OPENACC DATA MANAGEMENT

Speaker

OpenACC
More Science, Less Programming

NVIDIA aws Linux Academy

LECTURE 2 OUTLINE

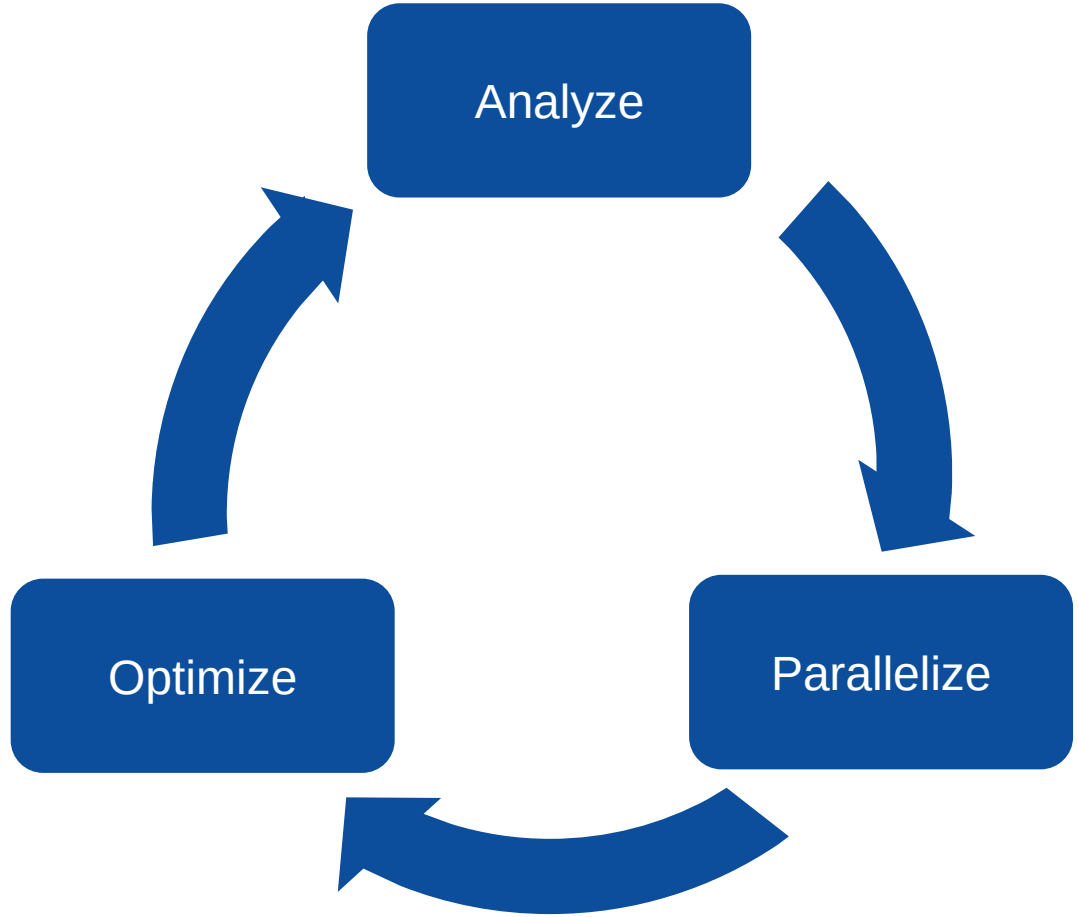
Topics to be covered

- CPU and GPU Memories
- CUDA Unified (Managed) Memory
- OpenACC Data Management
- Lab 2

WEEK 1 REVIEW

OPENACC DEVELOPMENT CYCLE

- **Analyze** your code to determine most likely places needing parallelization or optimization.
- **Parallelize** your code by starting with the most time consuming parts and check for correctness.
- **Optimize** your code to improve observed speed-up from parallelization.



OpenACC Directives

Manage Data Movement

Initiate Parallel Execution

Optimize Loop Mappings

```
#pragma acc data copyin(a,b) copyout(c)
{
  ...
  #pragma acc parallel
  {
  #pragma acc loop gang vector
      for (i = 0; i < n; ++i) {
          c[i] = a[i] + b[i];
          ...
      }
  }
  ...
}
```

OpenACC
Directives for Accelerators

- Incremental
- Single source
- Interoperable
- Performance portable
- CPU, GPU, Manycore

OpenACC Directives

This Week:
Manage
Data
Movement

Last Week:
Run loops in
parallel

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

- Incremental
- Single source
- Interoperable
- Performance portable
- CPU, GPU, Manycore

OpenACC
Directives for Accelerators

PARALLELIZE WITH OPENACC PARALLEL LOOP

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

#pragma acc parallel loop reduction(max:err)
  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]);

      err = max(err, abs(Anew[j][i] - A[j][i]));
    }
  }

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

Parallelize first loop nest, max *reduction* required.

Parallelize second loop.

We didn't detail *how* to parallelize the loops, just *which* loops to parallelize.

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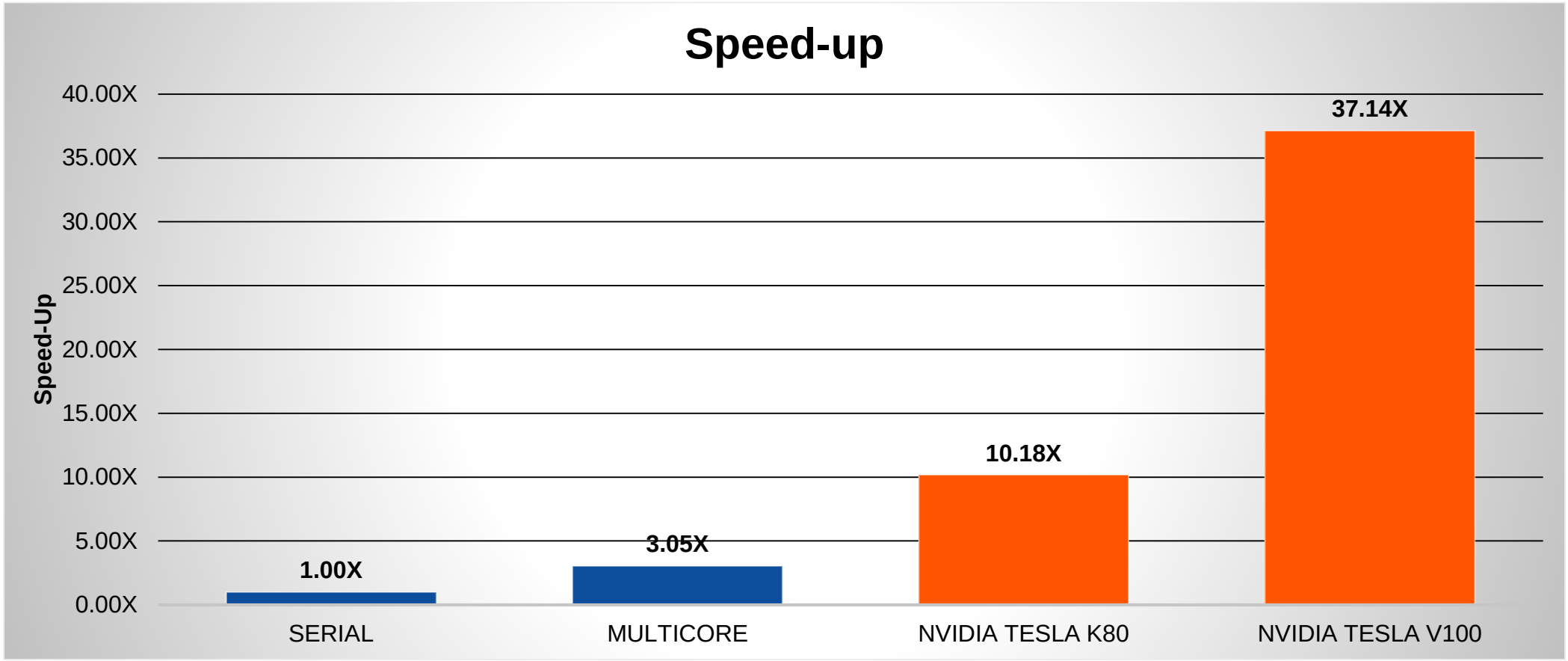
OPENACC SPEED-UP



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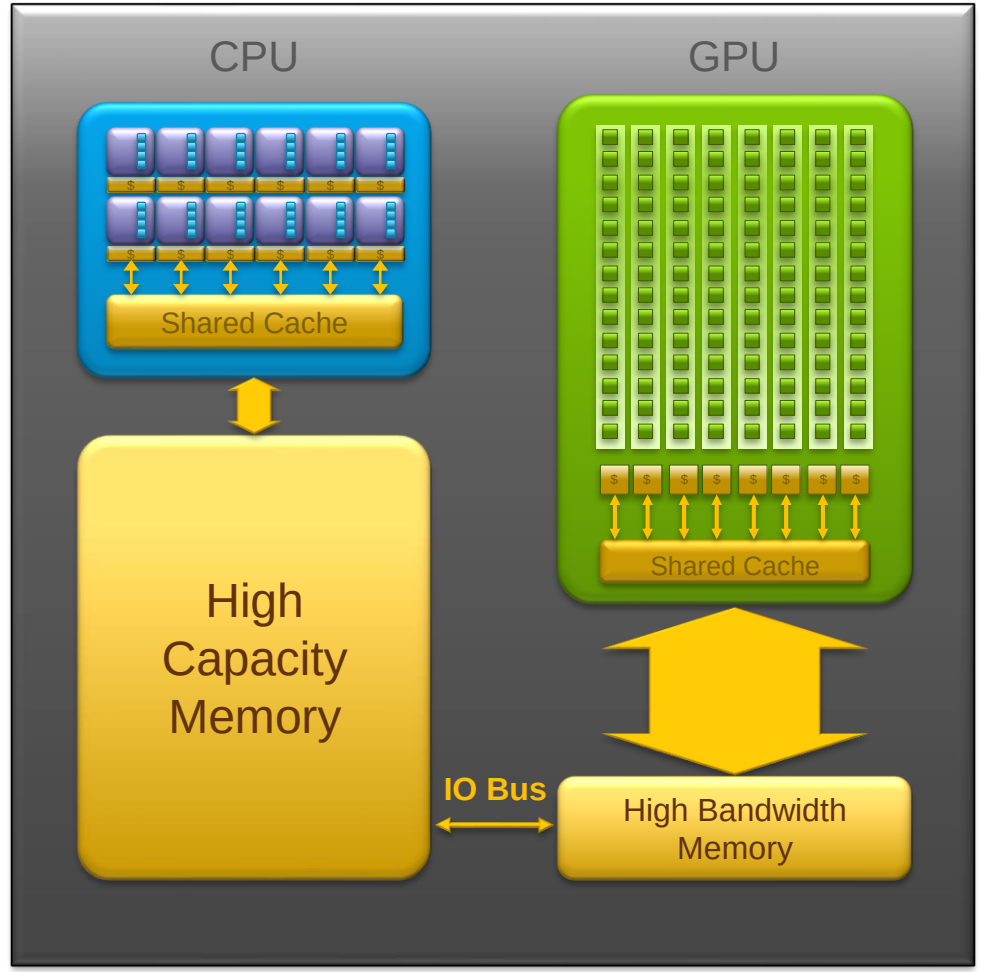
PGI 18.7, NVIDIA Tesla V100, Intel i9-7900X CPU @ 3.30GHz

CPU AND GPU MEMORIES

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



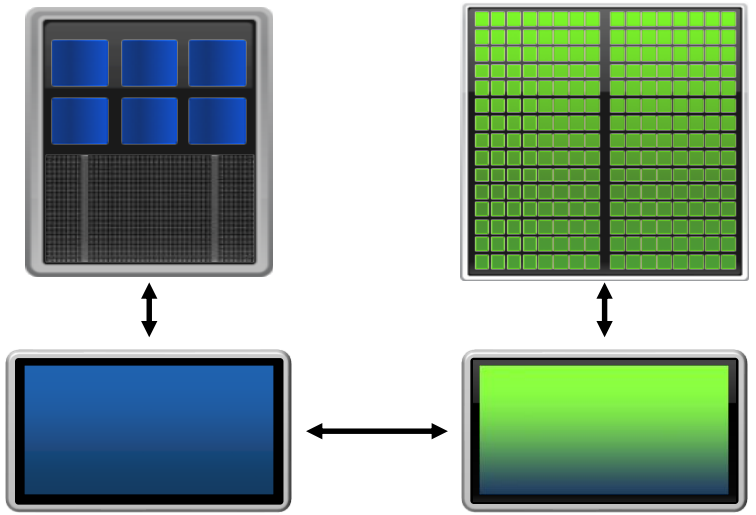
CUDA UNIFIED MEMORY

CUDA UNIFIED MEMORY

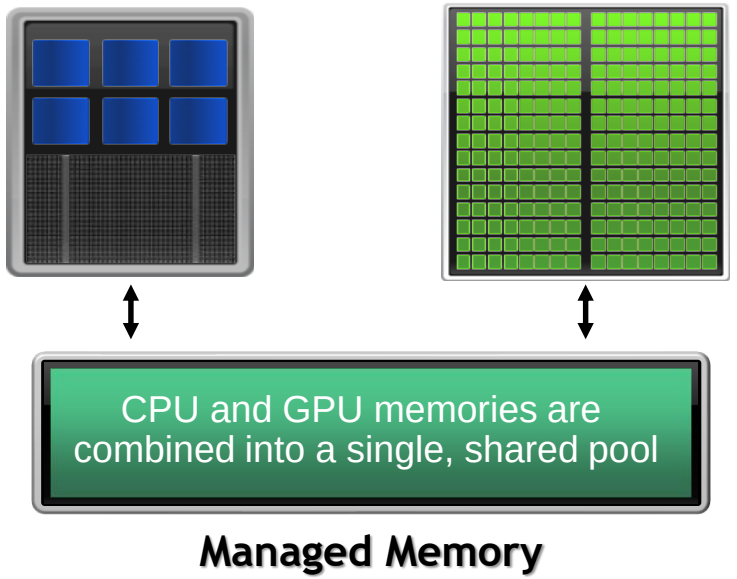
Simplified Developer Effort

Commonly referred to as
"managed 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

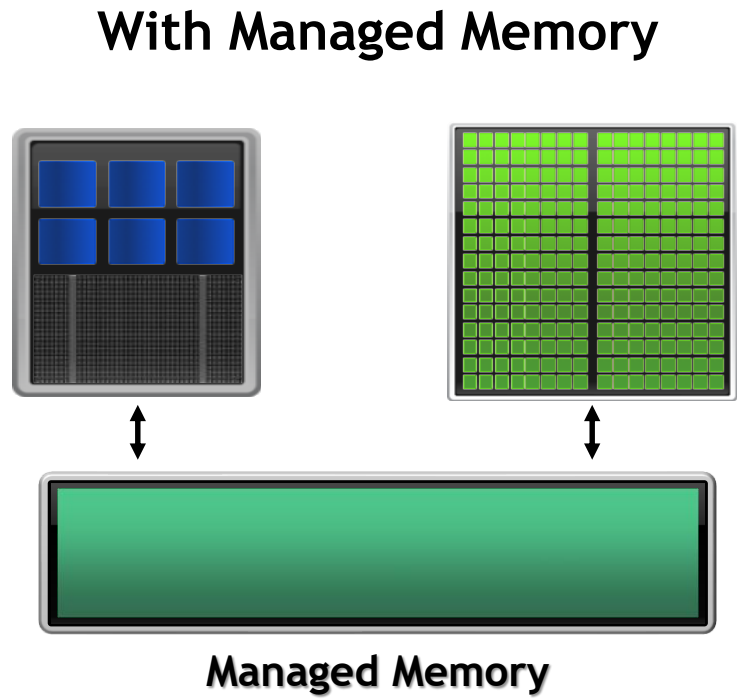
```
$ pgcc -fast -acc -ta=tesla:managed -Minfo=accel main.c
```

```
$ pgfortran -fast -acc -ta=tesla:managed -Minfo=accel main.f90
```

MANAGED MEMORY

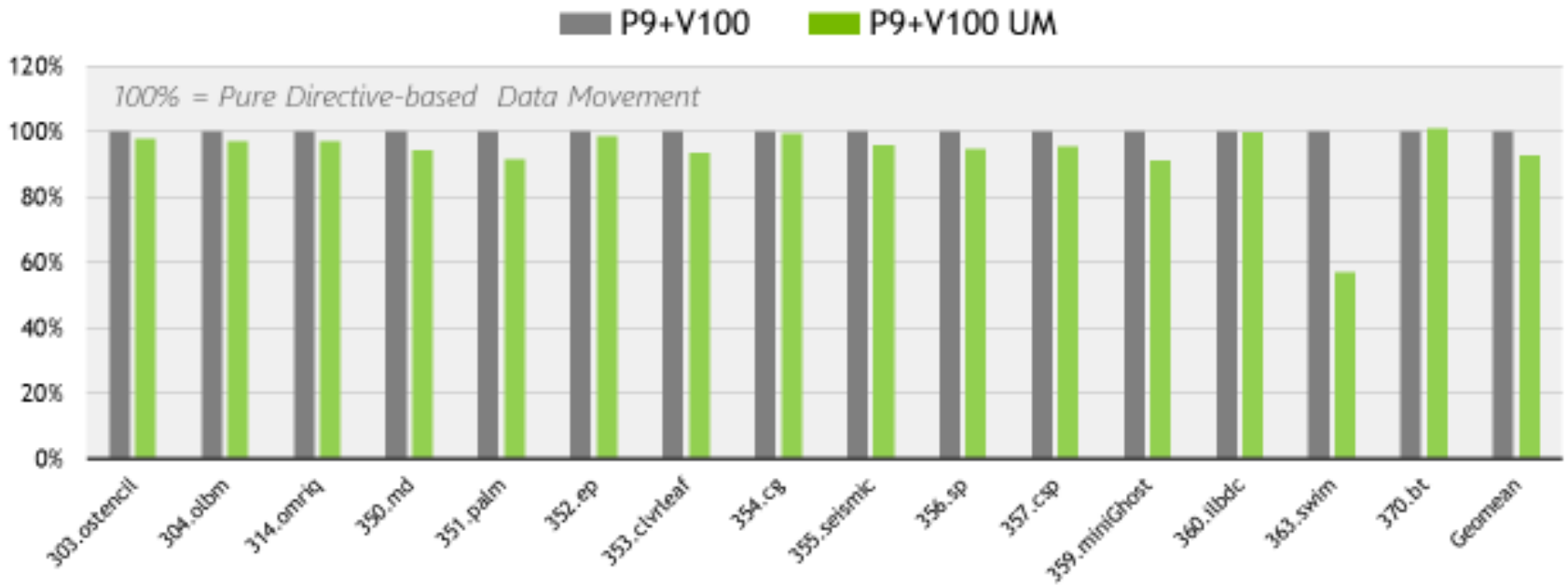
Limitations

- 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.



SPEC ACCEL 1.2 OPENACC BENCHMARKS

OpenACC with Unified Memory vs OpenACC Data Directives



PGI 18.4 Compilers OpenACC SPEC ACCEL™ 1.2 performance measured June, 2018
SPEC® and the benchmark name SPEC ACCEL™ are registered trademarks of the Standard Performance Evaluation Corporation.

PGI

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* Slide Courtesy of PGI

LAST WEEK WE USED UNIFIED MEMORY

Now let’s make our code run without.

Why?

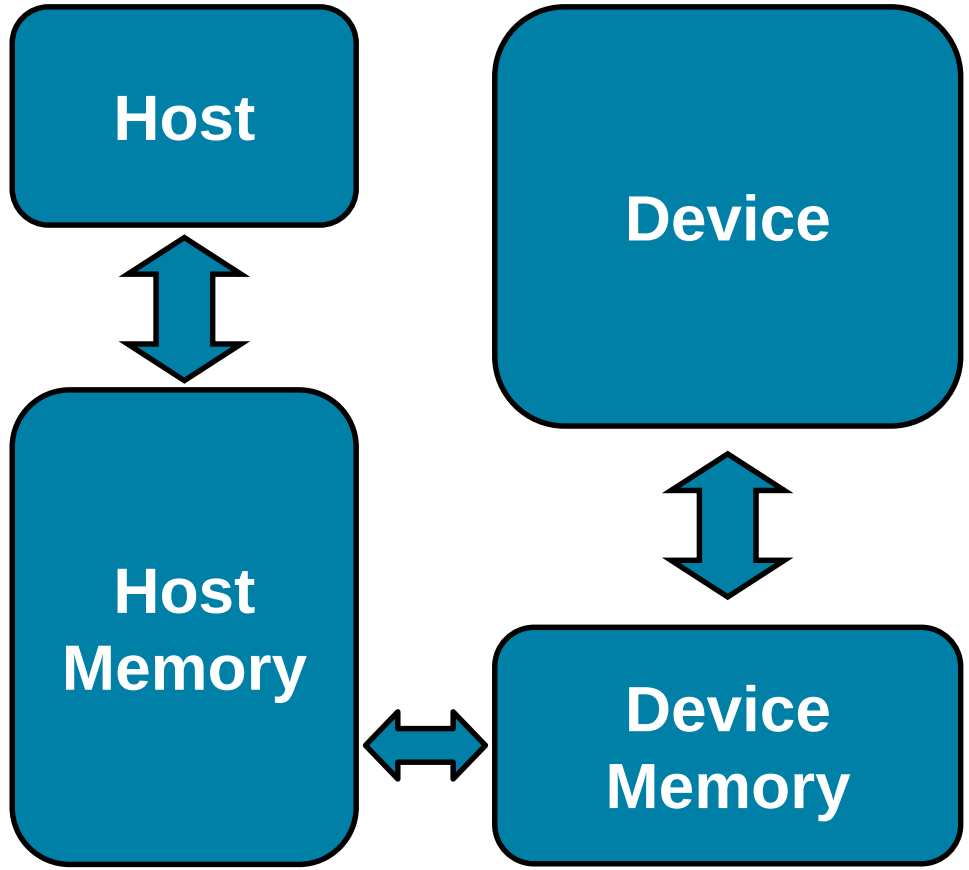
- Removes reliance on PGI and NVIDIA GPUs
- Currently the data always arrives “Just Too Late”, let’s do better

BASIC DATA MANAGEMENT

BASIC DATA MANAGEMENT

Between the host and device

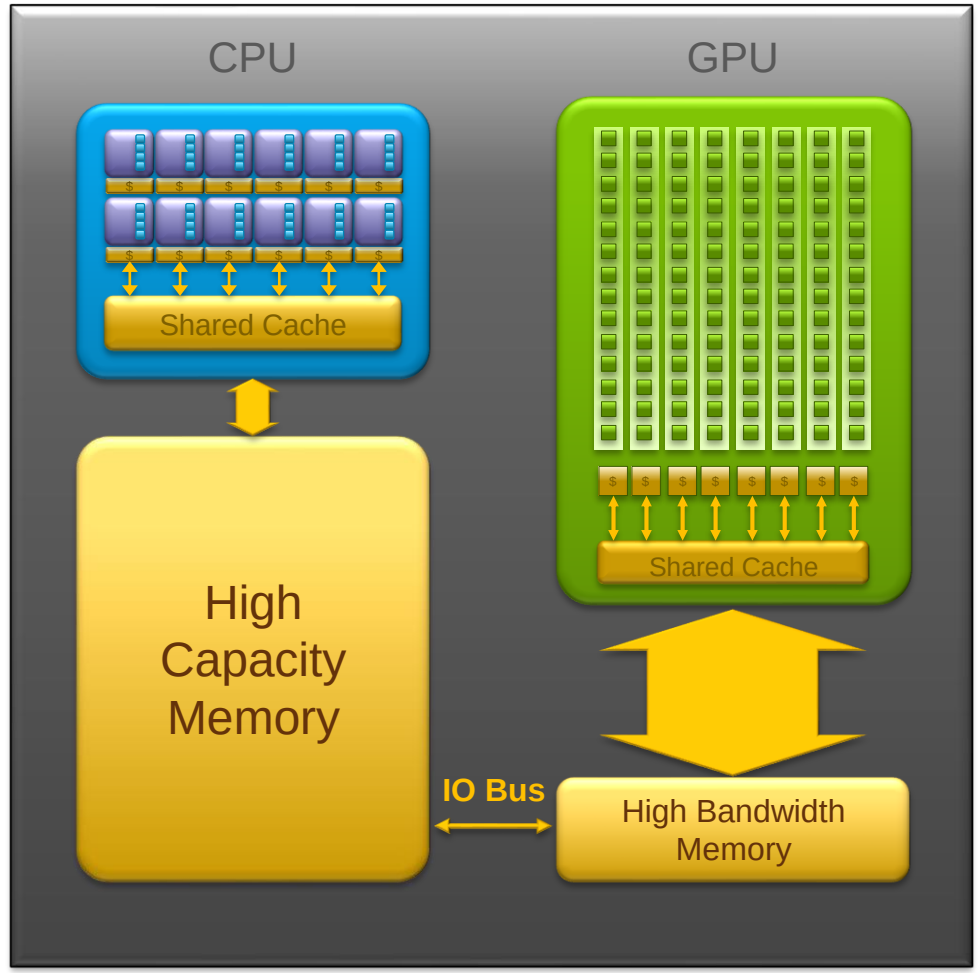
- The **host** is traditionally a CPU
- The **device** is some parallel accelerator
- When our target hardware is multicore, the host and device are the same, meaning that their memory is also the same
- There is no need to explicitly manage data when using a shared memory accelerator, such as the multicore target



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
- Each array used on the GPU must be allocated on the GPU
- When data changes on the CPU or GPU the other must be updated



TRY TO BUILD WITHOUT “MANAGED”

Change –ta=tesla:managed to remove “managed”

```
pgcc -ta=tesla -Minfo=accel laplace2d.c jacobi.c
laplace2d.c:
PGC-S-0155-Compiler failed to translate accelerator region (see -Minfo
messages): Could not find allocated-variable index for symbol (laplace2d.c: 47)
calcNext:
     47, Accelerator kernel generated
         Generating Tesla code
         48, #pragma acc loop gang /* blockIdx.x */
             Generating reduction(max:error)
         50, #pragma acc loop vector(128) /* threadIdx.x */
     48, Accelerator restriction: size of the GPU copy of Anew,A is unknown
     50, Loop is parallelizable
PGC-F-0704-Compilation aborted due to previous errors. (laplace2d.c)
PGC/x86-64 Linux 18.7-0: compilation aborted
jacobi.c:
```

DATA SHAPING

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
- In Fortran, the second number is the ending index

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

C/C++

```
copy(array(starting_index:ending_index))
```

Fortran

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

```
copy(array(1:N, 1:M))
```

Fortran

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

```
copy(array(i*N/4:i*N/4+N/4))
```

Fortran

OPTIMIZED DATA MOVEMENT

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

#pragma acc parallel loop reduction(max:err) copyin(A[0:n*m]) copy(Anew[0:n*m])
  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]);

      err = max(err, abs(Anew[j][i] - A[j][i]));
    }
  }

#pragma acc parallel loop copyin(Anew[0:n*m]) copyout(A[0:n*m])
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
  iter++;
}
```

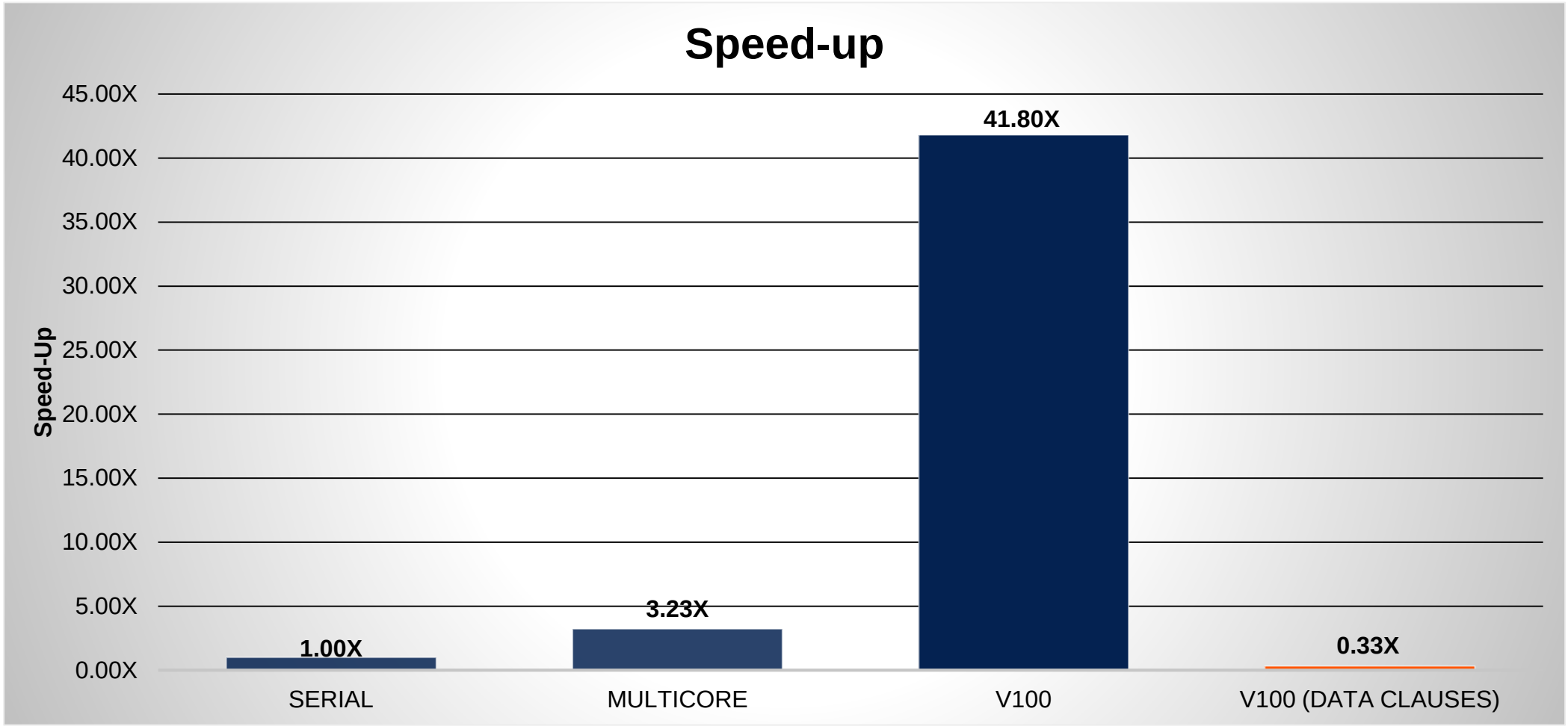
Data clauses provide necessary “shape” to the arrays.

TRY TO BUILD WITHOUT “MANAGED”

Change –ta=tesla:managed to remove “managed”

```
pgcc -ta=tesla -Minfo=accel laplace2d.c jacobi.c
laplace2d.c:
calcNext:
     47, Generating copyin(A[:m*n])
         Accelerator kernel generated
         Generating Tesla code
         48, #pragma acc loop gang /* blockIdx.x */
             Generating reduction(max:error)
         50, #pragma acc loop vector(128) /* threadIdx.x */
     47, Generating implicit copy(error)
         Generating copy(Anew[:m*n])
     50, Loop is parallelizable
swap:
     62, Generating copyin(Anew[:m*n])
         Generating copyout(A[:m*n])
         Accelerator kernel generated
         Generating Tesla code
         63, #pragma acc loop gang /* blockIdx.x */
         65, #pragma acc loop vector(128) /* threadIdx.x */
     65, Loop is parallelizable
jacobi.c:
```

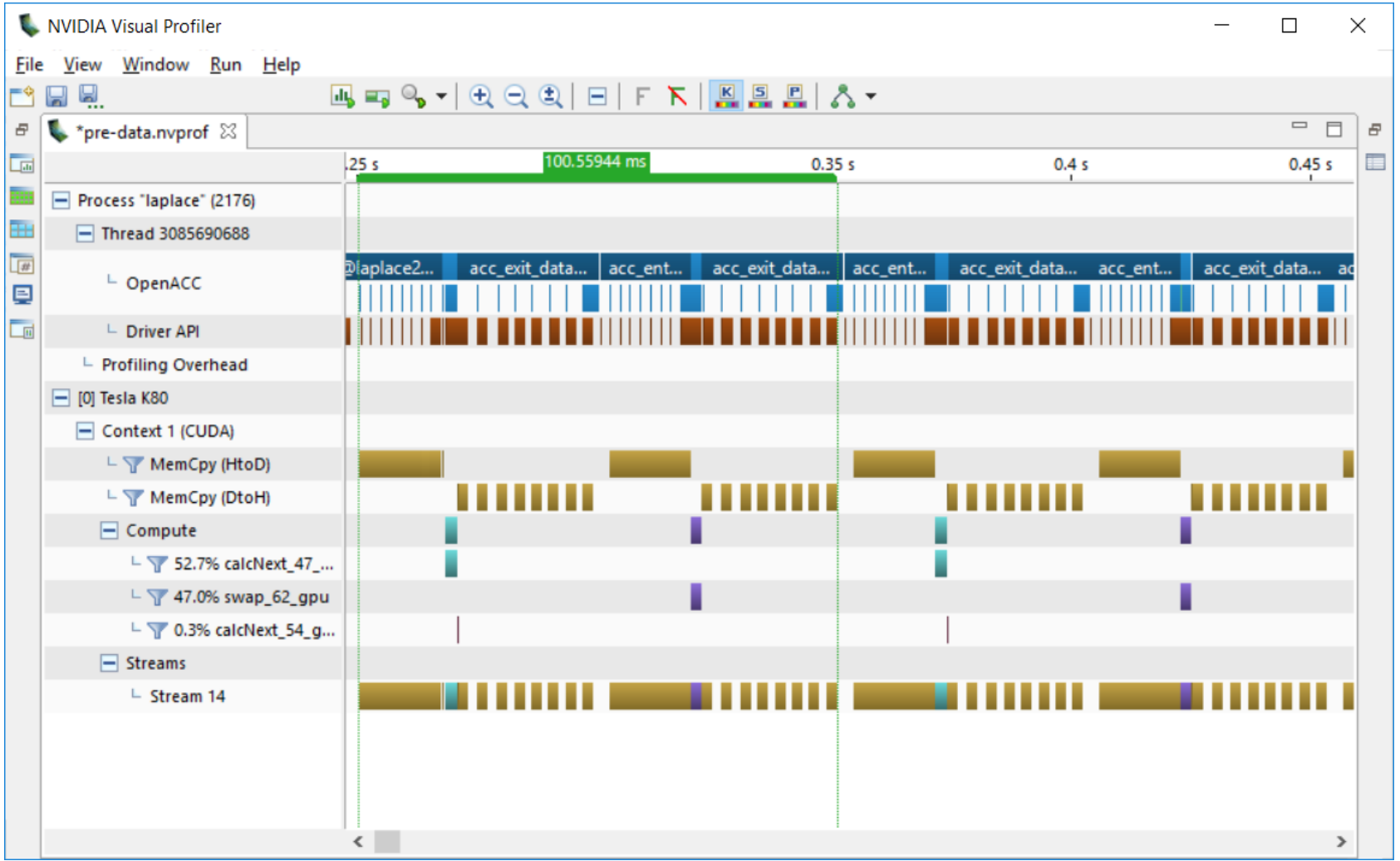
OPENACC ~~SPEED-UP~~ SLOWDOWN



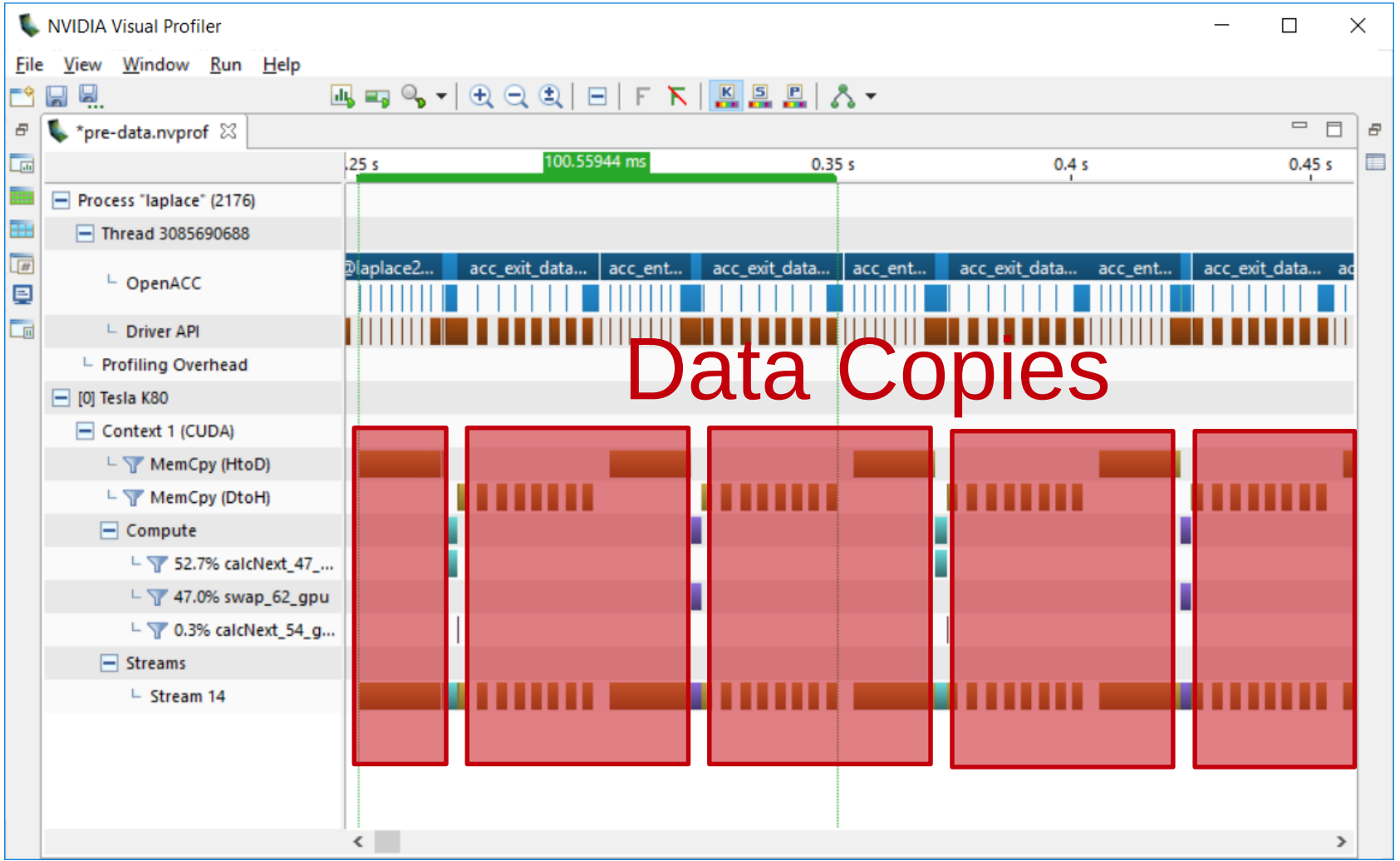
WHAT WENT WRONG?

- The code now has all of the information necessary to build without managed memory, but it runs much slower.
- Profiling tools are here to help!

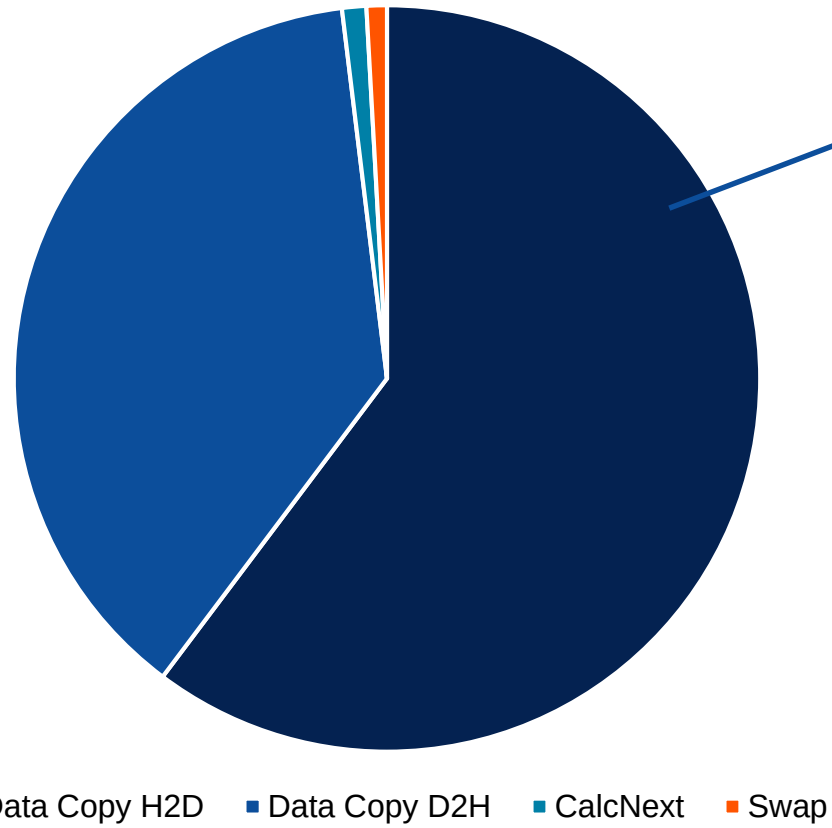
APPLICATION PROFILE (2 STEPS)



APPLICATION PROFILE (2 STEPS)



RUNTIME BREAKDOWN



Nearly all of our time is spent moving data to/from the GPU

OPTIMIZED DATA MOVEMENT

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

#pragma acc parallel loop reduction(max:err) copyin(A[0:n*m]) copy(Anew[0:n*m])
  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]);

      err = max(err, abs(Anew[j][i] - A[j][i]));
    }
  }

#pragma acc parallel loop copyin(Anew[0:n*m]) copyout(A[0:n*m])
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
  iter++;
}
```

Currently we're copying to/from the GPU for each loop, can we reuse it?

OPTIMIZE DATA MOVEMENT

OPENACC DATA DIRECTIVE

Definition

- The data directive defines a lifetime for data on the device beyond individual loops
- During the region data is essentially “owned by” the accelerator
- Data clauses express shape and data movement for the region

```
#pragma acc data clauses
{

  < Sequential and/or Parallel code >

}
```

```
!$acc data clauses

  < Sequential and/or Parallel code >

!$acc end data
```

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
[illegible]

OPTIMIZED DATA MOVEMENT

```
#pragma acc data copy(A[:n*m]) copyin(Anew[:n*m])
while ( err > tol && iter < iter_max ) {
  err=0.0;

#pragma acc parallel loop reduction(max:err) copyin(A[0:n*m])
  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]);

      err = max(err, abs(Anew[j][i] - A[j][i]));
    }
  }

#pragma acc parallel loop copyin(Anew[0:n*m]) copyout(A[0:n*m])
  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 to/from the accelerator only when needed.

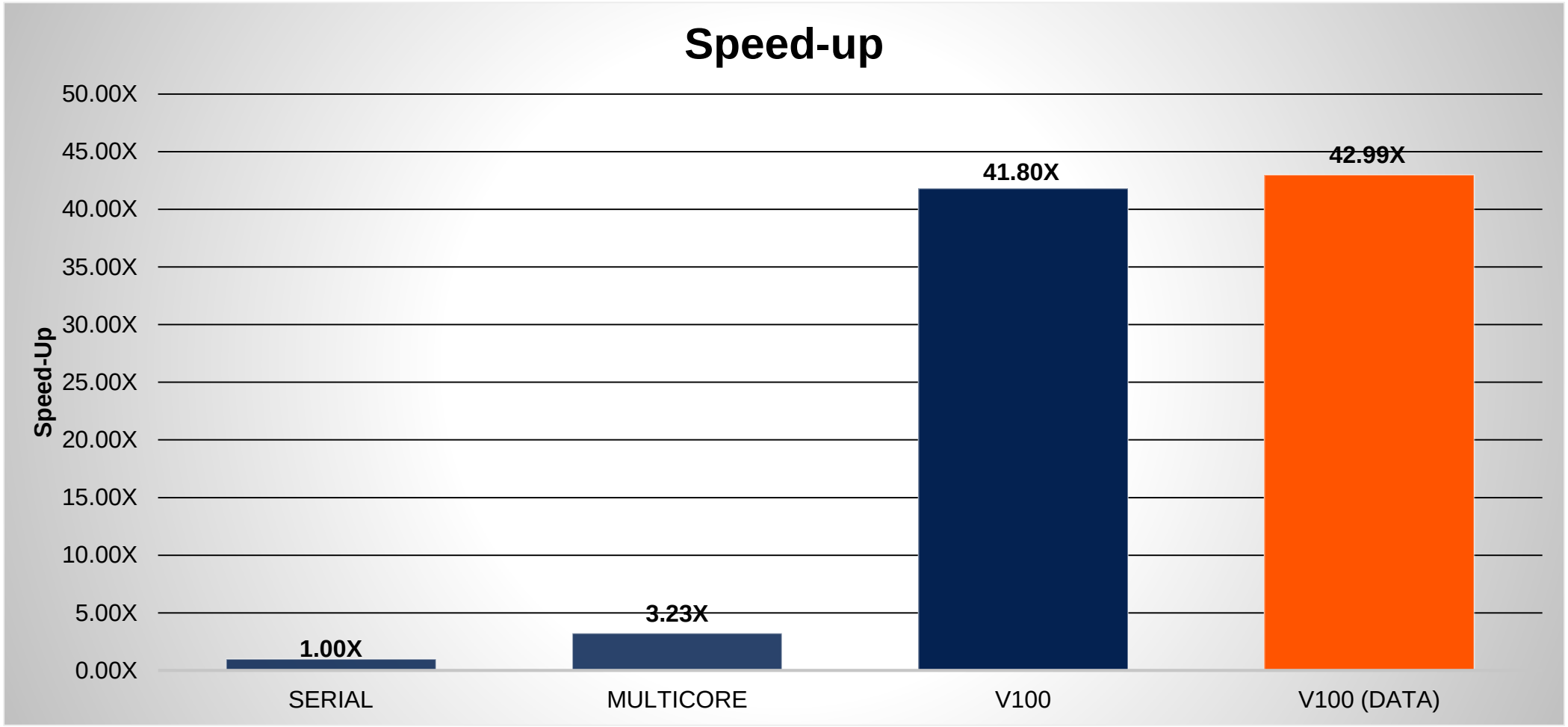
Copy initial condition of Anew, but not final value

REBUILD THE CODE

```
pgcc -fast -ta=tesla -Minfo=accel laplace2d_uvm.c
main:
     60, Generating copy(A[:m*n])
         Generating copyin(Anew[:m*n])
     64, Accelerator kernel generated
         Generating Tesla code
         64, Generating reduction(max:error)
         65, #pragma acc loop gang /* blockIdx.x */
         67, #pragma acc loop vector(128) /* threadIdx.x */
     67, Loop is parallelizable
     75, Accelerator kernel generated
         Generating Tesla code
         76, #pragma acc loop gang /* blockIdx.x */
         78, #pragma acc loop vector(128) /* threadIdx.x */
     78, Loop is parallelizable
```

Now data movement only happens at our data region.

OPENACC SPEED-UP



WHAT WE'VE LEARNED SO FAR

- CUDA Unified (Managed) Memory is a powerful porting tool
- GPU programming without managed memory often requires data shaping
- Moving data at each loop is often inefficient
- The OpenACC Data region can decouple data movement and computation

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])
```

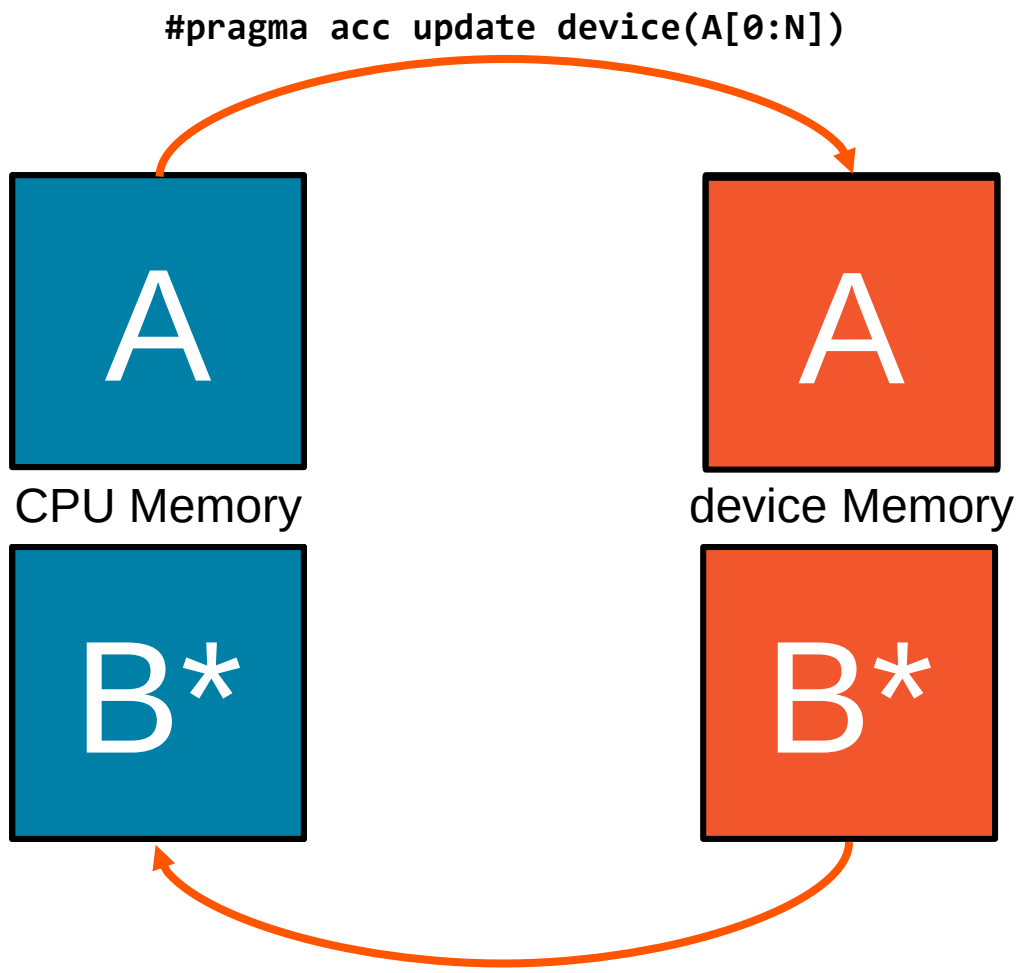
C/C++

```
!$acc update self(x(1:end_index))
!$acc update device(x(1:end_index))
```

Fortran

OPENACC UPDATE DIRECTIVE

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



SYNCHRONIZE DATA WITH UPDATE

```
int* A=(int*) malloc(N*sizeof(int)
#pragma acc data create(A[0:N])
while( timesteps++ < numSteps )
{
  #pragma acc parallel loop
  for(int i = 0; i < N; i++){
    a[i] *= 2;
  }

  if (timestep % 100 ) {
    #pragma acc update self(A[0:N])
    checkpointAToFile(A, N);
  }
}
```

- Sometimes data changes on the host or device inside a data region
- Ending the data region and starting a new one is expensive
- Instead, update the data so that the host and device data are the same
- Examples: File I/O, Communication, etc.

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
```

```
!$acc enter data clauses

  < Sequential and/or Parallel code >

!$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
```

```
!$acc enter data clauses

  < Sequential and/or Parallel code >

!$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]) delete(a,b)
```

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.

C/C++ STRUCTS/CLASSES

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);
}
```

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

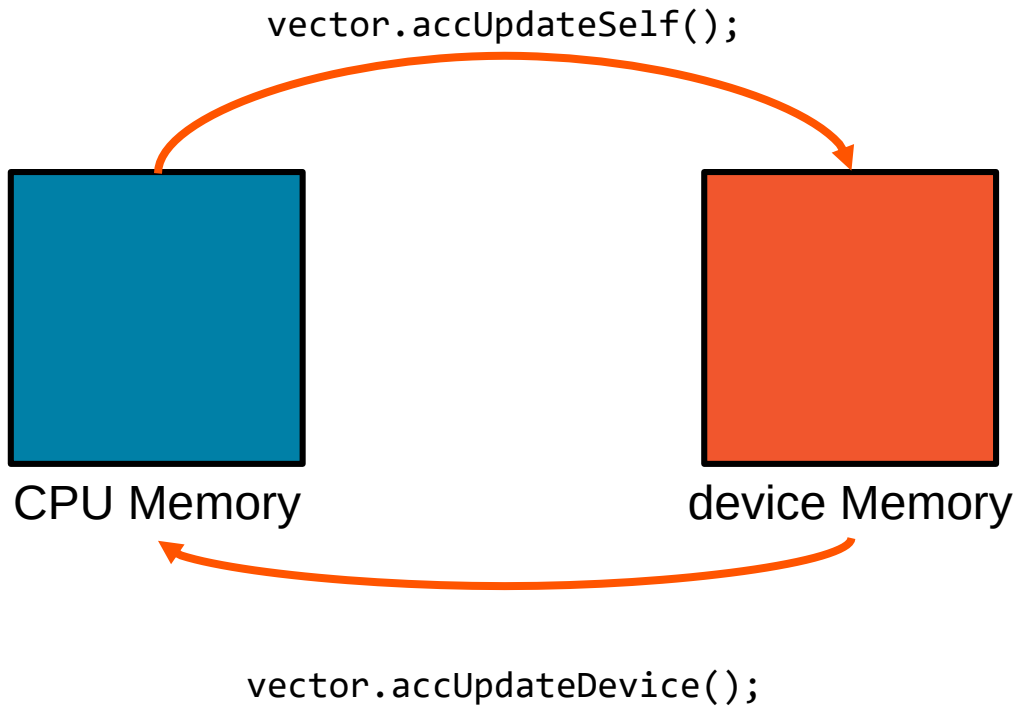
With dynamic data members

- 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);
    }
};
```

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])
}
```

OPENACC RESOURCES

Guides • Talks • Tutorials • Videos • Books • Spec • Code Samples • Teaching Materials • Events • Success Stories • Courses • Slack • Stack Overflow

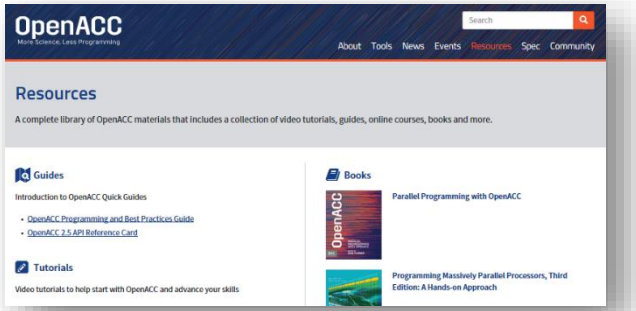
FREE Compilers

PGI® Community EDITION

OpenACC More Science, Less Programming | NVIDIA | aws | Linux Academy

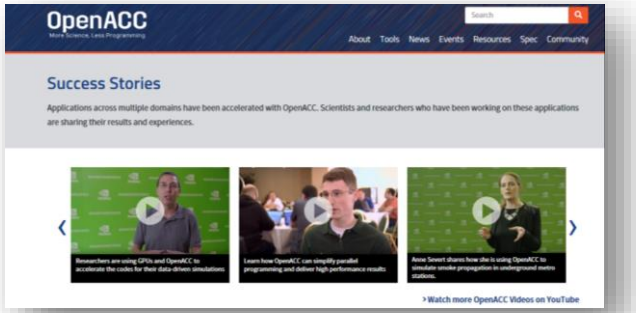
Resources

https://www.openacc.org/resources



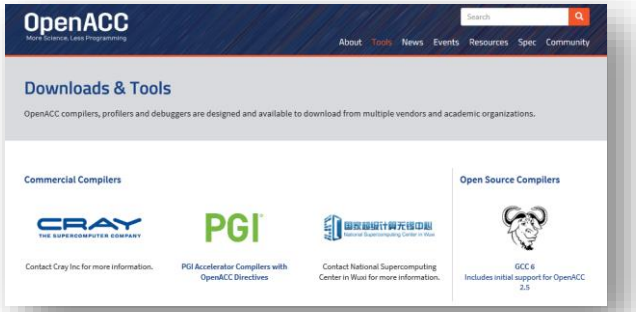
Success Stories

https://www.openacc.org/success-stories



Compilers and Tools

https://www.openacc.org/tools



Events

https://www.openacc.org/events

CLOSING REMARKS

KEY CONCEPTS

In this lecture we discussed…

- Differences between CPU, GPU, and Unified Memories
- OpenACC Array Shaping
- OpenACC Data Clauses
- OpenACC Structured Data Region
- OpenACC Update Directive
- OpenACC Unstructured Data Directives

Next Week: Loop Optimizations