

INF560 Algorithmique Parallèle et Distribuée

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Lecture Outline – GPU (1/2)

- Overview of Dedicated Hardware
- NVIDIA GPGPU architecture
- CUDA Programming
 - Host-Side
 - Device-Side

Dedicated Hardware

>>> Overview

Motivations

- Homogeneous clusters
 - Building blocks: on-the-shelves CPUs
 - Good performance for majority of codes, but dedicate many transistors to micro-architecture
- Limitations of such clusters
 - Homogeneous large cores
 - Relate to limitation of general purpose processors
- One possible solution
 - Towards dedicated hardware

Dedicated Hardware

Definition

Distinct resource dedicated to specific operations

Impact

- Aka accelerators
- Processor dedicated to a specific class of applications
 - Different goals from regular CPU
 - Enable better performance for this class
- Located on specific chip (or not)
 - Linked to CPU through some interconnect
 - Master/slave behavior

Interconnect Types

- Advantages
 - Low cost
 - Smooth integration
- Drawbacks
 - Moderate performance (generic bus)
 - Sub-optimal latency and bandwidth
- NVIDIA GPGPU, Intel Xe, AMD MI100

- Advantages
 - Fast access
 - Possibility to share resources w/ CPU
- Drawbacks
 - Complex integration
 - Processor dependency
- IBM Cell , AMD/ATI fusion architecture

System Bus

Processor Bus

Main Architecture

- Microarchitecture
 - Driven by target class of applications
 - Simplified compared to regular CPUs
 - No OoO execution
 - No branch predictor
 - •
- Exploited parallelism
 - Fine-grain parallelism (in general)
 - Mostly following the Single Instruction Multiple Data (SIMD) form
- But
 - Major work is let to software stack and code developer!

Main Architecture

Memory hierarchy

- Memory controlled by software/developer (scratchpad memory)
- Cache handled by hardware (part of microarchitecture like on regular CPU)
- Hardware connection between compute processors
- Large bandwidth between device on its global memory

Summary

- Interesting characteristics for HPC
- Many aspects to handle by hand
- Direct influence on programming and execution model

Accelerator Programming

- Accelerator can be seen as slave device
- Main processor controls accesses to dedicated hardware
 - Main processor (CPU): host
 - Accelerator: device
- Main concepts
 - Data transfers
 - Remote code execution with dedicated language
 - Manual management of execution
 - Queries to accelerators

Existing Accelerators

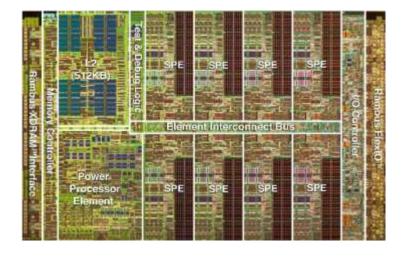
- Graphics-based processor
 - GPGPUs (General Purpose Graphics Processing Units)
 - NVIDIA
 - AMD
 - Intel Xe
- Dedicated accelerators
 - Cell (IBM)
 - Intel Xeon Phi (KNC/KNL)
- Reconfigurable architectures
 - FPGA

Graphics Processor

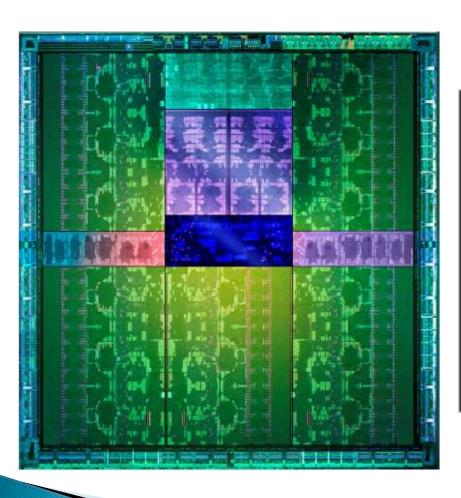
- Initially designed to print pixels on screen (for 2D or 3D graphics)
 - Dedicated processor for this purpose
- Large compute capabilities
 Optimized to image rendering
 Well adapted to regular data processing
- For scientific workloads
 - GPGPU (General Purpose Graphics Processing Unit)
 - Graphics cards on system bus
 - Connection to motherboard
 - Communication through PCI-E
 - Possibility to connect multiple graphics cards
 - Multi-GPU programming
 - Current configuration in heterogeneous supercomputers

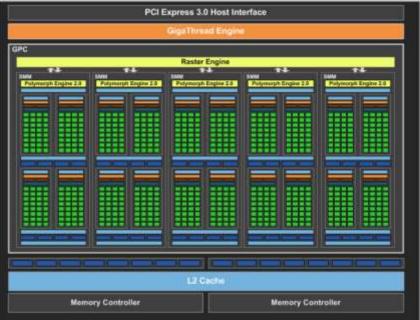
IBM Cell Processor

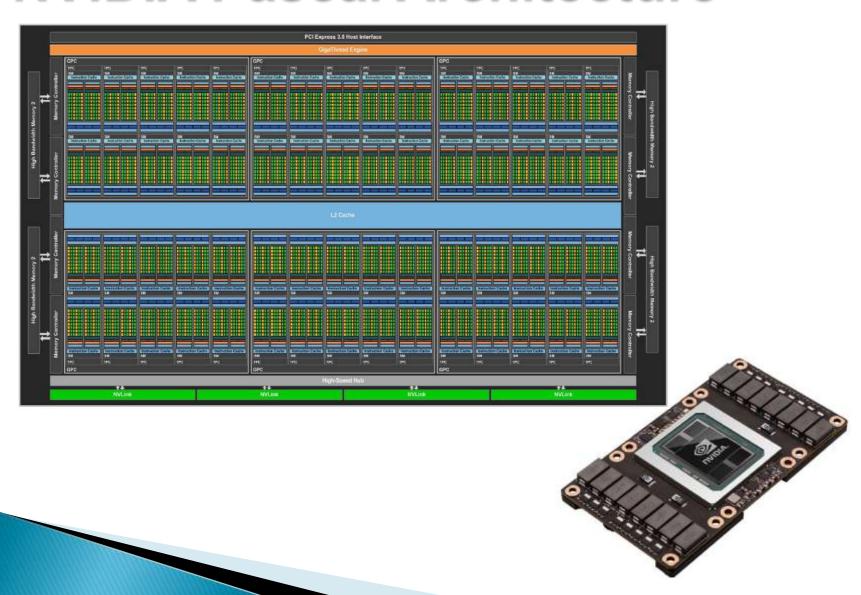
- Joint development between IBM, Sony and Toshiba
- 8 64-bit cores (w/ FP units)
 - Synergistic Processor Elements (SPEs).
 - SIMD: 128-bit register width (4 words of 32 bits)
- Master processor: 64-bit PowerPC
 - 2 logical threads
- Register file
 - 128 operands



NVIDIA Maxwell Architecture







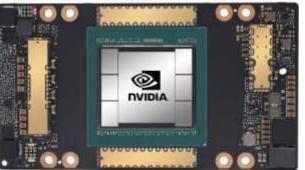
NVIDIA Volta Architecture



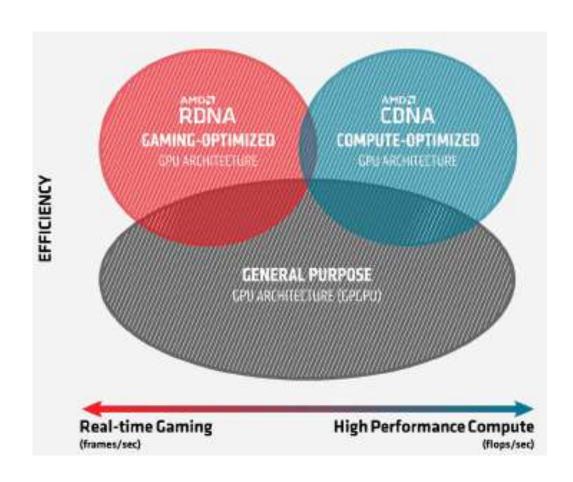


NVIDIA Ampere Architecture

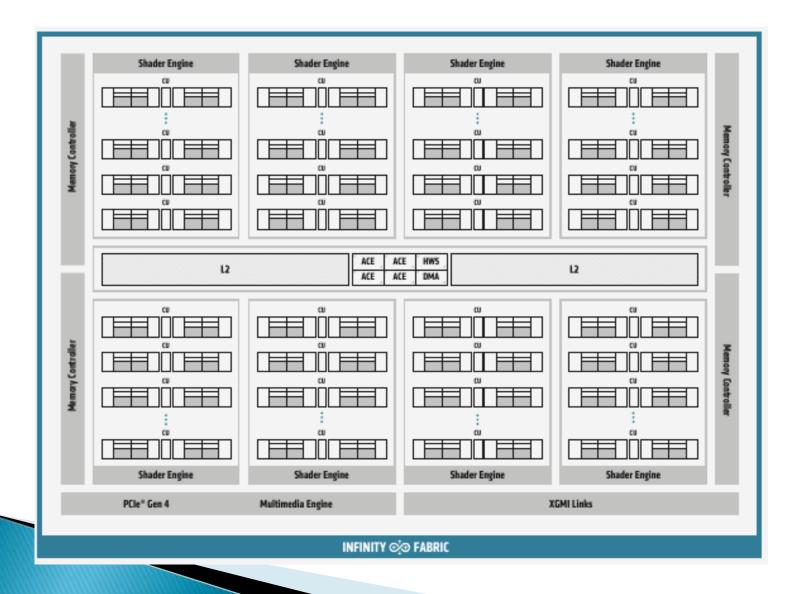




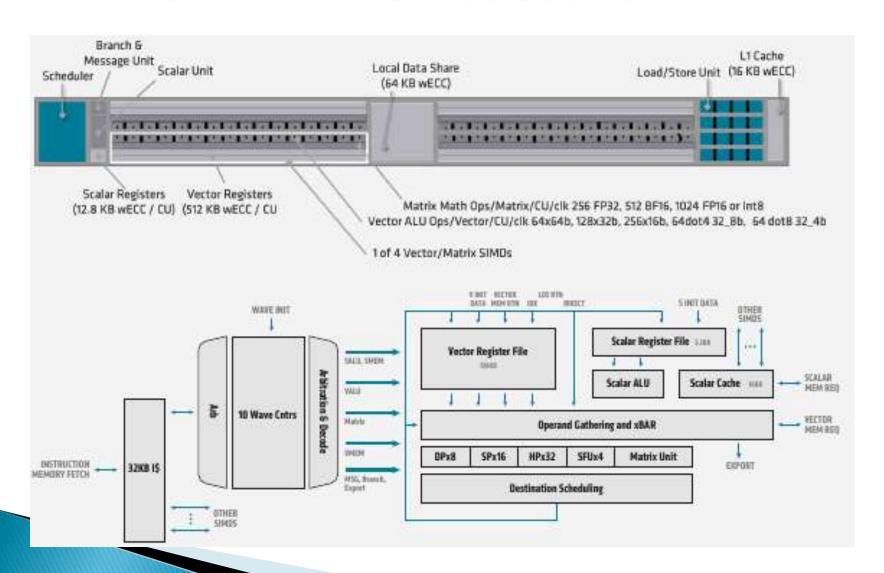
AMD CDNA Architecture



AMD CDNA Architecture

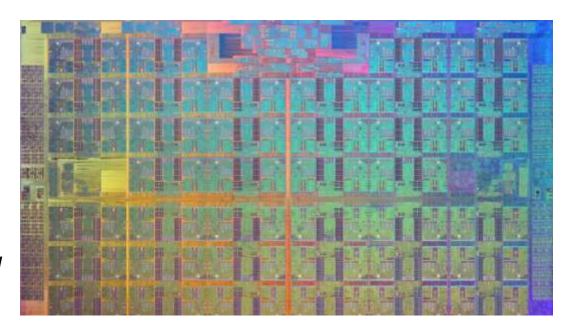


AMD CDNA Architecture



Intel Xeon Phi

- Accelerator designed by Intel
 - Many-Integrated Core (MIC)
- Introduced in 2008
 - @SigGraph 2008 conference
 - Codename at that time: Larabee
- Architecture
 - X86 cores
 - Support of hyperthreading
 - Cache coherency
- Current version: KNL
 - Exist in non-accelerator mode



Future Exascale Systems

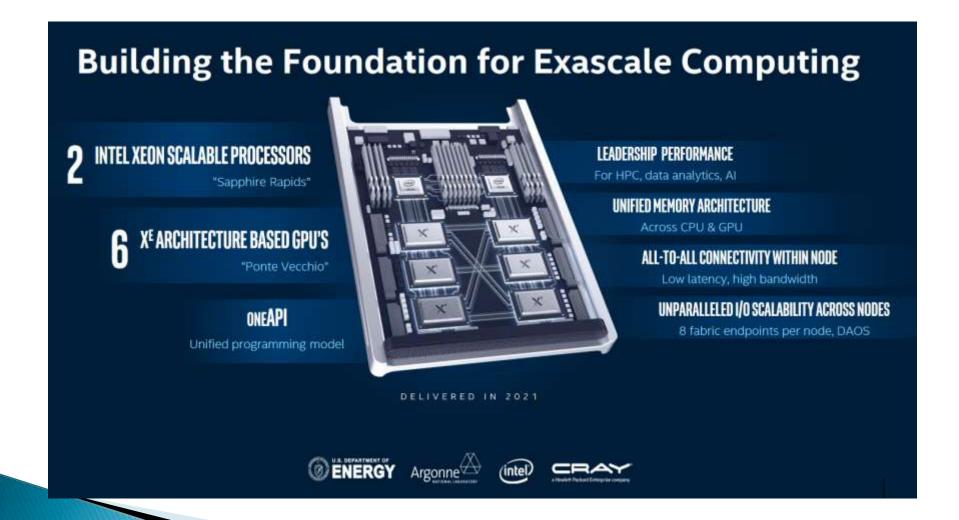
- Next year: first exascale machine!
- Funded by DoE, located in National Labs
- Argonne National Lab: Aurora
- Oakridge National Lab: Frontier
- Based on GPUs!

ANL - Aurora

- Sustained performance > 1 Exaflop
- Aggregate system memory > 10 PB
- Storage > 230 PB, 25 TB/s (DAOS)
- Compute node
 - 2 Intel Xeon processors
 - 6 Xe arch-based GP-GPUs
- Interconnect
 - CPU-GPU: PCIe
 - System : Cray Slingshot
- Software stack
 - Cray stack (+ Intel improvement)
 - Programming models : Intel OneAPI, OpenMP, SYCL/DPC++



ANL - Aurora



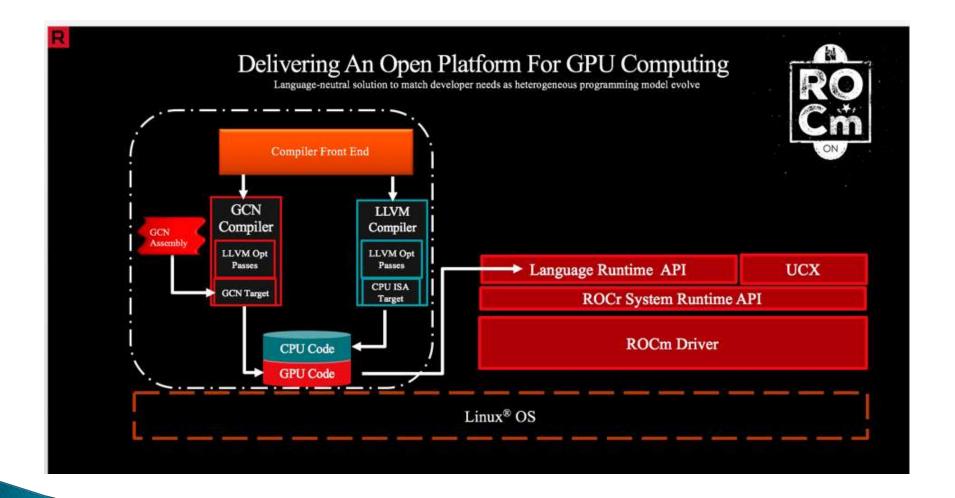
ONL - Frontier

- Peak Performance > 1.5 Exaflop
- More than 100 cabinets
- Node
 - 1 HPC and AI optimized AMD EPYC CPU
 - 4 AMD Radeon Instinct GPU
- Interconnect
 - CPU-GPUI: AMD infinity Fabrix (coherent memory across node)
 - System: Cray Slingshot
- Software stack
 - Cray + AMD ROCm
 - Programming models : MPI, OpenMP 5.X, HIP, ...





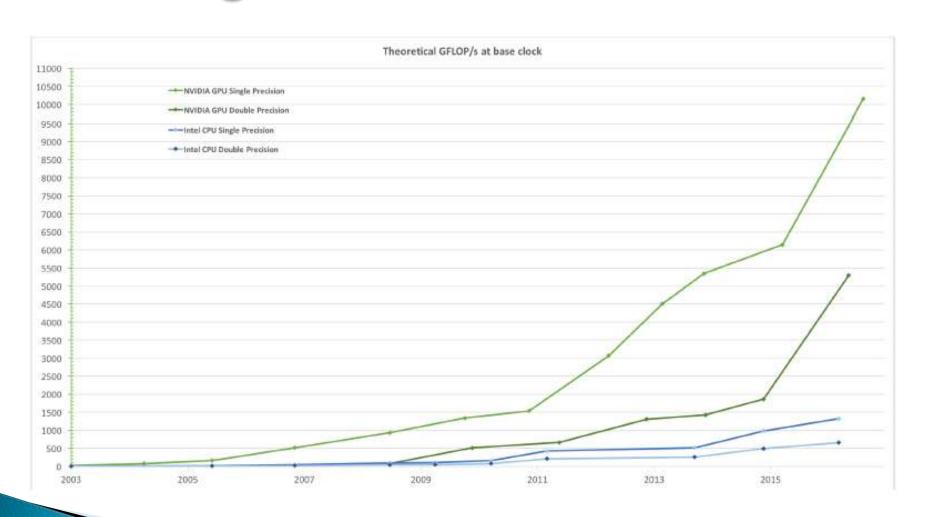
ONL - Frontier



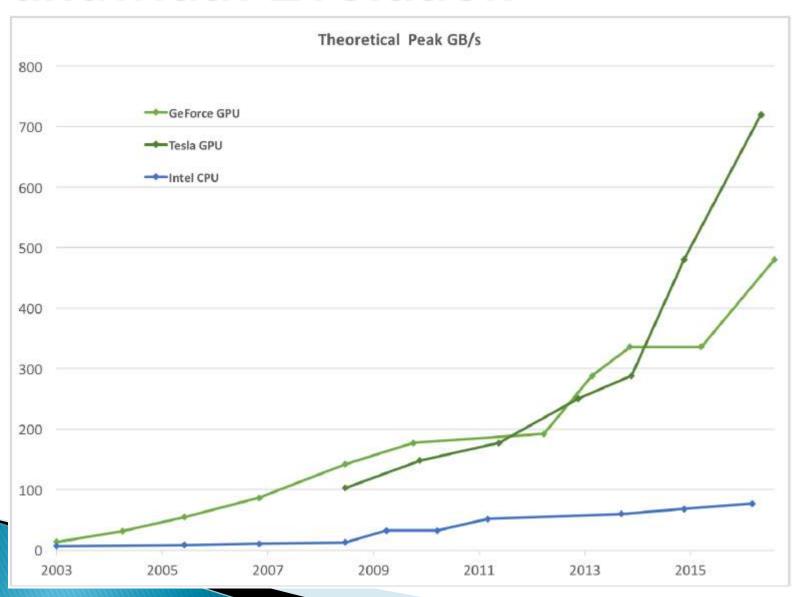
Dedicated Hardware

>>> NVIDIA GPGPU Architecture

Floating-Point Performance



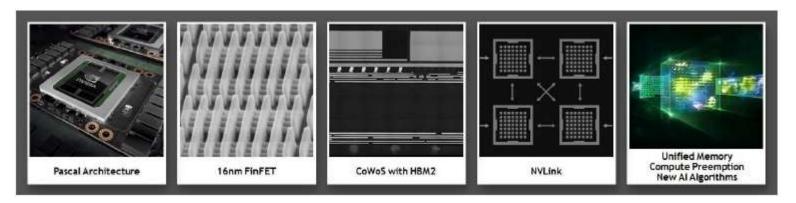
Bandwidth Evolution



NVIDIA Architecture Overview

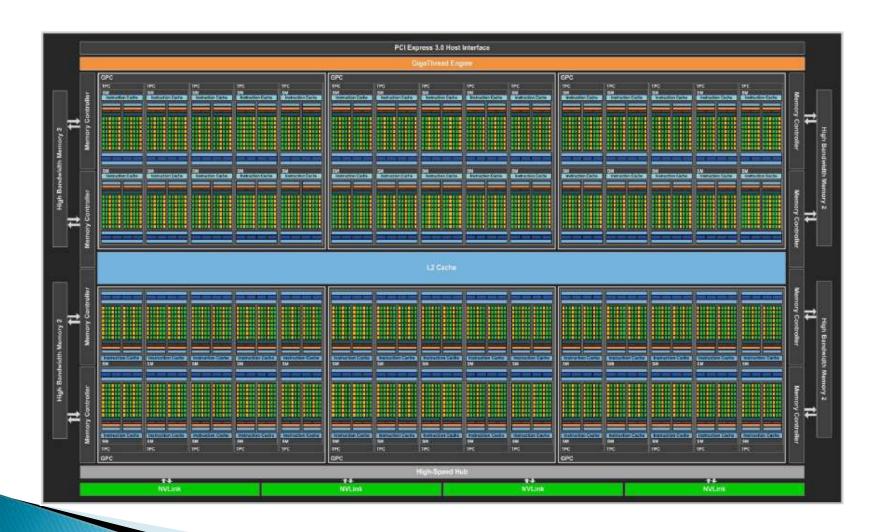
- Building block
 - Very simple compute core
 - Set of cores grouped inside a stream multiprocessor
- Why stream?
 - Made to handle data streams (contiguous flow of data)
 - Synchronous language on each multicore processor
- Designed for fine-grain parallelism

- Recent generation of NVIDIA architecture (w/ double-precision performance)
 - Codename: Pascal
- Tesla version
 - 15.3 billion transistors
 - 5.3 Tflops (double precision)



- ▶ GP100 → array of 6 GPCs (Graphics Processing Clusters)
 - 1 GPC → 10 SMs (Streaming Multiprocessors)
- Placement according to L2 cache
- Figure
 - Green → compute core
 - Double-precision unit in orange
 - Orange → scheduler and dispatcher
 - Light blue → register file and L1\$





Pascal: Streaming Multiprocessor

- 6th generation
- 64 CUDA-compatible cores
 - ALU unit
 - Simple-precision compute unit
- 32 double-precision units
- ▶ 16 special units (SFU)
- 16 load/store units



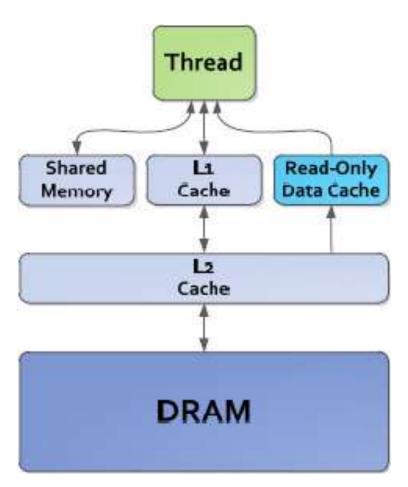
Pascal: Streaming Multiprocessor

- SIMT-based execution
 - Single-Instruction Multiple Thread
- Similar to SIMD
- Synchronous execution on compute cores
- Each SM manage threads through packs of 32
 - Notion of warp
 - 2 warp scheduler per SM
 - 2 dispatch units/scheduler →
 2 issued instruction per cycle



Pascal: Memory Hierarchy

- Threads are scheduled on one compute core (on one SM)
- Memory access through load/store instruction
- 2 possibilities
 - Shared-memory access → no cache
 - Access to global device memory → go through 2 levels of cache
- L1\$ and shared memory corresponds to the same physical memory or distinct space (depending on version)
- Read-only cache (48 KB)



CUDA Programming

>>> Host-Side Programming

Overview

- Kernel-based programming
- Two parts:
 - Host programming
 - Compute kernels
- Need to transfer data back and forth
- Compilation chain dedicated to computer kernels (slightly different source language)
- Link to an software ecosystem
 - Runtime system (user space)
 - Driver (kernel space)

Programming Steps

- Template of CUDA code
- Initialization
 - Memory allocation Read input data
- GPU memory allocation

 Dynamic allocation from host
- Host → device transfers
- Remote execution of compute kernel Possibility to launch multiple kernels
- Device → host transfers

Compilation Process

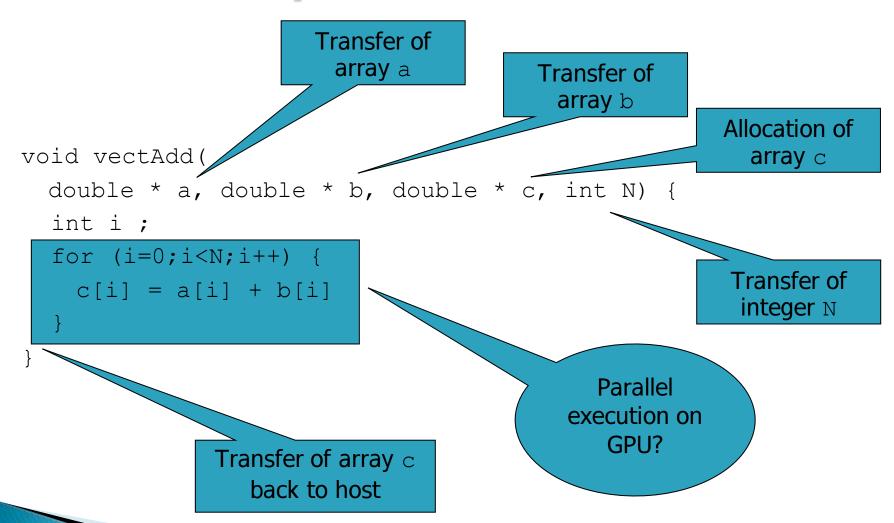
- Code structure
 - 2 parts
 - Host part
 - Device part
 - Two parts can be mixed inside same source file
- Host programming
 - C or C++
 - FORTRAN support developed by PGI
- Device programming
 - CUDA language
 - Superset of C99
- Compilation chain: NVCC
 - Use of nvcc compiler
 - Options available in the SDK documentation

First Example

- Example: vector addition
- Basic operation:
 - c[i] = a[i]+b[i]
- How to program this kernel in sequential?
 - Simple loop
 - Application of basic operation on each vector element

```
void vectAdd(
  double * a, double * b,
  double * c, int N) {
  int i;
  for (i=0;i<N;i++) {
    c[i] = a[i] + b[i];
  }
}</pre>
```

First Example



Host Programming

- Management from host (CPU)
 - Need to handle GPU global memory
 - Need to transfer data back and forth
 - Launch the remote device kernel
- Host-side CUDA API
 - CUDA high level / low level
 - Runtime or driver
 - cudaMalloc: allocate memory space on device
 - cudaMemcpy: transfer data with device
 - Multiple directions available

Host Programming

```
void vectAdd(
  double * a, double * b,
  double * c, int N) {
  double * d a ;
                       Device
                       pointers
  double * d b ;
  double * d c ;
  cudaMalloc((void **)&d a,
  N*sizeof(double));
  cudaMalloc(((void **)&d b,
  N*sizeof(double));
  cudaMalloc(((void **)&d c,
  N*sizeof(double);
```

Memory allocation on GPU

```
GPU
  cudaMemcpy(d a, a,
  N*sizeof(dou\overline{b}le),
  cudaMemcpyHostToDevice);
  cudaMemcpy(d b, b,
  N*sizeof(dou\overline{b}le),
  cudaMemcpyHostToDevice);
  cudaMemCpy(d c, c,
  N*sizeof(dou\overline{b}le),
  cudaMemcpyHostToDevice);
  vectAddKernel(d a, d b, d c,
  N);
                              Kernel
  cudaMemcpy(c, d c,
                             execution
  N*sizeof(double),
  cudaMemcpyDeviceToHost);
/* cudaFree... */
```

Transfer

to host

Transfe r to

Execution Model

- Device only has to execute kernel: vector addition
- How to program kernel on device?

```
for (i=0;i<N;i++)
c[i]=a[i]+b[i];
```

- CUDA model defines notion of thread
 - Each thread will run the kernel function
 - By default, CUDA programs are multithreaded
 - Point of view from threads, and not from loops
 - Different from regular sequential programming
- Kernel pseudo-code:

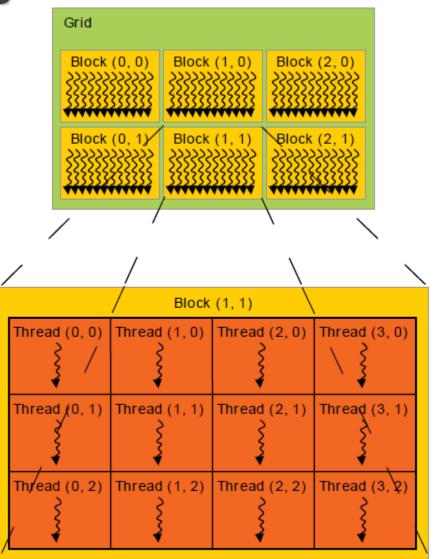
```
int i;
/* Update i with thread index */
c[i] = a[i] + b[i];
```

Thread Hierarchy

- How to get thread id?
 - Related to thread organization w/ execution model
- CUDA introduces notion of blocks and grid to organize threads in hierarchical manner
- Grid
 - Contains blocks
 - Contains threads
- Grid and blocks may be organized in 1D, 2D or 3D
 - Logical representation

Thread Hierarchy

- Example
 - 1 2D grid
 - 6 2D blocks
- 6 blocks in the grid and12 threads per block
 - → total of 72 threads
- How to compute thread id from this representation?



CUDA Programming

- Kernel declaration
 - Keyword: __global___
- Compute thread index according to grid/block geometry
 - Example w/ 1D grid and 1D blocks
 - Organization should map the computational part
- Test to check that threads do not write beyond array size
 - Corresponds to upper bound from sequential loop

```
global void
\overline{\text{vecAddKernel}} ( double *a,
double *b, double *c, int
N) {
int i ;
i = blockIdx.x *
blockDim.x + threadIdx.x
if ( i<N ) {
    c[i] = a[i] + b[i];
```

Kernel Integration

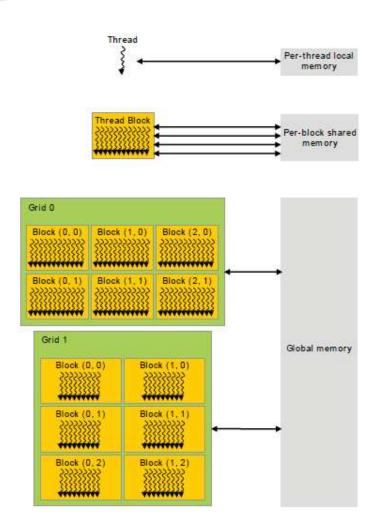
- How to choose representation of grid and blocks?
- Need to specify it during kernel remote launch
 - Host programming is in charge to define computational dimensions
- Syntax to launch a CUDA kernel from host to device

```
my kernel << Dg, Db>>> (arg1, arg2, arg3);
```

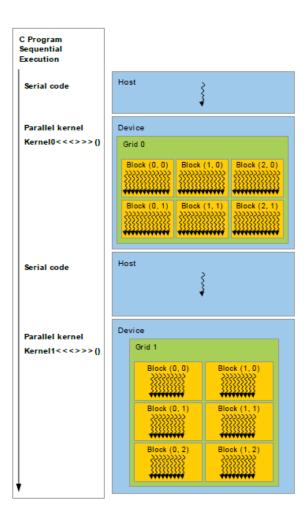
- Dg: dimensions and size of grid (dim3 type)
- Db: dimensions and size of blocks in grid (dim3 type)
- Total number of blocks?
- Number of thread per block?
- Total number of threads?

Memory Hierarchy

- Per-element vision
- Thread
 - Private local memory (stack)
 - Private register file
- Block
 - Private shared memory
- Grid
 - Global memory



Multi-Kernel Execution Model



Asynchronism

- By default some functions have asynchronous behavior
 - Kernel execution
 - Device-to-device copies
 - Memory initialization
- Possibility to wait for the end of operation execution
 - Sort of barriercudaThreadSynchronize();
- Force synchronism
 - CUDA_LAUNCH_BLOCKING=1
- Consecutive calls to kernel vecAdd
 - On different vectors?
 - If RAW dependencies exists?

Advanced Asynchronism

Motivations

- Ability to transfer data during kernel execution
- Ability to execute multiple compute kernels at the same type
 - If target device allows it (starting w/ Fermi)
 - If there are no data dependences between simultaneous kernels
- Solution: streaming
- Stream declaration
 - Interaction w/ device on a particular stream
 - Driver is aware of what can be done in parallel
 - o cudaMemCpy(d_c, c, N*sizeof(double), cudaMemcpyHostToDevice, stream[0]);
 - o my_kernel<<<Dg,Db,stream[0]>>>(arg1, arg2, arg3);

Profiling and Timers

- Profiling
 - Use provided tools like nvprof (see Lab)
 - Use CUDA events to track timing in CUDA functions
- Main type: cudaEvent t
- Event creation
 - cudaEventCreate(cudaEvent t * e)
- Event activation
 - cudaEventRecord(cudaEvent t e, cudaStream t s)
- Waiting for even to be activated
 - o cudaEventSynchronize(cudaEvent t e);
- Compute time spent between events
 - o cudaEventElapsedTime(float * ms, cudaEvent_t start, cudaEvent_t stop);

Error Handling

- In CUDA, almost all functions return an error code
 - Return type: cudaError_t
- ▶ If everything is ok → cudaSuccess
- Otherwise, possibility to access to error description
 - o const char * cudaGetErrorString (cudaError_t error);
- For functions not returning error information (e.g., kernel call)
 - Access to last error through cudaGetLastError()
 - Return type: cudaError t

Debugging

- How to debug a CUDA code?
- Add calls to printf?
 - Possible but not fully safe
- Add synchronization
- Check all error codes
 - Main way to check errors
- Transfer back to host on regular basis
 - Allow full checking w/ printing...

CUDA Programming

Device-Side Programming

CUDA Programming

- Compute kernel
 - Based on C99 standard
 - Some restrictions
 - Some extensions
- Extensions
 - New keywords
 - Variables defined by default
 - New function
- See CUDA C Programming Guide document
 - Appendix B for language extension
 - Appendix F for C/C++ standard support

Basic Kernel

- Basic syntax for a compute kernel
 - Function with void return type
 - Attribute to declare the function to execute on device
 - __global__
 - Input arguments

Example

Compilation

- Use dedicated compiler chain: NVCC
- Compiler will be in charge of splitting code parts for the host and device
- File extensions
 - .cu → file containing CUDA code (and host code)
 - .c / .cpp → file containing only host code (including CUDA API)

Extensions – Keywords

- Definition of new keywords
- Categories
 - Function attributes
 - Variable attributes
 - Types
- Set of variables defined by default
 - Rely on new defined data types

Function Attributes

- Keyword to add during function declaration and definition
 - Coherency between multiple declarations and definition!
 - Between return type and function name
- Function executed on device and callable from host (i.e., starting point for kernels)
 - o __global___
- Function dedicated to host or device (combinable)
 - host
 - o __device___
- ▶ Behavior by default → equivalent to __host__

Function Restrictions

- Functions with global attribute
 - Return type void
 - Call with execution context (number/dimensions of blocks, number of threads per block...)
 - Asynchronous call
 - Arguments stores in shared memory (256B) or constant memory (4KB)
 - Depends on CUDA capabilities of the target device
 - Impossible to get its address (function pointer)
- Functions executing on device
 - No static variable
 - No variable number of arguments
 - Restricted recursion (only for functions declared with ___device___ attribute)

Variable Attribute

- New variable attributes to handle placement
- Device-resident variable
 - o __device__
 - By default in global memory (shared by all threads during application lifetime)
- Constant memory resident variable
 - constant
 - Lifetime of application
 - Cannot be defined on device
- Shared-memory variable
 - shared
 - Shared between threads in the same block
 - One copy per block
 - Lifetime of block
- By default, variable declared on device is stored in a register

Volatile Variables

- Shared-data synchronization
- Example of concurrent accesses

```
// myArray is an array of non-zero integers
// located in global or shared memory
__global___ void MyKernel(int* result) {
   int tid = threadIdx.x;
   int ref1 = myArray[tid] * 1;
   myArray[tid + 1] = 2;
   int ref2 = myArray[tid] * 1;
   result[tid] = ref1 * ref2;
}
```

- What contains result [tid] ?
 - myArray[tid] is stored in a register → ref1==ref2
- If declared volatile → ok (or put a memory fence)
 - No guarantee on execution order

Variable Restrictions

 Dynamic management of variables in shared memory

```
extern __shared__ char array[];
_device__ void func() {
   short* array0 = (short*)array;
   float* array1 = (float*)&array[128];
   int* array2 = (int*)&array[64];
}
```

- Need to handle by hand placement of data in shared memory
 - No dynamic allocation
 - Need to respect alignment rules

Data Types

- New types
 - Vectors
 - Multi-dimension integers
- Vectors
 - Name convention: base type + width
 - **Examples**: int2, float4
 - Need to respect alignment rules
 - Functions available to create such types
 - Example: int2 make_int2(int x, int y);

Data Types

- 3D integers
 - dim3
 - Equivalent to vector type uint3
 - Access to coordinates through fields x, y and z
 - By default, initialized to 1

Example

```
dim3 a ;
a.x = 4 ;
```

Predefined Variables

Grid dimensions

- dim3 gridDim
- Contains number of blocks along 3 dimensions

Index of block in grid

- o dim3 blockIdx
- Contains coordinates of current block in grid

Block dimensions

- dim3 blockDim
- Contains number of threads along 3 dimensions

Index of thread in block

- uint3 threadIdx
- Contains coordonaites of current thread in its blocks

Warp size

• int warpSize

Available Functions

- Memory barrier
- Synchronizations
- Math operations
- Atomic operations
- Timing
- I/O

Memory Barrier

- Weakly-ordered memory model
 - Order of store instructions may be viewed as different from one thread to another
- Memory barrier
 - Mechanism to guarantee that memory accesses performed before the barrier appear to all threads as launched before the barrier
- Different levels of barrier

```
    Block: void __threadfence_block();
    Device: void __threadfence();
    Device + host: void threadfence system();
```

Synchronization

- Synchronization among all threads in the same block
 - o void syncthreads();
 - Include data synchronization
 - Be careful of control flow!
 - Act as a collective operations within a block
- For devices w/ CUDA capabilities >= 2.0

```
int __syncthreads_count(int predicate);
int __syncthreads_and(int predicate);
int __syncthreads_or(int predicate);
```

Math Operations

- Set of math functions optimized for GPU
 - Ex: sin(float), cos(double), ...
 - Less instructions but less accurate!
- Functions with prefix
 - $sinf(x) \rightarrow sinf(x)$
- Compilation option to automatically use these functions
 - Transform regular calls to optimized ones
 - -use fast math
 - Mainly available for single-precision computations

Atomic Operations

- Operation in one instruction that guarantee atomicity
 - E.g., int atomicAdd(int* address, int val);

Available functions

- Addition: atomicAdd
- Substraction: atomicSub
- Exchange: atomicExch
- Min/Max: atomicMin
- Increment/Decrement: atomicInc
- CAS, ...

Restrictions

- Available for integers
- Available for single-precision floats (capabilities 2.X)
- Since 6.X, double-precision operations

Timing & I/O

- Multiprocessor timestamp
 - o clock t clock();
 - Number of cycles
 - Possibility to check number of clocks for a thread

Formatted output

- int printf(const char *format[, arg,
 ...]);
- Require at least CUDA capabilities 2.X
- Per-thread context
- Final formatting on the host

Example

- Matrix multiply
- Rely on C data structure
 - Available on CPU and GPU
- Use variables w/ 2 dimensions
- Every thread computes one element of resulting matrix

```
typedef struct {
  int width;
  int height;
  float* elements;
} Matrix;
```

What if matrices are larger than maximum number of allowed threads?

```
global void MatMulKernel(Matrix
  A, Matrix B, Matrix C)
float Cvalue = 0;
int row = blockIdx.y * blockDim.y +
  threadIdx.y;
int col = blockIdx.x * blockDim.x +
  threadIdx.x;
for (int e = 0; e < A.width; ++e)
  Cvalue += A.elements[row *
  A.width + el
       * B.elements[e * B.width +
  coll;
C.elements[row * C.width + col] =
  Cvalue;
```

Example

```
global void MatMulKernel (Matrix A, Matrix B, Matrix C)
float Cvalue = 0:
int row = blockIdx.y * blockDim.y + threadIdx.y;
int col = blockIdx.x * blockDim.x + threadIdx.x;
for (int r = row ; r < C.height ; r += blockDim.y )</pre>
 for (int c = col ; c < C.width ; c += blockDim.x )
      for (int e = 0; e < A.width; ++e)
            Cvalue += A.elements[row * A.width + e]
                   * B.elements[e * B.width + col];
            C.elements[row * C.width + col] = Cvalue;
```

Register Allocation

- Each compute kernel uses several registers
- Depending on instructions inside the kernel body
 - Compiler transformations/optimizations
 - Register allocation
- But
 - Limited size of register file
 - Register file is shared among threads inside the same Streaming Multiprocessor
- Relation w/ number of threads?

Register Allocation

- Option to set an upper bound to compiler
 - -maxrregcount=N
- Attribute to indicate max number of threads and blocks when calling target function

```
__global___ void
__launch_bounds___(maxThreadsPerBlock,
    minBlocksPerMultiprocessor)
MyKernel(...)
{
    ...
}
```

Memory Access

- Because of synchronous execution
 - Thread executing load operation may lower other's speed
 - Several memory accesses may be serialized
 - Long-latency access need more warps to recover latency
- Possible optimizations
 - Load coalescing
 - Avoid bank conflicts

Load coalescing

- Access to global memory
- Concurrent accesses emitted by threads inside the same warp
 - All threads inside the same warp execute the same instruction at the same time
- Memory requests are serialized w/ chunks of 128B
 - Size of cache line
 - Optimization is memory accesses are contiguous

Load coalescing and shared memory

- Shared memory
 - Need to explicitly declare variables inside shared memory
 - Data transfers at the beginning of kernel
 - Update to global memory at the end of kernel
- Optimization: benefit from memory-to-memory transfers to change data layout
 - Even if all data are not necessary
- Be careful to bank conflicts

Best Practices

Higher priority

- Think parallel
- Minimize data transfers between host and device
- Access main device memory w/ coalesced operations
- Use shared memory when possible
- Avoid path divergence

Lower priority

- Avoid bank conflict when accessing shared memory
- Avoid too large number of threads per blocks (multiple of 32)
- Rely on optimized math functions