Introduction to Programming with OpenMP

Kent Milfeld; Lars Koesterke

Yaakoub El Khamra (presenting)

milfeld | lars | yye00@tacc.utexas.edu

October 2012, TACC



Outline

- What is OpenMP?
- How does OpenMP work?
 - Architecture
 - Fork-Join model of parallelism
 - Communication
- OpenMP Syntax
 - Compiler Directives
 - Runtime Library Routines
 - Environment variables
- What's new? OpenMP 3.1

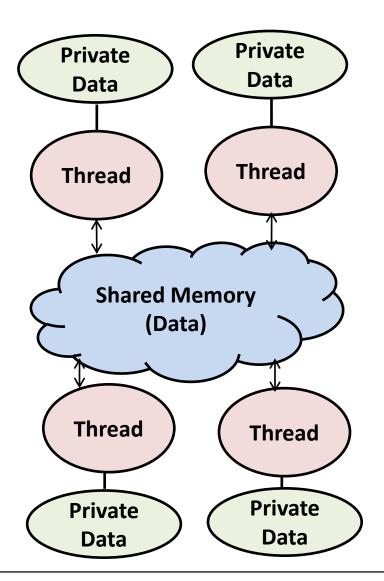


What is OpenMP?

- OpenMP stands for Open Multi-Processing
- An Application Programming Interface (API) for developing parallel programs for shared memory architectures
- Three primary components of the API are:
 - Compiler Directives
 - Runtime Library Routines
 - Environment Variables
- Standard specifies C, C++, and FORTRAN Directives & API
- http://www.openmp.org/ has the specification, examples, tutorials and documentation



Architecture

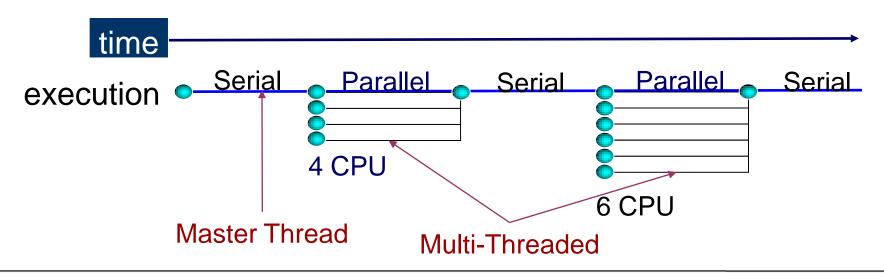


- Data: shared or private
- Shared data: all threads can access data in shared memory
- Private data: can only be accessed by threads that own it
- Data transfer is transparent to the programmer



OpenMP Fork-Join Parallelism

- Programs begin as a single process: master thread
- Master thread executes in serial mode until the parallel region construct is encountered
- Master thread creates a team of parallel threads (fork) that simultaneously execute statements in the parallel region
- After executing the statements in the parallel region, team threads synchronize and terminate (join) but master continues





How Do Threads Communicate?

- Every thread has access to "global" memory (shared)
- All threads share the same address space
- Threads communicate by reading/writing to the global memory
- Simultaneous updates to shared memory can create a race condition. Results change with different thread scheduling
- Use mutual exclusion to avoid data sharing but don't use too many because this will serialize performance



OpenMP Syntax

Most of the constructs in OpenMP are compiler directives

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

Example

```
#pragma omp parallel num_threads(4) C
```

!\$omp parallel num_threads(4) F90

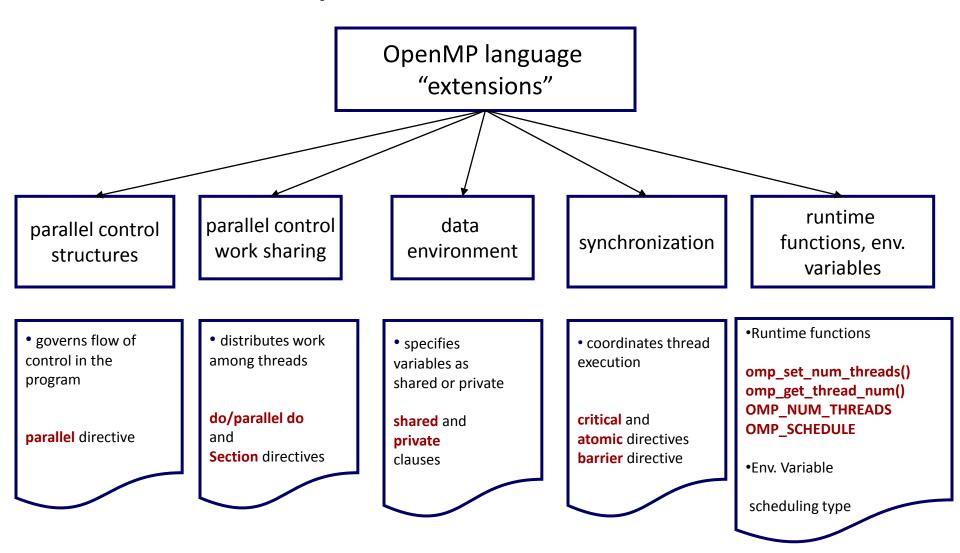
Function prototypes and types are in the file:

```
#include <omp.h> C
use omp_lib 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 Directives

 OpenMP directives are comments in source code that specify parallelism for shared memory machines

FORTRAN: directives begin with the !\$OMP, C\$OMP or *\$OMP sentinel.

F90 : **!\$OMP** free-format

C/C++ : directives begin with the **# pragma omp** sentinel

- Parallel regions are marked by enclosing parallel directives
- Work-sharing loops are marked by parallel do/for

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

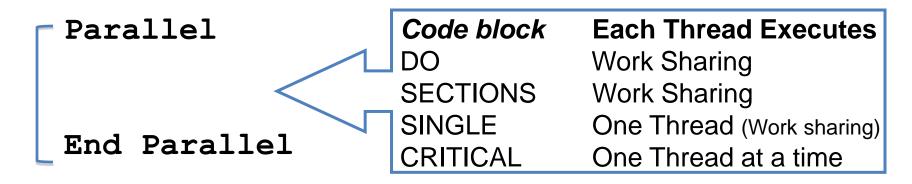
```
C/C++
# pragma omp parallel
{....}

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



Parallel Region & Work-Sharing

Use OpenMP directives to specify Parallel Region & Work-Sharing constructs



Parallel DO/for Parallel SECTIONS

Work-Sharing Parallel Region



Parallel Regions

Use the thread number to divide work among threads



Parallel Regions

- Line 1 Team of threads formed at parallel region.
- Lines 2-3 Each thread executes code block and subroutine calls. No branching (in or out) in a parallel region.
- Line 4 All threads synchronize at end of parallel region (implied barrier).

Use the thread number to divide work among.



Parallel Region & Number of Threads

For example, to create a 10-thread Parallel region:

```
double A[1000];
omp_set_num_threads(10);
#pragma omp parallel
{
  int ID = omp_get_thread_num();
  foo(ID, A);
}
```

But we need to make ID private to the thread-later...

- Each thread redundantly executes the code within the structured block
- Each thread calls foo(ID,A) for ID = 0 to 9



Parallel Regions & Modes

There are two OpenMP "modes"

- *static* mode
 - Fixed number of threads -- set in the OMP_NUM_THREADS env.
 Or the threads may be set by a function call (or clause) inside the code:
 - omp_set_num_threads runtime function
 num threads(#) clause
- **dynamic** mode:
 - Number of threads can change under OS control from one parallel region to another using:

Note: the user can only define the maximum number of threads, compiler can use a smaller number



Work sharing: Loop

- Line 1 Team of threads formed (parallel region).
- Line 2-4 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.



Work-Sharing: Loop

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

- Line 1 Team of threads formed (parallel region).
- Line 2-5 Loop iterations are split among threads. implied barrier at enddo

Each loop iteration must be independent of other iterations.



Work-Sharing: Sections

```
#pragma omp sections
{
    #pragma omp section
    {
        work_1();
    }
    #pragma omp section
    {
        work_2();
}
```

- Line 1 Team of threads formed (parallel region).
- Line 3-8 One thread is working on each section.
- Line 9 End of parallel sections with an implied barrier.

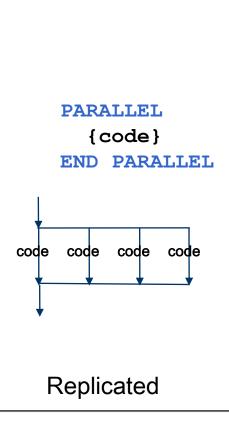
Scales only to the number of sections.

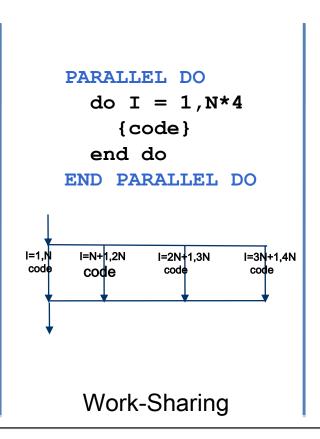


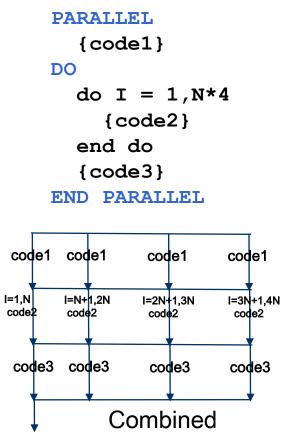
OpenMP Parallel Constructs

Replicated: Work blocks are executed by all threads.

Work-Sharing: Work is divided among threads.









OpenMP Clauses

Clauses control the behavior of an OpenMP directive:

- Data scoping (Private, Shared, Default)
- 2. Schedule (Guided, Static, Dynamic, etc.)
- Initialization (e.g. COPYIN, FIRSTPRIVATE)
- 4. Whether to parallelize a region or not (if-clause)
- Number of threads used (NUM_THREADS)



Schedule Clause

schedule(static)

Each CPU receives one set of contiguous iterations

schedule(static, C)

Iterations are divided round-robin fashion in chunks of size C

schedule(dynamic, C)

Iterations handed out in chunks of size C as CPUs become available

schedule(guided, C)

Each of the iterations are handed out in pieces of exponentially decreasing size, with C minimum number of iterations to dispatch each time

schedule (runtime)

Schedule and chunk size taken from the OMP_SCHEDULE environment variable



Comparison of Scheduling Options

name	type	chunk	chunk size	chunk#	static or dynamic	compute overhead
simple static	simple	no	N/P	Р	static	lowest
interleaved	simple	yes	С	N/C	static	low
simple dynamic	dynamic	optional	С	N/C	dynamic	medium
guided	guided	optional	decreasing from N/P	fewer than N/C	dynamic	high
runtime	runtime	no	varies	varies	varies	varies



Example - schedule(static, 16), threads = 4

```
thread0:
           do i=1,16
                                      thread2: do i=33,48
             A(i) = B(i) + C(i)
                                                   A(i) = B(i) + C(i)
           enddo
                                                 enddo
           do i=65,80
                                                 do i = 97,112
             A(i) = B(i) + C(i)
                                                   A(i) = B(i) + C(i)
           enddo
                                                 enddo
thread1:
           do i=17,32
                                      thread3: do i=49,64
             A(i) = B(i) + C(i)
                                                    A(i) = B(i) + C(i)
           enddo
                                                 enddo
           do i = 81,96
                                                 do i = 113,128
             A(i) = B(i) + C(i)
                                                   A(i) = B(i) + C(i)
           enddo
                                                 enddo
```



OpenMP Data Environment

- Data scoping clauses control the sharing behavior of variables within a parallel construct.
- These include shared, private, firstprivate,
 lastprivate, reduction clauses

Default variable scope:

- 1. Variables are shared by default
- 2. Global variables are shared by default
- Automatic variables within subroutines called from within a parallel region are private (reside on a stack private to each thread), unless scoped otherwise
- 4. Default scoping rule can be changed with **default** clause



Private & Shared Data

```
shared - Variable is shared (seen) by all processorsprivate - Each thread has a private instance (copy) of the variableDefaults: The for-loop index is private, all other variables are shared
```

All threads have access to the same storage areas for a, b, c, and n, but each loop has its own private copy of the loop index, i



Private Data Example

- In the following loop, each thread needs its own private copy of temp
- If temp were shared, the result would be unpredictable since each thread would be writing and reading to/from the same memory location

- 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) would copy the global temp value to each stack's temp.



Reduction

- Operation that combines multiple elements to form a single result
- A variable that accumulates the result is called a reduction variable
- In parallel loops reduction operators and variables must be declared

```
float asum, aprod;
asum = 0.;
aprod = 1.;
#pragma omp parallel for reduction(+:asum) reduction(*:aprod)
for (i=0; i<n; i++) {
   asum = asum + a[i];
   aprod = aprod * a[i];
}</pre>
```

Each thread has a private asum and aprod, initialized to the operator's identity

 After the loop execution, the master thread collects the private values of each thread and finishes the (global) reduction



Synchronization

- Synchronization is used to impose order constraints and to protect access to shared data
- High-Level Synchronization
 - critical
 - atomic
 - barrier
 - ordered
- Low-Level Synchronization
 - locks



Synchronization: Critical/Atomic Directives

- When each thread must execute a section of code serially the region must be marked with critical/end critical directives
- Use the #pragma omp atomic directive if executing only one operation serially

```
#pragma omp parallel shared(sum,x,y)
                                                 #pragma omp parallel shared(sum)
        #pragma omp critical
                                                 #pragma omp atomic
             update(x);
                                                       sum=sum+1;
             update(y);
             sum=sum+1;
              END PARALLEL
                                                                             time
Master Thread
                                 CRITICAL section or atomic operations
```



Synchronization: Barrier

Barrier: Each thread waits until all threads arrive

```
#pragma omp parallel shared (A, B, C) private(id)
   id=omp get thread num();
  A[id] = big calc1(id);
   #pragma omp barrier
   #pragma omp for
   for(i=0;i<N;i++){
         C[i]=big calc3(i,A);
   } < ____ Implicit barrier
   #pragma omp for nowait
   for(i=0;i<N;i++){
           B[i]=big calc2(C, i);
                                No implicit barrier due to nowait
  A[id] = big_calc4(id);
} ←
                              Implicit barrier
```



Mutual Exclusion: Lock Routines

When each thread must execute a section of code serially locks provide a more flexible way of ensuring serial access than **CRITICAL** and **ATOMIC** directives

```
call OMP_INIT_LOCK(maxlock)
!$OMP PARALLEL SHARED(X,Y)
...
call OMP_set_lock(maxlock)
call update(x)
call OMP_unset_lock(maxlock)
...
!$OMP END PARALLEL
call OMP_DESTROY_LOCK(maxlock)
```



Synchronization: Ordered

The ordered region executes in the sequential order

```
#pragma omp parallel private (tmp)
#pragma omp for ordered reduction(+:countVal)
for (i=0;i<N;i++) {
  tmp = foo(i);
  #pragma omp ordered
  countVal+= consume(tmp);
}</pre>
```



Mutual Exclusion Overhead

OMP exclusion directive	cycles
OMP_SET_LOCK	330
OMP_UNSET_LOCK	330
OMP_ATOMIC	480
OMP_CRITICAL	510

All measurements made in dedicated mode



NOWAIT

- When a work-sharing region is exited, a barrier is implied - all threads must reach the barrier before any can proceed.
- By using the NOWAIT clause at the end of each loop inside the parallel region, an unnecessary synchronization of threads can be avoided.

```
#pragma omp parallel
#pragma omp for nowait
         for (i=0; i<n; i++)
           {work(i);}
#pragma omp for schedule(dynamic,k)
         for (i=0; i<m; i++)
           {x[i]=y[i]+z[i];}
```



Runtime Library Routines

function	description
omp_get_num_threads()	Number of threads in team, N
omp_get_thread_num()	Thread ID {0 -> N-1}
omp_get_num_procs()	Number of machine CPUs
omp_in_parallel()	True if in parallel region & multiple thread executing
omp_set_num_threads(#)	Set the number of threads in the team
omp_get_dynamic()	True if dynamic threading is on
omp_set_dynamic()	Set state of dynamic threading (true/false)



Environment Variables

variable	description
OMP_NUM_THREADS int_literal	Set to default no. of threads to use
OMP_SCHEDULE "schedule[, chunk_size]"	Control how "omp for schedule(RUNTIME)" loop iterations are scheduled
OMP_DYNAMIC	TRUE/FALSE for enable/disable dynamic threading



OpenMP Wallclock Timers

```
real*8 :: omp_get_wtime, omp_get_wtick() (Fortran)
double omp_get_wtime(), omp_get_wtick(); (C)
```

```
double t0, t1, dt, res;
...
t0 = omp_get_wtime();
<work>
t1 = omp_get_wtime();
dt = t1 - t0;
res = 1.0/omp_get_wtick();
printf("Elapsed time = %lf\n",dt);
printf("clock resolution = %lf\n",res);
```



NUM_THREADS clause

 Use the NUM_THREADS clause to specify the number of threads to execute a parallel region

where scalar integer expression must evaluate to a positive integer

 NUM_THREADS supersedes the number of threads specified by the OMP_NUM_THREADS environment variable or that set by the OMP_SET_NUM_THREADS function



OpenMP 3.0

- First update to the spec since 2005
- Tasking: move beyond loops with generalized tasks and support complex and dynamic control flows
- Loop collapse: combine nested loops automatically to expose more concurrency
- Enhanced loop schedules: Support aggressive compiler optimizations of loop schedules and give programmers better runtime control over the kind of schedule used
- Nested parallelism support: better definition of and control over nested parallel regions, and new API routines to determine nesting structure



Tasks Parallelism

- Allows to parallelize irregular problems
 - Recursive loops
 - Unbounded algorithms
 - Threads can jump between tasks



What is a Task?

- A specific instance of executable code and its data environment, generated when a thread encounters a task construct or a parallel construct
- Tasks consist of
 - Code to execute
 - Data environment
 - Internal control variables (new from 2.5)
- Each encountering thread creates a new task which packages its own code and data
- Execution of the new task could be immediate, or deferred until later
- Can be nested into
 - Another task or a work sharing construct



What is a Task?

- Tasks have been fully integrated into OpenMP
- Note: OpenMP has always had tasks but they were never called that way before the 3.0 release!
 - Thread encountering parallel construct packages up a set of implicit tasks, one per thread
 - Team of threads is created
 - Each thread in team is assigned to one of the tasks (and tied to it)
 - Barrier holds original master thread until all implicit tasks are finished
- Now we have a way to create a task explicitly for the team to execute



Tasks: Usage

Task Construct:

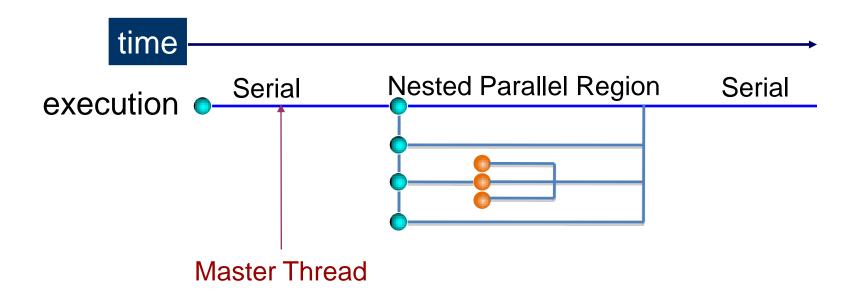
```
#pragma omp task [clause[[,]clause] ...]
structured-block
```

where clause can be

- Data scoping clauses
 - shared (list), private (list), firstprivate (list), default(shared | none)
- Scheduling clauses
 - untied
- Other clauses
 - if (expression)



Loop Nesting



While OpenMP 3.0 supports nested parallelism, many implementations may ignore the nesting by serializing the inner parallel regions



References

- http://www.openmp.org/
- Parallel Programming in OpenMP, by Chandra, Dagum, Kohr, Maydan, McDonald, Menon
- Using OpenMP, by Chapman, Jost, Van der Pas (OpenMP2.5)
- http://www.nic.uoregon.edu/iwomp2005/iwomp2005_tutorial_openmp_rvdp.pdf
- http://webct.ncsa.uiuc.edu:8900/public/OPENMP/



FOR FORTRAN USERS



Work sharing: Sections

```
!$OMP PARALLEL SECTIONS
!$OMP SECTION

call work_1()
!$OMP SECTION

call work_2()
!$OMP END SECTIONS
```

- Line 1 Team of threads formed (parallel region).
- Line 2-5 One thread is working on each section.
- Line 6 End of parallel sections with an implied barrier.

Scales only to the number of sections.



PRIVATE and SHARED Data

SHARED - Variable is shared (seen) by all processors.

PRIVATE - Each thread has a private instance (copy) of the variable.

Defaults: All DO LOOP indices are private, all other variables are shared.

```
!$OMP PARALLEL DO SHARED(A,B,C,N) PRIVATE(i)
do i=1,N
     A(i) = B(i) + C(i)
enddo
!$OMP END PARALLEL DO
```

All threads have access to the same storage areas for A, B, C, and N, but each loop has its own private copy of the loop index, i.



PRIVATE data example

- In the following loop, each thread needs its own PRIVATE copy of TEMP.
- If TEMP were shared, the result would be unpredictable since each processor would be writing and reading to/from the same memory location.

- 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) would copy the global temp value to each stack's temp.



Default variable scoping (Fortran example)

```
Program Main
Integer, Parameter :: nmax=100
Integer :: n, j
Real*8 :: x(n,n)
Common /vars/ y(nmax)
n=nmax; y=0.0
!$OMP Parallel do
   do j=1,n
   call Adder(x,n,j)
   end do
End Program Main
```

```
Subroutine Adder(a,m,col)
Common /vars/ y(nmax)
SAVE array sum
Integer :: i, m
Real*8 :: a(m,m)
do i=1, m
   y(col) = y(col) + a(i, col)
end do
array sum=array sum+y(col)
End Subroutine Adder
```



Default data scoping in Fortran (cont.)

Variable	Scope	Is use safe?	Reason for scope
n	shared	yes	declared outside parallel construct
j	private	yes	parallel loop index variable
X	shared	yes	declared outside parallel construct
У	shared	yes	common block
i	private	yes	parallel loop index variable
m	shared	yes	actual variable <i>n</i> is shared
а	shared	yes	actual variable x is shared
col	private	yes	actual variable <i>j</i> is private
array_sum	shared	no	declared with SAVE attribute



REDUCTION

- Operation that combines multiple elements to form a single result, such as a summation.
- A variable that accumulates the result is called a reduction variable.
- In parallel loops reduction operators and variables must be declared.

```
real*8 asum, aprod
    asum = 0.
    aprod = 1.
!$OMP PARALLEL DO REDUCTION(+:asum) REDUCTION(*:aprod)
    do i=1,N
        asum = asum + a(i)
        aprod = aprod * a(i)
    enddo
!$OMP END PARALLEL DO
    print*, asum, aprod
```

- Each thread has a private **ASUM** and **APROD**, initialized to the operator's identity, 0 & 1, respectively.
- After the loop execution, the master thread collects the private values of each thread and finishes the (global) reduction.



NOWAIT

- When a work-sharing region is exited, a barrier is implied - all threads must reach the barrier before any can proceed.
- By using the NOWAIT clause at the end of each loop inside the parallel region, an unnecessary synchronization of threads can be avoided.

```
!$OMP PARALLEL
!$OMP DO
      do i=1,n
         work(i)
      enddo
!$OMP END DO NOWAIT
!$OMP DO schedule(dynamic,k)
      do i=1,m
         x(i)=y(i)+z(i)
      enddo
!$OMP
     END DO
!$OMP END PARALLEL
```

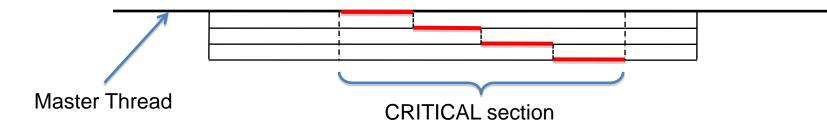


Mutual exclusion: critical/atomic directives

- When each thread must execute a section of code serially the region must be marked with CRITICAL / END
 CRITICAL directives.
- Use the !\$OMP ATOMIC directive if executing only one operation serially.

```
!$OMP PARALLEL SHARED(sum,X,Y)
...
!$OMP CRITICAL
    call update(x)
    call update(y)
    sum=sum+1
!$OMP END CRITICAL
...
!$OMP END PARALLEL
```

```
!$OMP PARALLEL SHARED(X,Y)
...
!$OMP ATOMIC
sum=sum+1
...
!$OMP END PARALLEL
```





Workshare directive

 WORKSHARE directive enables parallelization of Fortran 90 array expressions and FORALL constructs

- Enclosed code is separated into units of work
- All threads in a team share the work
- Each work unit is executed only once
- A work unit may be assigned to any thread



Reduction on array variables

- Supported in Fortran only!
- Array variables may now appear in the REDUCTION clause

- Assumed size and allocatable arrays are not supported
- Variable must be shared in the enclosing context



NUM_THREADS clause

Use the NUM_THREADS clause to specify the number of threads to execute a
parallel region

where **scalar integer expression** must evaluate to a positive integer

NUM_THREADS supersedes the number of threads specified by the
 OMP_NUM_THREADS environment variable or that set by the
 OMP_SET_NUM_THREADS function



Loop Collapse

Allow collapsing of perfectly nested loops

Will form a single loop and then parallelize it:

```
!$omp parallel do collapse(2)
do i=1,n
    do j=1,n
    ....
    end do
end do
```

