OPENACC ONLINE COURSE 2018

Week 3 – Loop Optimizations with OpenACC

Jeff Larkin, Senior DevTech Software Engineer, NVIDIA
ABOUT THIS COURSE

3 Part Introduction to OpenACC

- Week 1 – Introduction to OpenACC
- Week 2 – Data Management with OpenACC
- Week 3 – Loop Optimizations with OpenACC

Each week will have a corresponding lab, only an hour and a web browser is required.

Please ask questions in the Q&A box, our TA’s will answer as quickly as possible.
Enable **YOU** to accelerate **YOUR** applications with OpenACC.
WEEK 3 OUTLINE

Topics to be covered

- Gangs, Workers, and Vectors Demystified
- GPU Profiles
- Loop Optimizations
- Week 3 Lab
- Where to Get Help
WEEKS 1 & 2 REVIEW
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.
OpenACC Directives

- Incremental
- Single source
- Interoperable
- Performance portable
- CPU, GPU, Manycore

```c
#pragma acc data copyin(a,b) copyout(c) 
{
    ...
    #pragma acc parallel 
    {
        #pragma acc loop gang vector 
        for (i = 0; i < n; ++i) {
            c[i] = a[i] + b[i]; 
            ...
        }
    }
    ...
}
```
PARALLELIZE WITH OPENACC PARALLEL LOOP

```c
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++;
}
```

We didn’t detail how to parallelize the loops, just which loops to parallelize.
#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) copyin(A[0:n*m])
    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 copyin(Anew[0:n*m]) copyout(A[0:n*m])
    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.
OPENACC SPEED-UP

PGI 18.7, NVIDIA Tesla V100, Intel i9-7900X CPU @ 3.30GHz
GANGS, WORKERS, AND VECTORS DEMYSTIFIED
GANGS, WORKERS, AND VECTORS DEMYSTIFIED
GANGS, WORKERS, AND VECTORS DEMYSTIFIED
How much work 1 worker can do is limited by his speed.

A single worker can only move so fast.
GANGS, WORKERS, AND VECTORS DEMYSTIFIED

Even if we increase the size of his roller, he can only paint so fast.

We need more workers!
Multiple workers can do more work and share resources, if organized properly.
By organizing our workers into groups (gangs), they can effectively work together within a floor.

Groups (gangs) on different floors can operate independently.

Since gangs operate independently, we can use as many or few as we need.
GANGS, WORKERS, AND VECTORS DEMYSTIFIED

Even if there’s not enough gangs for each floor, they can move to another floor when ready.
Gangs, Workers, and Vectors Demystified

Our painter is like an OpenACC worker, he can only do so much.

His roller is like a vector, he can move faster by covering more wall at once.

Eventually we need more workers, which can be organized into gangs to get more done.
GPU PROFILES
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
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
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
PROFILING GPU CODE

Managed Memory

CPU Page Faults trigger Device to Host Migrations.

GPU Page Faults trigger Host to Device Migrations.

These may be hints that more needs to be parallelized and/or data optimization is needed.
CPU Page Faults trigger Device to Host Migrations.

GPU Page Faults trigger Host to Device Migrations.

These may be hints that more needs to be parallelized and/or data optimization is needed.
LOOP OPTIMIZATIONS
OPENACC LOOP DIRECTIVE

Expressing parallelism

- Mark a single for loop for parallelization
- Allows the programmer to give additional information and/or optimizations about the loop
- Provides many different ways to describe the type of parallelism to apply to the loop
- Must be contained within an OpenACC compute region (either a kernels or a parallel region) to parallelize loops

C/C++

```c
#pragma acc loop
for(int i = 0; i < N; i++)
  // Do something
```

Fortran

```fortran
!$acc loop
do i = 1, N
  ! Do something
```
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

```c
#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 )

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0)</td>
<td>(0,1)</td>
<td>(0,2)</td>
<td>(0,3)</td>
</tr>
<tr>
<td>(1,0)</td>
<td>(1,1)</td>
<td>(1,2)</td>
<td>(1,3)</td>
</tr>
<tr>
<td>(2,0)</td>
<td>(2,1)</td>
<td>(2,2)</td>
<td>(2,3)</td>
</tr>
<tr>
<td>(3,0)</td>
<td>(3,1)</td>
<td>(3,2)</td>
<td>(3,3)</td>
</tr>
</tbody>
</table>

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

When/Why to use it

- A single loop might not have enough iterations to parallelize
- Collapsing outer loops gives more scalable (gangs) parallelism
- Collapsing inner loops gives more tight (vector) parallelism
- Collapsing all loops gives the compiler total freedom, but may cost data locality
#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) collapse(2) \
        copyin(A[0:n*m]) copyin(Anew[0:n*m])
    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 collapse(2) \
        copyin(Anew[0:n*m]) copyout(A[0:n*m])
    for( int j = 1; j < n-1; j++) {
        for( int i = 1; i < m-1; i++) {
            A[j][i] = Anew[j][i];
        }
    }
    iter++;
}
OPENACC SPEED-UP

PGI 18.7, NVIDIA Tesla V100, Intel i9-7900X CPU @ 3.30GHz
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

```c
#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];
```
#pragma acc kernels loop tile(2,2)
for(int x = 0; x < 4; x++){
    for(int y = 0; y < 4; y++){
        array[x][y]++;
    }
}
#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) \
    copyin(A[0:n*m]) copyin(Anew[0:n*m])
    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) \
    copyin(Anew[0:n*m]) copyout(A[0:n*m])
    for( int j = 1; j < n-1; j++ ) {
        for( int i = 1; i < m-1; i++) {
            A[j][i] = Anew[j][i];
        }
    }
    iter++;
}
The collapse clause often requires an exhaustive search of options.

For our example code…

- CPU saw no benefit from tiling
- GPU saw anywhere from a 23% loss of performance to a 10% improvement
OPENACC SPEED-UP

PGI 18.7, NVIDIA Tesla V100, Intel i9-7900X CPU @ 3.30GHz
The developer can instruct the compiler which levels of parallelism to use on given loops by adding clauses:

- **gang** – Mark this loop for gang parallelism
- **worker** – Mark this loop for worker parallelism
- **vector** – Mark this loop for vector parallelism

These can be combined on the same loop.

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

#pragma acc parallel loop \ 
collapse(3) gang vector
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];
```
**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 as well.

```c
#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];
```
ADJUSTING GANGS, WORKERS, AND VECTORS

The compiler will choose a number of gangs, workers, and a vector length for you, but you can change it with clauses.

- **num_gangs(N)** – Generate N gangs for this parallel region
- **num_workers(M)** – Generate M workers for this parallel region
- **vector_length(Q)** – Use a vector length of Q for this parallel region

```c
#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]++;
        }
    }
}
```
#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) collapse(2) vector_length(1024) \
        copyin(A[0:n*m]) copy(A[0:n*m])
    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 collapse(2) vector_length(1024) \
        copyin(Anew[0:n*m]) copyout(A[0:n*m])
    for( int j = 1; j < n-1; j++ ) {
        for( int i = 1; i < m-1; i++ ) {
            A[j][i] = Anew[j][i];
        }
    }
    iter++;
OPENACC SPEED-UP

PGI 18.7, NVIDIA Tesla V100, Intel i9-7900X CPU @ 3.30GHz
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
- Gangs should come from outer loops, vectors from inner
CLOSING REMARKS
KEY CONCEPTS

In this lab we discussed…

- Some details that are available to use from a GPU profile
- Gangs, Workers, and Vectors Demystified
- Collapse clause
- Tile clause
- Gang/Worker/Vector clauses
OPENACC RESOURCES

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

FREE Compilers