Tutorial
Scientific Programming in CUDA

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Intermediate Level:
Writing an Optimized Kernel
using
Shared Memory and Streams

CUDA
Overview

- Tutorial is not meant for absolute beginners
- Focus on basic setup, performance optimization, and techniques that are beneficial under most circumstances
- Hardware overview
- Simple kernel: 'Hello World' equivalent for GPUs
- Stencil update
  1. Using main memory on card
  2. Using shared memory of each SM (Streaming Multiprocessor)
  3. Interleaving data transfer and calculations
     - Using the host as well
     - Using multiple nodes with MPI

Programming GPUs

A bit different, but not too difficult

- A bit of a learning curve at the beginning
  - This will guide you towards writing fast code
- 3 concepts
  - Hardware → constraints on the code
  - Shared (fast) memory
  - Data transfer between host and device (communication)
- Concepts are (relatively) easy to understand --- this is what this course is about
- Writing high performance, parallel code is always complicated, but the concepts are a recurring theme

Why NVIDIA GPUs?

- The market for computer hardware is tough. Vendors are competing ferociously. At times one vendor gets ahead for a short time.
- NVIDIA got ahead by
  - "converting" their graphics chips for compute
  - Adding a (proprietary) language: CUDA,

    Compute Unified Device Architecture
- Other vendors are catching up on Hardware and Software
  - AMD (bought ATI), Intel, etc.
  - Intel has launched its MIC (Many Integrated Core) technology (First product: Intel Xeon Phi)

Why CUDA?

- GPUs from a variety of vendors can be programmed in OpenCL
  - The industry standard for GPU programming
  - Language evolution through a language committee with GPU vendors, Compiler vendors, Industry, Software developers, etc.
- NVIDIA selected a different path
  - Proprietary Hardware
  - Proprietary Language: CUDA
- Advantages and Disadvantages
  - Supposedly faster language evolution
  - How does CUDA translate to the standard (OpenCL)?
  - CUDA is supported by C and Fortran compilers

This class will be bi-lingual: C & Fortran

CUDA, C and Fortran

- CUDA (from NVIDIA) is an addition to C
- The Portland group (PGI) provides a separate compiler for Fortran
- User profile at TACC: 50% C/C++ and 50% Fortran
- Student profile in our classes is usually the same!
- Being able to teach both languages is a big plus!
- C + CUDA: all code is written in C
- PGI CUDA Fortran Compiler: all code is written in Fortran
- There is also is PGI CUDA C compiler available

Why are we using Accelerators after all?

- The speed of one CPU (core) has been stagnant (sort of)
  - Cluster revolution in the 90's
- Capability comes from using multiple CPUs
  - With multiple cores in in CPU: multi-core CPU
  - And multiple CPUs in a computer
- Cluster: A lot of computers plus an Interconnect
  - Multi-core (4-8), multi-socket (2-4) → 10,000-100,000 cores
  - Connection through a fast (and very expensive) network
  - and a parallel file system, etc.
- Many clusters are build from commodity hardware
  - X86 from Intel and AMD, etc.

How can we make Supercomputers faster and more capable?

Accelerators and Co-Processors

- Several options:
  - Increase of the cluster size, more compute nodes
  - Increase capability of cluster components: make nodes “bigger”; more CPUs, more cores
  - Add Accelerators (GPU) or Co-processors (MIC) to the individual computer nodes

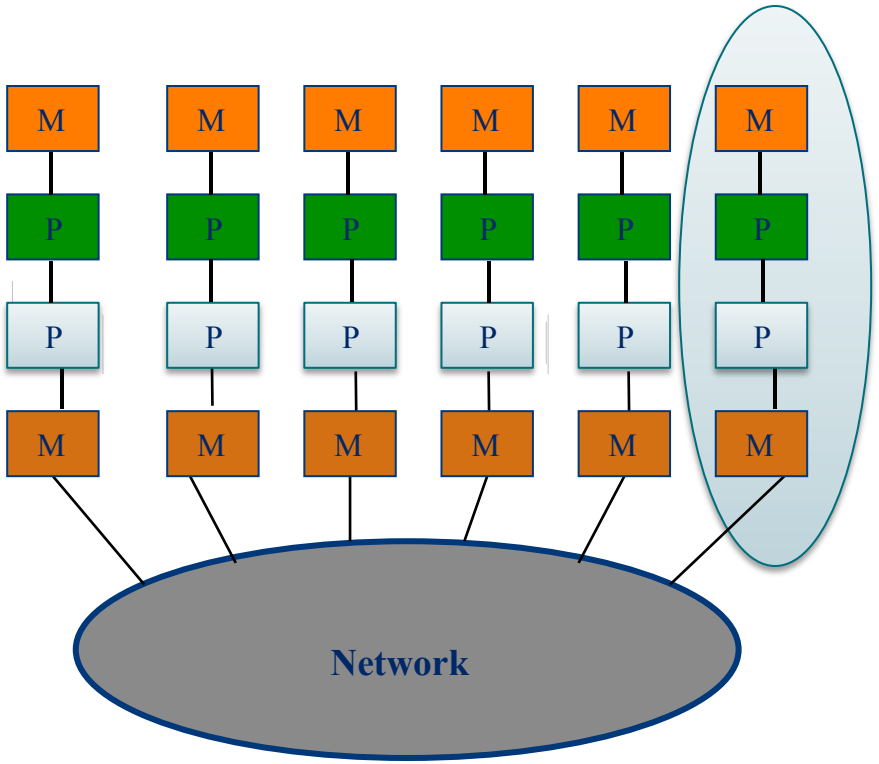
Cluster with GPUs

Memory GPU

GPU

CPU

Memory CPU



Step 1:
One node

Step 2:
Multiple nodes

Programming for a CPU/GPU pair is like programming for a small CPU cluster

GPU Overview

- GPUs have multiple independent compute units: SMs
  - SM: Streaming Multiprocessors
  - Rough equivalent of CPU cores
- GPUs have multiple memories
- Main Memory: accessible by all Threads executing on the SMs (Streaming Multiprocessors)
  - Relatively large: ≥4GB
  - Relatively fast (faster than CPU memory)
- Each SM has shared memory that is local to an SM
  - Very small: ~16KB per SM
  - Very fast (compared to the Main GPU Memory)
- Additional Memories: Texture, Constants, etc.

Resources

Kirk and Hwu:

Programming Massively Parallel Processors

Rob Farber:

CUDA Application Design and Development

Hwu:

GPU Computing Gems

Jason Sanders and Edward Kandrot:

CUDA by Example

Hardware Overview: CPU vs. GPU characteristics

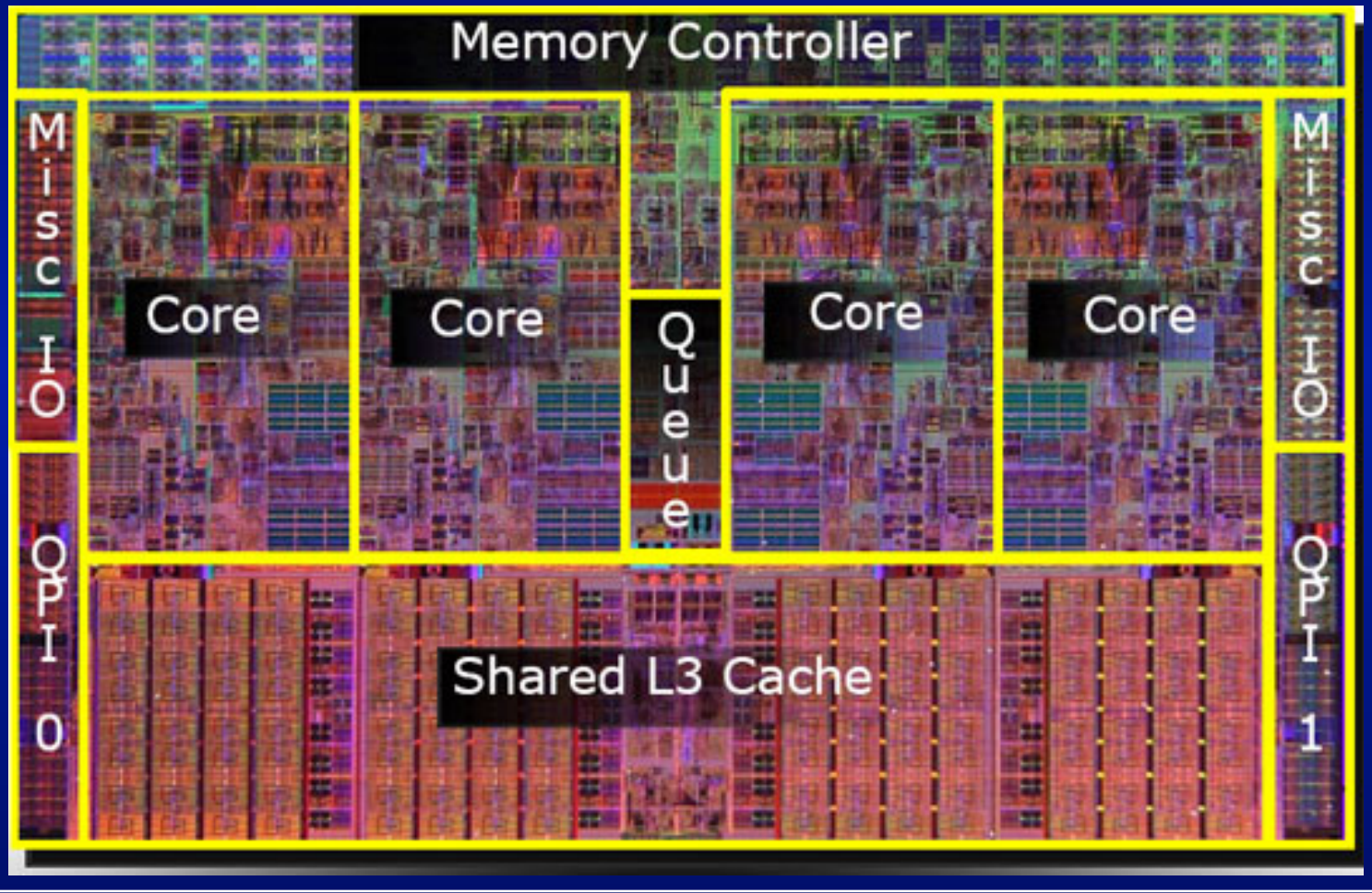
CPU

- Few compute cores
  - Supports many instruction streams, but keep few for performance
- More complex pipeline
  - Out-of-order processing
  - Deep (tens of stages)
  - Became simpler (Pentium 4 was complexity peak)
  - Pipelining
- Optimized for serial execution
  - But SIMD execution becomes more important

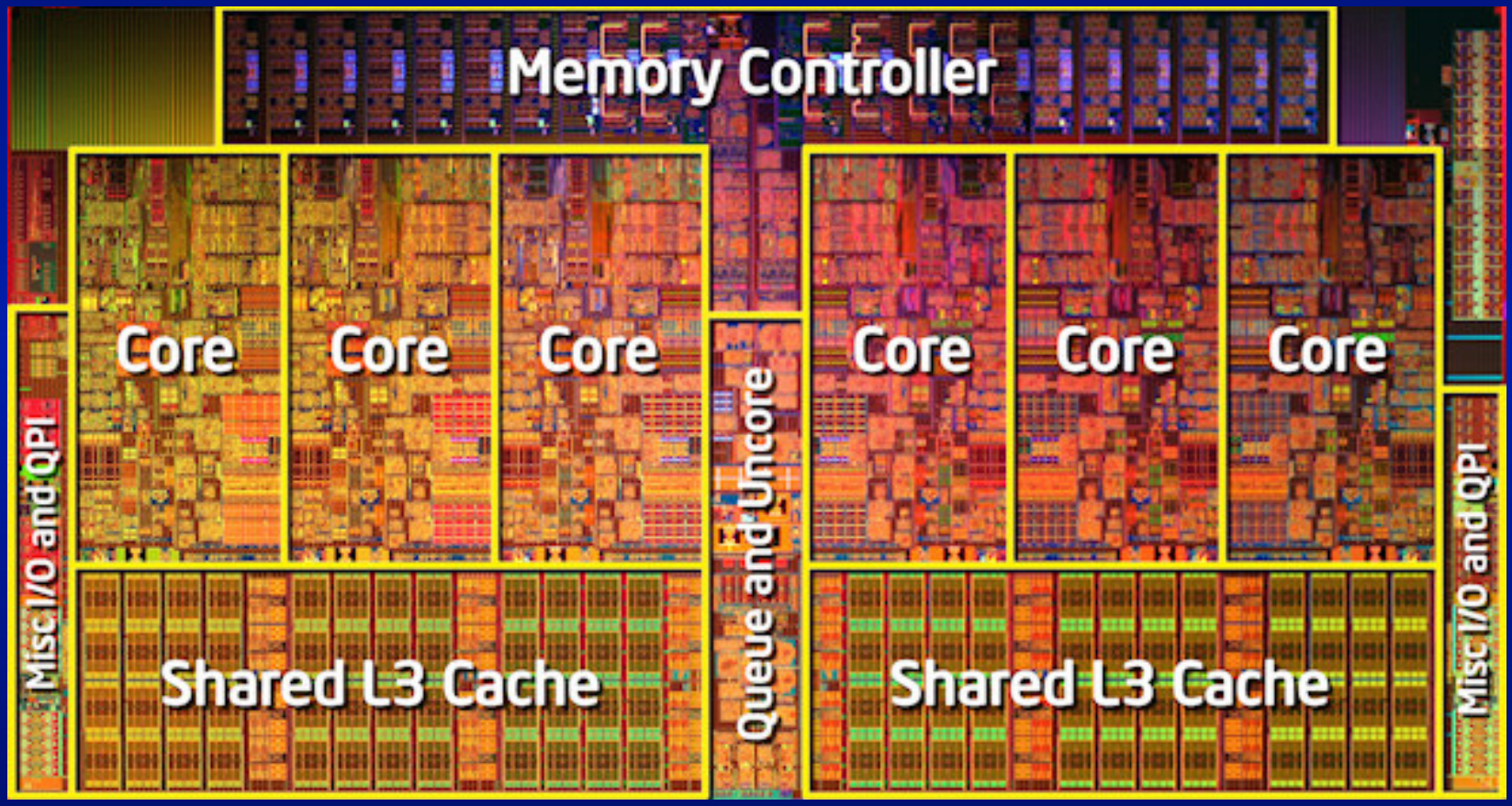
GPU

- Many compute cores
  - Few instruction streams
- Simple pipeline
  - In-order processing
  - Shallow (< 10 stages)
  - Became more complex
  - No pipelining
- Optimized for parallel execution
  - Instruction executed by 32 CUDA cores (warp)

Intel Nehalem
(Longhorn nodes)

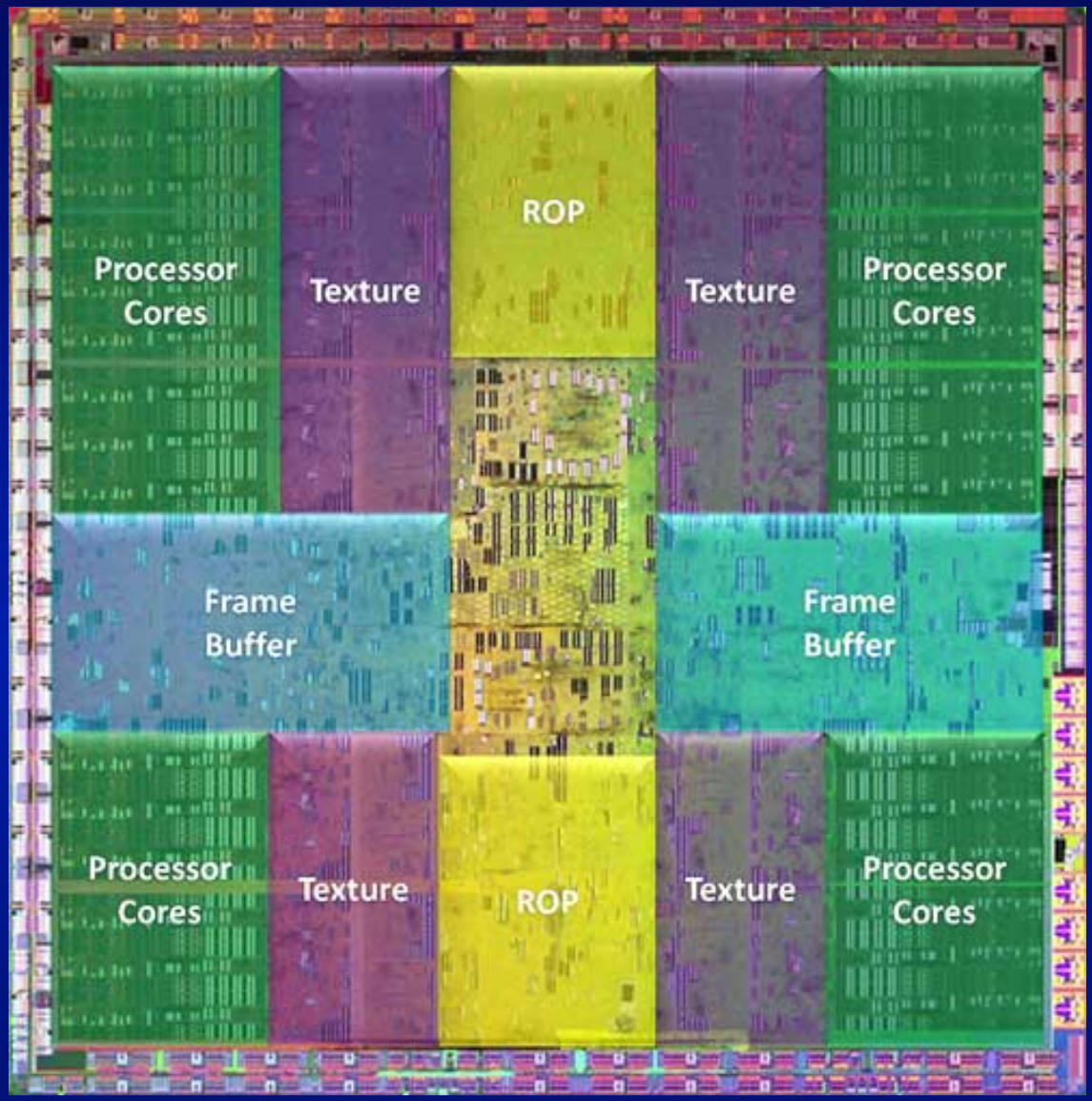


Intel Westmere (Lonestar nodes)



TACC

NVIDIA GT200 (Longhorn nodes)

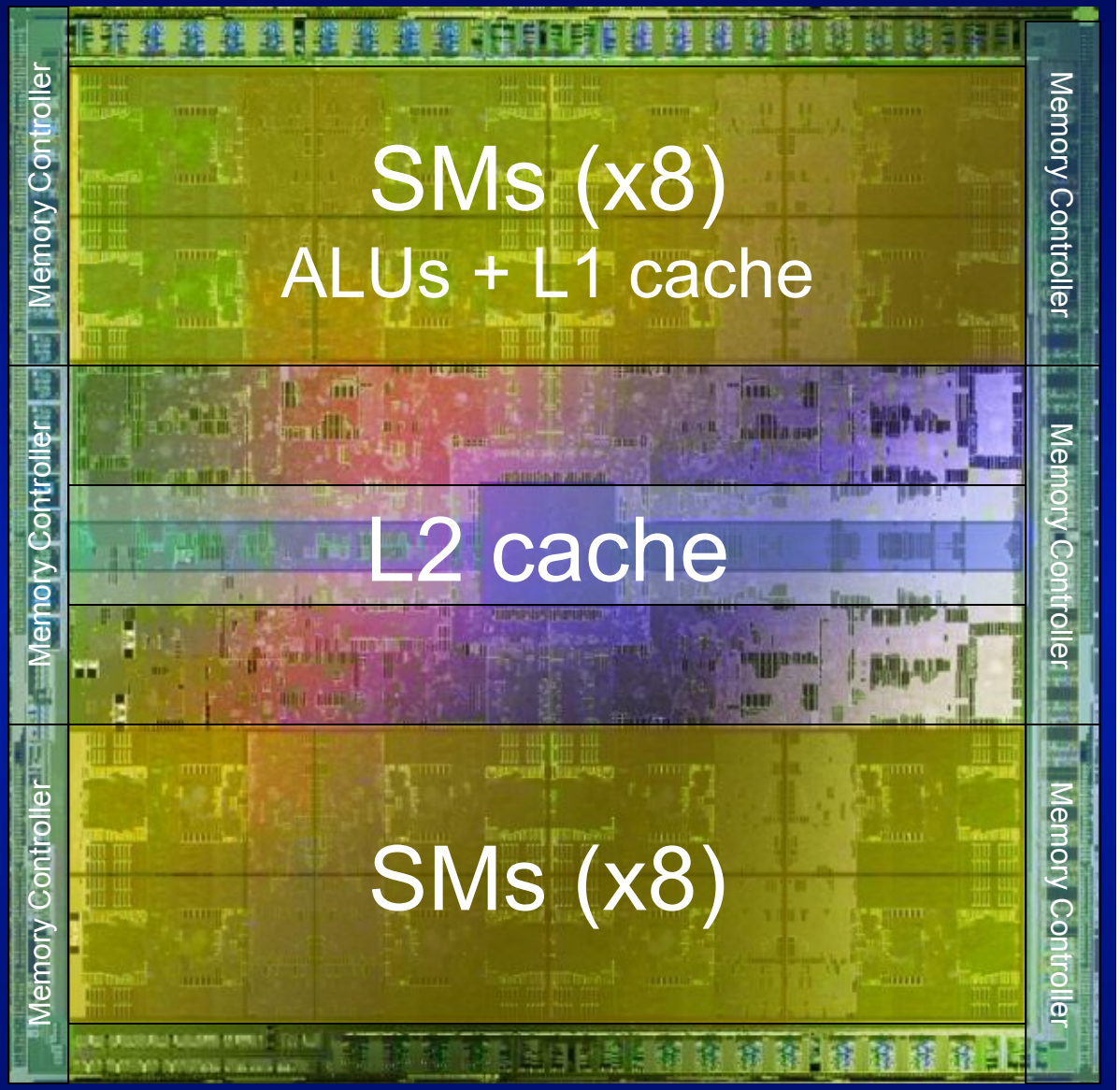


TACC

NVIDIA GF100

Fermi

(Lonestar nodes)



TACC


Instruction Cache
Warp Scheduler
Warp Scheduler
Dispatch Unit
Dispatch Unit
Register File (4096 x 32-bit)
Core
LD/ST
SFU
Interconnect Network
64 KB Shared Memory / L1 Cache
Uniform Cache
Memory Controller
CUDA Core
Dispatch Port
Operand Collector
FP Unit
INT Unit
Result Queue

Hardware Comparison

(Stampede- and Lonestar-deployed versions)

	Sandy-Bridge	Westmere X5680	K20	MIC
Functional Units	8	6	15	61
Speed (GHz)	2.8	3.33	0.71	≩1
SIMD / SIMT width	4	2	32	8
Instruction Streams	16	24	240	
Peak Bandwidth DRAM->Chip (GB/s)	40	35	160	160

Programming GPUs
A bit different, but not too difficult

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- Writing high performance, parallel code is always complicated, but the concepts are a recurring theme

Code has to match the hardware: Thread configuration

- Two-tiered hierarchy: grids and blocks (to match hardware)
  - A kernel contains one grid *"The grid executes on all SMs"*
  - A grid is a grid of blocks *"Each block executes on one SM"*
  - A block contains threads *"The threads in a block are configured to Warps"*
- When CPU code is translated into GPU code:
  - A specific thread (typically) executes one specific "loop iteration"
    - Example: Thread "#1202" may execute loop iteration i=12, j=27
    - Only one thread is mapped to a specific loop iteration
    - Only one loop iteration is mapped to a specific thread
    - This is called a bijection
  - Thread-# is not a linear construct, but has 6 components
    - Grid:3; block:3; confusing in the beginning but quite helpful later

Thread configuration

- Why is the hierarchy two-tiered?
  - All threads of a block (an element of the grid) execute on one SM
  - The hardware provides multiple SMs, so a grid must contain multiple blocks to keep the SMs busy
  - If your hardware has 8 SMs (Longhorn), you should select a setup with at least 8 blocks. For performance you'll need (many) more!
- The blocks in a grid match the HW parallelism on the SM level → multiple blocks
- An SM is also executing in parallel: "CUDA" cores
- Multiple threads have to execute concurrently on an SM
  - Longhorn's SMs have 8 "CUDA" cores → 8 threads simultaneously?
  - **No!** You need one warp (32), and for performance many warps

Thread configuration

- All blocks in a grid are configured the same
- A specific thread has
  - A block-identifier (it's position in the block)
  - A grid-identifier (the position of the block in the grid)
- Let's assume that both identifiers are linear indices of type integer:
  - **`threadidx`**: index of thread in block
  - **`blockidx`**: index of block in the grid
- And the blocks and the grid have "sizes"
  - **`blocksize`**: size of the block, i.e. number of threads in a block
  - **`gridsize`**: number of blocks in the grid

Thread configuration

- Example:
  - `Blocksize` = 32 (one warp)
  - `Gridsize` = 8 (for the 8 SMs in Longhorn's GPUs)
  - Total number of threads = 256 (32 x 8)
- What block/grid position does thread #72 have?
  - Block 1: 32 threads (32 total)
  - Block 2: 32 threads (64 total)
  - #72 is in Block 3 and has the position 8
- What is the thread-# for the 7th thread in 5th block?
  - (5-1) x 32 + 7 = 135
- Note, that I have carefully used "position" and not "index"
- Indices in C/Fortran start at 0 and 1, respectively

Thread configuration

- Example:
  - **`Blocksize`** = 32 (one warp)
  - **`Gridsize`** = 8 (for the 8 SMs in Longhorn's GPUs)
- What block/grid index does thread #72 have?
  - C: #72 is in Block w/ index 2 and has the index 7 in the block
  - Fortran: #72 is in Block w/ index 3 and has the index 8 in the block
- What is the thread-# for the 7th thread in 5th block?
  - C: **`threadidx=6, blockidx=4`**

    thread-# = **`blockidx * blocksize + threadidx`**

    Fortran: **`threadidx=7, blockidx=5`**

    thread-# = **`(blockidx-1) * blocksize + threadidx`**

    C, Fortran: thread-# starts at 0 and 1, respectively

Thread configuration

- Linear configuration → Cubes
- A grid contains a cube of blocks: 3 axes, x/y/z
- A block contains a cube of threads: 3 axes, x/y/z
- There is some freedom on what axes to use
  - Constraints are discussed later
  - minimum: 1 axis for the blocks, 1 axis for the grid
- Why x/y/z?

  Maps nicely to numerical code that uses a 1d (x), 2d (x/y), or 3d (x/y/z) grid

Thread configuration

- The thread configuration is specified in the host code (code that is executed on the host)
- You are free to choose a name
  - Here I use **`blocksize`** and **`gridsize`**
- The configuration variables are structures of type **`dim3`**
  - **`dim3`** is predefined in the header file **`cuda_runtime.h`** and the module **`mod_gpu`**, respectively
  - **`dim3`** contains the integer components **`x`**, **`y`** and **`z`**

```
use mod_gpu
type(dim3) :: blocksize, gridsize

gridsize  = dim3(8,1,1)
blocksize = dim3(32,1,1)
```

```
#include <cuda_runtime.h>

dim3 gridsize(8,1,1)
dim3 blocksize(32,1,1)
```

  - Same example as before: 32 threads in a block (x), 8 blocks in the grid (x)

Thread configuration

- **`blocksize = 32,2,1; gridsize = 8,3,1`**
- Total threads in a block: 64 = 32 x 2 (x 1)
- Total number of blocks in the grid: 24 = 8 x 3 (x 1)
- Threads are arranged: first x, then y, then z;
  "threads in block" before "blocks in grid"

	"thread in block"	"block in grid"
• 1st thread: position	(1,1,1)	(1,1,1)
• 2nd thread:	(2,1,1)	(1,1,1)
• 32nd thread:	(32,1,1)	(1,1,1)
• 33rd:	(1,2,1)	(1,1,1)
• 64th:	(32,2,1)	(1,1,1)
• 65th:	(1,1,1)	(2,1,1)

Thread configuration: uneven setup

- **`blocksize = 17,4,1`**`; gridsize = 2,1,1`
- Total threads in a block: 68 = 17 x 4 (x 1)
- How are the warps formed? — again in chunks of 32

```
                              f=full, p=partial row in x
```

- **1st warp: 32 = 17+15 y=1(f) y=2(p)**
- **2nd warp: 32 = 2+17+13 y=2(p) y=3(f) y=4(p)**
- **3rd warp: 4 = 4 y=4(p)**

- Two full warps, one partial warp
  - The partial warp contains also 32 threads, but 28 are doing nothing
  - No spill-over to the next block in the grid

Kernel launch, Chevron syntax

- A kernel is a routine that is executed on the GPU
- Calling a kernel (from the host) is called "launching a kernel"
- Calling a kernel uses familiar syntax (function/subroutine call) augmented by Chevron syntax
- The Chevron syntax (<<<…>>>) communicates the thread configuration to the kernel
  - First argument: grid configuration
  - Second argument: block configuration

No arguments passed to function in this example!

```
use mod_gpu
type(dim3) :: blocksize, gridsize

gridsize  = dim3(8,1,1)
blocksize = dim3(32,1,1)

call do_this<<<gridsize,blocksize>>>()
```

```
#include <cuda_runtime.h>

dim3 gridsize(8,1,1)
dim3 blocksize(32,1,1)

do_this<<<gridsize,blocksize>>>()
```

Thread configuration on the GPU

- How does this information appear on the GPU?
  - Kernel launched with:
    `blocksize = 32,2,1; gridsize = 8,3,1`: 1536 threads total
- 1536 threads are started on the GPU
- Inside the kernel: The size of the blocks and the grid is stored in: `blockdim` and `griddim`
- Every thread holds a unique position in the block and grid space
- Every thread has unique identifiers: `threadidx, blockidx`
- All these variables are again of type `dim3`, and they are predefined in the kernel code

Kernel

- Routine (kernel) carries a special attribute: **`global`**
- Every thread executes the same code in parallel
- Block/grid variables are filled with different content

host kernel

- 1st Chevron argument: **`gridsize`** → **`griddim`**
- 2nd Chevron argument: **`blocksize`** → **`blockdim`**

```
module mod_gpu

!***  Use CUDA module
use, intrinsic :: cudafor

contains

attributes(global) subroutine do_this()

!  blockdim, griddim, blockidx, threadidx
!    are predefined and of type dim3
```

```
#include <cuda_runtime.h>


__global__ void do_this(void)


/*  blockdim, griddim, blockidx, threadidx */
/*    are predefined and of type dim3      */
```

Thread configuration on the GPU

- 1st Chevron argument: **`gridsize → griddim`**
- 2nd Chevron argument: **`blocksize → blockdim`**
- Every thread as a unique position in the block and the grid
  - **`threadidx`** holds the 3 components of the position in the block
  - **`blockidx`** holds the 3 components of the position in the grid
- **`blockdim = 32,2,1; griddim = 8,3,1`**

```
Fortran          Thread-#
                 1   2   32  33  65

threadidx%x = 1   2   32   1   1
threadidx%y = 1   1    1   2   1
threadidx%z = 1   1    1   1   1
 blockidx%x = 1   1    1   1   2
 blockidx%y = 1   1    1   1   1
 blockidx%z = 1   1    1   1   1
```

```
C                Thread-#
                 0   1   31  32  64

threadidx.x = 0   1   31   0   0
threadidx.y = 0   0    0   1   0
threadidx.z = 0   0    0   0   0
 blockidx.x = 0   0    0   0   1
 blockidx.y = 0   0    0   0   0
 blockidx.z = 0   0    0   0   0
```

Why is this so important?

- The thread-# relates to the loop indices in CPU code
- The translation of loop index to thread indices is crucial
- Remember, a specific thread executes only one loop iteration

First Kernel

- Let's consider this operation: $x_i = x_i + 1.1$
- Vector x holds 256 elements
  - Pseudo code using variables x_f and x_c
    - x_f: 1 - 256
    - x_c: 0 - 255

```
*** 1d arrays with 256 elements
x_f{1..256}
x_c(0..255}

* Fortran
Loop i from 1 to 256
  x_f{i} = x_f{i) + 1.1
Loop end

* C
Loop i from 0 to 255
  x_c{i} = x_c{i} + 1.1
Loop end
```

How do we translate this into CUDA?

First kernel

- Pseudo code and kernels in C and Fortran
- Loop index i from the CPU code translates to index i in the kernel
- Thread configuration variables are used

```
*** 1d arrays with 256 elements
x_f{1..256}
x_c(0..255}

* Fortran
Loop i from 1 to 256
  x_f{i} = x_f{i) + 1.1
Loop end

* C
Loop i from 0 to 255
  x_c{i} = x_c{i} + 1.1
Loop end


Blocksize: x/y/x = 32,1,1
Gridsize:  x/y/z =  8,1,1
```

```
#include <cuda_runtime.h>

__global__ void add(float *x, int n)
{
/*  blockdim, griddim, blockidx, threadidx */
/*    are predefined and of type dim3      */

i = threadidx.x + blockidx.x * blockdim.x

x[i] = x[i] + 1.1
}
```

```
attributes(global) subroutine add(x,n)

!  blockdim, griddim, blockidx, threadidx
!    are predefined and of type dim3

real, dimension(n) :: x
integer, value     :: n

i = threadidx%x + (blockidx%x-1) * blockdim%x

x(i) = x(i) + 1.1

end subroutine
```

Stencil Update

Homework example that I give to my students

A common operation in scientific computing is digital convolution, by which each element in a multi-dimensional grid is replaced by a weighted sum of its neighbors. This has applications in graphics, in which such operations are done to both blur and sharpen images, and in numerical simulations, in which this may be a single step in a Poisson solver.
Write serial code for CPUs either in Fortran90 or in C. In the next homework you will port the code to the GPU and will compare timings on the CPU and the GPU.
Outline:
Define two 2D arrays (x, y) in your code. Initialize one array (x) with random numbers between 0 and 1. Derive the elements of the second array (y) from the first array by smoothing over the elements of the first array, using the constants a, b and c:

```
y(i,j) = a · (x(i-1,j-1) + x(i-1,j+1) + x(i+1,j-1) + x(i+1,j+1)) +
         b · (x(i-1,j+0) + x(i+1,j+0) + x(i+0,j-1) + x(i+0,j+1)) +
         c ·  x(i+0,j+0)
```

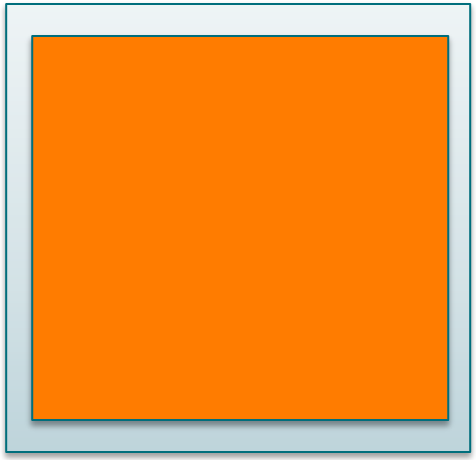
Count the elements that are smaller than a threshold t in both arrays and print the number for both arrays.

Serial Code: Stencil Update

- I'll show the whole source code for a serial CPU version on the slides, so that you'll be able to look at the complete code later on.
- I'll focus on the "smoothing" routine, which we will port to the GPU using CUDA

Data Layout

- Arrays x and y with (n+2) times (n+2) elements



- Inner elements (n by n) are going to be modified
- Ghost-layers used in x and y direction
- Provided boundaries “eliminates” the need for if statements in the code

Data Allocation

- Allocation on the heap:
  - More flexible
  - Stack size is limited
- Allocation in 1 step (for C programmers: no array of pointers pointing to non-consecutively stored rows or columns)

```
!***  Number of array elements in one direction
  integer                          :: n = 2**14
!***  Smothing constants
  real                             :: a = 0.05, &
                                      b = 0.1,  &
                                      c = 0.4
!***  Threshold
  real                             :: t = 0.1
!***  Input and output array
  real, dimension(:,:), allocatable :: &
                                       x, y

!***  Allocate input array
  allocate(x(0:n+1,0:n+1), stat=istat)
  allocate(y(0:n+1,0:n+1), stat=istat)
```

```
int n,nbx,nby;
    float a,b,c,
        t,
        *x, *y;
    Timer timer;

/* n - number of elements in one direction */
    n = 1 << 14;  /* 2^14 == 16384 */

/* a,b,c - smoothing constants */
    a = 0.05;
    b = 0.1;
    c = 0.4;

/* t - threshold */
    t = 0.1;

/* allocate x */
    x = new float[(n+2)*(n+2)];

/* allocate y */
    y = new float[(n+2)*(n+2)];
```

Calls to Initialize, Smooth, Count

- All are subroutine / void function calls
- All information through subprogram parameters
- No global variables!

```
!***  Initialize array x
call initialize(x, n)

!***  Derive first array from second array
call smooth(y, x, n, a, b, c)

!***  Count elements in first array
call count(x, n, t, nbx)

!***  Count elements in second array
call count(y, n, t, nby)
```

```
 /* initialize x */
initialize(x, n);

/* smooth x into y */
smooth(y, x, n, a, b, c);

/* count elements in first array */
count(x, n, t, nbx);

/* count elements in second array */
count(y, n, t, nby);
```

Initialization and Smoothing

- In C: Index calculation “by hand”
- $x_{i,j}$ = `x[ (n-1)*i + j ]`
- Fortran: `random_number` is an elemental function

The function/subroutine *smooth* will become a kernel later!

```
!***  Initialize with random numbers
subroutine initialize(x, n)
real, dimension(0:n+1,0:n+1) :: x
call random_number(x)
end subroutine

!***  Smooth data
subroutine smooth(y, x, n, a, b, c)
real, dimension(0:n+1,0:n+1) :: x, y
do j=1, n
  do i=1, n
    y(i,j) = a * (x(i-1,j-1) + x(i-1,j+1) + &
                  x(i+1,j-1) + x(i+1,j+1)) + &
             b * (x(i-0,j-1) + x(i-0,j+1) + &
                  x(i-1,j-0) + x(i+1,j+0)) + &
             c * x(i,j)
  enddo
enddo

end subroutine
```

```
void initialize( float* x, int n )
{
  int n2 = n+2;
  for (int i=0; i<n2; ++i)
    for (int j=0; j<n2; ++j)
      x[i*n2 + j] = random() / (float) RAND_MAX;
}
void smooth( float* y, float* x, int n,
             float a, float b, float c )
{
  int n2 = n+2;
  for (int i=1; i<=n; ++i)
    for (int j=1; j<=n; ++j)
      y[i*n2 + j] = a * (x[(i-1)*n2 + (j-1)] +
                         x[(i-1)*n2 + (j+1)] +
                         x[(i+1)*n2 + (j-1)] +
                         x[(i+1)*n2 + (j+1)])
                  + b * (x[i*n2+(j-1)] +
                         x[i*n2+(j+1)] +
                         x[(i-1)*n2 + j] +
                         x[(i+1)*n2 + j])
                  + c * x[i*n2 +j];
}
```

Counting

- Count could have been a function!
- Return value is communicated through an argument

```
!***  Count elements below threshold
subroutine count(x, n, t, nbx)

real, dimension(0:n+1,0:n+1) :: x

nbx = 0

do j=1, n
  do i=1, n
    if (x(i,j) < t) then
      nbx = nbx + 1
    endif
  enddo
enddo

end subroutine
```

```
void count( float* x, int n, float t, int &nbx )
{
  nbx = 0;
  int n2 = n+2;
  for (int i=1; i <= n; ++i)
    for (int j=1; j <= n; ++j)
      if (x[i*n2 + j] < t)
        ++nbx;
}
```

Sample Output

The output of your code may look like this:

```
Summary
-------
Number of elements in a row/column       :: 16386
Number of inner elements in a row/column :: 16384
Total number of elements                 :: 268500996
Total number of inner elements           :: 268435456
Memory (GB) used per array               :: 1.00024
Threshold                                :: 0.10
Smoothing constants (a, b, c)            :: 0.05 0.10 0.40
Number of elements below threshold (X)   :: 26847453
Fraction of elements below threshold     :: 1.00015E-01
Number of elements below threshold (Y)   :: 2950
Fraction of elements below threshold     :: 1.09896E-05

Action       :: time/s Time resolution = 1.0E-04
------
CPU: Alloc-X :: 0.000
CPU: Alloc-Y :: 0.000
CPU: Init-X  :: 3.904
CPU: Smooth  :: 1.434
CPU: Count-X :: 0.397
CPU: Count-Y :: 0.384
```

Formatted Output (Fortran)

```
!***  Print number of elements below threshold
write (0,*)
write (0,'(a)')         'Summary'
write (0,'(a)')         '-------'
write (0,'(a,i14)')     'Number of elements in a row/column       :: ', n+2
write (0,'(a,i14)')     'Number of inner elements in a row/column :: ', n
write (0,'(a,i14)')     'Total number of elements                 :: ', (n+2)**2
write (0,'(a,i14)')     'Total number of inner elements           :: ', n**2
write (0,'(a,f14.5)')   'Memory (GB) used per array               :: ', real((n+2))**2 * 4. / (1024.
write (0,'(a,f14.2)')   'Threshold                                :: ', t
write (0,'(a,3(f4.2,1x))')  'Smoothing constants (a, b, c)             :: ', a, b, c
write (0,'(a,i14)')     'Number   of elements below threshold (X) :: ', nbx
write (0,'(a,es14.5)') 'Fraction of elements below threshold     :: ', real(nbx) / n**2
write (0,'(a,i14)')     'Number   of elements below threshold (Y) :: ', nby
write (0,'(a,es14.5)') 'Fraction of elements below threshold     :: ', real(nby) / n**2
```

Formatted Output (C++ & C)

```
std::cout << std::endl;
std::cout << "Summary" << std::endl;
std::cout << "-------" << std::endl;
std::cout << "Number of elements in a row/column          :: " << n+2 << std::endl;
std::cout << "Number of inner elements in a row/column    :: " << n << std::endl;
std::cout << "Total number of elements                    :: " << (n+2)*(n+2) << std::endl;
std::cout << "Total number of inner elements              :: " << n*n << std::endl;
std::cout << "Memory (GB) used per array                  :: " << (n+2)*(n+2)*sizeof(float) / (float
std::cout << "Threshold                                   :: " << t << std::endl;
std::cout << "Smoothing constants (a, b, c)               :: " << a << " " << b << " " << c << std::
std::cout << "Number   of elements below threshold (X)    :: " << nbx << std::endl;
std::cout << "Fraction of elements below threshold        :: " << nbx / (float)(n*n) << std::endl;
std::cout << "Number   of elements below threshold (Y)    :: " << nby << std::endl;
std::cout << "Fraction of elements below threshold        :: " << nby / (float)(n*n) << std::endl;
```

```
printf("\n");
printf("Summary\n");
printf("-------\n");
printf("Number of elements in a row/column        :: %d\n", n+2);
printf("Number of inner elements in a row/column  :: %d\n", n);
printf("Total number of elements                  :: %d\n", (n+2)*(n+2));
printf("Total number of inner elements            :: %d\n", n*n);
printf("Memory (GB) used per array                :: %g\n", (n+2)*(n+2)*sizeof(float) / (float)(1024
printf("Threshold                                 :: %g\n", t);
printf("Smoothing constants (a, b, c)             :: %g %g %g\n", a,b,c);
printf("Number   of elements below threshold (X)  :: %d\n", nbx);
printf("Fraction of elements below threshold      :: %g\n", nbx / (float)(n*n));
printf("Number   of elements below threshold (Y)  :: %d\n", nby);
printf("Fraction of elements below threshold      :: %g\n", nby / (float)(n*n));
```

Timing

- We will be using timers left and right
- You can use a simple timer
- Our implementation uses a timer object.
- What is an object?
- How to declare an object?
- How to call an object?

```
!***  Timing information
class(cls_timer) :: timer

!***  Count elements in second array
call timer%start('CPU: Count-Y')
call count(y, n, t, nby)
call timer%stop
```

```
/* timer of class Timer */
Timer timer;

 /* count elements in second array */
timer.start("CPU: Count-Y");
count(y, n, t, nby);
timer.stop();
```

Timing

- An object is a special structure (called a class)
  - That contains data (instance variables)
  - That has ”procedures” attached (methods)
  - The data is hidden and can only be accessed through the methods
  - A method may have arguments
- Name-of-object: delimiter method
  - Fortran: **timer%start**
  - C: **timer.start**

```
!***  Timing information
class(cls_timer) :: timer

!***  Count elements in second array
call timer%start('CPU: Count-Y')
call count(y, n, t, nby)
call timer%stop
```

```
/* timer of class Timer */
Timer timer;

 /* count elements in second array */
timer.start("CPU: Count-Y");
count(y, n, t, nby);
timer.stop();
```

Timing

- A class contains private data and public methods

```
type, public :: cls_timer

private
integer                              :: n = 0
integer(8), dimension(2,m)           :: it
integer(8)                           :: itr
character(len=16), dimension(m)      :: c

contains

procedure, public :: reset
procedure, public :: start
procedure, public :: stop
procedure, public :: print

endtype cls_timer

contains

subroutine reset(this)

class(cls_timer) :: this
this%n  = 0
this%it = -1
this%c  = 'undef'

end subroutine

…
```

```
class Timer
{
public:
  Timer(): n(0) { }
  void start(std::string label)
  {
    if (n < 20)
      { labels[n] = label; times[2*n] = clock(); }
    else { std::cerr << "No more timers, " << label
      << " will not be timed." << std::endl; }
  }

  void stop() { times[2*n+1] = clock(); n++;}
  void reset() { n=0; }
  void print();
private:
  std::string labels[20];
  float times[40];
  int n;
};
…
```

Most important method: Printing

```
subroutine print(this)

      class(cls_timer) :: this

      write (0,*)
      write (0,'(a,es7.1)') 'Action           ::   time/s     Time resolution = ', 1./real(this%itr)
      write (0,'(a)')       '------'
      do i=1, this%n
        write (0,'(a16,a, f7.3)') this%c(i), ' :: ',                &
                                  (real(this%it(2,i) - this%it(1,i))) / real(this%itr)
      enddo

end subroutine
```

```
void Timer::print()
{
    std::cout << std::endl;
    std::cout << "Action           ::   time/s     Time resolution = " << 1.f/(float)CLOCKS_PER_SEC
    std::cout << "------" << std::endl;
    for (int i=0; i < n; ++i)
        std::cout << labels[i] << " :: " << (times[2*i+1] - times[2*i+0])/(float)CLOCKS_PER_SEC <<
}
```

Invoke printing by

- Invoking the method **`print`**

```
!***  Print timings
      call timer%print
```

```
/* Print timings */
timer.print();
```

- If you need another (probably nested) timer: create another object

```
!***  Timing information
class(cls_timer) :: timer, timer2

!***  Count elements in second array
call timer2%start('CPU: Count-XY')
  call timer%start('CPU: Count-X')
  call count(x, n, t, nbx)
  call timer%stop
  call timer%start('CPU: Count-Y')
  call count(y, n, t, nby)
  call timer%stop
call timer2%stop
```

```
/* timer of class Timer */
Timer timer timer2;

 /* count elements in second array */
timer2.start("CPU: Count-XY");
  timer.start("CPU: Count-X");
  Count(x, n, t, nbx);
  timer.stop();
  timer.start("CPU: Count-Y");
  count(y, n, t, nby);
  timer.stop();
timer2.stop();
```

Header files; Modules

- Fortran: Subroutines/Functions/Class are declared in Modules
  - Modules become available by use association
  - This implies also an order of compilation: Modules first, then code that uses the module
- C/C++: Header files are used to communicate the interface

```
! Example for a module
Module my_mod
Contains
Subroutine do_this(x, y, z)
…
End subroutine
End module

Program main
Use my_mod
Call do_this(a,b,c)
End program
```

```
/* Header files needed for HW0
   I/O
   timer
   strings */
#include <iostream>
#include <sys/time.h>
#include <string>
```

Converting the Serial Code to CUDA Code

Why a Stencil Update and not a Matrix-Matrix-Multiply

- Matrix-Matrix-Multiply (MMM) is a very simple example
  - Matrices are divided up into tiles
  - Operations on a tile require only data of that tile (no extra boundary layers needed)
  - Most books cover MMM
  - You will almost never code a MMM yourself, but rather use a library
- The setup of a Stencil update is more complex
  - A stencil update needs the boundaries around a tile
  - The operation is simpler, though

Pseudo Code

Simple execution scheme: CPU, Transfer, GPU

```
Loop until work is done
1.   Setup data on CPU
2.   Transfer input data to GPU
3.   Perform work on GPU
   1. using "Main Memory"
   2. using "Shared Memory"
   3. Two different ways to setup threads
4.   Transfer results back from GPU
EndLoop
```

Efficient Kernel Execution on GPU

Pseudo Code

Interleaved execution scheme: CPU, Transfer, GPU, …

```
Loop until work is done
1.   Setup(1)            Transfer-out(2)  (after first loop)
2.   Transfer-in(1)      Setup(2)
3.   GPU-work(1)         Transfer-in(2)
4.   Transfer-out(1)     GPU-work(2)
EndLoop
```

Efficient Kernel Execution on GPU

Efficient Data Transfer

Pseudo Code

Interleaved execution scheme with CPU: CPU, Transfer, GPU, …

```
Loop until work is done
1.   Setup(1)           Transfer-out(2)     CPU-work(3)
2.   Transfer-in(1)     Setup(2)            CPU-work(3)
3.   GPU-work(1)        Transfer-in(2)      CPU-work(3)
4.   Transfer-out(1)    GPU-work(2)         CPU-work(3)
EndLoop
```

Efficient Kernel Execution on GPU

Efficient Data Transfer

Simultaneous use of the GPU *and* CPU

Data Allocation: Fortran

- Declaration with special attribute: device
- Allocation with normal allocate

```
 real, dimension(:,:), allocatable, device :: d_x,  &
                                              d_y

!***  Allocate input array on device
      call timer%start('GPU: Alloc-D_X')
      allocate(d_x(0:n+1,0:n+1), stat=istat)
      call timer%stop
      if (istat /= 0) then
        write (*,*) 'Allocation of d_x failed'
        stop 'Fatal ERROR in Main Program HW2'
      endif



!***  Allocate output array on device
      call timer%start('GPU: Alloc-D_Y')
      allocate(d_y(0:n+1,0:n+1), stat=istat)
      call timer%stop
      if (istat /= 0) then
        write (*,*) 'Allocation of d_y failed'
        stop 'Fatal ERROR in Main Program HW2'
      endif
```

```
y_d;


device input array x_d */
t("GPU: Alloc-X_D  ");
((void**) &x_d, (n+2)*(n+2)*sizeof(float));
();

e device output array y_d */
t("GPU: Alloc-Y_D  ");
((void**) &y_d, (n+2)*(n+2)*sizeof(float));
();
```

Data Allocation: C

- Allocation with special malloc call: cudaMalloc()

```
 real, dimension(:,:), allocatable, device :: d_x,  &
                                              d_y

!***  Allocate input array on device
      call timer%start('GPU: Alloc-D_X')
      allocate(d_x(0:n+1,0:n+1), stat=is
      call timer%stop
      if (istat /= 0) then
        write (*,*) 'Allocation of d_x f
        stop 'Fatal ERROR in Main Progra
      endif



!***  Allocate output array on device
      call timer%start('GPU: Alloc-D_Y')
      allocate(d_y(0:n+1,0:n+1), stat=istat)
      call timer%stop
      if (istat /= 0) then
        write (*,*) 'Allocation of d_y failed'
        stop 'Fatal ERROR in Main Program HW2'
      endif
```

```
float *x_d, *y_d;



 /* allocate device input array x_d */
   timer.start("GPU: Alloc-X_D  ");
   cudaMalloc((void**) &x_d, (n+2)*(n+2)*sizeof(float));
   timer.stop();

   /* allocate device output array y_d */
   timer.start("GPU: Alloc-Y_D  ");
   cudaMalloc((void**) &y_d, (n+2)*(n+2)*sizeof(float));
   timer.stop();
```

Recap: Why Tiling?

- A GPU has multiple Streaming Multiprocessors (SMs), similar to the multiple cores of a CPU
- To use more than 1 SM, the problem has to be divided up
- Each SM will work on one (or more) tiles

Data Copy and Kernel Launch (F90)

- Block size: 16x16
- Assumption: Grid (n) is divisible by 16
- Coding for arbitrary grids adds a bit of complexity

```
!***  Copy first array to GPU
      call timer%start('GPU: Copy-in')
      d_x = x
      call timer%stop

!***  Kernel launch
      nblock    = 16
      blocksize = dim3(  nblock,   nblock, 1)
      gridsize  = dim3(n/nblock, n/nblock, 1)
      call timer%start('GPU: Smooth')
      call smooth_gpu<<<gridsize,blocksize>>>(d_y, d_x, n, a, b, c)
      ierr = cudaThreadSynchronize()
      call timer%stop


!***  Copy result back from GPU
      call timer%start('GPU: Copy-out')
      yd = d_y
      call timer%stop
```

```
, cudaMemcpyHostToDevice);

, n, a, b, c);

at), cudaMemcpyDeviceToHost);
```

Data Copy and Kernel Launch (C)

- Block size: 16x16
- Assumption: Grid (n) is divisible by 16
- Coding for arbitrary grid sizes adds a bit of complexity

```
!***  Copy first array to GPU
      call timer%start('GPU: Copy-in')
      d_x = x
      call timer%sto

!***  Kernel launch
      nblock    = 16
      blocksize = di
      gridsize  = di
      call timer%sta
      call smooth_gp
      ierr = cudaThr
      call timer%sto


!***  Copy result ba
      call timer%sta
      yd = d_y
      call timer%sto
```

```
/* copy x_h to x_d on GPU */
   timer.start("GPU: Copy-in    ");
   cudaMemcpy(x_d, x, (n+2)*(n+2)*sizeof(float), cudaMemcpyHostToDevice);
   timer.stop();

   /* launch smooth() on GPU */
   int nBlocks = 16;
   dim3 blockSize(nBlocks, nBlocks);
   dim3 gridSize(n/nBlocks, n/nBlocks);
   timer.start("GPU: Smooth     ");
   smooth_gpu<<<gridSize,blockSize>>>(y_d, x_d, n, a, b, c);
   cudaDeviceSynchronize();
   timer.stop();

   /* copy y_d to y_h on CPU */
   timer.start("GPU: Copy-out   ");
   cudaMemcpy(y_h, y_d, (n+2)*(n+2)*sizeof(float), cudaMemcpyDeviceToHost);
   timer.stop();
```

Fortran Kernel

- Kernel operates on the data stored in the main (GPU) memory
- Indices i and j are calculated from blockdim and blockidx
- Fortran example shown with full module environment

```
__global__ void smooth_gpu( float* y, float* x, int n, float a, float b, float c )
                                                                    rom index 1
```

```
 module mod_gpu
!***  Use CUDA module
      use, intrinsic :: cudafor

      contains
!***  Smooth data
      attributes(global) subroutine smooth_gpu(d_y, d_x, n, a, b, c)

      real, dimension(0:n+1,0:n+1) :: d_x, d_y
      real, value                  :: a, b, c
      integer, value               :: n
      integer                      :: i, j

      i = blockdim%x * (blockidx%x - 1) + threadidx%x
      j = blockdim%y * (blockidx%y - 1) + threadidx%y

      d_y(i,j) = a * (d_x(i-1,j-1) + d_x(i-1,j+1) + d_x(i+1,j-1) + d_x(i+1,j+1)) + &
                 b * (d_x(i-0,j-1) + d_x(i-0,j+1) + d_x(i-1,j-0) + d_x(i+1,j+0)) + &
                 c * d_x(i,j)

      end subroutine
end module mod_gpu
```

C Kernel

- Kernel operates on the data in the main (GPU) memory
- Indices i and j are calculated from blockdim and blockidx

```
__global__ void smooth_gpu( float* y, float* x, int n, float a, float b, float c )
{
    int n2 = n+2, i, j;

    i = blockDim.x * blockIdx.x + threadIdx.x + 1;  // add one to start from index 1
    j = blockDim.y * blockIdx.y + threadIdx.y + 1;

    y[i*n2 + j] = a * (x[(i-1)*n2 + (j-1)] + x[(i-1)*n2 + (j+1)] +
                       x[(i+1)*n2 + (j-1)] + x[(i+1)*n2 + (j+1)])
        +         b * (x[i*n2+(j-1)]   + x[i*n2+(j+1)] +
                       x[(i-1)*n2 + j] + x[(i+1)*n2 + j])
        +         c * x[i*n2 +j];
}
```

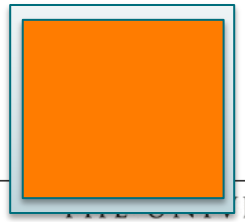
```
 module mod_
!***  Use CU
      use, i

      contai
!***  Smooth
      attrib

      real,
      real,
      intege
      intege

      i = blockdim%x * (blockidx%x - 1) + threadidx%x
      j = blockdim%y * (blockidx%y - 1) + threadidx%y

      d_y(i,j) = a * (d_x(i-1,j-1) + d_x(i-1,j+1) + d_x(i+1,j-1) + d_x(i+1,j+1)) + &
                 b * (d_x(i-0,j-1) + d_x(i-0,j+1) + d_x(i-1,j-0) + d_x(i+1,j+0)) + &
                 c * d_x(i,j)

      end subroutine
end module mod_gpu
```

Optimization with “Shared Memory”

- If data is re-used then a huge performance gain can be achieved by copying sections of the data into the (small) shared memory of the SM
- In the example every element is used 9 times to calculate smoothed values
- I will show how to allocate shared memory, and how to copy (inside the kernel), data from main GPU memory to the shared memory of an SM
- Note: In a Matrix-Matrix-Multiply every element is used n times

Using “Shared Memory”

- I will employ 3 different strategies
  - Simple, but very slow: Only one thread is copying the data
  - Fast (16x16 threads):
    - Most threads copy one element
    - Some threads are copying more than one element
    - All threads are calculating one result
  - Fast (18x18) threads:
    - All threads are copying exactly one element
    - Not all threads are calculating a result
  - Reminder: A tile contains 16x16 elements, but the data covers an 18x18 patch (Boundary condition)
    - 16x16 elements are calculated from 18x18 elements



Shared Memory: Fortran Kernel (sh1)

- Only the first thread copies data to shared memory
- Synchronization prevents threads from moving ahead
- Shared memory hold 18x18 elements

```
 attributes(global) subroutine smooth_gpu_sh1(d_y, d_x, n, a, b, c)
      integer, value                          :: n
      integer                                 :: i, j
      real, dimension(0:n+1,0:n+1)            :: d_x, d_y
      real, dimension(0:17,0:17), shared :: xb
      real, value                             :: a, b, c
      k = blockdim%x * (blockidx%x - 1) + threadidx%x
      l = blockdim%y * (blockidx%y - 1) + threadidx%y
      i = threadidx%x
      j = threadidx%y
!***  Data copy
      if (i == 1 .and. j == 1) then
        do n2=0, blockdim%y+1
          do n1=0, blockdim%x+1
            xb(n1,n2) = d_x(k+n1-1,l+n2-1)
          enddo
        enddo
      endif
!***  Synchronize
      call syncthreads()
!***  Action
      d_y(k,l) = a * (xb(i-1,j-1) + xb(i-1,j+1) + xb(i+1,j-1) + xb(i+1,j+1)) + &
                 b * (xb(i-0,j-1) + xb(i-0,j+1) + xb(i-1,j-0) + xb(i+1,j+0)) + &
                 c * xb(i,j)
end subroutine
```

Shared Memory: C Kernel (sh1)

- Only the first thread copies data to shared memory
- Synchronization prevents threads from moving ahead
- Shared memory hold 18x18 elements

```
__global__ void smooth_gpu_sh1( float* y, float* x, int n, float a, float b, float c )
{
    int n2 = n+2, i, j, k, l, block=18;
    __shared__ float xb[18*18];

    k = blockDim.x * blockIdx.x + threadIdx.x + 1; // add one to start from index 1
    l = blockDim.y * blockIdx.y + threadIdx.y + 1;
    i = threadIdx.x + 1;
    j = threadIdx.y + 1;

    /* copy data into shared buffer */
    if (i == 1 & j == 1)
    {
        for (int ii=0; ii <= (blockDim.x+1); ++ii)
            for (int jj=0; jj <= (blockDim.y+1); ++jj)
                xb[ii*block + jj] = x[(k+ii-1)*n2 + (l+jj-1)];
    }
    __syncthreads();

    y[l*n2 + k] = a * (xb[(j-1)*block+(i-1)] + xb[(j-1)*block+(i+1)] +
                       xb[(j+1)*block+(i-1)] + xb[(j+1)*block + (i+1)])\
                + b * (xb[j*block + (i-1)] + xb[j*block + (i+1)] +
                       xb[(j-1)*block + i] + xb[(j+1)*block + i])
                + c * xb[j*block + i];
}
```

Shared Memory: Calling the Kernel (sh1)

- Block size: 16x16
- Grid (n) is divisible by 16

```
!***  Block size: A tile must be 16x16!
        nblock    = 16
        blocksize = dim3(  nblock,   nblock, 1)
        gridsize  = dim3(n/nblock, n/nblock, 1)

        call smooth_gpu_sh1<<<gridsize,blocksize>>>(d_y, d_x, n, a, b, c)
```

```
 {
        nBlocks   = 16;
        blockSize = dim3(  nBlocks,    nBlocks);
        gridSize  = dim3( n/nBlocks), n/nBlocks) );
        smooth_gpu_sh1<<<gridSize,blockSize>>>(y_d, x_d, n, a, b, c);
}
```

Shared Memory: F90 Kernel (sh16)

```
attributes(global) subroutine smooth_gpu_sh16(d_y, d_x, n, a, b, c)
integer, value                          :: n
      integer                                 :: i, j
      real, dimension(0:n+1,0:n+1)            :: d_x, d_y
      real, dimension(0:17,0:17), shared :: xb
      real, value                             :: a, b, c
      k = blockdim%x * (blockidx%x - 1) + threadidx%x
      l = blockdim%y * (blockidx%y - 1) + threadidx%y
      i = threadidx%x
      j = threadidx%y
!***  Copy inner part: 16x16 elements
      xb(i,j) = d_x(k,l)
!***  Copy boundaries
!***  : x + corners
      if (i == 1) then
        xb(i-1,j) = d_x(k-1,l)
        if (j == 1) then
          xb(i-1,j-1) = d_x(k-1,l-1)
          xb(i-1,j+1) = d_x(k-1,l+1)
        else if (j == blockdim%y) then
          xb(i-1,j+1) = d_x(k-1,l+1)
        endif
```

```
      else if (i == blockdim%x) then
        xb(i+1,j) = d_x(k+1,l)
        if (j == 1) then
          xb(i+1,j-1) = d_x(k+1,l-1)
          xb(i+1,j+1) = d_x(k+1,l+1)
        else if (j == blockdim%y) then
          xb(i+1,j+1) = d_x(k+1,l+1)
        endif
      endif
!***  : y
      if (j == 1) then
        xb(i,j-1) = d_x(k,l-1)
      else if (j == blockdim%y) then
        xb(i,j+1) = d_x(k,l+1)
      endif

!***  Synchronize
      call syncthreads()

!***  Action
      d_y(k,l) = a * (xb(i-1,j-1) + xb(i-1,j+1) +
                 .etc, etc.

      end subroutine
```

Each thread copies one element

Threads close to boundary copy boundary

Threads close to the corner copy corner

TACC

Shared Memory: C Kernel (sh16)

```
__global__ void smooth_gpu_sh16( float* y, float* x, int n, float a, float b, float c )
{
    int n2 = n+2, i, j, k, l, block=18;
    __shared__ float xb[18*18];
    k = blockDim.x * blockIdx.x + threadIdx.x + 1; // add one to start from index 1
    l = blockDim.y * blockIdx.y + threadIdx.y + 1;
    i = threadIdx.x + 1;
    j = threadIdx.y + 1;
/* copy inner part: block x block elements */
    xb[j*block + i] = x[l*n2 + k];
/* copy boundaries */
/* x and corners */
if (i == 1)
    {
xb[j*block + (i-1)] = x[l*n2 + (k-1)];
if (j == 1)
 {
xb[(j-1)*block + (i-1)] = x[(l-1)*n2 + (k-1)];
xb[(j+1)*block + (i-1)] = x[(l+1)*n2 + (k-1)];
 }
else if (j == blockDim.y)
 {
xb[(j+1)*block + (i-1)] = x[(l+1)*n2 + (k-1)];
 }
 }
else if (i == blockDim.x)
  {
xb[j*block + (i+1)] = x[l*n2 + (k+1)];
if (j == 1)
  {
xb[(j-1)*block + (i+1)] = x[(l-1)*n2 + (k+1)];
xb[(j+1)*block + (i+1)] = x[(l+1)*n2 + (k+1)];
  }
else if (j == blockDim.y)
  {
xb[(j+1)*block + (i+1)] = x[(l+1)*n2 + (k+1)];
  }
  }
/* y */
if (j == 1)
xb[(j-1)*block + i] = x[(l-1)*n2 + k];
else if (j == blockDim.y)
xb[(j+1)*block + i] = x[(l+1)*n2 + k];
__syncthreads();
y[l*n2 + k] = a * (xb[(j-1)*18 + (i-1)] + etc.
}
```

Each thread copies one element

Threads close to boundary copy boundary

Threads close to the corner copy corner

Shared Memory: Calling the Kernel (sh16)

- Block size: 16x16
- Grid (n) is divisible by 16

```
!***  Block size: A tile must be 16x16!
        nblock    = 16
        blocksize = dim3(  nblock,   nblock, 1)
        gridsize  = dim3(n/nblock, n/nblock, 1)

        if (ckernel == 'global') then
          call timer%start('GPU: Smooth')
          call smooth_gpu16<<<gridsize,blocksize>>>(d_y, d_x, n, a, b, c)
```

```
 {
        nBlocks = 16;
        blockSize = dim3(nBlocks, nBlocks);
        gridSize = dim3( (int)ceilf(n/(float)nBlocks), (int)ceilf(n/(float)nBlocks) );
smooth_gpu_sh16<<<gridSize,blockSize>>>(y_d, x_d, n, a, b, c);
}
```

Calling the first three kernels

- No shared memory (16x16 threads)
- Shared memory (16x16 threads)
  - One thread copies data (sh1)
  - All threads are copying data (sh16); some multiple elements
- To call these three kernels the same block/grid structure is used
  - Blocksize : 16x16
  - Grid divided in tiles of 16x16 elements

Shared Memory: Calling the Kernel (sh18)

- Now we would like to have 18x18 threads
  - Each thread will copy exactly one data element
  - Threads will either calculate 1 or 0 elements
- Tile is still 16x16

```
!***  Block size: A tile must be 16x16, but the thread block holds 18x18 threads
        nblock    = 18
        blocksize = dim3(nblock, nblock, 1)
        gridsize  = dim3(n/16,   n/16,   1)

          call timer%start('GPU: Smooth')
          call smooth_gpu_sh18<<<gridsize,blocksize>>>(d_y, d_x, n, a, b, c)
          ierr = cudaThreadSynchronize()
          call timer%stop
```

```
 {
        nBlocks = 18;
        blockSize = dim3(nBlocks, nBlocks);
        gridSize = dim3( n/16, n/16 );
        smooth_gpu_sh18<<<gridSize,blockSize>>>(y_d, x_d, n, a, b, c);
}
```

Shared Memory: Fortran Kernel (sh18)

- Each thread copies exactly one element
- Only the first 256 threads calculate

```
attributes(global) subroutine smooth_gpu_sh18(d_y, d_x, n, a, b, c)
      integer, value                          :: n
      integer                                 :: i, j
      real, dimension(0:n+1,0:n+1)            :: d_x, d_y
      real, dimension(0:17,0:17), shared :: xb
      real, value                             :: a, b, c

      k = 16 * (blockidx%x - 1) + threadidx%x - 1
      l = 16 * (blockidx%y - 1) + threadidx%y - 1
      i = threadidx%x
      j = threadidx%y
!***  Copy tile from GPU memory to shared memory
      xb(i-1,j-1) = d_x(k,l)
!***  Synchronize
      call syncthreads()
!***  Linear thread index
      lind = blockdim%x * (threadidx%y - 1) + threadidx%x
!***  Select first 256 threads
      if (lind <= 256) then
        j = (lind-1) / 16 + 1
        i = lind - (j-1) * 16
        k = 16 * (blockidx%x - 1) + i
        l = 16 * (blockidx%y - 1) + j
!***  Action
        d_y(k,l) = a * (xb(i-1,j-1) + etc.
      endif
end subroutine
```

Shared Memory: C Kernel (sh18)

- Each thread copies exactly one element
- Only the first 256 threads calculate

```
__global__ void smooth_gpu_sh18( float* y, float* x, int n, float
a, float b, float c )
{
    int n2 = n+2, i, j, k, l, lind;
    __shared__ float xb[18*18];

    k = 16 * blockIdx.x + threadIdx.x;
    l = 16 * blockIdx.y + threadIdx.y;
    i = threadIdx.x + 1;
    j = threadIdx.y + 1;

    /* copy tile to shared memory */
    xb[threadIdx.y*18 + threadIdx.x] = x[l*n2 + k];

    __syncthreads();

    /* compute linear thread index */
    lind = blockDim.x * threadIdx.y + threadIdx.x + 1;

    if (lind <= 256)
    {
        i = (lind-1) / 16 + 1;
        j = lind - (i-1) * 16;
        k = 16 * blockIdx.x + i;
        l = 16 * blockIdx.y + j;

        y[l*n2 + k] = a * (xb[(j-1)*18 + (etc.
}
```

TACC

Performance

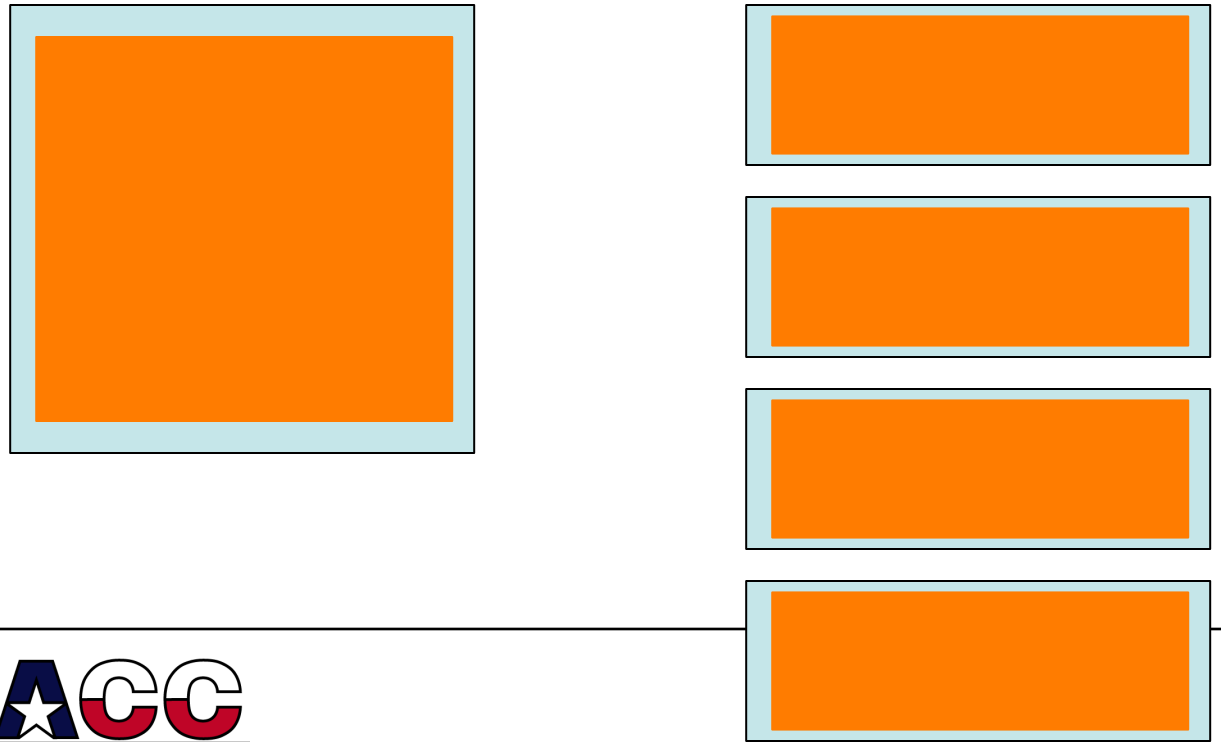
- Which kernel is the fastest?
- Obviously, using only 1 thread for the copy is slow
  - I added this one only for educational purposes
  - Any code that uses only 1 thread on an SM is slow
- But for the other 2 kernels it is not obvious, which one is faster
  - Analysis of the occupancy: registers, shared memory, etc.
  - Trial and error

Overlapping communication and computation

- With an efficient kernel at hand we can now do the second step
- To overlap communication with computation, we need
  - Break the problem into several pieces (4 in the example)
- This requires to go from a 2d array to a 3d array
  - 2d for the data, the last dimension (set to 4) is for the 4 pieces
- We can use the kernels that we have written, but we need to
  - Call the kernels for one 2d slab of the 3d array
  - Setup the data streams

Partitioning of the Problem

- Inner elements (n**x**n) are going to be modified
- “2D” array (square) → “3D” array (rectangles **x** “number of streams”)
- Example with 4 streams: ns = n/4; Inner elements: n**x**ns or ns**x**n
- All rectangles need their own “boundaries”



Streams

- CUDA allows you to execute multiple “streams” simultaneously in your code
- Parts of a stream are: (that we are interested in)
  - Asynchronous data transfer operations (default is synchronous)
  - Asynchronous kernel execution (default is asynchronous)
- How would this be executed if 4 streams are used?

```
“Pseudo code”

Loop over #-of streams: istream
  Asynchronous Copy xs{istream} to d_xs{istream}
  Kernel call for istream: smooth_gpu_sh16_p “Calculate d_ys from d_xs”
  Asynchronous Copy d_ys{istream} to ys{istream}
End Loop

Wait
```

- All 12 “operations” would be initiated at once
- GPU scheduler would decide in what order to execute
- The order inside a stream is maintained

Stream Creation

- Integer array that holds stream identifier
- Call to cudaStreamCreate creates a stream and returns an identifier, which is an integer number

```
Fortran

integer, dimension(4) :: id_stream

do istream=1, 4
  istat = cudaStreamCreate(id_stream(istream))
enddo
```

```
C/C++

int id_stream[4];

for (int istream=0; istream<4; ++i)
  cudaStreamCreate(id_stream[istream]);
```

Asynchronous copy

- Very similar the synchronous copy, but stream identifier is added

```
"istat = " cudaMemcpyAsync(destination, source, "size", direction, id_stream(istream))

Notes Fortran:
Call returns an integer
Size is the number of elements
Direction is optional

Notes C/C++:
Function has no return value
Size is in bytes
Direction is not optional
```

Kernel Invocation with Stream Reference

- Very similar to the normal Kernel launch
- 2 parameters added
- Size for shared memory transactions: Set this to 0 (zero) in HW4
- Stream ID

```
"call" kernel<<<gridsize, blocksize, 0, id_stream(istream)>>>()

Notes Fortran:
Subroutine call

Notes C/C++:
Function call
```

Events

- Events work like “Barriers”
- An event is recorded when the code “passes” the barrier
- A barrier can be passed when all streams have finished operating (stream number = 0)
- A barrier can be passed when a particular stream has finished (stream number >0)
- Events are of the type cudaEvent
- Syntax: “istat = “ cudaEventRecord(Event, stream-number)

Declaration: An event is of a special type

```
Fortran:
type(cudaEvent) :: startEvent, stopEvent

C/C++:
cudaEvent startEvent, stopEvent;
```

Example

```
“istat =“ cudaEventRecord(startEvent, 0)
“Start Timer”

“Do something with streams”

“Code will wait at the barrier until all
 stream operations are finished”
“istat =“ cudaEventRecord(stopEvent, 0)
“Stop timer”
```

Hardware and Scheduling

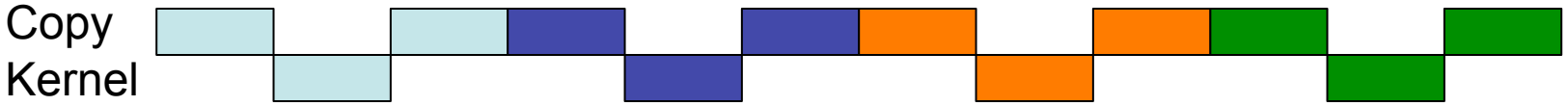
- Different scheduling ordering
- Scheme 1: One loop with Copy-Kernel-Copy
- Scheme 2: Three loops; Loop bodies are: Copy, Kernel, or Copy

```
"Pseudo code: Scheme 1"

Loop over #-of streams: istream
  Asynchronous Copy xs{istream} to d_xs{istream}
  Kernel call for istream: smooth_gpu_sh16_p "Calculate d_ys from d_xs"
  Asynchronous Copy d_ys{istream} to ys{istream}
End Loop
```

```
"Pseudo code: Scheme 2"

Loop over #-of streams: istream
  Asynchronous Copy xs{istream} to d_xs{istream}
End Loop

Loop over #-of streams: istream
  Kernel call for istream: smooth_gpu_sh16_p "Calculate d_ys from d_xs"
End Loop

Loop over #-of streams: istream
  Asynchronous Copy d_ys{istream} to ys{istream}
End Loop
```

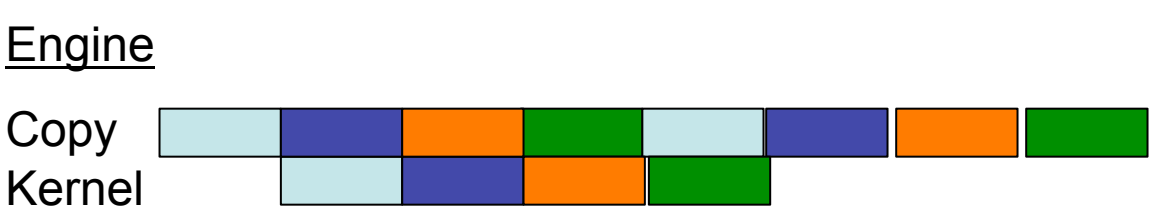
Longhorn

- Longhorn (Tesla) GPUs have
  - One copy engine
  - One Kernel engine
- Scheme 1: Copy-Kernel-Copy
- There is not overlap; Execution order of a non-stream implementation would be the same
  - The first copy-out is scheduled before the second copy-in
  - The first calculation cannot start before the first copy-in is finished
  - The first copy-out cannot start before the first kernel is finished
- The four streams have 4 different colors



Longhorn

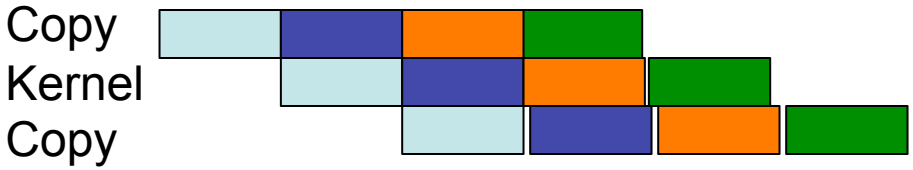
- Scheme 2: Loop-Copy, Loop-Kernel; Loop-Copy
- Now there is significant overlap
- The second copy-in is scheduled before the first copy-out
- Overlap is not perfect
  - Twice as many copy operations that kernel calls
  - Ratio of engines is 1:1



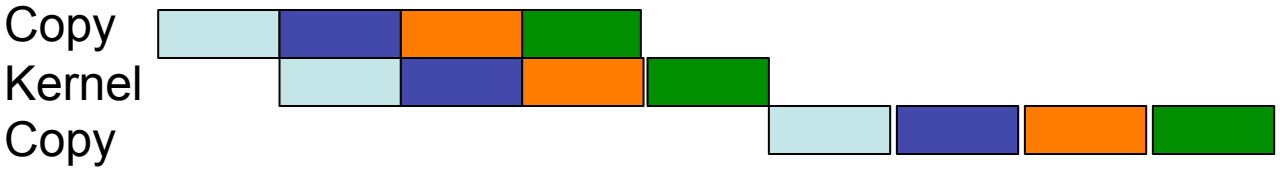
Lonestar

- Lonestar (Fermi) GPUs have
  - Two copy engines
  - One Kernel engine
- Scheme 1: Copy-Kernel-Copy
- Scheme 2: Loop-Copy, Loop-Kernel; Loop-Copy

Engine Scheme 1



Engine Scheme 2



Using Host and GPU together

- Simple expansion of the “overlap” concept
- Think of dividing the domain into 5 pieces
  - 4 would be executed on the GPU (w/ overlap)
  - The 5th piece is executed on the host
- Challenges
  - Load-balancing
  - For static problems
    - Determine the relative speeds
    - Adjust the tile sizes accordingly
- In real applications this will be a (big) challenge

Multiple nodes (MPI)

- One node with a GPU is already a cluster
  - Multiple memories, multiple address spaces
- Easiest way to expand to a cluster
  - Use MPI to divide the work among the nodes
  - Use CUDA to divide work assigned to a node between the host CPU(s) and the GPU(s)
  - A process on the host communicates with
    - Other nodes through MPI
    - The GPU(s) attached to the host through CUDA
- MPI is the outer frame-work
- CUDA kernels are on the inside
- Comparable to: MPI/OpenMP — Outside/Inside

Summary

- Writing efficient code for GPUs requires
  - An efficient kernel that uses (if applicable) shared memory (or texture/constant)
  - Efficient data transfer that overlaps with computations
  - Uses the cores of the CPU while also asynchronously executing on the GPU; applies to HPC clusters that have powerful hosts (most clusters available in XSEDE)
- Translation of host code to CUDA
  - Use a grid of blocks to keep all SMs busy; an SM executes one or more blocks
  - Use the blocks to keep all CUDA cores in an SM busy; execution in lockstep, similar to the Vector lanes of a CPU core

Programming GPUs

A bit different, but not too difficult

- A bit of a learning curve at the beginning
- 3 concepts
  - Hardware → constraints on the code
  - Shared (fast) memory
  - Data transfer between host and device (communication)
- Concepts are (relatively) easy to understand --- this is what this course is about
- Writing high performance, parallel code is always complicated, but the concepts are a recurring theme

Thank you very much

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Please participate in our survey

http://bit.ly/CSUXSEDE