
GPU Computing
Overview
UCAR SEA 2013
Tony Scudiero
NVIDIA

Outline

- Evolution of GPU Computing
- Parallelism
- Heterogeneous Computing Concepts
- Using GPUs to Accelerate Applications
  - Accelerated Libraries
  - Compiler Directives
  - Programming Languages

Once upon a time . . .

Quake Software Rendering

Quake Hardware Rendering

- GPU: Graphical Processing Unit
  - Originated as specialized hardware for 3D games.
- Why a different processor?
  - Rendering is the most computationally intense part of a game.
  - CPU is not an ideal device for computer graphics rendering
  - Freed CPU allows more complex AI, dynamic world generation, realistic dynamics.

Programmable GPUs

- Graphics research diverged from OpenGL pipeline.
- 2001 - Programmable vertex and fragment shaders. (Geforce3)
  - OpenGL 2.0 (2004) updates pipeline
  - *GPGPU* era begins

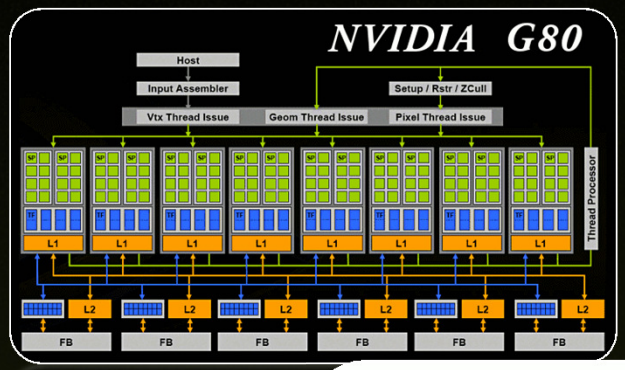
NVIDIA Geforce3

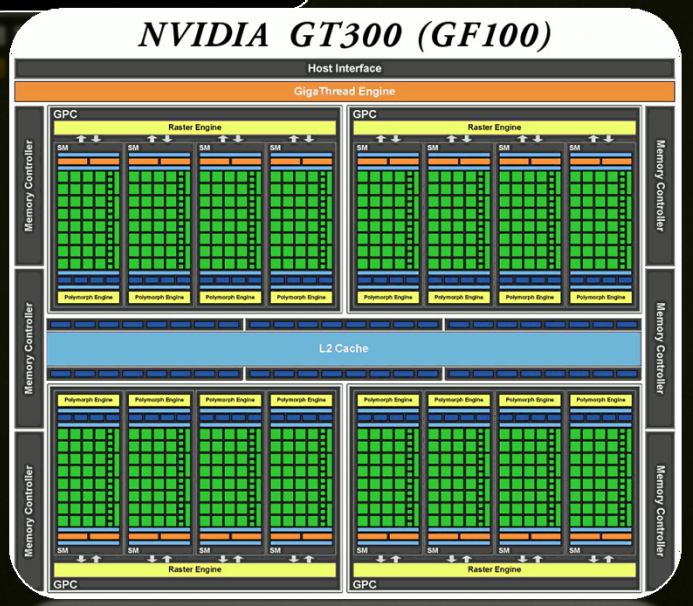
GPGPU: “Because It’s There”

Warning: Nerdy Movie Reference

GPU Computing Era: G80 and Fermi

- G80
  - Unified Shader Architecture
  - Double Precision
  - CUDA Introduced
- Fermi (GF100)
  - ECC
  - Enhanced Double precision
  - Memory hierarchy and expanded caching

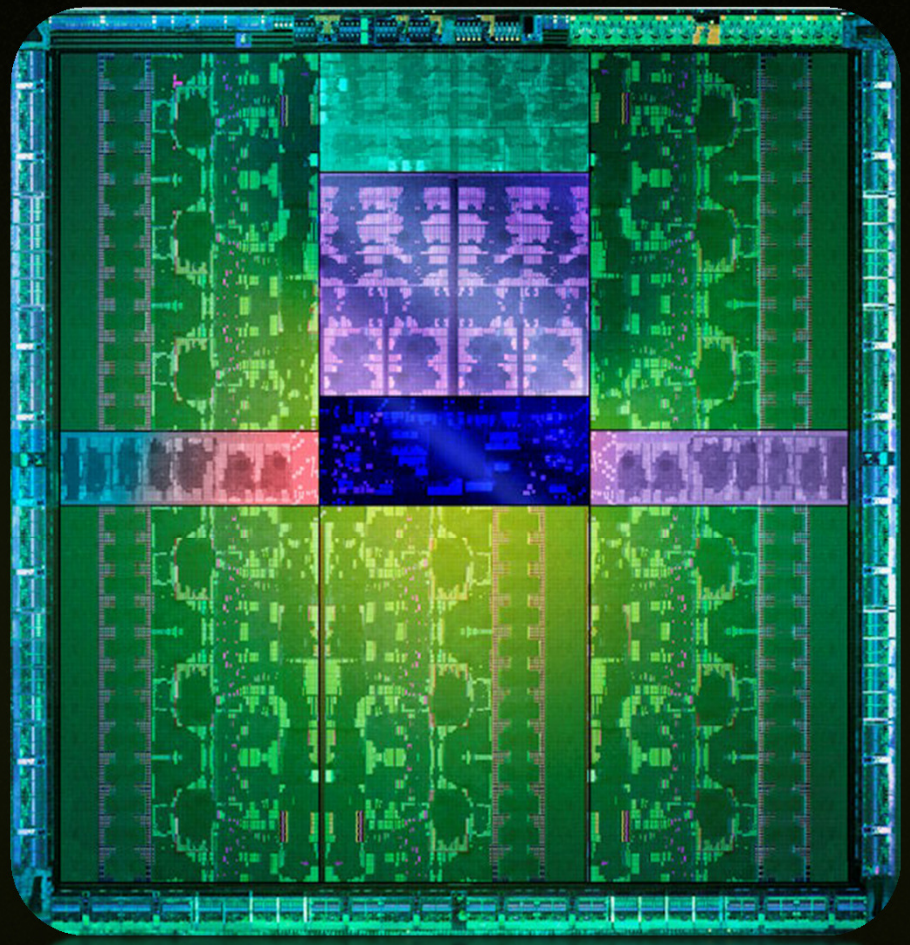




12 years later

- NVIDIA Kepler
  - 1.31 tflop double precision
  - 3.95 tflop single precision
  - 250 gb/sec memory bandwidth
  - 2,688 Functional Units (cores)
- ~= #1 on Top500 in 1997
- Can still play video games

NVIDIA GeForce Titan



NVIDIA GK110 - Kepler

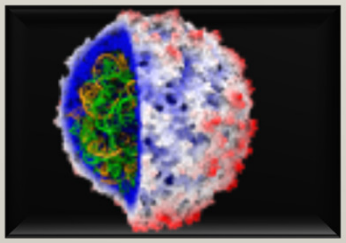
Not A Video Game

18,866 NVIDIA GK110 + AMD Interlagos
Rpeak: 27,112.5 TFLOPS

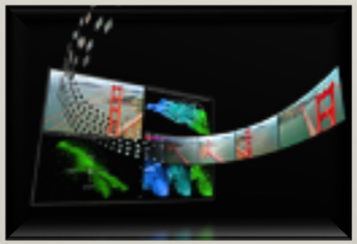
Top500 Rank: #1 Nov'12

Science Uses GPUs

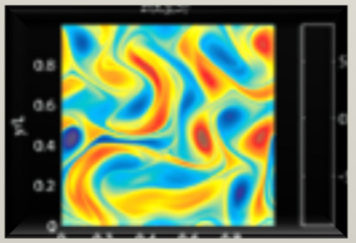
Medical Imaging
U of Utah



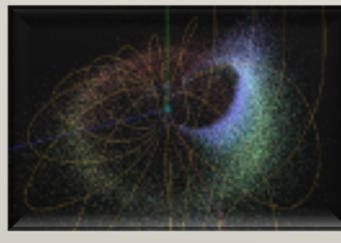
Molecular Dynamics
U of IL, Urbana



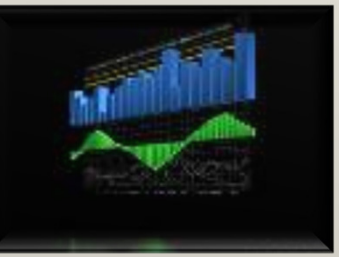
Video Transcoding
Elemental Tech



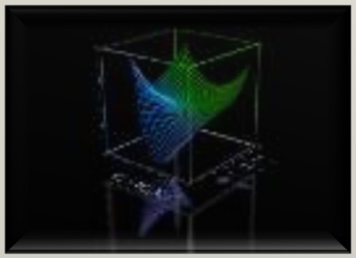
Matlab Computing
AccelerEyes



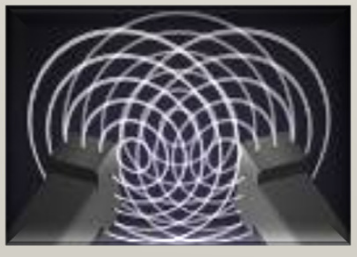
Astrophysics
RIKEN



Financial Simulation
Oxford

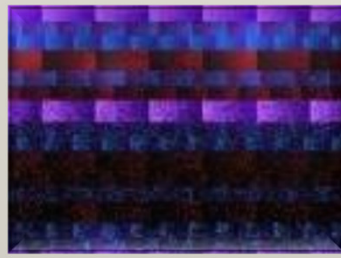


Linear Algebra
Universidad Jaime



3D Ultrasound
Techniscan

Quantum Chemistry
U of Illinois, Urbana



Gene Sequencing
U of Maryland

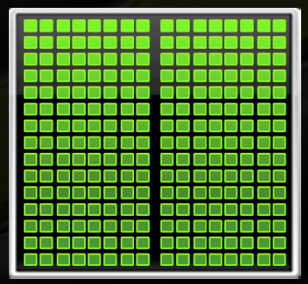
Outline

- Evolution of GPU Computing
- Parallelism
- Heterogeneous Computing Concepts
- Using GPUs to Accelerate Applications
  - Accelerated Libraries
  - Compiler Directives
  - Programming Languages

Latency vs. Throughput

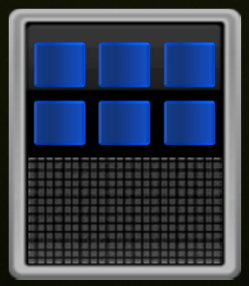
- Throughput
  - Work per unit time
  - Matrix operations, FFTs, signal processing, data analytics, rendering/visualization

GPU



- Latency
  - Time per unit work
  - Databases, web servers, transaction servers, Internet infrastructure.

CPU



A GPU is a Throughput Optimized Processor

- GPU Achieves high throughput by parallel execution
  - 2,688 cores (GK110)
  - Millions of resident threads
- GPU Threads are much lighter weight than CPU threads like pThreads
- Processing in Parallel is how GPU achieves performance

A GPU is a Throughput Optimized Processor

- GPU Achieves high throughput by parallel execution
  - 2,688 cores (GK110)
  - Millions of resident threads
- GPU Threads are much lighter weight than CPU threads like pThreads
- Processing in parallel is how ***HPC*** achieves performance

Parallelism

- Parallel Poll
  - Ideal Serial Processor: IPC 1.0, 8ghz, perfect pipeline: 8gflops/core

- Yellowstone: 1.5 Pflops @ 2.6ghz (#13 on Top 500 Nov'12!)
  - 4,512 Nodes
  - 2 Sockets per node
  - 8 cores per socket
  - Each Core: 2 x 256bit-wide pipelined FP units @ 2.6 ghz
    - Theoretical Peak: 20.8 gflops / core

Parallelism

- Exposing Parallelism is . . .

. . . a necessary part of GPU Computing

. . . essential to utilize current HPC systems

. . . going to be more important on future systems

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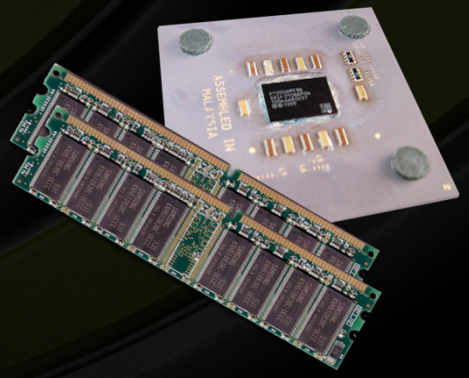
Heterogeneous Computing

- The CPU and its memory (host)
- The GPU and its memory (device)



CPU

GPU

Heterogeneous Computing

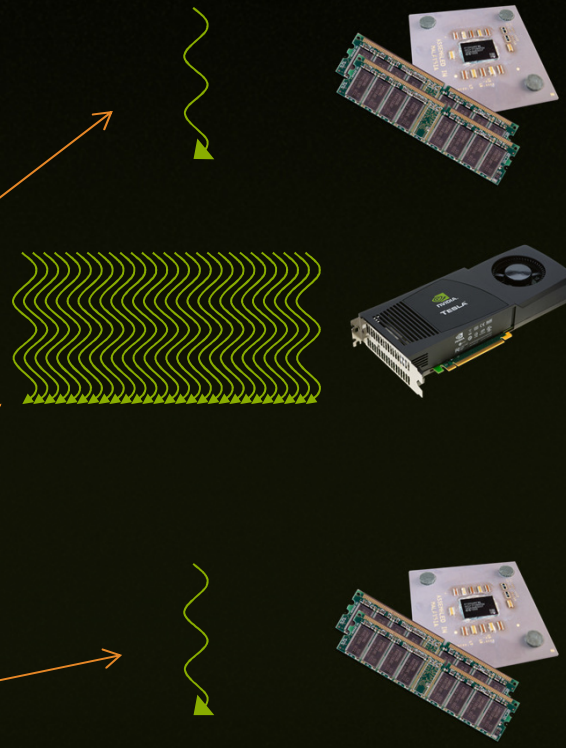
```
#include <iostream>
#include <algorithm>

using namespace std;

#define N          1024
#define RADIUS     3
#define BLOCK_SIZE 16

__global__ void stencil_1d(int *in, int *out) {
        __shared__ int temp[BLOCK_SIZE + 2 * RADIUS];
        int gindex = threadIdx.x + blockIdx.x * blockDim.x;
        int lindex = threadIdx.x + RADIUS;

        // Read input elements into shared memory
        temp[lindex] = in[gindex];
        if (threadIdx.x < RADIUS) {
                temp[lindex - RADIUS] = in[gindex - RADIUS];
                temp[lindex + BLOCK_SIZE] = in[gindex + BLOCK_SIZE];
        }

        // Synchronize (ensure all the data is available)
        __syncthreads();

        // Apply the stencil
        int result = 0;
        for (int offset = -RADIUS ; offset <= RADIUS ; offset++)
                result += temp[lindex + offset];

        // Store the result
        out[gindex] = result;
}

void fill_ints(int *x, int n) {
        fill_n(x, n, 1);
}

int main(void) {
        int *in, *out;          // host copies of a, b, c
        int *d_in, *d_out;      // device copies of a, b, c
        int size = (N + 2*RADIUS) * sizeof(int);

        // Alloc space for host copies and setup values
        in  = (int *)malloc(size); fill_ints(in,  N + 2*RADIUS);
        out = (int *)malloc(size); fill_ints(out, N + 2*RADIUS);

        // Alloc space for device copies
        cudaMalloc((void **)&d_in,  size);
        cudaMalloc((void **)&d_out, size);

        // Copy to device
        cudaMemcpy(d_in,  in,  size, cudaMemcpyHostToDevice);
        cudaMemcpy(d_out, out, size, cudaMemcpyHostToDevice);

        // Launch stencil_1d() kernel on GPU
        stencil_1d<<<N/BLOCK_SIZE,BLOCK_SIZE>>>(d_in + RADIUS, d_out + RADIUS);

        // Copy result back to host
        cudaMemcpy(out, d_out, size, cudaMemcpyDeviceToHost);

        // Cleanup
        free(in); free(out);
        cudaFree(d_in); cudaFree(d_out);
        return 0;
}
```

parallel fn

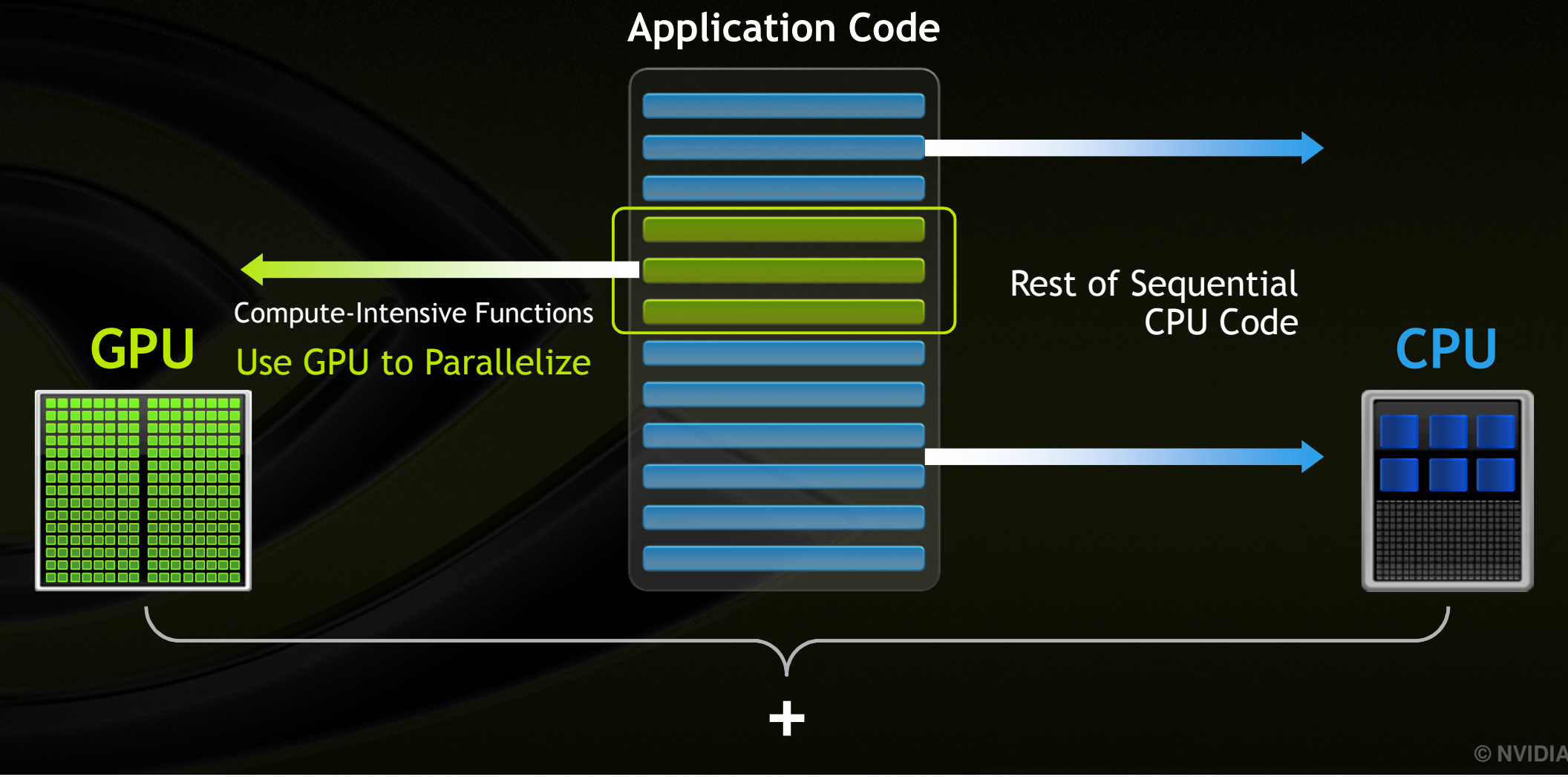
serial code

parallel code

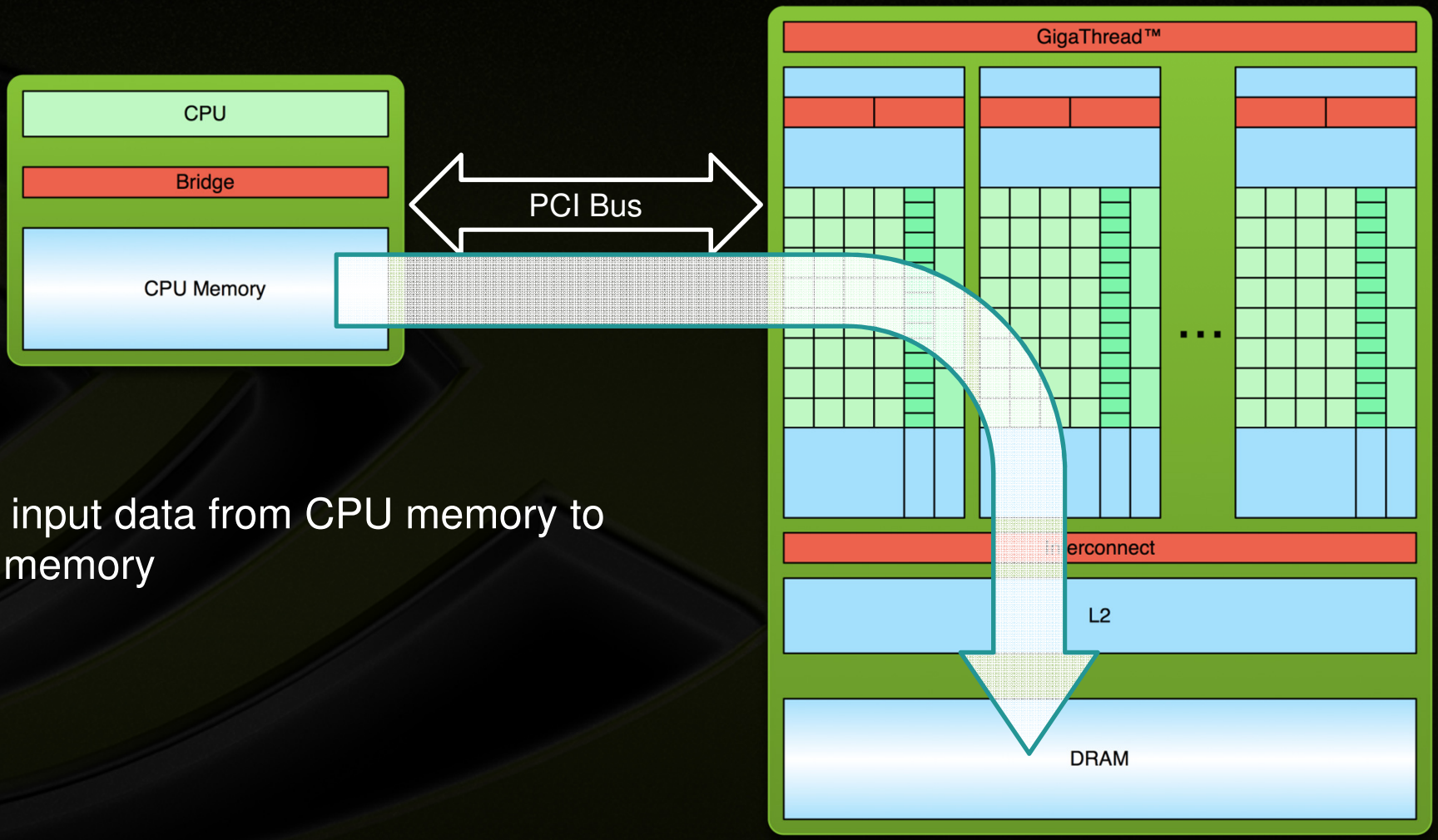
serial code



GPU Computing

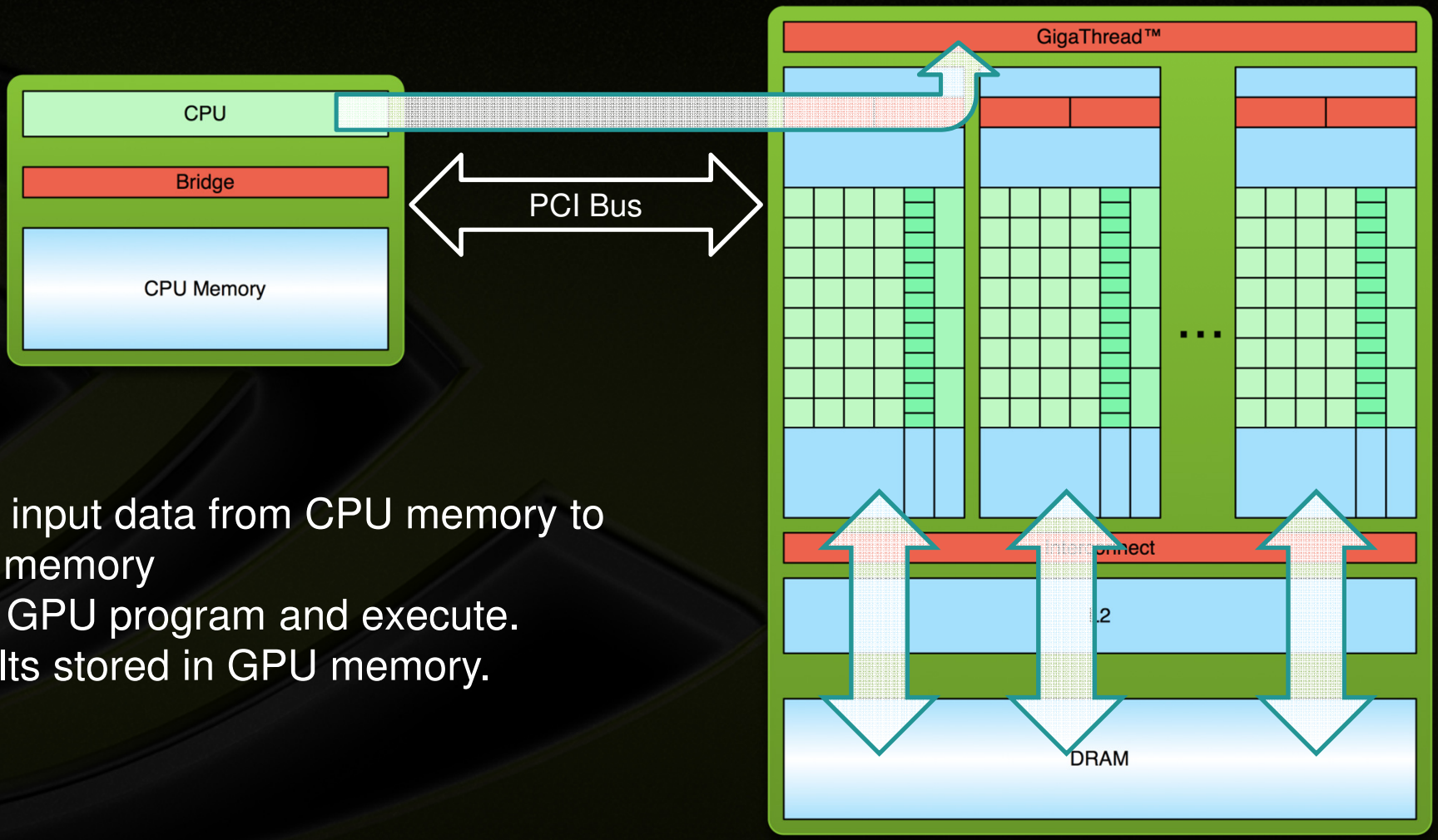


Simple Processing Flow



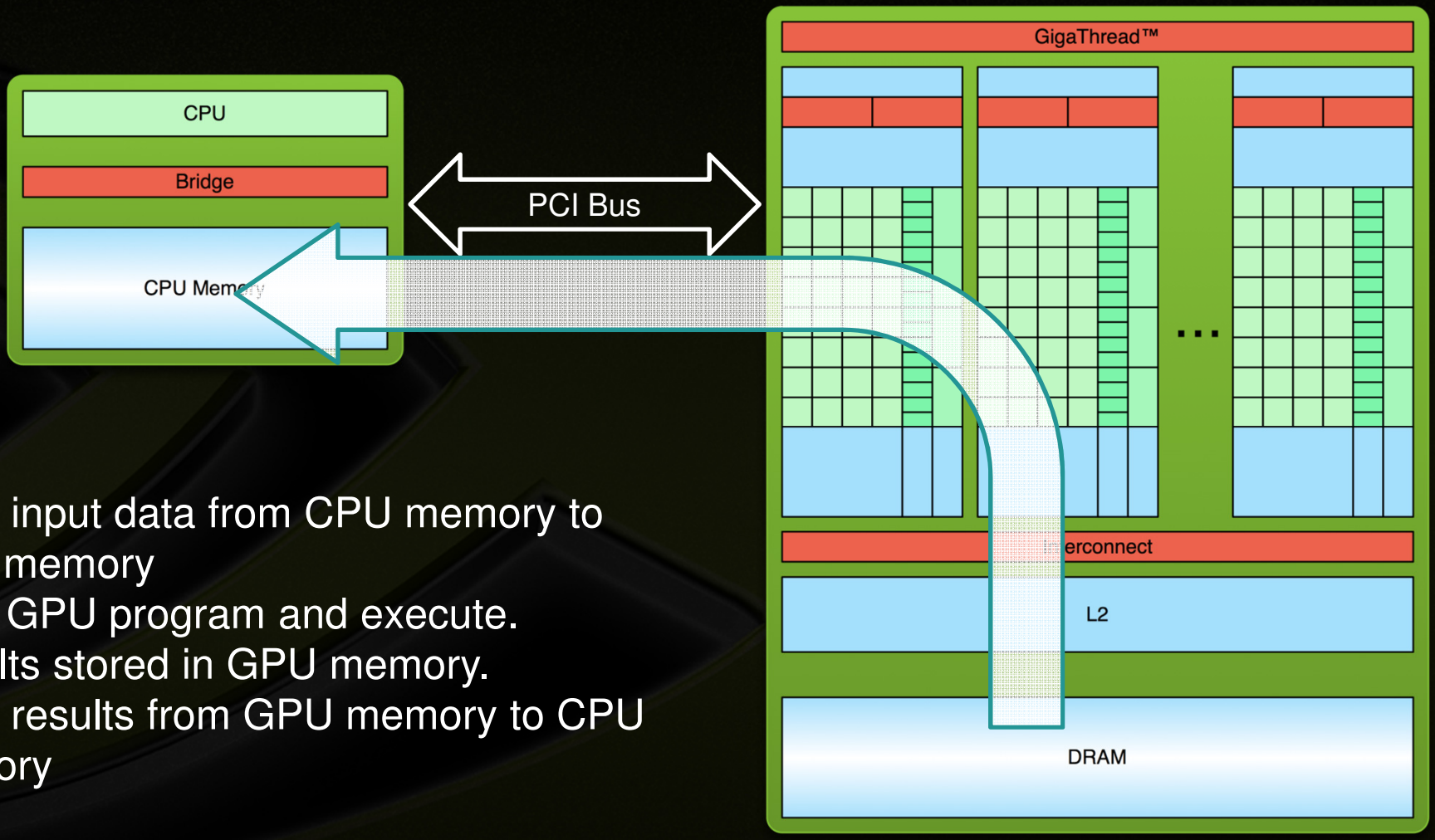
1. Copy input data from CPU memory to GPU memory

Simple Processing Flow



1. Copy input data from CPU memory to GPU memory
2. Load GPU program and execute. Results stored in GPU memory.

Simple Processing Flow



1. Copy input data from CPU memory to GPU memory
2. Load GPU program and execute. Results stored in GPU memory.
3. Copy results from GPU memory to CPU memory

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  - **Compiler Directives**
  - **Programming Languages**

Simple Example: SAXPY

- BLAS1 function
- Y = a*X+Y
  - Y and X are length N vectors
  - A is a scalar
  - single precision data (float)

```
void saxpy(int n, float a,
           float *x, float *y)
{
  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}

int N = 1<<20;



// Perform SAXPY on 1M elements
saxpy(N, 2.0, x, y);
```

3 Ways to Accelerate Applications

Applications

Libraries

OpenACC Directives

Programming Languages

"Drop-in" Acceleration

Easily Accelerate Applications

Maximum Flexibility

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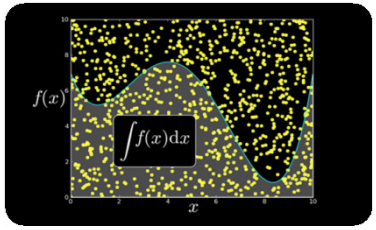
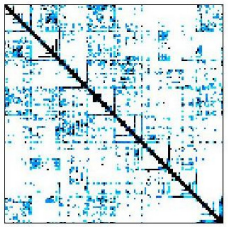
GPU Accelerated Libraries

NVIDIA cuBLAS



NVIDIA cuRAND



NVIDIA cuSPARSE

NVIDIA NPP

GPU VSIPL

Vector Signal Image Processing

CULA tools

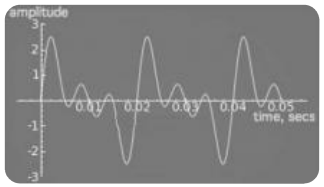
GPU Accelerated Linear Algebra

MAGMA

ICL UT

Matrix Algebra on GPU and Multicore

open source initiative



NVIDIA cuFFT

ROGUE WAVE SOFTWARE

IMSL Library

ArrayFire Matrix Computations

CUSP

Sparse Linear Algebra

open source initiative

Thrust

C++ STL Features for CUDA

open source initiative

SAXPY in cuBLAS

Serial BLAS Code

```
int N = 1<<20;

...

// Use your choice of blas library

// Perform SAXPY on 1M elements
blas_saxpy(N, 2.0, x, 1, y, 1);
```

Parallel cuBLAS Code

```
int N = 1<<20;

cublasInit();
cublasSetVector(N, sizeof(x[0]), x, 1, d_x, 1);
cublasSetVector(N, sizeof(y[0]), y, 1, d_y, 1);

// Perform SAXPY on 1M elements
cublasSaxpy(N, 2.0, d_x, 1, d_y, 1);

cublasGetVector(N, sizeof(y[0]), d_y, 1, y, 1);

cublasShutdown();
```

You can also call cuBLAS from Fortran, C++, Python, and other languages

http://developer.nvidia.com/cublas

3 Ways to Accelerate Applications

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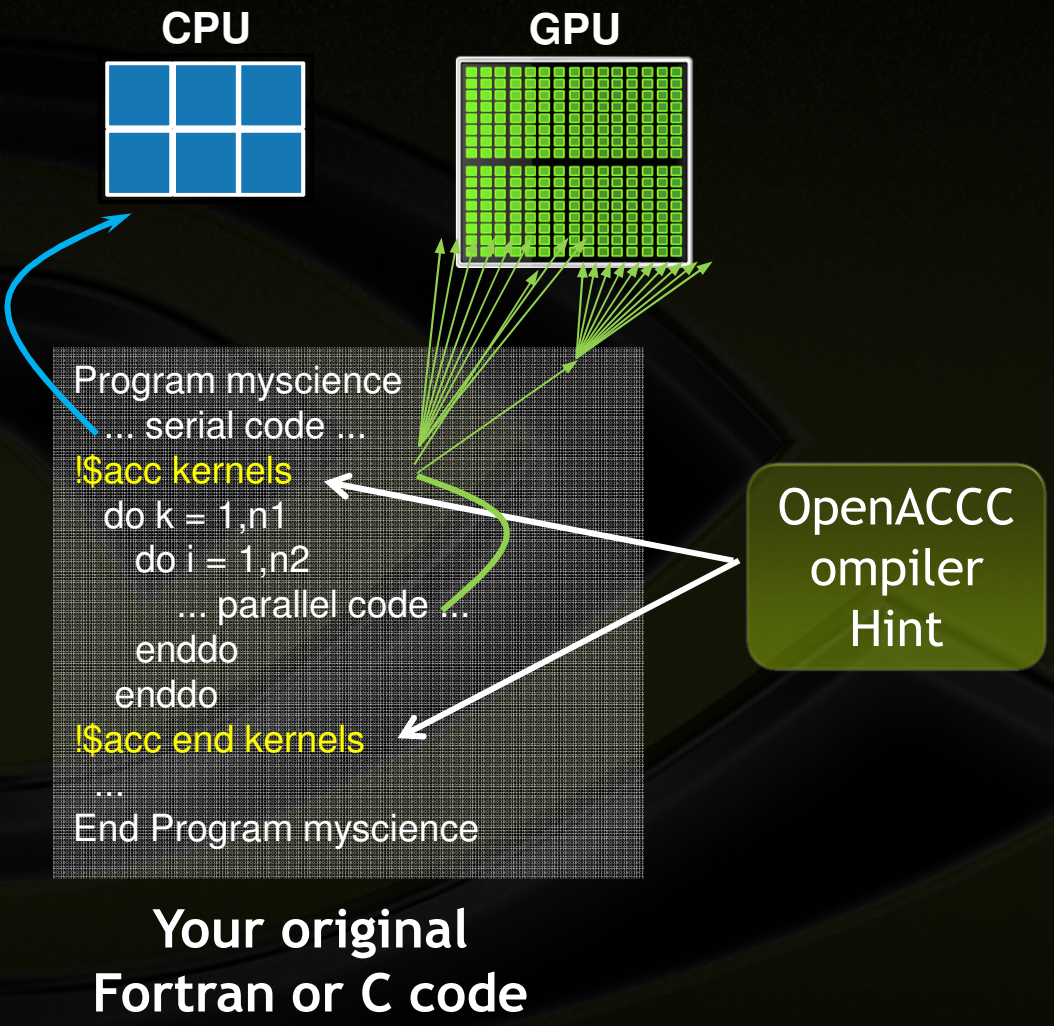
OpenACC Compiler Directives



Simple Compiler hints

Compiler Parallelizes code

Works on many-core GPUs & multicore CPUs

SAXPY with OpenACC Directives

Parallel C Code

```
void saxpy(int n,
           float a,
           float *x,
           float *y)
{
#pragma acc kernels
  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}

...
// Perform SAXPY on 1M elements
saxpy(1<<20, 2.0, x, y);
...
```

Parallel Fortran Code

```
subroutine saxpy(n, a, x, y)
  real :: x(:), y(:), a
  integer :: n, i
!$acc kernels
  do i=1,n
    y(i) = a*x(i)+y(i)
  enddo
!$acc end kernels
end subroutine saxpy


...
! Perform SAXPY on 1M elements
call saxpy(2**20, 2.0, x_d, y_d)
...
```

http://developer.nvidia.com/openacc or http://openacc.org

OpenACC Will be covered Friday

- Exposing Parallelism with OpenACC
- Profiling and Tuning OpenACC Applications
- Coding and profiling hands on

A Shameless Plug

3 Ways to Accelerate Applications

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"Drop-in" Acceleration

Easily Accelerate Applications

Maximum Flexibility

CUDA C/C++

CUDA C++ features enable sophisticated and flexible applications and middleware

- Class hierarchies
- __device__ methods
- Templates
- Operator overloading
- Functors (function objects)
- Device-side new/delete
- More…

```
template <typename T>
struct Functor {
  __device__ Functor(_a) : a(_a) {}
  __device__ T operator(T x) { return a*x; }
  T a;
}

template <typename T, typename Oper>
__global__ void kernel(T *output, int n) {
  Oper op(3.7);
  output = new T[n]; // dynamic allocation
  int i = blockIdx.x*blockDim.x + threadIdx.x;
  if (i < n)
    output[i] = op(i);  // apply functor
}
```

ttp://developer.nvidia.com/cuda-toolkit

CUDA Fortran

- Program GPU using Fortran
  - Key language for HPC
- Simple language extensions
  - Kernel functions
  - Thread / block IDs
  - Device & data management
  - Parallel loop directives
- Familiar syntax
  - Use allocate, deallocate
  - Copy CPU-to-GPU with assignment (=)

```
module mymodule contains
  attributes(global) subroutine saxpy(n,a,x,y)
    real :: x(:), y(:), a,
    integer n, i
    attributes(value) :: a, n
    i = threadIdx%x+(blockIdx%x-1)*blockDim%x
    if (i<=n) y(i) = a*x(i) + y(i);
  end subroutine saxpy
end module mymodule

program main
  use cudafor; use mymodule
  real, device :: x_d(2**20), y_d(2**20)
  x_d = 1.0; y_d = 2.0
  call saxpy<<<4096,256>>>(2**20,3.0,x_d,y_d,)
  y = y_d
  write(*,*) 'max error=', maxval(abs(y-5.0))
end program main
```

http://developer.nvidia.com/cuda-fortran

CUDA C/C++ will be covered Thursday

- Optimization and GPU Architecture
- Hands on development, optimization, and profiling

YASP: Yet Another Shameless Plug

SAXPY in CUDA C

Standard C

```
void saxpy(int n, float a,
           float *x, float *y)
{
  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}

int N = 1<<20;



// Perform SAXPY on 1M elements
saxpy(N, 2.0, x, y);
```

CUDA C

```
__global__
void saxpy(int n, float a,
           float *x, float *y)
{
  int i = blockIdx.x*blockDim.x + threadIdx.x;
  if (i < n) y[i] = a*x[i] + y[i];
}

int N = 1<<20;
cudaMemcpy(d_x, x, N, cudaMemcpyHostToDevice);
cudaMemcpy(d_y, y, N, cudaMemcpyHostToDevice);

// Perform SAXPY on 1M elements
saxpy<<<4096,256>>>(N, 2.0, d_x, d_y);

cudaMemcpy(y, d_y, N, cudaMemcpyDeviceToHost);
```

http://developer.nvidia.com/cuda-toolkit

SAXPY in CUDA Fortran

Standard Fortran

```
module mymodule contains
  subroutine saxpy(n, a, x, y)
    real :: x(:), y(:), a
    integer :: n, i
    do i=1,n
      y(i) = a*x(i)+y(i)
    enddo
  end subroutine saxpy
end module mymodule

program main
  use mymodule
  real :: x(2**20), y(2**20)
  x = 1.0, y = 2.0

  ! Perform SAXPY on 1M elements
  call saxpy(2**20, 2.0, x, y)

end program main
```

CUDA Fortran

```
module mymodule contains
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  call saxpy<<<4096,256>>>(2**20, 2.0, x_d, y_d)

end program main
```

http://developer.nvidia.com/cuda-fortran

Takeaways

- GPUs accelerate science
  - Increase throughput on parallel computations common to scientific applications.
  - GPUs have proven their worth in accelerating real science applications.
- Three ways to make use of GPUs in your application:
  - 1. Accelerated Libraries
  - 2. Compiler Directives – OpenACC in C, C++, Fortran
    - Tutorial - Friday
  - 3. Programming Languages- CUDA C/C++, CUDA Fortran
    - Tutorial – Thursday

Final Words:

- We live in a parallel universe
- Think in parallel about your problem in parallel


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Conference Progress: 60%
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Plenary Sessions: 100%
NVIDIA