OpenMP and GPUs

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OpenMP was designed to replace low-level and tedious multi-threaded programming solutions like POSIX threads, or Pthreads.

OpenMP was originally targeted towards controlling capable and completely independent processors, with shared memory. The most common such configurations today are the many multi-core chips we all use. You might have dozens of threads, each of which takes some time to start or complete.

In return for the flexibility to use those processors to their fullest extent, OpenMP assumes that you know what you are doing. You prescribe what how you want the threads to behave and the compiler faithfully carries it out.
Then Came This

CPU Memory

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

GPU Memory

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

CPU

GPU
GPUs are not CPUs

GPU require memory management. We do not simply have a single shared dataspace.

GPUs have thousands of cores.

But they aren't independent.

And they can launch very lightweight threads.

But it seems like the OpenMP approach provides a good starting point to get away from the low-level and tedious CUDA API...
Let OpenACC evolve rapidly without disturbing the mature OpenMP standard. They can merge somewhere around version 4.0.
Meanwhile...

Since the days of RISC vs. CISC, Intel has mastered the art of figuring out what is important about a new processing technology and saying “why can’t we do this in x86?”

The Intel Many Integrated Core (MIC) architecture is about large die, simpler circuit, and much more parallelism, in the x86 line.
What is was MIC?

Basic Design Ideas:

- Leverage x86 architecture (a CPU with many cores)
- Use x86 cores that are simpler, but allow for more compute throughput
- Leverage existing x86 programming models
- Dedicate much of the silicon to floating point ops., keep some cache(s)
- Keep cache-coherency protocol
- Increase floating-point throughput per core
- Implement as a separate device
- Strip expensive features (out-of-order execution, branch prediction, etc.)
- Widened SIMD registers for more throughput (512 bit)
- Fast (GDDR5) memory on card

Courtesy Dan Stanzione, TACC
Latest Last MIC Architecture

- Many cores on the die
- L1 and L2 cache
- Bidirectional ring network for L2 Memory and PCIe connection

Courtesy Dan Stanzone, TACC
Implications for the OpenMP/OpenACC Merge

Intel and NVIDIA have both influenced their favored approaches to make them more amenable to their own devices.
The OpenMP 4.0 standard did incorporate the features needed for accelerators, with an emphasis on Intel-like devices. We are left with some differences.

OpenMP takes its traditional prescriptive approach ("this is what I want you to do"), while OpenACC could afford to start with a more modern (compilers are smarter) descriptive approach ("here is some parallelizable stuff, do something smart"). This is practically visible in such things as OpenMP's insistence that you identify loop dependencies, versus OpenACC's kernel directive, and its ability to spot them for you.

OpenMP assumes that every thread has its own synchronization control (barriers, locks), because real processors can do whatever they want, whenever. GPUs do not have that at all levels. For example, NVIDIA GPUs have synchronization at the warp level, but not the thread block level. There are implications regarding this difference such as no OpenACC async/wait in parallel regions or kernels.

In general, you might observe that OpenMP was built when threads were limited and start up overhead was considerable (as it still is on CPUs). The design reflects the need to control for this. OpenACC starts with devices built around thousands of very, very lightweight threads.

They are also complementary and can be used together very well.
The most obvious improvements for accelerators are the data migration commands. These look very similar to OpenACC.

```
#pragma omp target device(0) map(tofrom:B)
```
## OpenMP vs. OpenACC Data Constructs

<table>
<thead>
<tr>
<th>OpenMP</th>
<th>OpenACC</th>
</tr>
</thead>
<tbody>
<tr>
<td>target data</td>
<td>data</td>
</tr>
<tr>
<td>target enter data</td>
<td>enter data</td>
</tr>
<tr>
<td>target exit data</td>
<td>exit data</td>
</tr>
<tr>
<td>target update</td>
<td>update</td>
</tr>
<tr>
<td>declare target</td>
<td>declare</td>
</tr>
</tbody>
</table>
OpenMP vs. OpenACC Data Clauses

**OpenMP**

- map(to:...)  
- map(from:...)  
- map(tofrom:...)  
- map(alloc:)  
- map(release:)  
- map(delete:)  

**OpenACC**

- copyin(...)  
- copyout(...)  
- copy(...)  
- create(...)  
- delete(...)  
- delete(...) finalize

OpenMP 5 has also embraced the NVIDIA "unified shared memory" paradigm

```c
#pragma omp requires unified_shared_memory
complex_deep_data * cdp = create_array_of_data();
#pragma omp target    //Notice no mapping clauses!
operate_on_data( cdp );
```

Just like with NVIDIA Unified Memory, this is hopelessly naïve and is not used in production code. It is often recommended for a "first pass" (but I find that counter-productive).

The closely related deep copy directives (*declare mapper*) can be useful to aid in moving pointer-based data. As can the *allocate* clauses.
## OpenMP vs. OpenACC Compute Constructs

<table>
<thead>
<tr>
<th>OpenMP</th>
<th>OpenACC</th>
</tr>
</thead>
<tbody>
<tr>
<td>target</td>
<td>parallel / kernels</td>
</tr>
<tr>
<td>teams</td>
<td>parallel / kernels</td>
</tr>
<tr>
<td>distribute</td>
<td>loop gang</td>
</tr>
<tr>
<td>parallel</td>
<td>parallel / kernels</td>
</tr>
<tr>
<td>for / do</td>
<td>loop worker or loop gang</td>
</tr>
<tr>
<td>simd</td>
<td>loop vector</td>
</tr>
<tr>
<td>is_device_ptr(...)</td>
<td>deviceptr(...)</td>
</tr>
</tbody>
</table>
## OpenMP vs. OpenACC Differences

<table>
<thead>
<tr>
<th>OpenMP</th>
<th>OpenACC</th>
</tr>
</thead>
<tbody>
<tr>
<td>device(n)</td>
<td>---</td>
</tr>
<tr>
<td>depend(to:a)</td>
<td>async(n)</td>
</tr>
<tr>
<td>depend(from:b)</td>
<td>async(n)</td>
</tr>
<tr>
<td>nowait</td>
<td>async</td>
</tr>
<tr>
<td>loops, tasks, sections</td>
<td>loops</td>
</tr>
<tr>
<td>atomic</td>
<td>atomic</td>
</tr>
<tr>
<td>master, single, critical, barrier, locks, ordered, flush, cancel</td>
<td>---</td>
</tr>
</tbody>
</table>
int main(int argc, const char* argv[]) {
    int n = 10240; float a = 2.0f; float b = 3.0f;
    float* x = (float*) malloc(n * sizeof(float));
    float* y = (float*) malloc(n * sizeof(float));

    // Run SAXPY TWICE inside data region
    #pragma omp target data map(to:x)
    {
        #pragma omp target map(tofrom:y)
        #pragma omp teams
        #pragma omp distribute
        #pragma omp parallel for
        for(int i = 0; i < n; ++i){
            y[i] = a*x[i] + y[i];
        }
        #pragma omp target map(tofrom:y)
        #pragma omp teams
        #pragma omp distribute
        #pragma omp parallel for
        for(int i = 0; i < n; ++i){
            y[i] = b*x[i] + y[i];
        }
    }
}

Courtesy Christian Terboven
Comparing OpenACC with OpenMP 4.0 on NVIDIA & Phi

First two examples
Courtesy Christian Terboven

OpenMP 4.0 for Intel Xeon Phi

```
#pragma omp target device(0) map(tofrom:B)
#pragma omp parallel for
for (i=0; i<N; i++)
    B[i] += sin(B[i]);
```

OpenMP 4.0 for NVIDIA GPU

```
#pragma omp target device(0) map(tofrom:B)
#pragma omp teams num_teams(num_blocks) num_threads(bsize) distribute
for (i=0; i<N; i += num_blocks)
    #pragma omp parallel for
    for (b = i; b < i+num_blocks; b++)
        B[b] += sin(B[b]);
```

OpenACC for NVIDIA GPU

```
#pragma acc kernels
for (i=0; i<N; ++i)
    B[i] += sin(B[i]);
```
OpenMP now has a number of OpenACC-like metadirectives to help cope with this confusion:

```c
#pragma omp target map(to:a,b) map(from:c)
#pragma omp metadrictive when (device={arch(nvptx}): teams loop) default (parallel loop)
for (i = 1; i<n; i++)
    c[i] = a[i] * b[i]
```

And also variant functions to substitute code for different targets.

```c
#pragma omp declare target
int some_routine(int a){
    //do things in serial way
}

#pragma omp declare variant ( int some_routine(int a) ) match(context={target} \ device={arch(nvptx)} )
int some_routine_gpu(int a){
    //gpu optimized code
}
```
OpenMP 4.0 Across Compilers

Cray C Compiler (v8.5)
#pragma omp target teams distribute
for(int ii = 0; ii < y; ++ii)

Clang Compiler (alpha)
#pragma omp target teams distribute \
parallel for schedule(static,1)
for(int ii = 0; ii < y; ++ii)

Intel C Compiler (v16.0)
#pragma omp target
#pragma omp parallel
for for(int ii = 0; ii < y; ++ii)

GCC C Compiler (v6.1))
#pragma omp target teams distribute \
parallel for
for(int ii = 0; ii < y; ++ii)

Subtle and confusing? You bet. For a nice discussion of these examples visit their authors at https://www.openmp.org/wp-content/uploads/Matt_openmp-booth-talk.pdf
In summary, using NPB benchmarks (FFT, Gauss Seidel, Multi-Grid) on leadership class platforms (Titan and Summit) using multiple compilers (clang, gcc, PGI, Cray, IBM), OpenMP is not yet competitive with OpenACC on GPUs.

A very interesting side-note is that OpenACC kernels and loop performed the same.
So, at this time...

- If you are using the fairly obsolete Phi Knights Corner or Knights Landing, you are probably going to be using the Intel OpenMP 4+ release. Unless you use it in cache mode, and then this is moot.

- If you are using NVIDIA GPUs, you are going to be using OpenACC.

Of course, there are other ways of programming both of these devices. You might treat Phi as MPI cores and use CUDA on NVIDIA, for example. But if the directive based approach is for you, then your path is clear. And as you should now suspect, even if it takes a while for these to merge as a standard, it is not a big jump for you to move between them.

The national labs have decided to deal with this by adding an additional layer of abstraction that will translate to the most usable lower level API with frameworks such as oneAPI (Includes DPC++ and extends SYCL) or Kokkos.

Right now, on Bridges you can try this out by using the \texttt{-mp=gpu} switch with the \texttt{nvc/nvfortran} compilers. Make sure you have the \texttt{nvhpc} and \texttt{cuda} modules loaded.