An Introduction to GPU Programming

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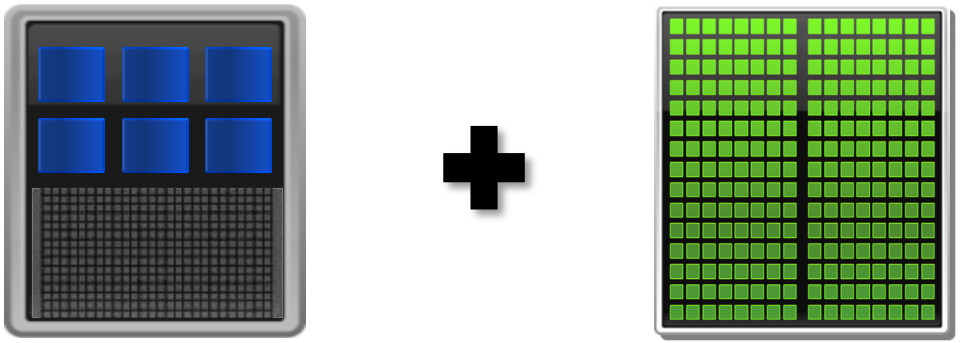
GPU Computing History

- The first GPU (Graphics Processing Unit)s were designed as graphics accelerators, supporting only specific fixed-function pipelines.
- Starting in the late 1990s, the hardware became increasingly programmable, culminating in NVIDIA's first GPU in 1999.
- Researchers were tapping its excellent floating point performance. The General Purpose GPU (GPGPU) movement had dawned.
- NVIDIA unveiled CUDA in 2006, the world's first solution for general-computing on GPUs.
- CUDA (Compute Unified Device Architecture) is a parallel computing platform and programming model created by NVIDIA and implemented by the GPUs that they produce.

Add GPUs: Accelerate Science Applications

CPU

GPU



Why is GPU this different from a CPU?

- **Different goals produce different designs**
  - GPU assumes work load is highly parallel
  - CPU must be good at everything, parallel or not

- **CPU: minimize latency experienced by 1 thread**
  - big on-chip caches
  - sophisticated control logic

- **GPU: maximize throughput of all threads**
  - # threads in flight limited by resources => lots of resources (registers, bandwidth, etc.)
  - multithreading can hide latency => skip the big caches
  - share control logic across many threads

Overview of the GPU nodes

- **CPU: Two 2.6 GHz 8-Core Sandy Bridge Xeon 64-bit Processors (16)**
  - 64GB 1666MHz Ram
- **GPU: Two NVIDIA Tesla K20Xm**
  - 14 Streaming Multiprocessor (SMX)
  - 2688 SP Cores
  - 896 DP Cores
  - 6G global memory

K20Xm GPU Architecture

SMX (192 SP, 64 DP)

Key Architectural Ideas

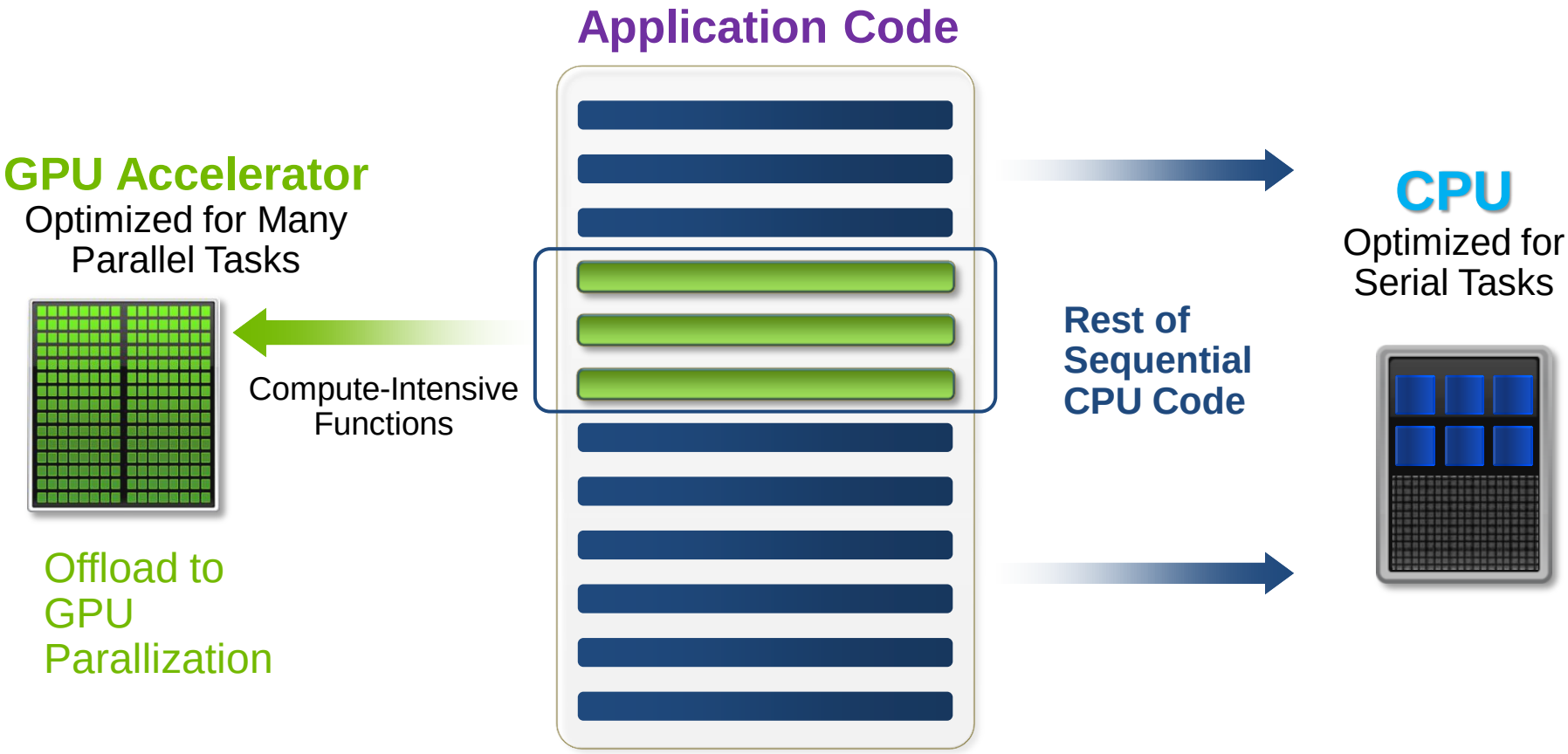
- **SIMT (**Single Instruction Multiple Thread**) execution**
  - threads run in groups of **32** called warps
  - threads in a warp share instruction unit (IU)
  - HW automatically handles divergence
- **Hardware multithreading**
  - HW resource allocation & thread scheduling
  - HW relies on threads to hide latency
- **Threads have all resources needed to run**
  - any warp not waiting for something can run
  - context switching is (basically) free

Enter CUDA

- **Scalable parallel programming model**
- **Minimal extensions to familiar C/C++ environment**
- **Heterogeneous serial-parallel computing**

CUDA Execution Model

- **Sequential code executes in a Host (CPU) thread**
- **Parallel code executes in many Device (GPU) threads across multiple processing elements**



Heterogeneous Computing

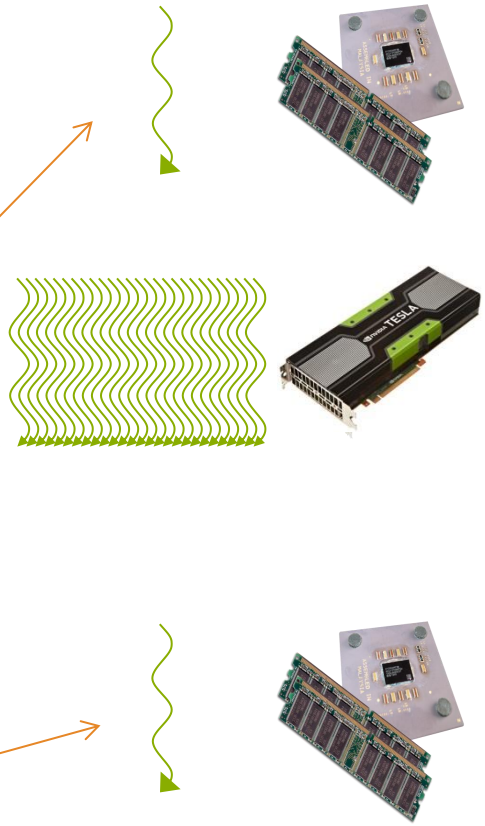
```
#include <iostream>
#include <algorithm>

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 function

serial code

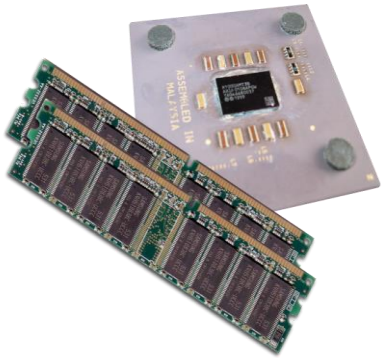
parallel code

serial code



Heterogeneous Computing

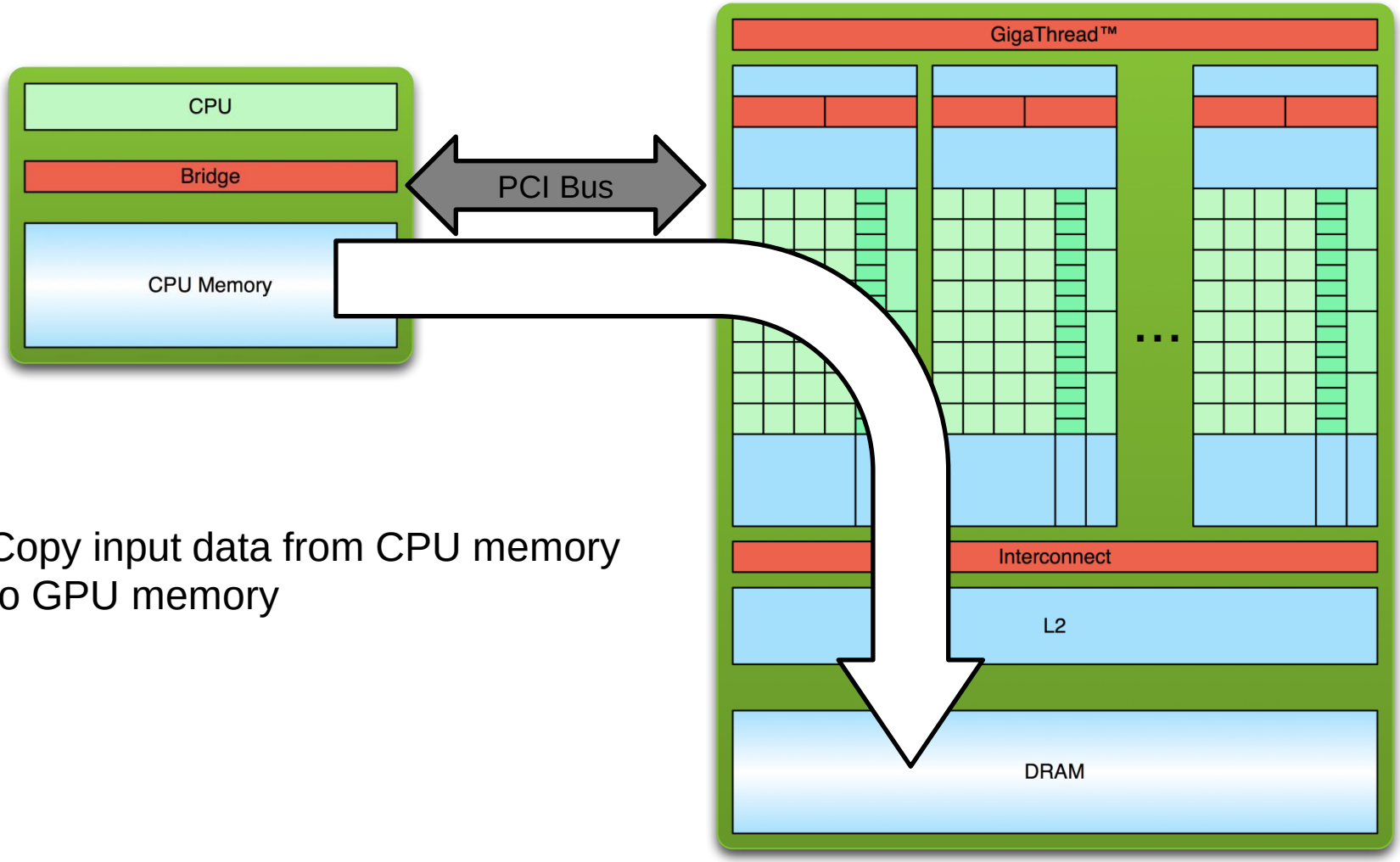
- Terminology:
  - *Host* The CPU and its memory (host memory)
  - *Device* The GPU and its memory (device memory)



Host

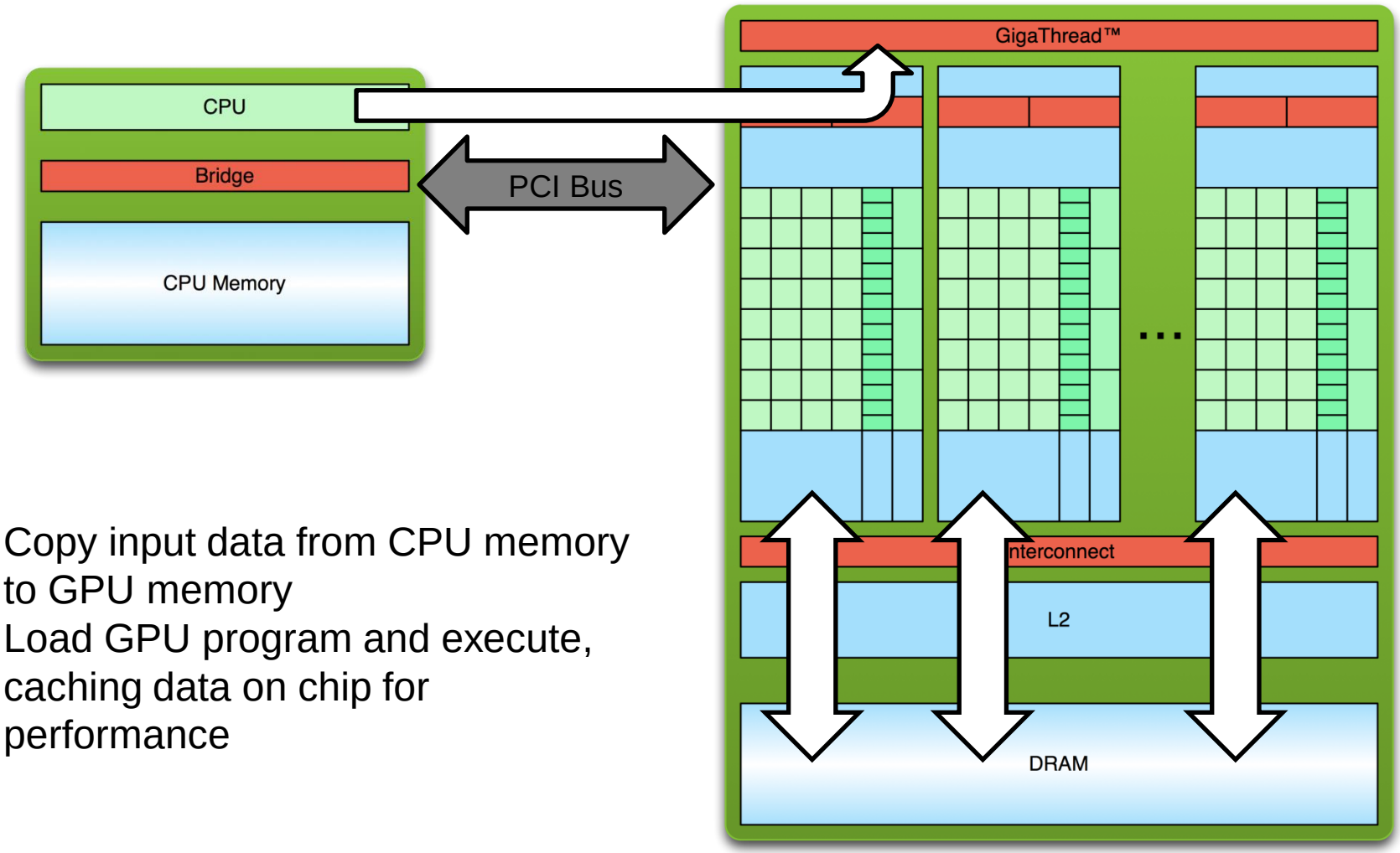
Device

Simple Processing Flow



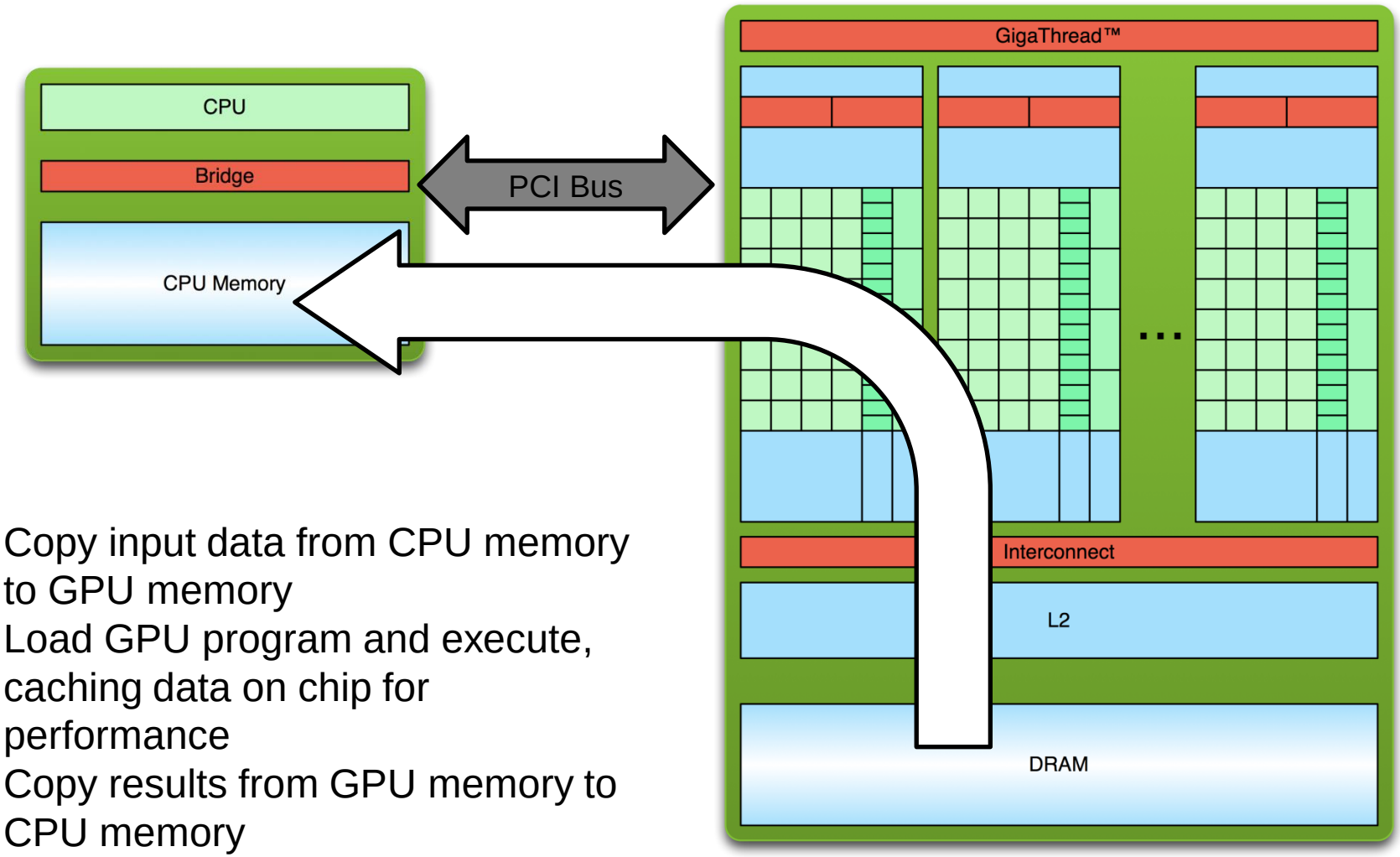
1. Copy input data from CPU memory to GPU memory

Simple Processing Flow



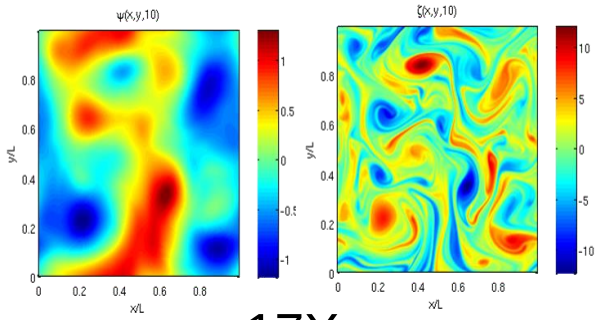
1. Copy input data from CPU memory to GPU memory
2. Load GPU program and execute, caching data on chip for performance

Simple Processing Flow

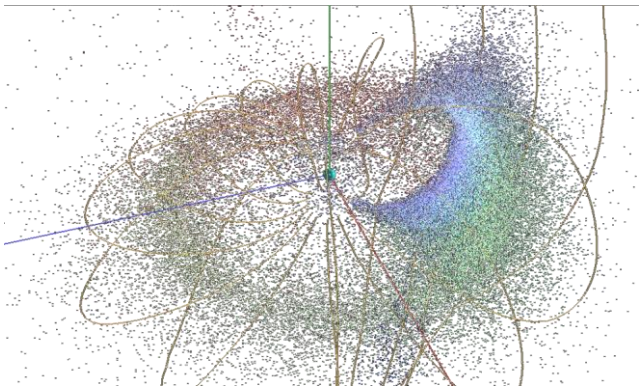


1. Copy input data from CPU memory to GPU memory
2. Load GPU program and execute, caching data on chip for performance
3. Copy results from GPU memory to CPU memory

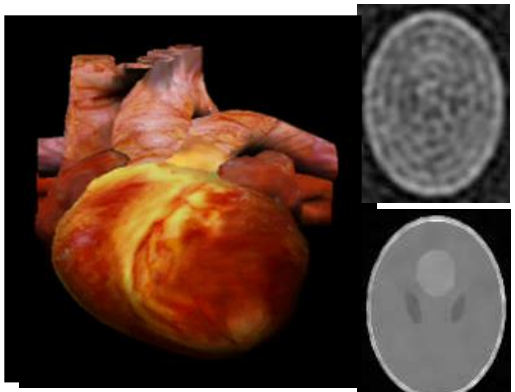
45X



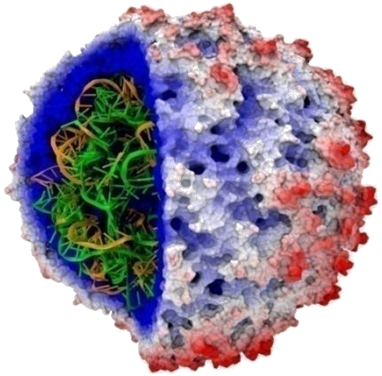
17X



100X

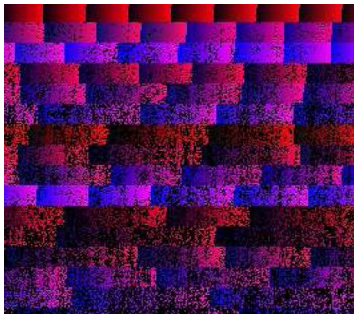


13–457x



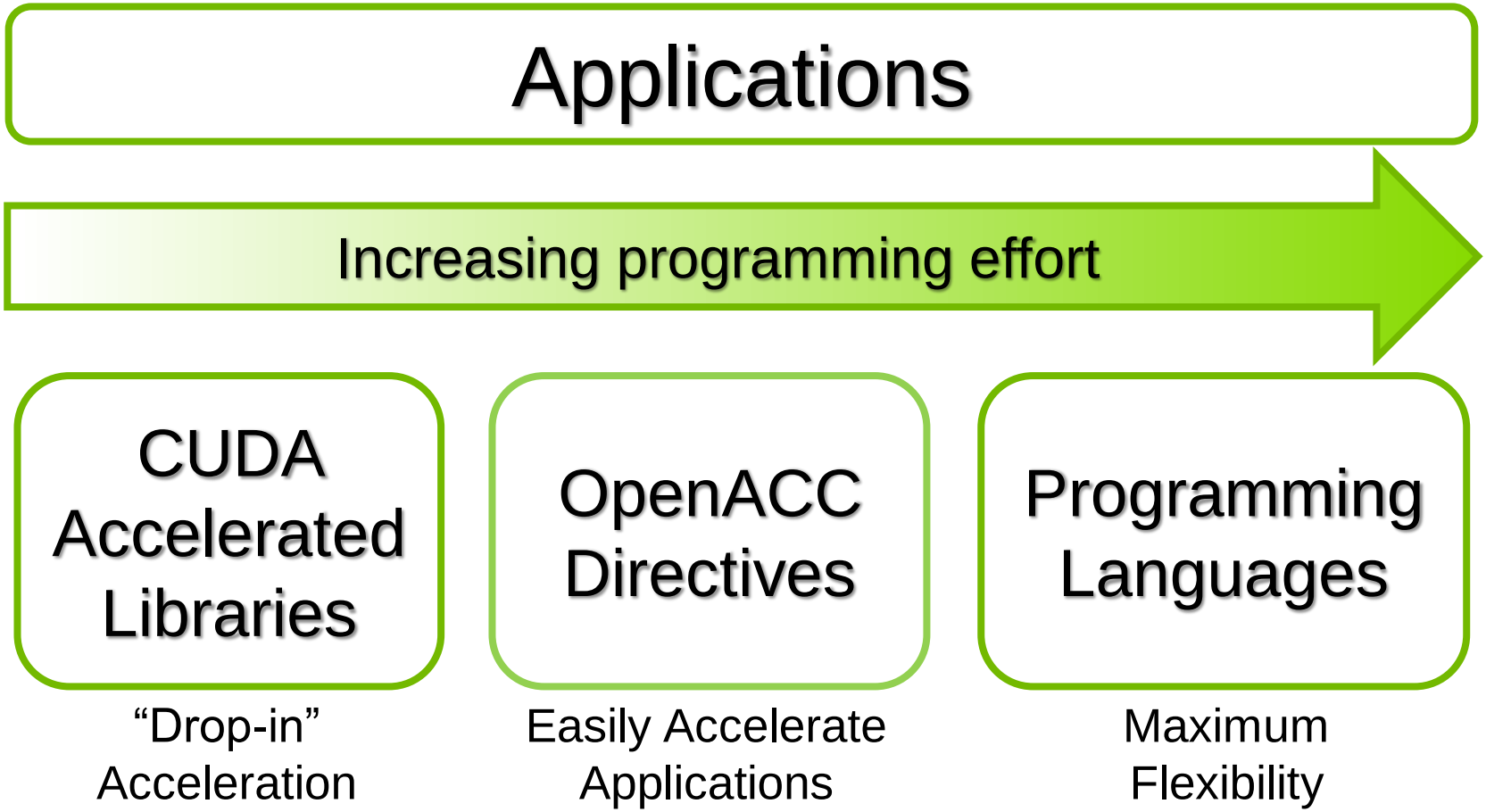
110-240X

Motivation



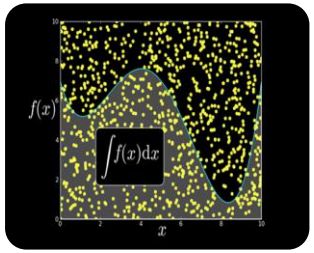
35X

3 Ways to Accelerate Applications

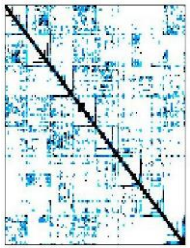


Some GPU-accelerated Libraries

NVIDIA cuBLAS



NVIDIA cuRAND



NVIDIA cuSPARSE

NVIDIA NPP

GPU VSIPL

Vector Signal Image Processing

CULA tools

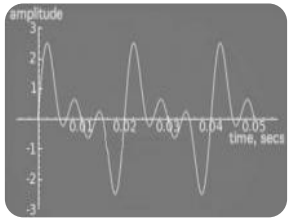
GPU Accelerated Linear Algebra

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

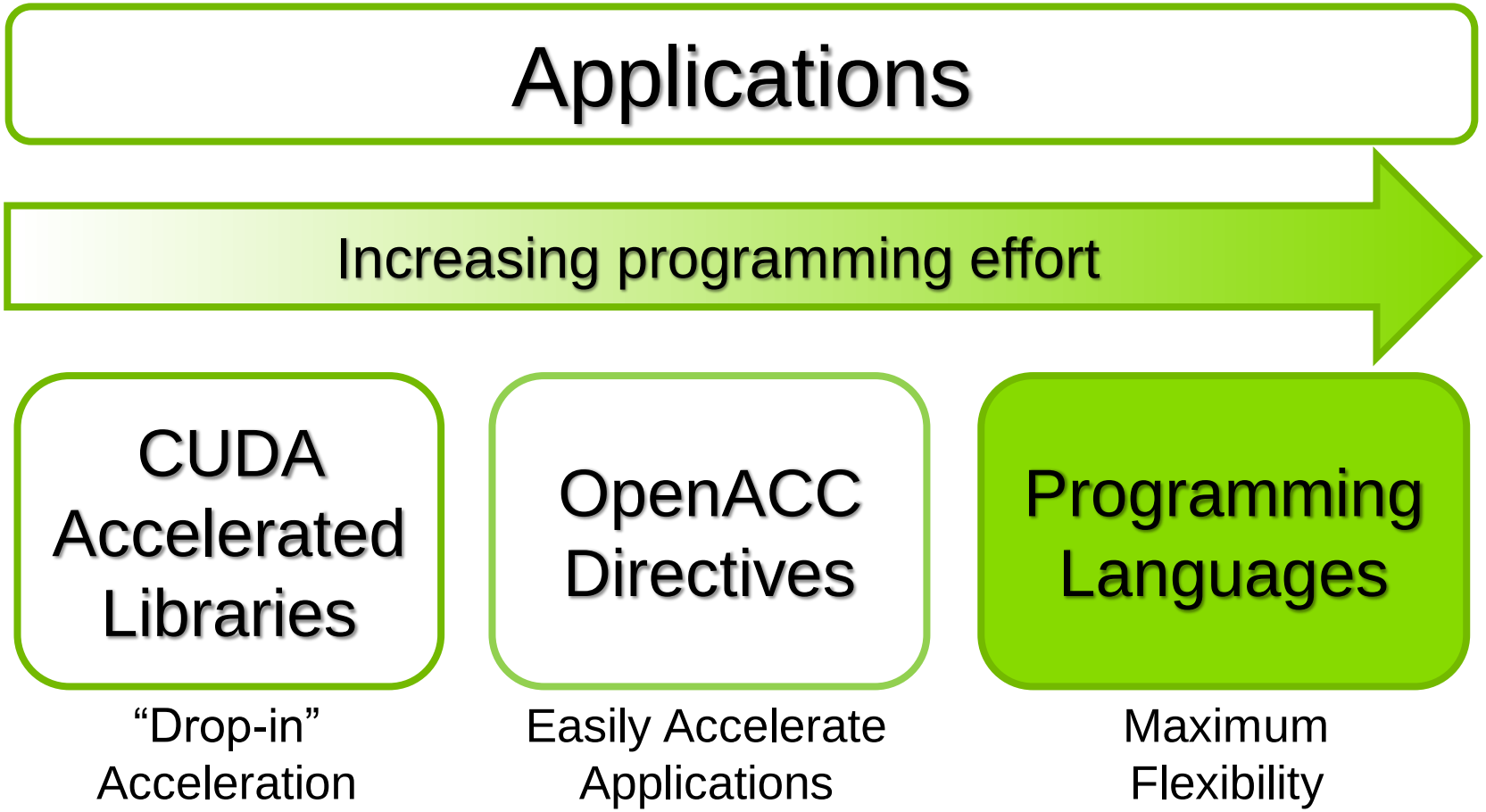
Thrust

C++ STL Features for CUDA

GPU Programming Languages

Numerical analytics	MATLAB, Mathematica, LabVIEW
Fortran	OpenACC, CUDA Fortran
C	OpenACC, CUDA C
C++	Thrust, CUDA C++
Python	PyCUDA, Copperhead
F#	Alea.cuBase

3 Ways to Accelerate Applications



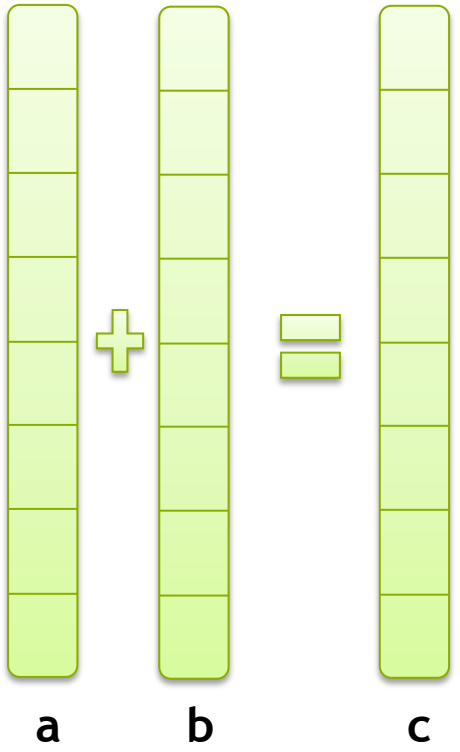
VECTOR ADDITION WITH CUDA

CONCEPTS

- Heterogeneous Computing
- Blocks
- Threads
- Indexing
- Shared memory
- __syncthreads()
- Asynchronous operation
- Handling errors
- Managing devices

Parallel Programming in CUDA C/C++

- We'll start by adding two integers and build up to vector addition



Addition on the Device

- **First recall how to write a pure C function:**

```
void add(int *a, int *b, int *c) {
    *c = *a + *b;
}
```

- **Then we have a simple kernel to add two integers**

```
__global__ void add(int *a, int *b, int *c) {
    *c = *a + *b;
}
```

- **As before `__global__` is a CUDA C/C++ keyword meaning**
  - `add()` is a kernel function that will execute on the device
  - `add()` will be called from the host

Addition on the Device

- Note that we use pointers for the variables

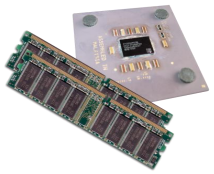
```
__global__ void add(int *a, int *b, int *c) {
        *c = *a + *b;
}
```

- `add()` runs on the device, so `a`, `b` and `c` must point to device memory

- We need to allocate memory on the GPU

Memory Management

- **Host and device memory are separate entities**
  - *Device* pointers point to GPU memory
    - May be passed to/from host code
    - May *not* be dereferenced in host code
  - *Host* pointers point to CPU memory
    - May be passed to/from device code
    - May *not* be dereferenced in device code



- **Simple CUDA API for handling device memory**
  - `cudaMalloc()`, `cudaFree()`, `cudaMemcpy()`
  - Similar to the C equivalents `malloc()`, `free()`, `memcpy()`

Addition on the Device: `add()`

- Returning to our `add()` kernel

```
__global__ void add(int *a, int *b, int *c) {
    *c = *a + *b;
}
```

- Let's take a look at main()…

Addition on the Device: `main()`

```
int main(void) {
        int a, b, c;         // host copies of a, b, c
        int *d_a, *d_b, *d_c;     // device copies of a, b, c
        int size = sizeof(int);

        // Allocate space for device copies of a, b, c
        cudaMalloc((void **)&d_a, size);
        cudaMalloc((void **)&d_b, size);
        cudaMalloc((void **)&d_c, size);

        // Setup input values
        a = 2;
        b = 7;
```

Addition on the Device: `main()`

```
    // Copy inputs to device
    cudaMemcpy(d_a, &a, size, cudaMemcpyHostToDevice);
    cudaMemcpy(d_b, &b, size, cudaMemcpyHostToDevice);

    // Launch add() kernel on GPU
    add<<<1,1>>>(d_a, d_b, d_c);

    // Copy result back to host
    cudaMemcpy(&c, d_c, size, cudaMemcpyDeviceToHost);

    // Cleanup
    cudaFree(d_a); cudaFree(d_b); cudaFree(d_c);
    return 0;
}
```

Compile and Run

- **Changes to the ~/.soft file:**

```
[fchen14@mike2 gpuex]$ cat ~/.soft
+cuda-5.5.22
+Intel-13.1.3
+portland-14.3
@default
```

- **Request an interactive session in GPU queue:**

```
qsub -I -X -l nodes=1:ppn=16 -l walltime=01:00:00 -q gpu -A
your_allocation_name
```

- **Compile and run the first vector addition:**

```
[fchen14@mike424 gpuex]$ nvcc my_vec_add.cu
[fchen14@mike424 gpuex]$ ./a.out
c=9
```

CONCEPTS

- Heterogeneous Computing
- Blocks
- Threads
- Indexing

RUNNING IN PARALLEL

Moving to Parallel

- **GPU computing is about massive parallelism**
  - So how do we run code in parallel on the device?

```
add<<< 1, 1 >>>();

add<<< N, 1 >>>();
```

- **Instead of executing `add()` once, execute N times in parallel**

Vector Addition on the Device

- **With `add()` running in parallel we can do vector addition**

- **Terminology: each parallel invocation of `add()` is referred to as a block**
  - The set of blocks is referred to as a grid
  - Each invocation can refer to its block index using `blockIdx.x`

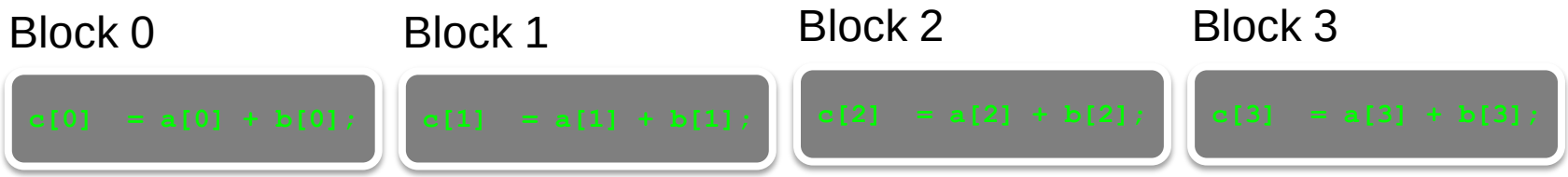
```
__global__ void add(int *a, int *b, int *c) {
    c[blockIdx.x] = a[blockIdx.x] + b[blockIdx.x];
}
```

- **By using `blockIdx.x` to index into the array, each block handles a different index**

Vector Addition on the Device

```
__global__ void add(int *a, int *b, int *c) {
        c[blockIdx.x] = a[blockIdx.x] + b[blockIdx.x];
}
```

- **On the device, each block can execute in parallel:**



Vector Addition on the Device: `add()`

- **Returning to our parallelized `add()` kernel**

```
__global__ void add(int *a, int *b, int *c) {
        c[blockIdx.x] = a[blockIdx.x] + b[blockIdx.x];
}
```

- **Let's take a look at main()…**

Vector Addition on the Device:

main()

```
#define N 512
int main(void) {
    int *a  *b  *c          // host copies of a, b, c
    int *d_a, *d_b, *d_c;  // device copies of a, b, c
    int size = N * sizeof(int);

    // Alloc space for device copies of a, b, c
    cudaMalloc((void **)&d_a, size);
    cudaMalloc((void **)&d_b, size);
    cudaMalloc((void **)&d_c, size);

    // Alloc space for host copies of a, b, c and setup input values
    a = (int *)malloc(size);
    b = (int *)malloc(size);
    c = (int *)malloc(size);
```

Vector Addition on the Device:

main()

```
    // Copy inputs to device
    cudaMemcpy(d_a, a, size, cudaMemcpyHostToDevice);
    cudaMemcpy(d_b, b, size, cudaMemcpyHostToDevice);

    // Launch add() kernel on GPU with N blocks
    add<<<N,1>>>(d_a, d_b, d_c);

    // Copy result back to host
    cudaMemcpy(c, d_c, size, cudaMemcpyDeviceToHost);

    // Cleanup
    free(a); free(b); free(c);
    cudaFree(d_a); cudaFree(d_b); cudaFree(d_c);
    return 0;
}
```

Review (1 of 2)

- **Difference between *host* and *device***
  - *Host* CPU
  - *Device* GPU

- **Using `__global__` to declare a function as device code**
  - Executes on the device
  - Called from the host

- **Passing parameters from host code to a device function**

Review (2 of 2)

- **Basic device memory management**
  - `cudaMalloc()`
  - `cudaMemcpy()`
  - `cudaFree()`

- **Launching parallel kernels**
  - Launch `N` copies of `add()` with `add<<<N,1>>>(…);`
  - Use `blockIdx.x` to access block index

CONCEPTS

- Heterogeneous Computing
- Blocks
- Threads
- Indexing

INTRODUCING THREADS

CUDA Threads

- **Terminology: a block can be split into parallel threads**
  - OR: **block is composed of threads**

- **Let's change `add()` to use parallel *threads* instead of parallel *blocks***

```
__global__ void add(int *a, int *b, int *c) {
    c[threadIdx.x] = a[threadIdx.x] + b[threadIdx.x];
}
```

- **We use threadIdx.x instead of blockIdx.x**

- **Need to make one change in main()…**

Vector Addition Using Threads:

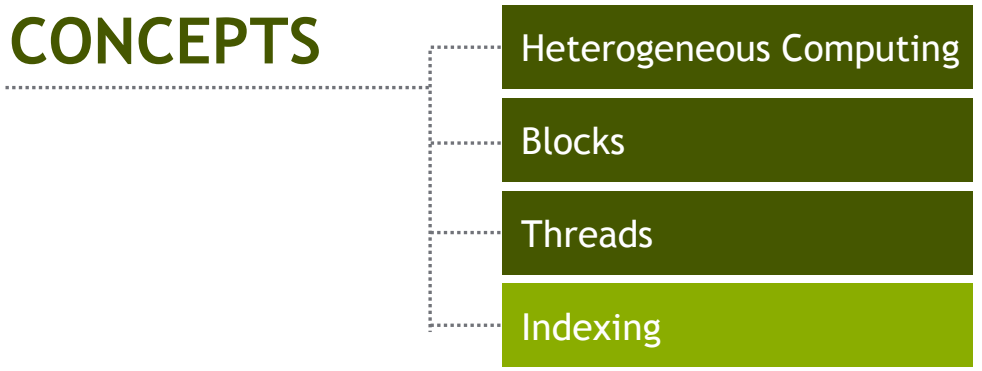
main()

```
#define N 512
int main(void) {
    int *a, *b, *c;                 // host copies of a, b, c
    int *d_a, *d_b, *d_c;           // device copies of a, b, c
    int size = N * sizeof(int);

    // Alloc space for device copies of a, b, c
    cudaMalloc((void **)&d_a, size);
    cudaMalloc((void **)&d_b, size);
    cudaMalloc((void **)&d_c, size);

    // Alloc space for host copies of a, b, c and setup input values
    a = (int *)malloc(size);
    b = (int *)malloc(size);
    c = (int *)malloc(size);

    for (int i=0; i<N; i++) a[i]=2, b[i]=7;
```

Vector Addition Using Threads:

main()

```
    // Copy inputs to device
    cudaMemcpy(d_a, a, size, cudaMemcpyHostToDevice);
    cudaMemcpy(d_b, b, size, cudaMemcpyHostToDevice);

    // Launch add() kernel on GPU with N threads
    add<<<1,N>>>(d_a, d_b, d_c);

    // Copy result back to host
    cudaMemcpy(c, d_c, size, cudaMemcpyDeviceToHost);

    // Cleanup
    free(a); free(b); free(c);
    cudaFree(d_a); cudaFree(d_b); cudaFree(d_c);
    return 0;
}
```



COMBINING THREADS AND BLOCKS

Combining Blocks and Threads

- **We've seen parallel vector addition using:**
  - Many blocks with one thread each
  - One block with many threads

- **Let's adapt vector addition to use both blocks and threads**

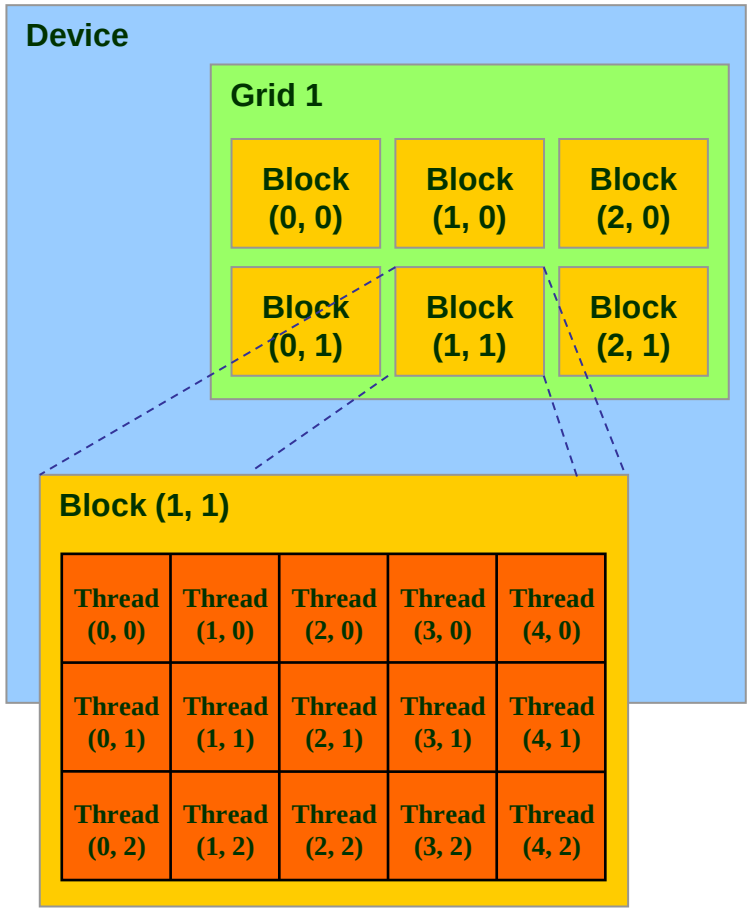
- **Why? We'll come to that…**

- **First let's discuss data indexing…**

IDs and Dimensions

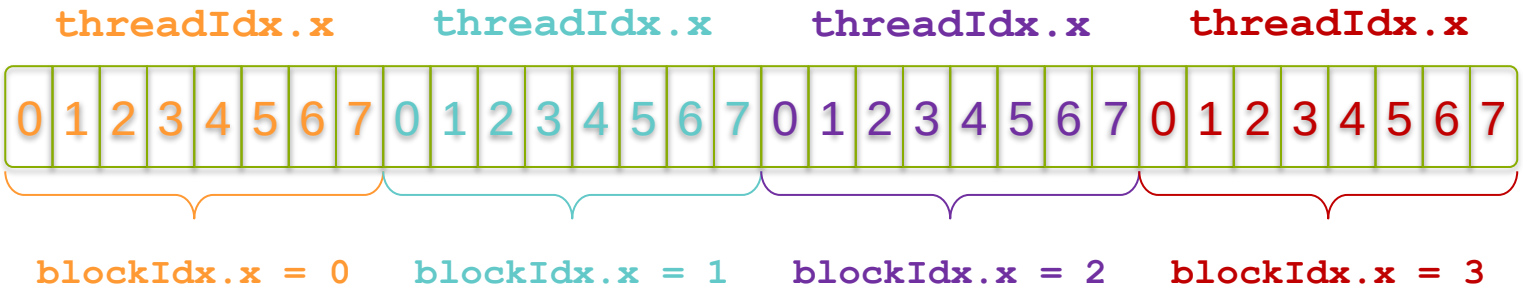
- **Threads:**
  - 3D IDs, unique within a block
- **Blocks:**
  - 2D IDs, unique within a grid
- **Dimensions set at launch**
  - Can be unique for each grid
- **Built-in variables:**
  - threadIdx, blockIdx
  - blockDim, gridDim

- **We will only discuss the usage of one dimension (x)**



Indexing Arrays with Blocks and Threads

- **No longer as simple as using blockIdx.x and threadIdx.x**
  - Consider indexing an array with one element per thread (8 threads/block)

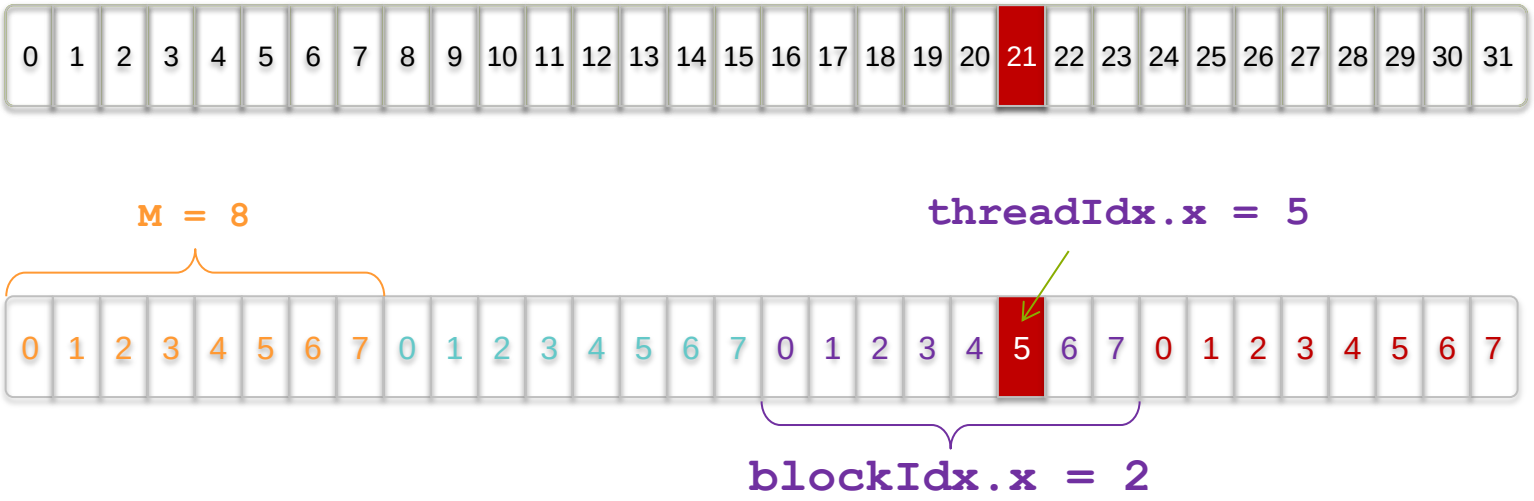


- **With M (M=8 here) threads per block a unique index for each thread is given by:**

```
int index = threadIdx.x + blockIdx.x * M;
```

Indexing Arrays: Example

- **Which thread will operate on the red element?**




```
int index = threadIdx.x + blockIdx.x * M;
          =       5     +     2      * 8;
          = 21;
```

Vector Addition with Blocks and Threads

- Use the built-in variable `blockDim.x` for threads per block

```
int index = threadIdx.x + blockIdx.x * blockDim.x;
```

- Combined version of `add()` to use parallel threads *and* parallel blocks

```
__global__ void add(int *a, int *b, int *c) {
    int index = threadIdx.x + blockIdx.x * blockDim.x;
    c[index] = a[index] + b[index];
}
```

- What changes need to be made in main()?

Addition with Blocks and Threads:

main()

```
#define N (2048*2048)
#define THREADS_PER_BLOCK 512
int main(void) {
    int *a, *b, *c;              // host copies of a, b, c
    int *d_a, *d_b, *d_c;        // device copies of a, b, c
    int size = N * sizeof(int);

    // Alloc space for device copies of a, b, c
    cudaMalloc((void **)&d_a, size);
    cudaMalloc((void **)&d_b, size);
    cudaMalloc((void **)&d_c, size);

    // Alloc space for host copies of a, b, c and setup input values
    a = (int *)malloc(size);
    b = (int *)malloc(size);
    c = (int *)malloc(size);
```

Addition with Blocks and Threads:

main()

```
    // Copy inputs to device
    cudaMemcpy(d_a, a, size, cudaMemcpyHostToDevice);
    cudaMemcpy(d_b, b, size, cudaMemcpyHostToDevice);

    // Launch add() kernel on GPU
    add<<<N/THREADS_PER_BLOCK,THREADS_PER_BLOCK>>>(d_a, d_b, d_c);

    // Copy result back to host
    cudaMemcpy(c, d_c, size, cudaMemcpyDeviceToHost);

    // Cleanup
    free(a); free(b); free(c);
    cudaFree(d_a); cudaFree(d_b); cudaFree(d_c);
    return 0;
}
```

Handling Arbitrary Vector Sizes

- **Typical problems are not friendly multiples of blockDim.x**

- **Avoid accessing beyond the end of the arrays:**

```
__global__ void add(int *a, int *b, int *c, int n) {
    int index = threadIdx.x + blockIdx.x * blockDim.x;
    if (index < n)
        c[index] = a[index] + b[index];
}
```

- **Update the kernel launch:**

```
add<<<(N + M-1) / M,M >>>(d_a, d_b, d_c, N);
```

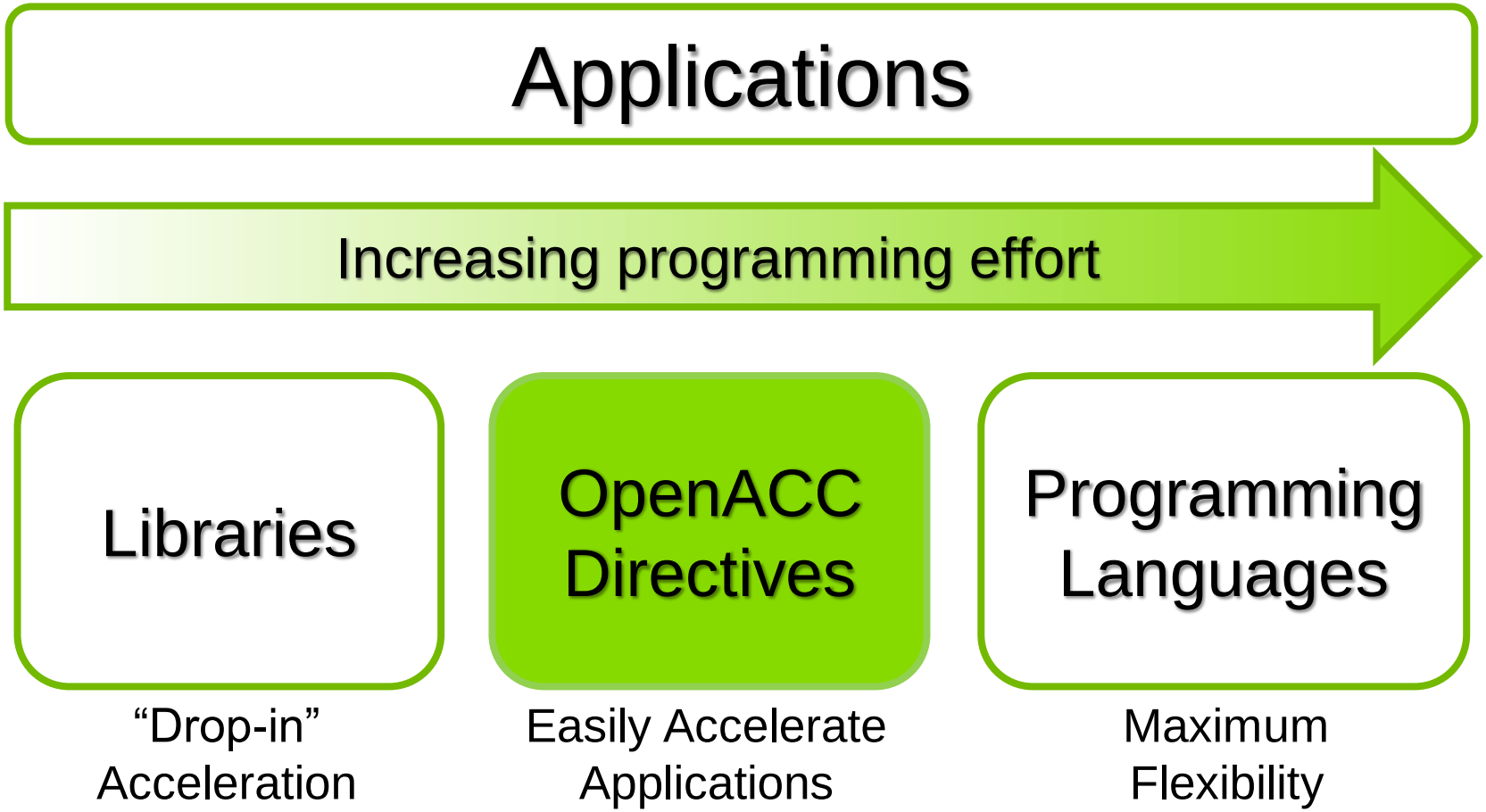
Review

- **Launching parallel kernels**
  - Launch `N` copies of `add()` with `add<<<N/M,M>>>(…);`
  - Use `blockIdx.x` to access block index
  - Use `threadIdx.x` to access thread index within block

- **Allocate elements to threads:**

```
int index = threadIdx.x + blockIdx.x * blockDim.x;
```

3 Ways to Accelerate Applications



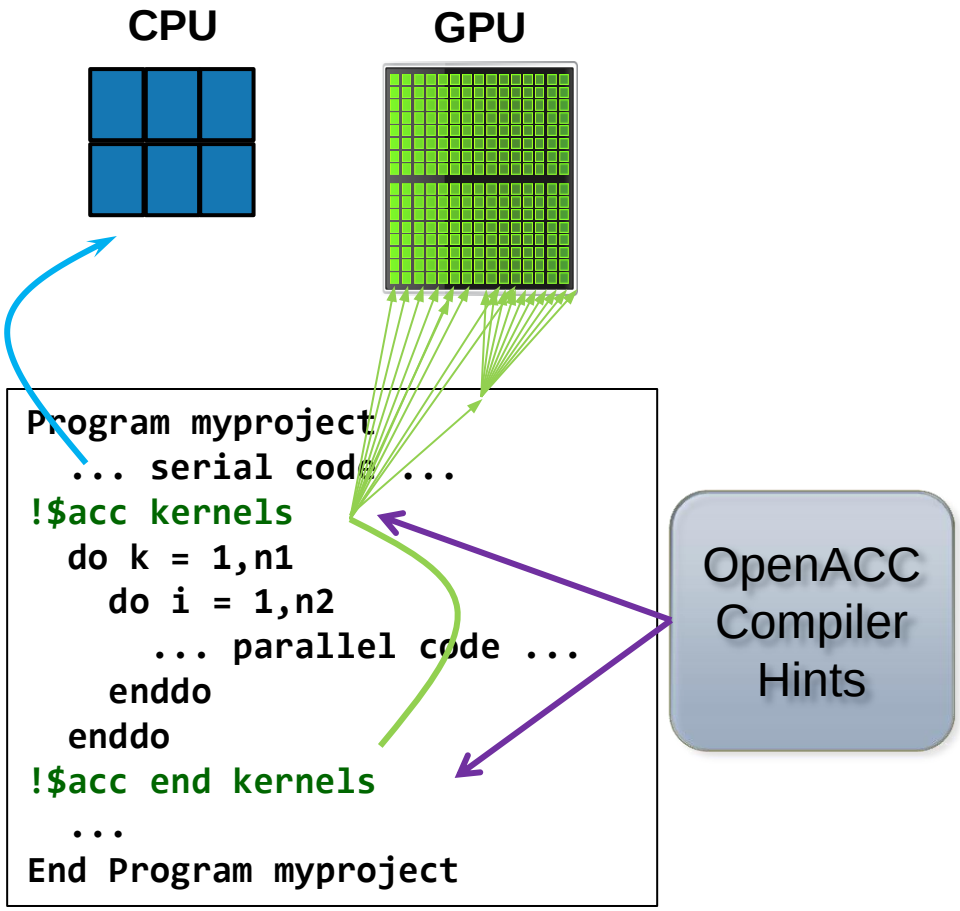
To be covered

- **OpenACC overview**
- **First OpenACC program and basic OpenACC directives**
- **Data region concept**
- **How to parallize our examples:**
  - Laplacian solver
- **Hands-on exercise**
  - Matrix Multiplication
  - SAXPY
  - Calculate π

What is OpenACC

- **OpenACC (for Open Accelerators) is a programming standard for parallel computing developed by Cray, CAPS, Nvidia and PGI. The standard is designed to simplify parallel programming of heterogeneous CPU/GPU systems.**
- **It provides a model for accelerator programming that is portable across operating systems and various types of host CPUs and *accelerators*.**
- **Full OpenACC 2.0 Specification available online**
  - http://www.openacc-standard.org/
  - Implementations available now from **PGI, Cray, and CAPS**

OpenACC Directives



Simple Compiler hints

Compiler Parallelizes code

Works on many-core GPUs & multicore CPUs

The Standard for GPU Directives

- **Simple and high-level :**
  - Directive are the easy path to accelerate compute intensive applications. Non-GPU programmers can play along.
  - Single Source: Compile the same program for accelerators or serial, No involvement of OpenCL, CUDA, etc.
- **Open and performance portable:**
  - OpenACC is an open GPU directives standard, making GPU programming straightforward and portable across parallel and multi-core processors
  - Supports GPU accelerators and co-processors from multiple vendors, current and future versions.
- **Powerful and Efficient:**
  - Directives allow complete access to the massive parallel power of GPU.
  - Experience shows very favorable comparison to low-level implementations of same algorithms.
  - Developers can port and tune parts of their application as resources and profiling dictates. No need to restructure the program.

Directive-based programming

- **Directives provide a high-level alternative**
  - Based on original source code (Fortran, C, C++)
  - Easier to maintain/port/extend code
  - Users with OpenMP experience find it a familiar programming model
  - Compiler handles repetitive coding (cudaMalloc, cudaMemcpy...)
  - Compiler handles default scheduling; user tunes only where needed
- **Possible performance sacrifice**
  - Small performance sacrifice is acceptable
  - trading-off portability and productivity against this
  - after all, who hand-codes in assembly for CPUs these days?
- **As researchers in science and engineering, you often need to balance between:**
  - ***Time needed to develop your code***
  - ***Time needed to focus on the problem itself***

General Directive Syntax and Scope

- **Fortran**

```
!$acc directive [clause [,] clause]...]
```

Often paired with a matching `end` directive surrounding a structured code block

```
!$acc end directive
```

- **C**

```
#pragma acc directive [clause [,] clause]...]
{
```

Often followed by a structured code block (compound statement)

```
}
```

The "restrict" keyword in C

- **Declaration of intent given by the programmer to the compiler**
  - Applied to a pointer, e.g. `float *restrict ptr;`
  - Meaning: "for the lifetime of `ptr`, only it or a value directly derived from it (such as ptr + 1) will be used to access the object to which it points"*
  - In simple, the `ptr` will only point to the memory space of itself
- **OpenACC compilers often require restrict to determine independence.**
  - Otherwise the compiler can't parallelize loops that access `ptr`
  - Note: if programmer violates the declaration, behavior is undefined.

THE RESTRICT CONTRACT

I, [insert your name], a PROFESSIONAL or AMATEUR [circle one] programmer, solemnly declare that writes through this pointer will not effect the values read through any other pointer available in the same context which is also declared as restricted.

* Your agreement to this contract is implied by use of the restrict keyword ;)

*http://en.wikipedia.org/wiki/Restrict

The First Simple Exercise: SAXPY

*restrict:
"y does not alias x"

```
void saxpy(int n,
           float a,
           float *x,
           float *restrict 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);
...
```

```
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)
...
```

Complete saxpy.c

- **Only a single line to the above example is needed to produce an OpenACC SAXPY in C.**

```
int main(int argc, char **argv)
{
    int n = 1<<20; // 1 million floats

    float *x = (float*)malloc(n*sizeof(float));
    float *y = (float*)malloc(n*sizeof(float));
    for (int i = 0; i < n; ++i) {
        x[i] = 2.0f;
        y[i] = 1.0f;
    }
    saxpy(n, 3.0f, x, y);
    free(x);
    free(y);
    return 0;
}
```

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

SAXPY code (only functions) in CUDA C

```
// define CUDA kernel function
__global__ void saxpy_kernel( float a, float* x, float* y, int n ){
    int i;
    i = blockIdx.x*blockDim.x + threadIdx.x;
    if( i <= n ) y[i] = a*x[i] + y[i];
}

void saxpy( float a, float* x, float* y, int n ){
    float *xd, *yd;
    // manage device memory
    cudaMalloc( (void**)&xd, n*sizeof(float) );
    cudaMalloc( (void**)&yd, n*sizeof(float) );
    cudaMemcpy( xd, x, n*sizeof(float), cudaMemcpyHostToDevice );
    cudaMemcpy( yd, y, n*sizeof(float), cudaMemcpyHostToDevice );
    // calls the kernel function
    saxpy_kernel<<< (n+31)/32, 32 >>>( a, xd, yd, n );
    cudaMemcpy( x, xd, n*sizeof(float), cudaMemcpyDeviceToHost );
    // free device memory after use
    cudaFree( xd );
    cudaFree( yd );
}
```

CUDA C/OpenACC – Big Difference

- **With CUDA, we changed the structure of the old code. Non-CUDA programmers can't understand new code. It is not even ANSI standard code.**
  - We have separate sections for the host code, and the GPU device code. Different flow of code. Serial path now gone forever.
  - Although CUDA C gives you maximum flexibility, the effort needed for restructuring the code seems to be high.
  - OpenACC seems ideal for researchers in science and engineering.

Compiler output of the first example

Emit information about accelerator region targeting.

- **C**

```
pgcc -acc -Minfo=accel -ta=nvidia,time saxpy_1stexample.c
```

- **Fortran**

```
pgf90 -acc -Minfo=accel -ta=nvidia,time saxpy_1stexample.c
```

- **Use "man pgcc/pgf90" to check the meaning of the compiler switches.**
- **Compiler output :**

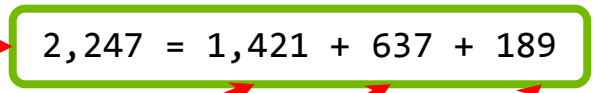
```
pgcc -acc -Minfo=accel -ta=nvidia,time saxpy_1stexample.c
saxpy:
     26, Generating present_or_copyin(x[:n])
         Generating present_or_copy(y[:n])
         Generating NVIDIA code
     27, Loop is parallelizable
         Accelerator kernel generated
         27, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
```

Add PGI compiler to your environment

```
[fchen14@mike424 gpuex]$ cat ~/.soft
# This is the .soft file.
# It is used to customize your environment by setting up environment
# variables such as PATH and MANPATH.
# To learn what can be in this file, use 'man softenv'.
+portland-14.3
@default
[fchen14@mike424 gpuex]$ resoft
[fchen14@mike424 gpuex]$ pgcc -V
pgcc 14.3-0 64-bit target on x86-64 Linux -tp sandybridge
The Portland Group - PGI Compilers and Tools
Copyright (c) 2014, NVIDIA CORPORATION.  All rights reserved.
[fchen14@mike424 gpuex]$ cp –r /home/fchen14/gpuex/ ./
[fchen14@mike424 gpuex]$ cd ~/gpuex
[fchen14@mike424 gpuex]$ cat saxpy.c
[fchen14@mike424 gpuex]$ pgcc -acc -Minfo=accel -ta=nvidia,time saxpy.c
```

Runtime output

```
[fchen14@mike424 gpuex]$ ./a.out

Accelerator Kernel Timing data
/home/fchen14/loniworkshop2014/laplace/openacc/c/saxpy_1stexample.c
  saxpy  NVIDIA  devicenum=0
    time(us): 2,247
    26: data region reached 1 time
        26: data copyin reached 2 times
             device time(us): total=1,421 max=720 min=701 avg=710
        29: data copyout reached 1 time
             device time(us): total=637 max=637 min=637 avg=637
    26: compute region reached 1 time
        26: kernel launched 1 time
            grid: [4096]  block: [256]
             device time(us): total=189 max=189 min=189 avg=189
            elapsed time(us): total=201 max=201 min=201 avg=201
```



OpenACC `kernels` directive

- **What is a kernel? A function that runs in parallel on the GPU.**
  - The kernels directive expresses that a region may contain parallelism and the compiler determines what can be safely parallelized.
  - The compiler breaks code in the kernel region into a sequence of kernels for execution on the accelerator device.
  - When a program encounters a `kernels` construct, it will launch a sequence of kernels in order on the device.
- **The compiler identifies 2 parallel loops and generates 2 kernels below.**

```
#pragma acc kernels
{
    for (i = 0; i < n; i++){
        x[i] = 1.0;
        y[i] = 2.0;
    }
    for (i = 0; i < n; i++){
        y[i] = a*x[i] + y[i];
    }
}
```

```
!$acc kernels
do i = 1, n
    x(i) = 1.0
    y(i) = 2.0
end do
do i = 1, n
    y(i) = y(i) + a * x(i)
end do
!$acc end kernels
```

OpenACC `parallel` directive

- **Similar to OpenMP, the parallel directive identifies a block of code as having parallelism.**
- **Compiler generates one parallel kernel for that loop.**
- **C**

```
#pragma acc parallel [clauses]
```

- **Fortran**

```
!$acc parallel [clauses]
```

```c
#pragma acc parallel
{
    for (i = 0; i < n; i++){
        x[i] = 1.0 ;
        y[i] = 2.0 ;
    }
    for (i = 0; i < n; i++){
        y[i] = a*x[i] + y[i];
    }
}
```

```fortran
!$acc parallel
do i = 1, n
    x(i) = 1.0
    y(i) = 2.0
end do
do i = 1, n
    y(i) = y(i) + a * x(i)
end do
!$acc end parallel
```

OpenACC loop directive

- **Loops are the most likely targets for parallelizing.**
  - The Loop directive is used within a parallel or kernels directive identifying a loop that can be executed on the accelerator device.
  - The loop directive can be combined with the enclosing parallel or kernels
  - The loop directive clauses can be used to optimize the code. This however requires knowledge of the accelerator device.
  - Clauses: gang, worker, vector, num_gangs, num_workers
- **C:** `#pragma acc [parallel/kernels] loop [clauses]`
- **Fortran:** `!$acc [parallel/kernels] loop [clauses]`

```c
#pragma acc loop
for (i = 0; i < n; i++){
    y[i] = a*x[i] + y[i];
}
```

```
!$acc loop
do i = 1, n
    y(i) = y(i) + a * x(i)
end do
!$acc end loop
```

OpenACC `kernels` vs `parallel`

- **`kernels`**
  - Compiler performs parallel analysis and parallelizes what it believes is safe.
  - Can cover larger area of code with single directive.
- **`parallel`**
  - Requires analysis by programmer to ensure safe parallelism.
  - Straightforward path from OpenMP
- **Both approaches are equally valid and can perform equally well.**

Clauses

- **data management clauses**
  - `copy(...),copyin(...), copyout(...)`
  - `create(...), present(...)`
  - `present_or_copy{,in,out}(...) or pcopy{,in,out}(...)`
  - `present_or_create(...) or pcreate(...)`
- **`reduction(operator:list)`**
- **`if (condition)`**
- **`async (expression)`**

Runtime Libraries

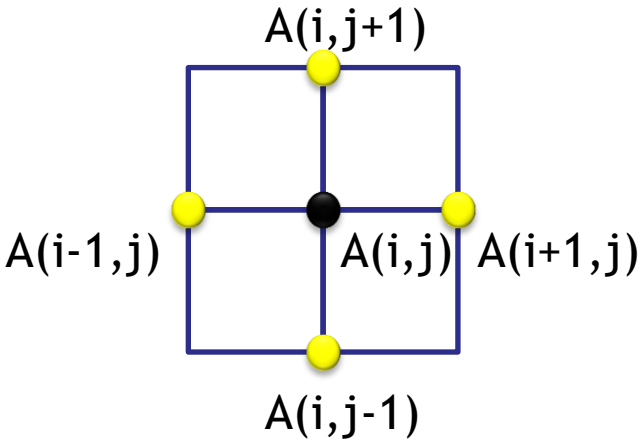
- **System setup routines**
  - `acc_init(acc_device_nvidia)`
  - `acc_set_device_type(acc_device_nvidia)`
  - `acc_set_device_num(acc_device_nvidia)`
- **Synchronization routines**
  - `acc_async_wait(int)`
  - `acc_async_wait_all()`
- **For more information, refer to the OpenACC standard**

Second example: Jacobi Iteration

- **Solve Laplace equation in 2D:**
  - Iteratively converges to correct value (e.g. Temperature), by computing new values at each point from the average of neighboring points.

$$\nabla^2 f(x,y) = 0$$

$$A_{k+1}(i,j) = \frac{A_k(i-1,j) + A_k(i+1,j) + A_k(i,j-1) + A_k(i,j+1)}{4}$$



Graphical representation for Jacobi iteration

Current Array: A

1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
1.0	2.0	4.0	6.0	8.0	10.0	12.0	1.0
1.0	3.0	5.0	7.0	9.0	11.0	13.0	1.0
1.0	2.0	6.0	1.0	3.0	7.0	5.0	1.0
1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

Next Array: Anew

1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
1.0	2.25	3.56	6.0				1.0
1.0		5.0					1.0
1.0							1.0
1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

Serial version of the Jacobi Iteration

```
while ( error > tol && iter < iter_max )
{
  error=0.0;

  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      error = fmax(error, abs(Anew[j][i] - A[j][i]);
    }
  }

  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
  iter++;
}
```

Iterate until converged

Iterate across matrix elements

Calculate new value from neighbors

Compute max error for convergence

Swap input/output arrays

First Attempt in OpenACC

```
// first attempt in C
while ( error > tol && iter < iter_max ) {
  error=0.0;
#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {
      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);
      error = max(error, abs(Anew[j][i] - A[j][i]);
    }
  }

#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
  iter++;
}
```

Execute GPU kernel for loop nest

Execute GPU kernel for loop nest

Compiler Output

```
pgcc -acc -Minfo=accel -ta=nvidia,time laplace_openacc.c -o laplace_acc.out
main:
     65, Generating present_or_copyin(Anew[1:4094][1:4094])
         Generating present_or_copyin(A[:4096][:4096])
         Generating NVIDIA code
     66, Loop is parallelizable
     67, Loop is parallelizable
         Accelerator kernel generated
         66, #pragma acc loop gang /* blockIdx.y */
         67, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
         70, Max reduction generated for error
     75, Generating present_or_copyin(Anew[1:4094][1:4094])
         Generating present_or_copyin(A[1:4094][1:4094])
         Generating NVIDIA code
     76, Loop is parallelizable
     77, Loop is parallelizable
         Accelerator kernel generated
         76, #pragma acc loop gang /* blockIdx.y */
         77, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
```

present_or_copyin

present_or_copyin

Performance of First Jacobi ACC Attempt

- **CPU: Intel(R) Xeon(R) CPU E5-2670 @ 2.60GHz**
- **GPU: Nvidia Tesla K20Xm**
- **The OpenACC code is even slower than the single thread/serial version of the code**
- **What is the reason for the significant slow-down?**

Execution	Time (sec)	Speedup
OpenMP 1 threads	45.64	--
OpenMP 2 threads	30.05	1.52
OpenMP 4 threads	24.91	1.83
OpenMP 8 threads	25.24	1.81
OpenMP 16 threads	26.19	1.74
OpenACC w/GPU	***190.32***	***0.24***

Output Timing Information from Profiler

- **Use compiler flag: `-ta=nvidia, time`**
  - Link with a profile library to collect simple timing information for accelerator regions.
- **OR set environmental variable: `export PGI_ACC_TIME=1`**
  - Enables the same lightweight profiler to measure data movement and accelerator kernel execution time and print a summary at the end of program execution.
- **Either way can output profiling information**

Accelerator Kernel Timing data (1st attempt)

```
time(us): 88,460,895
    60: data region reached 1000 times
        60: data copyin reached 8000 times
             device time(us): total=22,281,725 max=2,909 min=2,752 avg=2,785
        71: data copyout reached 8000 times
             device time(us): total=20,120,805 max=2,689 min=2,496 avg=2,515
    60: compute region reached 1000 times
        63: kernel launched 1000 times
            grid: [16x512]  block: [32x8]
             device time(us): total=2,325,634 max=2,414 min=2,320 avg=2,325
            elapsed time(us): total=2,334,977 max=2,428 min=2,329 avg=2,334
        63: reduction kernel launched 1000 times
            grid: [1]  block: [256]
             device time(us): total=25,988 max=90 min=24 avg=25
            elapsed time(us): total=35,063 max=99 min=33 avg=35
    71: data region reached 1000 times
        71: data copyin reached 8000 times
             device time(us): total=21,905,025 max=2,849 min=2,725 avg=2,738
        79: data copyout reached 8000 times
             device time(us): total=20,121,342 max=2,805 min=2,496 avg=2,515
    71: compute region reached 1000 times
        74: kernel launched 1000 times
            grid: [16x512]  block: [32x8]
             device time(us): total=1,680,376 max=1,758 min=1,670 avg=1,680
            elapsed time(us): total=1,689,640 max=1,768 min=1,679 avg=1,689
```

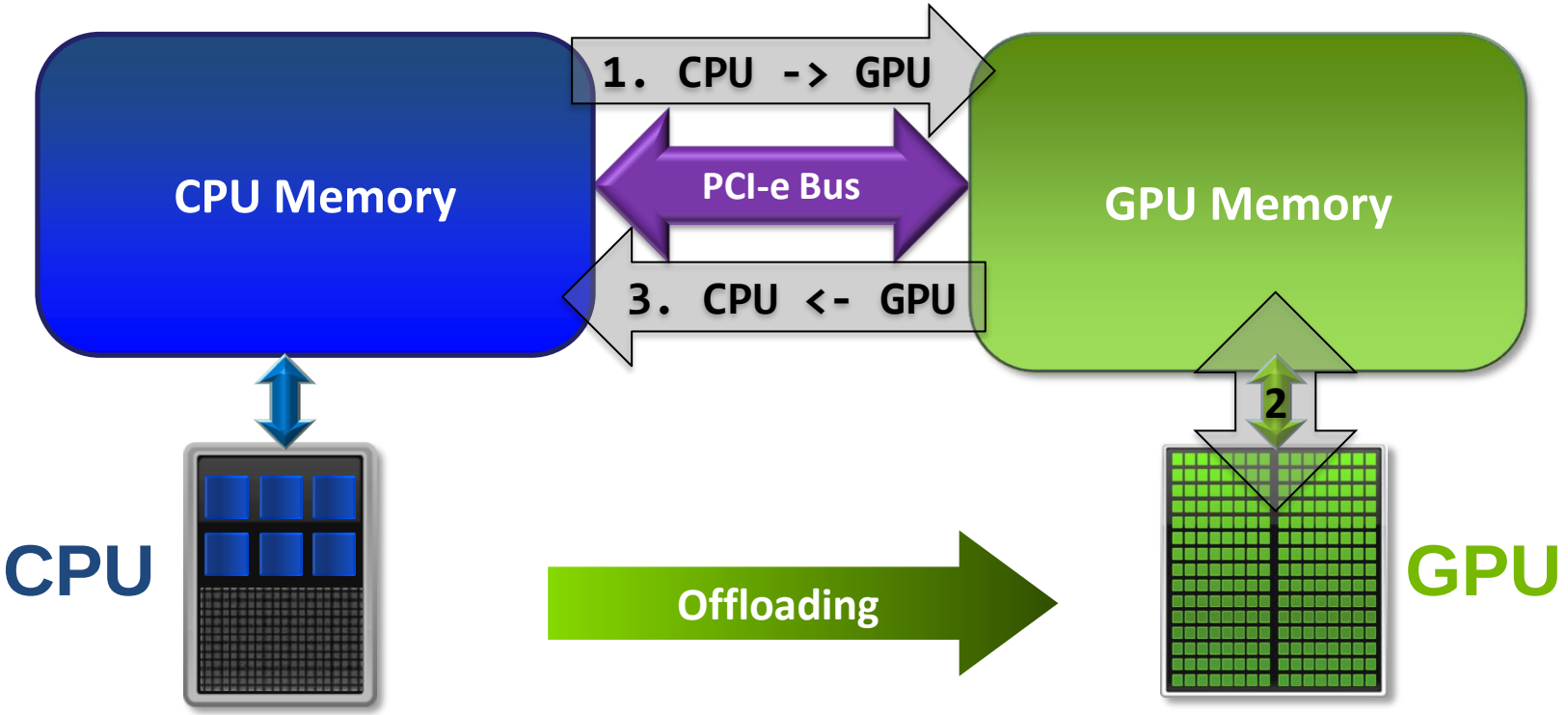
Total 42.4 sec spent on data transfer

Total 42.0 sec spent on data transfer

Around 84 sec on data transfer, huge bottleneck

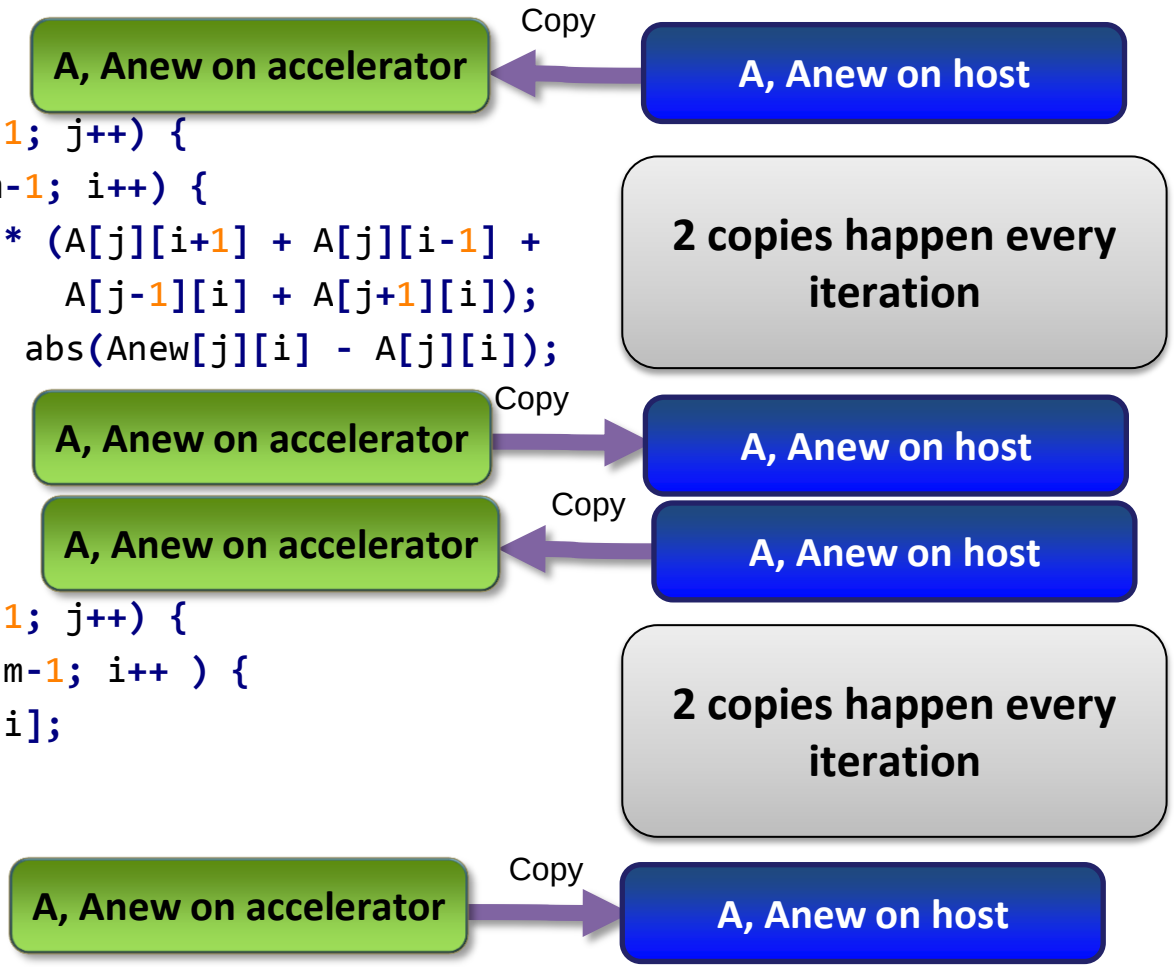
Recall Basic Concepts on Offloading

- **CPU and GPU have their respective memory, connected through PCI-e bus**
- **Processing Flow of the offloading**
  1. Copy input data from CPU memory to GPU memory
  2. Load GPU program and execute
  3. Copy results from GPU memory to CPU memory



Excessive Data Transfers

```
// first attempt in C
while ( error > tol && iter < iter_max ) {
  error=0.0;
#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {
      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);
      error = max(error, abs(Anew[j][i] - A[j][i]);
    }
  }

#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
  iter++;
}
```



Rules of Coprocessor (GPU) Programming

- **Transfer the data across the PCI-e bus onto the device and keep it there.**
- **Give the device enough work to do (avoid preparing data).**
- **Focus on data reuse within the coprocessor(s) to avoid memory bandwidth bottlenecks.**

OpenACC Data Management with Data Region

- **C syntax**

```
#pragma acc data [clause]
{ structured block/statement }
```

- **Fortran syntax**

```
!$acc data [clause]
structured block
!$acc end data
```

- **Data regions may be nested.**

Data Clauses

- **copy (list)**

```
/* Allocates memory on GPU and copies data from host to GPU
when entering region and copies data to the host when exiting region.*/
```

- **copyin (list)**

```
/* Allocates memory on GPU and copies data from host to GPU when
entering region. */
```

- **copyout (list)**

```
/* Allocates memory on GPU and copies data to the host when exiting
region. */
```

- **create (list)**

```
/* Allocates memory on GPU but does not copy. */
```

- **present (list)**

```
/* Data is already present on GPU from another containing data region.
*/
```

- **and present_or_copy[in|out], present_or_create, deviceptr.**

Second Attempt: OpenACC C

```
#pragma acc data copy(A), create(Anew)
while ( error > tol && iter < iter_max ) {
  error=0.0;

  #pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {
      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      error = max(error, abs(Anew[j][i] - A[j][i]);
    }
  }
#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
  iter++;
}
```

Copy A in at beginning of loop, out at end. Allocate Anew on accelerator

Second Attempt: OpenACC Fortran

```
!$acc data copy(A), create(Anew)
do while ( err > tol .and. iter < iter_max )
  err=0._fp_kind
!$acc kernels
  do j=1,m
    do i=1,n
      Anew(i,j) = .25_fp_kind * (A(i+1, j  ) + A(i-1, j  ) + &
                                 A(i  , j-1) + A(i  , j+1))
      err = max(err, Anew(i,j) - A(i,j))
    end do
  end do
!$acc end kernels
...
iter = iter +1
end do
!$acc end data
```

Copy A in at beginning of loop, out at end. Allocate Anew on accelerator

Second Attempt: Performance

- **Significant speedup after the insertion of the data region directive**
- **CPU: Intel Xeon CPU E5-2670 @ 2.60GHz**
- **GPU: Nvidia Tesla K20Xm**

Execution	Time (sec)	Speedup
OpenMP 1 threads	45.64	--
OpenMP 2 threads	30.05	1.52
OpenMP 4 threads	24.91	1.83
OpenACC w/GPU (data region)	***4.47***	***10.21*** **(serial)** ***5.57*** **(4 threads)**

Accelerator Kernel Timing data (2nd attempt)

```
time(us): 4,056,477
   54: data region reached 1 time
       54: data copyin reached 8 times
            device time(us): total=22,249 max=2,787 min=2,773 avg=2,781
       84: data copyout reached 9 times
            device time(us): total=20,082 max=2,510 min=11 avg=2,231
   60: compute region reached 1000 times
       63: kernel launched 1000 times
           grid: [16x512]  block: [32x8]
            device time(us): total=2,314,738 max=2,407 min=2,311 avg=2,314
           elapsed time(us): total=2,323,334 max=2,421 min=2,319 avg=2,323
       63: reduction kernel launched 1000 times
           grid: [1]  block: [256]
            device time(us): total=24,904 max=78 min=24 avg=24
           elapsed time(us): total=34,206 max=87 min=32 avg=34
   71: compute region reached 1000 times
       74: kernel launched 1000 times
           grid: [16x512]  block: [32x8]
            device time(us): total=1,674,504 max=1,727 min=1,657 avg=1,674
           elapsed time(us): total=1,683,604 max=1,735 min=1,667 avg=1,683
```

Only 42.2 ms spent on data transfer

Array Shaping

- **Compiler sometimes cannot determine size of arrays**
  - Sometimes we just need to use a portion of the arrays
  - we will see this example in the exercise
- **Under such case, we must specify explicitly using data clauses and array "shape" for this case**
- **C**

```
#pragma acc data copyin(a[0:size]), copyout(b[s/4:3*s/4])
```

- **Fortran**

```
!$pragma acc data copyin(a(1:size)), copyout(b(s/4:3*s/4))
```

- **The number between brackets are the beginning element followed by the number of elements to copy:**
  - [start_element:number_of_elements_to_copy]
  - In C/C++, this means start at `a[0]` and continue for `"size"` elements.
- **Note: data clauses can be used on `data, kernels or parallel`**

Update Construct

- **Fortran**

```
#pragma acc update [clause ...]
```

- **C**

```
!$acc update [clause ...]
```

- **Used to update existing data after it has changed in its corresponding copy (e.g. update device copy after host copy changes)**
- **Move data from GPU to host, or host to GPU. Data movement can be conditional, and asynchronous.**

Further Speedups

- **OpenACC gives us more detailed control over parallelization via gang, worker, and vector clauses**
  - PE (processing element) as a SM (streaming multiprocessor)
  - gang == CUDA threadblock
  - worker == CUDA warp
  - vector == CUDA thread
- **By understanding more about OpenACC execution model and GPU hardware organization, we can get higher speedups on this code**
- **By understanding bottlenecks in the code via profiling, we can reorganize the code for higher performance**

Finding Parallelism in your code

- **(Nested) for loops are best for parallelization**
  - Large loop counts needed to offset GPU/memcpy overhead
- **Iterations of loops must be independent of each other**
  - To help compiler:
    - `restrict` keyword
    - `independent` clause
- **Compiler must be able to figure out sizes of data regions**
  - Can use directives to explicitly control sizes
- **Pointer arithmetic should be avoided if possible**
  - Use subscripted arrays, rather than pointer-indexed arrays.
- **Function calls within accelerated region must be inlineable.**

Exercise 1

- **For the matrix multiplication code**

  $A \cdot B = C$

  where:

  $a_{i,j} = i + j$

  $b_{i,j} = i \cdot j$

  $$c_{i,j} = \sum_{k} a_{i,k} \cdot b_{k,j}$$

  1. For mm_acc_v0.c, speedup the matrix multiplication code segment using OpenACC directives
  2. For mm_acc_v1.c:
     - Change A, B and C to dynamic arrays, i.e., the size of the matrix can be specified at runtime;
     - Complete the function matmul_acc using the OpenACC directives;
     - Compare performance with serial and OpenMP results

Exercise 2

- **Complete the saxpy example using OpenACC directives.**

  $\vec{y} = a \cdot \vec{x} + \vec{y}$

- **Calculate the result of a constant times a vector plus a vector:**
  - where ***a*** is a constant, $\vec{x}$ and $\vec{y}$ are one dimensional vectors.

1. Add OpenACC directives for initialization of x and y arrays;
2. Add OpenACC directives for the code for the vector addition;
3. Compare the performance with OpenMP results;

Exercise 3

- **Calculate π value using the equation:**

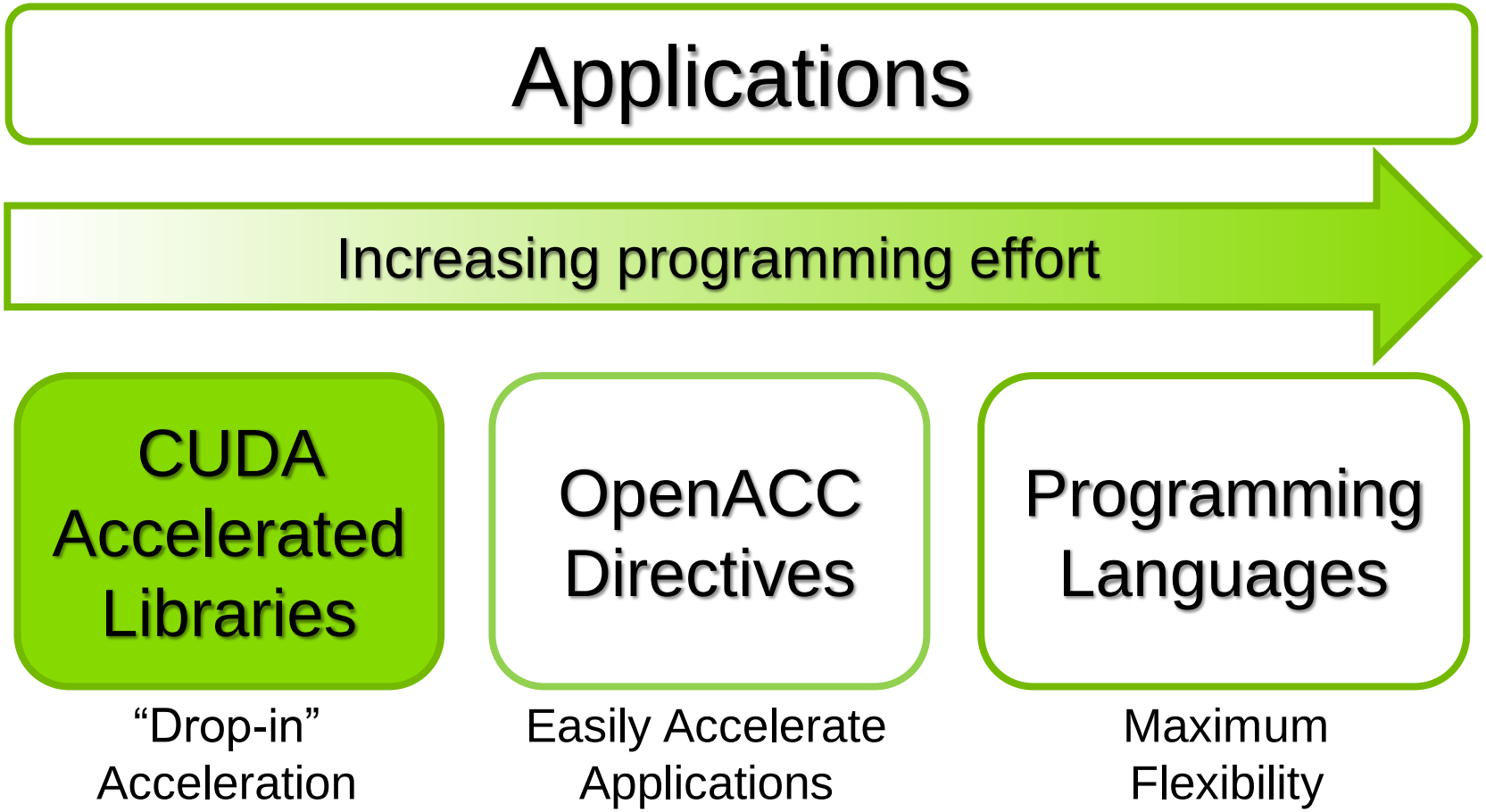
$$\int_0^1 \frac{4.0}{(1.0 + x^2)} = \pi$$

with the numerical integration:

$$\sum_{i=1}^{n} \frac{4.0}{(1.0 + x_i \cdot x_i)} \Delta x \approx \pi$$

1. Complete the code using OpenACC directives

3 Ways to Accelerate Applications



Drop-In Acceleration (Step 1)

```
int N = 1 << 20;
```

```
// Perform SAXPY on 1M elements: d_y[]=a*d_x[]+d_y[]

cublasSaxpy(h, N, &alpha, d_x, 1, d_y, 1);
```

Add “cublas” prefix and use device variables

Drop-In Acceleration (Step 2)

```
int N = 1 << 20;
cublasHandle_t h;
cublasCreate(&h);
```


```
// Perform SAXPY on 1M elements: d_y[]=a*d_x[]+d_y[]
cublasSaxpy(h, N, &alpha, d_x, 1, d_y, 1);
```

```
cublasDestroy(h);
cudaDeviceReset();
```

Drop-In Acceleration (Step 3)

```
int N = 1 << 20;
cublasHandle_t h;
cublasCreate(&h);
cudaMalloc((void**)&d_x, N*sizeof(float));
cudaMalloc((void**)&d_y, N*sizeof(float));
```

Allocate device vectors

```
// Perform SAXPY on 1M elements: d_y[]=a*d_x[]+d_y[]
cublasSaxpy(h, N, &alpha, d_x, 1, d_y, 1);
```

```
cudaFree(d_x);
cudaFree(d_y);
cublasDestroy(h);
cudaDeviceReset();
```

Deallocate device vectors

Drop-In Acceleration (Step 4)

```
int N = 1 << 20;
cublasHandle_t h;
cublasCreate(&h);
cudaMalloc((void**)&d_x, N*sizeof(float));
cudaMalloc((void**)&d_y, N*sizeof(float));
cudaMemcpy(d_x, &x[0], N*sizeof(float), cudaMemcpyHostToDevice);
cudaMemcpy(d_y, &y[0], N*sizeof(float), cudaMemcpyHostToDevice);

// Perform SAXPY on 1M elements: d_y[]=a*d_x[]+d_y[]
cublasSaxpy(h, N, &alpha, d_x, 1, d_y, 1);

cudaMemcpy(&y[0], d_y, N*sizeof(float), cudaMemcpyDeviceToHost);

cudaFree(d_x);
cudaFree(d_y);
cublasDestroy(h);
cudaDeviceReset();
```

Transfer data to GPU

Read data back GPU

Compile and Run

- **Need to link to the cublas library**

```
[fchen14@mike424 gpuex]$ nvcc cublas_vec_add.cu -l cublas
[fchen14@mike424 gpuex]$
```

- **Run example:**

```
[fchen14@mike424 gpuex]$ ./a.out
cublas time took 0.307 ms
x[0] = 7.200000
y[0] = 5.300000
z[0] = 12.500000
```