

PRACE Workshop: Deep Learning and GPU programming workshop

7 – 10 September 2020



MODUESX: LOOPOPIMIZATIONS

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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];</pre>
```



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];</pre>
```



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];</pre>
```



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 nonparallel 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];</pre>
```



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];</pre>
```



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];</pre>
```



PRIVATE AND FIRSTPRIVATE CLAUSES

- The private clause allows the programmer to define a list of variables as "thread-private".
- Each thread will be given a private copy of every variable in the commaseparated list
- firstprivate is like private except that the private values are initialized to the same value used on the host. private variables are uninitialized.

```
double tmp[3];
#pragma acc kernels loop private(tmp[0:3])
for( i = 0; i < size; i++ )
  tmp[0] = \langle value \rangle;
  tmp[1] = <value>;
  tmp[2] = <value>;
// note that the host value of "tmp"
// remains unchanged.
```



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] = \langle value \rangle;
  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:
- 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;</pre>
```



TILE CLAUSE

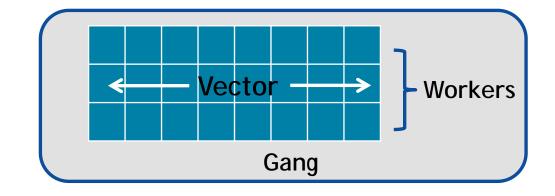
```
tile (x, y, z, ...)
```

- 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];</pre>
```

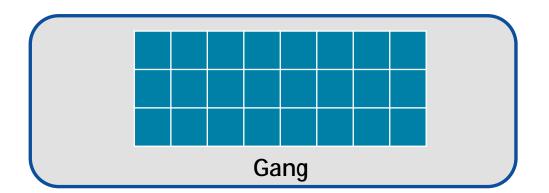


- Gang / Worker / Vector defines the various levels of parallelism we can achieve with OpenACC
- This parallelism is most useful when parallelizing multi-dimensional loop nests
- OpenACC allows us to define a generic Gang / Worker / Vector model that will be applicable to a variety of hardware, but we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



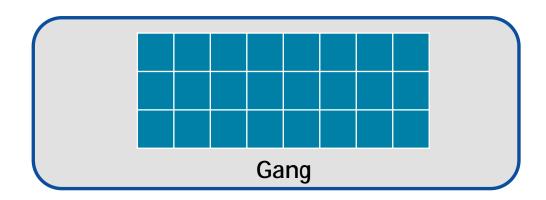


- When paralleling our loops, the highest level of parallelism is gang level parallelism
- When encountering either the kernels or parallel directive, multiple gangs will be generated, and loop iterations will be spread across the gangs
- These gangs are completely independent of each other, and there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





- In our code example, we see that we are applying the **gang** clause to an outerloop
- 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 >
```

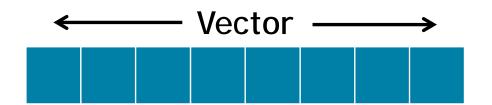


- A vector is the lowest level of parallelism
- Every gang will have at least 1 vector
- A vector has the ability to run a single instruction on multiple data elements
- Many different architectures can implement vectors in different ways, however, OpenACC allows for us to define them in a general, non-hardwarespecific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





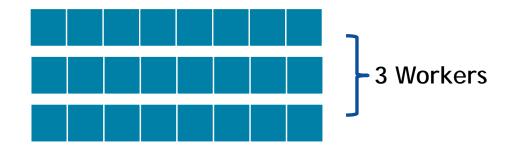
- In our code example, the inner-loop iterations will be evenly divided across a vector
- This means that those loop iterations will be executing in parallel with one-another
- Any loop that is **inside** of our vector loop cannot be parallelized further



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

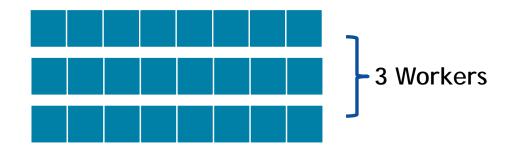


- The worker clause is a way for the programmer to have multiple vectors within a gang
- The primary use of the worker clause is to split up one large vector into multiple smaller vectors
- This can be useful when our inner parallel loops are very small, and will not benefit from having a large vector





- In our sample code, we apply both gang and worker level parallelism to our outerloop
- 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]++;
        }
    }
}</pre>
```



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



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



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

```
OpenACC
```

```
#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]++;
```

WARPS

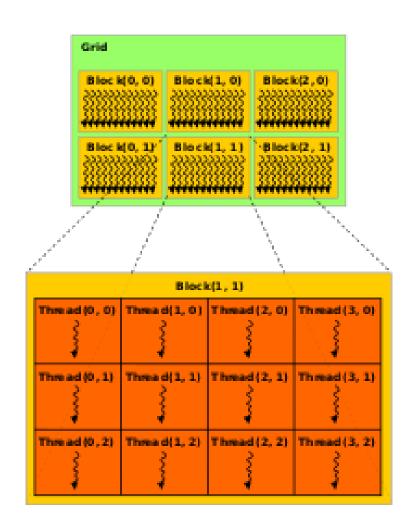
- So far we have been using a very small number of gangs/worker/vectors, simply because they're easier to understand
- When actually programming, the number of gangs/worker/vectors will be much larger
- When specifically programming for an NVIDIA GPU, you will always want your vectors large enough to 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



CUDA PROGRAMMING MODEL REVIEW

- A grid is composed of blocks which are completely independent
- A block is composed of threads which can communicate within their own block
- 32 threads form a warp
- Instructions are issued per warp
- If an operand is not ready the warp will stall
- Context switch between warps when stalled





- Gang is a general term that can mean a few different things. In short, it depends on your architecture.
 - On a multicore CPU, generally gang=thread.
 - On a GPU, generally gang=thread block.

The way I like to think of it is that gang represents my outer-most level of parallelism for any architecture I am running on.



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.



LAB ASSIGNMENT

In this module's lab you will...

- Update the code from the previous module in attempt to improve the performance
- Use PGProf to analyze the performance difference when changing your loops
- Experiment with the device_type clause to ensure GPU optimizations don't slow down the multicore speed-up, or vice versa

