ZEROJOGPUHEROWIII 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



ABOUT THIS LECTURE

- The objective of this lecture is to give you a brief introduction of OpenACC programming for NVIDIA GPUs
- This is an instructor-led session, there will be no hands on portion
- Feel free to interrupt with questions



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

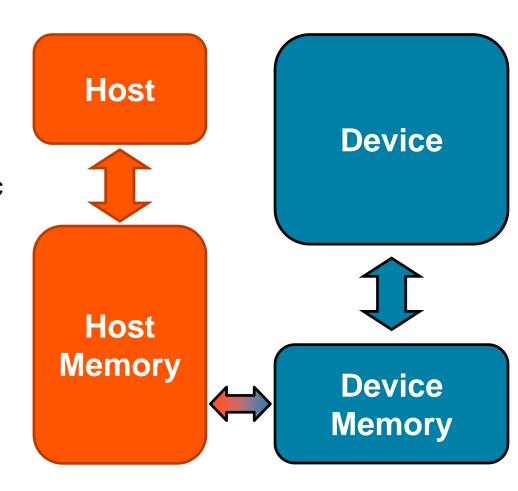
Most Performance Most Flexibility



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.

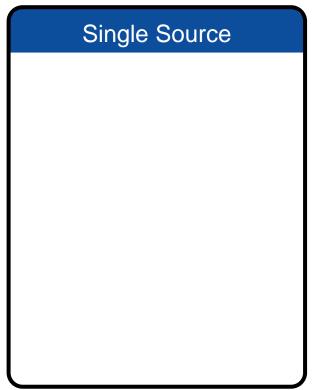


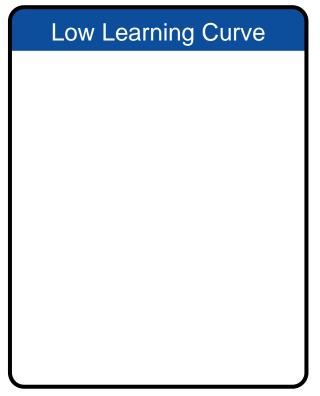




Three major strengths

Incremental







Incremental

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

Enhance Sequential 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

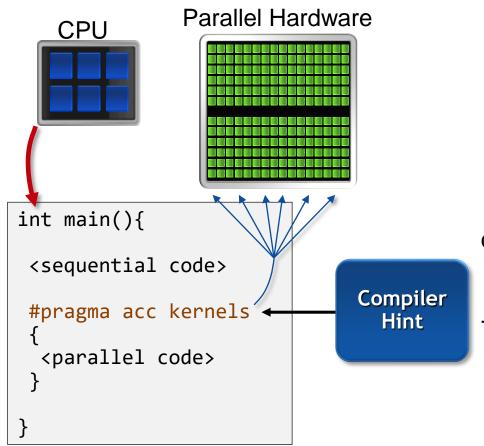
- Maintain existing sequential code
- Add annotations to expose parallelism
- After verifying correctness, annotate more of the code

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
- 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

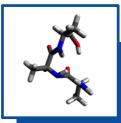
- OpenACC is meant to be easy to use, and easy to learn
- Programmer remains in familiar C, C++, or Fortran
- No reason to learn low-level details of the hardware.





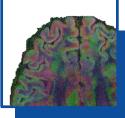


OPENACC SUCCESSES



LSDalton

Quantum Chemistry **Aarhus University** 12X speedup 1 week



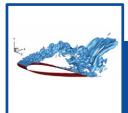
PowerGrid

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

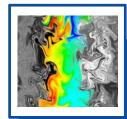
Comp Electromagnetics Argonne National Lab 2.5X speedup 60% less energy



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



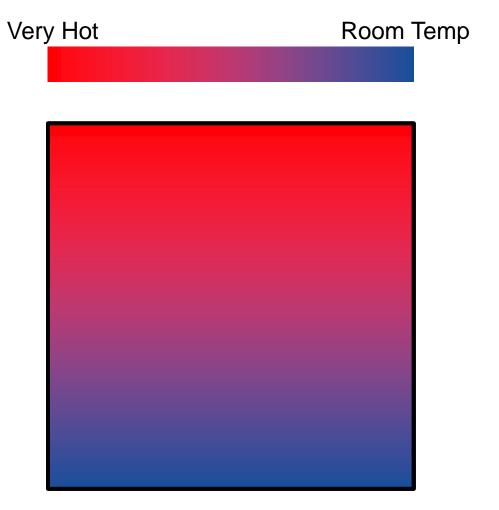


LAPLACE HEAT TRANSFER

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

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

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

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

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

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

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



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

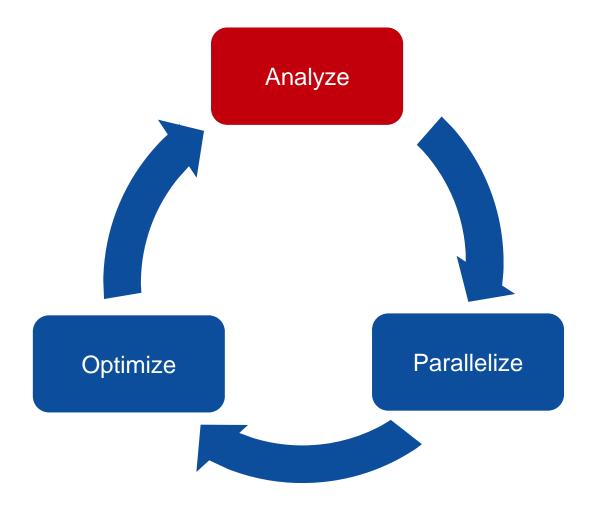
Swap input/output arrays

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.





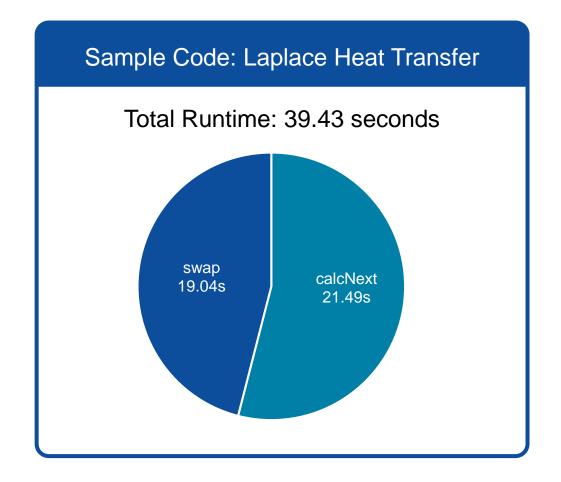
Profile Your Code

Obtain detailed information about how the code ran.

This can include information such as:

- Total runtime
- Runtime of individual routines
- Hardware counters

Identify the portions of code that took the longest to run. We want to focus on these "hotspots" when parallelizing.



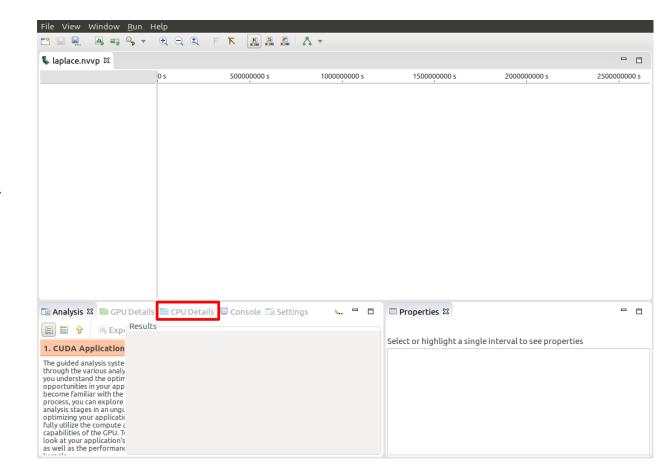






First sight when using PGPROF

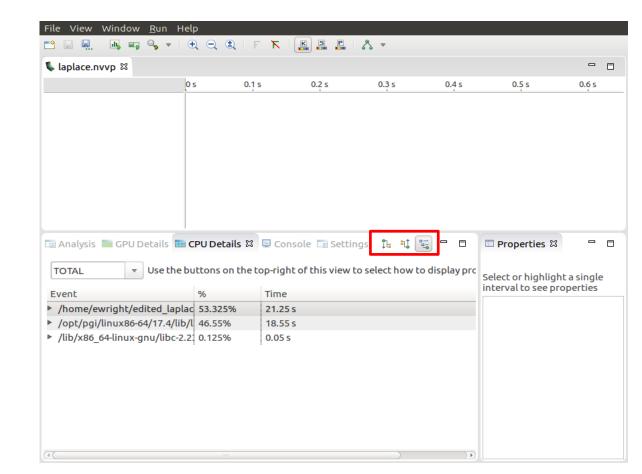
- Profiling a simple, sequential code
- Our sequential program will on run on the CPU
- To view information about how our code ran, we should select the "CPU Details" tab





CPU Details

- Within the "CPU Details" tab, we can see the various parts of our code, and how long they took to run
- We can reorganize this info using the three options in the top-right portion of the tab
- We will expand this information, and see more details about our code

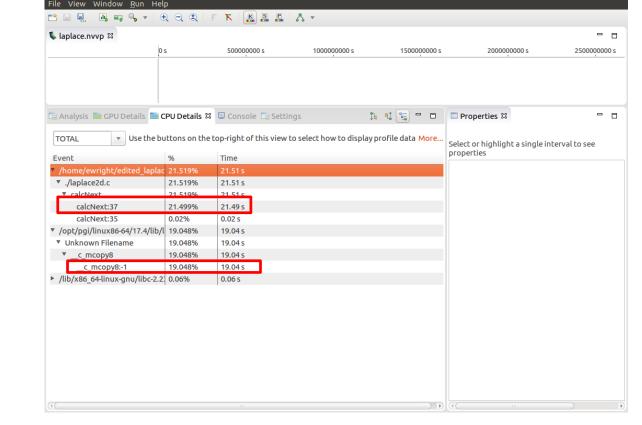






CPU Details

- We can see that there are two places that our code is spending most of its time
- 21.49 seconds in the "calcNext" function
- 19.04 seconds in a memcpy function
- The c_mcopy8 that we see is actually a compiler optimization that is being applied to our "swap" function

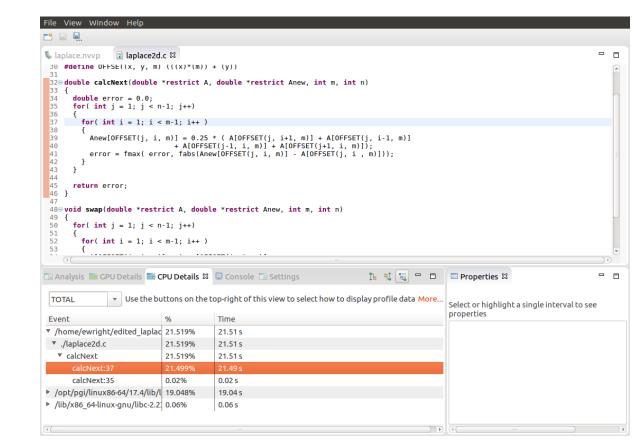






PGPROF

- We are also able to select the different elements in the CPU Details by double-clicking to open the associated source code
- Here we have selected the "calcNext:37" element, which opened up our code to show the exact line (line 37) that is associated with that element







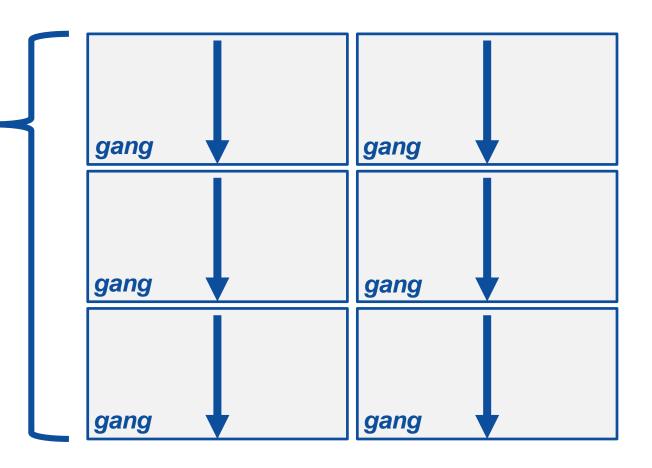




Expressing parallelism

```
#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

entire loop

DEEP LEARNING INSTITUTE

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

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

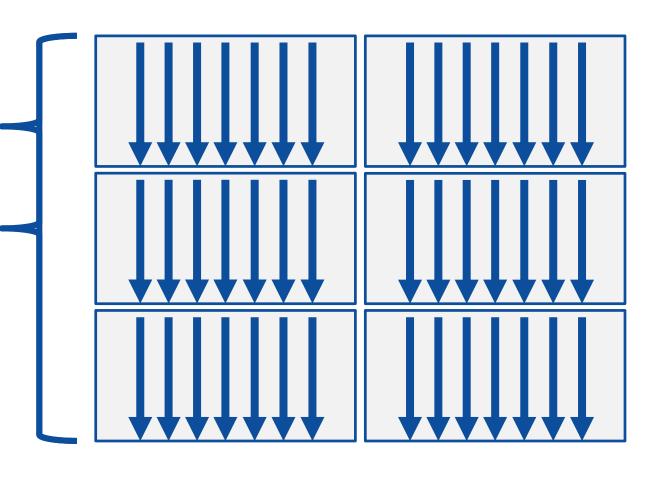
```
!$acc parallel loop
do i = 1, N
   a(i) = 0
end do
```

- 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 ) {</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++;
```

OpenACC

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)

```
$ pgcc -fast -ta=tesla:managed -Minfo=accel laplace2d uvm.c
main:
     63, Accelerator kernel generated
         Generating Tesla code
         64, #pragma acc loop gang /* blockIdx.x */
             Generating reduction(max:error)
         66, #pragma acc loop vector(128) /* threadIdx.x */
     63, Generating implicit copyin(A[:])
         Generating implicit copyout(Anew[:])
         Generating implicit copy(error)
     66, Loop is parallelizable
     74, Accelerator kernel generated
         Generating Tesla code
         75, #pragma acc loop gang /* blockIdx.x */
         77, #pragma acc loop vector(128) /* threadIdx.x */
     74, Generating implicit copyin(Anew[:])
         Generating implicit copyout(A[:])
     77, Loop is parallelizable
```

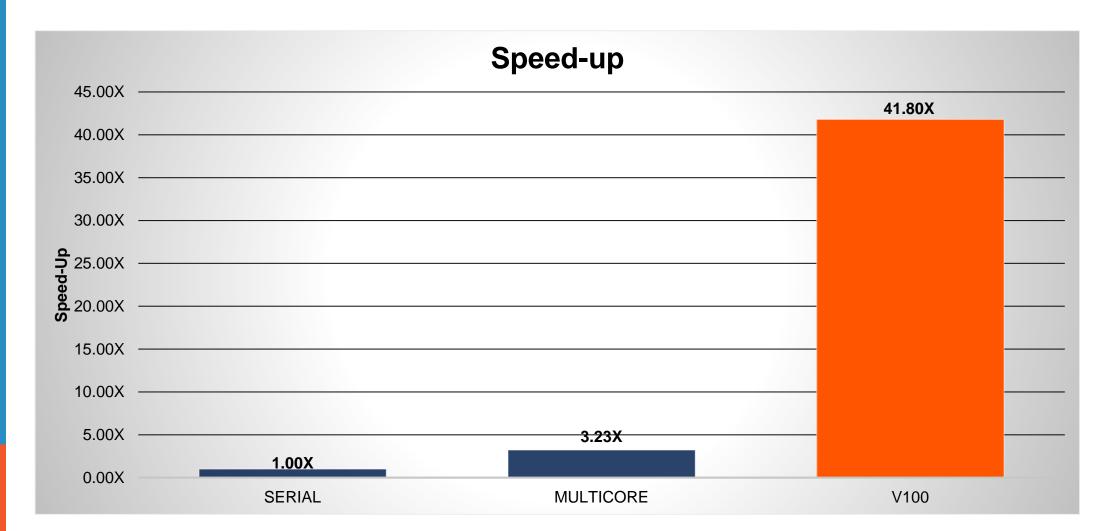


BUILDING THE CODE (MULTICORE)

```
$ pgcc -fast -ta=multicore -Minfo=accel laplace2d_uvm.c
main:
    63, Generating Multicore code
    64, #pragma acc loop gang
64, Accelerator restriction: size of the GPU copy of Anew, A is unknown
    Generating reduction(max:error)
66, Loop is parallelizable
74, Generating Multicore code
    75, #pragma acc loop gang
75, Accelerator restriction: size of the GPU copy of Anew, A is unknown
77, Loop is parallelizable
```



OPENACC SPEED-UP



BUILDING THE CODE (GPU)

```
$ pgcc -fast -ta=tesla -Minfo=accel laplace2d uvm.c
PGC-S-0155-Compiler failed to translate accelerator region (see -Minfo messages):
Could not find allocated-variable index for symbol (laplace2d uvm.c: 63)
PGC-S-0155-Compiler failed to translate accelerator region (see -Minfo messages):
Could not find allocated-variable index for symbol (laplace2d uvm.c: 74)
main:
     63, Accelerator kernel generated
         Generating Tesla code
         63, Generating reduction (max:error)
         64, #pragma acc loop gang /* blockIdx.x */
         66, #pragma acc loop vector(128) /* threadIdx.x */
     64, Accelerator restriction: size of the GPU copy of Anew, A is unknown
     66, Loop is parallelizable
     74, Accelerator kernel generated
         Generating Tesla code
         75, #pragma acc loop gang /* blockIdx.x */
         77, #pragma acc loop vector(128) /* threadIdx.x */
     75, Accelerator restriction: size of the GPU copy of Anew, A is unknown
     77, Loop is parallelizable
```



OPTIMIZE DATA MOVEMENT

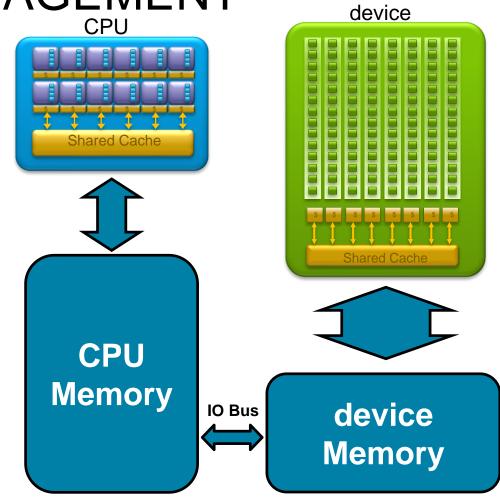




EXPLICIT MEMORY MANAGEMENT

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.





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



Host Memory



Device memory







OPTIMIZED DATA MOVEMENT

```
#pragma acc data copy(A[:n*m]) copyin(Anew[:n*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++;
OpenACC
```

Copy A to/from the accelerator only when needed.

Copy initial condition of Anew, but not final value

REBUILD THE CODE

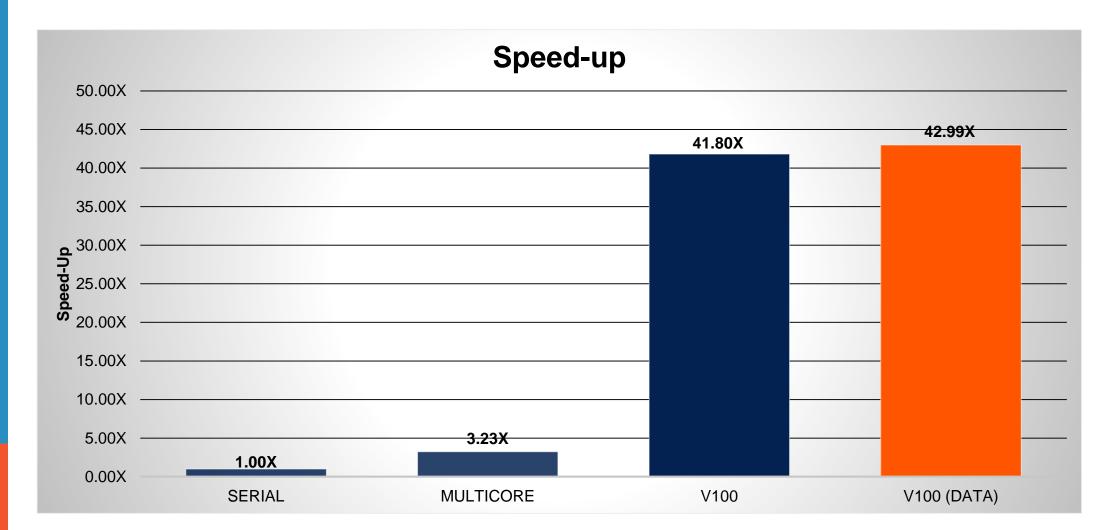
```
pqcc -fast -ta=tesla -Minfo=accel laplace2d uvm.c
main:
     60, Generating copy(A[:m*n])
         Generating copyin (Anew[:m*n])
     64, Accelerator kernel generated
         Generating Tesla code
         64, Generating reduction (max:error)
         65, #pragma acc loop gang /* blockIdx.x */
         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



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

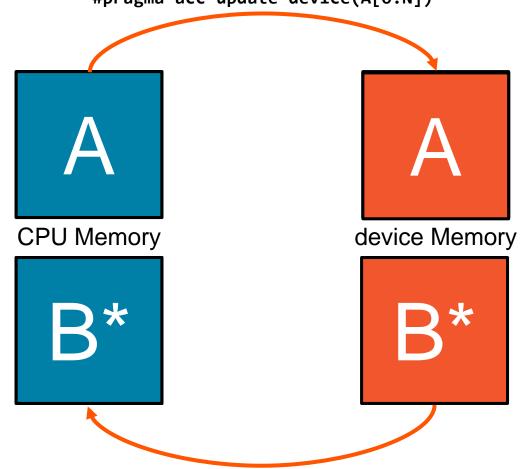




OPENACC UPDATE DIRECTIVE

#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.







FURTHER OPTIMIZATIONS

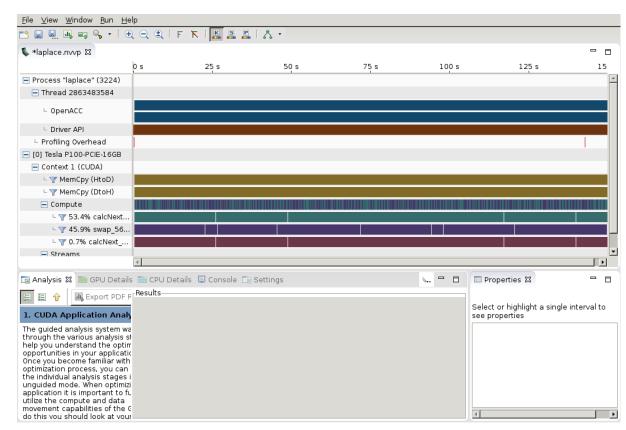




PROFILING GPU CODE (PGPROF)

Using PGPROF to profile GPU code

- PGPROF presents far more information when running on a GPU
- We can view CPU Details, GPU Details, a Timeline, and even do Analysis of the performance



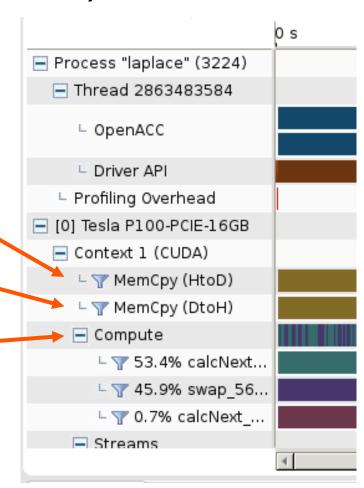




PROFILING GPU CODE (PGPROF)

Using PGPROF to profile GPU code

- MemCpy(HtoD): This includes data transfers from the Host to the Device (CPU to GPU)
- **MemCpy(DtoH):** These are data transfers from the Device to the Host (GPU to CPU)
- Compute: These are our computational functions. We can see our calcNext and swap function









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++ )
    for( 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;</pre>
```

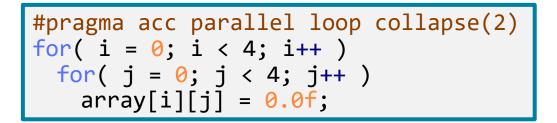




COLLAPSE CLAUSE

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++ )
  for( j = 0; j < size; j++ )</pre>
    for( k = 0; k < size; k++
      c[i][j] += a[i][k] * b[k][j];
```

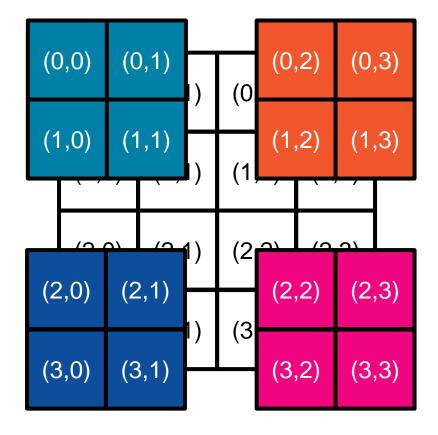




TILE CLAUSE

```
#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)

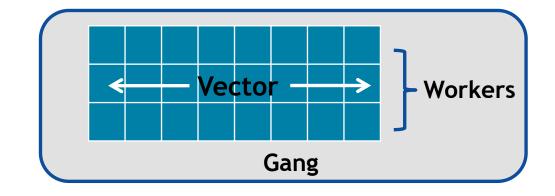






GANG WORKER VECTOR

- 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







OPTIMIZED LOOP

```
#pragma acc data copy(A[:n*m]) copyin(Anew[:n*m])
     while ( err > tol && iter < iter max ) {</pre>
       err=0.0;
     #pragma acc parallel loop reduction(max:err) tile(32,32)
       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 tile(32,32)
       for ( int j = 1; j < n-1; j++) {
         for( int i = 1; i < m-1; i++ ) {
           A[j][i] = Anew[j][i];
       iter++;
OpenACC
```

Create 32x32 tiles of the loops to better exploit data locality.

REBUILD THE CODE

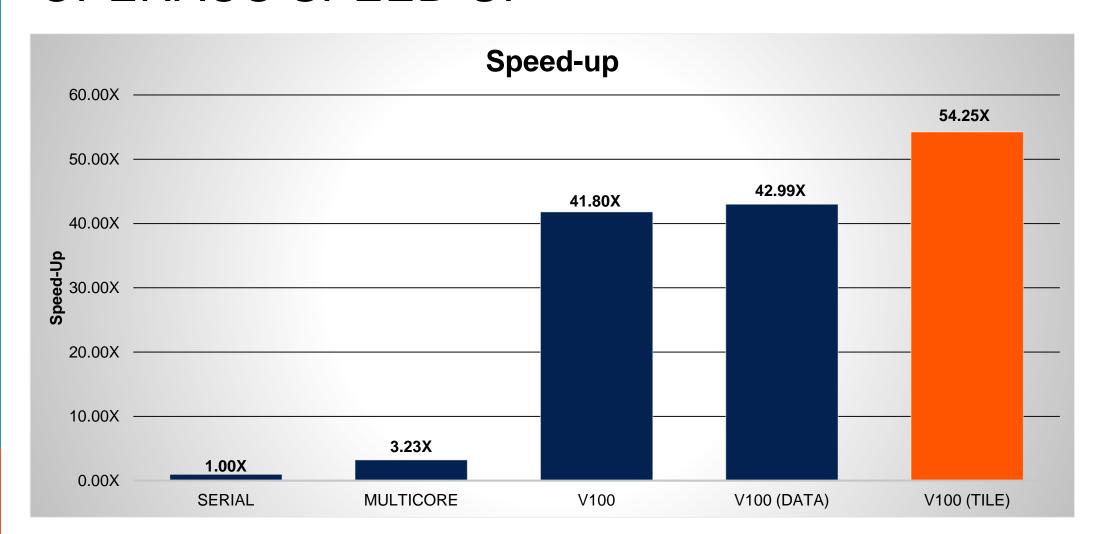
```
pqcc -fast -ta=tesla -Minfo=accel laplace2d uvm.c
main:
     60, Generating copy(A[:m*n])
         Generating copyin (Anew[:m*n])
     64, Accelerator kernel generated
         Generating Tesla code
         64, Generating reduction (max:error)
         65, #pragma acc loop gang /* blockIdx.x */
         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



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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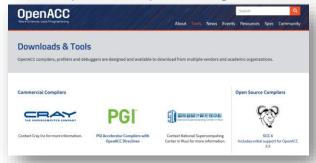
Resources

https://www.openacc.org/resources



Compilers and Tools

https://www.openacc.org/tools



Success Stories

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



Events

https://www.openacc.org/events





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