# ZEROTOGPULEROWITH OPENACO

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### OUTLINE

### Topics to be covered

- What is OpenACC
- Profile-driven Development
- OpenACC with CUDA Unified Memory
- OpenACC Data Directives
- OpenACC Loop Optimizations
- Where to Get Help







# INTRODUCTION TO OPENACC





**OpenACC** is a directivesbased programming approach to parallel computing designed for performance and portability on CPUs and GPUs for HPC.

```
Add Simple Compiler Directive
main()
  <serial code>
  #pragma acc kernels
    <parallel code>
```





# 3 WAYS TO ACCELERATE APPLICATIONS

# Applications

Libraries

Easy to use Most Performance Compiler Directives

Easy to use Portable code

**OpenACC** 

Programming Languages

Most Performance Most Flexibility

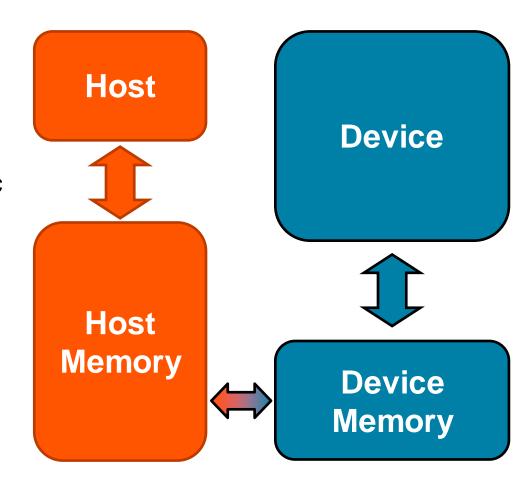




# **OPENACC PORTABILITY**

### Describing a generic parallel machine

- OpenACC is designed to be portable to many existing and future parallel platforms
- The programmer need not think about specific hardware details, but rather express the parallelism in generic terms
- An OpenACC program runs on a *host* (typically a CPU) that manages one or more parallel devices (GPUs, etc.). The host and device(s) are logically thought of as having separate memories.



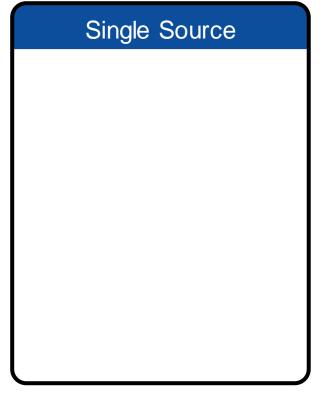


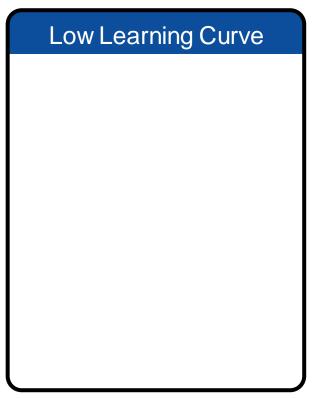




### Three major strengths

Incremental









#### Incremental

- Maintain existing sequential code
- Add annotations to expose parallelism
- After verifying correctness, annotate more of the code

Begin with a working sequential code.

Parallelize it with OpenACC.

Rerun the code to verify correct behavior, remove/alter OpenACC code as needed.







#### Incremental

- Maintain existing sequential code
- Add annotations to expose parallelism
- After verifying correctness, annotate more of the code

#### Single Source





#### Supported Platforms

**POWER** 

Sunway

x86 CPU

x86 Xeon Phi

**NVIDIA GPU** 

PEZY-SC

#### Single Source

- Rebuild the same code on multiple architectures
- Compiler determines how to parallelize for the desired machine
- Sequential code is maintained

The compiler can **ignore** your OpenACC code additions, so the same code can be used for **parallel** or **sequential** execution.





#### Incremental

- Maintain existing sequential code
- Add annotations to expose parallelism
- After verifying correctness, annotate more of the code

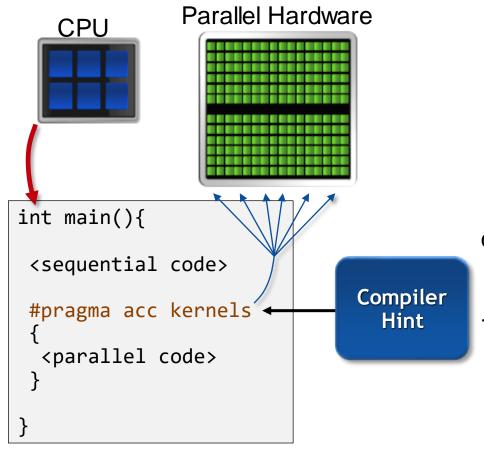
#### Single Source

- Rebuild the same code on multiple architectures
- Compiler determines how to parallelize for the desired machine
- Sequential code is maintained









The programmer will give hints to the compiler about which parts of the code to parallelize.

The compiler will then generate parallelism for the target parallel hardware.

- OpenACC is meant to be easy to use, and easy to learn
- Programmer remains in familiar C, C++, or Fortran
- No reason to learn low-level details of the hardware.







#### Incremental

- Maintain existing sequential code
- Add annotations to expose parallelism
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#### Single Source

- Rebuild the same code on multiple architectures
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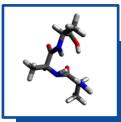
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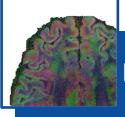


## OPENACC SUCCESSES



#### **LSDalton**

Quantum Chemistry
Aarhus University
12X speedup
1 week



#### **PowerGrid**

Medical Imaging
University of Illinois
40 days to
2 hours



#### COSMO

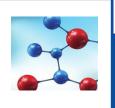
Weather and Climate MeteoSwiss, CSCS 40X speedup 3X energy efficiency



#### **INCOMP3D**

CFD NC State University

4X speedup



#### **NekCEM**

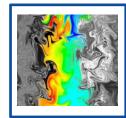
Comp Electromagnetics
Argonne National Lab
2.5X speedup
60% less energy



#### MAESTRO CASTRO

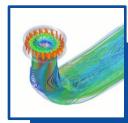
Astrophysics Stony Brook University

> 4.4X speedup 4 weeks effort



#### CloverLeaf

Comp Hydrodynamics
AWE
4X speedup
Single CPU/GPU code



FINE/Turbo

CFD
NUMECA
International
10X faster routines
2X faster app







# OPENACC SYNTAX





### OPENACC SYNTAX

Syntax for using OpenACC directives in code

C/C++

#pragma acc directive clauses <code>

**Fortran** 

!\$acc directive clauses <code>

- A *pragma* in C/C++ gives instructions to the compiler on how to compile the code. Compilers that do not understand a particular pragma can freely ignore it.
- A *directive* in Fortran is a specially formatted comment that likewise instructions the compiler in it compilation of the code and can be freely ignored.
- "acc" informs the compiler that what will come is an OpenACC directive
- **Directives** are commands in OpenACC for altering our code.
- **Clauses** are specifiers or additions to directives.







# EXAMPLE CODE



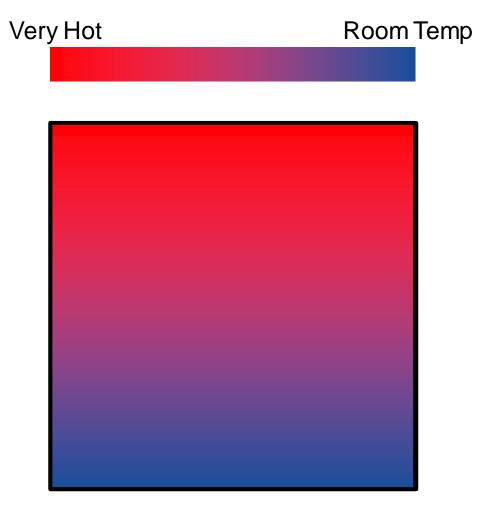


### LAPLACE HEAT TRANSFER

We will observe a simple simulation of heat distributing across a metal plate.

We will apply a consistent heat to the top of the plate.

Then, we will simulate the heat distributing across the plate.









### **EXAMPLE: JACOBI ITERATION**

- Iteratively converges to correct value (e.g. Temperature), by computing new values at each point from the average of neighboring points.
- Common, useful algorithm
- Example: Solve Laplace equation in 2D:  $\nabla^2 f(x, y) = 0$

A(i,j+1)
$$A(i-1,j)$$

$$A(i,j-1)$$

$$A(i+1,j)$$

$$A(i+1,j)$$

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



### JACOBI ITERATION: C CODE

```
while ( err > tol && iter < iter max ) {</pre>
        err=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]);
            err = max(err, 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++;
OpenACC
```

Iterate until converged

Iterate across matrix elements

Calculate new value from neighbors

Compute max error for convergence

Swap input/output arrays

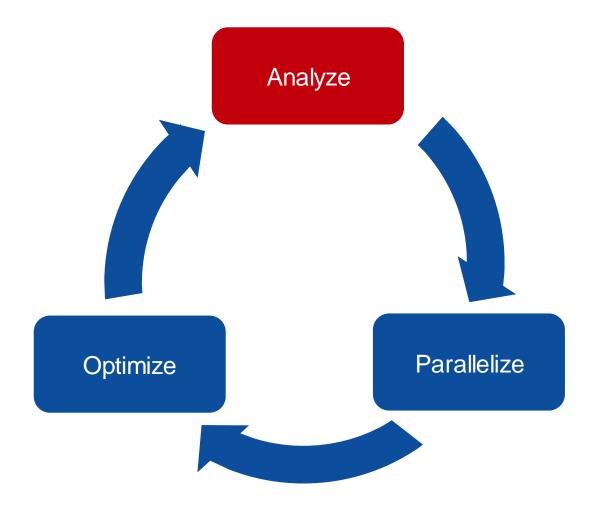
# PROFILE-DRIVEN DEVELOPMENT





### 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.





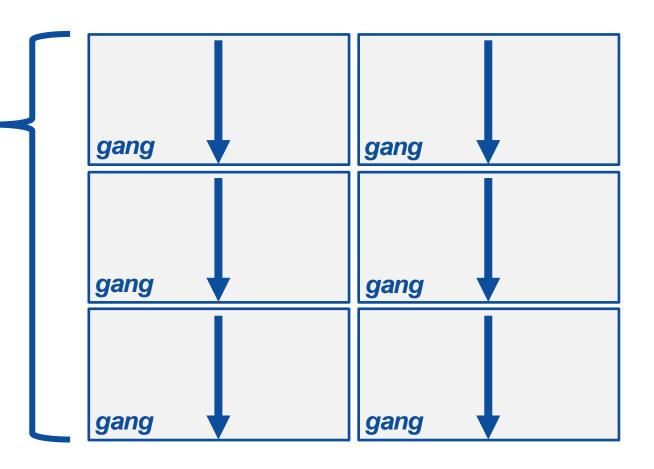




Expressing parallelism

```
#pragma acc parallel
{
```

When encountering the *parallel* directive, the compiler will generate 1 or more parallel gangs, which execute redundantly.







on each gang

**OpenACC** 

Expressing parallelism #pragma acc parallel gang gang loop for(int i = 0; i < N; i++) gang gang // Do Something This loop will be gang gang executed redundantly

OpenACC

Expressing parallelism #pragma acc parallel gang gang for(int i = 0; i < N; i++) gang gang // Do Something This means that each gang gang gang will execute the entire loop DEEP LEARNING

### Parallelizing a single loop

#### C/C++

```
#pragma acc parallel
{
    #pragma acc loop
    for(int i = 0; j < N; i++)
    a[i] = 0;
}</pre>
```

#### Fortran

```
!$acc parallel
  !$acc loop
  do i = 1, N
   a(i) = 0
  end do
!$acc end parallel
```

- Use a parallel directive to mark a region of code where you want parallel execution to occur
- This parallel region is marked by curly braces in C/C++ or a start and end directive in Fortran
- The loop directive is used to instruct the compiler to parallelize the iterations of the next loop to run across the parallel gangs







### Parallelizing a single loop

#### C/C++

```
#pragma acc parallel loop
for(int i = 0; j < N; i++)
  a[i] = 0;</pre>
```

#### Fortran

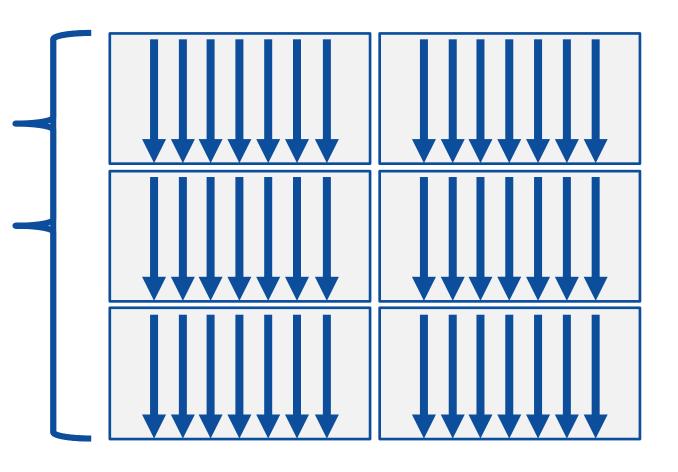
```
!$acc parallel loop
do i = 1, N
   a(i) = 0
end do
```

- This pattern is so common that you can do all of this in a single line of code
- In this example, the parallel loop directive applies to the next loop
- This directive both marks the region for parallel execution and distributes the iterations of the loop.
- When applied to a loop with a data dependency, parallel loop may produce incorrect results



Expressing parallelism

```
#pragma acc parallel
   #pragma acc loop
   for(int i = 0; i < N; i++)</pre>
       // Do Something
          The loop directive
         informs the compiler
            which loops to
              parallelize.
```







### Parallelizing many loops

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

#pragma acc parallel loop
for(int j = 0; j < M; j++)
  b[j] = 0;</pre>
```

- To parallelize multiple loops, each loop should be accompanied by a parallel directive
- Each parallel loop can have different loop boundaries and loop optimizations
- Each parallel loop can be parallelized in a different way
- This is the recommended way to parallelize multiple loops. Attempting to parallelize multiple loops within the same parallel region may give performance issues or unexpected results



### 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.

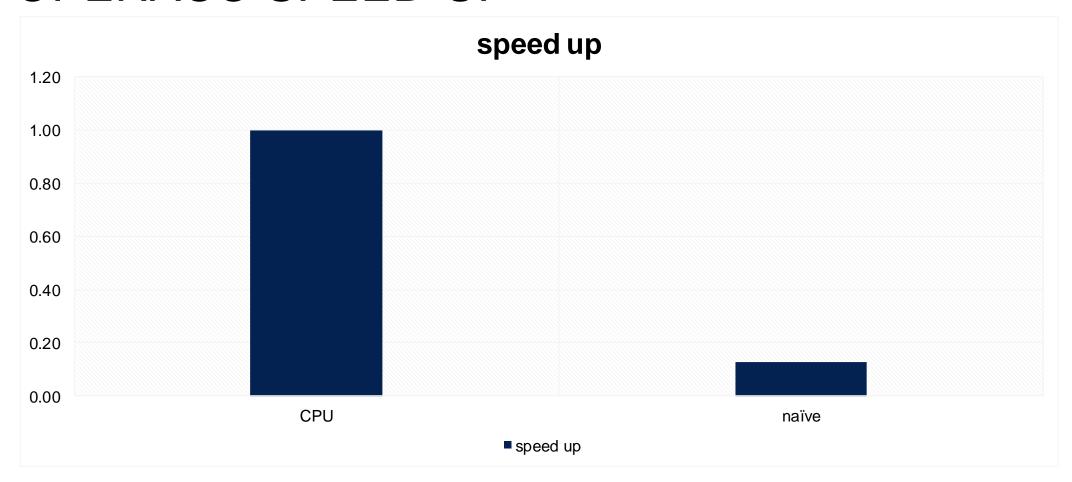
We didn't detail *how* to parallelize the loops, just *which* loops to parallelize.

# BUILDING THE CODE (GPU)

```
pgc++ -acc -fast -Minfo=accel -ta=nvidia,cc75 heat acc naive.cpp -03 -o
heat acc naive.x
main:
     39, Generating Tesla code
         42, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
             Generating reduction (max:error)
         43, #pragma acc loop seg
     39, Generating implicit copyin(A[:1000][:1000]) [if not already present]
         Generating implicit copy(error) [if not already present]
         Generating implicit copyout(Anew[1:998][1:998]) [if not already present]
     43, Complex loop carried dependence of A->, A->->, Anew->-> prevents
parallelization
     48, Generating Tesla code
         51, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
         52, #pragma acc loop seg
     48, Generating implicit copyin (Anew[1:998][1:998]) [if not already present]
         Generating implicit copyout(A[1:998][1:998]) [if not already present]
     52, Complex loop carried dependence of Anew->->, Anew->, A->->, A-> prevents
parallelization
```



# **OPENACC SPEED-UP**







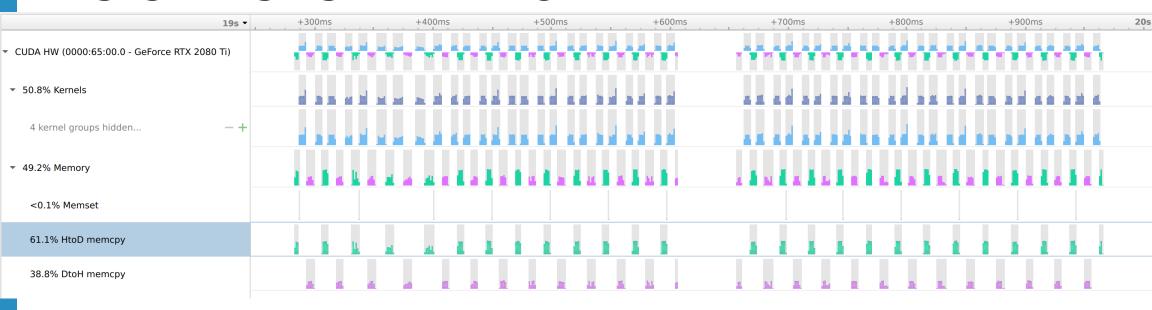
### ... THIS IS EMBARRASSING ...

- Nsight system is your (first) friend when you don't know what's going on with (NVIDIA) GPUs
- Command line way of profiling with nsight system

```
nsys profile -o heat_acc_naive ./heat_acc_naive.x
```

Then open the output file with the GUI interface

### **NSIGHT SYSTEM PROFILE**



- Data movements blobs (red/pink for device to host transfer, green for host to device transfer): for every iteration, data is copied from host to device in small chunks, and after compute they are copied back to host.
- (This should be avoided.)
- Most of the CUDA kernels here aren't the actual compute kernels rather they are some `fill` kernels OpenACC generates.





### ... THIS IS EMBARRASSING ...

- We want to keep data on the device until all computations are done.
- We can tell the compiler to, either:
- 1. "You can use unified virtual memory" (UVM/CUDA managed memory)
- 2. "Please move these data to device when I *tell* you to do so" (explicit data movement)
- Managed memory: compiler prepare two copies of the same data, one on host and one on device. Synchronization between these two copies are managed automatically.
- If for a period all data accesses are from the device, no data movement will be performed in practice.

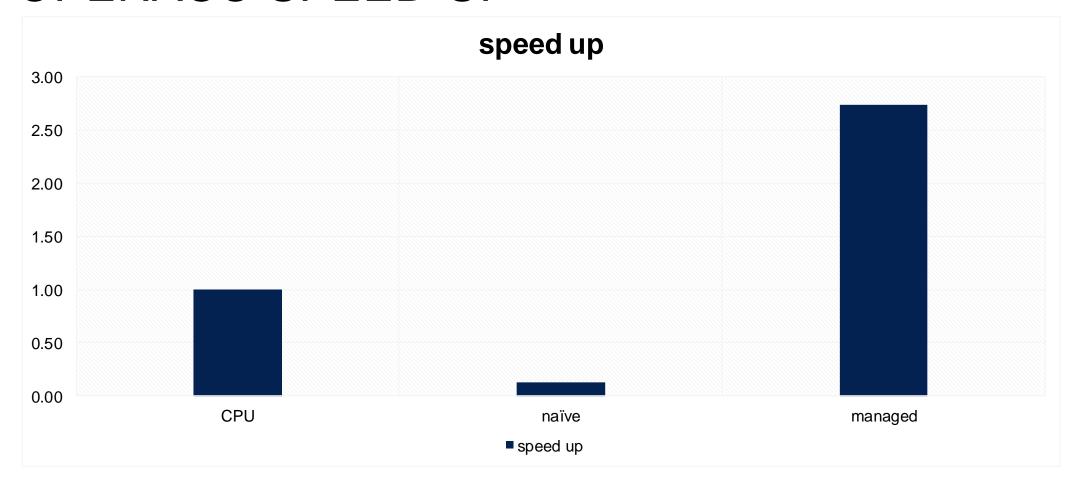


# BUILDING THE CODE (GPU)

```
pgc++ -acc -fast -Minfo=accel -ta=nvidia,cc75,managed heat acc naive.cpp -03 -o
heat acc naive.x
main:
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     52, Complex loop carried dependence of Anew->->, Anew->, A->->, A-> prevents
parallelization
```



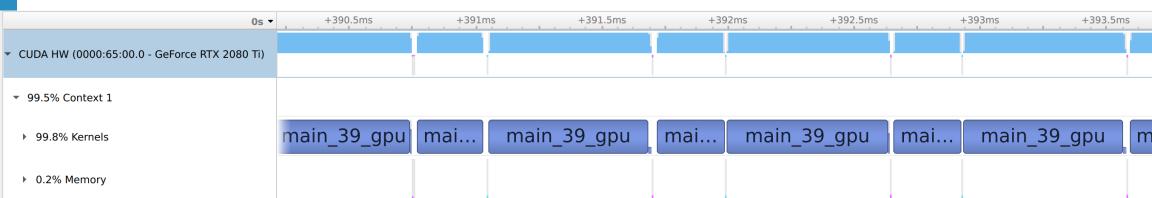
# **OPENACC SPEED-UP**







## **NSIGHT SYSTEM PROFILE**



 Now the only data movements in the main loop are small memset's and memcpy's (for the reduction on error)





# OPTIMIZE DATA MOVEMENT

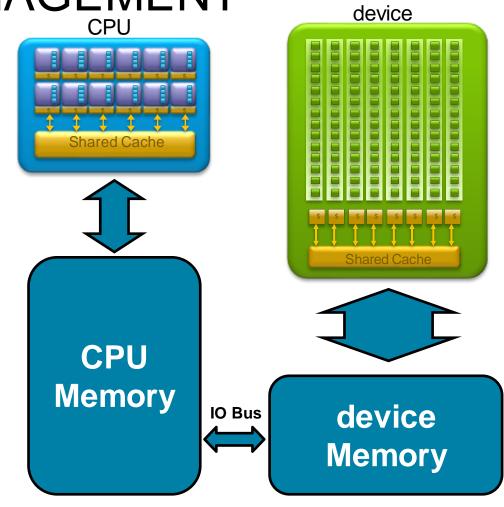




## EXPLICIT MEMORY MANAGEMENT

#### Key problems

- Many parallel accelerators (such as devices) have a separate memory pool 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





## 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 >
}
```

```
!$acc data clauses
  < Sequential and/or Parallel code >
!$acc end data
```





## 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.

OpenACC

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





### 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];
  }
}</pre>
```



#### **Host Memory**











#### OPTIMIZED DATA MOVEMENT

```
#pragma acc data copyin(A[0:n][0:m]) copyout(Anew[0:n][0:m])
while ( err > tol && iter < iter max ) {</pre>
  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++;
```

Copy A to/from the accelerator only when needed.

Copy initial condition of Anew, but not final value

#### REBUILD THE CODE

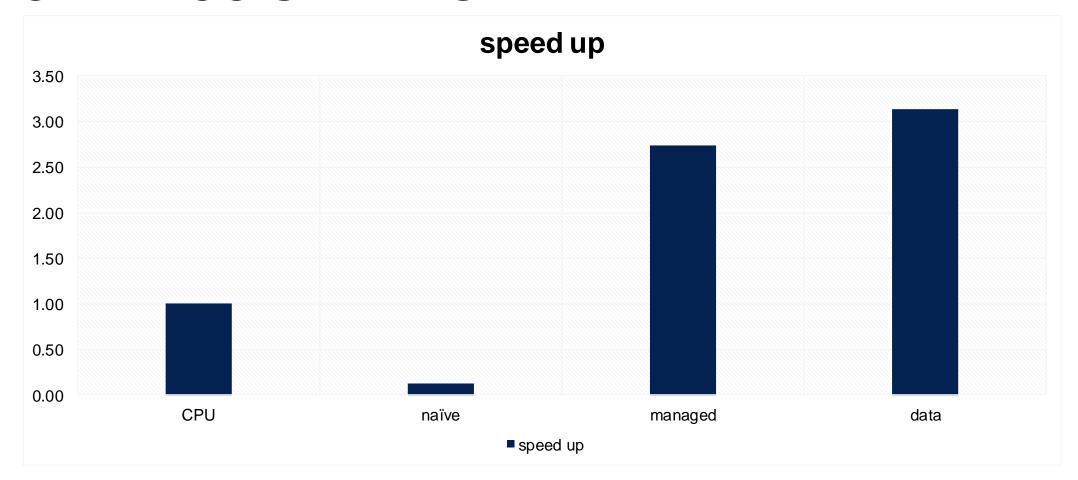
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pgc++ -acc -fast -Minfo=accel -ta=nvidia,cc75 heat acc data.cpp -03 -o
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main:
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     40, Generating Tesla code
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         53, #pragma acc loop seg
     53, Complex loop carried dependence of Anew->->, Anew->, A->->, A-> prevents
parallelization
```



Now data movement only happens at our data region.



# **OPENACC SPEED-UP**







# 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

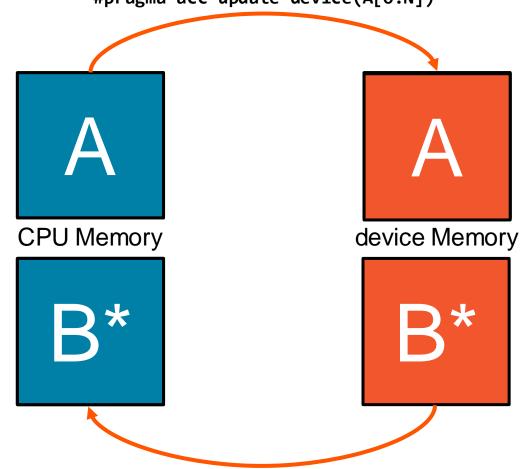




## OPENACC UPDATE DIRECTIVE

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

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







### 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.







# LOOP OPTIMIZATIONS





## COLLAPSE CLAUSE

- collapse( N )
- Combine the next N tightly nested loops
- Can turn a multidimensional loop nest into a single-dimension loop
- This can be extremely useful for increasing memory locality, as well as creating larger loops to expose more parallelism

```
#pragma acc parallel loop collapse(2
for( i = 0; i < size; i++ )</pre>
       j = 0; j < size; j++
    double tmp = 0.0f;
    #pragma acc loop reduction(+:tmp)
    for( k = 0; k < size; k++ )
      tmp += a[i][k] * b[k][j];
    c[i][j] = tmp;
```

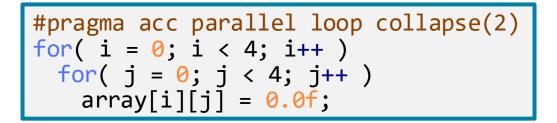




## COLLAPSE CLAUSE

#### collapse( 2 )

(0,0)	(0,1)	(0,2)	(0,3)
(1,0)	(1,1)	(1,2)	(1,3)
(2,0)	(2,1)	(2,2)	(2,3)
(3,0)	(3,1)	(3,2)	(3,3)







### TILE CLAUSE

```
tile (x, y, z, ...)
```

- Breaks multidimensional loops into "tiles" or "blocks"
- Can increase data locality in some codes
- Will be able to execute multiple "tiles" simultaneously

```
#pragma acc kernels loop tile(32, 32
for( i = 0; i < size; i++ )</pre>
  for( j = 0; j < size; j++ )</pre>
    for( k = 0; k < size; k++ )
      c[i][j] += a[i][k] * b[k][j];
```

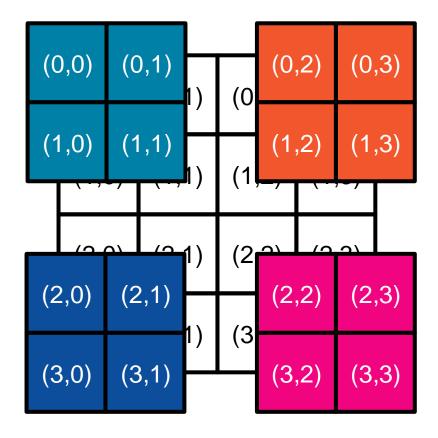




## TILE CLAUSE

```
#pragma acc kernels loop tile(2,2)
for(int x = 0; x < 4; x++){
  for(int y = 0; y < 4; y++){
    array[x][y]++;
  }
}</pre>
```

#### tile (2,2)

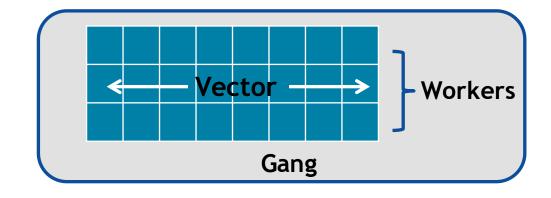






## GANG WORKER VECTOR

- Gang / Worker / Vector defines the various levels of parallelism we can achieve with OpenACC
- This parallelism is most useful when parallelizing multi-dimensional loop nests
- OpenACC allows us to define a generic Gang / Worker / Vector model that will be applicable to a variety of hardware, but we fill focus a little bit on a GPU specific implementation







#### BACK TO THE EXAMPLE

```
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heat acc data.x
main:
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         43, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
             Generating reduction (max:error)
         44, #pragma acc loop seg
     40, Generating implicit copy(error) [if not already present]
     44, Complex loop carried dependence of A->, A->->, Anew->-> prevents
parallelization
     49, Generating Tesla code
         52, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
         53, #pragma acc loop seg
     53, Complex loop carried dependence of Anew->->, Anew->, A->->, A-> prevents
parallelization
```



Now data movement only happens at our data region.



#### OPTIMIZED LOOP

```
#pragma acc data copyin(A[0:n][0:m]) copyout(Anew[0:n][0:m])
while ( err > tol && iter < iter max ) {</pre>
  err=0.0;
  #pragma acc parallel loop reduction(max:err)
  for ( int j = 1; j < n-1; j++) {
    #pragma acc loop independent
    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++) {
    #pragma acc loop independent
    for ( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  iter++;
```

Tell compiler that these inner loop and really independent from each other

#### REBUILD THE CODE

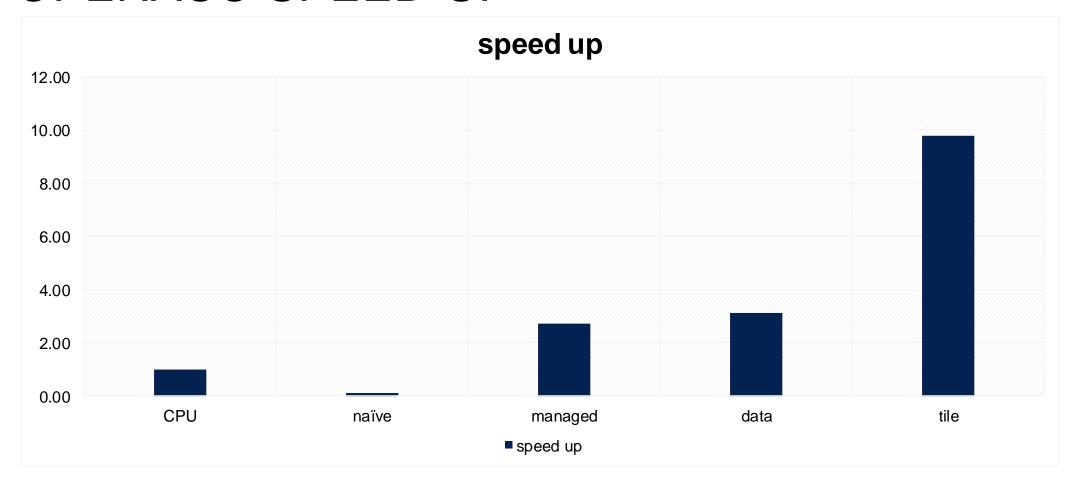
```
pgc++ -acc -fast -Minfo=accel -ta=nvidia,cc75 heat acc tile.cpp -03 -o
heat acc tile.x
main:
     39, Generating copyout(Anew[:n][:m]) [if not already present]
         Generating copyin(A[:n][:m]) [if not already present]
     40, Generating Tesla code
         43, #pragma acc loop gang /* blockIdx.x */
             Generating reduction (max:error)
         45, #pragma acc loop vector(128) /* threadIdx.x */
     40, Generating implicit copy(error) [if not already present]
     45, Loop is parallelizable
     50, Generating Tesla code
         53, #pragma acc loop gang /* blockIdx.x */
         55, #pragma acc loop vector(128) /* threadIdx.x */
     55, Loop is parallelizable
```



Now data movement only happens at our data region.



# **OPENACC SPEED-UP**







# NSIGHT SYSTEM PROFILE



Now the compute kernels are much shorter.





## LOOP OPTIMIZATION RULES OF THUMB

- It is rarely a good idea to set the number of gangs in your code, let the compiler decide.
- Most of the time you can effectively tune a loop nest by adjusting only the vector length.
- It is rare to use a worker loop. When the vector length is very short, a worker loop can increase the parallelism in your gang.
- When possible, the vector loop should step through your arrays
- Use the device\_type clause to ensure that tuning for one architecture doesn't negatively affect other architectures.





## OPENACC RESOURCES

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#### Resources

https://www.openacc.org/resources



#### **Compilers and Tools**

https://www.openacc.org/tools



#### **Success Stories**

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



#### **Events**

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# **CLOSING REMARKS**





#### KEY CONCEPTS

In this lecture we discussed...

- How to profile a serial code to identify loops that should be accelerated
- How to use OpenACC's parallel loop directive to parallelize key loops
- How to use OpenACC's data clauses to control data movement
- How to optimize loops in the code for better performance