An Introduction to OpenACC - Part 1

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Outline of today's topic

- **GPU accelerated computing overview**
- **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

GPU Accelerated Computing

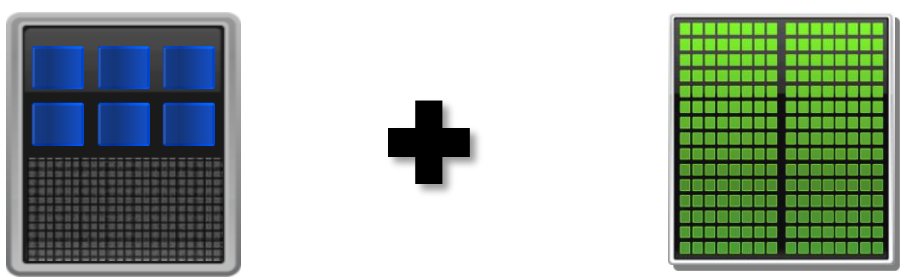
- **What is GPU**
  - A graphics processing unit (GPU) is a computer chip that performs rapid mathematical calculations, primarily for the purpose of rendering images.
  - A GPU cluster (Shelob and QB2) /queue is a computer cluster/queue in which each node is equipped with a Graphics Processing Unit (GPU).

GPU Accelerated Computing

- **What is GPU Accelerated Computing**
  – GPU-accelerated computing is the use of a graphics processing unit (GPU) together with a CPU to accelerate scientific, analytics, engineering, consumer, and enterprise applications.

CPU

GPU



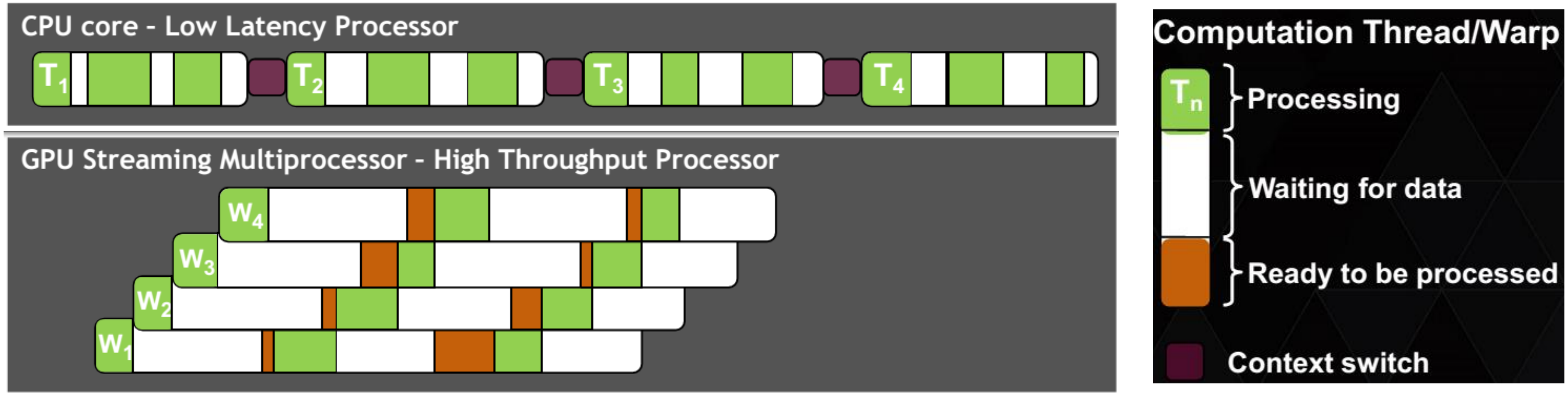
GPU Computing History

- 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.

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 architecture must minimize latency within each thread**
- **GPU architecture hides latency with computation from other threads**



Latency v.s. Throughput

- **F-22 Raptor**
  - 1500 mph
  - Baton Rouge to New York City in 1h 25h
  - Seats 1

- **Boeing 737**
  - 485 mph
  - Baton Rouge to New York City in 4:20h
  - Seats 200

Latency v.s. Throughput

- **F-22 Raptor**
  - Latency
    - **1:25**
  - Throughput
    - **1 / 1.42 hours = 0.7 people/hr.**

- **Boeing 737**
  - Latency
    - **4:20**
  - Throughput
    - **200 / 4.33 hours = 46.2 people/hr.**

Accelerator Fundamentals

- **We must expose enough parallelism to fill the device**
  - Accelerator threads are slower than CPU threads
  - Accelerators have orders of magnitude more threads
  - Accelerators tolerate resource latencies by cheaply context switching threads

3 Ways to Accelerate Applications

Applications

Increasing programming effort

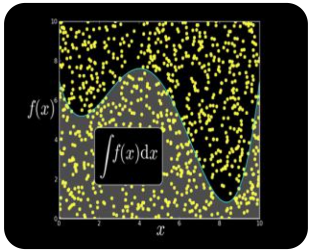
Libraries	OpenACC Directives	Programming Languages
"Drop-in" Acceleration	Easily Accelerate Applications	Maximum Flexibility

CUDA Libraries are interoperable with OpenACC

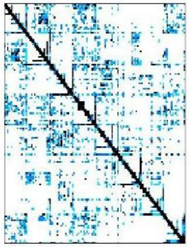
CUDA Languages are also interoperable with OpenACC

Some GPU-accelerated Libraries

NVIDIA cuBLAS



NVIDIA cuRAND



NVIDIA cuSPARSE

NVIDIA NPP

GPU VSIPL

Vector Signal Image Processing

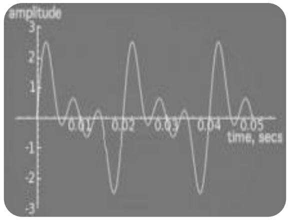
CULA tools

GPU Accelerated Linear Algebra

MAGMA

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

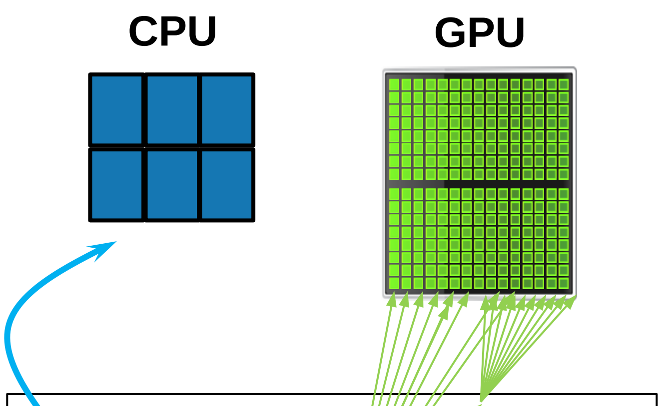
GPU Programming Languages

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

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*.**

OpenACC Directives




```
Program myproject
  ... serial code ...
!$acc kernels
  do k = 1,n1
    do i = 1,n2
      ... parallel code ...
    enddo
  enddo
!$acc end kernels
  ...
End Program myproject
```

Your original Fortran or C code

OpenACC compiler Hints

Simple Compiler hints

Compiler Parallelizes code

Works on many-core GPUs & multicore CPUs

History of OpenACC

- **OpenACC was developed by The Portland Group (PGI), Cray, CAPS and NVIDIA. PGI, Cray, and CAPs have spent over 2 years developing and shipping commercial compilers that use directives to enable GPU acceleration as core technology.**
- **The small differences between their approaches allowed the formation of a group to standardize a single directives approach for accelerators and CPUs.**
- **Full OpenACC 2.0 Specification available online**
  - http://www.openacc-standard.org/
  - Implementations available now from **PGI, Cray, and CAPS**

The Standard for GPU Directives

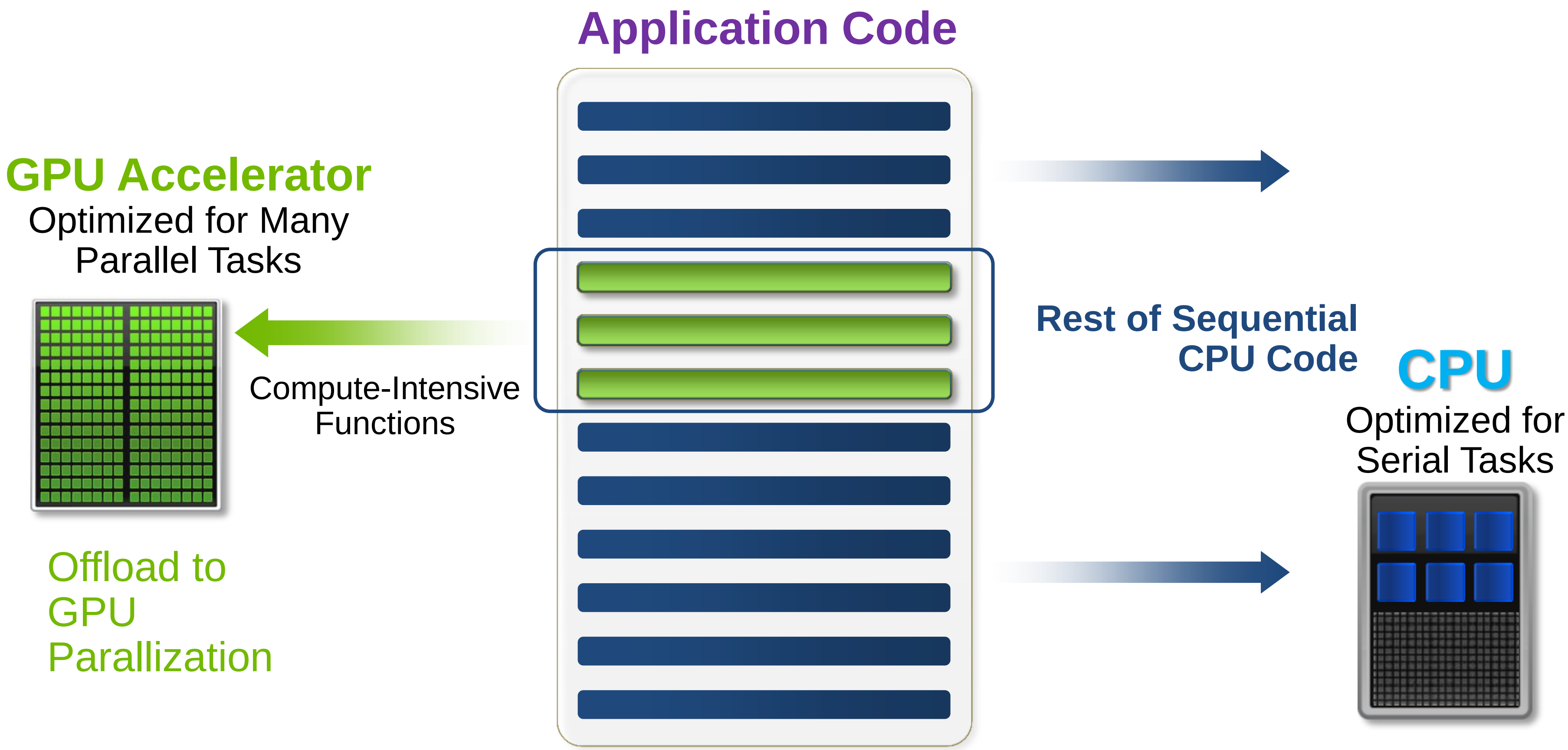
- **Simple and high-level :**
  - Directive are the easy path to accelerate compute intensive applications. Non-GPU programmers can play along.
  - Single Source: Compile the same program for accelerators or serial, No involvement of OpenCL, CUDA, etc.
- **Open and performance portable:**
  - OpenACC 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***

OpenACC Execution Model

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



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”

```c
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);
...
```

```fortran
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.

```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;
}
```

```c
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.

Add PGI compiler to your environment

Get an interactive session before running your jobs:

qsub -I -l nodes=1:ppn=16,walltime=4:00:00 -A hpc_train_2015

```
[hpctrn01@shelob001 ~]$ 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
[hpctrn01@shelob001 ~]$ resoft
[hpctrn01@shelob001 ~]$ pgcc -V
[hpctrn01@shelob001 ~]$ cp -r /home/fchen14/loniworkshop2015/ ./
[hpctrn01@shelob001 ~]$ cd ~/loniworkshop2015/saxpy/openacc/exercise
[hpctrn01@shelob001 ~]$ vi saxpy_1stexample.c
[hpctrn01@shelob001 ~]$ pgcc -acc -Minfo=accel -ta=nvidia,time saxpy_1stexample.c
```

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 */
```

Runtime output

```
[hpctrn01@shelob001 c]$ ./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
```

2,247 = 1,421 + 637 + 189

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.**

```c
#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];
    }
}
```

```fortran
!$acc kernels
do i = 1, n
    x(i) = 1.0
    y(i) = 2.0
end do
do i = 1, n
    y(i) = y(i) + a * x(i)
end do
!$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 [kernels/parallel] loop [clauses]`
- **Fortran:** `!$acc [kernels/parallel] loop [clauses]`

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

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

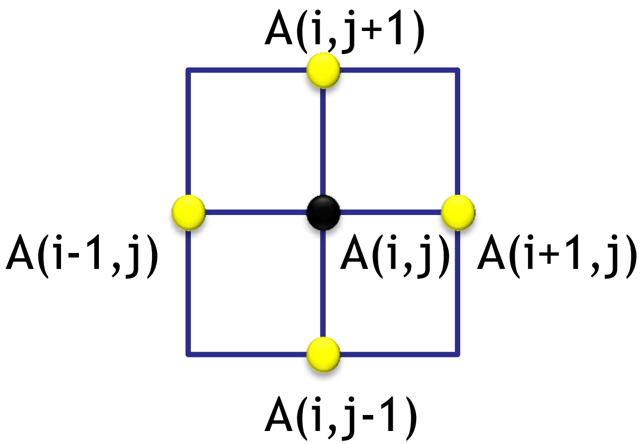
- **System setup routines**
  - `acc_init(acc_device_nvidia)`
  - `acc_set_device_type(acc_device_nvidia)`
  - `acc_set_device_num(acc_device_nvidia)`
- **Synchronization routines**
  - `acc_async_wait(int)`
  - `acc_async_wait_all()`
- **For more information, refer to the OpenACC standard**

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

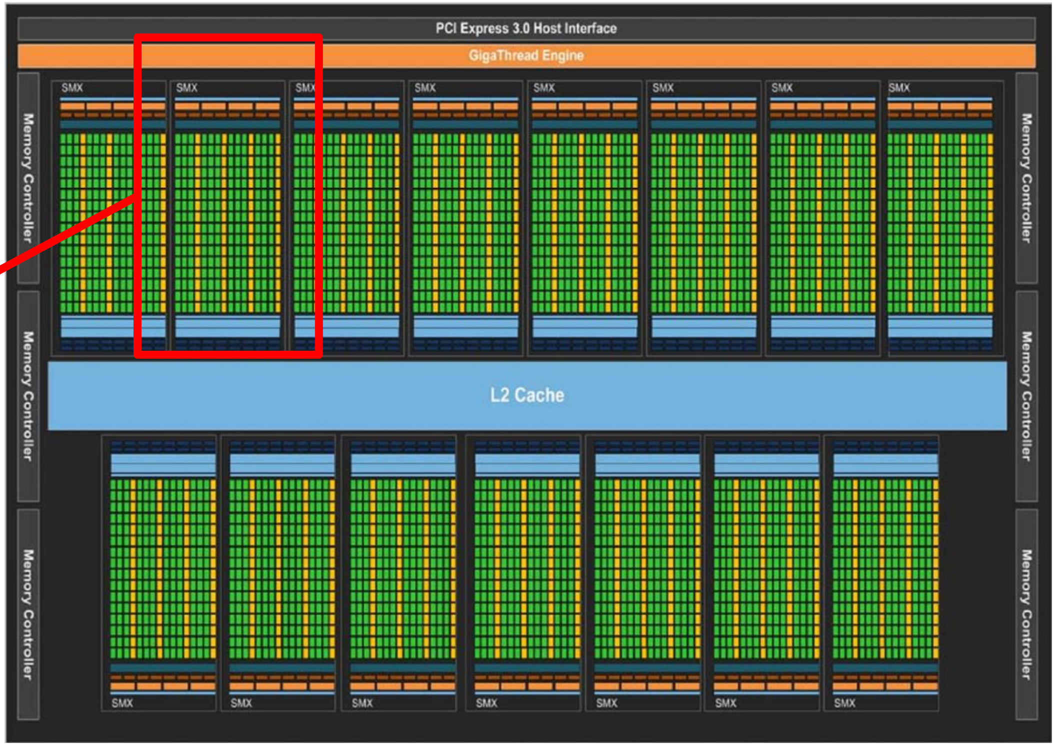
Total 42.0 sec spent on data transfer

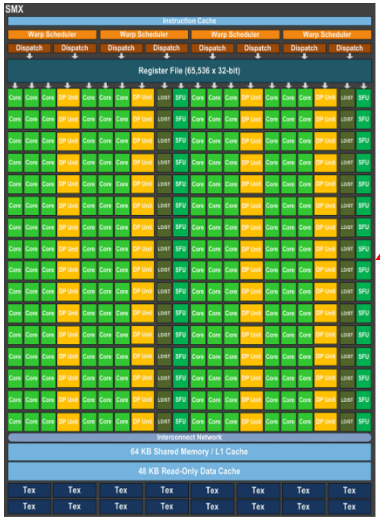
Around 84 sec on data transfer, huge bottleneck

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 SMX
  - 2688 SP Cores
  - 896 DP Cores
  - 6G global memory

K20Xm Full chip block diagram

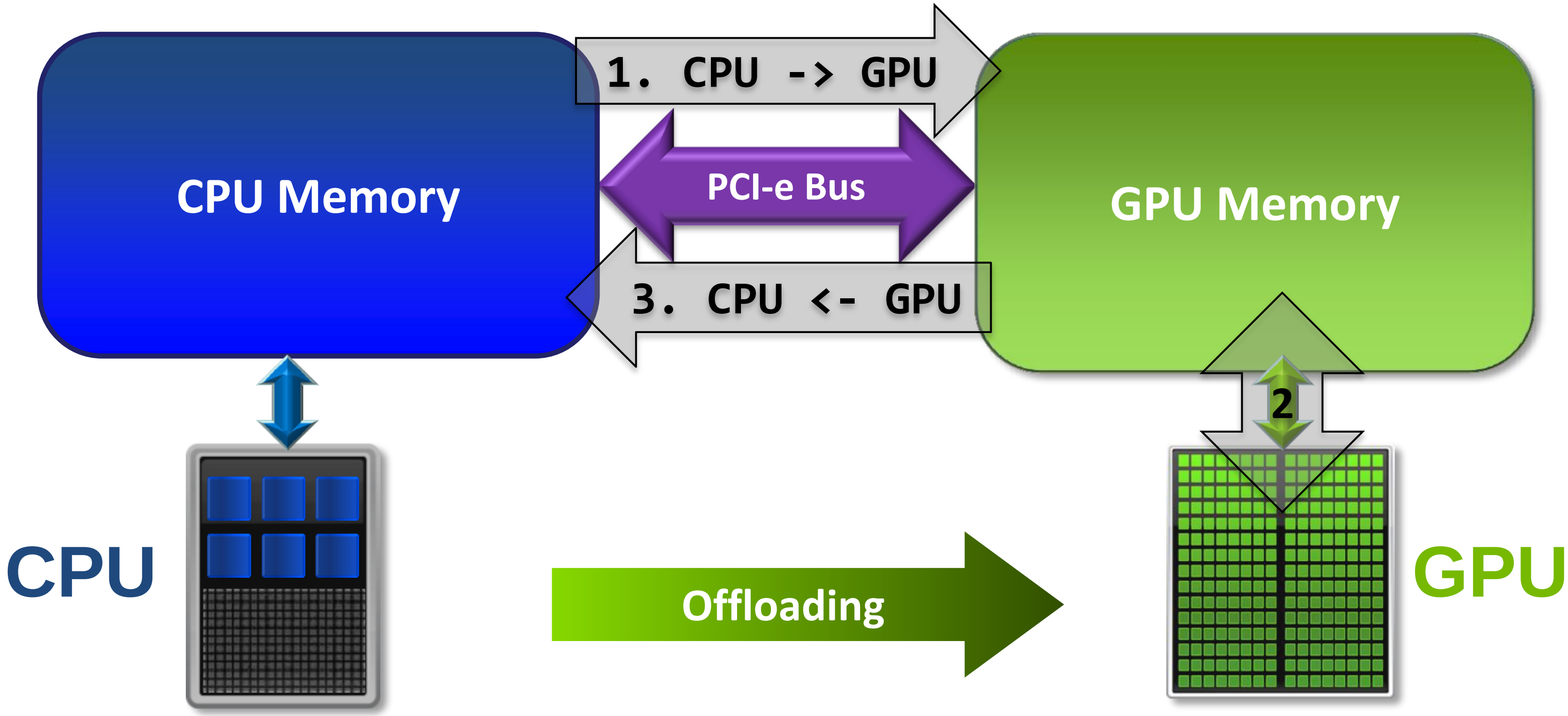




SMX (192 SP, 64 DP)

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++;
}
```

A, Anew on accelerator ← Copy ← A, Anew on host

2 copies happen every iteration

A, Anew on accelerator → Copy → A, Anew on host

A, Anew on accelerator ← Copy ← A, Anew on host

2 copies happen every iteration

A, Anew on accelerator → Copy → A, Anew on host

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 $\boldsymbol{a}$ 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