

Advanced OpenMP Tutorial

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Agenda – 09:00 through 13:00 ISC Time ©



- OpenMP Overview (~20 min.)
- Techniques to Obtain High Performance with OpenMP: Memory Access (~30 min.)
- Techniques to Obtain High Performance with OpenMP: Loops (~30 min.)
- Techniques to Obtain High Performance with OpenMP: Vectorization (~20 min.)
- OpenMP for Attached Compute Accelerators (~90 min.)
- Future OpenMP Directions (~20 min.)

Break:

• Coffee: 11:00 – 11:30



Updated slides

OpenMP

- Slides are never perfect ...
- ... but we offer a free update service :-)



https://bit.ly/isc25-adv-omp





Core Concepts: Worksharing and Tasking





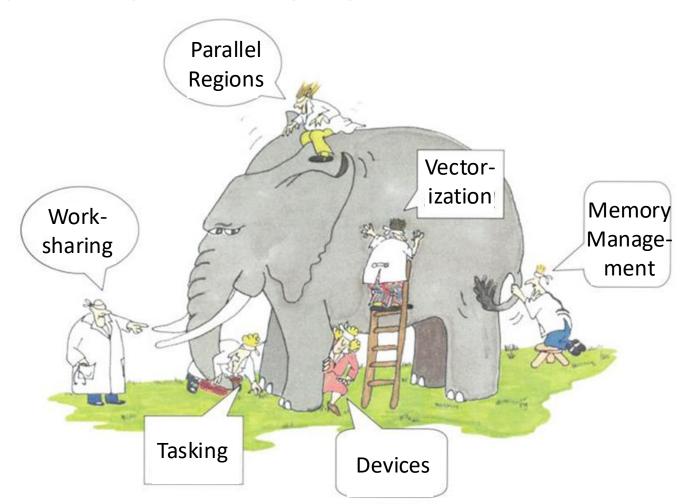
What is OpenMP?



■ De-facto standard Application Programming Interface (API) to write

shared memory parallel applications in C, C++, and Fortran

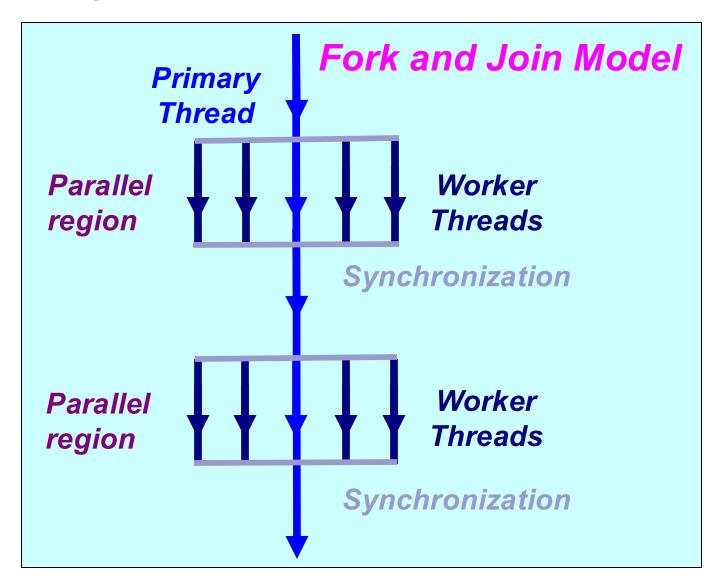
- Consists of compiler directives, runtime routines and environment variables
- Version 5.0 was released at SC18
- Version 5.2 was released at SC21
- Version 6.0 was released at SC24





The OpenMP Execution Model





```
#pragma omp parallel
{
    ....
}
```

```
#pragma omp parallel
{
    ....
}
```



The Worksharing Constructs



- The work is distributed over the threads
- Must be enclosed in a parallel region
- Must be encountered by all threads in the team, or none at all
- No implied barrier on entry
- Implied barrier on exit (unless the nowait clause is specified)
- A work-sharing construct does not launch any new threads

```
#pragma omp for
{
    ....
}
```

```
#pragma omp sections
{
          ....
}
```

```
#pragma omp single
{
     ....
}
```



The task construct



Deferring (or not) a unit of work (executable for any member of the team)

```
#pragma omp task [clause[[,] clause]...]
{structured-block}
```

!\$omp task [clause[[,] clause]...]
...structured-block...
!\$omp end task

Where clause is one of:

→ private(list)		
→ firstprivate(list)		
→ shared(list)	Data Environment	
→ default(shared none)		
→ in_reduction(r-id: list)		
→ allocate([allocator:] list)	Miscellaneous	
→ detach(event-handler)	iviiscenameous	

→ if(scalar-expression)	
→ mergeable	Cutoff Strategies
→ final(scalar-expression)	
→ depend(dep-type: list)	Synchronization
→ untied	
→ priority(priority-value)	Task Scheduling



Tasking execution model

OpenMP

- Supports unstructured parallelism
 - → unbounded loops

```
while ( <expr> ) {
    ...
}
```

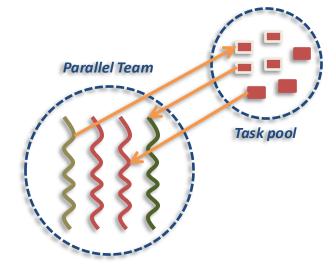
→ recursive functions

```
void myfunc( <args> )
{
    ...; myfunc( <newargs> ); ...;
}
```

- Several scenarios are possible:
 - → single creator, multiple creators, nested tasks (tasks & WS)
- All threads in the team are candidates to execute tasks

Example (unstructured parallelism)

```
#pragma omp parallel
#pragma omp single
while (elem != NULL) {
    #pragma omp task
        compute(elem);
    elem = elem->next;
}
```





Single and Masked / 1



Single: only one thread in the team executes the code enclosed

Masked: rule-based selection of threads for region execution

```
#pragma omp masked [filter(integer-expression)]
{<code-block>}
```

There is no implied barrier on entry or exit!







Single: only one thread in the team executes the code enclosed

Masked: rule-based selection of threads for region execution

```
#pragma omp masked [filter(integer-expression)]
{<code-block>}
```

→ Replacement of master construct:

```
#pragma omp masked [filter(0)]
{<code-block>}
```





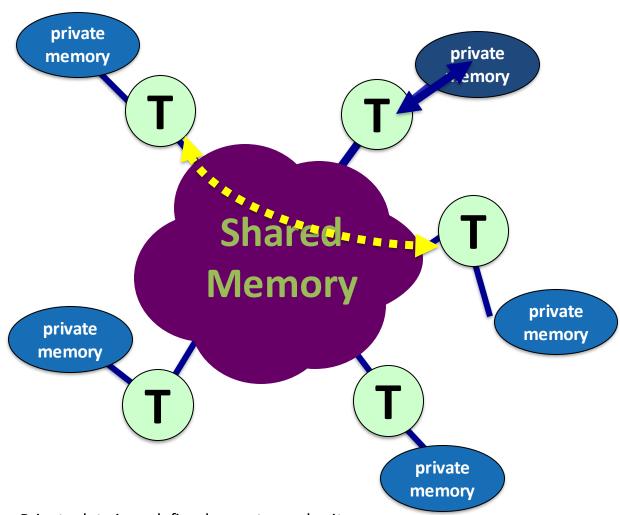
Synchronization





The OpenMP Memory Model





Private data is undefined on entry and exit

Can use firstprivate and lastprivate to address this

- All threads have access to the same, globally shared memory
- Data in <u>private memory</u> is only accessible by the thread owning this memory
- No other thread sees the change(s) in private memory
- ◆ Data transfer is through shared memory and is 100% transparent to the application

Barrier and Taskwait Constructs



- OpenMP barrier (implicit or explicit)
 - →All tasks created by any thread of the current *Team* are guaranteed to be completed at barrier exit

```
C/C++
#pragma omp barrier
```

- Task barrier: taskwait
 - →Encountering task is suspended until child tasks are complete
 - →Applies only to direct childs, not descendants!

```
C/C++
#pragma omp taskwait
```



The nowait Clause



- To minimize synchronization, some directives support the optional nowait clause
 - → If present, threads do not synchronize/wait at the end of that particular construct
- In C, it is one of the clauses on the pragma
- In Fortran, it is appended at the closing part of the construct



Task depend clause



With task dependencies, a task cannot be executed until all its predecessor tasks are completed

```
int x = 0;
#pragma omp parallel
#pragma omp single
  #pragma omp task depend(inout: x) //T1
  { . . . }
  #pragma omp task depend(in: x)
                                       //T2
                                                      T2
                                                                T3
  { . . . }
  #pragma omp task depend(in: x)
                                       //T3
                                                           T4
  { . . . }
  #pragma omp task depend(inout: x) //T4
  { . . . }
```



The taskgroup Construct



```
#pragma omp taskgroup
... structured block ...
!$omp taskgroup
... structured block ...
!$omp end taskgroup
```

- Specifies a wait on completion of child tasks and their descendent tasks
 - → ",deeper" sychronization than taskwait, but
 - with the option to restrict to a subset of all tasks (as opposed to a barrier)





User Defined Reductions



User Defined Reductions (UDRs) expand OpenMP's usability



- Use declare reduction directive to define operators
- Operators used in reduction clause like predefined ops

```
#pragma omp declare reduction (reduction-identifier :
typename-list : combiner) [initializer(initializer-expr)]
```

- reduction-identifier gives a name to the operator
 - → Can be overloaded for different types
 - → Can be redefined in inner scopes
- typename-list is a list of types to which it applies
- combiner expression specifies how to combine values
- initializer specifies the operator's identity value
 - → initializer-expression is an expression or a function





A simple UDR example

Declare the reduction operator

```
#pragma omp declare reduction (mindex : index_struct:
    (omp_in.value < omp_out.value) ? omp_in : omp_out)
    initializer(omp_priv = {.value = MAX_INT, .index = 0})</pre>
```

Use the reduction operator in a reduction clause

```
index_struct min_value = (.value = MAX_INT, .index = 0);
#pragma omp parallel for reduction (mindex : min_value)
for (i = 0; I < NUM_ELEMENTS; i++)
   if (a[i] < min_value.value) {
      min_value.value = a[i]; min_value.index = i;}</pre>
```

- Private copies created for a reduction are initialized to the identity that was specified for the operator and type
 - → Default identity defined if identity clause not present
- Compiler uses combiner to combine private copies
 - → omp out refers to private copy that holds combined value
 - → omp in refers to the other private copy





Atomics



The atomic construct supports efficient parallel accesses



Use atomic construct for mutually exclusive access to a single memory location

#pragma omp atomic [read|write|update] [capture] [compare|weak] [fail|seq_cst]
 expression-stmt

- expression-stmt restricted based on type of atomic
- update, the default behavior, reads and writes the single memory location atomically
- read reads location atomically
- write writes location atomically
- capture updates or writes location and captures its value (before or after update) into a private variable





OpenMP supports several atomic operations

Early versions did not support atomic capture

```
int schedule (int upper) {
   static int iter = 0; int ret;
   ret = iter;
   #pragma omp atomic
       iter++;
   if (ret <= upper) { return ret; }
   else { return -1; } //no more iters
}</pre>
```

Atomic capture provides the needed functionality



User-level synchronization supported by

OpenMP.

memory ordering clauses

- Naive attempt to write user-level critical section
 - → Assume shared * are all shared variables
 - → Assume only two threads access shared_lock

```
int local, do_not_have_lock = 1;

while (do_not_have_lock) {
    #pragma omp atomic capture
    do_not_have_lock = shared_lock++;
}

local = shared_a;
shared_a = shared_b;
shared_b = local;

#pragma omp atomic write
shared_lock = 0;
```

What's wrong with this code?



User-level synchronization must ensure that



memory is consistent

- Correct user-level critical section must include flushes
 - → Assume shared * are all shared variables
 - → Assume only two threads access shared lock

```
int local, do_not_have_lock = 1;
while (do_not_have_lock) {
    #pragma omp atomic capture seq_cst
    do_not_have_lock = shared_lock++;
}

local = shared_a;
shared_a = shared_b;
shared_b = local;

#pragma omp atomic write seq_cst
shared_lock = 0;
```

Alternatively, must add several flushes (more than 2)





Understanding Memory Access







Memory Affinity



Non-uniform Memory

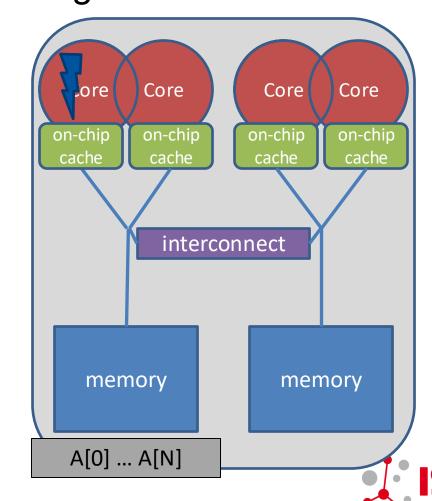


Serial code: all array elements are allocated in the memory of the NUMA node closest to the core executing the initializer thread (first

touch)

```
double* A;
A = (double*)
    malloc(N * sizeof(double));

for (int i = 0; i < N; i++) {
    A[i] = 0.0;
}</pre>
```



First Touch Memory Placement



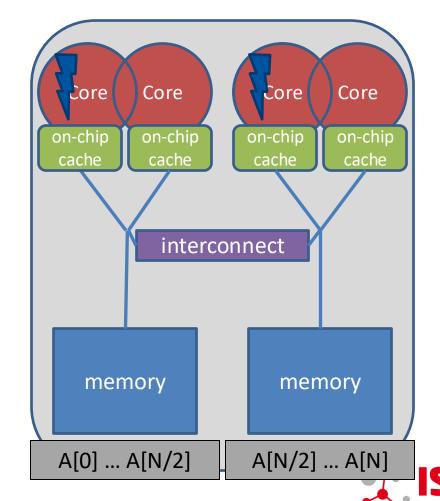
■ First Touch w/ parallel code: all array elements are allocated in the memory of the NUMA node that contains the core that executes the

thread that initializes the partition

```
double* A;
A = (double*)
    malloc(N * sizeof(double));

omp_set_num_threads(2);

#pragma omp parallel for proc_bind(spread)
for (int i = 0; i < N; i++) {
    A[i] = 0.0;
}</pre>
```

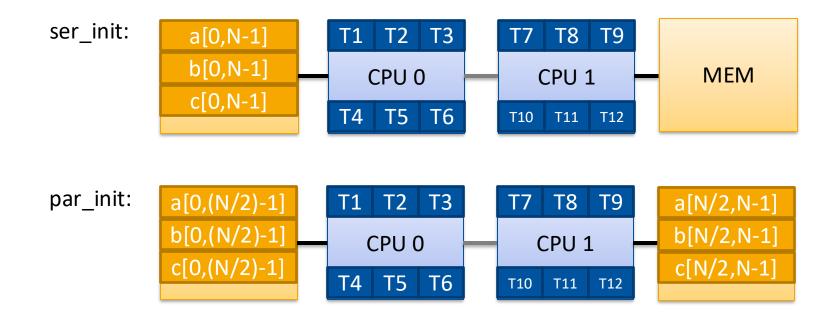


Serial vs. Parallel Initialization



- Stream example with and without parallel initialization.
 - → 2 socket sytem with Xeon X5675 processors, 12 OpenMP threads

	сору	scale	add	triad
ser_init	18.8 GB/s	18.5 GB/s	18.1 GB/s	18.2 GB/s
par_init	41.3 GB/s	39.3 GB/s	40.3 GB/s	40.4 GB/s







Thread Binding and Memory Placement





Get Info on the System Topology



- Before you design a strategy for thread binding, you should have a basic understanding of the system topology:
 - → Intel MPI's cpuinfo tool
 - → module switch openmpi intelmpi
 - → cpuinfo
 - → Delivers information about the number of sockets (= packages) and the mapping of processor IDs to CPU cores used by the OS
 - → hwlocs' hwloc-ls tool
 - → hwloc-ls
 - → Displays a representation of the system topology, separated into NUMA nodes, along with the mapping of processor IDs to CPU cores used by the OS and additional information on caches



Decide for Binding Strategy



- Selecting the "right" binding strategy depends not only on the topology, but also on the characteristics of your application.
 - → Putting threads far apart, i.e., on different sockets
 - → May improve the aggregated memory bandwidth available to your application
 - → May improve the combined cache size available to your application
 - → May decrease performance of synchronization constructs
 - → Putting threads close together, i.e., on two adjacent cores that possibly share some caches
 - → May improve performance of synchronization constructs
 - → May decrease the available memory bandwidth and cache size
- If you are unsure, just try a few options and then select the best one.



Since OpenMP 4.0: Places + Policies

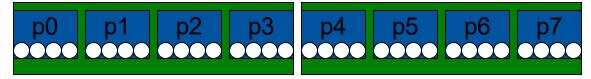


- Define OpenMP places
 - → set of OpenMP threads running on one or more processors
 - → can be defined by the user, i.e., OMP_PLACES=cores
- Define a set of OpenMP thread affinity policies
 - → SPREAD: spread OpenMP threads evenly among the places, partition the place list
 - → CLOSE: pack OpenMP threads near primary thread
 - → PRIMARY: collocate OpenMP thread with primary thread
- Goals
 - → user has a way to specify where to execute OpenMP threads for locality between OpenMP threads / less false sharing / memory bandwidth

OMP_PLACES env. variable



Assume the following machine:



- → 2 sockets, 4 cores per socket, 4 hyper-threads per core
- Abstract names for OMP_PLACES:
 - → threads: Each place corresponds to a single hardware thread.
 - → cores: Each place corresponds to a single core (having one or more hardware threads).
 - → sockets: Each place corresponds to a single socket (consisting of one or more cores).
 - → Il_caches (5.1): Each place corresponds to a set of cores that share the last level cache.
 - → numa_domains (5.1): Each places corresponds to a set of cores for which their closest memory is: the same memory; and at a similar distance from the cores.

OpenMP 4.0: Places + Policies

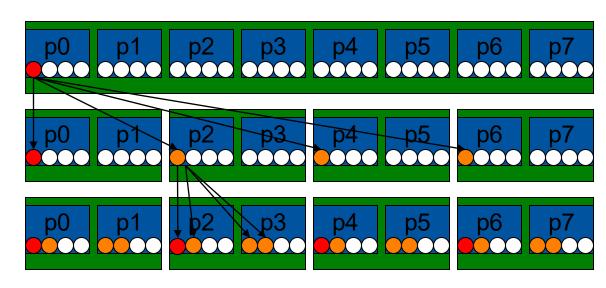


- Example's Objective:
 - → separate cores for outer loop and near cores for inner loop
- Outer Parallel Region: proc_bind(spread), Inner: proc_bind(close)
 - → spread creates partition, compact binds threads within respective partition

```
OMP_PLACES=(0,1,2,3), (4,5,6,7), ... = (0-4):4:8 = cores #pragma omp parallel proc_bind(spread) num_threads(4) #pragma omp parallel proc bind(close) num threads(4)
```

Example

- → initial
- → spread 4
- → close 4

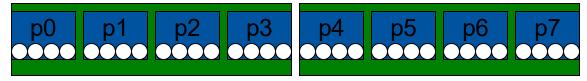




More Examples (1/3)



Assume the following machine:



→ 2 sockets, 4 cores per socket, 4 hyper-threads per core

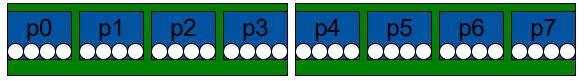
- Parallel Region with two threads, one per socket
 - → OMP_PLACES=sockets
 - → #pragma omp parallel num_threads(2) proc_bind(spread)



More Examples (2/3)



Assume the following machine:



→ 2 sockets, 4 cores per socket, 4 hyper-threads per core

- Parallel Region with four threads, one per core, but only on the first socket
 - → OMP PLACES=cores
 - → #pragma omp parallel num_threads(4) proc_bind(close)



More Examples (3/3)



Spread a nested loop first across two sockets, then among the cores within each socket, only one thread per core

```
→ OMP_PLACES=cores
```

- → #pragma omp parallel num_threads(2) proc_bind(spread)
- → #pragma omp parallel num_threads(4) proc_bind(close)

Places API routines allow to

- → query information about binding...
- → query information about the place partition...



Places API: Example



Simple routine printing the processor ids of the place the calling thread is bound to:

```
void print binding info() {
     int my place = omp get place num();
     int place num procs = omp get place num procs (my place);
     printf("Place consists of %d processors: ", place num procs);
     int *place processors = malloc(sizeof(int) * place num procs);
     omp get place proc ids(my place, place processors)
     for (int i = 0; i < place num procs - 1; <math>i++) {
             printf("%d ", place processors[i]);
     printf("\n");
     free(place processors);
```



OpenMP 5.x way to do this



- Set OMP DISPLAY AFFINITY=TRUE
 - →Instructs the runtime to display formatted affinity information
 - → Example output for two threads on two physical cores:
 - →Output (nesting_level= 1, thread_num= 0, thread_affinity= 0,1 nesting_level= 1, thread_num= 1, thread_affinity= 2,3

 CORRESPONDING TOURING
 - → Formatted affinity information can be printed with omp display affinity (const char* format)



Affinity format specification



t	omp_get_team_num()
Т	omp_get_num_teams()
L	omp_get_level()
n	omp_get_thread_num()
N	omp_get_num_threads()

а	omp_get_ancestor_thread_num() at level-1
Н	hostname
Р	process identifier
i	native thread identifier
Α	thread affinity: list of processors (cores)

Example:

```
OMP_AFFINITY_FORMAT="Affinity: %0.3L %.8n %.15{A} %.12H"
```

→ Possible output:

Affinity: 0	01	0	0-1,16-17	host003
Affinity: 0	01	1	2-3,18-19	host003



Fine-grained control of Memory Affinity



- Explicit NUMA-aware memory allocation:
 - →By carefully touching data by the thread which later uses it
 - → By changing the default memory allocation strategy
 - → Linux: numactl command
 - →By explicit migration of memory pages
 - →Linux: move pages()

- Example: using numactl to distribute pages round-robin:
 - → numactl -interleave=all ./a.out





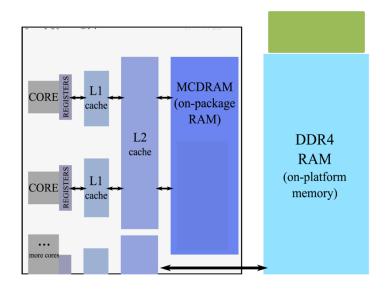
Memory Management



Different kinds of memory

OpenMP

- Traditional DDR-based memory
- High-bandwidth memory
- Non-volatile memory
- ...



Cascade Lake (Leonide at INRIA)

```
CPU: Intel(R) Xeon(R) Gold 6230 CPU @ 2.10GHz
Freq Govenor: performance
available: 4 \text{ nodes } (0-3)
node 0 cpus: 0 2 4 6 8 10 12 14 16 18
             20 22 24 26 28 30 32 34 36 38
node 0 size: 191936 MB
node 0 free: 178709 MB
node 1 cpus: 1 3 5 7 9 11 13 15 17 19 21 23
             25 27 29 31 33 35 37 39
node 1 size: 192016 MB
node 1 free: 179268 MB
node 2 cpus:
node 2 size: 759808 MB
node 2 free: 759794 MB
node 3 cpus:
node 3 size: 761856 MB
node 3 free: 761851 MB
node distances:
                           DRAM + Optane
```



Memory Management



- Allocator := an OpenMP object that fulfills requests to allocate and deallocate storage for program variables
- OpenMP allocators are of type omp_allocator_handle_t
- Default allocator for host
 - → via OMP ALLOCATOR env. var. or corresponding API
- OpenMP 5.0 supports a set of memory allocators



OpenMP allocators



Selection of a certain kind of memory

Allocator name	Storage selection intent
omp_default_mem_alloc	use default storage
omp_large_cap_mem_alloc	use storage with large capacity
omp_const_mem_alloc	use storage optimized for read-only variables
omp_high_bw_mem_alloc	use storage with high bandwidth
omp_low_lat_mem_alloc	use storage with low latency
omp_cgroup_mem_alloc	use storage close to all threads in the contention group of the thread requesting the allocation
omp_pteam_mem_alloc	use storage that is close to all threads in the same parallel region of the thread requesting the allocation
omp_thread_local_mem_alloc	use storage that is close to the thread requesting the allocation



Using OpenMP allocators



New clause on all constructs with data sharing clauses:

```
→ allocate( [allocator:] list )
```

Allocation:

```
→ omp alloc(size t size, omp allocator handle t allocator)
```

Deallocation:

```
→ omp_free(void *ptr, const omp_allocator_handle_t allocator)
```

allocate directive: standalone directive for allocation, or declaration of allocation stmt.





sync_hint	contended, uncontended, serialized, private	default: contended
alignment	positive integer value that is a power of two	default: 1 byte
access	all, memspace, device, cgroup, pteam, thread	default: memspace
pool_size	positive integer value	
fallback	default_mem_fb, null_fb, abort_fb, allocator_fb	default: default_mem_fb
fb_data	an allocator handle	
pinned	true, false	default: false
partition	environment, nearest, blocked, interleaved	default: environment
pin_device	conforming device number	
preferred_device	conforming device number	
target access	single, multiple	default: single
atomic_scope	all, device	default: device
part_size	positive integer value	
partitioner	a memory partitioner handle	
partitioner_arg	an integer value	0



- fallback: describes the behavior if the allocation cannot be fulfilled
 - → default_mem_fb: return system's default memory
 - →Other options: null, abort, or use different allocator
- pinned: request pinned memory, i.e. for GPUs,
 - → device may be specified





- partition: partitioning of allocated memory of physical storage resources (think of NUMA)
 - →environment: use system's default behavior
 - →nearest: most closest memory
 - →blocked: partitioning into approx. same size with at most one block per storage resource
 - →interleaved: partitioning in a round-robin fashion across the storage resources, in which part_size specifies the size of individual partitions
 - partitioner: definition of memory parts and distribution across storage are defined by a memory partitioner





Example code:

→ Distributes chunks of memory:





ontended, uncontended, serialized, private	default: contended
ositive integer value that is a power of two	default: 1 byte
II, memspace, device, cgroup, pteam, thread	default: memspace
ositive integer value	
lefault_mem_fb, null_fb, abort_fb, allocator_fb	default: default_mem_fb
n allocator handle	
rue, false	default: false
nvironment, nearest, blocked, interleaved	default: environment
onforming device number	
onforming device number	
ingle, multiple	default: single
II, device	default: device
ositive integer value	
memory partitioner handle	
n integer value	0
	ositive integer value that is a power of two I, memspace, device, cgroup, pteam, thread ositive integer value efault_mem_fb, null_fb, abort_fb, allocator_fb in allocator handle ue, false invironment, nearest, blocked, interleaved onforming device number onforming device number ingle, multiple I, device ositive integer value memory partitioner handle



- partition: partitioning of allocated memory of physical storage resources (think of NUMA)
 - →environment: use system's default behavior
 - →nearest: most closest memory
 - →blocked: partitioning into approx. same size with at most one block per storage resource
 - →interleaved: partitioning in a round-robin fashion across the storage resources, in which part size specifies the size of individual partitions
 - partitioner: definition of memory parts and distribution across storage are defined by a memory partitioner



OpenMP Memory Partitioner



- Memory Partitioner := an OpenMP object that represents mechanisms to create and destroy memory partitions
 - → Memory Partition := a definition how an allocator divides memory into parts
 - → Memory Part := a storage block in a single storage resource within a memory space
- omp_init_mempartitioner routine: initializes a partitioner that ...
 - → ... can be used with an OpenMP allocator
 - → ... takes the argument compute_proc to determine the number of memory parts and their distribution across the storage resources
 - →+ further management and cleanup routines
- Memory Space Retrieving Routines: return memory space handles



Using OpenMP allocator traits



Construction of allocators with traits via

```
>omp_allocator_handle_t omp_init_allocator(
  omp_memspace_handle_t memspace,
  int ntraits, const omp_alloctrait_t traits[]);
```

- → Selection of memory space mandatory
- →Empty traits set: use defaults
- Allocators have to be destroyed with *_destroy_*
- Custom allocator can be made default with omp set default allocator (omp allocator handle t allocator)



Memory Management Status (status: 11/2024) OpenMP



- LLVM OpenMP runtime internally already uses libmemkind (libnuma, numactl)
 - → Support for various kinds of memory: DDR, HBW and Persistent Memory (Optane)
 - → Library loaded at initialization (checks for availability)
 - → If requested memory space for allocator is not available → fallback to DDR.

Memory Management implementation in LLVM still not complete

- → Some allocator traits not implemented yet
- → Some partition values not implemented yet (environment, interleaved, nearest, blocked)
- → Semantics of omp high bw mem space and omp large cap mem space unclear. Which memory should be used?
 - → Explicitly target HBM → currently implemented in LLVM

LLVM has custom implementation of aligned memory allocation

→ Allocation covers → {Allocator Information + Requested Size + Buffer based on alignment}





Loop Transformations





Loop Unrolling



Loop unrolling is a standard tuning practice to reduce loop overhead and increase potential for pipeline.

```
subroutine loop()
   do i = 1, 4
        call body(i)
   end do
end subroutine loop
```

```
subroutine loop()
    call body(i + 0)
    call body(i + 1)
    call body(i + 2)
    call body(i + 3)
end subroutine loop
```

```
subroutine loop()
  !$omp unroll full
  do i = 1, 4
          call body(i)
  end do
end subroutine loop
```

- full" completely unrolls the loop
 - → Needs a compile-time constant upper bound.
 - → Loop is no longer present after unrolling took place.



Loop Unrolling



Loop unrolling is a standard tuning practice to reduce loop overhead and increase potential for pipeline.

```
subroutine loop()
   do i = 1, n
       call body(i)
   end do
end subroutine loop
```

```
subroutine loop()
  !$omp unroll partial(4)
  do i = 1, n
       call body(i)
  end do
end subroutine loop
```

- "partial(f)" unrolls the loop with
 unroll factor f
 - → Upper bound can now be a runtime value
 - Compiler will introduce remainder loops as necessary

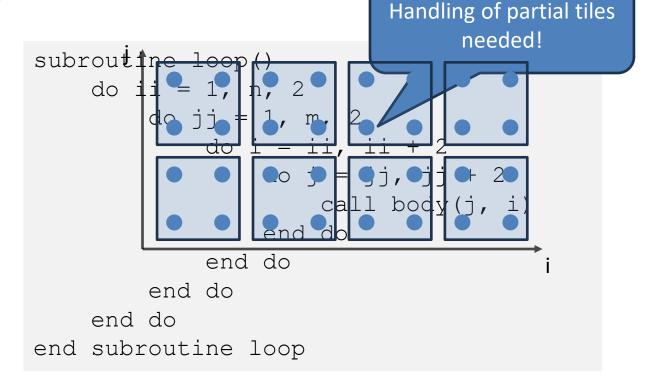


Tiling



■ Tiling is a useful to optimize a loop nest for the cache hierarchy and

exploiting temporal/spatial locality





Tiling



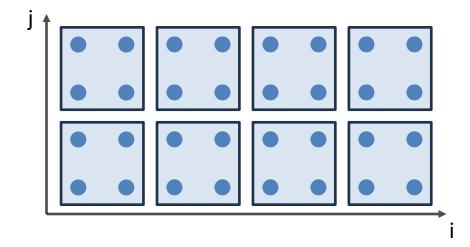
Handling of partial tiles

Tiling is a useful to optimize a loop nest for the cache hierarchy and exploiting temporal/spatial locality

Tiling



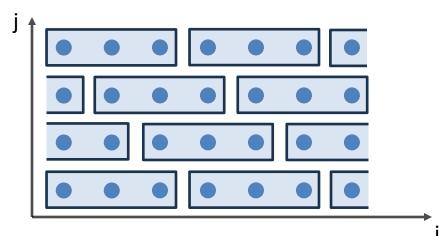
Tiling is a useful to optimize a loop nest for the cache hierarchy and exploiting temporal/spatial locality



Tiling and Chunking



One can think of tiling as "multi-dimensional" chunking:



```
!$omp tile sizes(3,3)
do i = 1, n
    do j = 1, m
        call body(j, i)
    end do
end do
```

Other Loop Transformations /1



Loop Interchange

Loop Reversal

```
!$omp reverse
do i = 1, n
    call body(i)
end do
```

```
do i = 1, n
     call body(n - (i - 1))
end do
```



Other Loop Transformations /2



Loop Fusion

```
!$omp fuse
do i = 1, n
    call body1(i)
end do
do i = 1, n
    call body2)(i)
end do
!$omp end fuse
do i = 1, n
    call body1(i)
    call body2(i)
end do
```

Loop Reversal



Other Loop Transformations /3



Loop Index Splitting

```
!$omp split counts(k, omp_fill)
do i = 1, n
    call body(i)
end do

end do

call body(i)
end do

call body(i)
end do
```

- All these transformations can be useful:
 - → Fusion: reduce loop overhead and get more work per loop iteration
 - → Reversal: create forward memory references
 - →Index splitting: peel off loop iterations, e.g., for better SIMD/memory alignment







Loop transformations can be composed, e.g., tiling and unrolling:





Vectorization





Topics



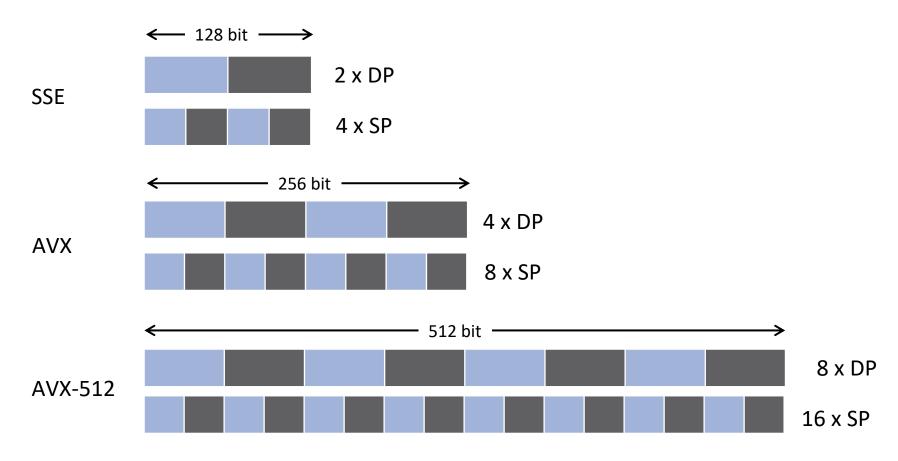
- Exploiting SIMD parallelism with OpenMP
- Using SIMD directives with loops
- Creating SIMD functions



SIMD on x86 Architectures



Width of SIMD registers has been growing in the past:



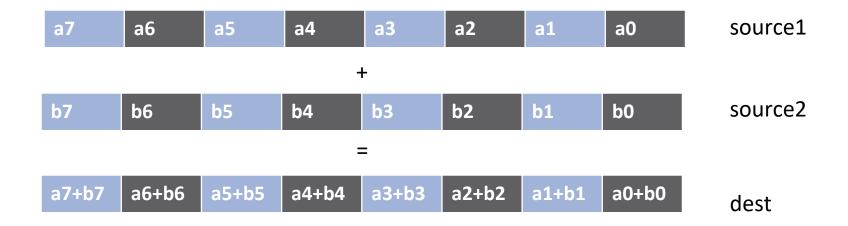


More Powerful SIMD Units



SIMD instructions become more powerful

vadd dest, source1, source2



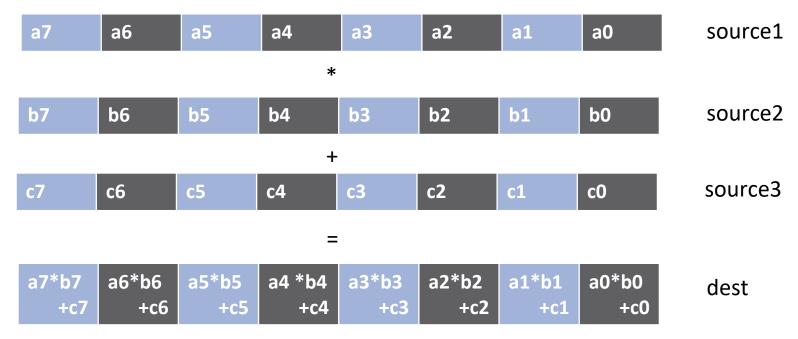


More Powerful SIMD Units



SIMD instructions become more powerful

vfma source1, source2, source3



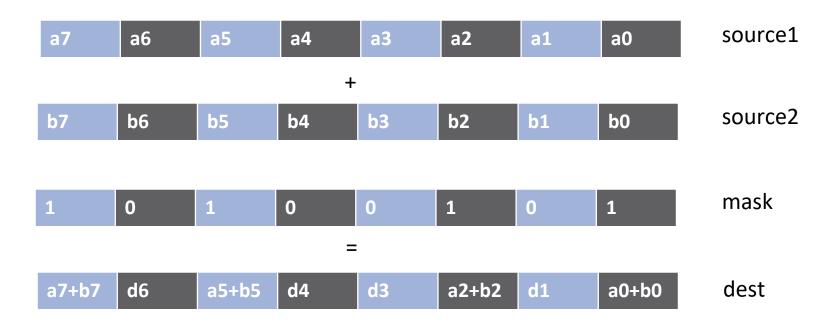


More Powerful SIMD Units



SIMD instructions become more powerful

vadd dest{k1}, source2, source3



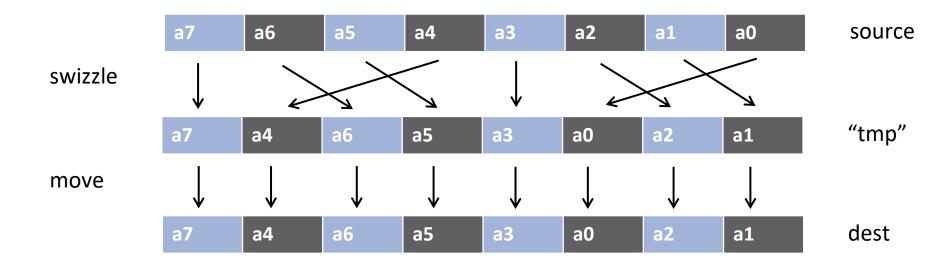


More Powerful SIMD Units



SIMD instructions become more powerful

vload dest, source{dacb}





Auto-vectorization



- Compilers offer auto-vectorization as an optimization pass
 - → Usually, part of the general loop optimization passes
 - → Code analysis detects code properties that inhibit SIMD vectorization



- → Heuristics determine if SIMD execution might be beneficial
- → If all goes well, the compiler will generate SIMD instructions
- Example: clang/LLVM GCC Intel Compiler
 - →-fvectorize -ftree-vectorize -vec (enabled w/ -O2)
 - →-Rpass=loop-.* -ftree-loop-vectorize -qopt-report=vec
 - →-mprefer-vector-width=<width> -fopt-info-vec-all



Why Auto-vectorizers Fail



- Data dependencies
- Other potential reasons
 - →Alignment
 - → Function calls in loop block
 - → Complex control flow / conditional branches
 - → Loop not "countable"
 - →e.g., upper bound not a runtime constant
 - → Mixed data types
 - → Non-unit stride between elements
 - → Loop body too complex (register pressure)
 - → Vectorization seems inefficient
- Many more ... but less likely to occur



Data Dependencies



- Suppose two statements S1 and S2
- S2 depends on S1, iff S1 must execute before S2
 - → Control-flow dependence
 - → Data dependence
 - → Dependencies can be carried over between loop iterations
- Important flavors of data dependencies

FLOW s1: a = 40 b = 21 s2: c = a + 2

ANTI
$$b = 40$$

s1: $a = b + 1$
 $s2: b = 21$



Loop-Carried Dependencies



- Dependencies may occur across loop iterations
 - → Loop-carried dependency
- The following code contains such a dependency:

```
void lcd_ex(float* a, float* b, size_t n, float c1, float c2)
{
    size_t i;
    for (i = 0; i < n; i++) {
        a[i] = c1 * a[i + 17] + c2 * b[i];
    }
}</pre>
Loop-carried dependency for a[i] and
```

- Some iterations of the loop have to complete before the next iteration can run
 - → Simple trick: Can you reverse the loop w/o getting wrong results?



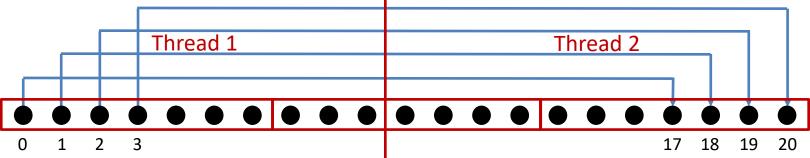
a[i+17]; distance is 17.

Loop-carried Dependencies



Can we parallelize or vectorize the loop?

```
void lcd_ex(float* a, float* b, size_t n, float c1, float c2) {
   for (int i = 0; i < n; i++) {
      a[i] = c1 * a[i + 17] + c2 * b[i];
}
</pre>
```



- Parallelization: no (except for very specific loop schedules)
- → Vectorization: yes (iff vector length is shorter than any distance of any dependency)



In a Time Before OpenMP 4.0



- Support required vendor-specific extensions
 - → Programming models (e.g., Intel® Cilk Plus)
 - → Compiler pragmas (e.g., #pragma vector)
 - → Low-level constructs (e.g., mm add pd())

```
#pragma omp parallel for
#pragma vector always
#pragma ivdep

for (int i = 0; i < N; i++) {
   a[i] = b[i] + ...;
}</pre>
```

You need to trust your compiler to do the "right" thing.



SIMD Loop Construct



- Vectorize a loop nest
 - → Cut loop into chunks that fit a SIMD vector register
 - →No parallelization of the loop body

■ Syntax (C/C++)

```
#pragma omp simd [clause[[,] clause],...]
for-loops
```

Syntax (Fortran)

```
!$omp simd [clause[[,] clause],...]
do-loops
[!$omp end simd]
```

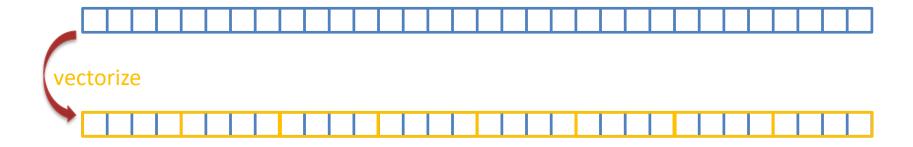


Example



```
float sprod(float *a, float *b, int n) {
  float sum = 0.0f;

#pragma omp simd reduction(+:sum)
  for (int k=0; k<n; k++)
    sum += a[k] * b[k];
  return sum;
}</pre>
```





Data Sharing Clauses



private(var-list):

Uninitialized vectors for variables in *var-list*



firstprivate(var-list):
Initialized vectors for variables in var-list

reduction(op:var-list):

Create private variables for *var-list* and apply reduction operator *op* at the end of the construct





SIMD Loop Clauses



- safelen (length)
 - Maximum number of iterations that can run concurrently without breaking a dependence
 - →In practice, maximum vector length
- linear (list[:linear-step])
 - The variable's value is in relationship with the iteration number $\rightarrow x_i = x_{orig} + i$ * linear-step
- aligned (list[:alignment])
 - → Specifies that the list items have a given alignment
 - → Default is alignment for the architecture
- \blacksquare collapse (n)



SIMD Worksharing Construct



- Parallelize and vectorize a loop nest
 - → Distribute a loop's iteration space across a thread team
 - → Subdivide loop chunks to fit a SIMD vector register

Syntax (C/C++)

```
#pragma omp for simd [clause[[,] clause],...]
for-loops
```

Syntax (Fortran)

```
!$omp do simd [clause[[,] clause],...]
do-loops
[!$omp end do simd [nowait]]
```

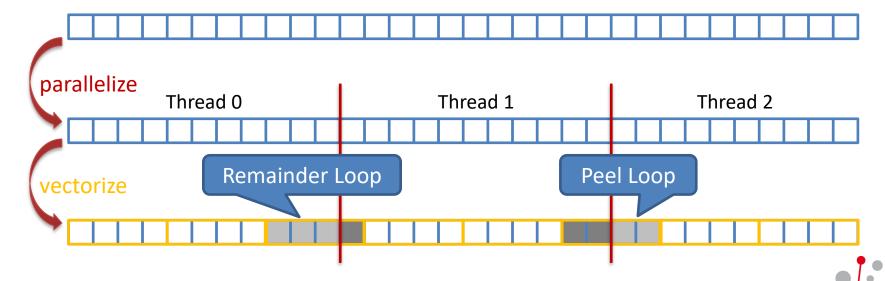


Example



```
float sprod(float *a, float *b, int n) {
  float sum = 0.0f;

#pragma omp for simd reduction(+:sum)
  for (int k=0; k<n; k++)
    sum += a[k] * b[k];
  return sum;
}</pre>
```







- You should choose chunk sizes that are multiples of the SIMD length
 - → Remainder loops are not triggered
 - → Likely better performance
- In the above example ...
 - → and AVX2, the code will only execute the remainder loop!
 - → and SSE, the code will have one iteration in the SIMD loop plus one in the remainder loop!







- Chooses chunk sizes that are multiples of the SIMD length
 - → First and last chunk may be slightly different to fix alignment and to handle loops that are not exact multiples of SIMD width
 - → Remainder loops are not triggered
 - → Likely better performance







```
float min(float a, float b) {
    return a < b ? a : b;
float distsq(float x, float y) {
    return (x - y) * (x - y);
void example() {
#pragma omp parallel for simd
    for (i=0; i< N; i++) {
        d[i] = min(distsq(a[i], b[i]), c[i]);
```



SIMD Function Vectorization



Declare one or more functions to be compiled for calls from a SIMDparallel loop

■ Syntax (C/C++):

```
#pragma omp declare simd [clause[[,] clause],...]
[#pragma omp declare simd [clause[[,] clause],...]]
[...]
function-definition-or-declaration
```

Syntax (Fortran):

```
!$omp declare simd (proc-name-list)
```







```
#pragma omp declare simd
                                 ZGVZN16vv min(%zmm0, %zmm1):
float min(float a, float b)
                                    vminps %zmm1, %zmm0, %zmm0
    return a < b ? a : b;
                                    ret
#pragma omp declare simd
                                 ZGVZN16vv distsq(%zmm0, %zmm1):
float distsq(float x, float y)
                                    vsubps %zmm0, %zmm1, %zmm2
    return (x - y) * (x - y)
                                    vmulps %zmm2, %zmm2, %zmm0
                                    ret
void example() {
#pragma omp parallel for simd
    for (i=0; i< N; i++) {
        d[i] = min(distsq(a[i], b[i]), c[i]);
                               vmovups (%r14,%r12,4), %zmm0
                               vmovups (%r13,%r12,4), %zmm1
                               call ZGVZN16vv distsq
                               vmovups (%rbx,%r12,4), %zmm1
                                                                  High Performance
                               call ZGVZN16vv min
```

SIMD Function Vectorization



- simdlen (length)
 - → generate function to support a given vector length
- uniform (argument-list)
 - → argument has a constant value between the iterations of a given loop
- inbranch
 - → function always called from inside an if statement
- notinbranch
 - → function never called from inside an if statement
- linear (argument-list[:linear-step])
- aligned (argument-list[:alignment])



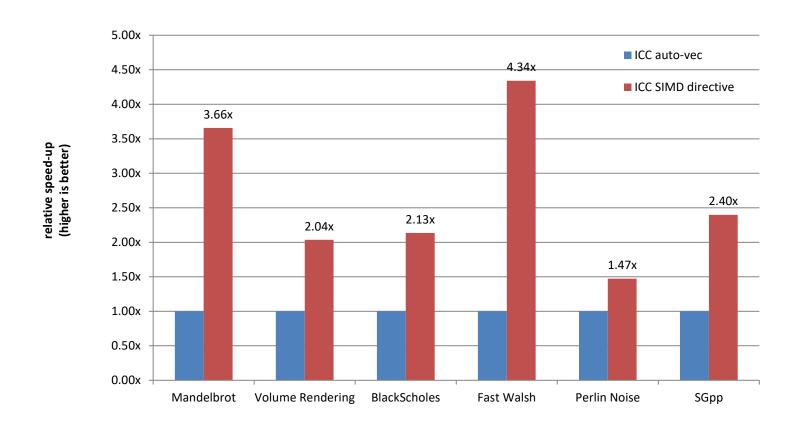




```
#pragma omp declare simd inbranch
float do stuff(float x)
                            vec8 do stuff v(vec8 x, mask m) {
    /* do something */
                                /* do something */
    return x * 2.0;
                                vmulpd x\{m\}, 2.0, tmp
                                return tmp;
void example() {
#pragma omp simd
    for (int i = 0; i < N; i++)
        if (a[i] < 0.0)
            b[i] = do stuff(a[i]);
                          for (int i = 0; i < N; i+=8) {
                              vcmp lt &a[i], 0.0, mask
                              b[i] = do stuff v(&a[i], mask);
```

SIMD Constructs & Performance





M.Klemm, A.Duran, X.Tian, H.Saito, D.Caballero, and X.Martorell. Extending OpenMP with Vector Constructs for Modern Multicore SIMD Architectures. In Proc. of the Intl. Workshop on OpenMP, pages 59-72, Rome, Italy, June 2012. LNCS 7312.





OpenMP Offload Programming





Topics



- OpenMP device and execution model
- Offload basics and exploiting parallelism
- Asynchronous offloading
- Hybrid OpenMP and HIP
- Advanced Task Synchronization
- Case Study: NWChem TCE CCSD(T)





Introduction to OpenMP Offload Features





Running Example for this Presentation: saxpy

```
void saxpy() {
   float a, x[SZ], y[SZ];
   // left out initialization
    double t = 0.0;
    double tb, te;
   tb = omp_get_wtime();
#pragma omp parallel for firstprivate(a)
    for (int i = 0; i < SZ; i++) {
       y[i] = a * x[i] + y[i];
   te = omp_get_wtime();
   t = te - tb;
    printf("Time of kernel: %lf\n", t);
```

Timing code (not needed, just to have a bit more code to show ☺)

This is the code we want to execute on a target device (i.e., GPU)

Timing code (not needed, just to have a bit more code to show ③)

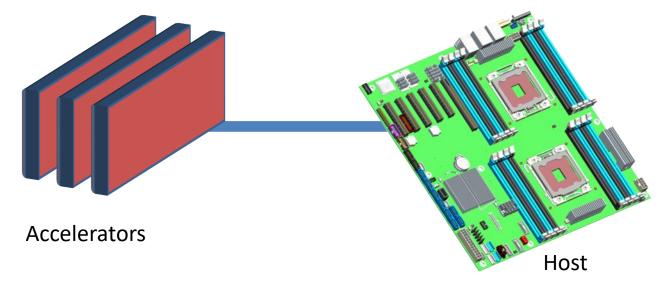
Don't do this at home!
Use a BLAS library for this!



Device Model



- As of version 4.0 the OpenMP API supports accelerators/coprocessors
- Device model:
 - →One host for "traditional" multi-threading
 - → Multiple accelerators/coprocessors of the same kind for offloading





OpenMP Execution Model for Devices



- Offload region and its data environment are bound to the lexical scope of the construct
 - → Data environment is created at the opening curly brace
 - → Data environment is automatically destroyed at the closing curly brace
 - → Data transfers (if needed) are done at the curly braces, too:
 - →Upload data from the host to the target device at the opening curly brace.
 - → Download data from the target device at the closing curly brace.

```
!$omp target &
!$omp map(alloc:A) &
!$omp map(to:A) &
!$omp map(from:A) &
    call compute(A)
!$omp end target
```

Device mem.







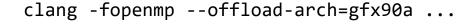
- Transfer control and data from the host to the device
- Syntax (C/C++)
 #pragma omp target [clause[[,] clause],...]
 structured-block
- Syntax (Fortran)
 !\$omp target [clause[[,] clause],...]
 structured-block
 !\$omp end target
- Clauses
 device(scalar-integer-expression)

```
map([{alloc | to | from | tofrom}:] list)
if(scalar-expr)
```





```
The compiler identifies variables that are
                                                                    used in the target region.
void saxpy() {
    float a, x[SZ], y[SZ];
                                                                        All accessed arrays are copied from
    double t = 0.0;
                                                                             host to device and back
    double tb, te;
                                                             x[0:SZ]
    tb = omp_get_wtime();
                                                             y[0:SZ]
#pragma omp target "map(tofrom:y[0:SZ])"
    for (int i = 0; i < SZ; i++) {
         y[i] = a * x[i] + y[i];
                                                                             Presence check: only transfer
    te = omp_get_wtime();
                                                                              if not yet allocated on the
                                                             x[0:SZ]
    t = te - tb;
                                                             y[0:SZ]
                                                                                      device.
    printf("Time of kernel: %lf\n", t);
                                                                         Copying x back is not necessary: it
                                                                                was not changed.
```







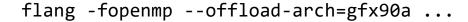
The compiler identifies variables that are used in the target region.

```
subroutine saxpy(a, x, y, n)
    use iso_fortran_env
    integer :: n, i
    real(kind=real32) :: a
    real(kind=real32), dimension(n) :: x
                                                      x(1:n)
    real(kind=real32), dimension(n) :: y
                                                      y(1:n)
!$omp target "map(tofrom:y(1:n))"
    do i=1,n
        y(i) = a * x(i) + y(i)
    end do
!$omp end target
                                                      x(1:n)
end subroutine
                                                      y(1:n)
```

All accessed arrays are copied from host to device and back

Presence check: only transfer if not yet allocated on the device.

Copying x back is not necessary: it was not changed.







```
void saxpy() {
    double a, x[SZ], y[SZ];
    double t = 0.0;
    double tb, te;
                                                      x[0:SZ]
   tb = omp_get_wtime();
                                                      y[0:SZ]
#pragma omp target map(to:x[0:SZ]) \
                   map(tofrom:y[0:SZ])
    for (int i = 0; i < SZ; i++) {
        y[i] = a * x[i] + y[i];
                                                     y[0:SZ]
   te = omp_get_wtime();
   t = te - tb;
    printf("Time of kernel: %lf\n", t);
```

```
clang -fopenmp --offload-arch=gfx90a ...
```





```
The compiler cannot determine the size
                                                               of memory behind the pointer.
void saxpy(float a, float* x, float* y,
            int sz) {
    double t = 0.0;
    double tb, te;
                                                         x[0:sz]
    tb = omp_get_wtime();
                                                         y[0:sz]
#pragma omp target map(to:x[0:sz]) \
                     map(tofrom:y[0:sz])
    for (int i = 0; i < sz; i++) {
        y[i] = a * x[i] + y[i];
                                                         v[0:sz]
    te = omp_get_wtime();
    t = te - tb;
    printf("Time of kernel: %lf\n", t);
                                                          Programmers have to help the compiler
                                                         with the size of the data transfer needed.
```

clang -fopenmp --offload-arch=gfx90a





Exploiting (Multilevel) Parallelism



Creating Parallelism on the Target Device



- The target construct transfers the control flow to the target device
 - → Transfer of control is sequential and synchronous
 - →This is intentional!

- OpenMP separates offload and parallelism
 - → Programmers need to explicitly create parallel regions on the target device
 - →In theory, this can be combined with any OpenMP construct
 - →In practice, there is only a useful subset of OpenMP features for a target device such as a GPU, e.g., no I/O, limited use of base language features.



Example: saxpy



GPUs are multi-level devices: SIMD, threads, thread blocks

Create a team of threads to execute the loop in parallel using SIMD instructions.

clang -fopenmp --offload-arch=gfx90a



teams Construct



- Support multi-level parallel devices
- Syntax (C/C++):
 #pragma omp teams [clause[[,] clause],...]
 structured-block
- Syntax (Fortran):
 !\$omp teams [clause[[,] clause],...]
 structured-block
- Clauses
 num_teams(integer-expression), thread_limit(integer-expression)
 expression)
 default(shared | firstprivate | private none)
 private(list), firstprivate(list), shared(list),
 reduction(operator:list)



Multi-level Parallel saxpy



- Manual code transformation
 - → Tile the loop into an outer loop and an inner loop.
 - → Assign the outer loop to "teams".
 - → Assign the inner loop to the "threads".
 - → (Assign the inner loop to SIMD units.)



Multi-level Parallel saxpy



For convenience, OpenMP defines composite constructs to implement the required code transformations

```
subroutine saxpy(a, x, y, n)
  ! Declarations omitted
!$omp omp target teams distribute parallel do simd &
!$omp& num_teams(num_blocks) map(to:x) map(tofrom:y)
  do i=1,n
      y(i) = a * x(i) + y(i)
  end do
!$omp end target teams distribute parallel do simd
end subroutine
```





Optimizing Data Transfers



Optimizing Data Transfers is Key to Performance



- Connections between host and accelerator are typically lower-bandwidth, higher-latency interconnects
 - → Bandwidth host memory: hundreds of GB/sec
 - → Bandwidth accelerator memory: TB/sec
 - → PCIe Gen 4 bandwidth (16x): tens of GB/sec
- Unnecessary data transfers must be avoided, by
 - →only transferring what is actually needed for the computation, and
 - →making the lifetime of the data on the target device as long as possible.



Role of the Presence Check



■ If map clauses are not added to target constructs, presence checks determine if data is already available in the device data environment:

```
subroutine saxpy(a, x, y, n)
    use iso_fortran_env
    integer :: n, i
    real(kind=real32) :: a
    real(kind=real32), dimension(n) :: x
    real(kind=real32), dimension(n) :: y
!$omp target
    do i=1,n
        y(i) "=præs*enxt(?i()y)+" y"(pir)esent?(x)"
    end do
!$omp end target
end subroutine
```

- OpenMP maintains a mapping table that records what memory pointers have been mapped.
- That table also maintains the translation between host memory and device memory.
- Constructs with no map clause for a data item then determine if data has been mapped and if not, a map(tofrom:...) is added for that data item.



Optimize Data Transfers



- Reduce the amount of time spent transferring data:
 - → Use map clauses to enforce direction of data transfer.
 - →Use target data, target enter data, target exit data constructs to keep data environment on the target device.

```
subroutine saxpy(a, x, y, n)
  ! Declarations omitted

!$omp target "present?(y)" "present?(x)"
  do i=1,n
      y(i) = a * x(i) + y(i)
  end do
!$omp end target
end subroutine
```



Optimize Data Transfers



- Reduce the amount of time spent transferring data:
 - → Use map clauses to enforce direction of data transfer.
 - →Use target data, target enter data, target exit data constructs to keep data environment on the target device.

```
void zeros(float* a, int n) {
#pragma omp target teams distribute parallel for
   for (int i = 0; i < n; i++)
        a[i] = 0.0f;
}</pre>
```

```
void saxpy(float a, float* y, float* x, int n) {
#pragma omp target teams distribute parallel for
   for (int i = 0; i < n; i++)
      y[i] = a * x[i] + y[i];
}</pre>
```







- Create scoped data environment and transfer data from the host to the device and back
- Syntax (C/C++)
 #pragma omp target data [clause[[,] clause],...]
 structured-block
- Syntax (Fortran)
 !\$omp target data [clause[[,] clause],...]
 structured-block
 !\$omp end target data
- Clauses
 device(scalar-integer-expression)
 map([{alloc | to | from | tofrom | release | delete}:]

```
list)
  if(scalar-expr)
```







- Issue data transfers to or from existing data device environment
- Syntax (C/C++)
 #pragma omp target update [clause[[,] clause],...]
- Syntax (Fortran)
 !\$omp target update [clause[[,] clause],...]
- Clauses

```
device(scalar-integer-expression)
to(list)
from(list)
if(scalar-expr)
```



ğ

Example: target data and target update OpenMP

```
#pragma omp target data device(0) map(alloc:tmp[:N]) map(to:input[:N)) map(from:res)
#pragma omp target device(0)
#pragma omp parallel for
    for (i=0; i<N; i++)
      tmp[i] = some computation(input[i], i);
    update input array on the host(input);
#pragma omp target update device(0) to(input[:N])
#pragma omp target device(0)
#pragma omp parallel for reduction(+:res)
    for (i=0; i<N; i++)
      res += final_computation(input[i], tmp[i], i)
```





Asynchronous Offloading



Asynchronous Offloads



- OpenMP target constructs are synchronous by default
 - → The encountering host thread awaits the end of the target region before continuing
 - → The nowait clause makes the target constructs asynchronous (in OpenMP speak: they become an OpenMP task)

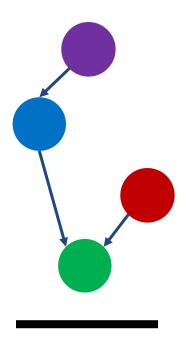
```
#pragma omp task
    init_data(a);

#pragma omp target map(to:a[:N]) map(from:x[:N]) nowait depend(in:a) depend(out:x)
    compute_1(a, x, N);

#pragma omp target map(to:b[:N]) map(from:y[:N]) nowait depend(out:y)
    compute_2(b, y, N);

#pragma omp target map(to:x[:N],y[:N]) map(to:z[:N]) nowait depend(in:x) depend(in:y)
    compute_3(z, x, y, N);

#pragma omp taskwait
```







Hybrid Programming



Hybrid Programming



- Hybrid programming here stands for the interaction of OpenMP with a lower-level programming model, e.g.
 - →OpenCL
 - → CUDA
 - →HIP
- OpenMP supports these interactions
 - → Calling low-level kernels from OpenMP application code
 - → Calling OpenMP kernels from low-level application code



Example: Calling saxpy



```
void example() {
    float a = 2.0;
                                                                  Let's assume that we want to
    float * x;
                                                                 implement the saxpy() function
    float * y;
                                                                    in a low-level language.
    // allocate the device memory
    #pragma omp target data map(to:x[0:count])
                                                map(tofrom:y[0:count])
                                                void saxpy(size_t n, float a,
        compute_1(n, x);
                                                            float * x, float * y) {
        compute 2(n, y);
                                                #pragma omp target teams distribute \
                                                                    parallel for simd
        saxpy(n, a, x, y)
                                                    for (size t i = 0; i < n; ++i) {
        compute 3(n, y);
                                                        y[i] = a * x[i] + y[i];
```



HIP Kernel for saxpy()



Assume a HIP version of the SAXPY kernel:

```
__global__ void saxpy_kernel(size_t n, float a, float * x, float * y) {
    size_t i = threadIdx.x + blockIdx.x * blockDim.x;
    y[i] = a * x[i] + y[i];
}

void saxpy_hip(size_t n, float a, float * x, float * y) {
    assert(n % 256 == 0);
    saxpy_kernel<<<<n/256,256,0,NULL>>>(n, a, x, y);
}
```

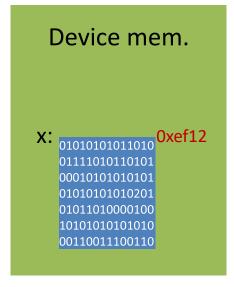
We need a way to translate the host pointer that was mapped by OpenMP directives and retrieve the associated device pointer.

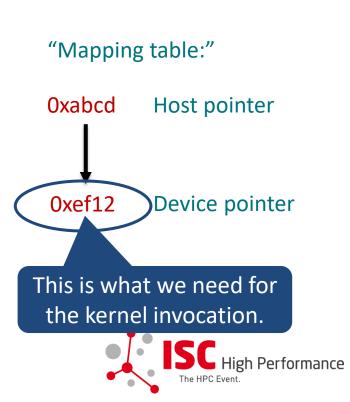


Pointer Translation /1



- When creating the device data environment, OpenMP creates a mapping between
 - → the (virtual) memory pointer on the host and
 - → the (virtual) memory pointer on the target device.
- This mapping is established through the data-mapping directives and their clauses.





Pointer Translation /2



- The target data construct defines the use_device_addr clause to perform pointer translation.
 - →The OpenMP implementation searches for the host pointer in its internal mapping tables.
 - → The associated device pointer is then returned.

```
type * x = 0xabcd;
#pragma omp target data use_device_addr(x[:0])
{
    example_func(x); // x == 0xef12
}
```

Note: the pointer variable shadowed within the target data construct for the translation.



Putting it Together...



```
void example() {
    float a = 2.0;
    float * x = ...; // assume: x = 0xabcd
    float * y = ...;
    // allocate the device memory
   #pragma omp target data map(to:x[0:count]) map(tofrom:y[0:count])
    {
        compute_1(n, x); // mapping table: x:[0xabcd,0xef12], x = 0xabcd
        compute_2(n, y);
        #pragma omp target data use_device_addr(x[:0],y[:0])
            saxpy_hip(n, a, x, y) // mapping table: x:[0xabcd,0xef12], x = 0xef12
        compute_3(n, y);
```



Advanced Task Synchronization



Asynchronous API Interaction



- Some APIs are based on asynchronous operations
 - → MPI asynchronous send and receive
 - → Asynchronous I/O
 - → HIP, CUDA and OpenCL stream-based offloading
 - → In general: any other API/model that executes asynchronously with OpenMP (tasks)
- Example: HIP memory transfers

```
do_something();
hipMemcpyAsync(dst, src, nbytes, hipMemcpyDeviceToHost, stream);
do_something_else();
hipStreamSynchronize(stream);
do_other_important_stuff(dst);
```

- Programmers need a mechanism to marry asynchronous APIs with the parallel task model of OpenMP
 - → How to synchronize completions events with task execution?







```
void hip_example() {
#pragma omp task
                   // task A
        do something();
        hipMemcpyAsync(dst, src,
                                   bytes, hipMemcpyDeviceToHost, stream);
                                      Race condition between the tasks A & C,
    #pragma omp task // task B
                                      task C may start execution before
        do_something_else();
                                      task A enqueues memory transfer.
    #pragma omp task // task C
        hipStreamSynchronize(stream);
        do_other_important_stuff(dst);
```

This solution does not work!





Try 2: Use just OpenMP Tasks Dependences

```
void hip_example() {
#pragma omp task depend(out:stream)
                                         // task A
        do something();
        hipMemcpyAsync(dst, src, nbytes, hipMemcpyDeviceToHost, stream);
                                                       Synchronize execution of tasks through dependence.
    #pragma omp task
                                         // task B
                                                       May work, but task C will be blocked waiting for
        do something else();
                                                       the data transfer to finish
    #pragma omp task depend(in:stream) // task (
        hipStreamSynchronize(stream);
        do other important stuff(dst);
```

- This solution may work, but
 - → takes a thread away from execution while the system is handling the data transfer.
 - → may be problematic if called interface is not thread-safe



Detachable



- OpenMP 5.0 introduces the concept of a detachable task
 - → Task can detach from executing thread without being "completed"
 - → Regular task synchronization mechanisms can be applied to await completion of a detached task
 - → Runtime API to complete a task
- Detached task events: omp_event_handle_t datatype
- Detached task clause: detach(event)
- Runtime API: void omp_fulfill_event(omp_event_handle_t *event)



Detaching Tasks



```
omp_event_handle_t *event;
void detach_example() {
    #pragma omp task detach(event)
    {
        important_code();
    }
    #pragma omp taskwait ② 4
}
Some other thread/task:
    omp_fulfill_event(event);
```

- 1. Task detaches
- 2. taskwait construct cannot complete

- 3. Signal event for completion
- 4. Task completes and taskwait can continue



Putting It All Together



```
void callback(hipStream t stream, hipError t status, void *cb dat) {
 (3) omp_fulfill_event(* (omp_event_handle_t *) cb_data);
void hip example() {
    omp_event_handle_t hip_event;
#pragma omp task detach(hip_event) // task A
        do something();
        hipMemcpyAsync(dst, src, nbytes, hipMemcpyDeviceToHost, stream);
        hipStreamAddCallback(stream, callback, &hip event, 0);
                                     // task B
#pragma omp task
        do_something_else();
                                                         Task A detaches
#pragma omp taskwait(2)(4)
                                                      taskwait does not continue
                                     // task C
#pragma omp task
                                                      3. When memory transfer completes, callback is
                                                         invoked to signal the event for task completion
        do other important stuff(dst);
                                                      4. taskwait continues, task C executes
```

Removing the taskwait Construct



```
void callback(hipStream t stream, hipError t status, void *cb dat) {
 Omp_fulfill_event(* (omp_event_handle_t *) cb_data);
void hip_example() {
    omp_event_handle_t hip_event;
#pragma omp task depend(out:dst) detach(hip_event) // task A
        do something();
        hipMemcpyAsync(dst, src, nbytes, hipMemcpyDeviceToHost, stream);
        hipStreamAddCallback(stream, callback, &hip_event, 0);
                                    // task B
#pragma omp task
        do something else();
#pragma omp task depend(in:dst)
        do_other_important_stuff(dst);
```

- Task A detaches and task C will not execute because of its unfulfilled dependency on A
- 2. When memory transfer completes, callback is invoked to signal the event for task completion
- Task A completes and C's dependency is fulfilled





Case Study: NWChem TCE CCSD(T)

 TCE: Tensor Contraction Engine CCSD(T): Coupled-Cluster with Single, Double, and perturbative Triple replacements



NWChem



- Computational chemistry software package
 - →Quantum chemistry
 - → Molecular dynamics
- Designed for large-scale supercomputers
- Developed at the EMSL at PNNL
 - → EMSL: Environmental Molecular Sciences Laboratory
 - → PNNL: Pacific Northwest National Lab
- URL: http://www.nwchem-sw.org



Finding Offload Candidates



- Requirements for offload candidates
 - → Compute-intensive code regions (kernels)
 - → Highly parallel
 - → Compute scaling stronger than data transfer, e.g., compute O(n³) vs. data size O(n²)



Example Kernel (1 of 27 in total)



```
subroutine sd t d1 1(h3d,h2d,h1d,p6d,p5d,p4d,
                     h7d, triplesx, t2sub, v2sub)
     Declarations omitted.
     double precision triplesx(h3d*h2d,h1d,p6d,p5d,p4d)
     double precision t2sub(h7d,p4d,p5d,h1d)
     double precision v2sub(h3d*h2d,p6d,h7d)
!$omp target ,,presence?(triplesx,t2sub,v2sub)"
!$omp teams distribute parallel do private(p4,p5,p6,h2,h3,h1,h7)
     do p4=1, p4d
     do p5=1,p5d
                            1.5GB data transferred
     do p6=1,p6d
     do h1=1,h1d
                                (host to device)
     do h7=1,h7d
     do h2h3=1,h3d*h2d
      triplesx(h2h3,h1,p6,p5,p4)=triplesx(h2h3,h1,p6,p5,p4)
    1 - t2sub(h7,p4,p5,h1)*v2sub(h2h3,p6,h7)
     end do
     end do
                       1.5GB data transferred
     end do
                           (device to host)
     end do
     end do
     end do
                    Toute parallel do
!$omp end teams dis
!$omp end target
     end subroutine
```

- All kernels have the same structure
- 7 perfectly nested loops
- Some kernels contain inner product loop (then, 6 perfectly nested loops)
- Trip count per loop is equal to "tile size" (20-30 in production)
- Naïve data allocation (tile size 24)
 - Per-array transfer for each target construct
 - triplesx: 1458 MB
 - t2sub, v2sub:2.5 MB each



Invoking the Kernels / Data Management



Simplified pseudo-code

```
!$omp target enter data map(alloc:triplesx(1:tr_size))
     for all tiles
     do ...
       call zero_triplesx(triplesx)
                                                Allocate 1.5GB data once,
       do ...
                                                     stays on device.
         call comm and sort(t2sub, v2sub)
!$omp target data map(to:t2sub(t2_size)) map(to:v2sub(v2_size))
         if (...)
            call sd t d1 1(h3d,h2d,h1d,p6d,p.
                                             1d_h7,triplesx,t2sub,v2sub)
          end if
         same for sd t d1 2 until sd t d1 9
                                                 Update 2x2.5MB of data for
!$omp target end data
                                                (potentially) multiple kernels.
       end do
       do ...
         Similar structure for sd_t_d2_1 until sd_t_d2_9, incl. target data
       end do
       call sum energy(energy, triplesx)
     end do
!$omp target exit data map(release:triplesx(1:size))
```

- Reduced data transfers:
 - triplesx:
 - allocated once
 - always kept on the target
 - t2sub, v2sub:
 - allocated after comm.
 - kept for (multiple) kernel invocations



Invoking the Kernels / Data Management



```
    Simplified pseudo-code

                                                                         subroutine sd_t_d1_1(h3d,h2d,h1d,p6d,p5d,p4d,
                                                                                       h7d, triplesx, t2sub, v2sub)
                                                                         Declarations omitted.
  !$omp target enter data map(alloc:triplesx(1:tr_size
                                                                         double precision triplesx(h3d*h2d,h1d,p6d,p5d,p4d)
        for all tiles
                                                                         double precision t2sub(h7d,p4d,p5d,h1d)
        do ...
                                                                         double precision v2sub(h3d*h2d,p6d,h7d)
          call zero_triplesx(triplesx
                                                                         target "presence?(triplesx,t2sub,v2sub)"
                                                     Allocate 1.5G
          do ...
                                                                         teams distribute parallel do private(p4,p5,p6,h2,h3,h1,h7)
                                                          stays on
            call comm and sort (t2sub, v2sub)
                                                                         do p4=1,p4d
                                                                         do p5=1,p5d
  !$omp target data map(to:t2sub(t2_size)) map(to:v2sub(v2_size)
                                                                         do p6=1,p6d
            if (...
                                                                         do h1=1,h1d
                                                    4d.h7,triplesx
               call sd t d1 1(h3d,h2d,h1d,p6d,p.
                                                                         do h7=1,h7d
                                                                                        Presence check determines that arrays
            end if
                                                                         do h2h3=1,h3d^{3}
                                                                                        have been allocated in the device data
            same for sd t d1 2 until
                                                                          triplesx(h2h)
                                                     Update 2x2.5
                                                                        1 - t2sub(h7
  !$omp target end data
                                                                                                  environment already.
                                                     (potentially) r
                                                                         end do
          end do
                                                                         end do
          do ...
                                                                         end do
            Similar structure for sd_t_d2_1 until sd_t_d2_9, inc
                                                                         end do
          end do
                                                                         end do
                                                                         end do
          call sum_energy(energy, triplesx)
                                                                    $omp end teams distribute parallel do
        end do
                                                                         end target
  !$omp target exit data map(release:triplesx(1:size))
                                                                         end subroutine
```





Future OpenMP Directions





OpenMP 6.0 includes many major new features



- Officially released on November 14, 2024
 - → Reflects three years of work since release of OpenMP 5.2
 - →Includes 416 enacted issues, covering a wide range of content and complexity
- Free-agent threads significantly change execution model, implementations
- New concept for task dependences: transparent tasks
 - → Enables asynchronous target data (also enables other future extensions)
- User-defined induction and induction clause expand parallelism support
- Many significant device support improvements (e.g., workdistribute)
- Several additional (sequential) loop transforming directives
- Supported compound constructs are now defined based on a grammar
- Significant improvements to usability and correctness of specification



OpenMP tasking advances have pervasive impact



- Other major additions to 6.0 include:
 - → Support for dependences and affinity of tasks generated by taskloop directives
 - → A new taskgraph directive that enables optimized task generation
- Task-generating constructs are fundamental to OpenMP offload model
 - → Most device constructs (e.g., target and target update directives) already generate them
 - → Another major change: target data is now a dependence sequence of three tasks
 - → Middle task is transparent by default
 - → The construct now is also a taskgroup region by default
 - → Can specify no wait and no group to rely only on dependences for ordering
- Other constructs (e.g., parallel and teams) are composed of implicit tasks
 - → While not adopted for 6.0, expect to add transparent clause to many of them eventually
 - → Will enable no_wait to be supported for parallel construct



Topics



- Current OpenMP Language Committee Activities
- OpenMP Organizational Overview
- Final Review of OpenMP 5.0, 5.1, 5.2 and 6.0 (included for reference)





OpenMP Language Committee Current Activities: TR14 and OpenMP 6.1



OpenMP 6.1 will refine and amend OpenMP 6.0



- Significant progress has already been made
 - → 18 issues have been adopted, mostly covering small updates to 6.0 additions
 - → Language committee face-to-face meeting week after next will result in many more issues moving forward
- Targeting some significant improvements for device support
 - → Support for dynamic groupprivate memory (e.g., small, optimized GPU memory pool) (done!)
 - → Support for explicit control of pointer attachment (done!)
 - → Improved support for implicit declare target in Fortran
 - → Beginning work on "kernel language", which will provide more low-level device control
- Expect continued refinement in many other areas
 - → More loop transformations, refinements of other ones
 - → Working on mechanism to control OpenMP defaults used for a translation unit
 - → Considering additional extensions that build on transparent tasks (e.g., parallel nowait)
 - → Many other small changes, particularly related to tasking and tool support, are likely



Things likely to be deferred to beyond 6.1



- True support for using multiple devices
 - → Device-to-device scoping support for atomic and other memory operations
 - → Support for bulk launch
 - → Support to update data on multiple devices (broadcast/multicast, other collectives)
 - → Support for work distribution across devices
 - → Considering relaxing restrictions on nested target regions
- Support for pipelining, data-flow, other parallelization models
- Support for event-based parallelism
- Characterizing loop-based work distribution constructs as transformations
- Efficient use of multiple compilation units (i.e., support for efficient IPO)



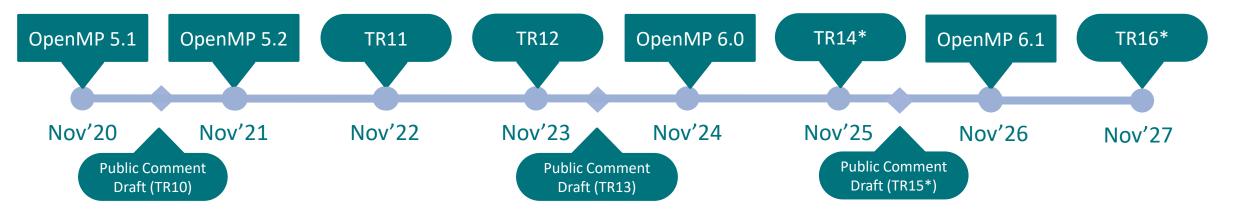
OpenMP Organizational Overview



OpenMP Roadmap



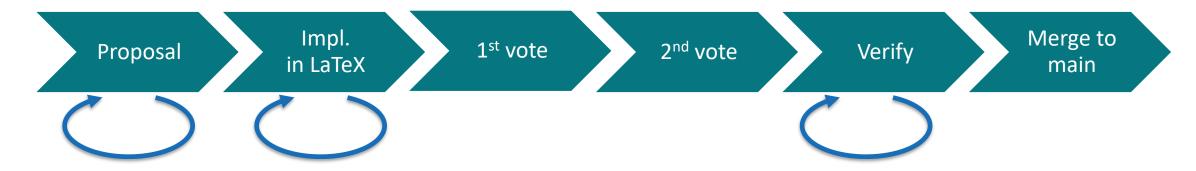
- OpenMP has a well-defined roadmap:
 - →5-year cadence for major releases
 - →One minor release in between
 - →OpenMP 5.2 was added as a second minor release before OpenMP version 6.0
 - →(At least) one Technical Report (TR) with feature previews in every year



Development Process of the Specification



Modifications to the OpenMP specification follow a (strict) process:



Release process for specifications:





User Outreach & Education













Check out openmp.org/news/events-calendar/



Help Us Shape the Future of OpenMP



- OpenMP continues to grow
 - →32 members currently
- You can contribute to our annual releases
- Attend IWOMP, understand and shape research directions
- OpenMP membership types now include less expensive memberships
 - → Please let us know if you would be interested





Final Review of OpenMP 5.0, 5.1, 5.2 and 6.0 Included for Reference



Ratified OpenMP 5.0 in November 2018, Ratified OpenMP 5.1 in November 2020



- OpenMP 5.0
 - →Addressed several major open issues for OpenMP
 - →Included 293 passed tickets
- OpenMP 5.1
 - →Includes many refinements to 5.0 additions
 - →Included 254 passed GitHub issues
- OpenMP 5.2
 - → Mostly address quality of specification issues but also refines 5.0 and 5.1 additions
 - →Included 131 passed GitHub issues



Major new features in OpenMP 5.0



- Significant extensions to improve usability
 - →OpenMP contexts, metadirective and declare variant
 - → Addition of requires directive, including support for unified shared memory
 - → Memory allocators and support for deep memory hierarchies
 - → Descriptive loop construct
 - → Ability to quiesce OpenMP threads
 - → Support to print/inspect affinity state
 - → Release/acquire semantics added to memory model
 - → Support for C/C++ array shaping
- First (OMPT) and third (OMPD) party tool support



Major new features in OpenMP 5.0



- Some significant extensions to existing functionality
 - → Verbosity reducing changes such as implicit declare target directives
 - → User defined mappers provide deep copy support for map clauses
 - → Support for reverse offload
 - → Support for task reductions, including on taskloop construct, task affinity, new dependence types, depend objects and detachable tasks
 - → Allows teams construct outside of target construct (i.e., on host)
 - → Supports collapse of non-rectangular loops
 - → Scan extension of reductions
- Major advances for base language normative references
 - → Completed support for Fortran 2003
 - → Added initial support of Fortran 2008, C11, C++11, C++14 and C++17







- Supports collapse of imperfectly nested loops
- Supports != on C/C++ loops
- Adds conditional modifier to lastprivate
- Support use of any C/C++ Ivalue in depend clauses
- Permits declare target on C++ classes with virtual members
- Clarification of declare target C++ initializations
- Adds task modifier on many reduction clauses
- Adds depend clause to taskwait construct





OpenMP 5.1 refines existing functionality

- Adds full support for C11, C++11, C++14, C++17, C++20 and Fortran 2008 and partial support for Fortran 2018
- Extends directive syntax to C++ attribute specifiers
- The scope construct supports reductions within parallel regions
 - → Christian discussed this enhancement in another session
- Extends atomic construct to support compare-and-swap, min and max
 - → Detailed these enhancements in another session
- Adds many clauses and clause modifiers including:
 - → nowait **to** taskwait **construct**
 - → strict modifier to clauses on the taskloop construct





OpenMP 5.1 refines existing functionality

- Support for mapping (translated) function pointers
- Device-specific environment variables to control their ICVs
- nothing directive supports metadirective clarity and completeness
- Several new runtime routines, including more memory allocation flavors
- Deprecations include:
 - → The master affinity policy and master construct
 - → Cray pointers
 - → Many enum values, most related to OMPT (first-party tool interface)





OpenMP 5.1 adds some significant extensions

- The interop construct
 - →Improves native device support (e.g., CUDA streams)
 - → Also supports interoperability with CPU-based libraries (e.g., TBB)
- The new dispatch construct, improved declare variant directive
 - → Enable use of variants with device-specific arguments
 - →Elision of "unrecognized" code





OpenMP 5.1 adds some significant extensions

- The assume directive
 - → Supports optimization hints based on invariants
 - → Supports promise to limit OpenMP usage to (optimizable) subsets
- Loop transformation directives: The tile and unroll directives
 - → Control use of traditional sequential optimizations
 - →Ensure that they are applied when, where appropriate relative to parallelization



The error directive supports user-defined warnings and errors



Use error directive to interact with the compiler

- Compiler displays msg-string as part of implementation-defined message
- The at clause determines when the effect of the directive occurs
 - → compilation: If encountered during compilation in a declarative context (useful along with metadirective) or is reachable at runtime
 - → execution: If the code location is encountered during execution (similar to assert ())
- The severity clause determines compiler action
 - → warning: Print message only (default)
 - → fatal: Stop compilation or execution



The masked construct supports filtering execution per thread



Use masked construct to limit parallel execution (low cost: no data environ.)

#pragma omp masked [filter(integer-expression)]
 structured-block

- Encountering thread executes if filter clause matches its thread number
- Default (i.e., no clause) is equivalent to deprecated master construct
- Future (i.e., OpenMP 6.0) enhancements planned
 - → Define concept of thread groups, a subset of the threads in a team
 - → Extend masked to filter based on thread groups or booleans (via clause modifier)
 - → filter clause added to other constructs, relying on thread group concept



OpenMP 5.2 improves quality of the specification



- Large portions of specification now generated from JSON-based database
 - → Section headers and directive and clause format
 - → Cross references, index entries, hyperlinks and many other document details
 - → Long-term plan will capture sufficient information in database to generate much more, including grammar, quick reference guide, and header and runtime library routine stub files
- Improves specification of OpenMP syntax
 - → Ensuring syntax of directives and clauses is well-specified and consistent
 - → Ensuring restrictions are consistent and not just implied by syntax
 - → Deprecating one-off syntax choices, many other inconsistencies (12 new deprecation entries)
 - → Makes C++ attribute syntax a first-class citizen
- Many other minor improvements



OpenMP 6.0 includes many major new features



- Free-agent threads significantly change execution model, implementations
- New concept for task dependences: transparent tasks
 - → Enables asynchronous target data (also enables other future extensions)
- The target data directive is now a dependence sequence of three task
- Support for dependences and affinity of tasks generated by taskloop
- The taskgraph directive enables optimized task generation
- User-defined induction and induction clause expand parallelism support
- Many significant device support improvements (e.g., workdistribute)
- Several additional (sequential) loop transforming directives
- Supported compound constructs are now defined based on a grammar
- Significant improvements to usability and correctness of specification







```
xi = x0;
result = 0.0;
#pragma omp parallel for reduction(+: result) induction(step(x), *: xi)
for (I = 0; I < N; i++) {
   result += c[i] * xi;
   xi *= x;
}</pre>
```

- Simple inductions are similar to reductions, particulary with use of inscan
 - → Avoids complexity needed to avoid serialization for parallel scan computations
- User-defined induction greatly expands expressible loop parallelism
 - → Can define complex functions to perform computations with dependences
 - → Can use collector clause to specify closed form function to enable starting at arbitrary iterations (typically used for start of chunks but can allow arbitrarily)



What is the effect of the following code?



```
// assume in main with initialization omitted
// assume no OpenMP directives omitted

TS = 4096;
#pragma omp taskloop grainsize(TS)
for (i = 0; i < SIZE; i++) {
   A[i] = A[i] * B[i] * s;
}</pre>
```

■ Pre-6.0 need parallel masked directive so multiple threads execute tasks

```
// assume in main with initialization omitted
// assume no OpenMP directives omitted

TS = 4096;
#pragma omp parallel masked
#pragma omp taskloop grainsize(TS)
for (i = 0; i < SIZE; i++) {
   A[i] = A[i] * B[i] * s;
}</pre>
```







```
// assume in main with initialization omitted
// assume no OpenMP directives omitted

TS = 4096;
#pragma omp taskloop grainsize(TS) threadset(omp_pool)
for (i = 0; i < SIZE; i++) {
   A[i] = A[i] * B[i] * s;
}</pre>
```

- OpenMP 6.0 defines OpenMP threads as members of logical thread pool
 - → Pool size can be specified by OMP THREAD LIMIT environment variable
- OpenMP 6.0 also adds the concept of free-agent threads
 - → Do not need parallel masked directive
 - →Instead threadset clause can specify that unassigned threads may execute tasks







```
// assume library must ensure fine-grain dependences are honored
int my_func(double *M, double *v) {
  int i, j, k;

  for (i = 0; i < N_ROWS; i += ROWS_PER_TASK) {
    #pragma omp task depend(inout:M[i*N_COLS])
    for (j = 0; j < ROWS_PER_TASK; j++) {
        for (k = 0; k < N_COLS; k++) {
            M[(i+j)*N_COLS + k] = M[(i+j)*N_COLS + k] * v[k]; } }
    return 0;
}</pre>
```

- Successive calls to my_func with the same M are ordered correctly in OpenMP 5.2 and earlier if they are issued in the same task
 - → Ensures all uses of task construct will not deadlock
 - →Other synchronization can alleviate constraint by eliminating concurrency of tasks from different calls so this solution does not provide the desired result

Transparency supports rich dependence graphs OpenMP

```
// assume my func as in previous example
double M[N ROWS*NCOLS], v[NUM VS][N COLS];
int i;
// code to initialize M and v omitted for brevity
for (i = 0; i < NUM VS; i++) {
  #pragma omp task depend(inout:i) transparent(omp impex)
  my func(M, &v[i*N COLS]);
```

- The calls to my func are ordered because of the dependence shown
- These tasks are transparent importing and exporting ("omp impex") tasks
 - → Dependences expressed in the calls are now imported and exported
 - → Deadlock freedom is still guaranteed



Extended parallel directive to support complete user control of number of threads



The parallel directive will accept a new modifier and two "new" clauses

- Using strict prescriptiveness requires nthreads to be provided
- Clauses, previously available on error directive, effective with strict if cannot provide nthreads
 - → Display msg-string as part of implementation-defined message
 - → If severity is fatal execution is terminated
 - → If severity is warning message is displayed but execution continues
- Also now allowed to provide a list for nthreads to support nested parallelism

