OPENACC ONLINE COURSE

Module 2 – OpenACC Data Management

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NVIDIA Corporation

OpenACC

More Science, Less Programming

NVIDIA

ABOUT THIS COURSE

3 Part Introduction to OpenACC

- Module 1 – Introduction to OpenACC ✓
- Module 2 – Data Management with OpenACC
- Module 3 – Optimizations with OpenACC

Each module will have a corresponding lab

COURSE OBJECTIVE

Enable ***YOU*** to accelerate ***YOUR*** applications with OpenACC.

MODULE 2 OUTLINE

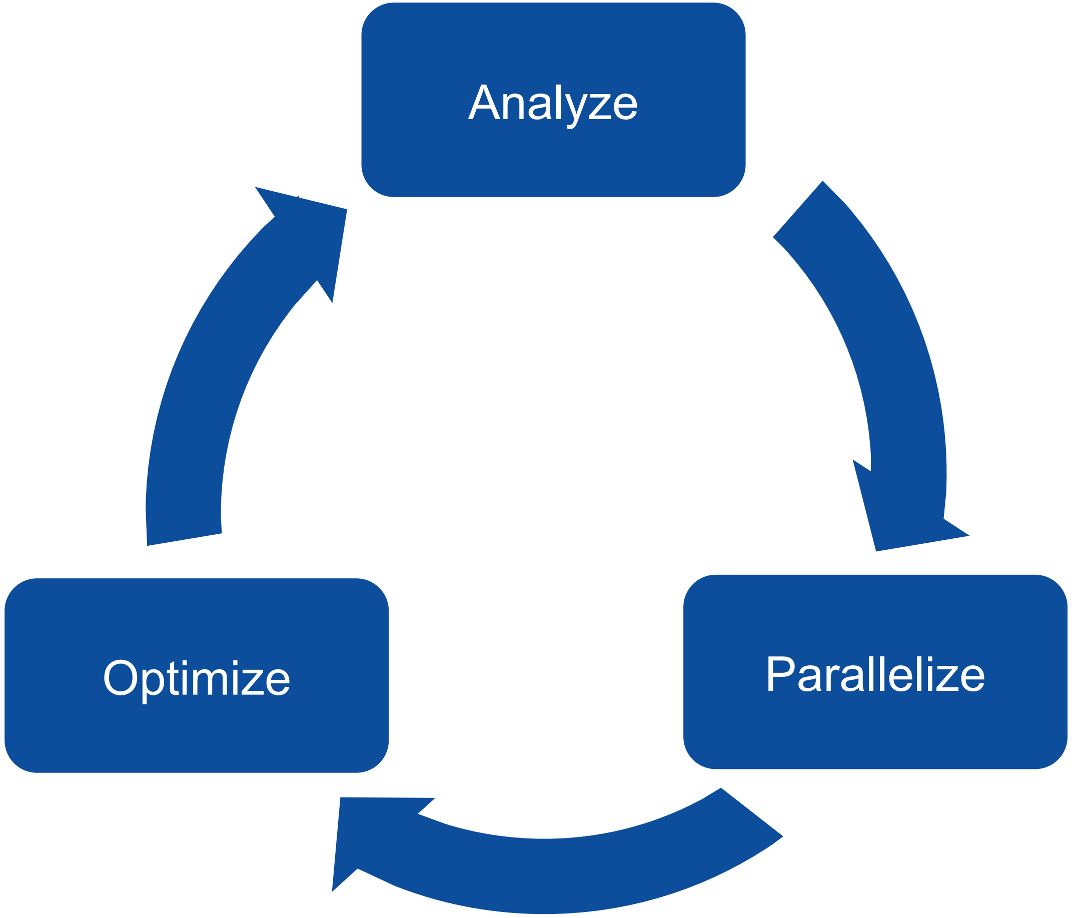
Topics to be covered

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

MODULE 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
      for (i = 0; i < n; ++i) {
  #pragma acc loop vector
        for (j = 0; j < n; ++j) {
          c[i][j] = a[i][j] + b[i][j];
          ...
        }
      }
  }
  ...
}
```

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

OpenACC
Directives for Accelerators

OpenACC Directives

This Module:
Manage Data Movement

Last Module:
Run loops in parallel

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

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

OpenACC
Directives for Accelerators

PARALLELIZE WITH OPENACC PARALLEL LOOP

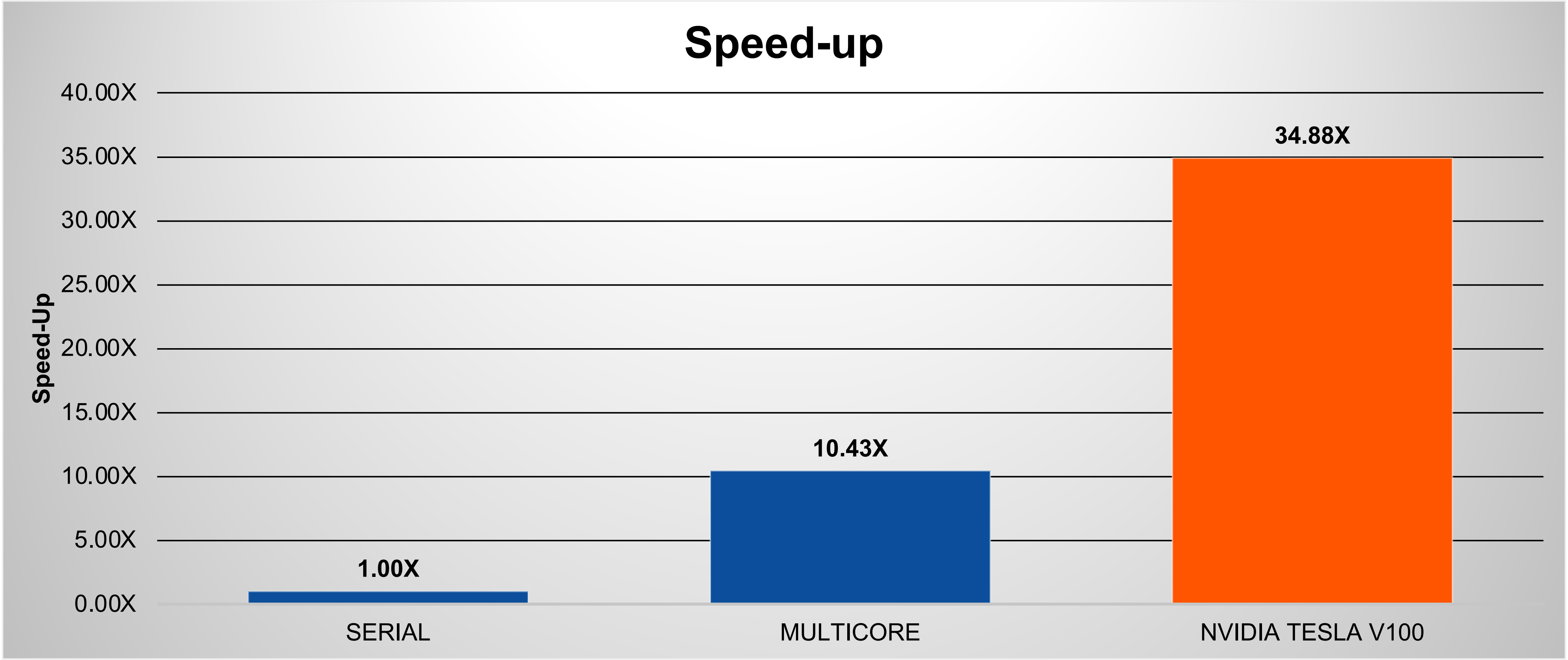
```
while ( err > tol && iter < iter_max ) {
  err=0.0;

#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.

OPENACC SPEED-UP

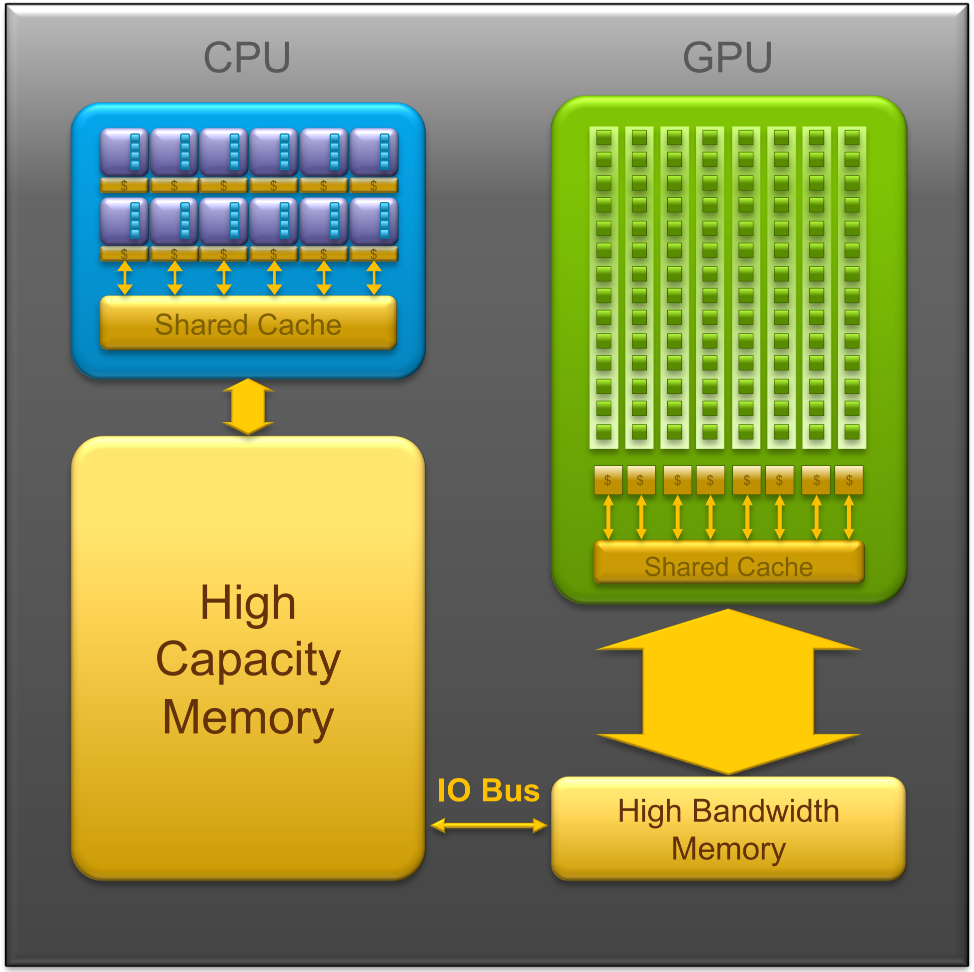


PGI 19.10, NVIDIA Tesla V100, IBM POWER9 22-core CPU @ 3.07GHz

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 PCIe)
- 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



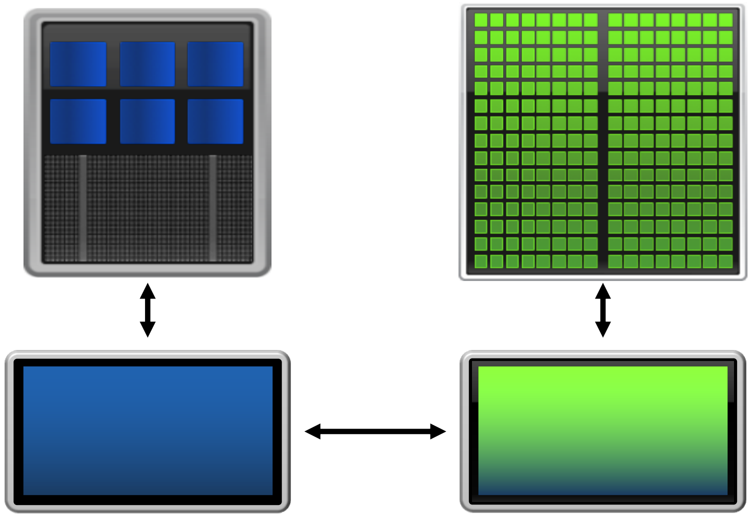
CUDA UNIFIED MEMORY

CUDA UNIFIED MEMORY

Simplified Developer Effort

Commonly referred to as *"managed memory."*

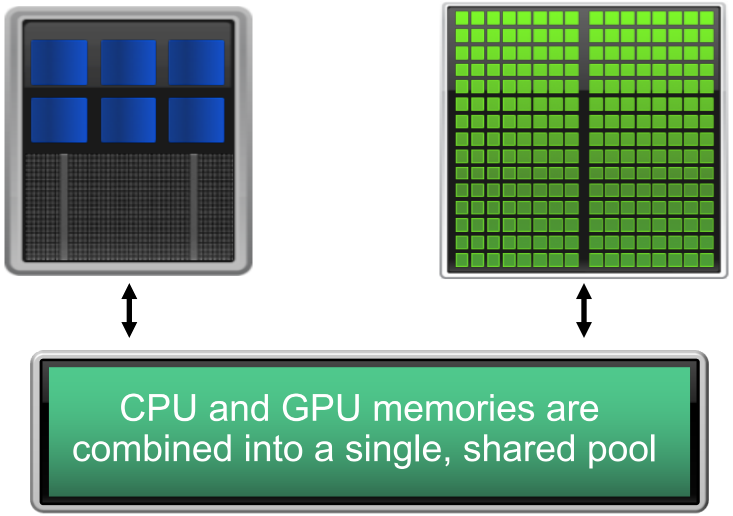
Without Managed Memory



System Memory

GPU Memory

With Managed Memory



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

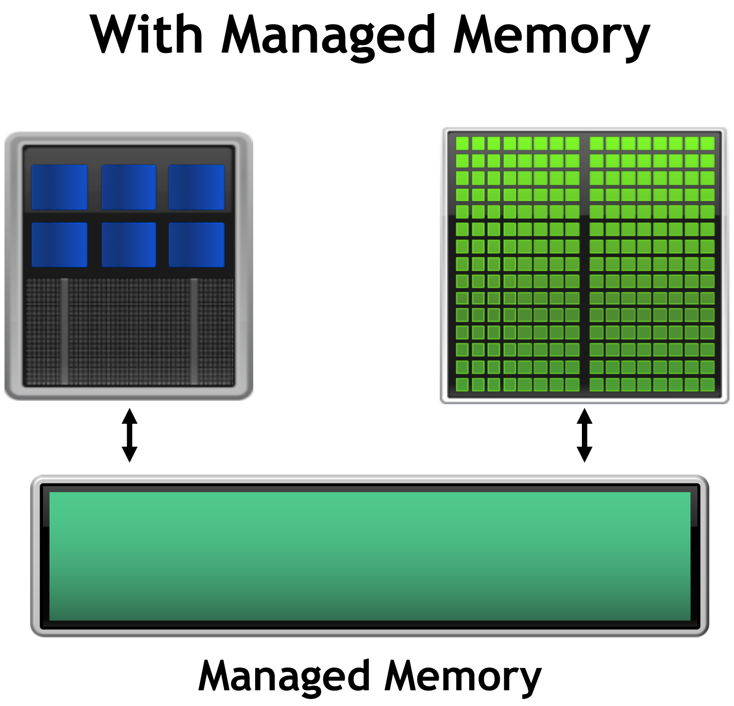
```
$ pgcc -fast -ta=tesla:managed -Minfo=accel main.c
```

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

MANAGED MEMORY

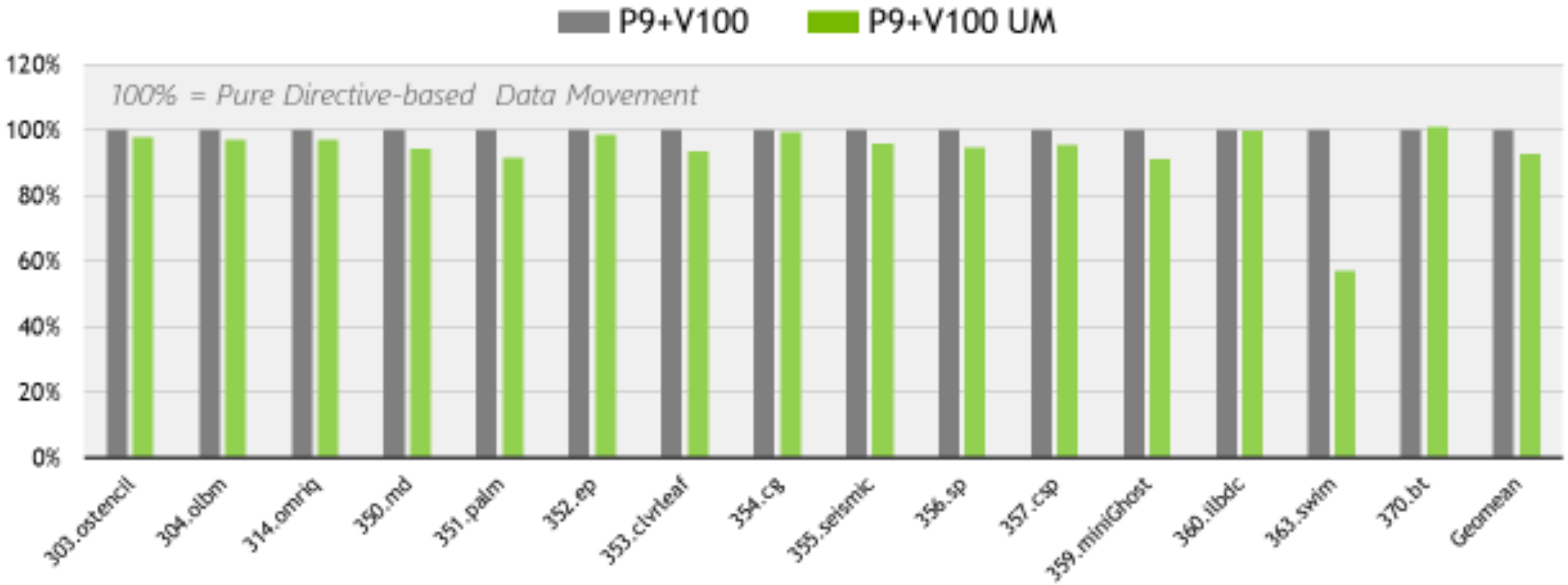
Limitations

- 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.

* Slide Courtesy of NVIDIA

LAST MODULE WE USED UNIFIED MEMORY

Now let’s make our code run without.

Why?

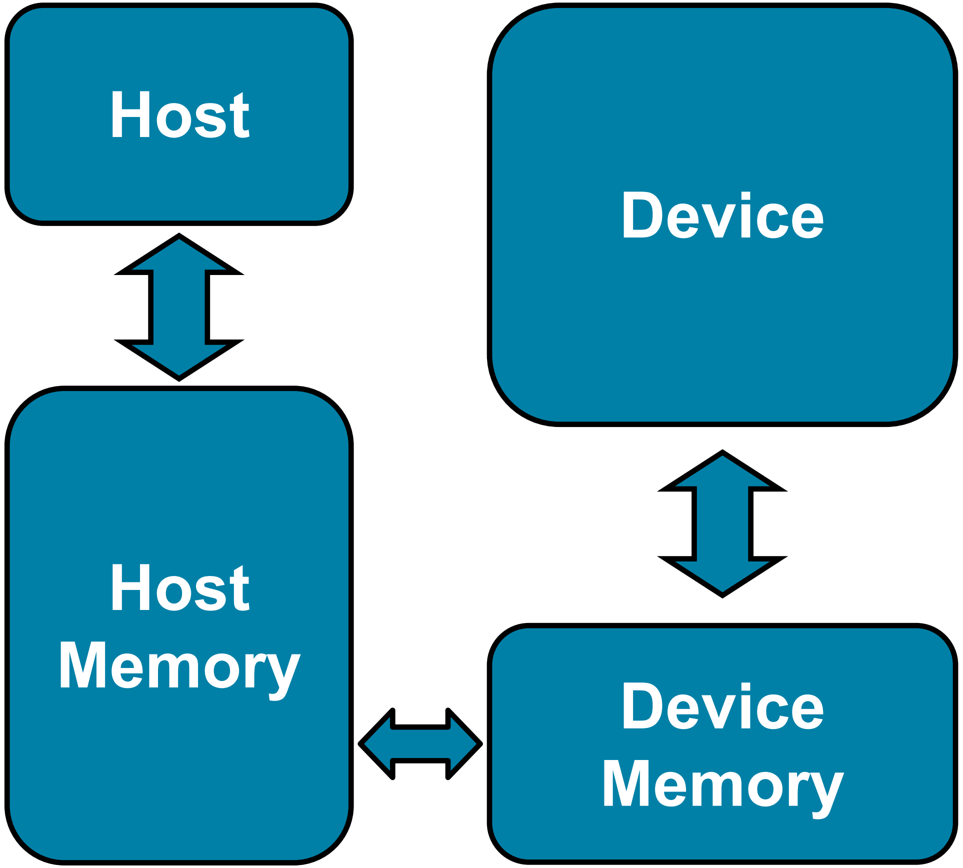
- Removes reliance on PGI and NVIDIA GPUs
- Currently the data always arrives “Just Too Late”, let’s do better

BASIC DATA MANAGEMENT

BASIC DATA MANAGEMENT

Between the host and device

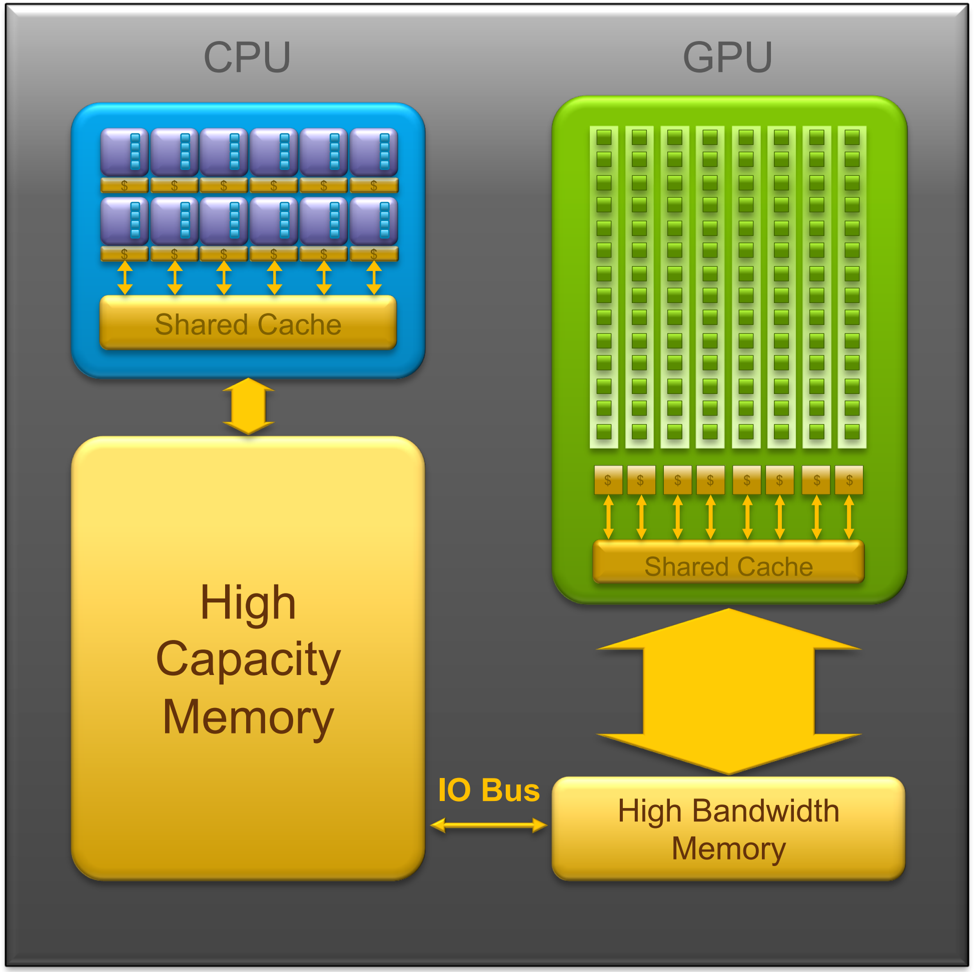
- The **host** is traditionally a CPU
- The **device** is some parallel accelerator
- When our target hardware is multicore, the host and device are the same, meaning that their memory is also the same
- There is no need to explicitly manage data when using a shared memory accelerator, such as the multicore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

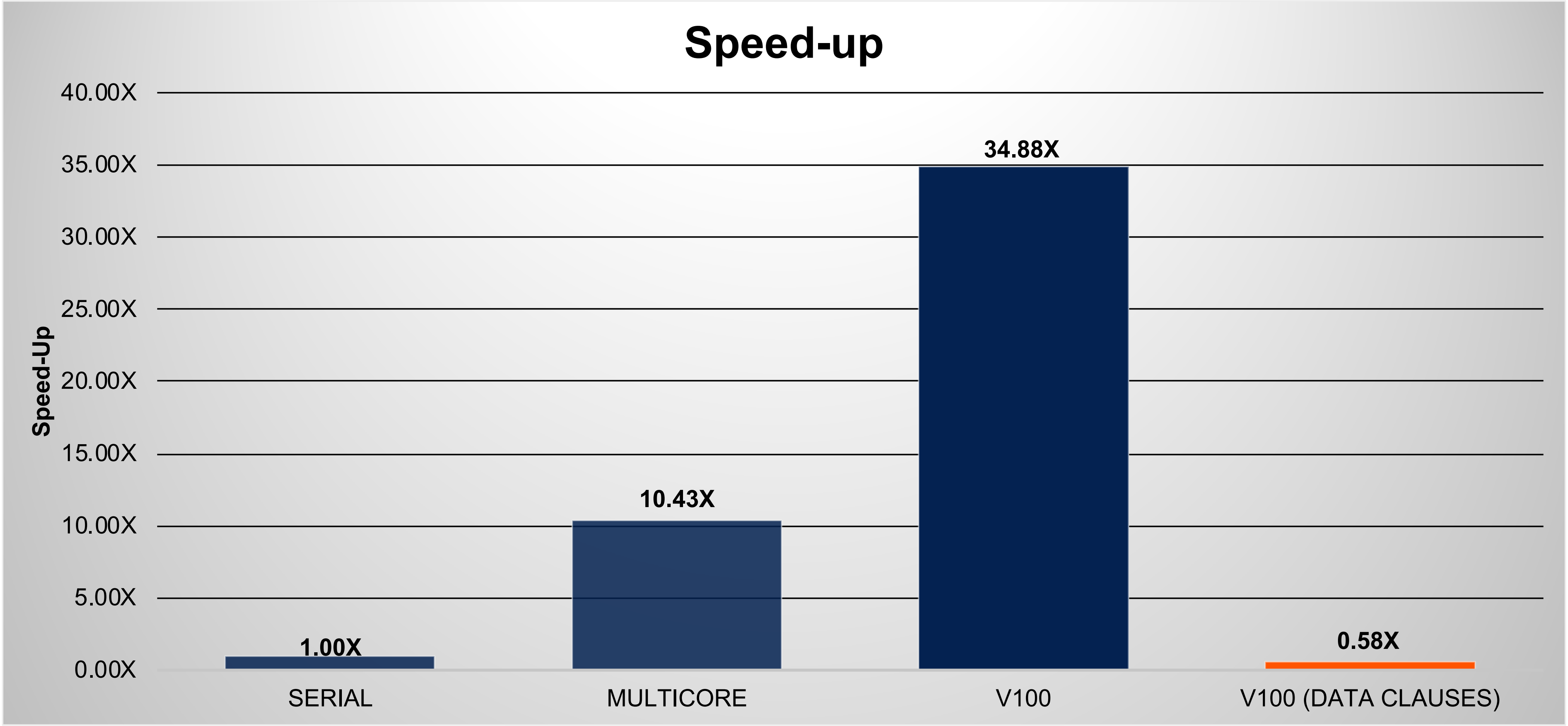
Data clauses provide necessary “shape” to the arrays.

TRY TO BUILD WITHOUT “MANAGED”

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

```
pgcc -ta=tesla -Minfo=accel -Mcuda -lnvToolsExt 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:
```

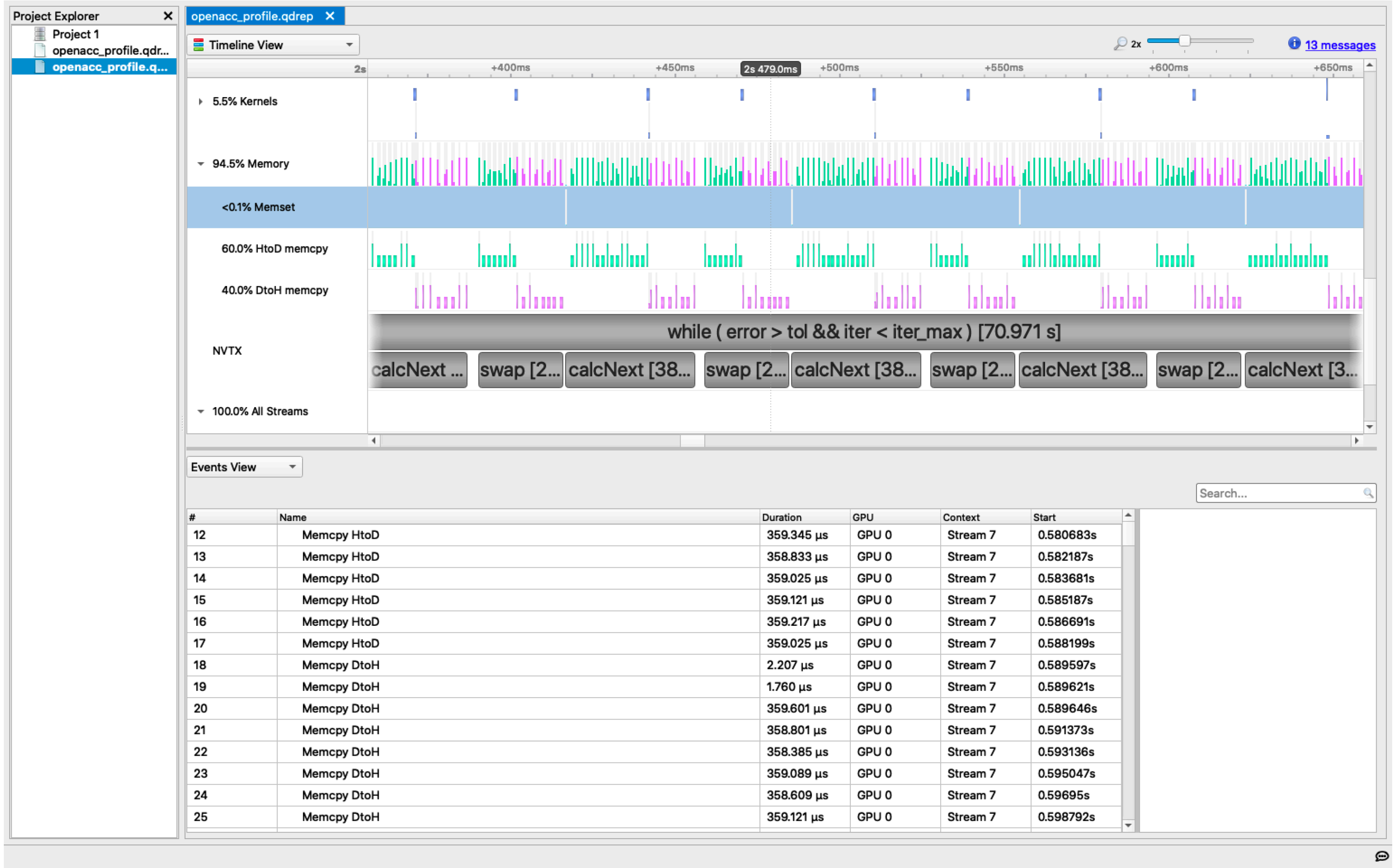
OPENACC ~~SPEED-UP~~ SLOWDOWN



WHAT WENT WRONG?

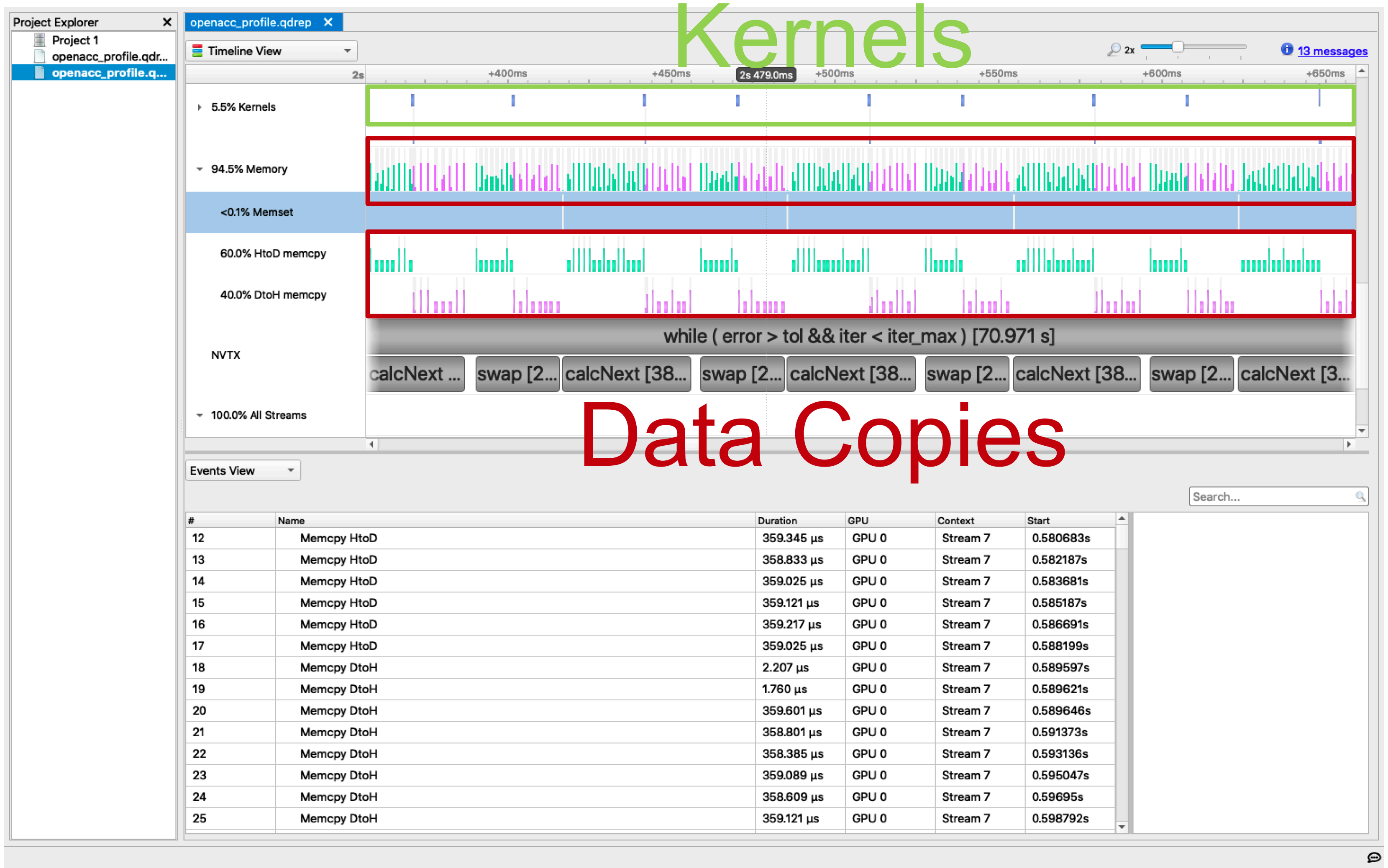
- The code now has all of the information necessary to build without managed memory, but it runs much slower.
- Profiling tools are here to help!

APPLICATION PROFILE

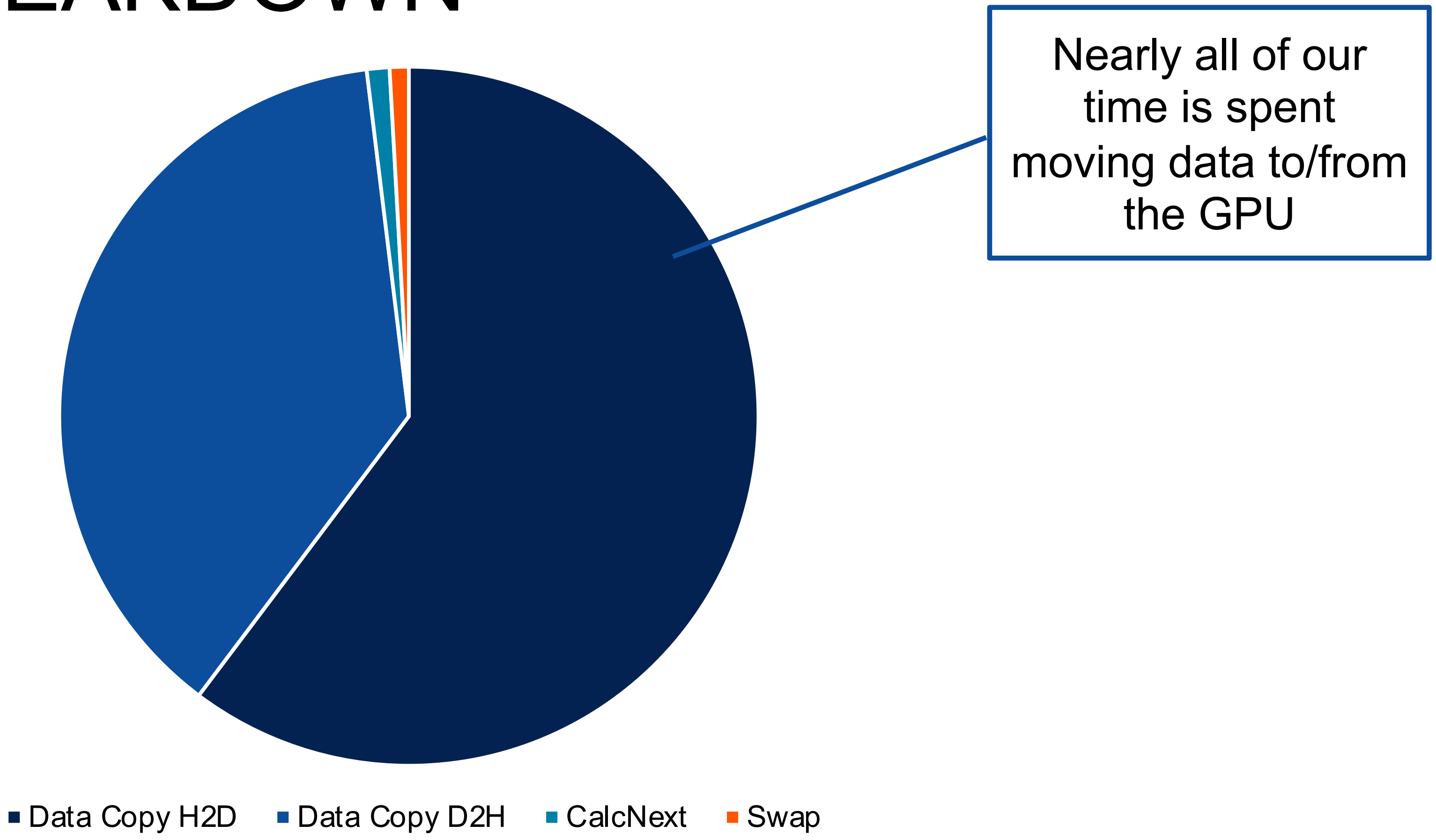


#	Name	Duration	GPU	Context	Start
12	Memcpy HtoD	359.345 µs	GPU 0	Stream 7	0.580683s
13	Memcpy HtoD	358.833 µs	GPU 0	Stream 7	0.582187s
14	Memcpy HtoD	359.025 µs	GPU 0	Stream 7	0.583681s
15	Memcpy HtoD	359.121 µs	GPU 0	Stream 7	0.585187s
16	Memcpy HtoD	359.217 µs	GPU 0	Stream 7	0.586691s
17	Memcpy HtoD	359.025 µs	GPU 0	Stream 7	0.588199s
18	Memcpy DtoH	2.207 µs	GPU 0	Stream 7	0.589597s
19	Memcpy DtoH	1.760 µs	GPU 0	Stream 7	0.589621s
20	Memcpy DtoH	359.601 µs	GPU 0	Stream 7	0.589646s
21	Memcpy DtoH	358.801 µs	GPU 0	Stream 7	0.591373s
22	Memcpy DtoH	358.385 µs	GPU 0	Stream 7	0.593136s
23	Memcpy DtoH	359.089 µs	GPU 0	Stream 7	0.595047s
24	Memcpy DtoH	358.609 µs	GPU 0	Stream 7	0.59695s
25	Memcpy DtoH	359.121 µs	GPU 0	Stream 7	0.598792s

APPLICATION PROFILE



RUNTIME BREAKDOWN



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

Host Memory

A | B | C'

Device memory

A | B | C'

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.

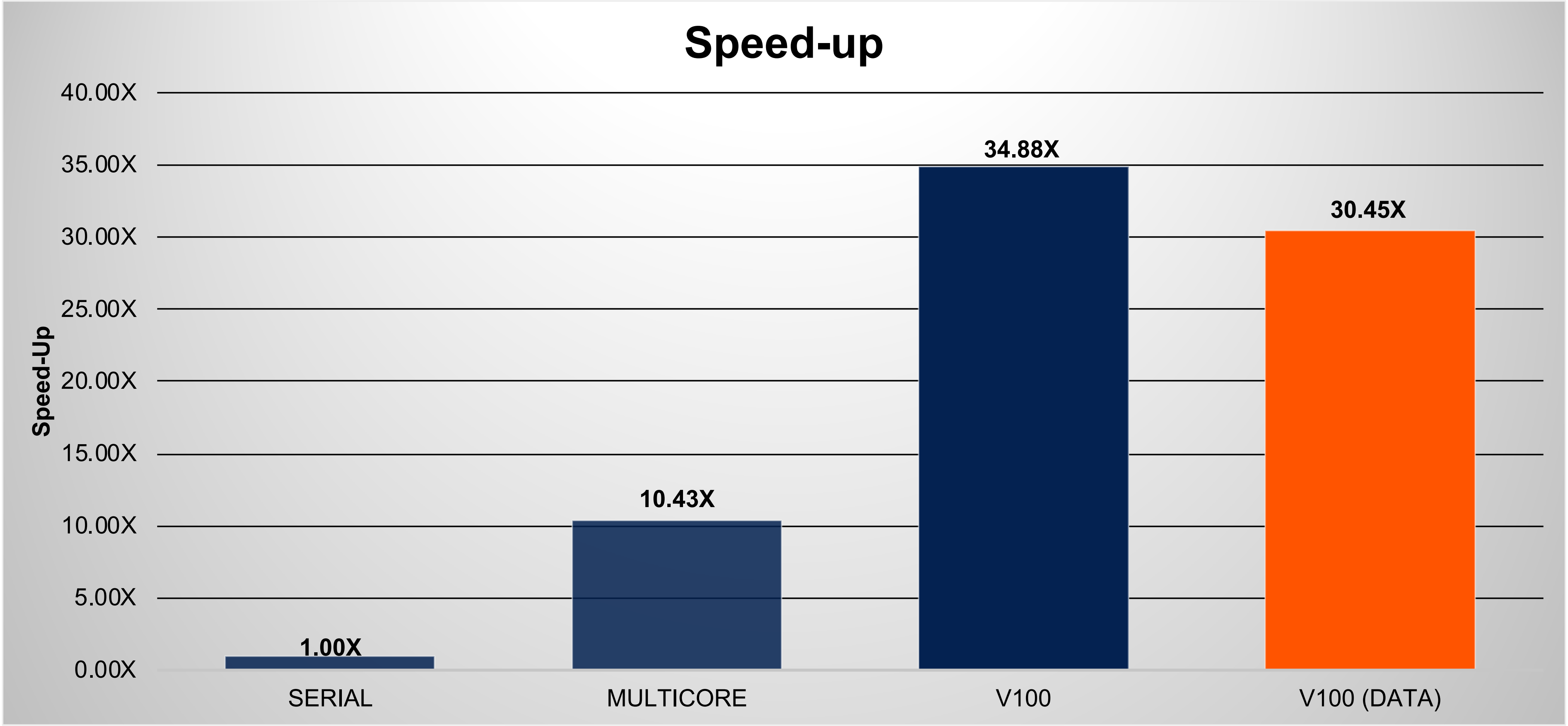
Copy initial condition of Anew, but not final value

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 outer 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

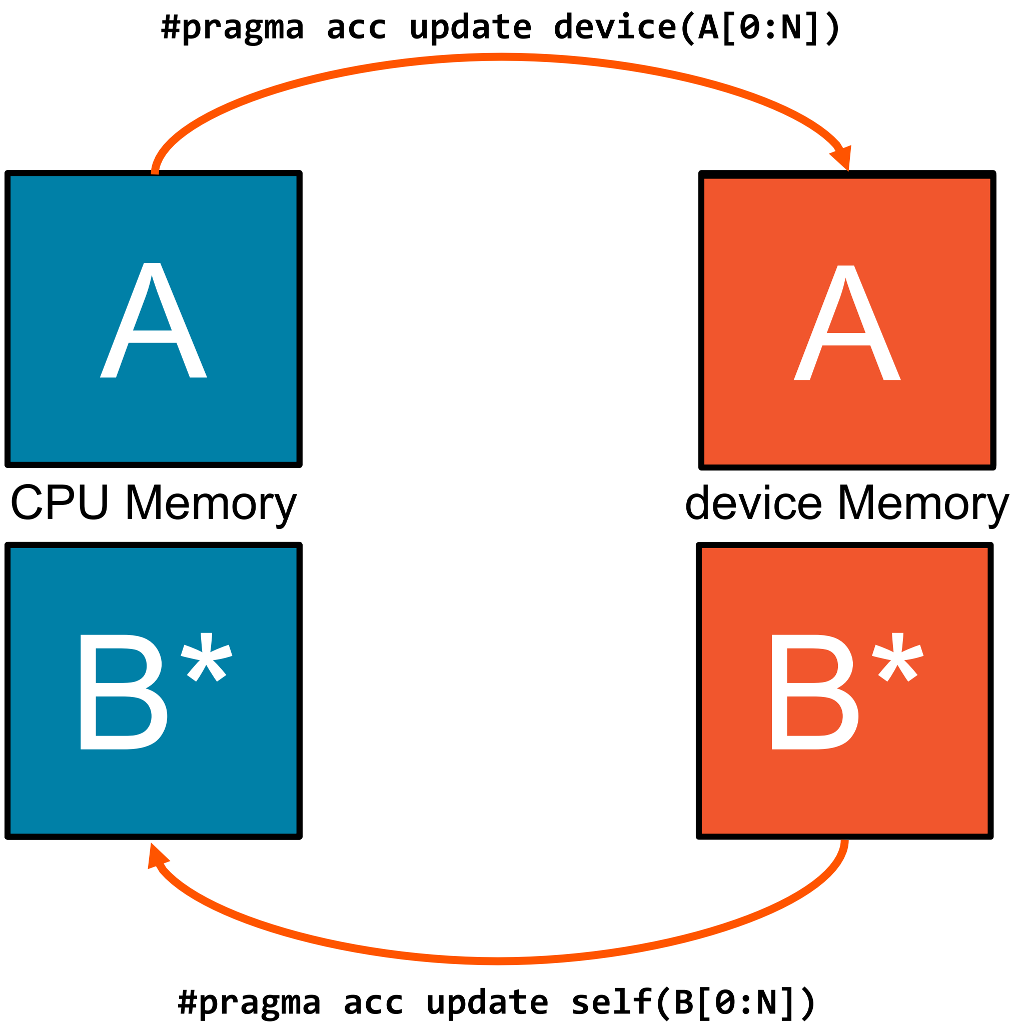
```c
#pragma acc update self(x[0:count])
#pragma acc update device(x[0:count])
```

C/C++

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

OpenACC More Science, Less Programming NVIDIA.

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.

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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
```

```
!$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

Enter data:

`copyin ( list )`	Allocates memory on device and copies data from host to device on enter data.
`create ( list )`	Allocates memory on device without data transfer on enter data.

Exit data:

`copyout ( list )`	Allocates memory on device and copies data back to the host on exit 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];
  }

}
```

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);
    }
};
```

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.

OPENACC RESOURCES

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

FREE Compilers

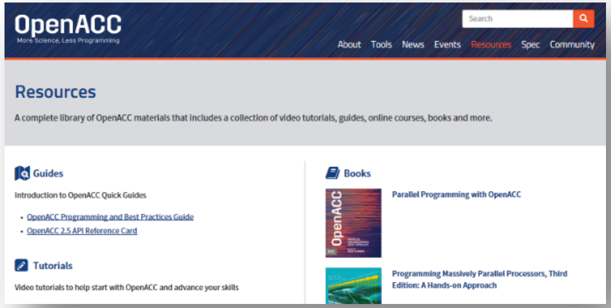
PGI Community EDITION

slack

https://www.openacc.org/community#slack

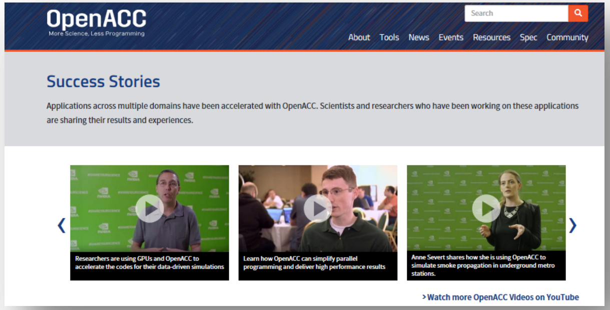
Resources

https://www.openacc.org/resources



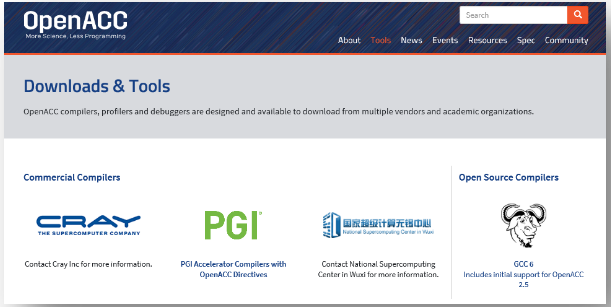
Success Stories

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



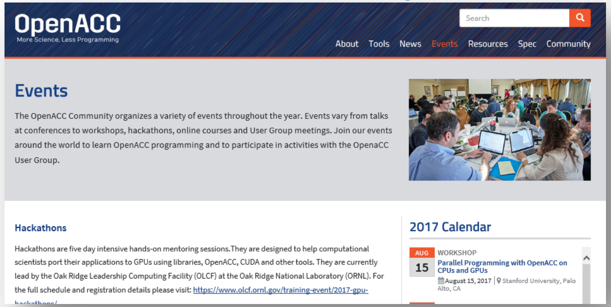
Compilers and Tools

https://www.openacc.org/tools



Events

https://www.openacc.org/events



OpenACC More Science, Less Programming

NVIDIA

CLOSING REMARKS

KEY CONCEPTS

In this module 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 Module: Loop Optimizations