OpenMP (with Labs)

Steve Lantz

Senior Research Associate

Cornell University Center for Advanced Computing (CAC)

slantz@cac.cornell.edu

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What is OpenMP?

- OpenMP is an acronym for Open Multi-Processing
- An Application Programming Interface (API) for developing parallel programs in shared-memory architectures
- Three primary components of the API are:
  - Compiler Directives
  - Runtime Library Routines
  - Environment Variables
- De facto standard -- specified for C, C++, and FORTRAN
- http://www.openmp.org/ has the specification, examples, tutorials and documentation
- OpenMP 4.0 specified July 2013

OpenMP = Multithreading

- All about executing concurrent work (tasks)
  - Tasks execute as independent *threads*
  - Threads access the same *shared memory* (no message passing!)
  - Threads synchronize only at *barriers*
- Simplest way to do multithreading – run tasks on multiple cores/units
  - Insert OpenMP *parallel directives* to create tasks for concurrent threads
  - So, shared-memory parallel programming is super-easy with OpenMP?
  - Nope! Updates to a shared variable, e.g., need special treatment…

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

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

Role of the Compiler

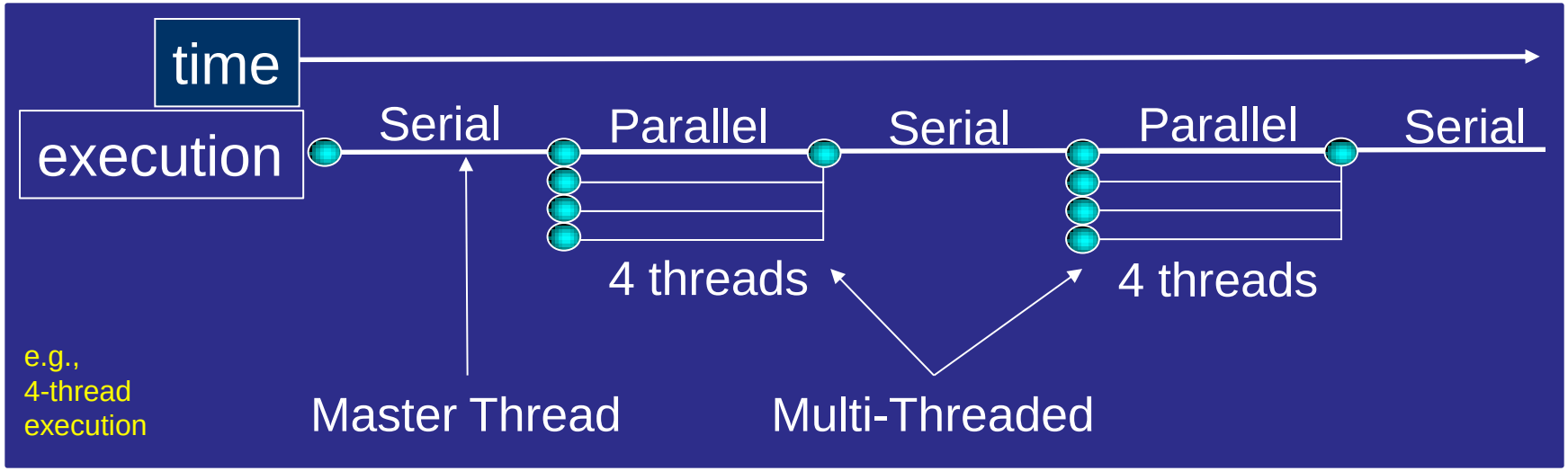
- OpenMP relies on the compiler to do the multithreading
  - Compiler recognizes OpenMP directives, builds in appropriate code
- A special flag is generally required to enable OpenMP
  - GNU: `gcc -fopenmp`
  - Intel: `icc -openmp`
- On Stampede, extra flags may be required for Intel Xeon Phi
  - May need to tell the Intel compiler to enable MIC instructions
  - Build OpenMP code native to MIC: `icc -openmp -mmic`
  - Offload marked sections to MIC: `icc -openmp`
  - Must do multithreading to make full use of the Phi!

Stampede OpenMP Use Cases

- **Two distinct pools of shared memory** exist on a Stampede node:
  - 32 GB for the Intel Xeon E5 host processors
  - 8 GB for the Intel Xeon Phi (MIC) coprocessor
- Thus, many possibilities exist for single-node OpenMP applications:
  - **Host only**: compile for E5, run threads on E5 cores
  - **MIC only**: compile natively for Phi, run threads on Phi cores
  - **Offload**: compile so code runs on E5 but offloaded sections run on Phi
- More possibilities exist for multi-node MPI/OpenMP *hybrid* codes:
  - **Symmetric**: compile separately for E5 and Phi, launch MPI tasks on both, spawn local OpenMP threads for all tasks
  - **Offload**: compile for E5, launch all MPI tasks on E5, offload some OpenMP sections to Phi

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

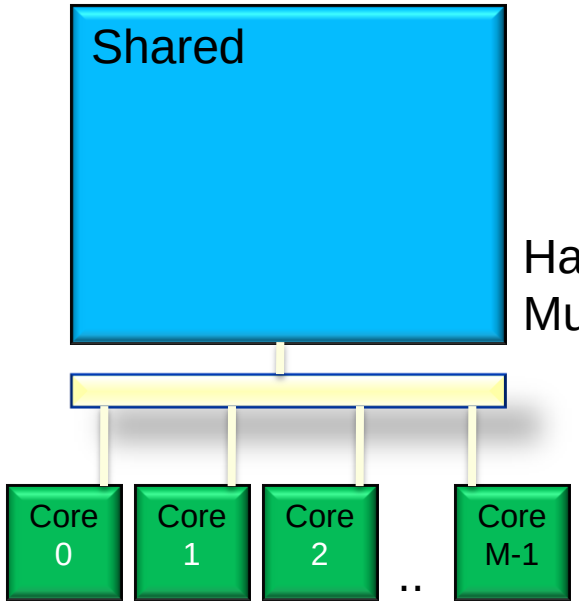
Parallel Region: C/C++ and Fortran

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

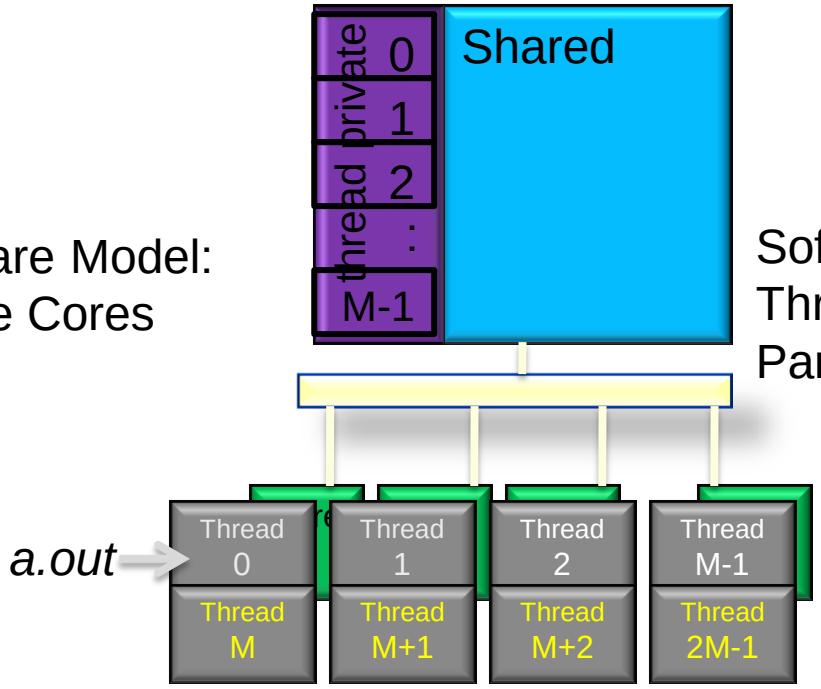
```
!$omp parallel
  code block
  call work(...)
!$omp end parallel
```

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)

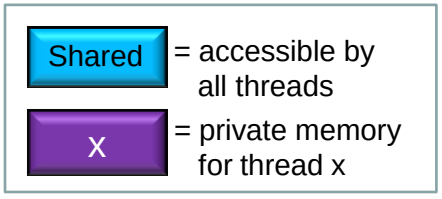
OpenMP on Shared Memory Systems



Hardware Model:
Multiple Cores



Software Model:
Threads in
Parallel Region



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.

OpenMP Directives

- OpenMP directives are comments in source code that specify parallelism for shared-memory parallel (SMP) machines
- FORTRAN compiler directives begin with one of the sentinels `!$OMP`, `C$OMP`, or `*$OMP` – use `!$OMP` for free-format F90
- C/C++ compiler directives begin with the sentinel `#pragma omp`

Fortran 90

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

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

C/C++

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

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

OpenMP 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"

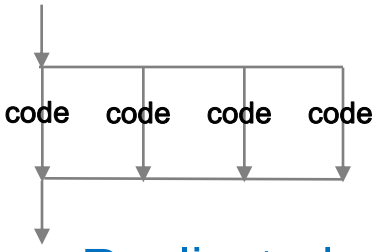
parallel control	work-sharing	control of one task	data access	synchron-ization	runtime environment

• 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 Directives

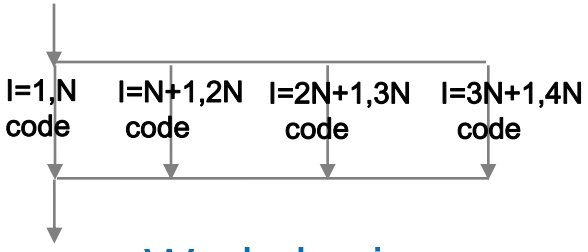
- Replicated – executed by all threads
- Worksharing – divided among threads

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



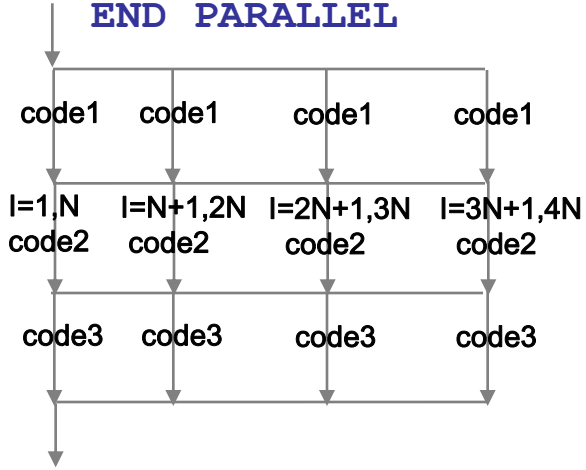
Replicated

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



Worksharing

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



Combined

OpenMP Worksharing

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

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

Code block	*Thread action*
`for`	Worksharing
`sections`	Worksharing
`single`	One thread
`master`	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

- 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
```

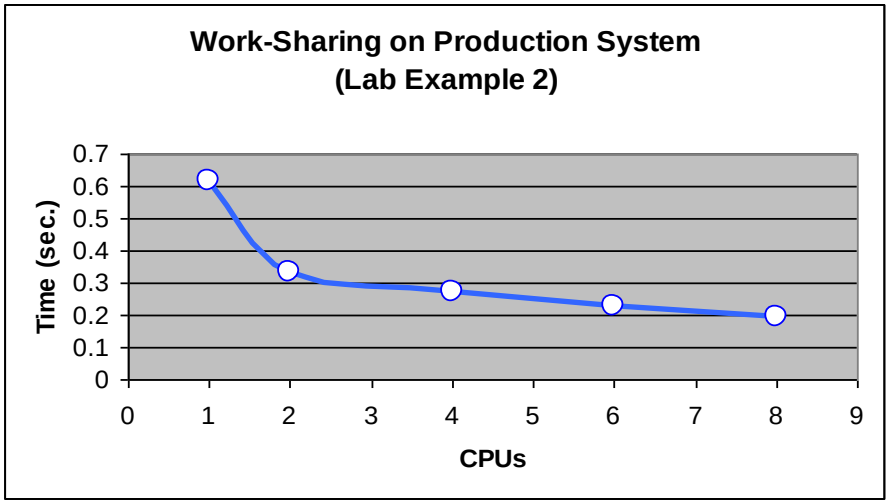
  - A “lastprivate(temp)” clause will copy the last loop (stack) value of temp to the (global) temp storage when the parallel DO is complete
  - A “firstprivate(temp)” initializes each thread’s temp to the global value

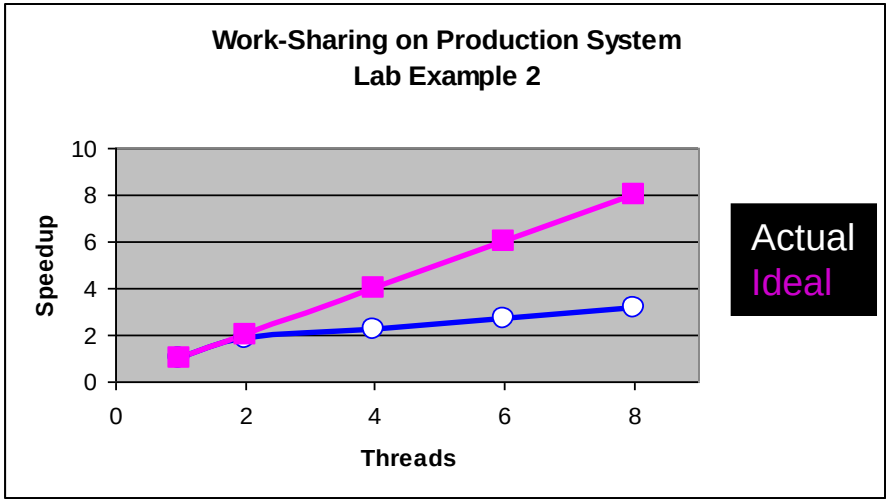
Worksharing Results

Speedup =
cputime(1) / cputime(N)

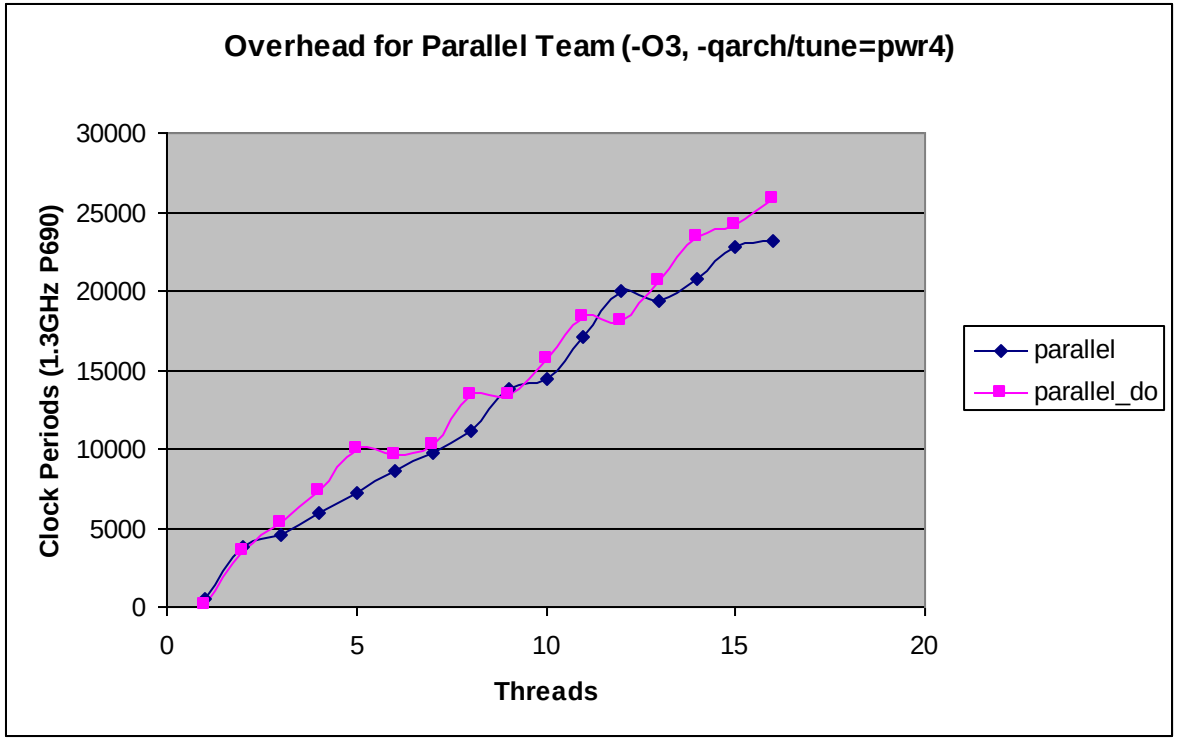
If work is completely parallel, scaling is linear.

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





Overhead to Fork a Thread Team



- Increases roughly linearly with number of threads

Merging Parallel Regions

The !$OMP PARALLEL directive declares an entire region as parallel; therefore, merging work-sharing constructs into a single parallel region eliminates the overhead of separate team formations

```
!$OMP PARALLEL DO
      do i=1,n
         a(i)=b(i)+c(i)
      enddo
!$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
```

Thread Memory Access: Race Conditions

- Every thread accesses “global” or shared memory
  - All threads share the same address space except for private variables
  - Thus, threads have no need to pass messages like MPI processes…
- But race conditions can occur with shared memory. Examples:
  - The last writer “wins”, if no order is imposed on multiple writers
  - The reader who “loses” to a writer will acquire the newly-updated value
- A race condition leads to unpredictable results!
  - Avoid introducing one; usually it’s a bug which is hard to debug
- What do you do to prevent a race condition? Synchronize!
  - 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)

Illustration of a Race Condition

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 Reduction

- Recall previous example of parallel dot product
  - Simple parallel-for doesn't work due to race condition on shared **sum**
  - Best solution is to apply OpenMP's reduction clause
  - Doing private partial sums is fine too; add a critical section for **sum** of **ps**

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

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

```
// repetitive updates: OK
#pragma omp parallel \
     firstprivate(ps)
{
#pragma omp for
  for (i=0; i<N; i++)
     ps = ps + b[i]*c[i];
#pragma omp critical
  sum = sum + ps; }
```

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 are executing
`omp_set_num_threads(#)`	Changes number of threads for parallel region, if dynamic threading is enabled

Environment Variables, More Functions

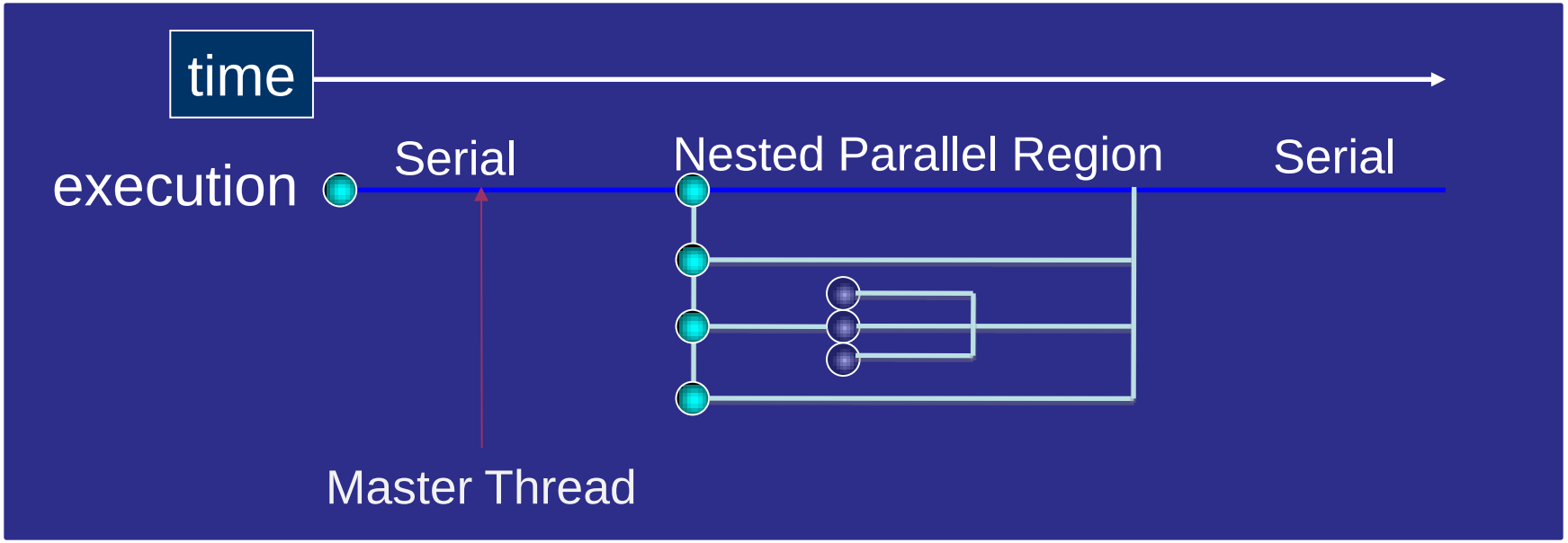
- To control the OpenMP runtime environment

`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

Loop Nesting in 3.0



- 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.

Additional Topics to Explore…

- 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)`

Some Programming Models for Intel MIC

- Intel Threading Building Blocks (TBB)
  - For C++ programmers
- Intel Cilk Plus
  - Task-oriented add-ons for OpenMP
  - Currently for C++ programmers, may become available for Fortran
- Intel Math Kernel Library (MKL)
  - Automatic offloading by compiler for some MKL features
  - MKL is inherently parallelized with OpenMP
- **OpenMP**
  - On Stampede, TACC expects that this is the most interesting programming model for HPC users

MIC Programming with OpenMP

- Compile with the Intel compiler (icc)
- 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 from disk
  - Also very helpful when debugging (print statements)
- Specific subroutines can be offloaded, including MKL subroutines

Example 1

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

Data handling is done <u>automatically</u> 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), &          ! Parallel -
  private(x, i, j), schedule(dynamic)     ! region
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; }}
```

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);
  }
}
```

LAB: Hand-Coding vs. MKL

Example 3

Two routines, MKL's **sgemm** and **my_sgemm**

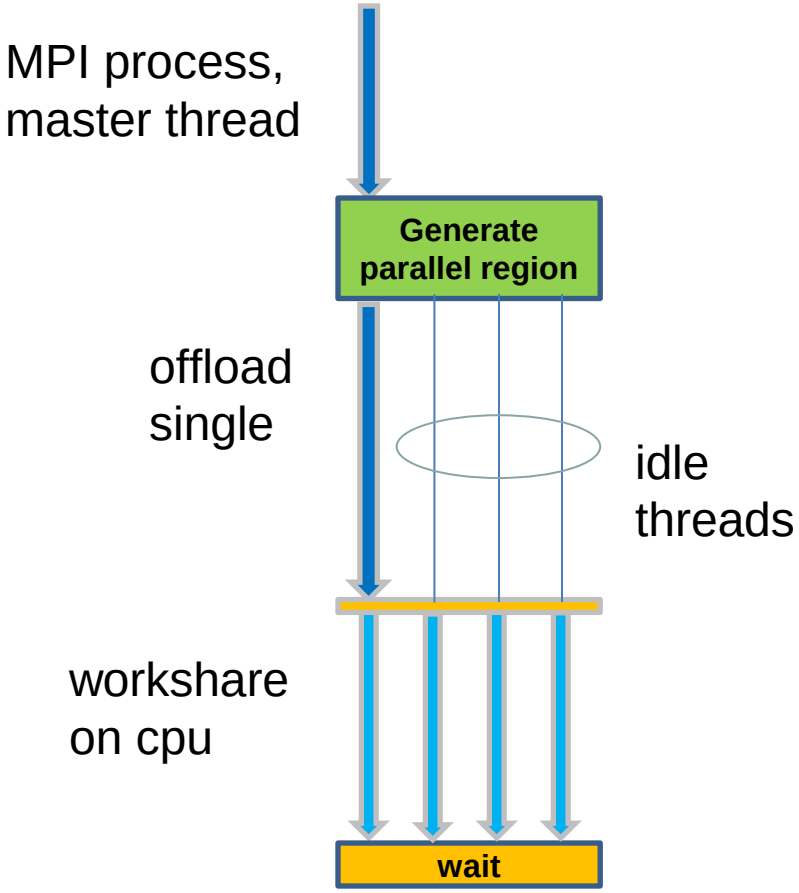
- Both are called with **offload** directive
- **my_sgemm** specifies explicit **in** and **out** data movement

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

```
! snippet from the caller...
! offload MKL routine to accelerator
!dir$ attributes offload:mic :: sgemm
!dir$ offload target(mic)
Call sgemm('N','N',n,n,n,alpha,a,n,b,n,beta,c,n)
! 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++

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

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

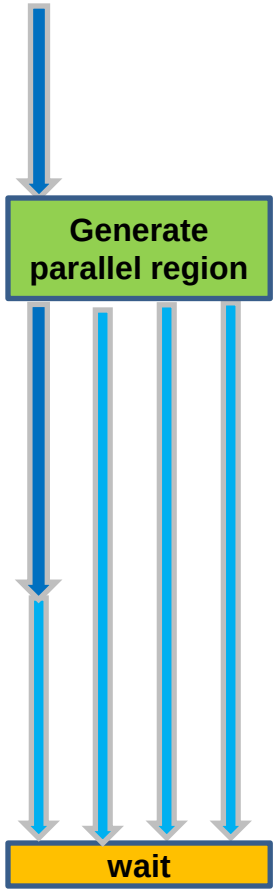
F90

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

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

Heterogeneous Threading, Concurrent

MPI process, master thread



offload single **nowait**

workshare on cpu

assist when done in single

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
```