ZERO TO GPU HERO WITH OPENACC

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OpenACC
More Science, Less Programming

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 directives-based 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

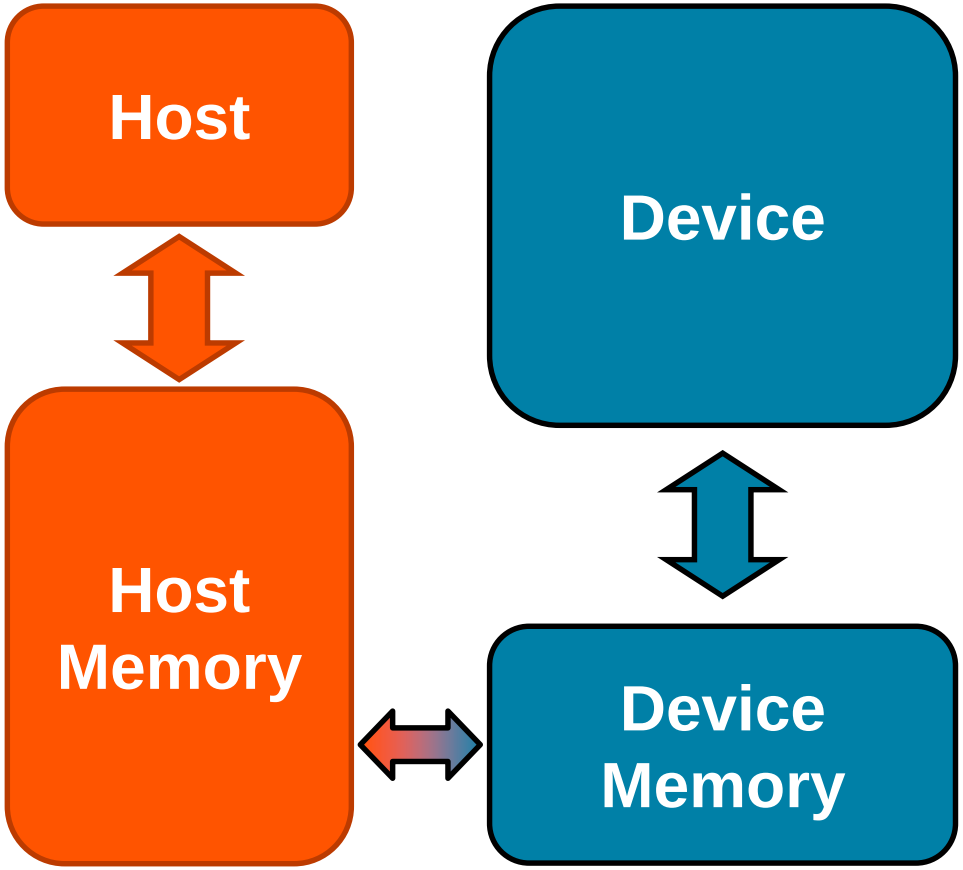
Applications

Libraries	Compiler Directives	Programming Languages
Easy to use **Most Performance**	**Easy to use** **Portable code**	**Most Performance** **Most Flexibility**
	OpenACC	

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.



OPENACC

Three major strengths

Incremental	Single Source	Low Learning Curve

OPENACC

Incremental

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

Enhance Sequential Code

```
#pragma acc parallel loop
for( i = 0; i < N; i++ )
{
    < loop code >
}

#pragma acc parallel loop
for( i = 0; i < N; i++ )
{
    < loop code >
}
```

Begin with a working sequential code.

Parallelize it with OpenACC.

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

OPENACC

Incremental

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

Single Source

Low Learning Curve

OPENACC

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.

```
int main(){

...

   #pragma acc parallel loop
   for(int i = 0; i < N; i++)
     < loop code >

}
```

OPENACC

Incremental

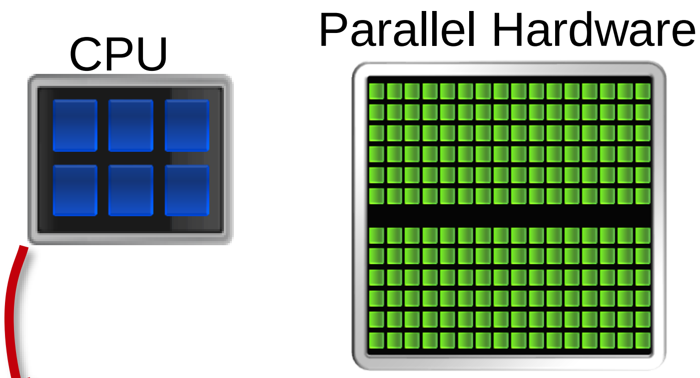
- Maintain existing sequential code
- Add annotations to expose parallelism
- After verifying correctness, annotate more of the code

Single Source

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

Low Learning Curve

OPENACC




```
int main(){

 <sequential code>

 #pragma acc kernels
 {
  <parallel code>
 }

}
```

Compiler Hint

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.

Low Learning Curve

- 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

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
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Low Learning Curve

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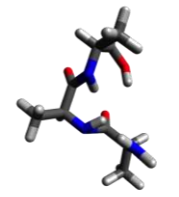
- No reason to learn low-level details of the hardware.

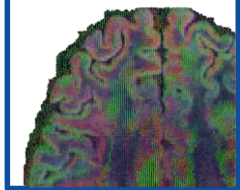
OPENACC SUCCESSES



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

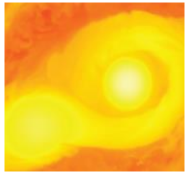
CFD
NC State University

4X speedup

NekCEM

Comp Electromagnetics
Argonne National Lab

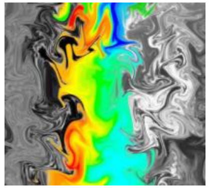
2.5X speedup
60% less energy



MAESTRO CASTRO

Astrophysics
Stony Brook University

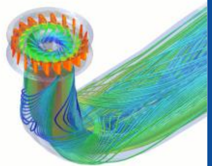
4.4X speedup
4 weeks effort



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>
```

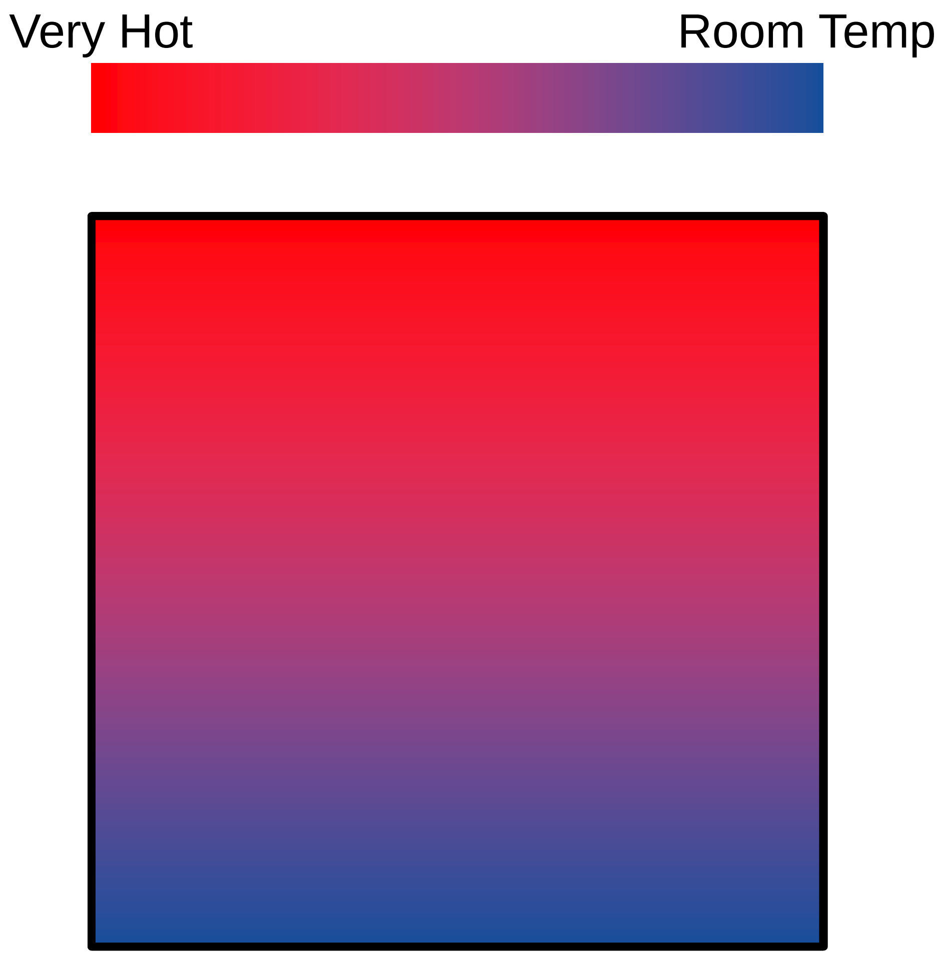
Fortran

```
!$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



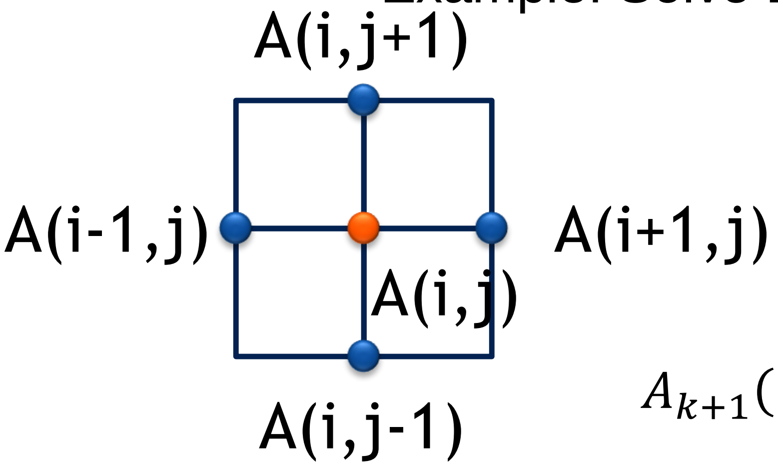
We will observe a simple simulation of heat distributing across a metal plate.

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: $\boldsymbol{\nabla^2 f(x,y) = 0}$



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

JACOBI ITERATION: C CODE

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

Iterate until converged

Iterate across matrix elements

Calculate new value from neighbors

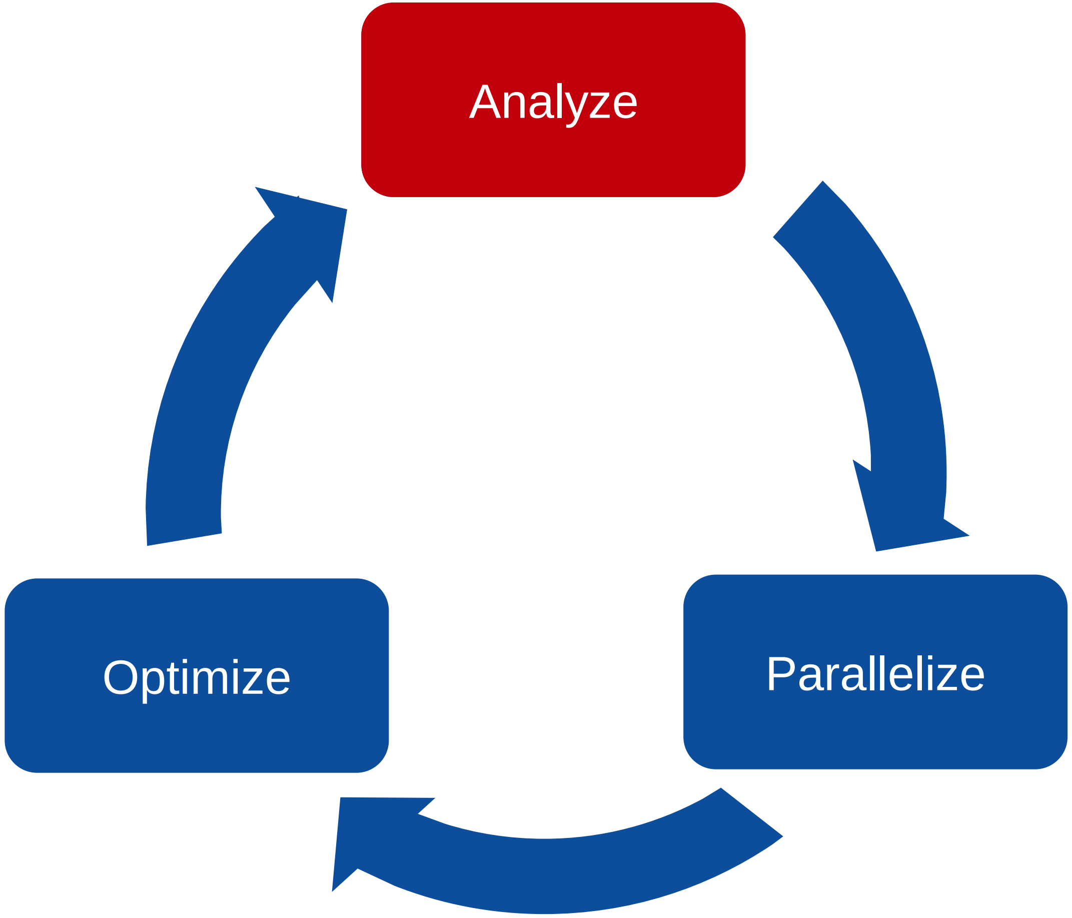
Compute max error for convergence

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.



PROFILING SEQUENTIAL CODE

Profile Your Code

Obtain detailed information about how the code ran.

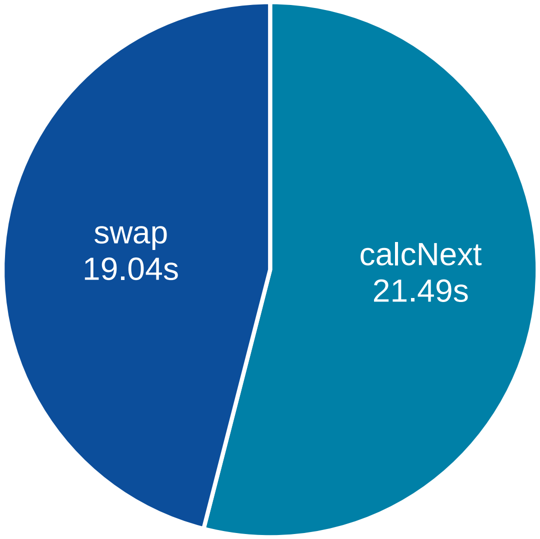
This can include information such as:

- 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.

Sample Code: Laplace Heat Transfer

Total Runtime: 39.43 seconds



OPENACC PARALLEL DIRECTIVE

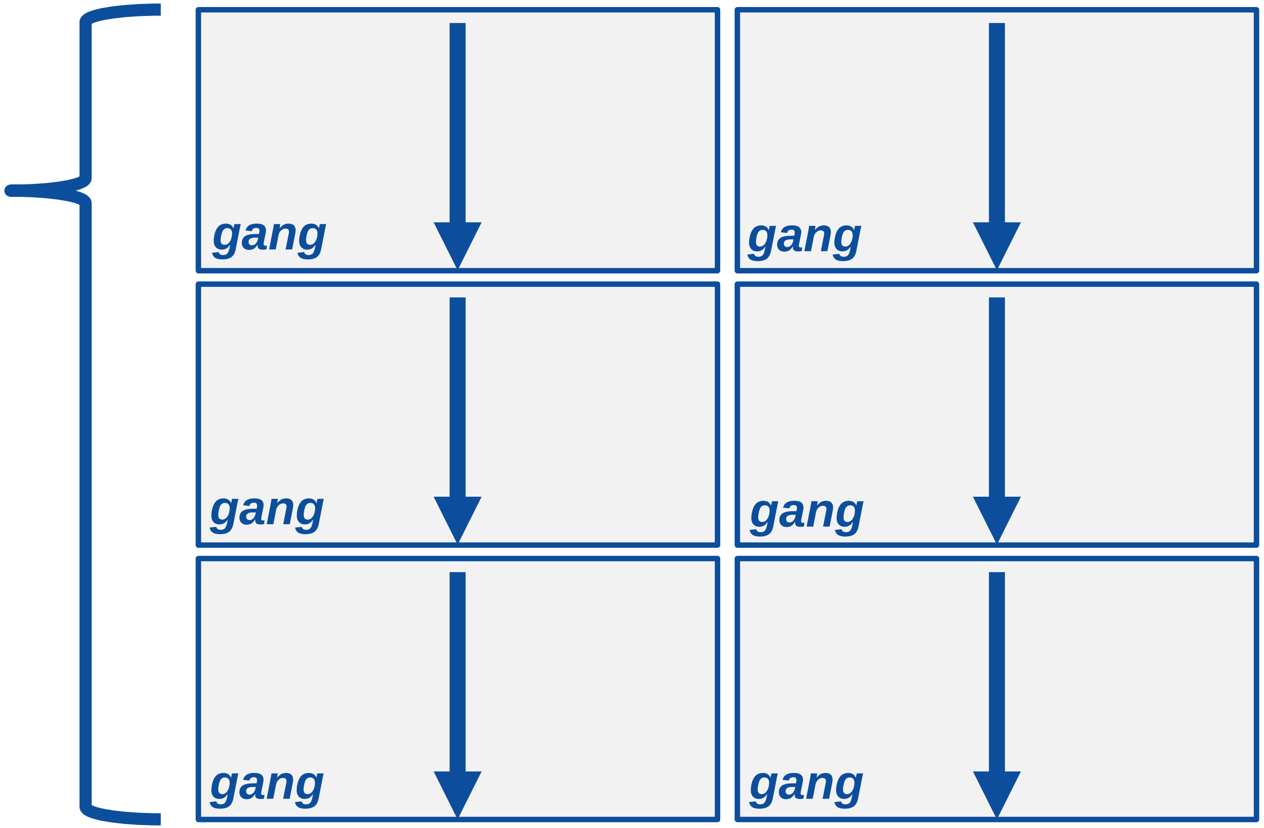
OPENACC PARALLEL DIRECTIVE

Expressing parallelism

```
#pragma acc parallel
{
```

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

```
}
```



OPENACC PARALLEL DIRECTIVE

Expressing parallelism

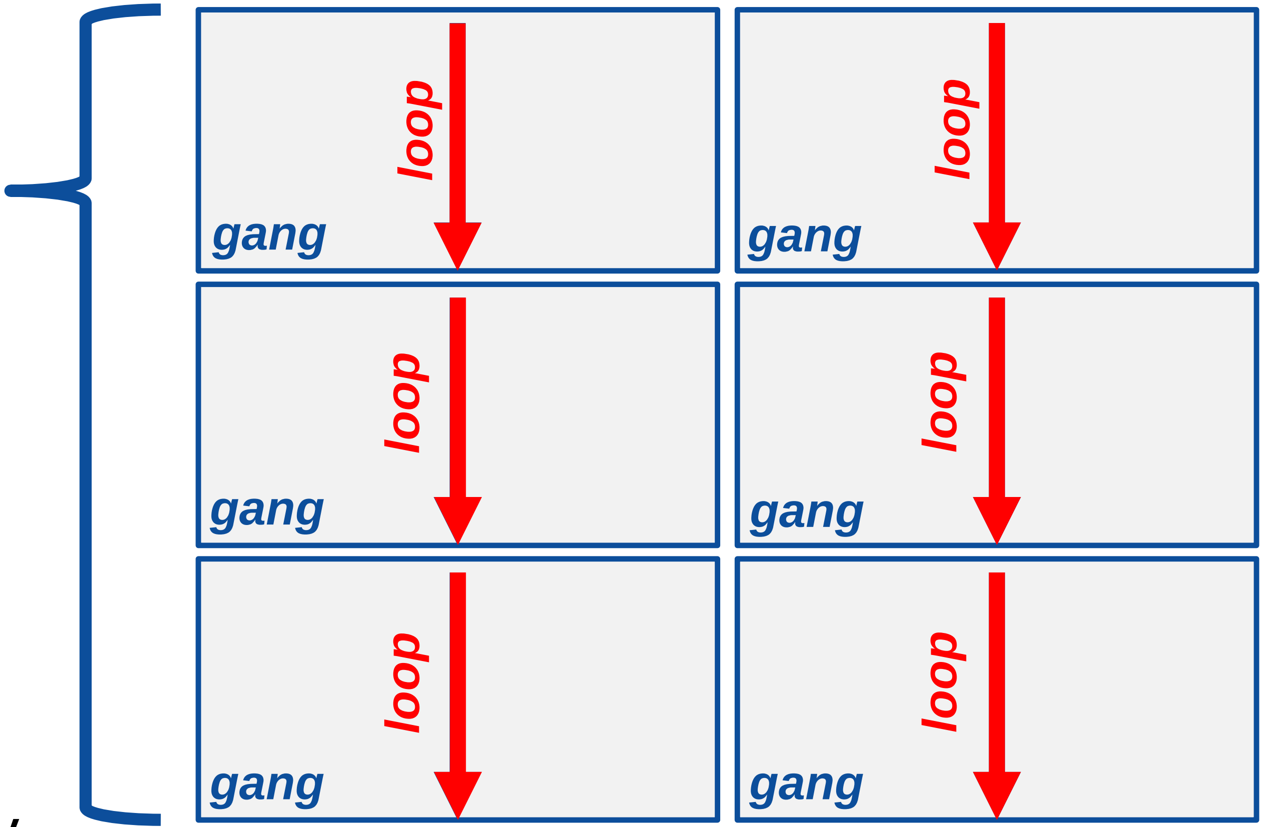
```
#pragma acc parallel
{

    for(int i = 0; i < N; i++)
    {
        // Do Something
    }

}
```

loop

This loop will be executed redundantly on each gang



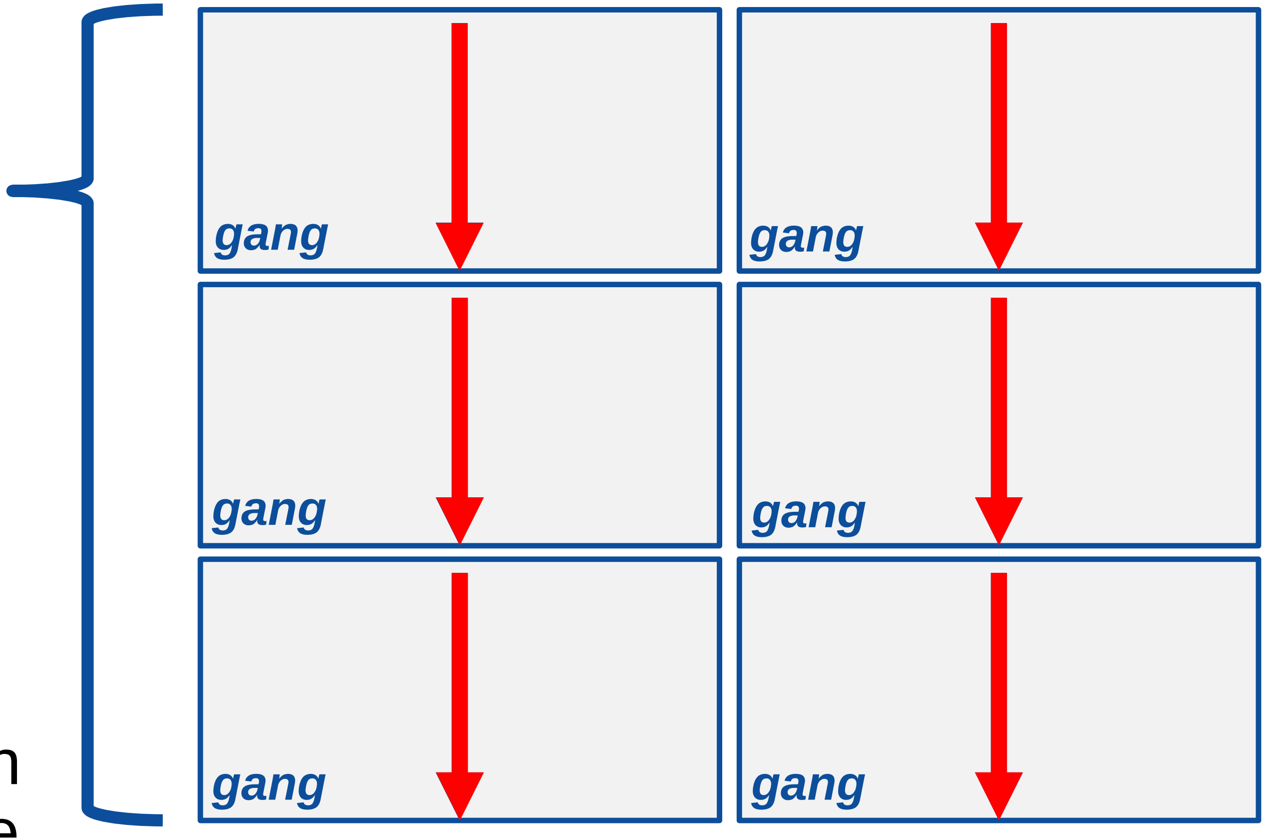
OPENACC PARALLEL DIRECTIVE

Expressing parallelism

```
#pragma acc parallel
{

    for(int i = 0; i < N; i++)
    {
        // Do Something
    }

}
```



This means that each ***gang*** will execute the entire loop

OPENACC PARALLEL DIRECTIVE

Parallelizing a single loop

C/C++

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

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

OPENACC PARALLEL DIRECTIVE

Parallelizing a single loop

C/C++

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

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

OPENACC PARALLEL DIRECTIVE

Expressing parallelism

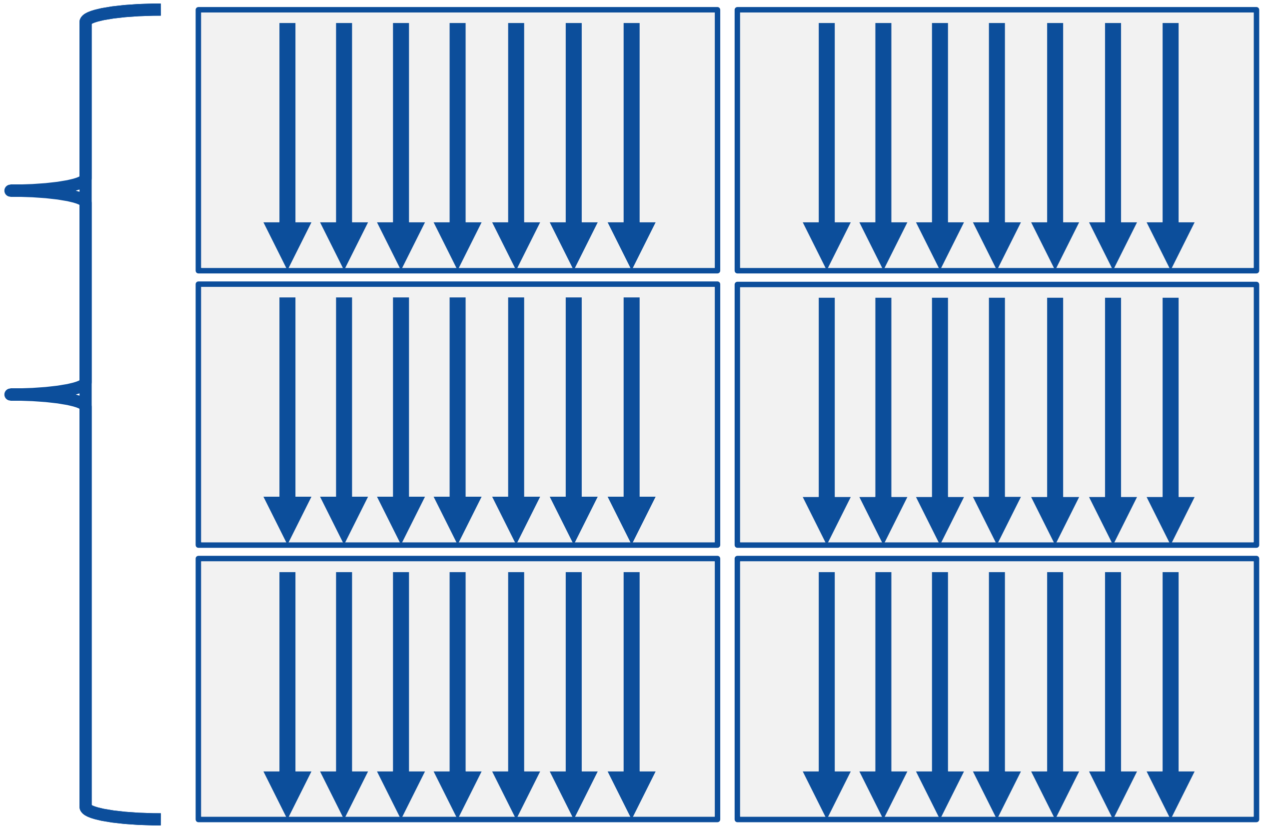
```
#pragma acc parallel
{


    #pragma acc loop
    for(int i = 0; i < N; i++)
    {
        // Do Something
    }



}
```

The ***loop*** directive informs the compiler which loops to parallelize.



OpenACC More Science, Less Programming NVIDIA DEEP LEARNING INSTITUTE

OPENACC PARALLEL LOOP DIRECTIVE

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;
```

- 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.

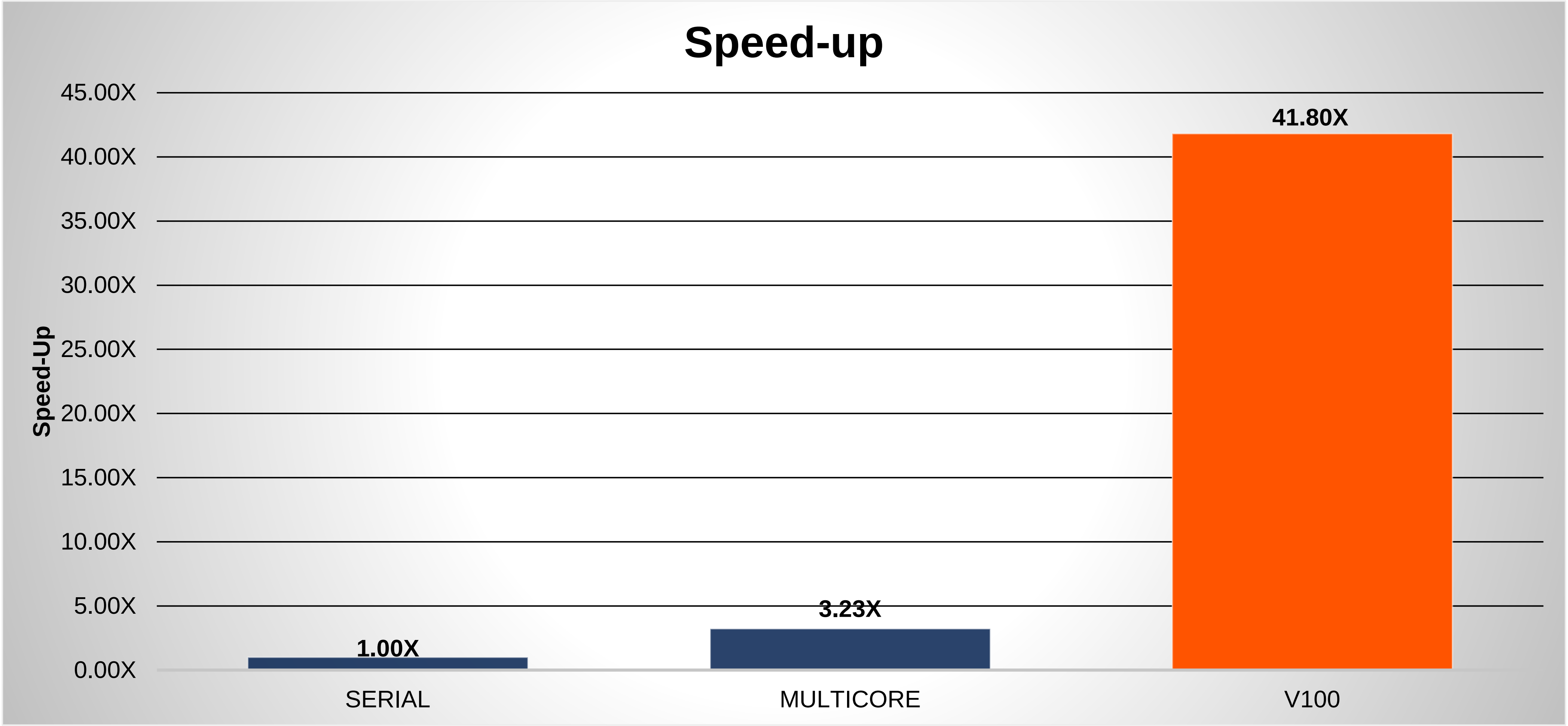
BUILDING THE CODE (GPU)

```
$ pgcc -fast -ta=tesla:managed -Minfo=accel laplace2d_uvm.c
main:
     63, 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, 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:
     55, Generating Multicore code
         56, #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)

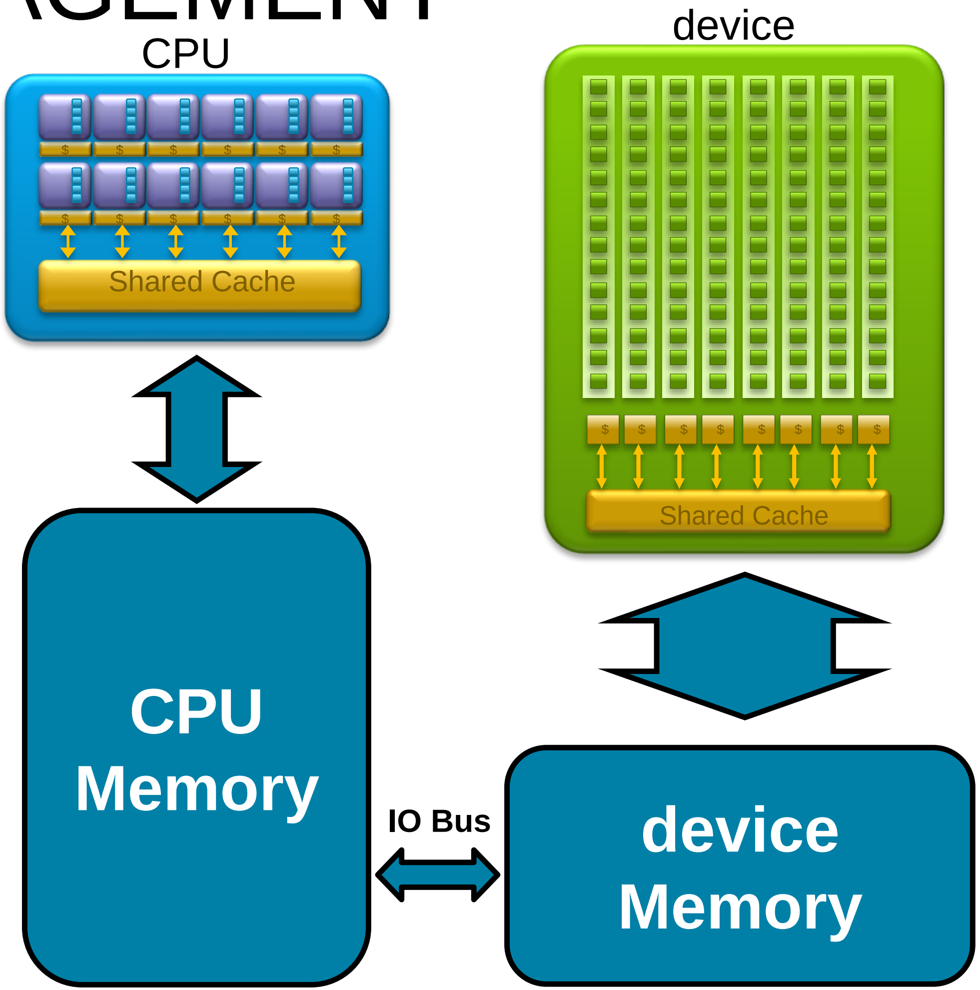
```
$ pgcc -fast -ta=tesla -Minfo=accel laplace2d_uvm.c
PGC-S-0155-Compiler failed to translate accelerator region (see -Minfo messages):
Could not find allocated-variable index for symbol (laplace2d_uvm.c: 63)
PGC-S-0155-Compiler failed to translate accelerator region (see -Minfo messages):
Could not 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]) 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)
  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.

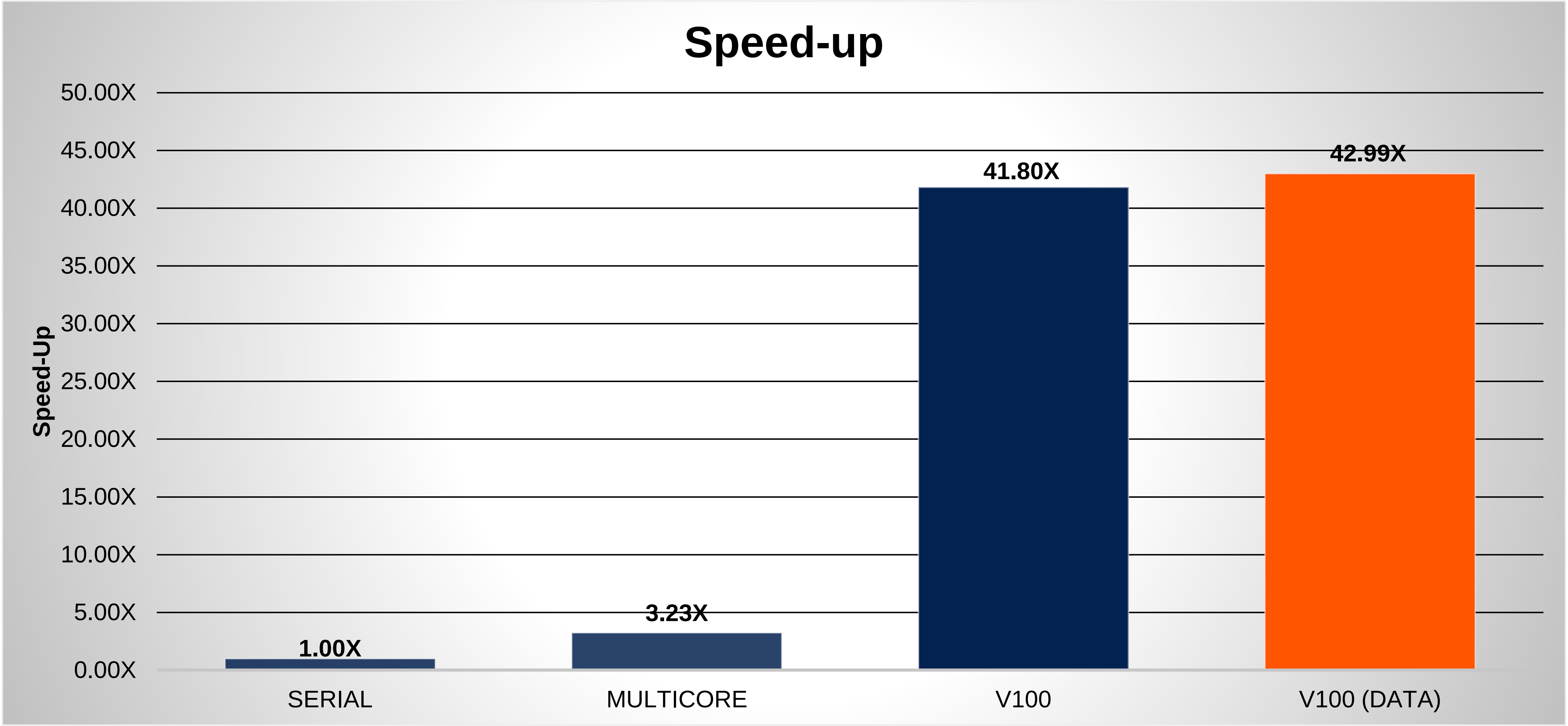
Copy initial condition of Anew, but not final value

REBUILD THE CODE

```
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



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])
```

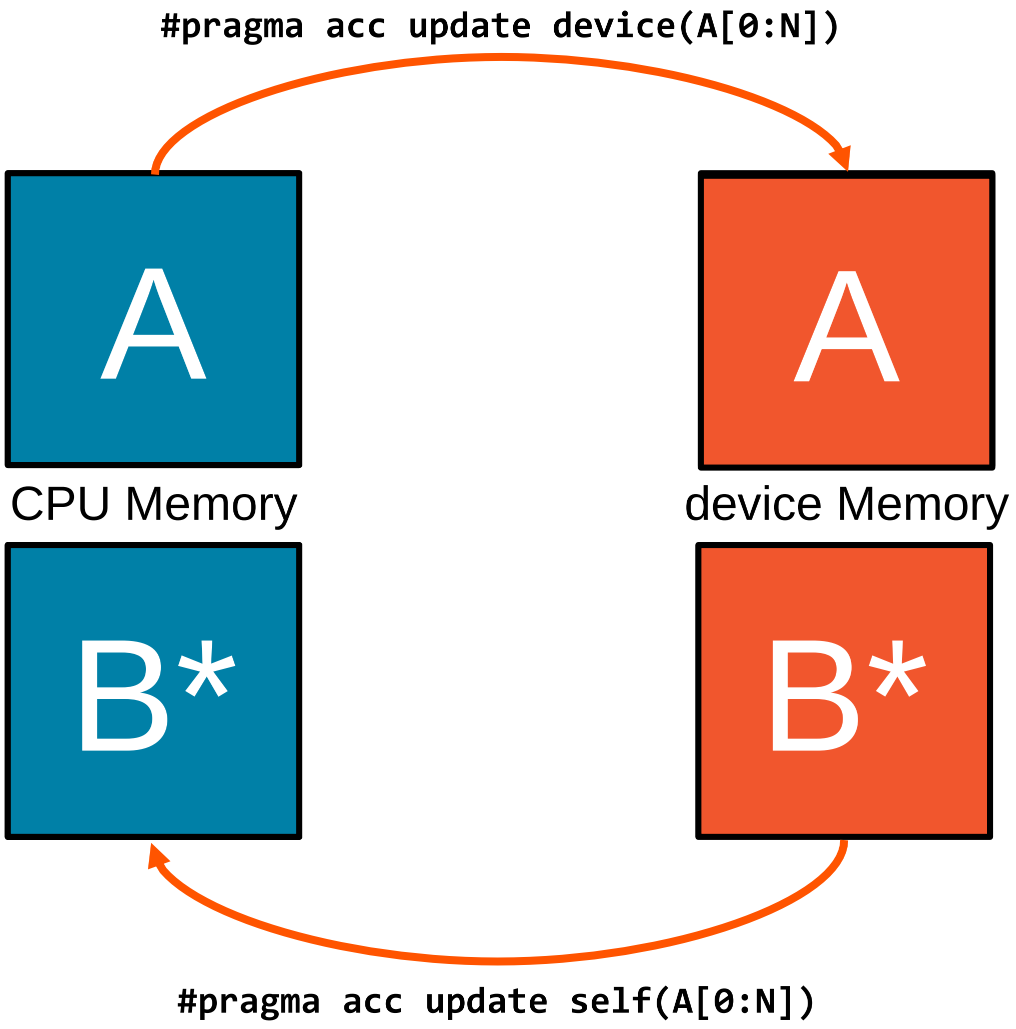
C/C++

```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.



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++ )
  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;
```

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)

```
#pragma acc parallel loop collapse(2)
for( i = 0; i < 4; i++ )
  for( j = 0; j < 4; j++ )
    array[i][j] = 0.0f;
```

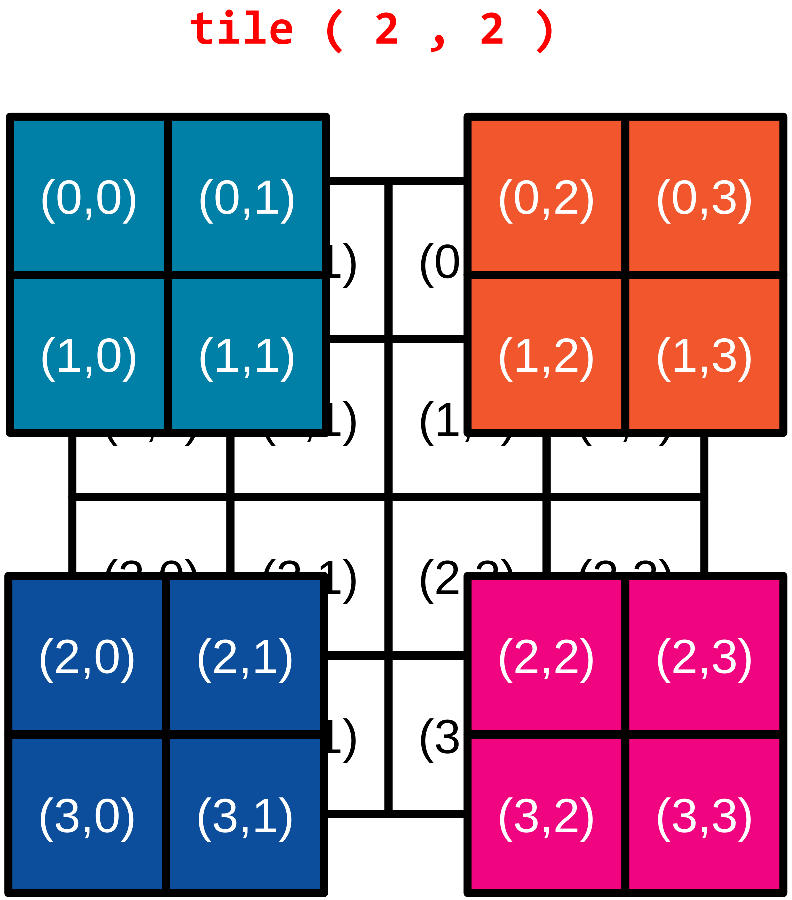
TILE CLAUSE

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

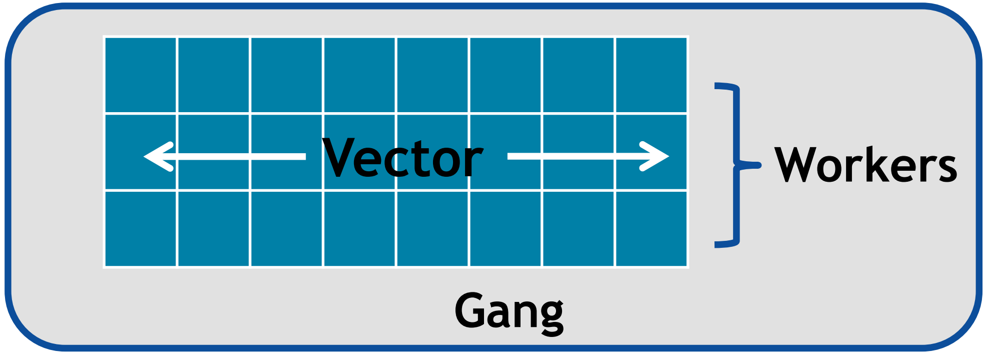
TILE CLAUSE

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



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 ) {
  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++;
}
```

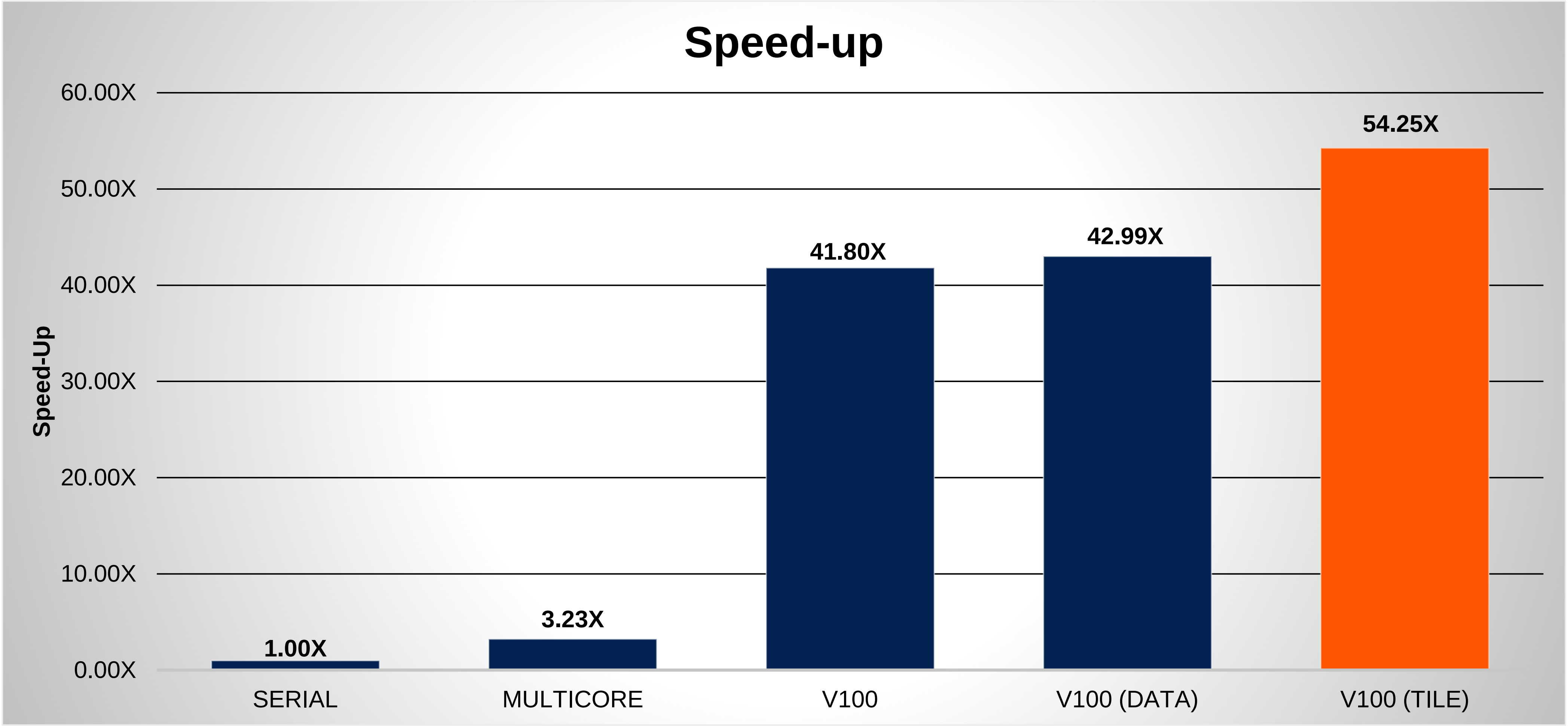
Create 32x32 tiles of the loops to better exploit data locality.

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



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

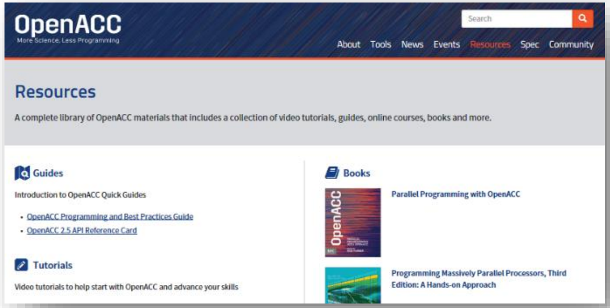
Guides ● Talks ● Tutorials ● Videos ● Books ● Spec ● Code Samples ● Teaching Materials ● Events ● Success Stories ● Courses ● Slack ● Stack Overflow

FREE Compilers

PGI Community EDITION

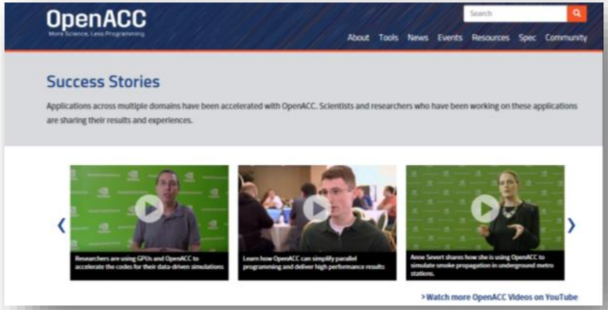
Resources

https://www.openacc.org/resources



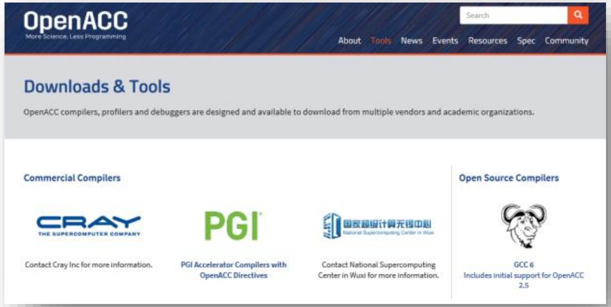
Success Stories

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



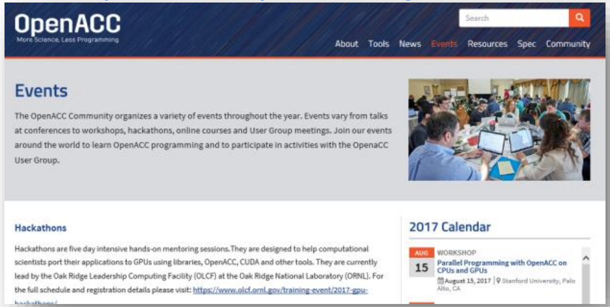
Compilers and Tools

https://www.openacc.org/tools



Events

https://www.openacc.org/events



OpenACC More Science, Less Programming

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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