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OpenMP (with Labs)

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Parallel Computing at TACC: Stampede

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Based on materials developed by Kent Milfeld at TACC

Multithreading

- A programming model that allows multiple *threads* to exist in a single process, sharing the same memory space
- Thread – A single sequence of programming instructions

- Why multithreading?
  - Speedup – For an application that scales well, the speedup increases linearly with number of threads, theoretically

Goal

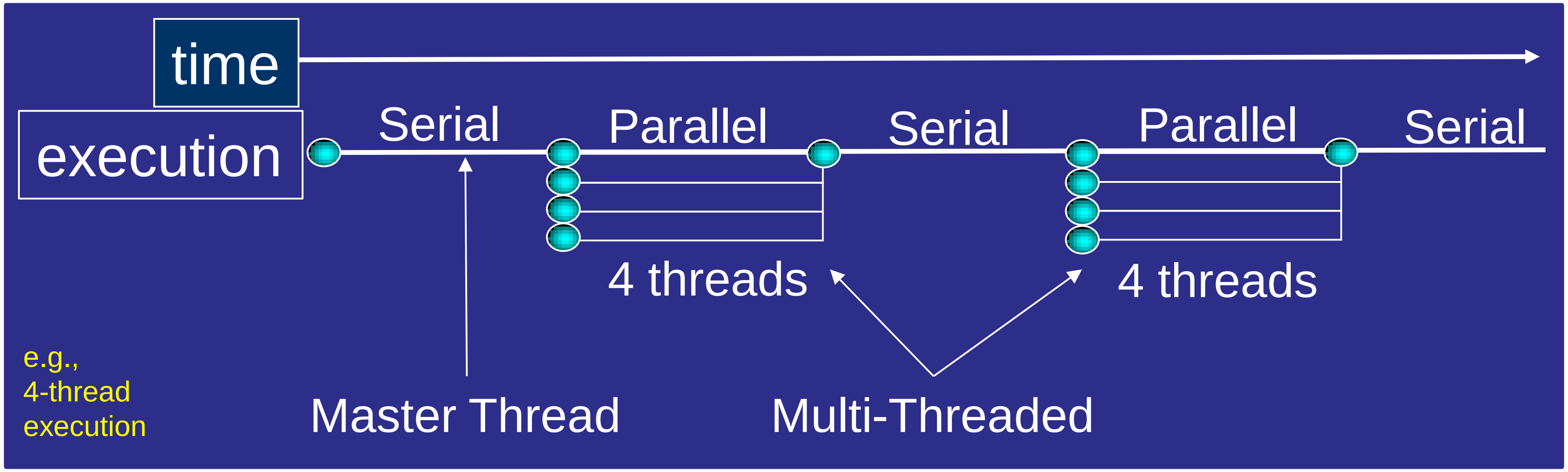
- In this talk, you will learn how to:
  - Parallelize portions of your application
  - Use the OpenMP API
  - Avoid common pitfalls in shared memory programming

What is OpenMP?

- OpenMP is an acronym for Open Multi-Processing
- An Application Programming Interface (API) for developing multithreading parallel program in shared memory architecture
- Three primary components of the API are:
  - Compiler Directives
  - Runtime Library Routines
  - Environment Variables
- OpenMP standard is maintained by the OpenMP Architecture Review Board
- http://www.openmp.org/ has the specification, examples, tutorials and documentation

OpenMP Fork-Join Parallelism

- Programs begin as a single process: master thread
- Master thread executes until a parallel region is encountered
  - Master thread creates (forks) a team of parallel threads
  - Threads in team simultaneously execute tasks in the parallel region
  - Team threads synchronize and terminate (join); master continues



LAB: OMP Hello World

Parallel Region: C/C++ and Fortran

```
1 #pragma omp parallel
2  { code block
3     a = work(...);
4  }
```

```
!$omp parallel
   code block
   call work(...)
!$omp end parallel
```

Line 1	Team of threads is formed at parallel region
Lines 2–3	Each thread executes code block and subroutine call, no branching into or out of a parallel region
Line 4	All threads synchronize at end of parallel region (implied barrier)

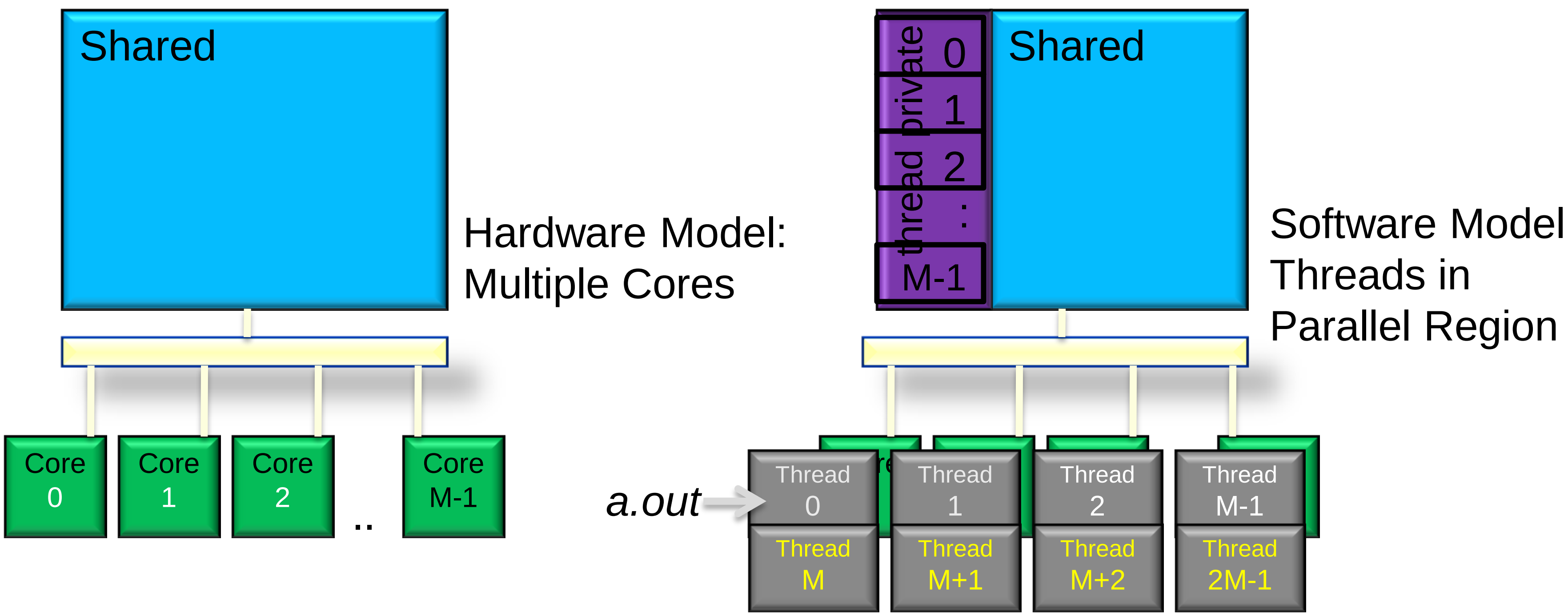
OpenMP: Multithreading

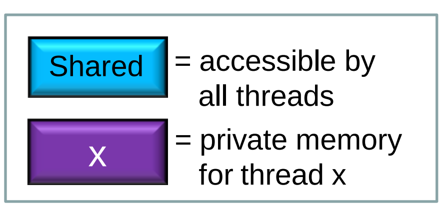
- All about executing concurrent work (tasks)
  - Tasks execute independently
  - Tasks access the same shared memory
  - Shared variable updates must be mutually exclusive
  - Synchronization through barriers

```
// repetitive work
#pragma omp parallel for
for (i=0; i<N; i++)
     a[i] = b[i] + c[i];
```

```
// repetitive updates
#pragma omp parallel for
for (i=0; i<N; i++)
     sum = sum + b[i]*c[i];
```

OpenMP: Shared Memory Systems





M threads are usually mapped to M cores.

For HyperThreading, 2 SW threads are mapped to 2 HW threads on each core.

On the Intel Xeon Phi Coprocessors, there are 4 HW threads/core.

Thread Memory Access

- Every thread has access to "global" (shared) memory
  - All threads share the same address space
  - Threads don't communicate like MPI processes
- But need to avoid race conditions with shared memory. Examples:
  1. If multiple writers are going in no particular order, last writer "wins"
  2. A reader may either precede or follow a writer – lack of synchronization
  3. Threads may overlap in a code block, causing conditions 1 *and* 2
- What do you with a race condition?
  - Don't introduce one in the first place: it's a bug, hard to debug
  - Impose order with barriers (explicit/implicit synchronization)
  - Use mutual exclusion (mutex) directives to protect critical sections, where one thread must run at a time (at a performance penalty)

Example of a Critical Section

Intended

Thread 0		Thread 1		Value
read	←			0
increment				0
write	→			1
		read	←	1
		increment		1
		write	→	2

Possible…

Thread 0		Thread 1		Value
				0
read	←			0
increment		read	←	0
write	→	increment		1
		write	→	1
				1

- In a critical section, need *mutual exclusion* to get intended result
- The following OpenMP directives prevent this race condition:

#pragma omp critical – for a code block (C/C++)
#pragma omp atomic – for single statements

OpenMP Directives

- OpenMP directives:
  - specify parallelism for shared-memory parallel (SMP) machines
  - Appear like comments in source code
- FORTRAN compiler: `!$OMP`, `C$OMP`, or `*$OMP` – use `!$OMP` for free-format F90
- C/C++ compiler directive: `#pragma omp`

C/C++

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

#pragma omp parallel for
    for(...){...
    }
```

Fortran 90

```
!$OMP parallel
  ...
!$OMP end parallel

!$OMP parallel do
  DO ...
!$OMP end parallel do
```

Role of the Compiler

- OpenMP relies on the compiler to do the multithreading
  - Compiler recognizes OpenMP directives, builds in appropriate code
- A special flag is generally required to enable OpenMP
  - GNU: `gcc -fopenmp`
  - Intel: `icc -openmp`

OpenMP Compiler Directive Syntax

- OpenMP Directives: Sentinel, construct, and clauses

```
#pragma omp construct [clause [[,]clause]…]        C
!$omp       construct [clause [[,]clause]…]        F90
```

- Example

```
#pragma omp parallel private(i) reduction(+:sum)   C
!$omp       parallel private(i) reduction(+:sum)   F90
```

- Most OpenMP constructs apply to a “structured block”, that is, a block of one or more statements with one point of entry at the top and one point of exit at the bottom.

OpenMP Constructs

OpenMP language "extensions"

parallel control	work-sharing	control of one task	data access	synchron-ization	runtime environment
• governs flow of control in the program **`parallel`** directive	• distributes work among threads **`do/for`** **`sections`** **`single`** directives	• assigns work to a thread **`task`** directive (OpenMP 3.0)	• specifies scoping of variables **`shared`** **`private`** **`reduction`** clauses	• coordinates execution of threads **`critical`** **`atomic`** **`barrier`** directives	• sets/gets environment **`schedule`** **`omp_set_num_threads()`** **`omp_get_thread_num()`** **`OMP_NUM_THREADS`** **`OMP_SCHEDULE`** clause, API, env. variables

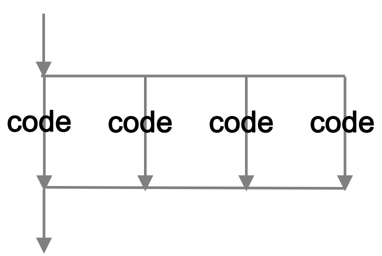
OpenMP Parallel Construct

- Replicated – executed by all threads
- Worksharing – divided among threads

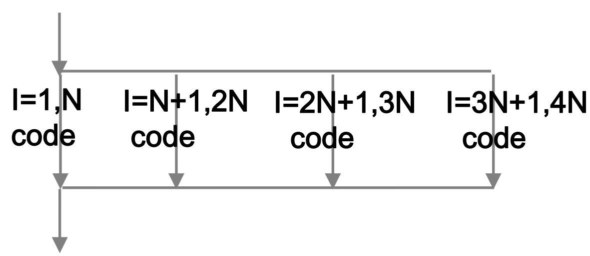
```
PARALLEL
    {code1}
DO
  do I = 1,N*4
    {code2}
  end do
    {code3}
END PARALLEL
```

```
PARALLEL DO
  do I = 1,N*4
    {code}
  end do
END PARALLEL DO
```

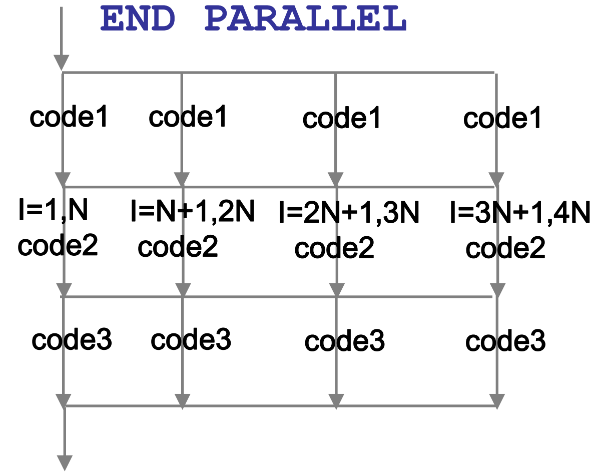
```
PARALLEL
  {code}
END PARALLEL
```



Replicated



Worksharing



Combined

OpenMP Worksharing, Mutual Exclusion

Use OpenMP directives to specify worksharing in a parallel region, as well as mutual exclusion

```
#pragma omp parallel
{
        #pragma omp
} // end parallel
```

Code block	*Thread action*
for	Worksharing
sections	Worksharing
single	One thread
critical	One thread at a time

```
parallel do/for
parallel sections
```

Directives can be combined, if a parallel region has just one worksharing construct.

Worksharing Loop: C/C++

```
1 #pragma omp parallel for
2  for (i=0; i<N; i++)
3  {
4    a[i] = b[i] + c[i];
5  }
6
```

General form:

```
#pragma omp parallel
{
  #pragma omp for
  for (i=0; i<N; i++)
  {a[i] = b[i] + c[i];}
}
```

Line 1	Team of threads formed (parallel region).
Lines 2–6	Loop iterations are split among threads. Implied barrier at end of block(s) {}.

Each loop iteration must be independent of other iterations.

Worksharing Loop: Fortran

```
1 !$omp parallel do
2  do i=1,N
3     a(i) = b(i) + c(i)
4  enddo
5 !$omp end parallel do
6
```

General form:

```
!$omp parallel
!$omp do
 do i=1,N
  a(i) = b(i) + c(i)
 enddo
!$omp end parallel
```

Line 1	Team of threads formed (parallel region).
Lines 2–5	Loop iterations are split among threads.
Line 5	(Optional) end of parallel loop (implied barrier at enddo).

Each loop iteration must be independent of other iterations.

OpenMP Clauses

- *Directives* dictate what the OpenMP thread team will do
- Examples:
  - *Parallel regions* are marked by the **`parallel`** directive
  - *Worksharing loops* are marked by **`do`**, **`for`** directives (Fortran, C/C++)
- *Clauses* control the behavior of any particular OpenMP directive
- Examples:
  1. Scoping of variables: **`private`**, **`shared`**, **`default`**
  2. Initialization of variables: **`copyin`**, **`firstprivate`**
  3. Scheduling: **`static`**, **`dynamic`**, **`guided`**
  4. Conditional application: **`if`**
  5. Number of threads in team: **`num_threads`**

LAB: Worksharing Loop

Private, Shared Clauses

- Private : Variable is private to each thread
- Shared : Variable is shared among all threads
- In the following loop, each thread needs a private copy of temp
  - The result would be unpredictable if temp were shared, because each processor would be writing and reading to/from the same location

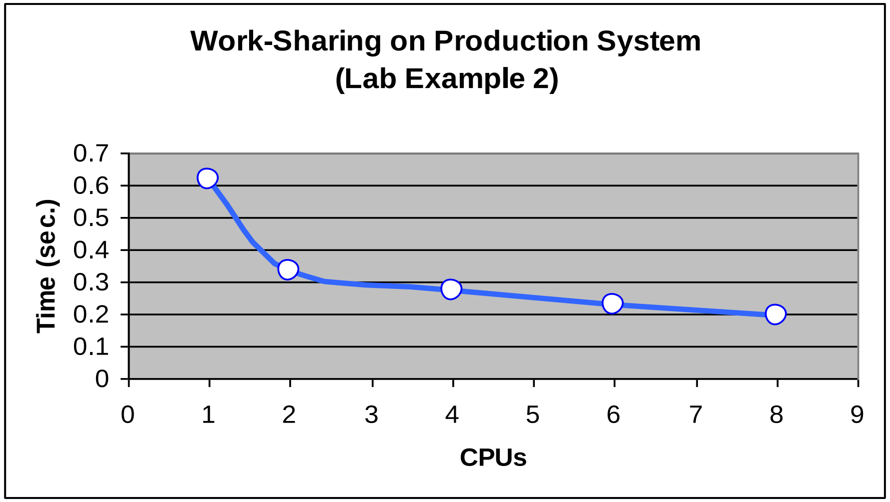
```
!$omp parallel do private(temp,i) shared(A,B,C)
      do i=1,N
         temp = A(i)/B(i)
         C(i) = temp + cos(temp)
      enddo
!$omp end parallel do
```

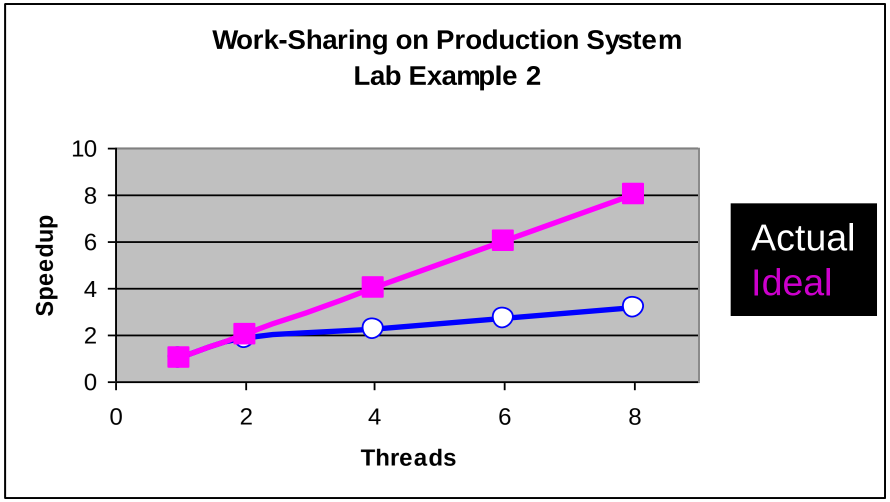
Worksharing Results

Speedup =
cputime(1) / cputime(N)

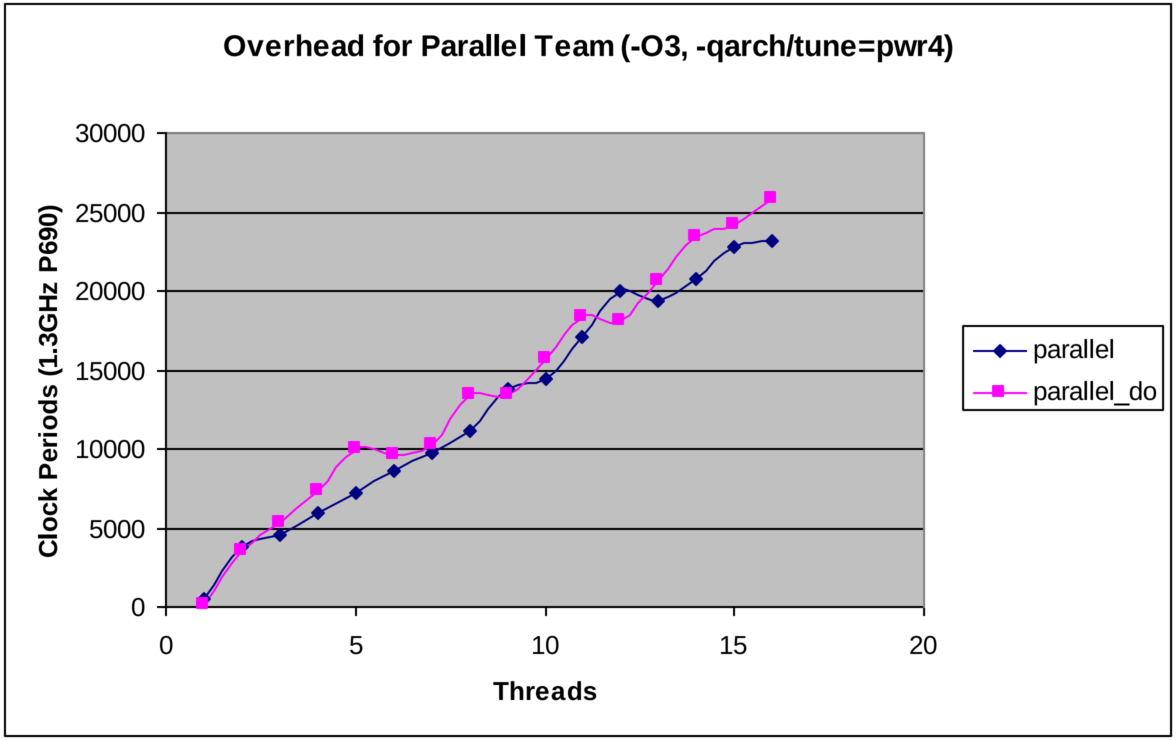
If work is completely parallel, scaling is linear.

Scheduling, memory contention and overhead can impact speedup and Mflop/s rate.





Overhead to Fork a Thread Team



- Increases roughly linearly with number of threads

Merging Parallel Regions

Merging work-sharing constructs eliminates the overhead

```
!$OMP PARALLEL DO
      do i=1,n
         a(i)=b(i)+c(i)
      enddo
!$OMP END PARALLEL DO
!$OMP PARALLEL DO
      do i=1,m
         x(i)=y(i)+z(i)
      enddo
!$OMP END PARALLEL DO
```

```
!$OMP PARALLEL
  !$OMP DO
      do i=1,n
        a(i)=b(i)+c(i)
      enddo
  !$OMP END DO
  !$OMP DO
      do i=1,m
          x(i)=y(i)+z(i)
      enddo
  !$OMP END DO
!$OMP END PARALLEL
```

LAB: OMP Functions

Runtime Library Functions

`omp_get_num_threads()`	Number of threads in current team
`omp_get_thread_num()`	Thread ID, {0: N-1}
`omp_get_max_threads()`	Number of threads in environment, **`OMP_NUM_THREADS`**
`omp_get_num_procs()`	Number of machine CPUs
`omp_in_parallel()`	True if in parallel region & multiple threads executing
`omp_set_num_threads(#)`	Changes number of threads for parallel region, if dynamic threading is enabled

Environment Variables, More Functions

- To control the OpenMP runtime environment

OMP_NUM_THREADS	Set to permitted number of threads: this is the value returned by **omp_get_max_threads()**
OMP_DYNAMIC	TRUE/FALSE for enable/disable dynamic threading (can also use the function below)

- To enable dynamic thread count (*not* dynamic scheduling!)

omp_set_dynamic()	Set state of dynamic threading: if equal to "true", **omp_set_num_threads()** controls thread count
omp_get_dynamic()	True if dynamic threading is on

Additional OpenMP Features

- Schedule clause: specify how to divide work among threads

  `schedule(static)` `schedule(dynamic,M)`

- Reduction clause: perform collective operations on shared variables

  `reduction(+:asum)` `reduction(*:aprod)`

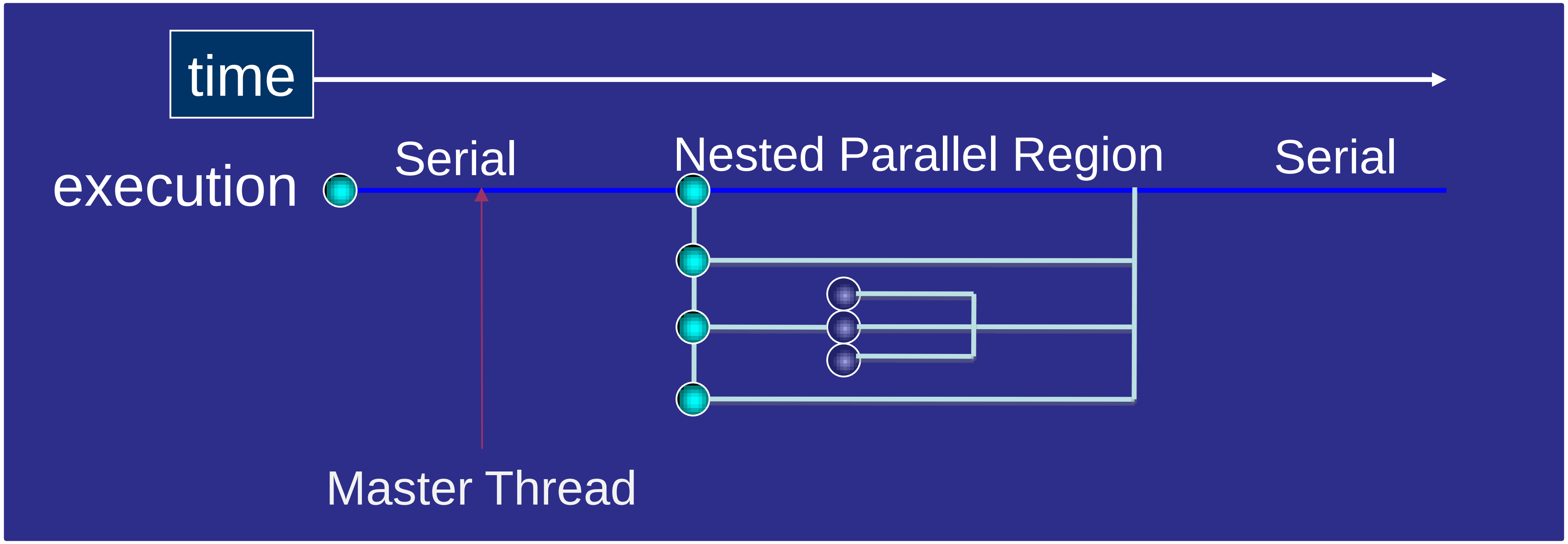
- Nowait clause: remove the barrier at the end of a parallel section

  `for ... nowait` `end do nowait`

- Lock routines: make mutual exclusion more lightweight and flexible

  `omp_init_lock(var)` `omp_set_lock(var)`

Loop Nesting



- OpenMP 3.0 supports nested parallelism, older implementations may ignore the nesting and serialize inner parallel regions.
- A nested parallel region can specify any number of threads to be used for the thread team, new id’s are assigned.

MIC Programming with OpenMP

- Intel compiler, *icc*, is needed
- OpenMP pragma is preceded by MIC-specific **pragma**
  - Fortran: **!dir$ omp offload target(mic) <...>**
  - C: **#pragma offload target(mic) <...>**
- All data transfer is handled by the compiler
  - User control provided through **optional keywords**
- I/O can be done from within offloaded region
  - Data can “stream” through the MIC; no need to leave MIC to fetch new data
  - Also very helpful when debugging (print statements)
- Specific subroutines are automatically offloaded, including MKL subroutines

Example 1

2-D array (**a**) is filled with data on the coprocessor

Data management done automatically by compiler

- Memory is allocated on coprocessor for (**a**)
- Private variables (**i,j,x**) are created
- Result is copied back

```
use omp_lib                                ! OpenMP
integer              :: n = 1024           ! Size
real, dimension(:,:), allocatable :: a     ! Array
integer              :: i, j               ! Index
real                 :: x                  ! Scalar
allocate(a(n,n))                         ! Allocation
!dir$ omp offload target(mic)            ! Offloading
!$omp parallel do shared(a,n), &         ! Par. region
  private(x, i, j), schedule(dynamic)
do j=1, n
  do i=j, n
    x = real(i + j); a(i,j) = x
```

```
#include <omp.h>       /* C example */
  const int n = 1024; /* Size of the array */
  int     i, j;       /* Index variables   */
  float a[n][n], x;
#pragma offload target(mic)
#pragma omp parallel for shared(a), \
        private(x), schedule(dynamic)
  for(i=0;i<n;i++) {
    for(j=i;j<n;j++) {
      x = (float)(i + j); a[i][j] = x; }}
```

LAB: Hand-coding vs. MKL

Example 2

Hand-coded routine, **my_sgemm**:

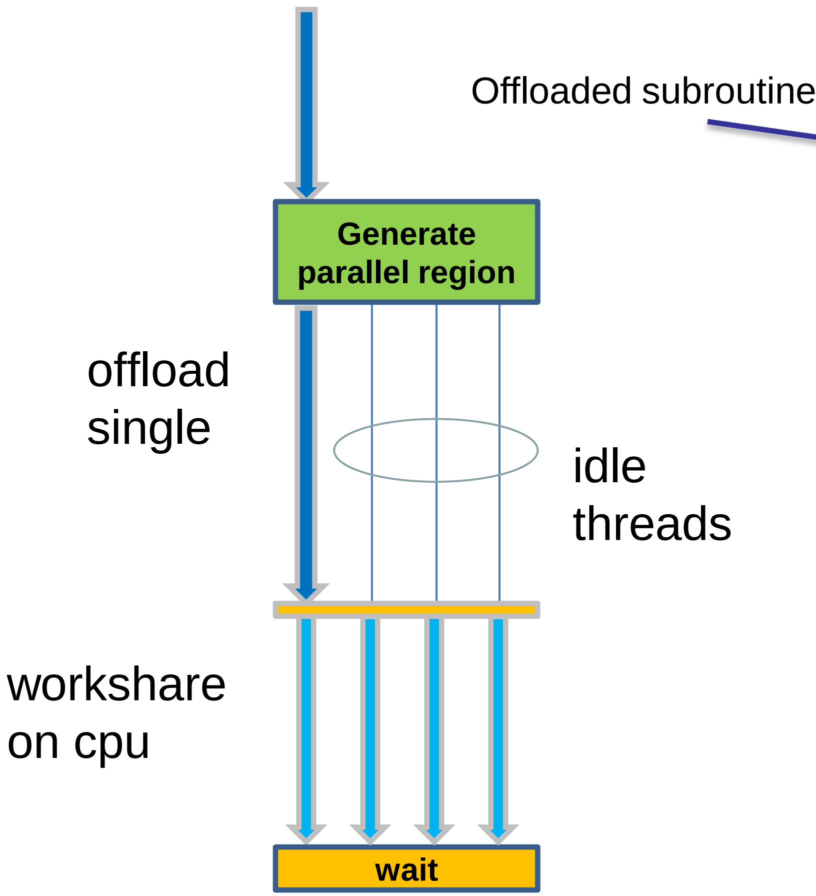
- specifies explicit **in** and **out** data movement

Use **attributes** to have routine compiled for the coprocessor, or link coprocessor-based MKL

```
! snippet from the caller...
! offload MKL routine to accelerator
! offload hand-coded routine with data clauses
!dir$ offload target(mic) in(a,b) out(d)
call my_sgemm(d,a,b)
```

```
! snippet from the hand-coded subprogram...
!dir$ attributes offload:mic :: my_sgemm
subroutine my_sgemm(d,a,b)
real, dimension(:,:) :: a, b, d
!$omp parallel do
do j=1, n
  do i=1, n
    d(i,j) = 0.0
    do k=1, n
      d(i,j) = d(i,j)+a(i,k)*b(k,j)
    enddo; enddo; endo
end subroutine
```

Heterogeneous Threading, Sequential



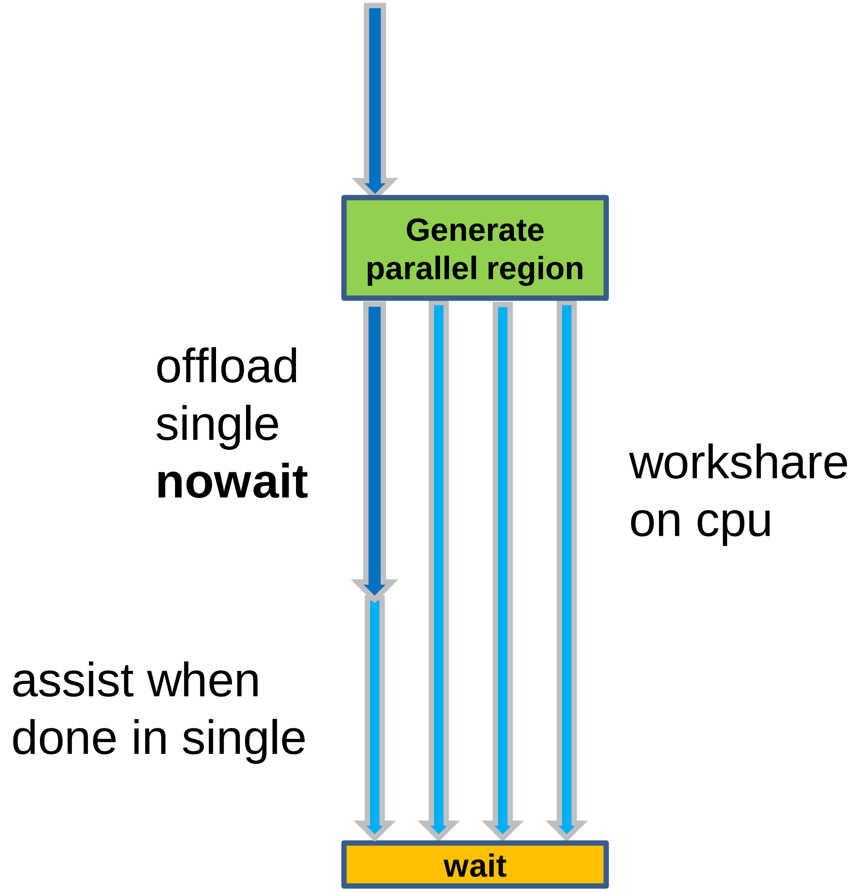
C/C++

```c
#pragma omp parallel
 {
#pragma omp single
   { offload(); }

#pragma omp for
   for(i=0; i<N; i++){...}
 }
```

F90

```fortran
!$omp parallel
   !$omp single
     call offload();
   !$omp end single

   !$omp do
     do i=1,N; ...
     end do
!$omp end parallel
```

Heterogeneous Threading, Concurrent



C/C++

```
#pragma omp parallel
 {
#pragma omp single nowait
   { offload(); }

#pragma omp for schedule(dynamic)
   for(i=0; i<N; i++){...}
 }
```

F90

```
!$omp parallel
   !$omp single
     call offload();
   !$omp end single nowait

   !$omp do schedule(dynamic)
     do i=1,N; ...
     end do
!$omp end parallel
```

Example 2

I/O from offloaded region:

- File is opened and closed by one thread (**omp single**)
- All threads take turns reading from the file (**omp critical**)

Threads may also read in parallel (not shown)

- Parallel file system
- Threads read parts from different targets

```
#pragma offload target(mic) //Offload region
#pragma omp parallel
{
  #pragma omp single /* Open File */
  {
  printf("Opening file in offload region\n");
  f1 = fopen("/var/tmp/mydata/list.dat","r");
  }

  #pragma omp for
  for(i=1;i<n;i++) {
    #pragma omp critical
    { fscanf(f1,"%f",&a[i]);}
    a[i] = sqrt(a[i]);
  }

  #pragma omp single
  {
  printf("Closing file in offload region\n");
  fclose (f1);
  }
}
```