OpenMP Advanced Overview
SIMD and Target Offload

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Topics

• We Will Cover:
  • Accelerated OpenMP* basics review
  • Vectorization and OpenMP* SIMD
  • OpenMP* Device Usage (target)

• We will NOT Cover:
  • Detailed OpenMP* basics usage
  • OpenMP* Tasking
  • Affinity
  • NUMA effects

• Reference material in backup:
  • Interface descriptions for all described constructs
  • Brief Introduction to OpenMP* 5.0 Changes
OpenMP* Review
OpenMP*: 
- Application Program Interface (API) focused on the expression of parallelism within an application
- Provides methods for creating multi-threaded, heterogeneous device, and vectorized applications
- Contains standardized directives and library functions
- Supports C, C++, and Fortran
- Was established in 1997
Threads are the original and most basic concept within OpenMP*.

A master thread spawns a team of threads when it encounters a parallel region.

Threads can distribute work among themselves to accomplish the same task faster, or can work on independent tasks in parallel.
### OpenMP* Directive Overview

<table>
<thead>
<tr>
<th>Directive</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>#pragma omp parallel !$omp parallel</code></td>
<td>Create threads in a parallel region</td>
</tr>
<tr>
<td><code>#pragma omp for !$omp do</code></td>
<td>Distribute iterations of a loop among threads</td>
</tr>
<tr>
<td><code>#pragma omp for reduction(+:sum) !$omp do reduction(+:sum)</code></td>
<td>Distribute iterations of a loop among threads, and reduce the thread private ‘sum’ after the loop is complete.</td>
</tr>
<tr>
<td><code>#pragma omp single !$omp single</code></td>
<td>Execute code with a single thread</td>
</tr>
<tr>
<td><code>#pragma omp master !$omp master</code></td>
<td>Execute code only on the master thread</td>
</tr>
<tr>
<td><code>#pragma omp barrier !$omp barrier</code></td>
<td>Wait for all threads in current team before proceeding</td>
</tr>
</tbody>
</table>
# OpenMP* Data Sharing Attributes

<table>
<thead>
<tr>
<th>Data Sharing Level</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>shared</td>
<td>Variables are shared among all members. If one thread updates the value, all members see the new value.</td>
</tr>
<tr>
<td>private</td>
<td>Variables are private among members. If one member updates the value, no other member sees that update.</td>
</tr>
<tr>
<td>firstprivate</td>
<td>Same as private, but all members are initialized with the value before the scope changed.</td>
</tr>
<tr>
<td>lastprivate</td>
<td>Same as private, but the logically last iteration of a loop is used to set the value of the variable after the region ends.</td>
</tr>
</tbody>
</table>
Modern computational architectures include everything from traditional CPUs, to Vector Processing Units, to Graphics Processing Units, and beyond.

OpenMP* is constantly evolving to help developers properly utilize the features of their underlying hardware.

The remainder of this talk will focus on more advanced topics from OpenMP*. These topics include:

- SIMD (Vectorization)
- Target Teams (Heterogeneous Devices)
Introduction to SIMD
Introduction to SIMD

Scalar Code
- Executes code one element at a time.
- Not all scalar instructions have a vector equivalent (e.g. cpuid)

Vector Code
- Executes code multiple elements at a time.
- Single Instruction Multiple Data.
- Not all vector instructions have a scalar equivalent (e.g. shuffle)

[Scalar] 1 elem at a time
addss xmm1, xmm2

[SSE] 4 elems at a time
addps xmm1, xmm2

[AVX] 8 elems at a time
vaddps ymm1, ymm2, ymm3

[MIC / AVX-512] 16 elems at a time
vaddps zmm1, zmm2, zmm3
Introduction to SIMD

Hardware (Colors represent SIMD lanes)

Software (Vectorization)

```c
int i = 0;
for (; i < size; i += 4) {
    for (int j = 0; j < 4; j++)
        C[i+j] = A[i+j] + B[i+j];
}
for (; i < size; i++) {
    C[i] = A[i] + B[i];
}
```
Utilizing SIMD Instructions
Utilizing SIMD Instructions

SIMD Libraries

- Use a library that is already SIMD-optimized (e.g. Intel® Math Kernel Library)

Implicit (Auto) Vectorization

- Use a compiler that recognises vectorization opportunities (e.g. Intel® Composer XE)
- Possibly annotate with vendor specific pragmas (i.e. #pragma ivdep)

Explicit (Manual) Vectorization

- Express vectorization opportunities to a compiler (e.g. OpenMP* 4.0)
- Write intrinsics code (or inline assembly!)
Very powerful, but a compiler cannot make unsafe assumptions.

- a, b and c point to different arrays.
- Value of global g_size is constant.
- ind[i] is a one-to-one mapping.

```c
int* g_size;
void not_vectorizable(float* a, float* b, float* c, int* ind)
{
    for (int i = 0; i < *g_size; i++)
    {
        int j = ind[i];
        c[j] += a[i] + b[i];
    }
}
```
Utilizing SIMD Instructions – Auto-vectorization

Very powerful, but a compiler cannot make unsafe assumptions.

\[
\begin{align*}
\text{int} & \ast \text{g}_\text{size}; \\
\text{void vectorizable} & (\text{float} \ast \text{restrict a, float} \ast \text{restrict b, float} \ast \text{restrict c, int} \ast \text{ind}) \\
\{ & \\
\quad & \text{int size} = *\text{g}_\text{size}; \\
\quad & \text{#pragma ivdep} \\
\quad & \text{for (int } i = 0; i < \text{size}; i++) \\
\quad & \{ \\
\quad & \quad \text{int } j = \text{ind}[i]; \\
\quad & \quad \text{c}[j] += \text{a}[i] + \text{b}[i]; \\
\quad & \} \\
\}
\end{align*}
\]

- Safe Assumptions:
  - a, b and c point to different arrays. (restrict)
  - Value of global g_size is constant. (pointer dereference outside loop)
  - ind[i] is a one-to-one mapping. (#pragma ivdep)
Utilizing SIMD Instructions – Compiler Pragmas

```c
float sum = 0.0f;
float *p = a;
int step = 4;

#pragma omp simd reduction(+:sum) linear(p:step)
for (int i = 0; i < N; ++i) {
    sum += *p;
    p += step;
}
```

- The same constructs can have different meaning from each other:
  - The two `+=` operators have a different purpose.
  - The variables `sum` and `p` relate differently to the iteration space.

- The compiler has to generate different code.
- OpenMP* 4.0 pragmas allow programmers to express this.
Implicit vs Explicit Vectorization

**Implicit**
- Automatic dependency analysis. (e.g. recognises SIMD reductions)
- Recognizes idioms with data dependencies. (e.g. array[i++] = x; -> vcompress)
- Non-inline functions will be scalarized.
- Limited support for outer-loop vectorization (only with –O3).

**Explicit**
- No dependency analysis. (e.g. SIMD reductions must be declared)
- Recognizes idioms without data dependencies.
- Non-inline functions can be vectorized.
- Outer loops can be vectorized.
Let's say we want to measure achievable bandwidth.

In order to achieve the highest bandwidth we can, we need to move a maximum number of bytes per cycle.

The STREAM Triad benchmark is typically used to measure this, it is a simple vector multiply and add of the form:

```c
for ( int i = 0; i < N; i++ ) {
    a[i] = b[i] * scalar + c[i];
}
```
OpenMP* SIMD Example: STREAM Triad

In this example, the 16 is tuned for single precision on AVX512
OpenMP* Target
OpenMP* Target

Introduced in OpenMP* 4.0

The **target** construct is used to create a target task that should be offloaded to a device.

We’ll carry the STREAM triad example with us to show device execution.
OpenMP* Target Example: STREAM Triad

**Always Move Everything**

```c
#pragma omp target map(tofrom:a[0:N], b[0:N], c[0:N], scalar)
for (i = 0, i < N, i++)
    a[i] = b[i] * scalar + c[i];
```

**Only Move What's Needed**

```c
#pragma omp target map(to:b[0:N], c[0:N], scalar) map(tofrom:a[0:N])
for (i = 0, i < N, i++)
    a[i] = b[i] * scalar + c[i];
```
OpenMP* Target Example: STREAM Triad

Structured Data Management

```c
#pragma omp target data map(to:b[0:N], c[0:N], scalar) \ 
    map(from:a[0:N])
{
    #pragma omp target
    for (i = 0, i < N, i++){
        a[i] = b[i] * scalar + c[i];
    }
}
```

Unstructured Data Management

```c
#pragma omp target enter data map(to:a[0:N], b[0:N], 
    c[0:N], scalar)
#pragma omp target
for (i = 0, i < N, i++){
    a[i] = b[i] * scalar + c[i];
}
#pragma omp target exit data map(from:a[0:N])
```
OpenMP* Target Example: STREAM Triad

```c
#pragma omp target enter data \
    map(to:a[0:N],b[0:N],c[0:N])

#pragma omp target 
for (i = 0, i < N, i++){
    a[i] = b[i] * scalar + c[i];
}

#pragma omp target exit data map(from:a[0:N])
```

At the beginning of the target region, b, c, and scalar will be copied onto the device and after the target region is complete, a will be copied back to the host. The target region will be executed on the device.

However....

All of the examples so far have a **serial** execution!

The target construct only creates a target task which is executed by a **single** thread!
OpenMP* Teams

To utilize multiple threads on a device, we need to first use the teams construct.

A teams construct creates a league of teams. Each team consists of some number of threads, and to begin with the master thread of each team executes the code in the teams region.

```
#pragma omp target teams
```

![Diagram showing teams construct and execution on host and device]
OpenMP* Teams Example: STREAM Triad

```c
#pragma target teams
for (i = 0, i < N, i++){
a[i] = b[i] * scalar + c[i];
}
```

Now we have multiple threads executing on the device, however they are all performing the **same** work.

Additionally, only the **master** thread of each team is doing anything.
OpenMP* Distribute

Right now we have:

- Multiple thread teams working on a device
- All thread teams performing the same work
- Only the master thread of each team executing anything

When we encounter a loop, we can spread the iterations among teams using the **distribute** construct.
At this point, we have teams performing independent iterations of this loop, however each team is only executing serially.

In order to work in parallel within a team we thread as we normally would with the basic OpenMP usage.

However, there are composite constructs that can help.
OpenMP* Distribute Full Example: STREAM Triad

```c
#pragma target teams distribute parallel for
for (i = 0, i < N, i++){
    a[i] = b[i] * scalar + c[i];
}
```

Now, we have teams splitting the work into large chunks on the device, while threads within the team will further split the work into smaller chunks and execute in parallel.
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Notice revision #20110804
OpenMP* References
#pragma omp simd / !$omp simd => for/do loop is a SIMD loop.

<table>
<thead>
<tr>
<th>Clause</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>private(list)</td>
<td>Listed variables are scoped as private</td>
</tr>
<tr>
<td>lastprivate(list)</td>
<td>Listed variables are scoped as lastprivate</td>
</tr>
<tr>
<td>reduction(reduction-identifier:list)</td>
<td>Reduce listed variables according to reduction-identifier</td>
</tr>
<tr>
<td>collapse(n)</td>
<td>Associate loop construct with n following nested loops</td>
</tr>
<tr>
<td>safelen(n)</td>
<td>Maximum allowed 'distance' between SIMD lanes in a single execution</td>
</tr>
<tr>
<td>aligned(list)</td>
<td>Hint to the run-time to use aligned loads and stores on listed variables</td>
</tr>
<tr>
<td>linear(list)</td>
<td>Described later</td>
</tr>
</tbody>
</table>
Explicit Vectorization – OpenMP* 5.0 SIMD Loops

#pragma omp simd / !$omp simd => for/do loop is a SIMD loop.

<table>
<thead>
<tr>
<th>Clause</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>nontemporal(list)</td>
<td>Hint to the runtime to use accesses with no temporal locality, i.e. there is no need to cache the data</td>
</tr>
<tr>
<td>order(concurrent)</td>
<td>Hint to the run-time that iterations of the loop can be executed in any order, including concurrently</td>
</tr>
</tbody>
</table>
Explicit Vectorization – OpenMP* SIMD Functions

#pragma omp declare simd / !$omp declare simd => function called from a SIMD loop.

<table>
<thead>
<tr>
<th>Clause</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>simdlen(n)</td>
<td>Preferred SIMD width is n</td>
</tr>
<tr>
<td>aligned(list)</td>
<td>Listed variables should use aligned accesses</td>
</tr>
<tr>
<td>uniform(list)</td>
<td>Listed variables have an invariant value for all concurrent calls to the SIMD function</td>
</tr>
<tr>
<td>inbranch</td>
<td>Function is always called from within a branch</td>
</tr>
<tr>
<td>notinbranch</td>
<td>Function is never called from within a branch</td>
</tr>
<tr>
<td>linear(list)</td>
<td>Described later</td>
</tr>
</tbody>
</table>
OpenMP* Linear Clause

The linear clause provides the compiler additional information about variables.

linear(linear-list:step)

<table>
<thead>
<tr>
<th>Linear List Options</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>variable val(variable)</td>
<td>Variable listed have linear values with a distance between consecutive SIMD lanes of step.</td>
</tr>
<tr>
<td>ref(variable)</td>
<td>Variable listed have linear memory addresses with a distance between consecutive SIMD lanes of step.</td>
</tr>
<tr>
<td>uval(variable)</td>
<td>Variable listed have linear values with a distance between consecutive SIMD lanes of step. Variable uses the same storage location across all SIMD lanes, and the logically last iteration is stored out.</td>
</tr>
</tbody>
</table>
#pragma omp target !$omp target !$omp end target

=> Create a *target task*, and execute on a device

<table>
<thead>
<tr>
<th>Clause</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>if(scalar-expression)</td>
<td>If scalar-expression is false, device used is host</td>
</tr>
<tr>
<td>device(integer-expression)</td>
<td>Controls the device used, as described in data management</td>
</tr>
<tr>
<td></td>
<td>constructs</td>
</tr>
<tr>
<td>private(list)</td>
<td>Listed variables are scoped as private</td>
</tr>
<tr>
<td>firstprivate(list)</td>
<td>Listed variables are scoped as firstprivate</td>
</tr>
<tr>
<td>map([[map-type-modifier[],]map-type:]list)</td>
<td>Described later</td>
</tr>
<tr>
<td>is_device_ptr(list)</td>
<td>Listed variables are already device pointers (allocated</td>
</tr>
<tr>
<td></td>
<td>before the target construct)</td>
</tr>
<tr>
<td>depend(dependence-type:list)</td>
<td>Follows task dependencies, as previously described.</td>
</tr>
<tr>
<td>nowait</td>
<td>If present, execution of the target task may be deferred. If</td>
</tr>
<tr>
<td></td>
<td>not, the task is an undeferred task.</td>
</tr>
</tbody>
</table>
## OpenMP* 5.0 Target Construct

```
#pragma omp target !$omp target !$omp end target
```

=> Create a *target task* task, and execute on a device

<table>
<thead>
<tr>
<th>Clause</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>in_reduction(reduction-identifier:list)</td>
<td>The generated target task will participate in a previously defined task_reduction</td>
</tr>
<tr>
<td>defaultmap(implicit-behavior:[variable-category])</td>
<td>Implicit behavior can be one of alloc, to, from, tofrom, firstprivate, none, or default and variable category can be one of scalar, aggregate, pointer, or allocatable (in fortran)</td>
</tr>
<tr>
<td>allocate([allocator:]list)</td>
<td>Allocates listed variables using the specified allocator (or a default device allocator)</td>
</tr>
<tr>
<td>uses_allocators(allocator[ (allocator-traits-arrays) ], ...)</td>
<td>Each allocator listed will be made available in the target region.</td>
</tr>
<tr>
<td>device([device-modifier:]integer-expression)</td>
<td>Modifier can be ancestor, or device_num. Used to determine which device will be selected. ancestor:1 executes on the parent device of the target region.</td>
</tr>
</tbody>
</table>
## OpenMP* Target Data Mapping

map([[map-type-modifier[,]]]map-type:]list)

<table>
<thead>
<tr>
<th>Clause</th>
<th>Valid for construct</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>to</td>
<td>target enter data, target data, target</td>
<td>Copies data from listed variables into device data region</td>
</tr>
<tr>
<td>from</td>
<td>target exit data, target data, target</td>
<td>Copies data from listed variables out of the device data region</td>
</tr>
<tr>
<td>tofrom</td>
<td>target data, target</td>
<td>Copies data into and out of the device data region for listed variables</td>
</tr>
<tr>
<td>alloc</td>
<td>target enter data, target data, target</td>
<td>Allocates memory for listed variables in the device data region</td>
</tr>
<tr>
<td>release</td>
<td>target exit data</td>
<td>Releases device pointers for listed variables in the device data region</td>
</tr>
<tr>
<td>delete</td>
<td>target exit data</td>
<td>Frees memory for listed variables in the device data region</td>
</tr>
</tbody>
</table>

Structured data regions trigger events upon entry and exit.

In 5.0 requires(unified_shared_memory) can make map() optional
OpenMP* Target Structured Data Management

#pragma omp target data / !$omp target data
!$omp end target data => Create a data region for a device

<table>
<thead>
<tr>
<th>Clause</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>if(scalar-expression)</td>
<td>If scalar-expression is false, device used is host</td>
</tr>
<tr>
<td>device(integer-expression)</td>
<td>Integer expression for the device to use. Must be a non-negative integer less than the value of \texttt{omp_get_num_devices()}</td>
</tr>
<tr>
<td>map([[map-type-modifier[,]\text{map-type:}list])</td>
<td>Described previously</td>
</tr>
<tr>
<td>use_device_ptr(list)</td>
<td>Listed items are converted to device pointers in the device data environment</td>
</tr>
<tr>
<td>\texttt{use_device_addr(list)} (in 5.0)</td>
<td>Listed items have the address of the corresponding object in the device data environment.</td>
</tr>
</tbody>
</table>
#pragma omp enter target data / !$omp enter target data
#pragma omp exit target data / !$omp exit target data

=> Manage data associated with a device

<table>
<thead>
<tr>
<th>Clause</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>if(scalar-expression)</td>
<td>If scalar-expression is false, device used is host</td>
</tr>
<tr>
<td>device(integer-expression)</td>
<td>Integer expression for the device to use. Must be a non-negative integer less than the value of omp_get_num_devices() If not specified, device is determined from the default-device-var icv.</td>
</tr>
<tr>
<td>map([map-type-modifier[,]map-type:]list)</td>
<td>Described previously</td>
</tr>
<tr>
<td>depend(dependence-type:list)</td>
<td>Follows task dependencies, as previously described.</td>
</tr>
<tr>
<td>nowait</td>
<td>If present, execution of the target task may be deferred. If not, the task is an undeferred task.</td>
</tr>
</tbody>
</table>
OpenMP* Teams Construct

#pragma omp teams/ !$omp teams !$omp end teams => Create a league of thread teams. The master thread of each team executes the region.

<table>
<thead>
<tr>
<th>Clause</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_teams(integer-expression)</td>
<td>Sets the maximum number of teams to create within a target task</td>
</tr>
<tr>
<td>thread_limit(integer_expression)</td>
<td>Sets the maximum number of threads to create within each team</td>
</tr>
<tr>
<td>default(shared</td>
<td>firstprivate</td>
</tr>
<tr>
<td>private(list)</td>
<td>Listed variables are scoped as private</td>
</tr>
<tr>
<td>firstprivate(list)</td>
<td>Listed variables are scoped as firstprivate</td>
</tr>
<tr>
<td>shared(list)</td>
<td>Listed variables are scoped as shared</td>
</tr>
<tr>
<td>reduction(reduction-identifier:list)</td>
<td>Perform a reduction on listed variables across teams using reduction-identifier.</td>
</tr>
</tbody>
</table>
OpenMP* Distribute Construct

#pragma omp distribute / !$omp distribute
$omp end distribute  =>  Distribute the iterations of one or more loops across the master threads of a league of teams

<table>
<thead>
<tr>
<th>Clause</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>private(list)</td>
<td>Listed variables are scoped as private</td>
</tr>
<tr>
<td>firstprivate(list)</td>
<td>Listed variables are scoped as firstprivate</td>
</tr>
<tr>
<td>lastprivate(list)</td>
<td>Listed variables are scoped as lastprivate</td>
</tr>
<tr>
<td>collapse(n)</td>
<td>Specifies how many loops are associated with a particular distribute construct</td>
</tr>
<tr>
<td>dist_schedule(kind[, chunk_size])</td>
<td>Kind must be static, chunk_size specifies the division of iterations. Chunks are assigned to teams in a round-robin fashion</td>
</tr>
</tbody>
</table>
OpenMP* Distribute Composite Constructs

In addition to using a vanilla *distribute* construct, there are also composite constructs that allow more parallelism.

<table>
<thead>
<tr>
<th>Construct</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>#pragma omp distribute simd !omp [end] distribute simd</td>
<td>Distribute loop chunks among teams, and execute those iterations using SIMD instructions</td>
</tr>
<tr>
<td>#pragma omp distribute parallel for !omp [end] distribute parallel do</td>
<td>Distribute loop chunks among teams, then distribute iterations within each chunk among threads within the team and execute in parallel</td>
</tr>
<tr>
<td>#pragma omp distribute parallel for simd !omp [end] distribute parallel for simd</td>
<td>Distribute loop chunks among teams, then distribute iterations within each chunk among threads within the team and execute in parallel using SIMD instructions</td>
</tr>
</tbody>
</table>
OpenMP* 5.0 adds several new features which can be useful in achieving a performance portable application. We won't go over these in detail, but some items to look into are:

<table>
<thead>
<tr>
<th>Construct</th>
<th>Description</th>
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<tbody>
<tr>
<td>#pragma omp metadirective !$omp metadirective</td>
<td>Conditionally apply a directive from a set to a location.</td>
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<tr>
<td>#pragma omp declare variant !$omp declare variant</td>
<td>Define variants of a function to use on different architectures or devices.</td>
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<tr>
<td>#pragma omp requires !$omp requires</td>
<td>Specify that an implementation requires a specific hardware feature</td>
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<tr>
<td>#pragma omp teams loop !$omp teams loop</td>
<td>Specify a teams construct that contains a loop and nothing else. Equivalent to #pragma omp teams distribute parallel for !$omp teams distribute parallel for</td>
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<tr>
<td>#pragma omp scan !$omp scan</td>
<td>Tells the compiler that the following statement is a scan that can be performed in parallel</td>
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<tr>
<td>Memory Management #pragma omp allocate !$omp allocate</td>
<td>More explicit control over memory spaces for host and device, and the ability to define and use custom memory allocators</td>
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