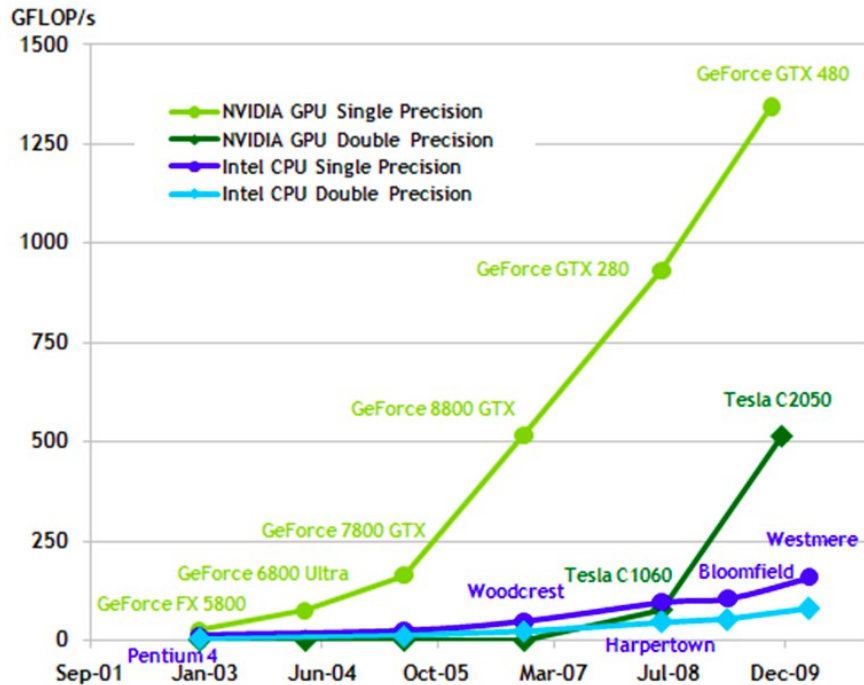
- A typical GPU architecture consists of:
 - Main global memory
 - high bandwidth
 - Streaming Processor
 - grouping independent cores and control units
- Each SM unit has
 - Many ALU cores
 - Instruction scheduler dispatchers
 - Shared memory with very fast access to data



The concurrency revolution

A new direction in microprocessor design roadmaps

- CPU vendors tend to increase the computational power of single processing unit by increasing the working frequency and adding more higher level control logic and pipelines
- GPU increased the number of processing units, less logic, lowering frequency and dropping down power consumption



Peak GFlops (left) and bandwidth (right) trends of some nVIDIA GPU compared to Intel CPU products

GPGPU (General Purpose GPU) and GPU computing

- many applications that process large data sets can use a data-parallel programming model to speed up the computations
- many algorithms outside the field of image rendering are accelerated by data-parallel processing
- ... so why not using GPU power for applications out of the 3D graphics domain?
- many attempts were made by brave programmers and researchers in order to force GPU APIs to treat their scientific data (atoms, signals, events, etc) as pixel or vertex in order to be computed by the GPU.
- not many survived, still the era of GPGPU computing was just begun ...

AMD HPC GPU Solutions

Model	FP32 [TFlops]	cores	RAM [GB]	Bandwidth [GB/s]	Link
Radeon MI8	8.2	4096	4 HBM	512	PCIe 3.0 x 16
Radeon MI25	12.3	4096	16 HBM2	484	PCIe 3.0 x 16
Radeon MI50	13.4	3840	16 HBM2	1024	PCIe 4.0 x 16
Radeon MI60	14.7	4096	32 HBM2	1024	PCIe 4.0 x 16

- VEGA Processor is the AMD top gamma GPU solution for HPC
 - the Radeon RX VEGA/500/400 series are for gaming
- HBM2: gen2 high-performance RAM interface for 3D-stacked DRAM with Error-correcting (ECC)
- Infinity Fabric™ Links per GPU deliver up to 200 GB/s of peer-to-peer bandwidth
- very high TDP factor sustainable on HPC server blades

NVIDIA HPC GPU Solutions

Model	FP32 [TFlops]	cores	RAM [GB]	Bandwidth [GB/s]	Link
Kepler K40	4.3	2280	12 GDDR5	240	PCIe 3.0 x 16
Pascal P100	10.6	3584	16 HBM2	732	PCIe 3.0 x 16
Volta V100	14.0	5120	32 HBM2	900	PCIe 3.0 x 16

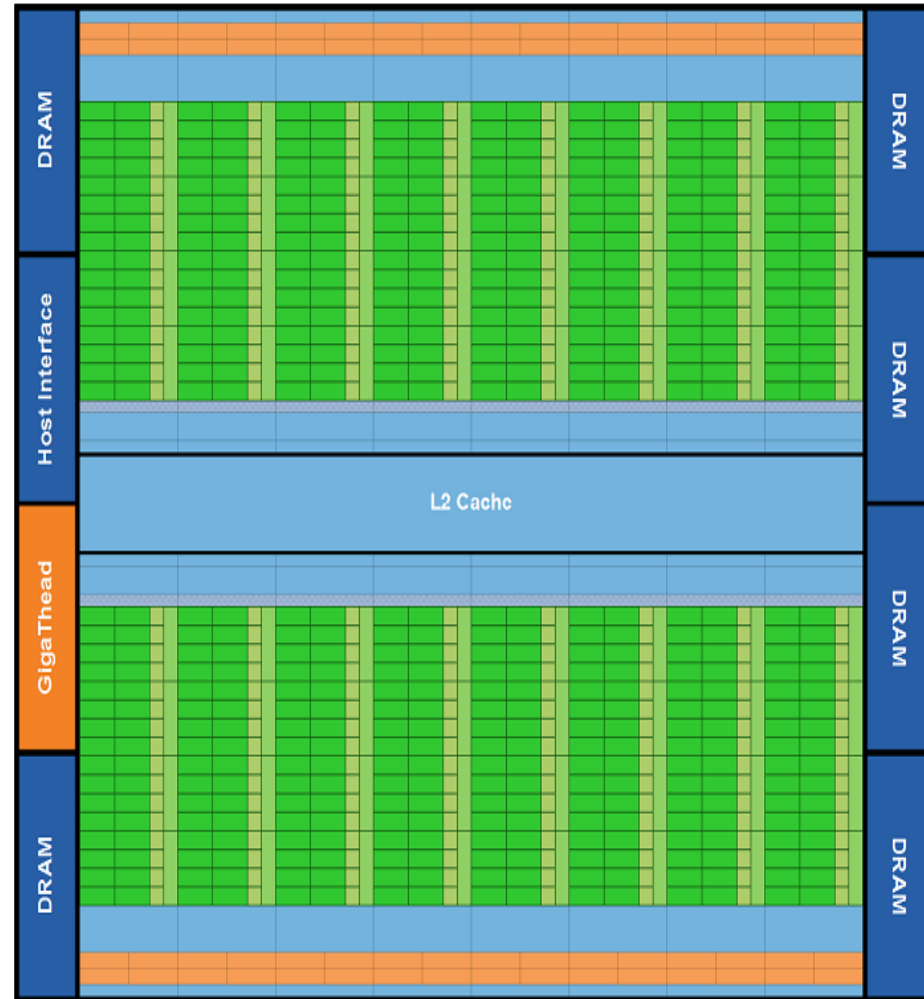
- Tesla serie is the NVIDIA top gamma GPU solution for HPC
 - the GeForce series are for gaming
- HBM2: gen2 high-performance RAM interface for 3D-stacked DRAM with Error-correcting (ECC)

NVIDIA Architectures naming

- Mainstream & laptops: GeForce
 - Target: videogames and multi-media
- Workstation: Quadro
 - Target: professional graphic applications such as CAD, modeling 3D, animation and visual effects
- GPGPU: Tesla
 - Target: High Performance Computing

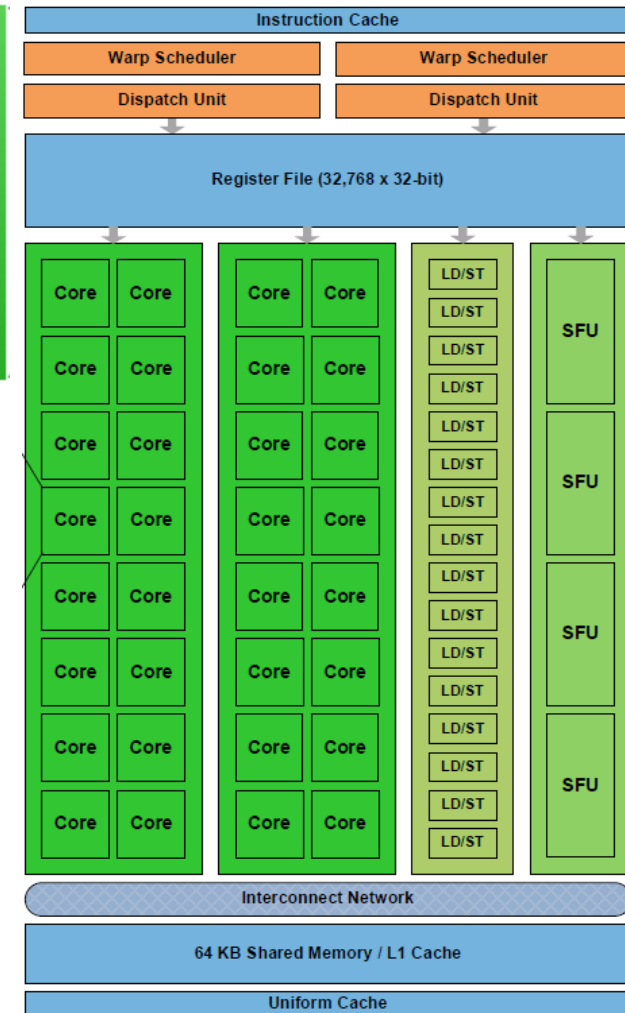
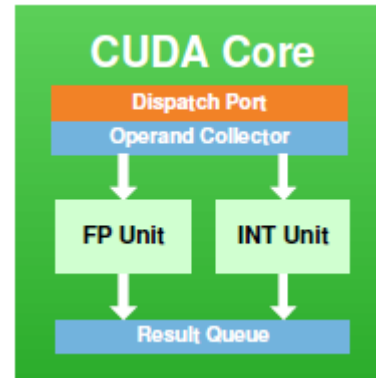
NVIDIA Fermi Architecture (2009)

- 16 Streaming Multiprocessors (SM)
- DDR3 Memory
 - 4-6 GB global memory with ECC
- First model with a cache hierarchy:
 - L1 (16-48KB) per SM
 - L2 (768KB) shared among all SM
- 2 independent controllers for data transfer from/to host through PCI-Express
- Global thread scheduler (GigaThread global scheduler) which manage and distribute thread blocks to be processed on SM resources



Fermi Streaming Multiprocessor (SM)

- 32/48 CUDA cores with an arithmetic logic unit (ALU) and a floating point unit (FPU) fully pipelined
- floating point operations are fully IEEE 754-2008 a 32-bit e a 64-bit
- fused multiply-add (FMA) for both single and double precision
- 32768 registers (32-bit)
- 64KB configurable L1
- shared-memory/cache
- 48-16KB or 16-48KB shared/L1 cache
- 16 load/store units
- 4 Special Function Unit (SFU) to handle transcendental mathematical functions (sin, sqrt, recp-sqrt,...)



NVIDIA Kepler Architecture (2012)

- x3 performance/watt with respect to FERMI
- 28nm lithography
- 192 CUDA cores
- 4 warp scheduler (2 dispatcher)
 - 2 independent instruction/warp
- 65536 registers per SM (32-bit)
- 32 load/store units
- 32 Special Function Unit
- 1534KB L2 cache (x2 vs Fermi)
- 64KB shared-memory/cache + 48KB read-only L1 cache
- 16 texture units (x4 vs Fermi)
 - Read-only cache
- Hyper-Q technology
 - Enable dynamic parallelism



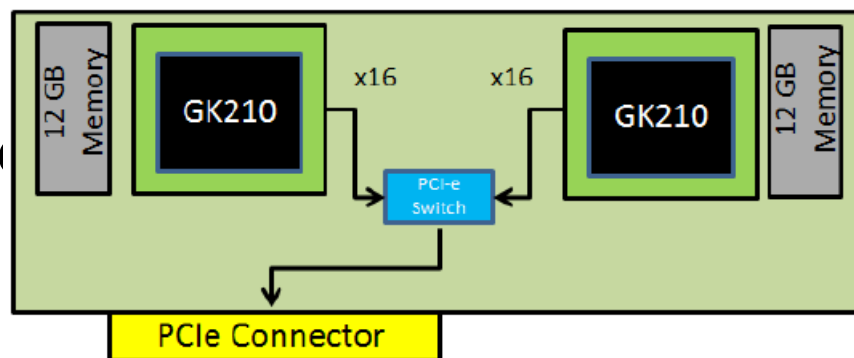
GPU nVIDIA K80 (2013)

- Two GPUs (K40) per device

- 12GB RAM per GPU
- 480 GB/s memory bandwidth



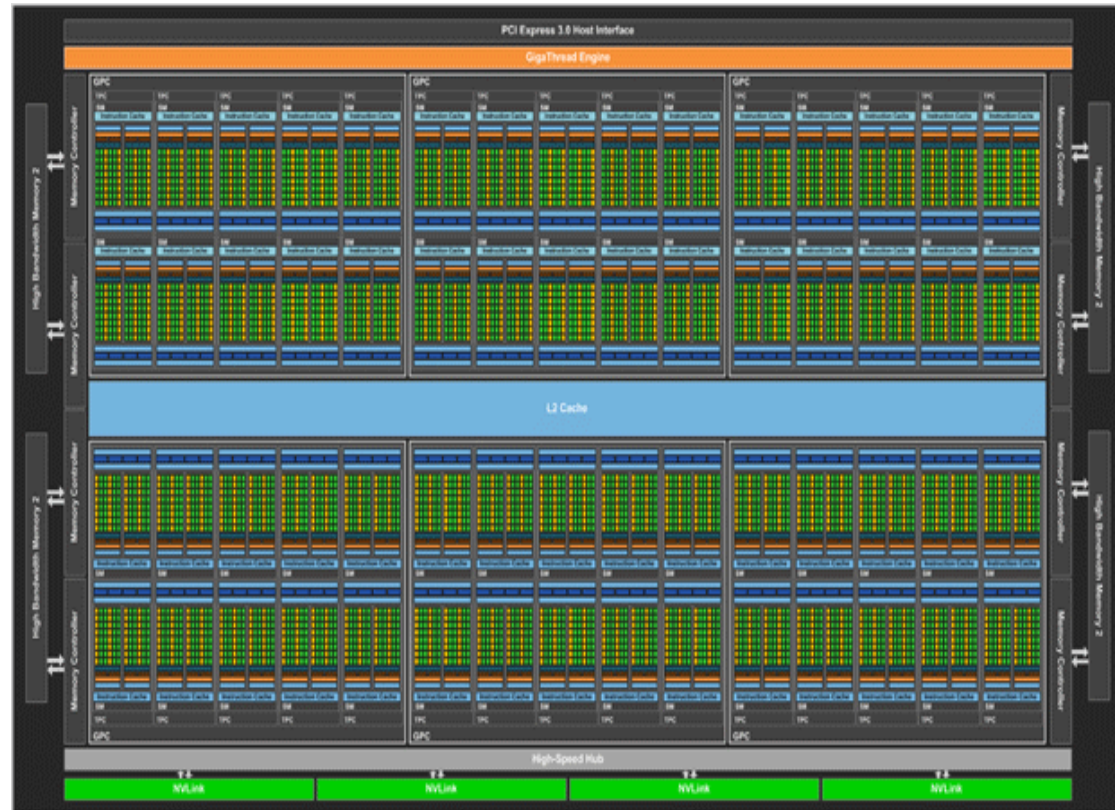
- 15 SM per GPU
- 192 CUDA cores/SM
 - total of 2880 cuda cores



- 500-800 MHz clock

NVIDIA Pascal Architecture (2016)

- 6 Compute Graphic Clusters (CGC) with 10 SM each
- 16nm lithography
 - 2X Watt/Flop respect Kepler architecture
- 4MB L2 cache
- 3D stacked RAM HDDR5
- High Bandwidth Memory
 - 16GB RAM
 - 760 GB/s bandwidth
- NVLink technology
 - 80GB/s bandwidth to host data transfers
 - 5X respect PCIe Gen3 16x



Peak Performance: 5,7 TFlops

NVIDIA Pascal Architecture (2016)

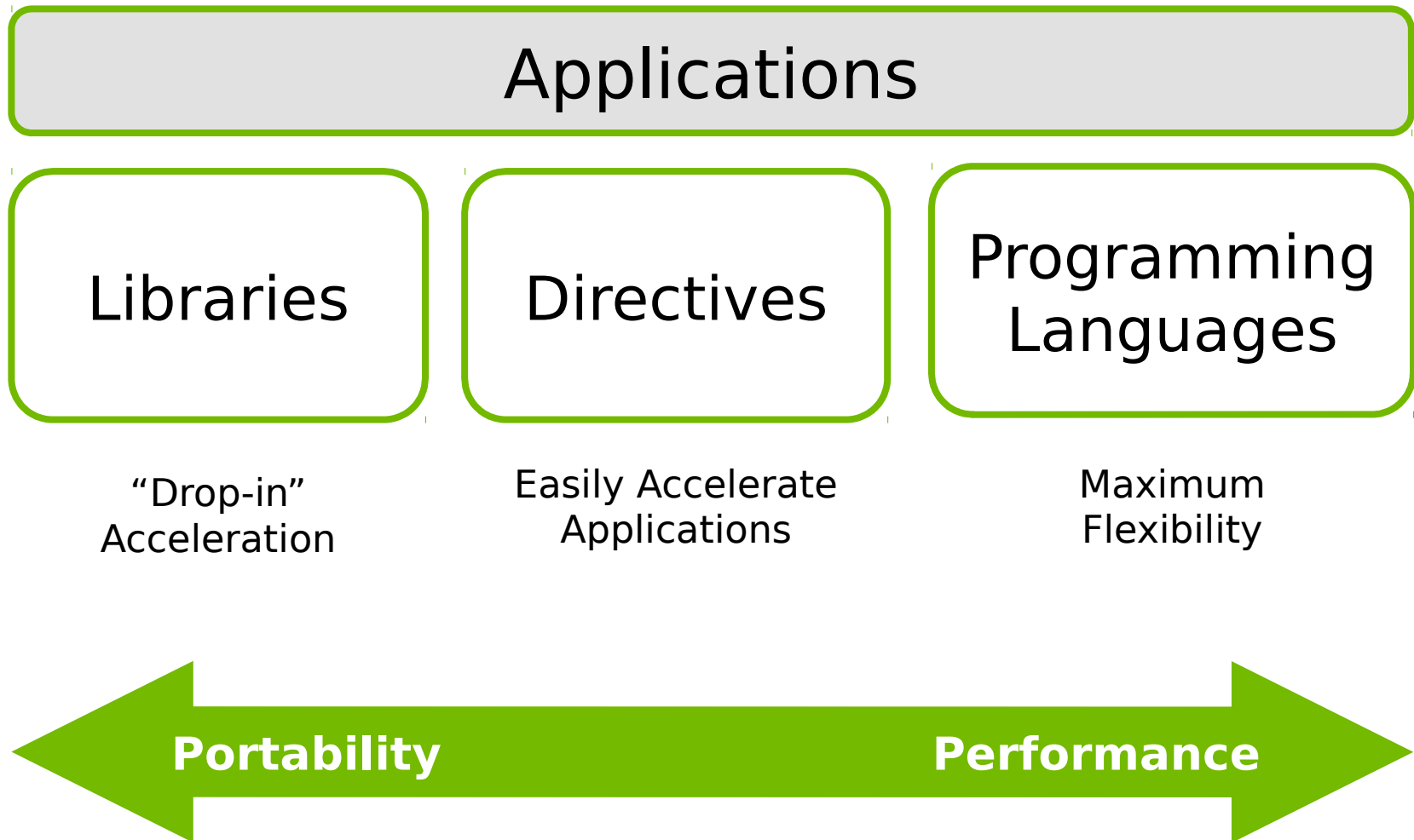
- SM composed of two independent blocks
- Each block sports:
 - 1 warps x 2 dispatchers
 - 32 ALU SIMD units
 - 16FP64 units
 - 8 Load/Store units
 - 8 SFU units
 - 32768 32bits registers
- Each block accesses:
 - 64KB shared memory
 - L1 64KB cache
 - 4 texture units



GPGPU Programming Model

- GPU is seen as an auxiliary coprocessor equipped with
 - thousands of cores
 - global memory with high bandwidth
- *computational-intensive data-parallel* regions of a program can be executed on the GPU device
 - thousands of threads will be executed on the GPU
 - each thread will insist on a different GPU core
 - each thread can acts on a different data element independently
 - the GPU parallelism is very close to the SPMD paradigm
- the more the working thread, the better are the performances
 - GPU threads are very *light*
 - no penalty is paid in case of *context-switch* (each thread has its own registers)
 - the more the threads, the more the chance to hide memory or computational latencies

3 Ways to Accelerate Applications



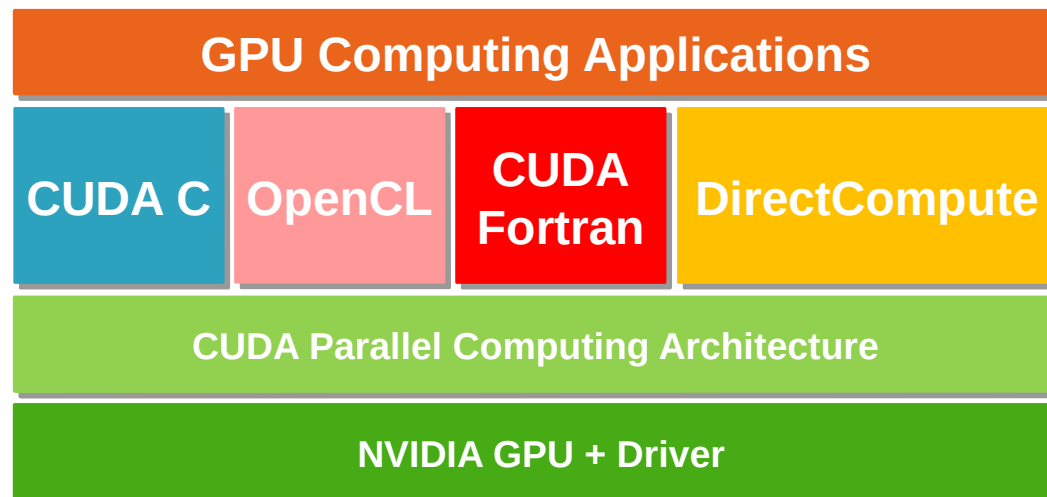
GPGPU Programming Approaches

- nVIDIA CUDA (Compute Unified Device Architecture)
 - a set of extensions to higher level programming language to use GPU as a coprocessor for heavy parallel task
 - a developer toolkit to compile, debug, profile programs and run them easily in a heterogeneous systems
- OpenCL (Open Computing Language):
 - a standard open-source programming model developed by major brands of hardware manufacturers (Apple, Intel, AMD/ATI, nVIDIA).
 - like CUDA, provides extensions to C/C++ and a developer toolkit
 - extensions for specific hardware (GPUs, FPGAs, MICs, etc)
 - it's very low level (verbose) programming
- Accelerator Directives Approach
 - OpenACC
 - OpenMP v4.x accelerator directives
 - you hope your compiler understand what you want, and do a good job
- Library Based:
 - MAGMA, CUDA Libraries, StarPu, ArrayFire, etc

General-Purpose Parallel Computing Architecture

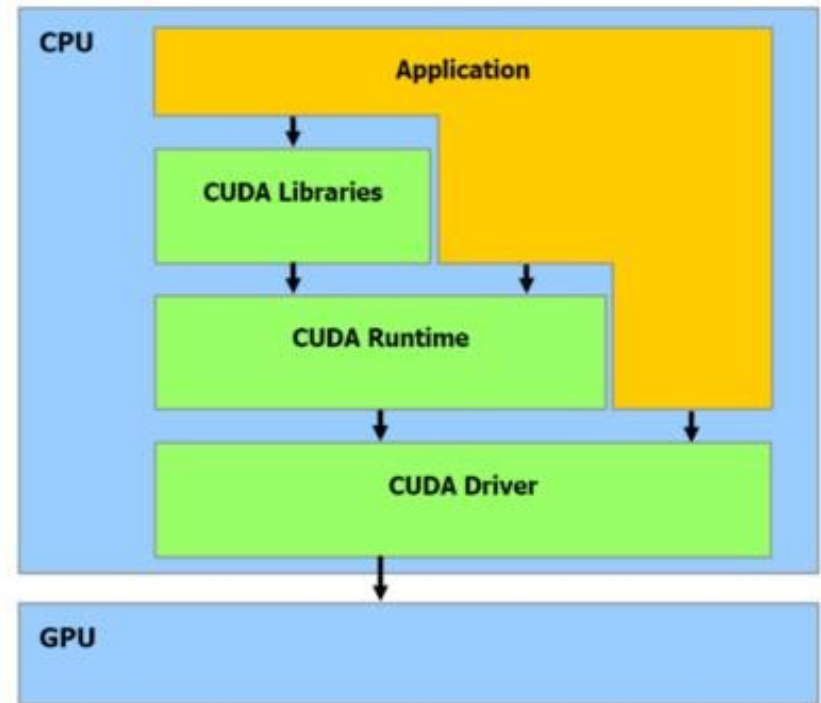
Compute Unified Device Architecture (CUDA)

- a general purpose parallel computing platform and programming model that easy GPU programming, which provides:
 - a new hierarchical multi-threaded programming paradigm
 - a new architecture instruction set called PTX (Parallel Thread eXecution)
 - a small set of syntax extensions to higher level programming languages (C, Fortran) to express thread parallelism within a familiar programming environment
 - A complete collection of development tools to compile, debug and profile CUDA programs.



CUDA Driver Vs Runtime API

- CUDA is composed of two APIs:
 - the CUDA runtime API
 - the CUDA driver API
- They are mutually exclusive
- Runtime API:
 - easier to program
 - it eases device code management: it's where the C-for-CUDA language lives
- Driver API:
 - requires more code: no syntax sugar for the kernel launch, for example
 - finer control over the device especially in multithreaded application
 - doesn't need nvcc to compile the host code.



CUDA Driver API

- The driver API is implemented in the nvcuda dynamic library. All its entry points are prefixed with cu.
- It is a handle-based, imperative API: most objects are referenced by opaque handles that may be specified to functions to manipulate the objects.
- The driver API must be initialized with cuInit() before any function from the driver API is called. A CUDA context must then be created that is attached to a specific device and made current to the calling host thread.
- Within a CUDA context, kernels are explicitly loaded as PTX or binary objects by the host code**.
- Kernels are launched using API entry points.
- **by the way, any application that wants to run on future device architectures must load PTX, not binary code

Compute Capability

- the *compute capability* of a device describes its architecture
 - *registers, memory sizes, features and capabilities*
- the compute capability is identified by a code like “compute_Xy”
 - major number (X): identifies base line chipset architecture
 - minor number (y): indentifies variants and releases of the base line chipset
- a compute capability select the set of usable PTX instructions

<i>compute capability</i>	<i>feature support</i>
compute_20	FERMI architecture
compute_30	KEPLER K10 architecture (only single precision)
compute_35	KEPLER K20, K20X, K40 architectures
compute_37	KEPLER K80 architecture (two K40 on a single board)
compute_53	MAXWELL GM200 architecture (only single precision)
compute_60	PASCAL GP100 architecture

Capability: resources constraints



Technical Specifications	Compute Capability						
	1.0	1.1	1.2	1.3	2.x	3.0	3.5
Maximum dimensionality of grid of thread blocks	2				3		
Maximum x-dimension of a grid of thread blocks	65535					2 ³¹ -1	
Maximum y- or z-dimension of a grid of thread blocks	65535						
Maximum dimensionality of thread block	3						
Maximum x- or y-dimension of a block	512				1024		
Maximum z-dimension of a block	64						
Maximum number of threads per block	512				1024		
Warp size	32						
Maximum number of resident blocks per multiprocessor	8					16	
Maximum number of resident warps per multiprocessor	24		32		48	64	
Maximum number of resident threads per multiprocessor	768		1024		1536	2048	
Number of 32-bit registers per multiprocessor	8 K		16 K		32 K	64 K	
Maximum number of 32-bit registers per thread	128				63		255
Maximum amount of shared memory per multiprocessor	16 KB				48 KB		
Number of shared memory banks	16				32		
Amount of local memory per thread	16 KB				512 KB		
Constant memory size	64 KB						
Cache working set per multiprocessor for constant memory	8 KB						
Cache working set per multiprocessor for texture memory	Device dependent, between 6 KB and 8 KB						
Maximum width for a 1D texture reference bound to a CUDA array	8192				65536		

- CUDA programming model
 - Heterogeneous execution
 - Writing a CUDA Kernels
 - Thread Hierarchy
- Getting started with CUDA programming:
 - Vector-Vector Add
 - Handling data transfers from CPU to GPU and back
 - Write and launch a CUDA program



GPU Programming Model

- GPU is seen as an auxiliary coprocessor with its own memory space
- *data-parallel, computational-intensive* portions of a program can be executed on the GPU
 - each *data-parallel* computational portion can be isolated into a function, called CUDA kernel, that is executed on the GPU
 - CUDA kernels are executed by many different threads in parallel
 - each thread can compute different data elements independently
 - the GPU parallelism is very close to the SPMD (Single Program Multiple Data) paradigm. Single Instruction Multiple Threads (SIMT) according to the Nvidia definition.
- GPU threads are extremely *light weight*
 - no penalty in case of a *context-switch* (each thread has its own registers)
 - the more are the threads *in flight*, the more the GPU hardware is able to hide memory or computational latencies, i.e better overall performances at executing the kernel function

GPGPU Programming Model

- CPU and GPU are **separate devices** with **separate memory** space addresses
- GPU is seen as an auxiliary coprocessor equipped with thousands of cores and a high bandwidth memory
- They should work together for best benefit and performances

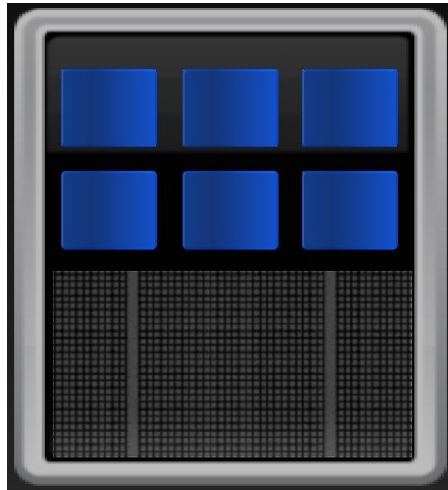


GPGPU Programming Model

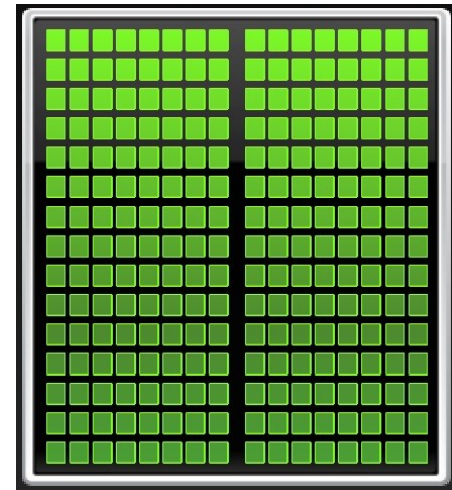
- Optimized for low-latency accesses to caches data sets
- Control logic for out-of-order and speculative execution

- Optimized for data-parallel, throughput computation
- Architecture tolerant of memory latency
- Best for data-parallel

CPU

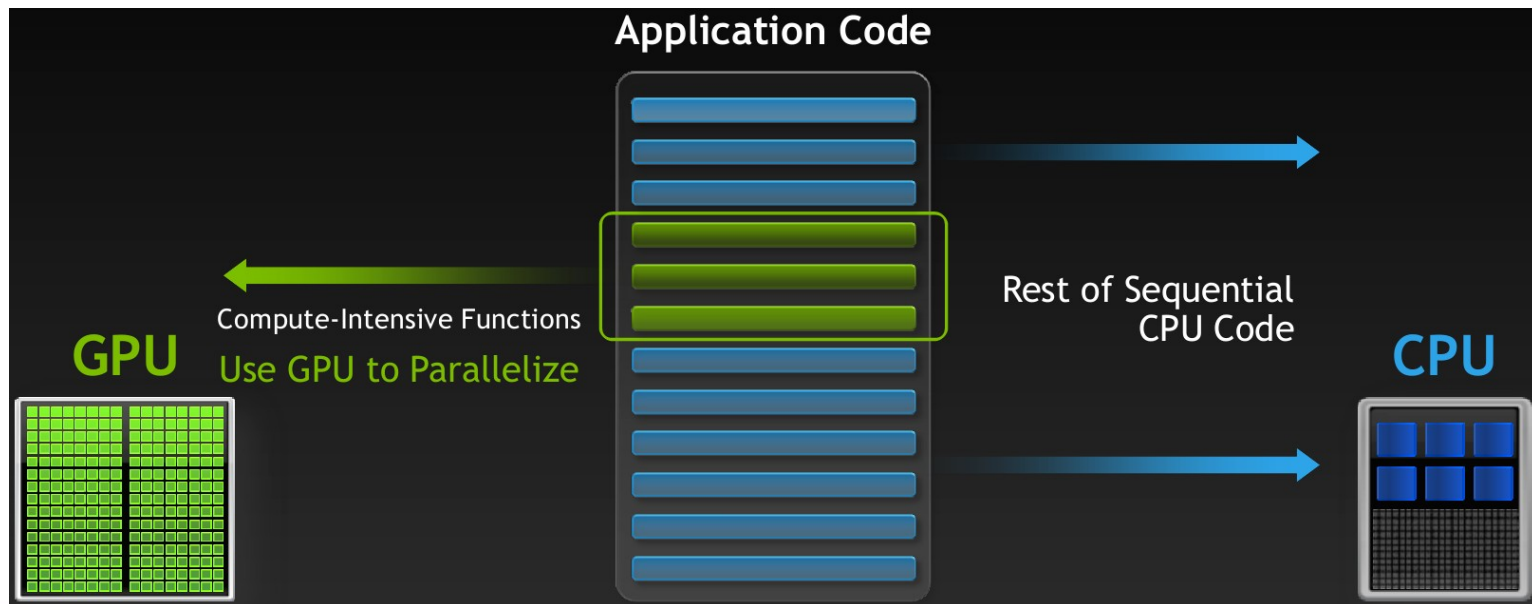


GPU



GPGPU Programming Model

- **serial parts** of a program, or those with low level of parallelism, keep running **on the CPU** (host)
- **computational-intensive data-parallel** regions are executed **on the GPU** (device)
 - required data is moved on GPU memory and back to HOST memory



GPGPU Programming Model

- A function which runs on a GPU is called “**kernel**”
 - when a kernel is launched on a GPU thousands of threads will execute its code
 - programmer chooses the number of threads to run
 - each thread act on a different data element independently
 - the GPU parallelism is very close to the SPMD paradigm

```
void vecAddCPU (int N, float *A,
               float *B, float *C)
{
    for ( int i = 0; i < N; i++ )
        c[i] = a[i] + b[i];
}

...

// call vecAddCPU on N elements
vecAddCPU ( N, a, b, c );
```

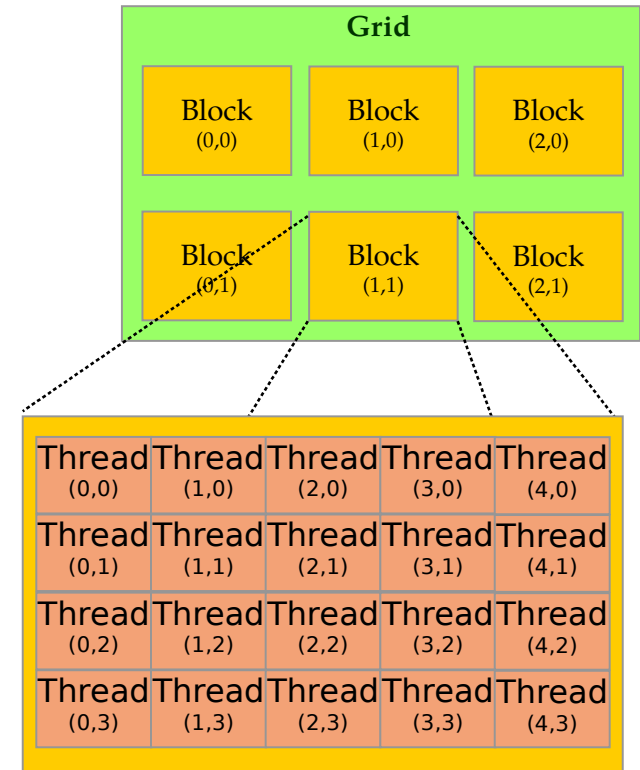
```
void vecAddGPU (int N, float *A,
               float *B, float *C)
{
    int i = threadIdx.x;
    if ( i < N )
        c[i] = a[i] + b[i];
}

...

// CUDA kernel vecAddGPU on N elems
vecAddGPU<<<1, N>>>( N, a, b, c );
```

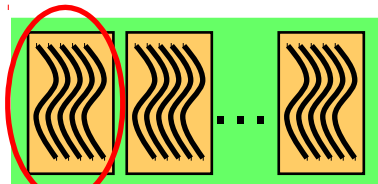
GPU Thread Hierarchy

- In order to compute N elements on the GPU in parallel, at least N concurrent threads must be created on the device
- GPU threads are grouped together in *teams* or *blocks* of threads
- Threads belonging to the same block or team can cooperate together exchanging data through the shared memory area



more on the GPU Execution Model

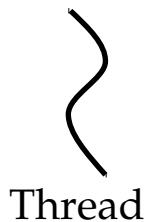
Software



Grid

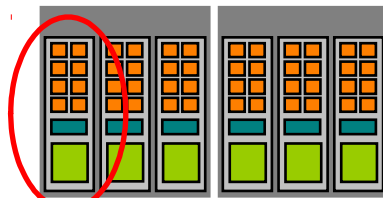


Thread Block



Thread

Hardware



GPU



Streaming Multiprocessor



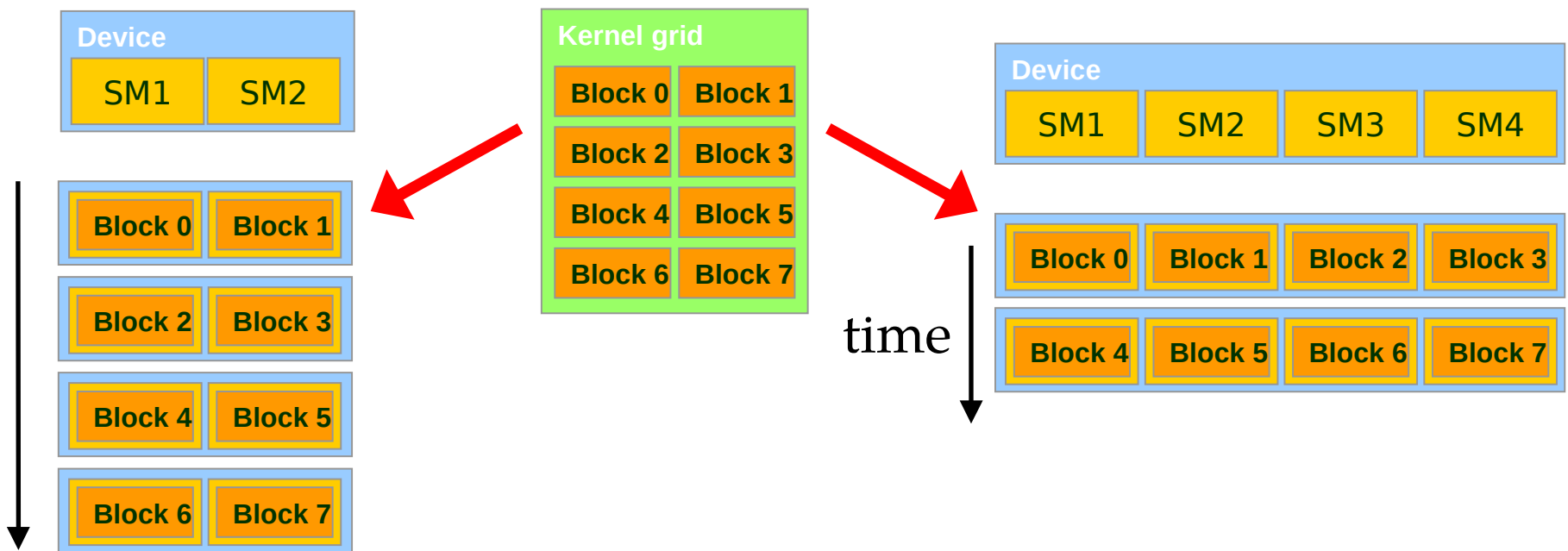
GPU core

when a kernel is invoked:

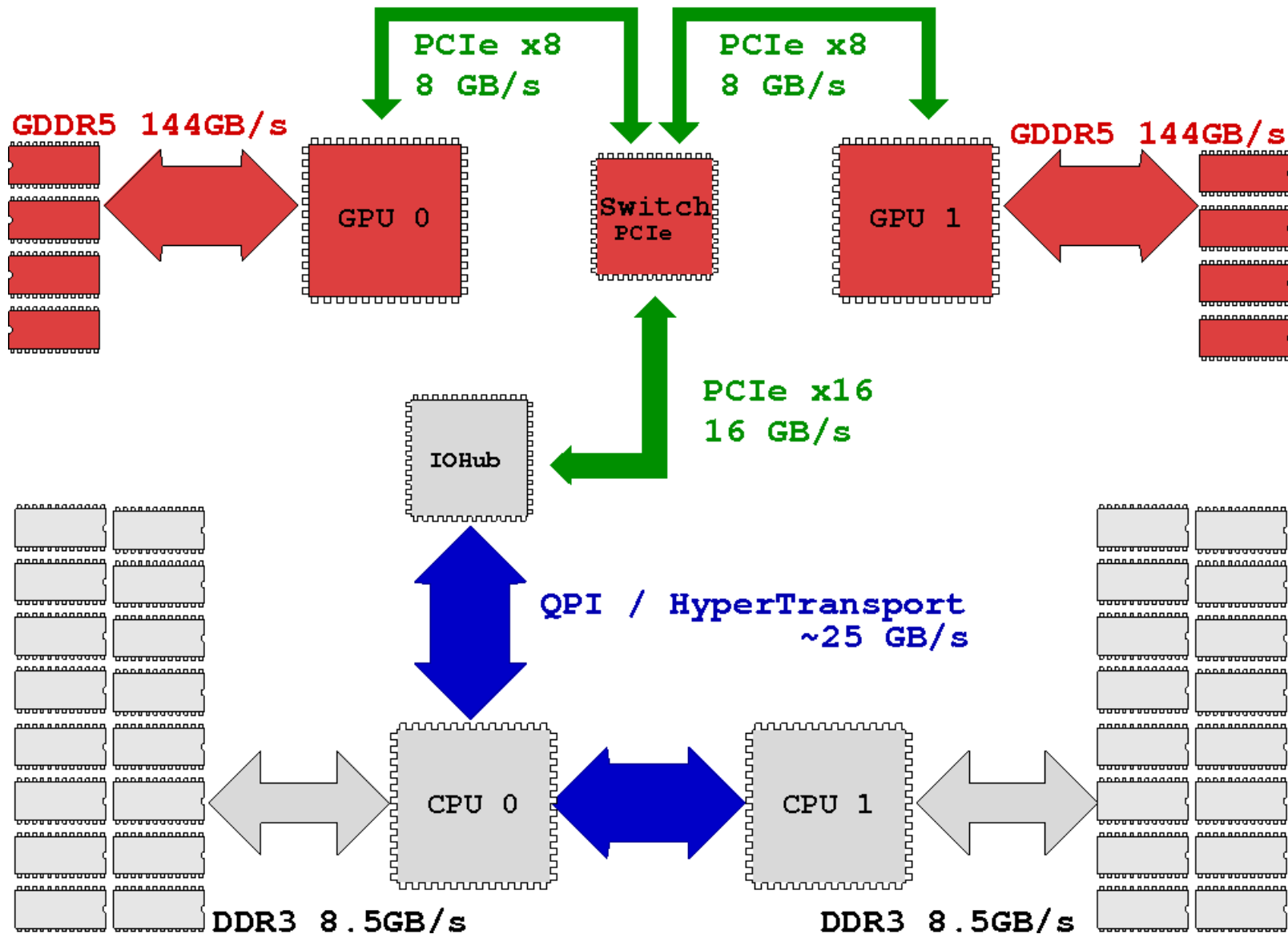
- each thread block is assigned to a SM in a round-robin mode
 - a maximum number of blocks can be assigned to each SM, depending on hardware generation and on how many resources each block needs to be executed (registers, shared memory, etc)
 - the runtime system maintains a list of blocks that need to execute and assigns new blocks to SMs as they complete the execution of blocks previously assigned to them.
 - once a block is assigned to a SM, it remains on that SM until the work for all threads in the block is completed
 - each block execution is independent from the other (no synchronization is possible among them)
- threads of each block are partitioned into warps of 32 *threads* each, so to map each thread with a unique consecutive thread index in the block, starting from index 0.
- the scheduler selects for execution a warp from one of the residing blocks in each SM.
- A warp executes one common instruction at a time
 - each GPU core takes care of one thread in the warp
 - fully efficient when all threads agree on their execution path

Transparent Scalability

- GPU runtime system can execute blocks in any order relative to each other.
- This flexibility enables to execute the same application code on hardware with different numbers of SM

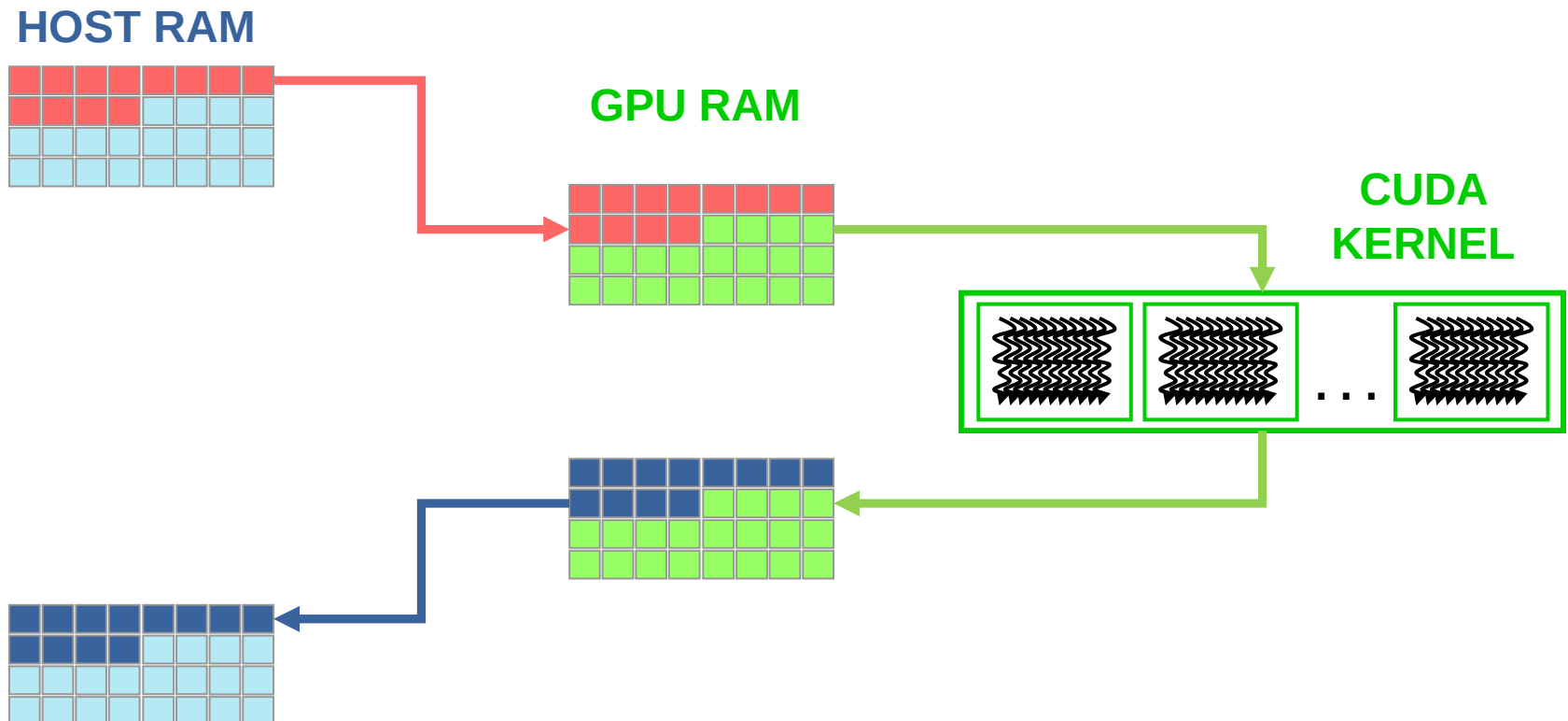


Connection Scheme of *host/device*



Data movement

- data must be moved from HOST to DEVICE memory in order to be processed by a CUDA kernel
- when data is processed, and no more needed on the GPU, it is transferred back to HOST



D2H and H2D Data Transfers

- GPU devices are connected to the host with a PCIe bus
 - PCIe bus is characterized by very low latency, but also by a low bandwidth with respect to other bus

Technology	Peak Bandwidth
PCIex GEN2 (16x, full duplex)	8 GB/s (peak)
PCIex GEN3 (16x, full duplex)	16 GB/s (peak)
DDR3 (full duplex)	26 GB/s (single channel)

- data transfer can easily become a bottleneck in heterogeneous environment equipped with accelerators
 - strive to minimize transfers or execute them in overlap with computations (advanced technique, more on this later)

NVLink NVIDIA Technology

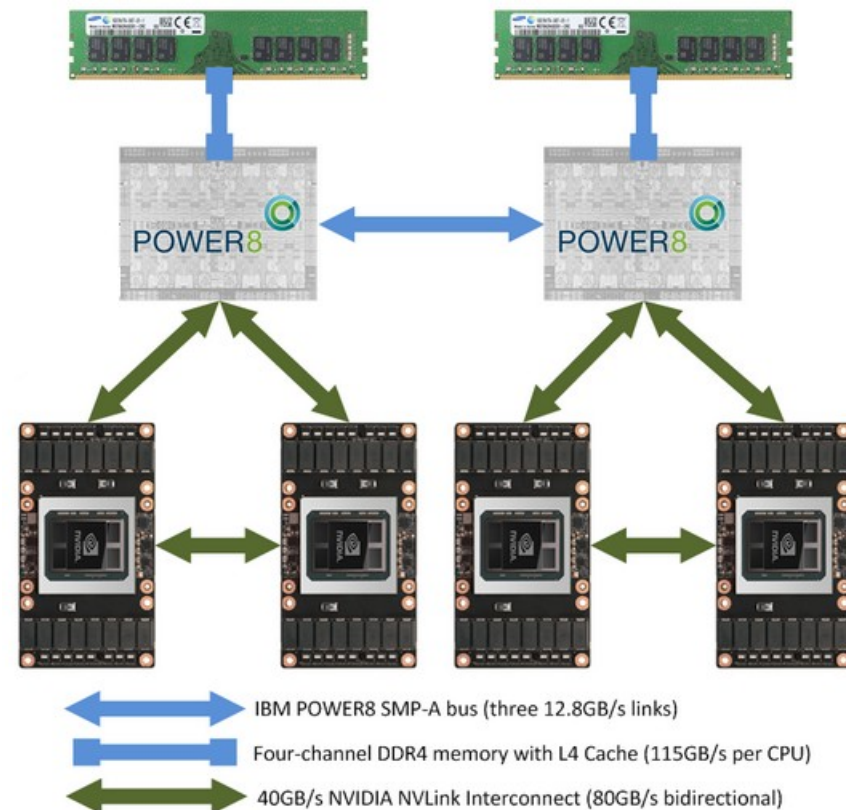
- NVLink is a wire-based communications protocol serial multi-lane near-range communication link developed by Nvidia.
- NVLink specifies a point-to-point connections with data rates of 20 and 25 Gbit/s (v1.0/v2.0) per data lane per direction.
- Total data rates in real world systems are 160 and 300 GByte/s (v1.0/v2.0) for the total system sum of input and output data streams.

NVLink Transfers on D.A.V.I.D.E.

	1	2	3	4
1	457.93	35.30	20.37	20.40
2	35.30	454.78	20.16	20.14
3	20.19	20.16	454.56	35.29
4	18.36	18.42	35.29	454.07

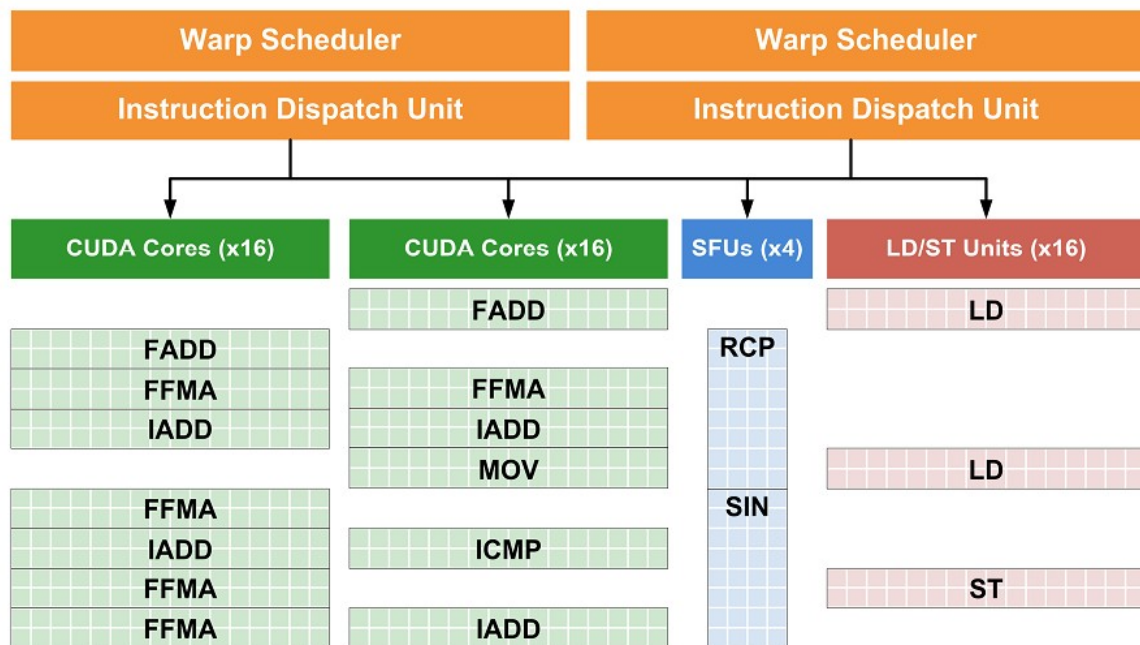
Bandwidth in GB/s transferring 1GB of data from device-to-device with peer-to-peer communications.

On each GPU, the available 80GB/s bandwidth was divided in half. One link goes to a POWER8 CPU and one link goes to the adjacent P100 GPU.



Warps

- The GPU multiprocessor creates, manages, schedules, and executes threads in groups of 32 parallel threads called *warps*.
- Individual threads composing a warp start together at the same program address, but they have their own instruction address counter and register state and are therefore free to branch and execute independently
- each *warp* can execute instructions on
 - SM cores
 - load/store units
 - SFUs units

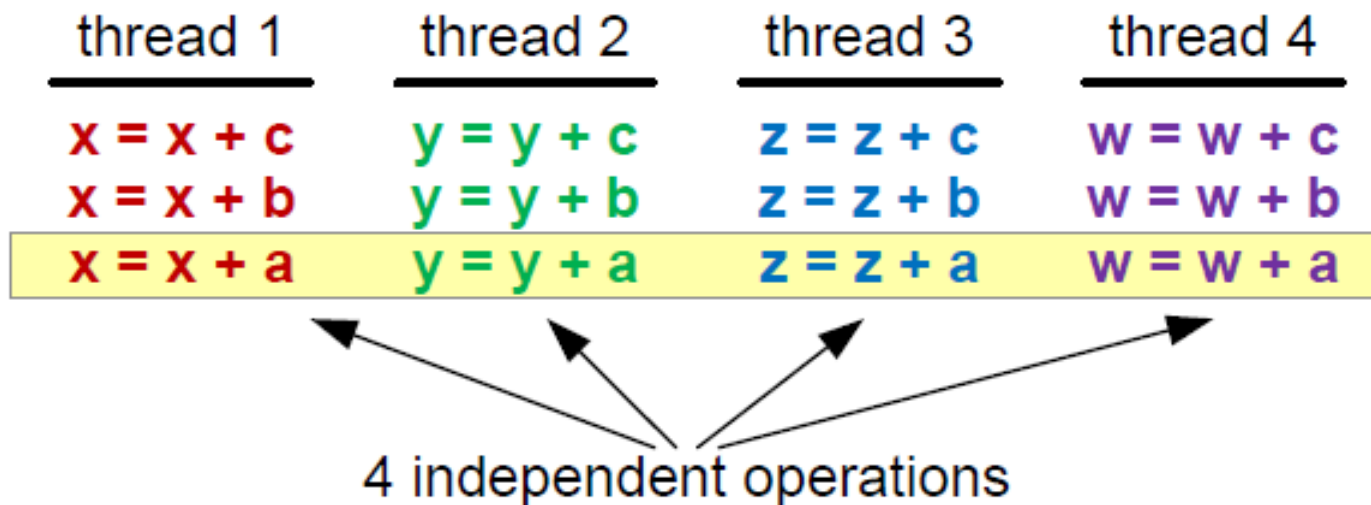


Hiding Latencies

- What is latency?
 - the number of clock cycles needed to complete an instruction
 - ... that is, the number of cycles I need to wait for before another **dependent operation** can start
 - arithmetic latency (~ 18-24 cycles)
 - memory access latency (~ 400-800 cycles)
- We cannot discard latencies (it's an hardware design effect), but we can lesser their effect and hide them.
 - saturating computational pipelines in computational bound problems
 - saturating bandwidth in memory bound problems
- We can organize our code so to provide the scheduler a sufficient number of **independent operations**, so that the more the warp are available, the more content-switch can hide latencies and proceed with other useful operations
- There are two possible ways and paradigms to use (can be combined too!)
 - Thread-Level Parallelism (TLP)
 - Instruction-Level Parallelism (ILP)

Thread-Level Parallelism (TLP)

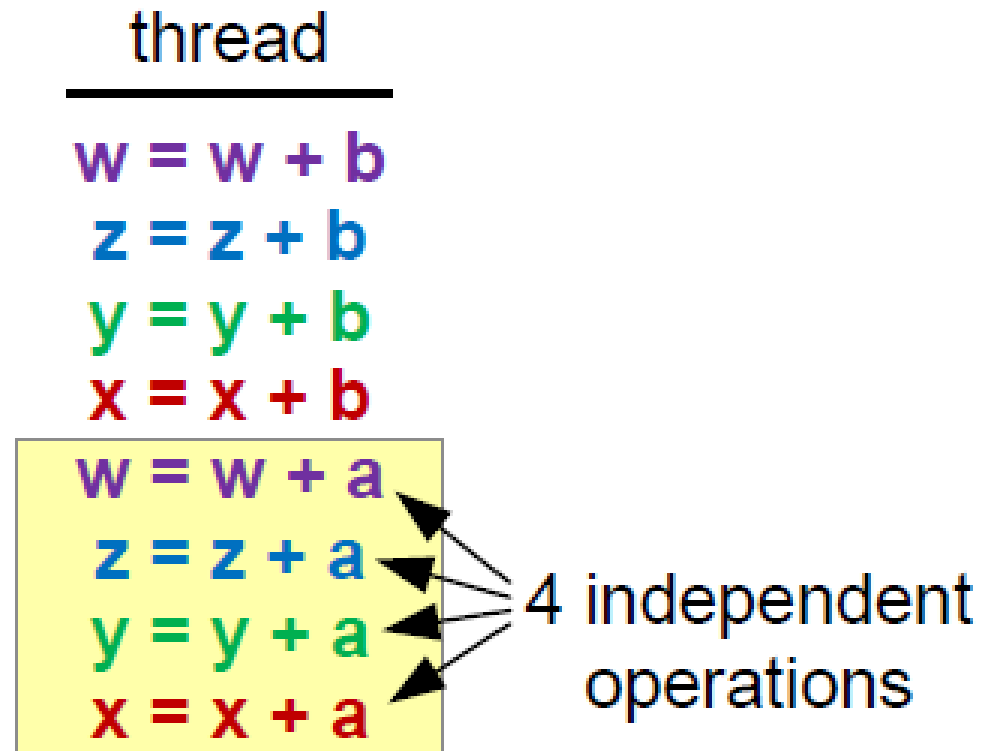
- Strive for high SM occupancy: that is try to provide as much threads per SM as possible, so to easy the scheduler find a warp ready to execute, while the others are still busy
- This kind of approach is effective when there is a low level of independent operations per CUDA kernels



Instruction-Level Parallelism (ILP)

- Strive for multiple independent operations inside you CUDA kernel: that is, let your kernel act on more than one data
- this will grant the scheduler to stay on the same warp and fully load each hardware pipeline

- note: the scheduler will not select a new warp until there are eligible instructions ready to execute on the current warp



■ GPU programming models

- GPU enabled libraries
- high level directives
- low level programming languages



3 Ways to Accelerate Applications

Applications

Libraries

Directives

Programming
Languages

“Drop-in”
Acceleration

Easily Accelerate
Applications

Maximum
Flexibility

Portability

Performance

3 Ways to Accelerate Applications

Applications

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Performance

Libraries: Easy, High-Quality GPU Ready

- **Ease of use:**

Using libraries enables GPU acceleration without in-depth knowledge of GPU programming

- **“Drop-in”:**

Many GPU-accelerated libraries follow standard APIs, thus enabling acceleration with minimal code changes

- **Quality:**

Libraries offer high-quality implementations of functions encountered in a broad range of applications

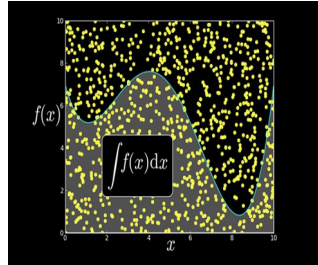
- **Performance:**

libraries are tuned by experts

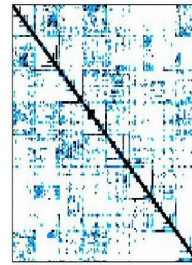
Some GPU-accelerated Libraries



cuBLAS



NVIDIA cuRAND



NVIDIA cuSPARSE



NVIDIA NPP

GPU VSIPL

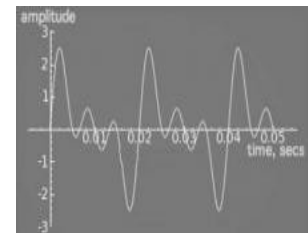
Vector Signal
Image
Processing

CULA|tools

GPU
Accelerated
Linear Algebra



Matrix Algebra
on GPU and
Multicore



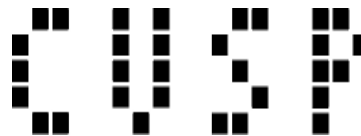
NVIDIA cuFFT



IMSL Library



ArrayFire
Matrix
Computations



Sparse Linear
Algebra



C++ STL
Features for
CUDA



3 Ways to Accelerate Applications

Applications

Libraries

Directives

Programming
Languages

“Drop-in”
Acceleration

Easily Accelerate
Applications

Maximum
Flexibility

Portability

Performance

Directive Based Approach

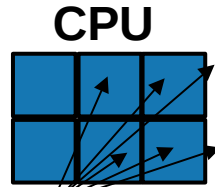
- Directives are added to serial source code
 - Manage loop parallelization
 - Manage data transfer between CPU and GPU memory
- Directives are formatted as comments
 - They don't interfere with serial execution
 - Maintains portability of original code
- Works with C/C++ or Fortran
- Can be combined with explicit CUDA C/Fortran usage

OpenACC

- OpenACC is a high-level specification with compiler directives for expressing parallelism for accelerators.
 - Portable to a wide range of accelerators.
 - One specification for Multiple Vendors and Multiple Devices
- OpenACC specification was released in November 2011.
 - Original members: CAPS, Cray, NVIDIA, Portland Group
- OpenACC 2.0 was released in June 2013
 - More functionality
 - Improve portability
- OpenACC 2.5 in November 2015
- OpenACC had more than 10 member organizations

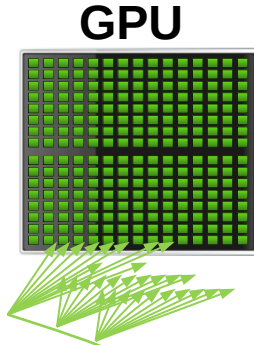
Familiar to OpenMP Programmers

OpenMP



```
main() {  
    double pi = 0.0; long i;  
  
    #pragma omp parallel for reduction(+:pi)  
    for (i=0; i<N; i++)  
    {  
        double t = (double)((i+0.05)/N);  
        pi += 4.0/(1.0+t*t);  
    }  
  
    printf("pi = %f\n", pi/N);  
}
```

OpenACC



```
main() {  
    double pi = 0.0; long i;  
  
    #pragma acc parallel loop reduction(+:pi)  
    for (i=0; i<N; i++)  
    {  
        double t = (double)((i+0.05)/N);  
        pi += 4.0/(1.0+t*t);  
    }  
  
    printf("pi = %f\n", pi/N);  
}
```

OpenMP 4.x

- Starting from OpenMP 4.x begins support for accelerator offload of high-parallel regions
- data movement and placement was refined with OpenMP v4.5
- OpenMP accelerator suites very well GPUs and efficient implementation runs on NVIDIA and AMD GPUs
- “OpenMP will be at a point where everything OpenACC has will have a direct analogy in OpenMP other than the kernels directive, which will probably never be in OpenMP.” *Bronis de Supinski - CTO and chair of the OpenMP language committee*

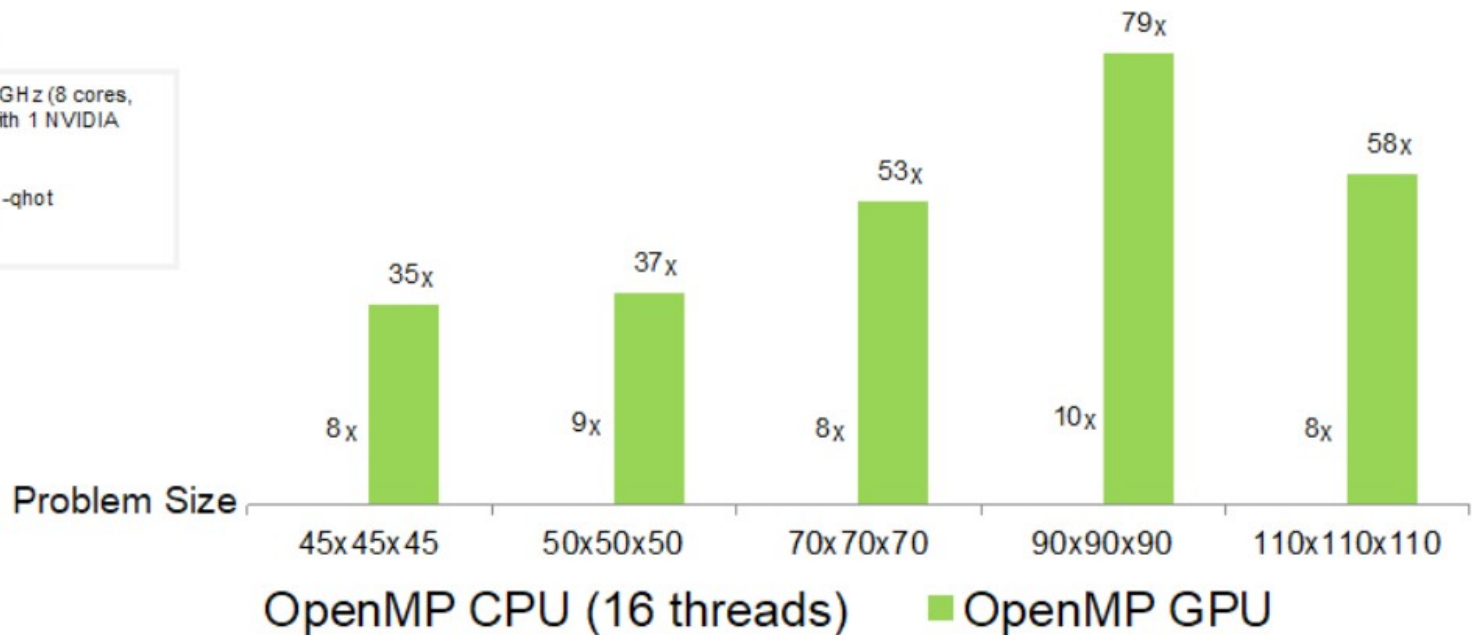
OpenMP v4.5 Benchmark on GPU

- LULESH represents a typical hydrocode, like ALE3D. LULESH approximates the hydrodynamics equations discretely by partitioning the spatial problem domain into a collection of volumetric elements defined by a mesh. A node on the mesh is a point where mesh lines intersect. LULESH is built on the concept of an unstructured hex mesh. Instead, indirection arrays that define mesh relationships are used. The default test case for LULESH appears to be a regular cartesian mesh, but this is for simplicity only – it is important to retain the unstructured data structures as they are representative of what a more complex geometry will require.

Test Specs

2 Power8 sockets @ 4GHz (8 cores, with 8 threads each) with 1 NVIDIA Pascal P100 GPU.

Compiler Options: -O3 -qhot
-qsm p=omp -qoffload*
* Where applicable



<https://codesign.llnl.gov/lulesh.php>

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GPU Programming Languages

- nVIDIA CUDA (Compute Unified Device Architecture)
 - a set of extensions to higher level programming language to use GPU as a coprocessor for heavy parallel task
 - a developer toolkit to compile, debug, profile programs and run them easily in a heterogeneous systems
- OpenCL (Open Computing Language):
 - a standard open-source programming model developed by major brands of hardware manufacturers (Apple, Intel, AMD/ATI, nVIDIA).
 - like CUDA, provides extensions to C/C++ and a developer toolkit
 - extensions for specific hardware (GPUs, FPGAs, MICs, etc)
 - it's very low level (verbose) programming

GPU Programming Languages

Fortran ▶

OpenMP, OpenACC, CUDA
Fortran

C ▶

OpenMP, OpenACC, CUDA C, OpenCL

C++ ▶

Thrust, CUDA C++, OpenCL

Python ▶

PyCUDA, Copperhead

Numerical analytics ▶

MATLAB, Mathematica, LabVIEW

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