Module III:
GPU PROGRAMMING

OpenACC More Science, Less Programming
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MODULE OVERVIEW

OpenACC Directives

- Multicore CPU vs GPU
- Introduction to GPU Data Management
- CUDA Managed Memory
- Explicit Data Management
- OpenACC Data Regions and Clauses
- Unstructured Data Lifetimes
- Data Synchronization

CPU VS GPU

CPU VS GPU

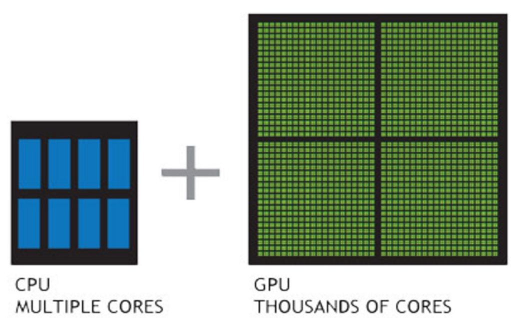
Number of cores and parallelism

Both are extremely popular parallel processors, but with different degrees of parallelism

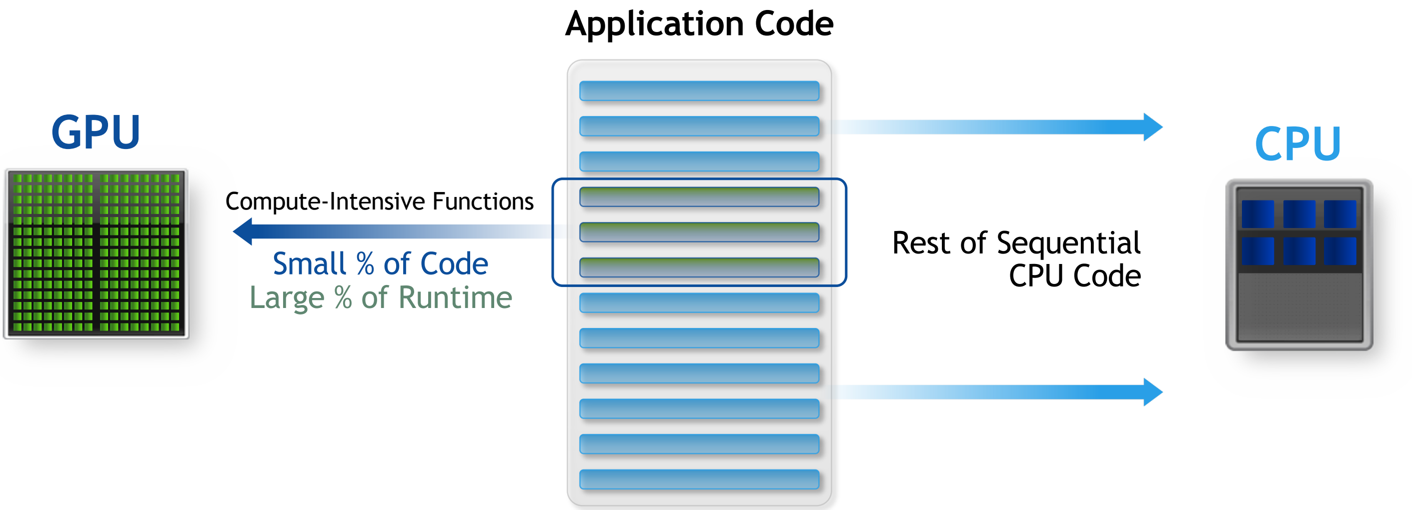
CPUs generally have a small number of very fast physical cores

GPUs have thousands of simple cores able to achieve high performance in aggregate

Both require parallelism to be fully utilized, but GPUs require much more



CPU + GPU WORKFLOW



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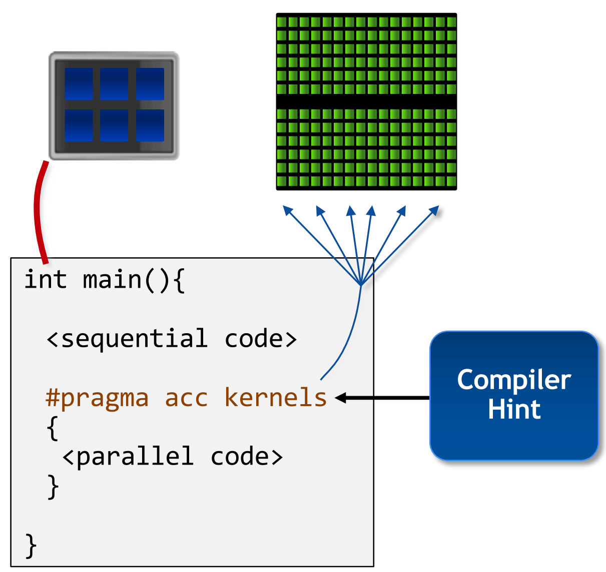
GPU PROGRAMMING IN OPENACC

Execution always begins and ends on the *host* CPU

Compute-intensive loops are offloaded to the GPU using directives

Offloading may or may not require data movement between the *host* and *device*.



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CPU + GPU
Physical Diagram

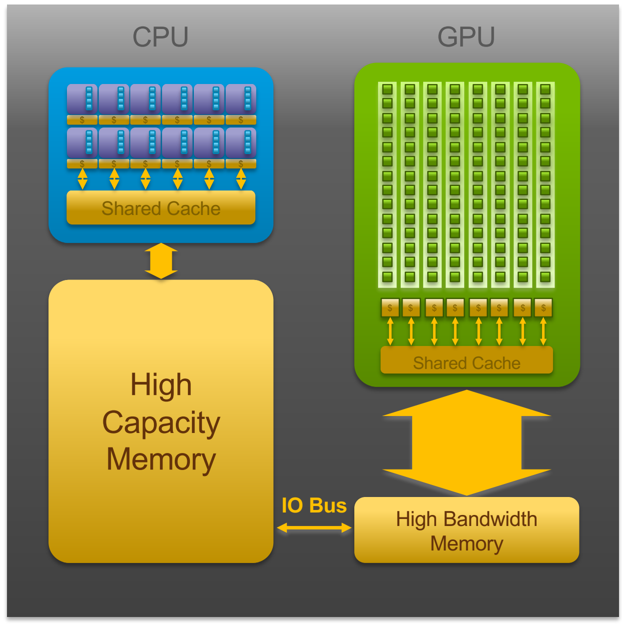
CPU memory is larger, GPU memory has more bandwidth

CPU and GPU memory are usually separate, connected by an I/O bus (traditionally PCI-e)

Any data transferred between the CPU and GPU will be handled by the I/O Bus

The I/O Bus is relatively slow compared to memory bandwidth

The GPU cannot perform computation until the data is within its memory



BASIC DATA MANAGEMENT

BASIC DATA MANAGEMENT

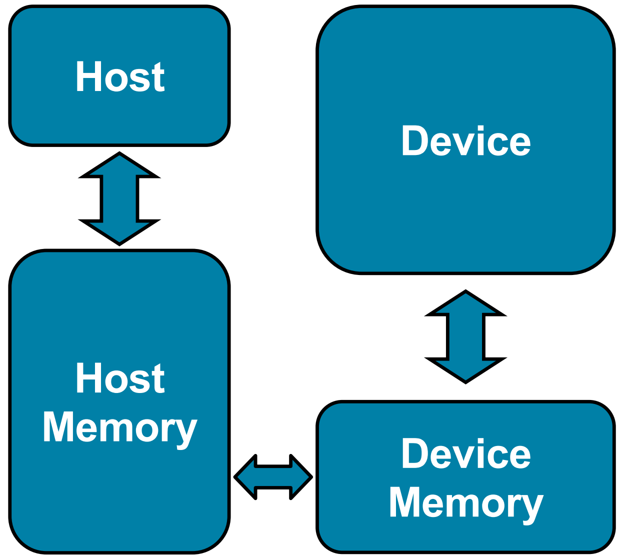
Between the host and device

The **host** is traditionally a CPU

The **device** is some parallel accelerator

When our target hardware is multicore, the host and device are the same, meaning that their memory is also the same

There is no need to explicitly manage data when using a shared memory accelerator, such as the multicore target



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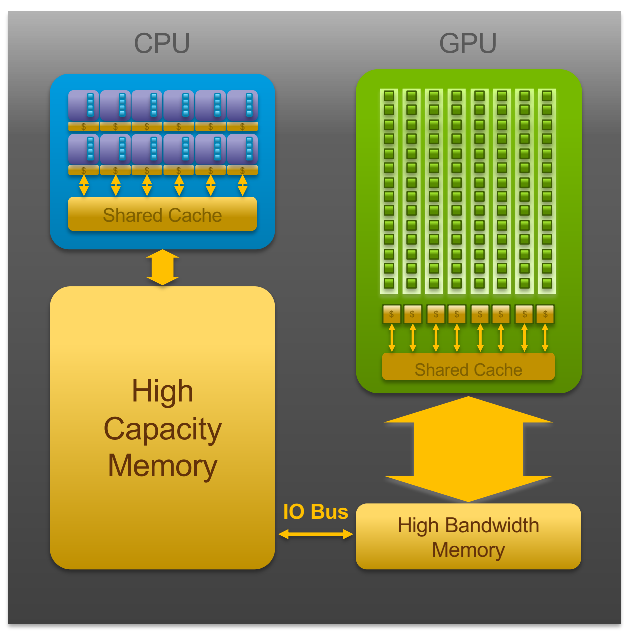
BASIC DATA MANAGEMENT

Between the host and device

When the target hardware is a GPU data will usually need to migrate between CPU and GPU memory

The next lecture will discuss OpenACC data management, for now we'll assume a unified Host/Accelerator memory



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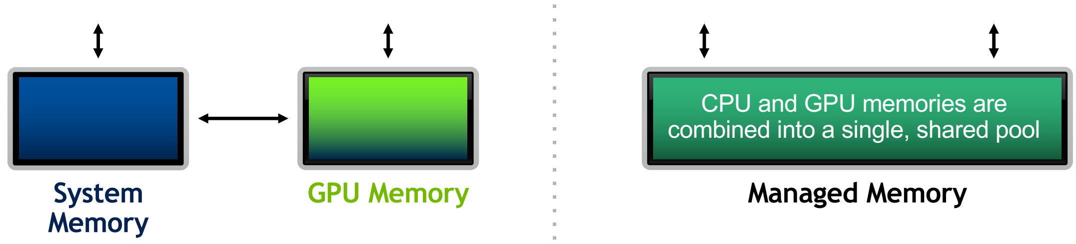
CUDA MANAGED MEMORY

CUDA MANAGED MEMORY

Simplified Developer Effort

Commonly referred to as "unified memory."

Without Managed Memory | **With Managed Memory**



CUDA MANAGED MEMORY

Usefulness

Handling explicit data transfers between the host and device (CPU and GPU) can be difficult

The PGI compiler can utilize CUDA Managed Memory to defer data management

This allows the developer to concentrate on parallelism and think about data movement as an optimization

```
$      pgcc -fast -acc -ta=tesla:managed -Minfo=accel main.c
```


MANAGED MEMORY

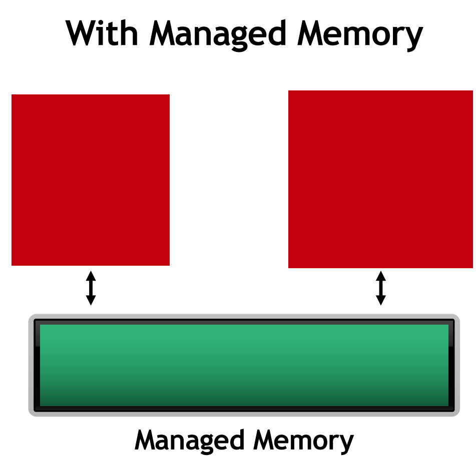
Limitations

The programmer will almost always be able to get better performance by manually handling data transfers

Memory allocation/deallocation takes longer with managed memory

Cannot transfer data asynchronously

Currently only available from PGI on NVIDIA GPUs.



OPENACC WITH MANAGED MEMORY

An Example from the Lab Code

```
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 = fmax( error, fabs(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];
      }
    }
  }
}
```

Without Managed Memory the compiler must determine the size of A and Anew and copy their data to and from the GPU each iteration to ensure correctness

With Managed Memory the underlying runtime will move the data only when needed

INTRODUCTION TO DATA CLAUSES

BASIC DATA MANAGEMENT

Moving data between the Host and Device using copy

Data clauses allow the programmer to tell the compiler which data to move and when

Data clauses may be added to **kernels** or **parallel** regions, but also **data**, **enter data**, and **exit data**, which will discussed shortly

C/C++

```
#pragma acc kernels
for(int i = 0; i < N; i++){
     a[i] = 0;
}
```

BASIC DATA MANAGEMENT

Moving data between the Host and Device using copy

Data clauses allow the programmer to tell the compiler which data to move and when

Data clauses may be added to **kernels** or **parallel** regions, but also **data**, **enter data**, and **exit data**, which will discussed shortly

C/C++

```
#pragma acc parallel loop copyout(a[0:n])
for(int i = 0; i < N; i++){
     a[i] = 0;
}
```

I don't need the initial value of a, so I'll only copy it out of the region at the end.

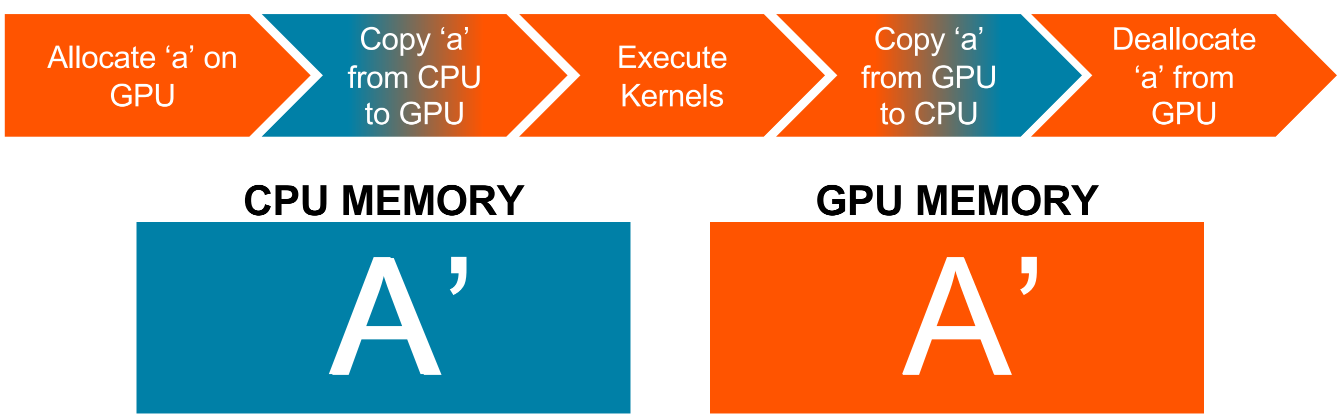
BASIC DATA MANAGEMENT

Moving data between the Host and Device using copy


```
#pragma acc parallel loop copy(a[0:N])
for(int i = 0; i < N; i++){
     a[i] = 2 * a[i];
}
```


BASIC DATA MANAGEMENT

Moving data between the Host and Device using copy



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.**

Principal use: For many important data structures in your code, this is a logical default to input, modify and return the data.

`copyin( list )` **Allocates memory on GPU and copies data from host to GPU when entering region.**

Principal use: Think of this like an array that you would use as just an input to a subroutine.

`copyout( list )` **Allocates memory on GPU and copies data to the host when exiting region.**

Principal use: A result that isn't overwriting the input data structure.

`create( list )` **Allocates memory on GPU but does not copy.**

Principal use: Temporary arrays.

ARRAY SHAPING

Sometimes the compiler needs help understanding the *shape* of an array

The first number is the start index of the array

In C/C++, the second number is how much data is to be transferred

```
copy(array[starting_index:length])
```

C/C++

BASIC DATA MANAGEMENT

Multi-dimensional Array shaping

```
copy(array[0:N][0:M])
```

C/C++

EXPLICIT MEMORY MANAGEMENT

EXPLICIT MEMORY MANAGEMENT

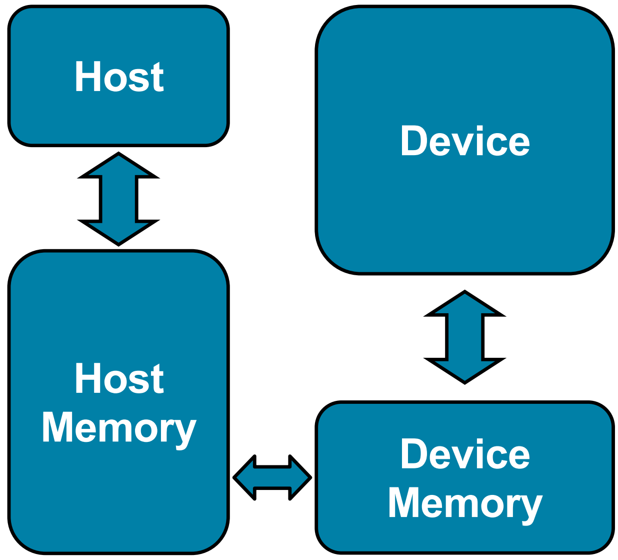
Requirements

Data must be visible on the **device** when we run our **parallel** code

Data must be visible on the **host** when we run our **sequential** code

When the host and device don't share memory, data movement must occur

To maximize performance, the programmer should avoid all unnecessary data transfers



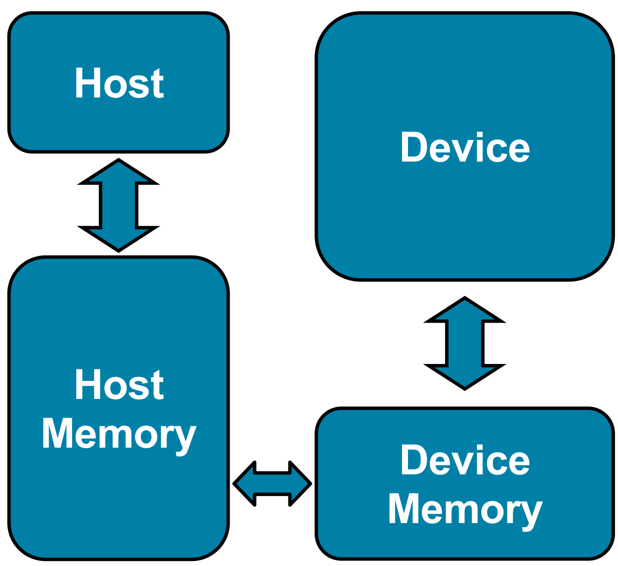
EXPLICIT MEMORY MANAGEMENT

Key problems

Many parallel accelerators (such as devices) have a separate memory space from the host

These separate memories can become out-of-sync and contain completely different data

Transferring between these two memories can be a very time consuming process



EXPLICIT MEMORY MANAGEMENT

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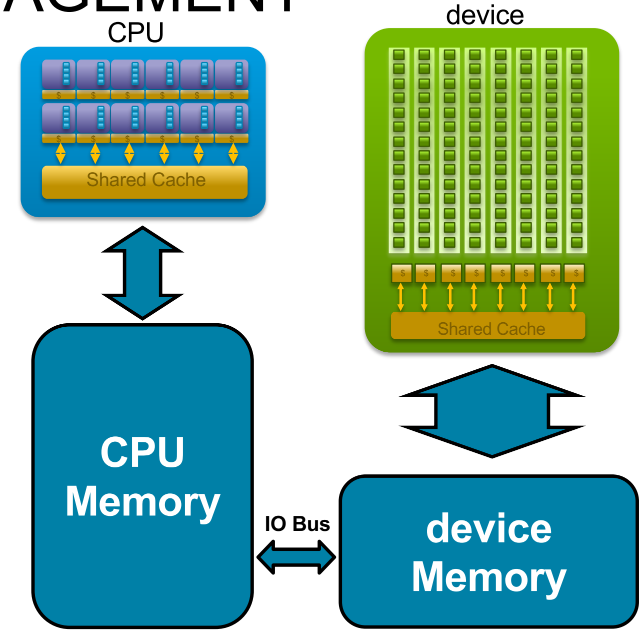

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OPENACC DATA DIRECTIVE

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OPENACC DATA DIRECTIVE

Definition

The data directive defines a lifetime for data on the device

During the region data should be thought of as residing on the accelerator

Data clauses allow the programmer to control the allocation and movement of data

```
#pragma acc data clauses
{

 < Sequential and/or Parallel code >

}
```

DATA CLAUSES

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```
copy(array[starting_index:length])
```

C/C++

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ARRAY SHAPING (CONT.)

Multi-dimensional Array shaping

```
copy(array[0:N][0:M])
```

C/C++

Both of these examples copy a 2D array to the device

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ARRAY SHAPING (CONT.)

Partial Arrays

```
copy(array[i*N/4:N/4])
```

C/C++

Both of these examples copy only ¼ of the full array

STRUCTURED DATA DIRECTIVE

Example

This **parallel loop** will execute on the **accelerator**, so **a, b, and c** must be visible on the accelerator.

```
#pragma acc parallel loop
for(int i = 0; i < N; i++){
 c[i] = a[i] + b[i];
}
```

STRUCTURED DATA DIRECTIVE

Example

Start of Data Region →

End of Data Region →

```
#pragma acc data copyin(a[0:N],b[0:N]) copyout(c[0:N])
{
 #pragma acc parallel loop
 for(int i = 0; i < N; i++){
  c[i] = a[i] + b[i];
 }
}
```

STRUCTURED DATA DIRECTIVE

Example

```
#pragma acc data copyin(a[0:N],b[0:N]) copyout(c[0:N])
{
 #pragma acc parallel loop
 for(int i = 0; i < N; i++){
  c[i] = a[i] + b[i];
 }
}
```

Action

IMPLIED DATA REGIONS

IMPLIED DATA REGIONS

Definition

Every **kernels** and **parallel** region has an implicit data region surrounding it

This allows data to exist solely for the duration of the region

All data clauses usable on a **data** directive can be used on a **parallel** and **kernels** as well

```
#pragma acc kernels copyin(a[0:100])
{
 for( int i = 0; i < 100; i++ )
 {
  a[i] = 0;
 }
}
```

IMPLIED DATA REGIONS

Explicit vs Implicit Data Regions

Explicit

```
#pragma acc data copyin(a[0:100])
{
 #pragma acc kernels
 {
  for( int i = 0; i < 100; i++ )
  {
   a[i] = 0;
  }
 }
}
```

Implicit

```
#pragma acc kernels copyin(a[0:100])
{
 for( int i = 0; i < 100; i++ )
 {
  a[i] = 0;
 }
}
```

These two codes are functionally the same.

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EXPLICIT VS. IMPLICIT DATA REGIONS

Limitation

Explicit **1 Data Copy**

```
#pragma acc data copyout(a[0:100])
{

 #pragma acc kernels
 {
a[i] = i;
 }

 #pragma acc kernels
 {
a[i] = 2 * a[i];
 }

}
```

Implicit **2 Data Copies**

```
#pragma acc kernels copyout(a[0:100])
{
 a[i] = i;
}

#pragma acc kernels copy(a[0:100])
{
 a[i] = 2 * a[i];
}
```

The code on the left will perform better than the code on the right.

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UNSTRUCTURED DATA DIRECTIVES

UNSTRUCTURED DATA DIRECTIVES

Enter Data Directive

Data lifetimes aren't always neatly structured.

The **enter data** directive handles device memory **allocation**

You may use either the **create** or the **copyin** clause for memory allocation

The enter data directive is **not** the start of a data region, because you may have multiple enter data directives

```
#pragma acc enter data clauses

 < Sequential and/or Parallel code >

#pragma acc exit data clauses
```

UNSTRUCTURED DATA DIRECTIVES

Exit Data Directive

The **exit data** directive handles device memory **deallocation**

You may use either the **delete** or the **copyout** clause for memory deallocation

You should have as many **exit data** for a given array as **enter data**

These can exist in different functions

```
#pragma acc enter data clauses

 < Sequential and/or Parallel code >

#pragma acc exit data clauses
```


UNSTRUCTURED DATA CLAUSES

`copyin ( list )`	Allocates memory on device and copies data from host to device on enter data.
`copyout ( list )`	Allocates memory on device and copies data back to the host on exit data.
`create ( list )`	Allocates memory on device without data transfer on enter data.
`delete ( list )`	Deallocates memory on device without data transfer on exit data

UNSTRUCTURED DATA DIRECTIVES

Basic Example

```
#pragma acc parallel loop
for(int i = 0; i < N; i++){
 c[i] = a[i] + b[i];
}
```

UNSTRUCTURED DATA DIRECTIVES

Basic Example

```
#pragma acc enter data copyin(a[0:N],b[0:N]) create(c[0:N])

 #pragma acc parallel loop
 for(int i = 0; i < N; i++){
  c[i] = a[i] + b[i];
 }

#pragma acc exit data copyout(c[0:N])
```

UNSTRUCTURED DATA DIRECTIVES

Basic Example

```
#pragma acc enter data copyin(a[0:N],b[0:N]) create(c[0:N])

#pragma acc parallel loop
for(int i = 0; i < N; i++){
 c[i] = a[i] + b[i];
}

#pragma acc exit data copyout(c[0:N])
```

Action

UNSTRUCTURED DATA DIRECTIVES

Basic Example – proper memory deallocation

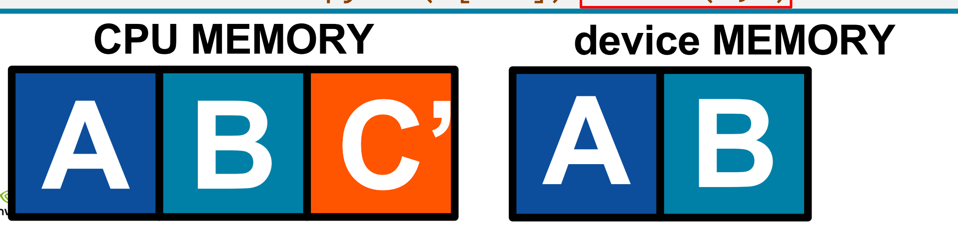
```
#pragma acc enter data copyin(a[0:N],b[0:N]) create(c[0:N])

      #pragma acc parallel loop
      for(int i = 0; i < N; i++){
            c[i] = a[i] + b[i];
      }

#pragma acc exit data copyout(c[0:N]) delete(a,b)
```

Action

Deallocate B from device



UNSTRUCTURED VS STRUCTURED

With a simple code

Unstructured

- Can have multiple starting/ending points
- Can branch across multiple functions
- Memory exists until explicitly deallocated

```
#pragma acc enter data copyin(a[0:N],b[0:N]) \
 create(c[0:N])

 #pragma acc parallel loop
 for(int i = 0; i < N; i++){
  c[i] = a[i] + b[i];
 }

#pragma acc exit data copyout(c[0:N]) \
 delete(a,b)
```

Structured

- Must have explicit start/end points
- Must be within a single function
- Memory only exists within the data region

```
#pragma acc data copyin(a[0:N],b[0:N]) \
 copyout(c[0:N])
{
 #pragma acc parallel loop
 for(int i = 0; i < N; i++){
  c[i] = a[i] + b[i];
 }

}
```


UNSTRUCTURED DATA DIRECTIVES

Branching across multiple functions

```
int* allocate_array(int N){
 int* ptr = (int *) malloc(N * sizeof(int));
 #pragma acc enter data create(ptr[0:N])
 return ptr;
}

void deallocate_array(int* ptr){
 #pragma acc exit data delete(ptr)
 free(ptr);
}

int main(){
 int* a = allocate_array(100);
 #pragma acc kernels
 {
  a[0] = 0;
 }
 deallocate_array(a);
}
```

In this example enter data and exit data are in different functions

This allows the programmer to put device allocation/deallocation with the matching host versions

This pattern is particularly useful in C++, where structured scopes may not be possible.

DATA SYNCHRONIZATION

OPENACC UPDATE DIRECTIVE

update: Explicitly transfers data between the host and the device

Useful when you want to synchronize data in the middle of a data region

Clauses:

- **self:** makes host data agree with device data
- **device:** makes device data agree with host data

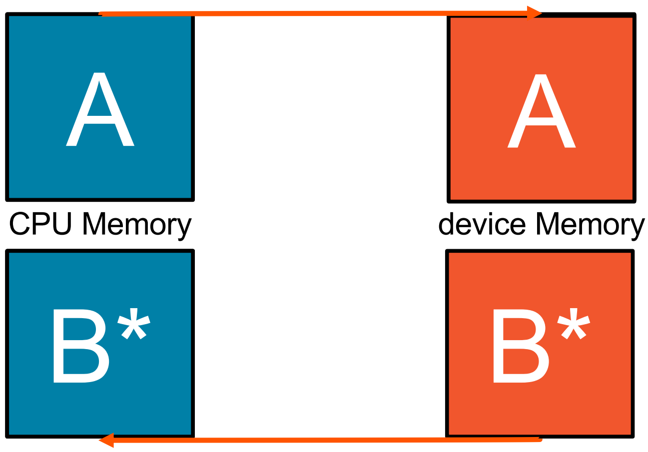
```
#pragma acc update self(x[0:count])
#pragma acc update device(x[0:count])
```

C/C++

OPENACC UPDATE DIRECTIVE

`#pragma acc update device(A[0:N])`

The data must exist on both the CPU and device for the update directive to work.



`#pragma acc update self(A[0:N])`

SYNCHRONIZE DATA WITH UPDATE

```
int* allocate_array(int N){
 int* A=(int*) malloc(N*sizeof(int));
 #pragma acc enter data create(A[0:N])
 return A;
}

void deallocate_array(int* A){
 #pragma acc exit data delete(A)
 free(A);
}

void initialize_array(int* A, int N){
 for(int i = 0; i < N; i++){
  A[i] = i;
 }
 #pragma acc update device(A[0:N])
}
```

Inside the **initialize** function we alter the host copy of **'A'**

This means that after calling **initialize** the host and device copy of **'A'** are out-of-sync

We use the **update** directive with the **device** clause to update the device copy of **'A'**

Without the **update** directive later compute regions will use incorrect data.

C/C++ STRUCTS/CLASSES

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C STRUCTS

Without dynamic data members

Dynamic data members are anything contained within a struct that can have a **variable size**, such as dynamically allocated arrays

OpenACC is easily able to copy our struct to device memory because everything in our float3 struct has a **fixed size**

But what if the struct had dynamically allocated members?

```
typedef struct {
 float x, y, z;
} float3;

int main(int argc, char* argv[]){
 int N = 10;
 float3* f3 = malloc(N * sizeof(float3));

 #pragma acc enter data create(f3[0:N])

 #pragma acc kernels
 for(int i = 0; i < N; i++){
  f3[i].x = 0.0f;
  f3[i].y = 0.0f;
  f3[i].z = 0.0f;
 }

 #pragma acc exit data delete(f3)
 free(f3);
}
```

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C STRUCTS

With dynamic data members

OpenACC does not have enough information to copy the struct and its dynamic members

You must first copy the struct into device memory, then allocate/copy the dynamic members into device memory

To deallocate, first deal with the dynamic members, then the struct

OpenACC will automatically *attach* your dynamic members to the struct

```
typedef struct {
 float *arr;
 int n;
} vector;

int main(int argc, char* argv[]){

 vector v;
 v.n = 10;
 v.arr = (float*) malloc(v.n*sizeof(float));

#pragma acc enter data copyin(v)
#pragma acc enter data create(v.arr[0:v.n])

 ...

#pragma acc exit data delete(v.arr)
#pragma acc exit data delete(v)
 free(v.arr);
}
```


C++ STRUCTS/CLASSES

With dynamic data members

C++ Structs/Classes work the same exact way as they do in C

The main difference is that now we have to account for the implicit “this” pointer

```
class vector {
 private:
  float *arr;
  int n;
 public:
  vector(int size){
   n = size;
   arr = new float[n];
   #pragma acc enter data copyin(this)
   #pragma acc enter data create(arr[0:n])
  }
  ~vector(){
   #pragma acc exit data delete(arr)
   #pragma acc exit data delete(this)
   delete(arr);
  }
};
```

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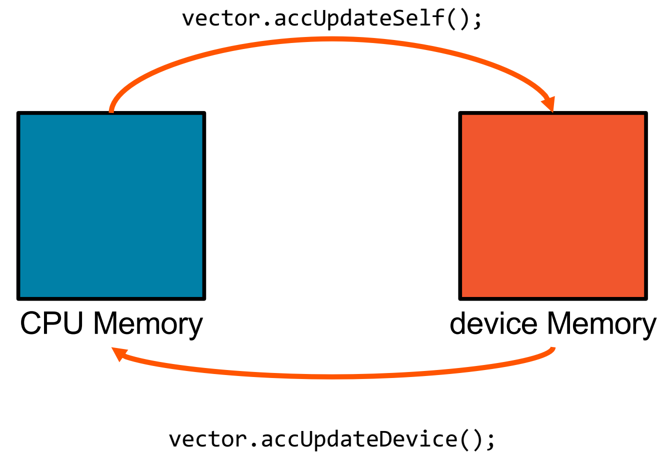
C++ CLASS DATA SYNCHRONIZATION

Since data is encapsulated, the class needs to be extended to include data synchronization methods

Including explicit methods for host/device synchronization may ease C++ data management

Allows the class to be able to naturally handle synchronization, creating less code clutter



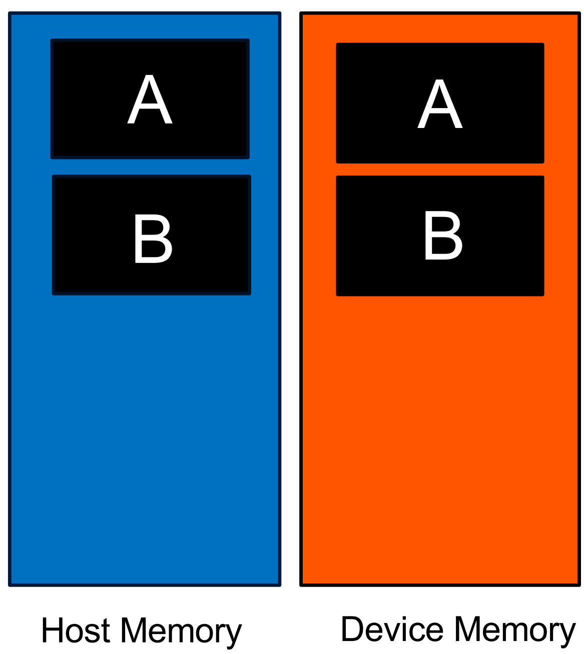

```
void accUpdateSelf() {
 #pragma acc update self(arr[0:n])
}
void accUpdateDevice() {
 #pragma acc update device(arr[0:n])
}
```

USING A OPENACC AWARE C++ CLASS

```
#include “vector.h"

int main() {

    vector A(N), B(N);
    for (int i=0; i < B.size(); ++i) {
        B[i]=2.5;
    }
    B.accUpdateDevice();
    #pragma acc parallel loop present(A,B)
    for (int i=0; i < A.size(); ++i) {
          A[i]=B[i]+i;
    }
    A.accUpdateSelf();
    for(int i=0; i<10; ++i) {
        cout << "A[" << i << "]: " << A[i] << endl;
    }
    exit(0);
}
```



MODULE REVIEW

KEY CONCEPTS

In this module we discussed…

- Why explicit data management is necessary for best performance
- Structured and Unstructured Data Lifetimes
- Explicit and Implicit Data Regions
- The **data**, **enter data**, **exit data**, and **update** directives
- Data Clauses

KEY CONCEPTS

In this module we discussed…

- The fundamental differences between CPUs and GPUs
- Assisting the compiler by providing information about array sizes for data management
- Managed memory