OpenMP* Threading

Dr. Mikko Byckling
Senior Application Engineer

Acknowledgements: Martyn Corden, Intel; Steve “Dr. Fortran” Lionel, ex-Intel

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Contents

- OpenMP* Threading Model
  - **`parallel`**, **`do`** and **`task`** constructs, **`barrier`**, data scoping, scheduling
- OpenMP* 4.0 Tasking
  - Task **`depend`**
  - OpenMP* 4.5 Tasking: **`taskloop`**
- OpenMP* performance aspects
  - Thread affinity
  - Non-uniform memory access

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  - OpenMP* 4.5 Tasking: **`taskloop`**
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OpenMP Threading Model

- In OpenMP, the description of ***parallelism*** and ***worksharing*** treated as separate entities
- Thread *parallelism* is described with `parallel` construct

  C/C++: `#pragma omp parallel [clauses]`

  Fortran: `!$omp parallel [clauses]`
- Loop *worksharing* is described with `loop` construct

  C/C++: `#pragma omp for [clauses]`

  Fortran: `!$omp do [clauses]`
- Task *worksharing* is described with `task` construct

  C/C++: `#pragma omp task [clauses]`

  Fortran: `!$omp task [clauses]`

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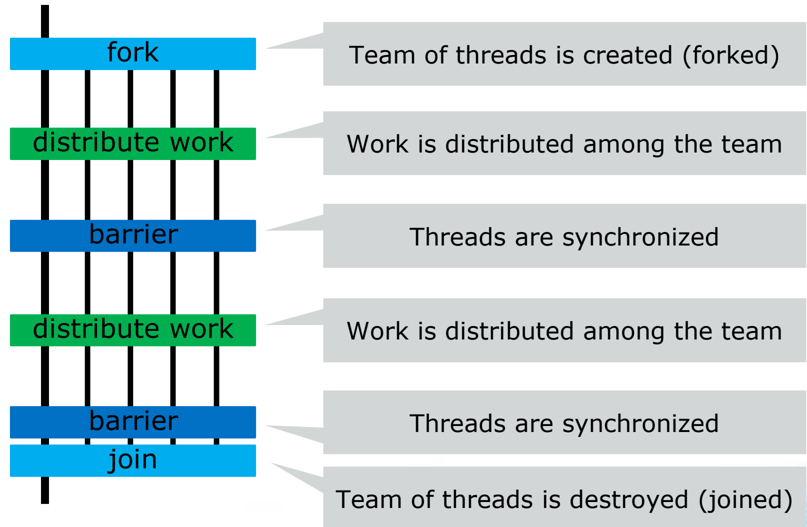
OpenMP `parallel`: Example

```
!$omp parallel
    !$omp do
    DO i=1,N
    …
    END DO
    !$omp end do
    !$omp do
    DO i=1,N
    …
    END DO
    !$omp end do
!$omp end parallel
```



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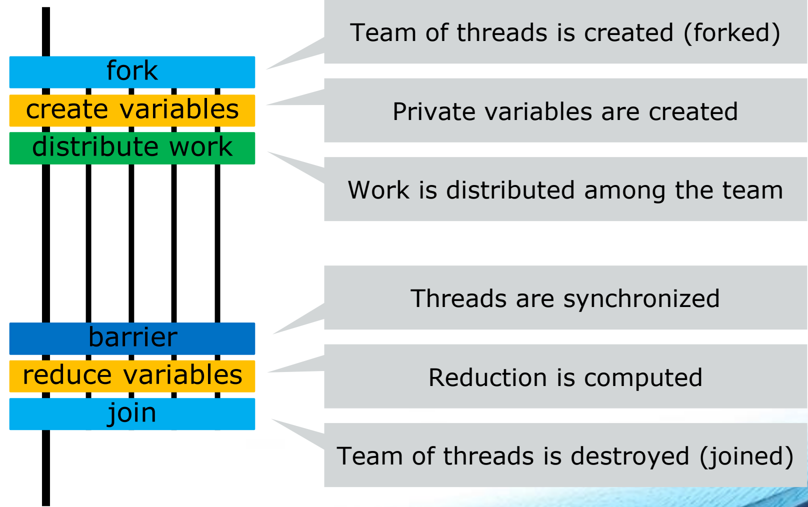
OpenMP `parallel do`: Example

```fortran
REAL :: a(N), l, s
s = 0.0
!$omp parallel do      &
  reduction(+:s)       &
  private(l)           &
  schedule(static,4)
  DO i=1,N
    l = sqrt(a(i))
    s = s + l
  END DO
!$omp end parallel do
```



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OpenMP `barrier` construct

- Specify an explicit barrier at the point at which the construct appears
  `!$omp barrier`
  - All threads executing the enclosing parallel region must execute the barrier before any are allowed to continue

```
INTEGER :: n
REAL :: global_data(n,n)
REAL, ALLOCATABLE :: private_data(:,:)
!$omp parallel private(private_data)
  CALL initialize(global_data, private_data)
  !$omp barrier
  CALL compute(data)
!$omp end parallel
```

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OpenMP `single` construct

- Execute a structured block with any single thread
  - Other threads wait at end of the construct

```
INTEGER :: n
REAL, ALLOCATABLE :: global_data(:,:), global_data_in(:,:)
REAL, ALLOCATABLE :: private_data(:,:)
!$omp parallel private(private_data)
  ! Initialize global data (in parallel)
  CALL initialize_global(global_data)
  !$omp single
  ! Read from file (serial)
  CALL initialize_global_in(global_data_in)
  !$omp end single
  CALL initialize_private(global_data, global_data_in, private_data)
  …
!$omp end parallel
```

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OpenMP `threadprivate` directive

- Declarative directive
  `!$omp threadprivate(list)`
  - Specify that variables in list are replicated, with each thread having its own copy

```
MODULE thread_data
  REAL, ALLOCATABLE :: data(:,:)
  !$omp threadprivate(data)
CONTAINS
  SUBROUTINE initialize_thread_private(global_data)
    REAL, CONTIGUOUS :: global_data(:,:)
    !$omp parallel
    ALLOCATE(data, SOURCE=global_data)
    !$omp end parallel
  END SUBROUTINE
! Rest of implementation omitted
```

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OpenMP `parallel` clauses

- `if(expression)`
  - When `expression` evaluates to `.TRUE.`, execute the construct in parallel
- `num_threads(num-threads)`
  - Execute the construct with `num-threads`
- `reduction(identifier:list)`
  - For variables in `list`, make a private copy and compute a reduction with `identifier` after the end of the region
- `proc_bind(master | close | spread)`
  - Execute region with the defined thread affinity

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OpenMP `parallel` clauses

- **`private(list)`**
  - Declare variables in **`list`** to be private to a thread
  - Implicitly private: variables in a private scope (a called function or **`BLOCK`** construct) within a parallel region
- **`firstprivate(list)`**
  - As private, but initialize the value according to the corresponding original item

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OpenMP `parallel` clauses

- **`shared(list)`**
  - Declare variable in **`list`** to be shared between threads
  - Implicitly shared: all variables with the **`SAVE`** attribute (incl. implicit SAVE), **`COMMON`** block and **`MODULE`** scope variables
- **`copyin(list)`**
  - Initialize a **`threadprivate`** variable to the value of the master thread

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OpenMP `parallel` clauses

- `default( firstprivate | none | private | shared )`
  - Set the data sharing attribute for variables which the data scoping would be otherwise implicitly defined
  - NOTE: **`none`** will require each variable referred in the scope of the parallel section to have its data sharing attribute defined

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OpenMP loop construct clauses

- `private, firstprivate, reduction`
  - As with parallel
- `lastprivate(list)`
  - As private, but set the value **after** the region according corresponding to the lexically last iteration index

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OpenMP loop construct clauses

- `collapse(n)`
  - Combine the iteration space of **n** subsequent tightly nested loops together
- `ordered[(n)]`
  - Execute **n** subsequent tightly nested loops in a sequential order
- `nowait`
  - No implicit barrier at the end of the construct

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OpenMP loop construct scheduling

- **`schedule(kind[, chunk_size])`**
  - Distribute work in chunks of **`chunk_size`** to threads with schedule kind, where **`kind`** is
    `static`: distribute chunks to threads in a round-robin fashion
    `dynamic`: chunks are distributed to threads dynamically
    `guided`: as dynamic, but decrease the **`chunk_size`** towards the end of the iteration
    `runtime`: choose schedule at run time (**`OMP_SCHEDULE`**)
  - Default **`chunk_size`** depends on the used schedule **`kind`**

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  - Task **depend**
  - OpenMP* 4.5 Tasking: **taskloop**
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OpenMP 4.0 Tasking

- OpenMP 3.0 introduced dynamic tasking in addition to static tasking (cf., `sections` construct)
- Implement irregular patterns through tasking
  - Recursion
  - Graph traversal
- OpenMP 4.0 added task dependencies to influence scheduling

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OpenMP `task` Construct

- Create a new task
  - Memorize data and code to be executed
  - Task constructs can be arbitrarily nested
  - By default tasks are *tied* to the thread that first executes them, not neccessarily the creator.
- Syntax (C/C++)

```
#pragma omp task [clause[[,] clause],…]
 structured-block
```

- Syntax (Fortran)

```
!$omp task[clause[[,] clause],…]
 block
!$omp end task
```


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OpenMP `task` clauses (1/2)

- Data scoping clauses:
  `shared(list)`, `private(list)`, `firstprivate(list)`,
  `default(private*|firstprivate*|shared|none)` * Fortran only
- Note: data scoping has a slightly different meaning than for threads
  - Private: variable is stored in the task's private memory

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OpenMP `task` clauses (2/2)

- Task scheduling clauses:
- `final(logical-expression)`
  The task is a *final task* if logical-expression evaluates to true. All tasks generated by final task are *included tasks*, i.e., will be evaluated immediately after their generation.
- `untied`
  The task is not tied to the thread that started its execution. Any thread in the team can resume the task region after a suspension.
- `mergeable`
  When the generated task is an *undeferred task* or an *included task*, the implementation may generate a *merged task*, i.e., a task for which the data environment is the same as its generating region.
- `depend(dependence-type:list)`

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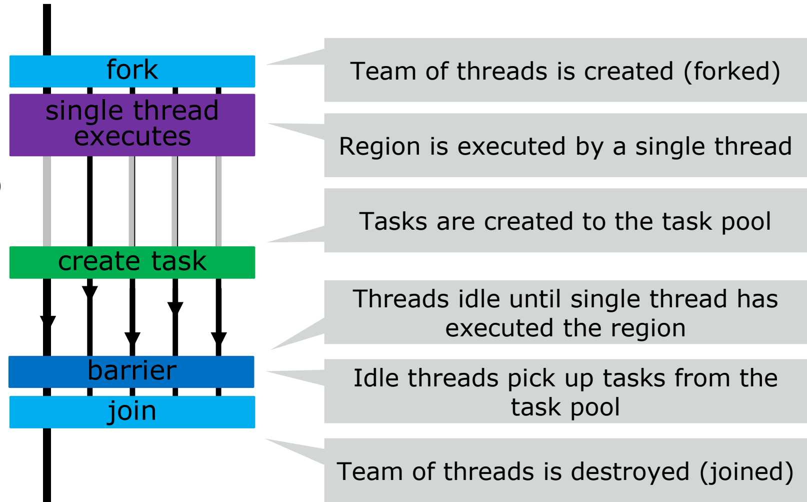
OpenMP `task`: Example (1/2)

```
!$omp parallel
  !$omp single
  e => l % head
  DO WHILE (ASSOCIATED(e))
    !$omp task &
    !$omp firstprivate(e)
      call process(e)
    !$omp end task
    e => e % next
  END DO
  !$omp end single
!$omp end parallel
```



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OpenMP Task Scheduling: `taskwait`, `barrier`

- Task scheduling constraints:
  - Only the binding thread of a task can execute it
  - A task can only be suspended at a task suspend point (creation, finish, `taskwait`, `barrier`)
  - If task is not suspended in a barrier, executing thread can only switch to a direct descendant of all tasks tied to the thread
- Task barrier: `taskwait`
  - Encountering task suspends until child tasks are complete
    - Only direct childs, not descendants!
- OpenMP `barrier` (implicit or explicit)
  - All tasks created by any thread of the current *thread team* are guaranteed to be completed at barrier exit

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OpenMP `task`: Example (2/2)

- Fibonacci numbers $F_n = F_{n-1} + F_{n-2}, F_0 = 0, F_1 = 1$ with OpenMP tasks

```
INTEGER(KIND=int64) :: fn
INTEGER :: n
! Set n
!$omp parallel
  !$omp single
    fn = fibonacci(n)
  !$omp end single
!$omp single
…
RECURSIVE FUNCTION fibonacci(n) RESULT(fn)
  IMPLICIT NONE
  INTEGER, INTENT(IN) :: n
  INTEGER(KIND=int64) :: fn, fnm1, fnm2

  IF (n<2) THEN
    fn=n
    RETURN
  END IF
```

```
  ! Compute Fibonacci number by recursion
  !$omp task shared(fnm1)
    fnm1 = fibonacci(n-1)
  !$omp end task
  !$omp task shared(fnm2)
    fnm2 = fibonacci(n-2)
  !$omp end task

  !$omp taskwait
  fn = fnm1+fnm2
END FUNCTION fibonacci
```

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OpenMP `taskgroup` Construct

- The `taskgroup` construct specifies a wait on the child tasks of the current task and their descendents at the end of construct
- Syntax (C/C++)

```
#pragma omp taskgroup
 structured block
```

- Syntax (Fortran)

```
!$omp taskgroup
 block
!$omp end taskgroup
```

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OpenMP `taskgroup`: Example

- Not waiting for all tasks currently in execution

```
!$omp parallel
  !$omp task
  CALL background_task()
  !$omp end task

  !$omp taskgroup
    !$omp task
    CALL compute_task()
   !$omp end task
  !$omp end taskgroup
  ! compute_task() and its siblings guaranteed to be finished
  !$omp taskwait
  ! background_task() guaranteed to be finished
!$omp end parallel
```

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OpenMP `depend` clause

- Idea: programmer defines the dependencies between the tasks, the OpenMP runtime extracts the parallelism from the dependency graph
- The `depend` clause can enforce constraints on the order of execution by enabling dependencies between sibling tasks
  - By default the order of execution for OpenMP tasks is arbitrary

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OpenMP `depend` clause

- Syntax:
  `depend(dependence-type:list)`
  where dependence-type is either `in`, `out` or `inout`, `list` describes one or more variables or non-zero length array sections.
- **Restriction:** any `list` items used in a `depend` clause of the same task or sibling tasks must indicate identical storage or disjoint storage, i.e., partially overlapping OpenMP array sections as dependencies are not allowed

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OpenMP `depend` dependency types

- Task dependency types:
- `in`

  The generated task will be a dependent task of all *previously generated* sibling tasks that reference at least one of the list items in an `out` or `inout` clause.
- `out, inout`

  The generated task will be a dependent task of all *previously generated* sibling tasks that reference at least one of the list items in an `in`, `out`, or `inout` clause.

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OpenMP array sections

- An OpenMP array section designates the elements in an array
  - Array sections must be contiguous in memory
- Syntax (C/C++)

  `array[lower-bound:length]`

  alternatively

  `array[:length]`, `array[lower-bound:]`, `array[:]`
- Syntax (Fortran)

  `array(start:end)`

  or alternatively any **contiguous** Fortran array section

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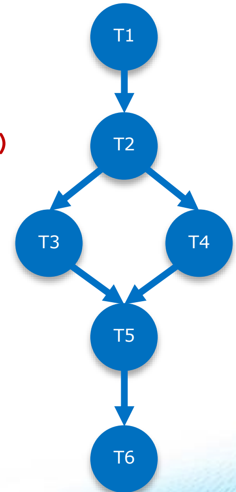
OpenMP depend: Example

```
INTEGER, TARGET :: a
INTEGER, POINTER :: b
b => a
!$omp task depend(in:a)
  ! T1
!$omp end task
!$omp task depend(out:b)
  ! T2
!$omp end task
!$omp task depend(in:a)
  ! T3
!$omp end task
```

```
!$omp task depend(in:b)
 ! T4
!$omp end task
!$omp task depend(inout:a)
 ! T5
!$omp end task
!$omp task depend(in:a)
 ! T6
!$omp end task
```



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OpenMP `taskloop` construct

- Motivation: OpenMP loop worksharing or using nested parallelism can lead to excessive fork/join overhead
  - Typical example: a call to a threaded numerical library such as BLAS from within an OpenMP parallel region

```
INTEGER :: N
REAL(kind=real64) :: A(N,N), B(N,N), C(N,N)
 !$omp parallel
 CALL compute_in_parallel_1(A,B,C)
 !$omp end parallel
 CALL DGEMM('N','N', n, n, n, &
                  real(1,real64), A, size(A,1), &
                  B, size(B,1), &
                  real(0,real64), C, size(C,1))
 !$omp parallel
 CALL compute_in_parallel_2(A,B,C)
 !$omp end parallel
```

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OpenMP `taskloop` construct

- OpenMP `taskloop` construct
  - Split iterations of a loop into chunks, execute the chunks in parallel by using OpenMP tasks
  - Defines an implicit `taskgroup`, i.e., tasks generated by `taskloop` are *undeferred*
- Syntax (C/C++)

```
#pragma omp taskloop [simd] [clauses]
 for-loops
```

- Syntax (Fortran)

```
!$omp taskloop [simd] [clauses]
 do-loops
!$omp end taskloop [simd]
```

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OpenMP `taskloop` clauses (1/2)

- Worksharing clauses
- **`grainsize`(`grain-size`)**
  Positive integer **`grain-size`** defines the number of iterations assigned to each created task to be at least **`grain-size`**, but less than two times the value of the **`grain-size`**.
- **`nogroup`**
  No implicit taskgroup region will be created.
- **`num_tasks`(`num-tasks`)**
  Positive integer **`num-tasks`** defines the number of created tasks as at least **`num-tasks`**. Each task must have at least one logical loop iteration.
- **`collapse`(`n`)**
  Positive integer **`n`** defines the number of nested loops associated with the taskloop construct.

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OpenMP `taskloop` clauses (2/2)

- Clauses inherited from `parallel` and `task`
- Data scoping clauses:
  `shared(list), private(list), firstprivate(list), default(private*|firstprivate*|shared|none)`
- Task scheduling clauses
  `final(logical-expr), untied, mergeable`

* Fortran only

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OpenMP `taskloop`: Example

- Mixing different types of tasks

```
!$omp parallel
!$omp task
  call background_task() ! Can execute concurrently
  !$omp end task

  !$omp taskloop grainsize(500) nogroup
  DO i=1,N
     CALL computation_task(i) ! Can execute concurrently
  END DO
  !$omp end taskloop
!$omp end parallel
```

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  - Task `depend`
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Thread or process pinning

- Pinning "assigns" a process or thread to a particular core for execution.
- If a thread/process is not pinned, the operating system is free to
  - initially start it on any core
  - freely move it around between cores
- Issues:
  - Might destroy memory locality (NUMA)
  - Sub-optimal placement might affect performance

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Thread affinity – processor binding

Success of processor binding strategies depend on the machine and the application!

- Putting threads far, i.e. on different packages
  - (May) improve the aggregated memory bandwidth
  - (May) improve the combined cache size
  - (May) decrease performance of synchronization constructs
- Putting threads close together, i.e. on two adjacent cores which possible share the cache
  - (May) improve performance of synchronization constructs
  - (May) decrease the available memory bandwidth and cache size (per thread)

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Thread affinity in OpenMP* 4.0

- OpenMP 4.0 introduces the concept of places
  - Set of threads running on one or more processors
  - Can be defined by the user
  - Pre-defined places available:
    - **threads** one place per hyper-thread
    - **cores** one place exists per physical core
    - **sockets** one place per processor package
- OpenMP 4.0 affinity policies
  - **spread** spread OpenMP threads evenly among the places
  - **close** pack OpenMP threads near master thread
  - **master** collocate OpenMP thread with master thread
- OpenMP 4.0 affinity control via
  - Environment variables **`OMP_PLACES`** and **`OMP_PROC_BIND`**
  - Clause **proc_bind** for parallel regions

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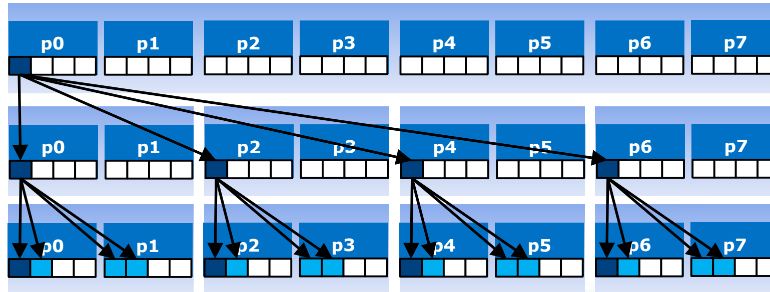
Thread affinity: example

- Example (Intel® Xeon Phi™ processor):
  Distribute outer region, keep inner regions close

```
OMP_PLACES=cores(8)
!$omp parallel proc_bind(spread)
   !$omp parallel proc_bind(close)
```



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(Almost) all HPC systems are NUMA

- **N**on-**U**niform **M**emory **A**ccess
- (Almost) all multi-socket compute servers are NUMA systems
  - Different access latencies for different memory locations
  - Different bandwidth observed for different memory locations
- Example: Intel® Xeon E5-2600v3 Series processor

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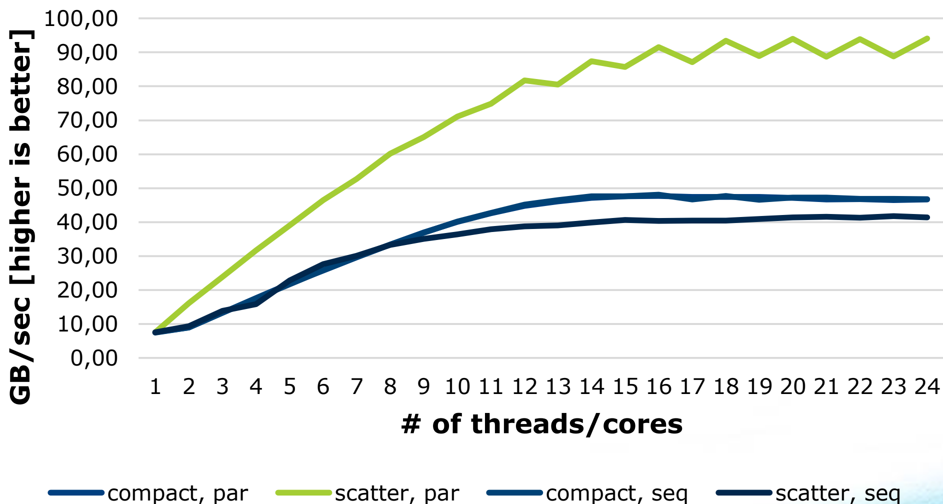
NUMA - Does it matter?



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First touch policy

- Modern operating systems all use virtual memory
- The OS typically optimizes memory allocations
  - `malloc()` or **`ALLOCATE`** does not allocate the memory directly
  - Only the memory management "knows" about the memory allocation, but no memory pages are made available
  - At first memory access (***write***), the OS physically allocates the corresponding page (First touch policy)
- On NUMA systems this might lead to performance issues in threaded or multi-process applications

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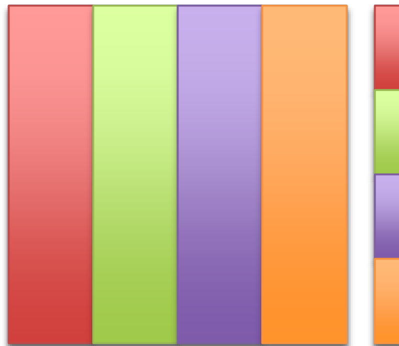
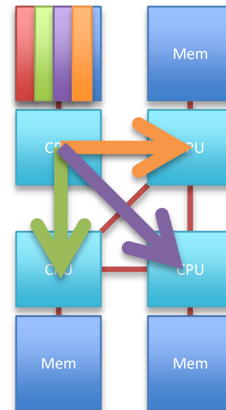
NUMA Optimization with OpenMP

```
! Initialize data

DO j=1,N
  DO i=1,M
  …
  END DO
END DO

! Perform work
!$omp parallel do private(j)
DO j=1,N
  DO i=1,M
  …
  END DO
END DO
!$omp end parallel do
```





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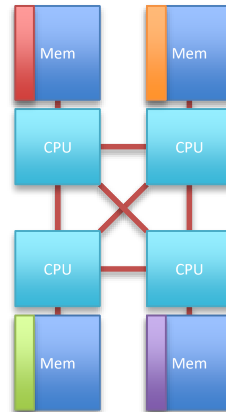
NUMA Optimization with OpenMP

```
! Initialize data
!$omp parallel do private(j)
DO j=1,N
  DO i=1,M
  …
  END DO
END DO
!$omp end parallel do
! Perform work
!$omp parallel do private(j)
DO j=1,N
  DO i=1,M
  …
  END DO
END DO
!$omp end parallel do
```



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Summary

- Use OpenMP tasks for irregular parallelism and for increased composability
- Task dependencies enable OpenMP runtime to extract the parallelism
- Task loops can be used to extract task parallelism from (nested) loops

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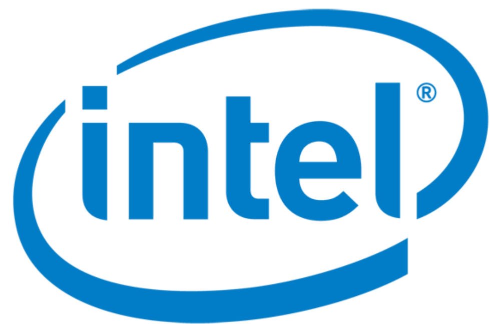
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