

Module IV: LOOP OPTIMIZATIONS

OpenACC
More Science, Less Programming



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INSTITUTE

LOOP OPTIMIZATIONS

- Majority of program runtime is spent in loops
- Every loop can execute in a very different way
- Using OpenACC loop optimization, we can speed-up our most time-consuming portions of code



SAMPLE LOOP CODE

Matrix multiplication

- Our code is a 3-Dimensional Matrix Multiplication code
- The code allows for many different levels and types of parallelism, and works well with all of our loop clauses

```
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];
```

PARALLELIZING LOOPS

AUTO CLAUSE

- The **auto** clause tells the compiler to decide whether or not the loop is parallelizable
- The auto clause can be very useful when you are unsure of whether or not a loop is safe to parallelize

```
#pragma acc parallel loop auto
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];
```

AUTO CLAUSE

- When using the **kernels directive**, the auto clause is **implied**
- This means that you do not need to include the auto clause when using the kernels directive
- However, the auto clause can be very useful when using the **parallel directive**

```
#pragma acc kernels loop auto
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];
```

INDEPENDENT CLAUSE

- The **independent** clause asserts to the compiler that the loop is parallelizable
- This will overwrite any decision that the compiler makes about the loop
- Adding the independent clause could force the compiler to parallelize a non-parallel loop
- Allows the programmer to force parallelism when using the kernels directive

```
#pragma acc kernels loop independent
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];
```

INDEPENDENT CLAUSE

- When using the **parallel directive**, the independent clause is **implied**
- With the parallel directive, the programmer is determining which loops are parallelizable and thus the independent clause is not needed

```
#pragma acc parallel loop independent
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];
```

LOOP CORRECTNESS

SEQ CLAUSE

- The **seq** clause (short for sequential) will tell the compiler to run the loop sequentially
- In the sample code, the compiler will parallelize the outer loops across the parallel threads, but each thread will run the inner-most loop sequentially
- The compiler may automatically apply the seq clause to loops that have too many dimensions

```
#pragma acc parallel loop
for( i = 0; i < size; i++ )
#pragma acc loop
for( j = 0; j < size; j++ )
#pragma acc loop seq
for( k = 0; k < size; k++ )
    c[i][j] += a[i][k] * b[k][j];
```

PRIVATE AND FIRSTPRIVATE CLAUSES

- Variables in **private** or **firstprivate** clause are private to the loop level on which the clause appears.
- Private variables on an outer loop are shared within inner loops.

```
double tmp[3];

#pragma acc kernels loop private(tmp[0:3])
for( i = 0; i < size; i++ ) {
    // the tmp array is private to each iteration
    // of the outer loop
    tmp[0] = <value>;
    tmp[1] = <value>;
    tmp[2] = <value>;
#pragma acc loop
for ( j = 0; j < size2; j++) {
    // but tmp is shared amongst the threads
    // in the inner loop
    array[i][j] = tmp[0]+tmp[1]+tmp[2];
}
}
```

SCALARS AND PRIVATE CLAUSE

- By default, scalars are **firstprivate** when used in a parallel region and **private** when used in a kernels region.
- Except in some cases, scalars do not need to be added to a private clause. These cases may include but are not limited to:
 1. Scalars with global storage such as global variables in C/C++, Module variables in Fortran
 2. When the scalar is passed by reference to a device subroutine
 3. When the scalar is used as an rvalue after the compute region, aka “live-out”
- Note that putting scalars in a private clause may actually hurt performance!

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

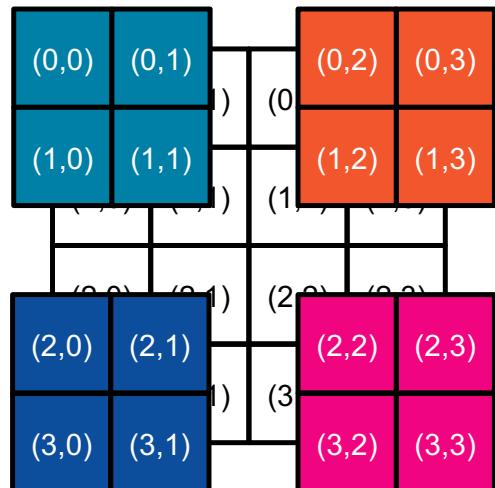
- **tile (x , y , z, ...)**
- Breaks multidimensional loops into “tiles” or “blocks”
- Can increase data locality in some codes
- Will be able to execute multiple “tiles” simultaneously

```
#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

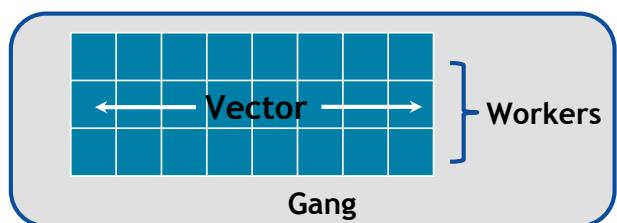
```
#pragma acc kernels loop tile(2,2)
for(int x = 0; x < 4; x++){
    for(int y = 0; y < 4; y++){
        array[x][y]++;
    }
}
```

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 will focus a little bit on a GPU specific implementation



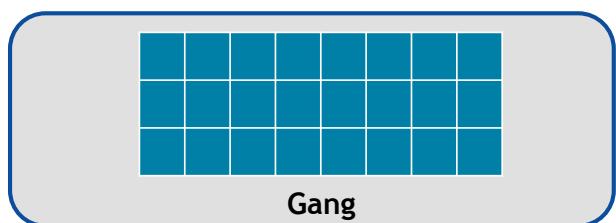
GANG WORKER VECTOR

- When parallelizing our loops, the highest level of parallelism is **gang level parallelism**
- When encountering either the kernels or parallel directive, multiple gangs will be generated, and loop iterations will be spread across the gangs
- These gangs are completely independent of each other, and there is no way for the programmer to know exactly how many gangs are running at a given time
- In many architectures, the gangs have completely separate (or private) memory



GANG WORKER VECTOR

- In our code example, we see that we are applying the **gang** clause to an outer-loop
- This means that the outer-loop iterations will be split across some number of gangs
- These gangs will then execute in parallel with each other
- Whenever a parallel compute region is encountered, some number of gangs will be created
- The programmer is able to specify exactly how many gangs to create



```
#pragma acc parallel loop gang
for( i = 0; i < N; i++ )
    for( j = 0; j < M; j++ )
        < loop code >
```

GANG WORKER VECTOR

- A **vector** is the lowest level of parallelism
- Every gang will have **at least 1 vector**
- A vector has the ability to **run a single instruction on multiple data elements**
- Many different architectures can implement vectors in different ways, however, OpenACC allows for us to define them in a general, non-hardware-specific way



GANG WORKER VECTOR

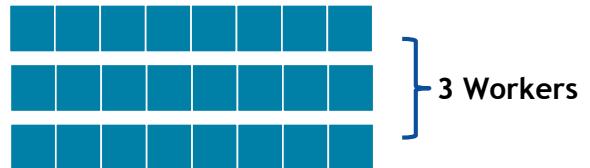
- In our code example, the inner-loop iterations will be evenly divided across a vector
- This means that those loop iterations will be executing in parallel with one-another
- Any loop that is **inside** of our vector loop cannot be parallelized further



```
#pragma acc parallel loop gang
for( i = 0; i < N; i++ )
    #pragma acc loop vector
        for( j = 0; j < M; j++ )
            < loop code >
```

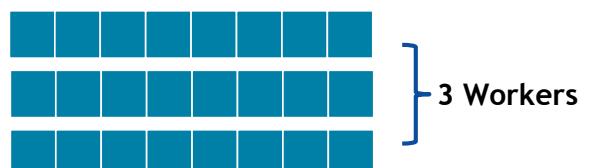
GANG WORKER VECTOR

- The **worker clause** is a way for the programmer to have **multiple vectors** within a gang
- The primary use of the worker clause is to split up one large vector into multiple smaller vectors
- This can be useful when our inner parallel loops are very small, and will not benefit from having a large vector



GANG WORKER VECTOR

- In our sample code, we apply both gang and worker level parallelism to our outer-loop
- The main difference this creates for our code is that we can now have smaller vectors running the inner loop
- This will most likely improve performance **if** the inner loop is relatively small



```
#pragma acc parallel loop gang worker
for( i = 0; i < N; i++ )
    #pragma acc loop vector
        for( j = 0; j < M; j++ )
            < loop code >
```

PARALLEL DIRECTIVE SYNTAX

- When using the parallel directive, you may define the number of gangs/workers/vectors with **num_gangs(N)**, **num_workers(M)**, **vector_length(Q)**
- Then, you may define where they belong in the loops using **gang**, **worker**, **vector**

```
#pragma acc parallel num_gangs(2) \
    num_workers(2) vector_length(32)
{
    #pragma acc loop gang worker
    for(int x = 0; x < 4; x++){
        #pragma acc loop vector
        for(int y = 0; y < 32; y++){
            array[x][y]++;
        }
    }
}
```

PARALLEL DIRECTIVE SYNTAX

- You may also apply gang/worker/vector when using the parallel loop construct

```
#pragma acc parallel loop num_gangs(2) num_workers(2) \
    vector_length(32) gang worker
for(int x = 0; x < 4; x++){
    #pragma acc loop vector
    for(int y = 0; y < 32; y++){
        array[x][y]++;
    }
}
```

KERNELS DIRECTIVE SYNTAX

- When using the kernels directive, the process is somewhat simplified
- You may define the location and number by using **gang(N)**, **worker(M)**, **vector(Q)**
- You may also define gang, worker, and vector using the same method as with the parallel directive
- If you do not specify a number, the compiler will decide one

```
#pragma acc kernels loop gang(2) worker(2)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(32)
    for(int y = 0; y < 32; y++){
        array[x][y]++;
    }
}
```

KERNELS DIRECTIVE SYNTAX

- When using the kernels directive, the process is somewhat simplified
- You may define the location and number by using **gang(N)**, **worker(M)**, **vector(Q)**
- You may also define gang, worker, and vector using the same method as with the parallel directive
- If you do not specify a number, the compiler will decide one
- Each loop nest can have different values for gang, worker, and vector

```
#pragma acc kernels
{
    #pragma acc loop gang(2) worker(2)
    for(int x = 0; x < 4; x++){
        #pragma acc loop vector(32)
        for(int y = 0; y < 32; y++){
            array[x][y]++;
        }
    }

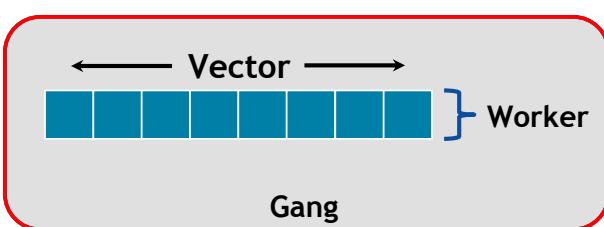
    #pragma acc loop gang(4) worker(4)
    for(int x = 0; x < 16; x++){
        #pragma acc loop vector(16)
        for(int y = 0; y < 16; y++){
            array2[x][y]++;
        }
    }
}
```

GANG WORKER VECTOR

```
#pragma acc kernels loop gang worker(1)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(8)
    for(int y = 0; y < 8; y++){
        array[x][y]++;
    }
}
```

- We have a simple 2-dimensional loop nest
- We have specified that there is **1 worker** and a **vector length of 8**
- We do not specify how many **gangs** to generate, so the compiler will create **enough gangs to cover the loop**

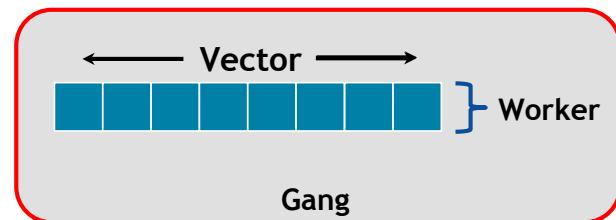
GANG WORKER VECTOR



```
#pragma acc kernels loop gang worker(1)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(8)
    for(int y = 0; y < 8; y++){
        array[x][y]++;
    }
}
```

- The diagram shows a single gang, though the compiler will be able to generate as many gangs as it wants
- These gangs are completely separate from each other, and are indistinguishable
- We will show these gangs apply to a physical loop diagram, but this representation may not be 100% accurate to what the compiler might decide

GANG WORKER VECTOR



```
#pragma acc kernels loop gang worker(1)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(8)
    for(int y = 0; y < 8; y++){
        array[x][y]++;
    }
}
```

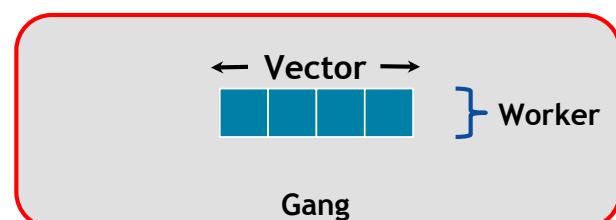
(0,0)	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)
(1,0)	(1,1)	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)
(2,0)	(2,1)	(2,2)	(2,3)	(2,4)	(2,5)	(2,6)	(2,7)
(3,0)	(3,1)	(3,2)	(3,3)	(3,4)	(3,5)	(3,6)	(3,7)

1 Worker

Gang

- The vectors are colored, so that we can observe which loop iterations they are being applied to
- Based on the size of this loop nest, the compiler will (theoretically) generate **4 gangs**

GANG WORKER VECTOR



```
#pragma acc kernels loop gang worker(1)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(4)
    for(int y = 0; y < 8; y++){
        array[x][y]++;
    }
}
```

- We have now reduced the **vector length to 4**, but have kept everything else the same
- The dimension of the outer-loop is still the same, and is still being distributed across the gangs, so the numbers of gangs will not change
- Let's observe how our code will function with a **smaller vector size**

GANG WORKER VECTOR

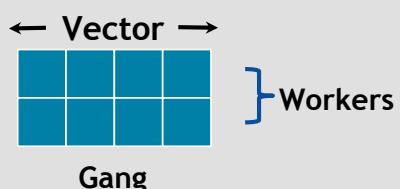


```
#pragma acc kernels loop gang worker(1)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(4)
    for(int y = 0; y < 8; y++){
        array[x][y]++;
    }
}
```

Gang	1 Worker	(0,0)	Vector	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)
		(1,0)		(1,1)	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)
		(2,0)		(2,1)	(2,2)	(2,3)	(2,4)	(2,5)	(2,6)	(2,7)
		(3,0)		(3,1)	(3,2)	(3,3)	(3,4)	(3,5)	(3,6)	(3,7)

- We are still generating 4 gangs, but now each vector is computing two loop iterations
- If we wanted to generate **more gangs**, we would need to increase the size of the outer-loop

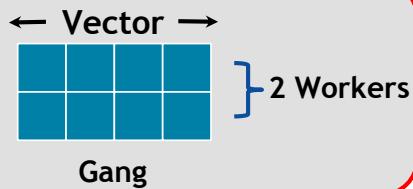
GANG WORKER VECTOR



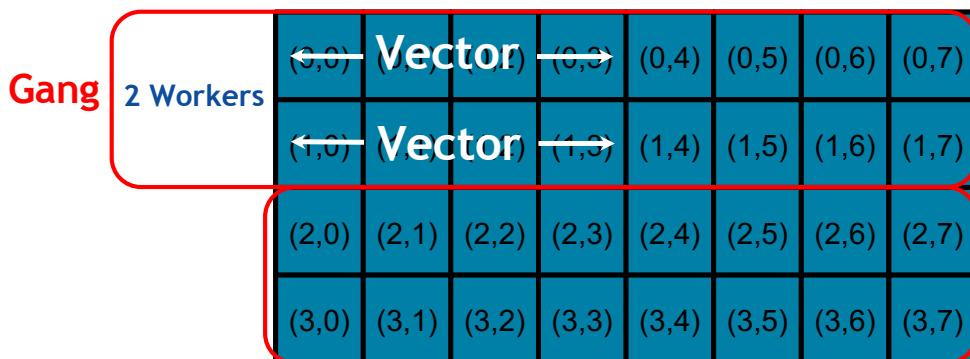
```
#pragma acc kernels loop gang worker(2)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(4)
    for(int y = 0; y < 8; y++){
        array[x][y]++;
    }
}
```

- For our last trivial example, let's increase the **number of workers to 2**
- There are now **two vectors per gang**, and each **vector is of length 4**

GANG WORKER VECTOR

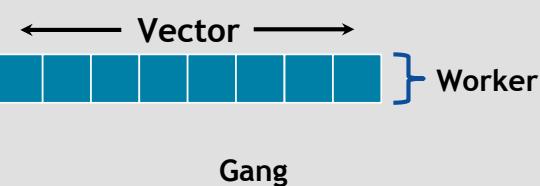


```
#pragma acc kernels loop gang worker(2)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(4)
    for(int y = 0; y < 8; y++){
        array[x][y]++;
    }
}
```



- Since we have increased the number of workers, we will now only generate **2 gangs**

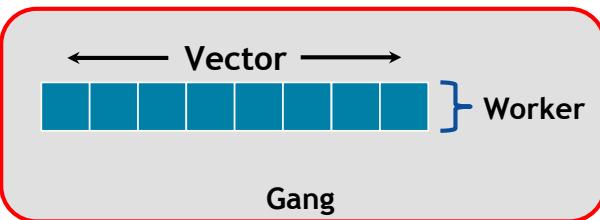
GANG WORKER VECTOR



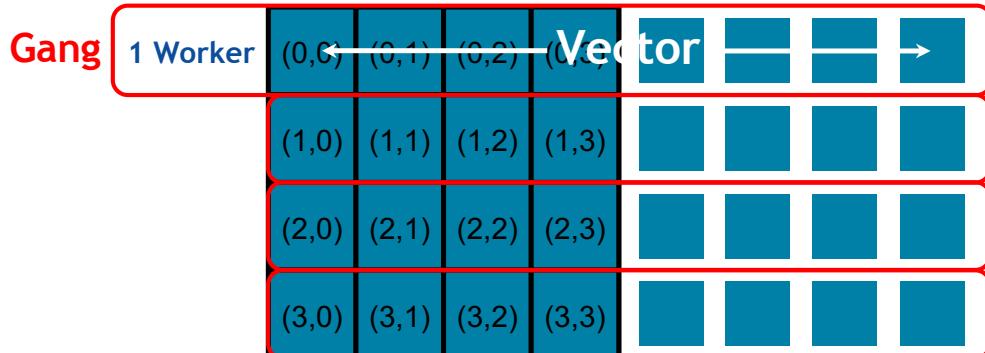
```
#pragma acc kernels loop gang worker(1)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(8)
    for(int y = 0; y < 4; y++){
        array[x][y]++;
    }
}
```

- Now let's look at a situation where the gang/worker/vector model is very useful
- We have reduced the size of our inner-loop to 4 iterations
- Let's try to run this loop with a vector length of 8

GANG WORKER VECTOR

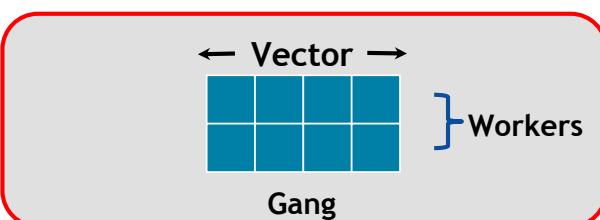


```
#pragma acc kernels loop gang worker(1)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(8)
    for(int y = 0; y < 4; y++){
        array[x][y]++;
    }
}
```



- We can see that our vector length is **much larger** than our inner-loop
- We are **wasting** half of our vector, meaning our code is performing half as well as it could

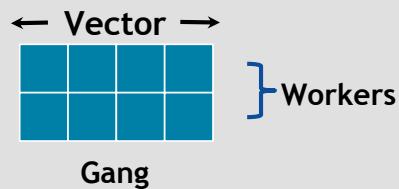
GANG WORKER VECTOR



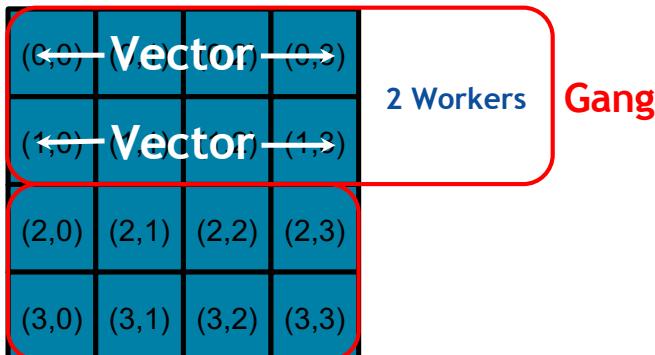
```
#pragma acc kernels loop gang worker(2)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(4)
    for(int y = 0; y < 4; y++){
        array[x][y]++;
    }
}
```

- We can fix this by **breaking our vector** up among **2 workers**
- Now instead of having 1 long vector, we have 2 shorter vectors
- This setup should fit the organization of our loop better

GANG WORKER VECTOR

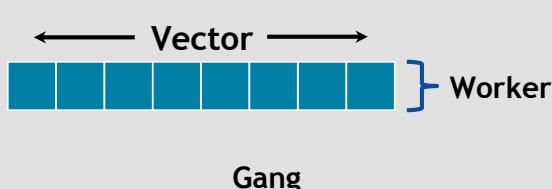


```
#pragma acc kernels loop gang worker(2)
for(int x = 0; x < 4; x++){
    #pragma acc loop vector(4)
    for(int y = 0; y < 4; y++){
        array[x][y]++;
    }
}
```



- We are no longer wasting a portion of our vectors, since the smaller vector size now fits our loop properly
- We always need to consider the size of the loop when choosing the gang worker vector dimensions

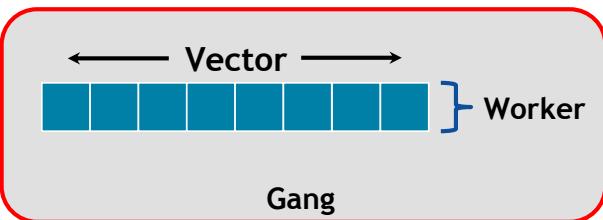
GANG WORKER VECTOR



- Another way we could have fixed this problem is by using the **collapse clause**

```
#pragma acc kernels loop collapse(2) gang worker(1) vector(8)
for(int x = 0; x < 4; x++){
    for(int y = 0; y < 4; y++){
        array[x][y]++;
    }
}
```

GANG WORKER VECTOR



```
#pragma acc kernels loop collapse(2) \
gang worker(1) vector(8)
for(int x = 0; x < 4; x++){
    for(int y = 0; y < 4; y++){
        array[x][y]++;
    }
}
```

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

- The **collapse clause** allows us to combine two small loops into a larger one
- This exposes **additional parallelism**, and allows us to use a **longer vector**

WARPS

- So far we have been using a very small number of gangs/worker/vectors, simply because they're easier to understand
- When actually programming, the number of gangs/worker/vectors will be much larger
- When specifically programming for an NVIDIA GPU, you will always want your vectors large enough to fully utilize **warps**
- A warp, simply put, is an optimized group of 32 threads
- To utilize warps in OpenACC, always make sure that your vector length is a **multiple of 32**

DEVICE_TYPE CLAUSE

- **device_type (<type>)**
- Clauses that follow only apply to the specified device type.
- This allows you to optimize for one type (GPU) without hurting the performance of another (CPU)
- Multiple device types can be specified on a single directive.

```
#pragma acc parallel loop collapse(3)\  
device_type(nvidia) \  
vector_length(256)  
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];
```

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.

MODULE REVIEW

KEY CONCEPTS

In this module we discussed...

- The loop directive enables the programmer to give more information to the compiler about specific loops
- This information may be used for correctness or to improve performance.
- The device_type clause allows the programmer to optimize for one device type without hurting others.