Practical stuff!

Ways of actually get stuff done in HPC:

- ➤ Message Passing (send, receive, broadcast, ...) ✓ MPI
- Shared memory (load, store, lock, unlock) -
- Directive-based (compiler needs help)
- > Task farming (scientific term for large transaction processing)

MapReduce/Hadoop etc

Usual confessions!

A lot of blatant plagiarism of BLAINE BARNEY's tutorial at LLNL!

https://computing.llnl.gov/tutorials/openMP

Other really good sources added to the webpage:

Parallel Programming in Fortran 95 using OpenMP, Miguel Hermanns, Universidad Politecnica de Madrid

Advanced OpenMP Topics, NAS seminar, NASA

OpenMP by Example, TACC training

etc

OpenMP - History

- Another specification: openmp.org
- "Open specifications for Multi-Processing via collaborative work between interested parties from the hardware and software industries, government and academia"
- Implementation of the shared memory programming model
- Is an Application Program Interface (API) that may be used to explicitly direct multi-threaded shared memory parallelism
- API = 3 parts:
 - Compiler directives
 - Runtime library routines
 - Environment variables

• Evolution:

- Early 90's, vendors made directive-driven Fortran extensions for shared mem machines
- 1994: standard ANSI X3H5 never adopted as distributed machines emerged
- Newer shared mem machines came along
- 1997: OpenMP standard took up where ANSI left off: OpenMP Architecture Review Board (ARB):
 Compaq, HP, Intel. IBM, Silicon Graphics, Sun, Fujitsu, DoE-ASCI, ...
- API specs separate releases for C and Fortran until combined in 2005
- Latest: OpenMP 5.0 Nov 2018

OpenMP - History

• OpenMP is **NOT**:

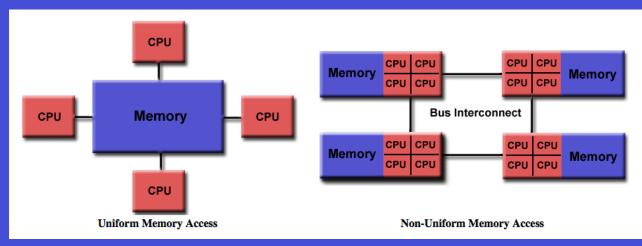
- Meant for distributed memory parallel systems (by itself)
- Implemented identically by all vendors
- Guaranteed to make most efficient use of shared memory
- Required to check for data dependencies, deadlocks etc (programmer!)

• OpenMP is:

- A standardization built and endorsed by many
- "lean and mean" and simple (although trend away with later versions ☺)
- portable
- C/C++, Fortran
- ⊗ OpenMP requires a compiler that supports OpenMP
- (a) Amdahl's law! Lot of the code is still sequential
- © Easy to build up code incrementally by adding directives
- Directives are like comments so sequential code still runs
- Code is lightweight
- © Data decomposition is largely invisible/automatic

Designed for multi-processor/core shared memory architectures, UMA or

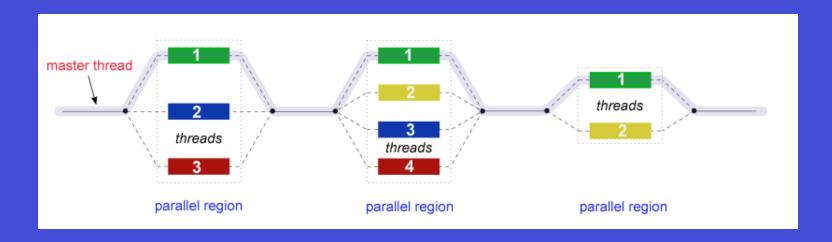
NUMA



- Parallelism by use of THREADS
- Threads are smallest units of processing
- Many threads share resources of a single process
- Typically, number of threads matches number of cores, but not necessarily (can overlap some work with virtual threads)

Programming model:

- Explicit not automatic (despite compiler-based; not Holy Grail!) => programmer has complete control over parallelism
- Easy: take sequential program and insert compiler directives to parallellize
- Complex: insert subroutines to set multiple levels of parallelism with locks etc
- Fork-join model:
 - Start as single process = master thread
 - Fork: master thread creates team of parallel threads
 - Join: when team threads complete parallel work, synchronize and terminate
 - Control returns to master thread



Programming model (cont)

Notice:

- Parallelism is achieved by marking sequential codes with embedded compiler directives
- Nested parallelism is allowed
- Threads are dynamically created and destroyed
- I/O is up to the programmer!
- Cache level coherency in threads needs to be ensured by the programmer (FLUSH often ©)

Programming model:

- Compiler directives (44)
- Runtime Library routines (35)
- Environment variables (13)

• Compiler directives

- Comments in source code, interpreted by compiler if required
- Spawn parallel region

Of !\$OMP directive

[structured block of code]
!\$OMP end directive

Programming model:

- Compiler directives (44)
- Runtime Library routines (35)
- Environment variables (13)
- <u>Compiler directives</u>

Extending lines: Note that there is ANOTHER sentinel:

```
!$OMP PAPALLEL DEFAULT(private) SHARED(vars..., &
!$OMP& more_vars..., &
!$OMP& more_vars... &
!$OMP& )
```

An OpenMP-compliant compiler interprets this as conditional text that should be included whereas a non-OpenMP-compliant compiler will interpret it as a comment.

Programming model:

- Compiler directives (44)
- Runtime Library routines (35)
- Environment variables (13)

• Runtime routines that you can call

- Setting and querying number of threads
- Querying thread identifiers
- Setting/querying nested parallelism
- etc etc

e.g.

Fortran	INTEGER FUNCTION OMP_GET_NUM_THREADS()
C/C++	<pre>#include <omp.h> int omp_get_num_threads(void)</omp.h></pre>

Programming model:

- Compiler directives (44)
- Runtime Library routines (35)
- Environment variables (13)

• Environment variables

- Set number of threads
- Specify how loop iterations are divided
- Binding threads to processors
- Enabling/disabling nested parallelism, dynamic threads

e.g.

csh/tcsh	setenv OMP_NUM_THREADS 8
sh/bash	export OMP_NUM_THREADS=8

OpenMP: Typical code

Fortran

```
PROGRAM HELLO
      INTEGER VAR1, VAR2, VAR3
       Serial code
       Beginning of parallel section. Fork a team of threads.
      Specify variable scoping
!$OMP PARALLEL PRIVATE(VAR1, VAR2) SHARED(VAR3)
      Parallel section executed by all threads
       Other OpenMP directives
      Run-time Library calls
      All threads join master thread and disband
ISOMP END PARALLEL
      Resume serial code
      END
```

C

```
#include <omp.h>
main () {
int var1, var2, var3;
Serial code
Beginning of parallel section. Fork a team of threads.
Specify variable scoping
#pragma omp parallel private(var1, var2) shared(var3)
  Parallel section executed by all threads
  Other OpenMP directives
  Run-time Library calls
  All threads join master thread and disband
Resume serial code
```

How to compile:

Compiler / Platform	Compiler	Flag	
Intel Linux Opteron/Xeon	icc icpc ifort	-openmp	
PGI Linux Opteron/Xeon	pgcc pgCC pgf77 pgf90	-mp	
GNU Linux Opteron/Xeon IBM Blue Gene	gcc g++ g77 gfortran	-fopenmp	
IBM Blue Gene	bgxlc_r, bgcc_r bgxlc_r, bgxlc++_r bgxlc89_r bgxlc99_r bgxlf_r bgxlf90_r bgxlf95_r bgxlf2003_r *Be sure to use a thread-safe compiler - its name ends with _r	-qsmp=omp	

· Compiler Documentation:

- o IBM BlueGene: www-01.ibm.com/software/awdtools/fortran/ and www-01.ibm.com/software/awdtools/xlcpp
- o Intel: www.intel.com/software/products/compilers/
- o PGI: www.pgroup.com
- o GNU: gnu.org
- o All: See the relevant man pages and any files that might relate in /usr/local/docs

OpenMP: Example – Hello World

Let's just do an example: Hello World!

```
Compiler
     PROGRAM HELLO
                                                                              directives
     implicit none
     INTEGER NTHREADS, TID, OMP_GET_NUM_THREADS, &
             OMP_GET_THREAD_NUM
     Fork a team of threads giving them their own copies of variables
!$OMP PARALLEL PRIVATE(NTHREADS, TID)
     Obtain thread number
     TID = OMP_GET_THREAD_NUM()
     PRINT *, 'Hello World from thread = '
                                                                               Parallel
     Only master thread does this
     IF (TID .EQ. 0) THEN
                                                                               region
       NTHREADS = OMR_GET_NUM_THREADS()
       PRINT *, 'Number of threads = ', NTHREAD
     END IF
     All threads join master thread and disband
!$OMP END PARALLEL
     END
                                                                           Library
                                                                          routine calls
                                          Notice master thread = 0
```

Example

Notice you needed a bunch of things:

```
gfortran -fopenmp <file.f90> -o file_exec
Setenv OMP_NUM_THREADS <nthreads>
```

Mencia, Muscat, Jerez (no qsub, interactive or Unix batch only):

```
./file_exec
```

Grape (qsub):

```
Qsub -q newest -I
./file_exec
```

OpenMP - Directives

Parallel region: A block of code that will execute on multiple threads

When a thread reaches a PARALLEL directive, thread creates team of threads and becomes master (0)

Implied barrier at END PARALLEL

If any thread terminates, all terminate

Region must be all in one routine/code file

Cannot branch (GOTO) out!

Number of threads set by

- IF (must be TRUE to create threads)
- NUM_THREADS clause
- library function OMP_NUM_THREADS
- env variable OMP_NUM_THREADS
- Default (no of procs on node)

```
!SOMP PARALLEL [clause ...]
                         IF (scalar logical expression)
                         PRIVATE (list)
                         SHARED (list)
                         DEFAULT (PRIVATE | FIRSTPRIVATE | SHARED |
                         FIRSTPRIVATE (list)
                         REDUCTION (operator: list)
Fortran
                         COPYIN (list)
                         NUM THREADS (scalar-integer-expression)
            block
          !$OMP END PARALLEL
         #pragma omp parallel [clause ...] newline
                               if (scalar expression)
                               private (list)
                               shared (list)
                               default (shared | none)
                               firstprivate (list)
C/C++
                               reduction (operator: list)
                               copyin (list)
                               num threads (integer-expression)
            structured block
```

Data scope attribute clauses like PRIVATE, SHARED dealt with later Implied synchronization at the end of the parallel region.

OpenMP - Directives

Work sharing constructs:

The main routines for telling the parallel region how to divide the work

DO – divides a DO loop amongst thread. Data parallelism

SECTIONS – divides work into discrete sections for each thread. Functional parallelism

SINGLE – forces region to execute on single thread. Sequential.

WORKSHARE – FORTRAN only! Specific types of Fortran work can be enclosed and forked

TASK – Task scheduling of code blocks

Go through these one by one ...

```
ISOMP DO Lala
                  SCHEDULE ( ype chunk])
                   ORDERED
                   PRIVATE (list)
                   FIRSTPRIVATE (list)
                   LASTPRIVATE (list)
                   SHARED (list)
Fortran
                   REDUCTION (operator | intrinsic : list)
                   COLLAPSE (n)
             do loop
          SOMP END DOO NOWAIT
         #pragma omp for [clause ...] newline
                          schedule (type [,chunk])
                          ordered
                          private (list)
                          firstprivate (list)
                          lastprivate (list)
C/C++
                          shared (list)
                          reduction (operator: list)
                          collapse (n)
                          nowait
            for loop
```

```
PROGRAM VEC ADD DO
      INTEGER N, CHUNKSIZE, CHUNK, I
      PARAMETER (N=1000)
      PARAMETER (CHUNKSIZE=100)
      REAL A(N), B(N), C(N)
      Some initializations
      DO I = 1, N
       A(I) = I * 1.0
        B(I) = A(I)
      ENDDO
      CHUNK = CHUNKSIZE
!$OMP PARALLEL SHARED(A,B,C,CHUNK) PRIVATE(I)
!$OMP DO SCHEDULE(DYNAMIC, CHUNK)
      DO I = 1, N
         C(I) = A(I) + B(I)
      ENDDO
!SOMP END DO NOWAIT
!SOMP END PARALLEL
      END
```

SCHEDULE:

Static – loop divided into pieces of size chunk (default: evenly) then statically assigned to threads

Dynamic – default chunk =1. Threads assigned dynamically i.e. start one chunk, and grab another when finished

Guided – dynamic but in blocks that decrease in size, since blocksize = n iter remaining/n threads

Runtime – schedule determined at runtime by env variable OMP SCHEDULE

AUTO – compiler decides!

NOWAIT: No implied barrier synch at end of loop (Note: be careful to FLUSH if re-use constructs from within loop etc)

Data dependency:

Simple test: Can serial loop be executed in reverse order with same result?

```
!$OMP DO
Do i=1,10
...
A(i)=A(i-1)
...
End Do
!$OMP END DO
```

```
!$OMP DO ORDERED
do i = 1, 1000
   !$OMP ORDERED
    A(i) = A(i-1)
   !$OMP END ORDERED
enddo
!$OMP END DO
```

BUT in this case, this serializes the code!

ORDERED construct only useful for ordering a nested segment really:

```
Read-after-write (RAW) data dependency
```

```
!$OMP DO ORDERED
do i = 1, 100
   block1

!$OMP ORDERED
   block2
!$OMP END ORDERED

block3
enddo
!$OMP END DO
```

Aside: Data dependencies

1. A=3

Read-After-Write (RAW, flow, true) dependency:

2. B=A

Instruction requires result from previous instruction

3. C=B

Instruction 3 truly depends on 2; 2 truly depends on 1; 3 truly depends on 1 No parallelism.

- 1. B=3
- Write-After-Read (WAR, anti-) dependency:
- 2. A=B+1

Instruction requires a result that is later updated

3. B=7

Instruction 3 anti-depends on 2

No parallelism; but can be fixed by renaming

- 1. B=3
- 2. B2=B
- 3. A=B2+1
- 4. B=7

WAR btw 3-4 removed

Now RAW btw 1-2-3

- 1. B=3
- Write-After-Write (WAW, output) dependency:
- 2. A=B+1
- Reording instruction changes final output of a variable
- 3. B=7
- WAW btw 1-3. Reordering changes final value of A

No parallelism; but can be fixed by renaming

- 1. B2=3
- 2. A=B2+1
- 3. B=7

Data dependency:

Simple test: Can serial loop be executed in reverse order with same result?

```
real(8) :: A(1000)

do i = 1, 999
   A(i) = A(i+1)
enddo
```

Write-after-read (WAR) data dependency

Solvable!

```
real(8) :: A(1000), dummy(2:1000:2)
!Saves the even indices
!$OMP DO
 do i = 2, 1000, 2
    dummy(i) = A(i)
  enddo
!$OMP END DO
!Updates even indices from odds
!$OMP DO
  do i = 0, 998, 2
    A(i) = A(i+1)
  enddo
!$OMP END DO
!Updates odd indices with evens
!$OMP DO
  do i = 1, 999, 2
    A(i) = dummy(i+1)
  enddo
!$OMP END DO
```

Which is better?

A

```
Do i=1,100
    Do j = 1,100
!$OMP DO

    Do k = 1,100
        A(i,j,k)=i*j*k
        End Do

!$OMP END DO

End Do

End Do
```

B

```
!$OMP DO
Do i=1,100
Do j = 1,100
Do k = 1,100
A(i,j,k)=i*j*k
End Do
End Do
End Do
!$OMP END DO
```

B.

- (i) Work per thread is a LOT more
- (ii) Less creation/destruction of threads => minimizes overhead too

Can do even better?

```
Do i=1,10
  Do j = 1,10
!$OMP DO
        Do k = 1,10
        A(i,j,k)=i*j*k
        End Do
!$OMP END DO
        End Do
End Do
```

```
!$OMP DO
Do i=1,10
    Do j = 1,10
        Do k = 1,10
        A(i,j,k)=i*j*k
        End Do
        End Do
End Do
!$OMP END DO
```

```
!$OMP DO
Do k=1,10
    Do j = 1,10
        Do i = 1,10
        A(i,j,k)=i*j*k
        End Do
    End Do
End Do
!$OMP END DO
```

Fortran arrays are stored in column-major format

i.e. columns (first dimension – rows - changing) are contiguous in memory

Better cache performance

DO THIS ALWAYS FOR FORTRAN!

OpenMP – Directives: SECTIONS

```
!$OMP SECTIONS [clause ...]
                        PRIVATE (list)
                        FIRSTPRIVATE (list)
                        LASTPRIVATE (list)
                        REDUCTION (operator | intrinsic : list)
         !SOMP SECTION
Fortran
            block
         !SOMP SECTION
             block
         !$OMP END SECTIONS [ NOWAIT ]
         #pragma omp sections [clause ...] newline
                              private (list)
                              firstprivate (list)
                              lastprivate (list)
                              reduction (operator: list)
C/C++
           #pragma omp section newline
              structured block
           #pragma omp section newline
              structured block
```

```
PROGRAM VEC ADD SECTIONS
      INTEGER N, I
      PARAMETER (N=1000)
      REAL A(N), B(N), C(N), D(N)
      Some initializations
      DO I = 1, N
       A(I) = I * 1.5
        B(I) = I + 22.35
      ENDDO
!$OMP PARALLEL SHARED(A,B,C,D), PRIVATE(I)
!$OMP SECTIONS
!SOMP SECTION
      DO I = 1, N
         C(I) = A(I) + B(I)
      ENDDO
!$OMP SECTION
      DO I = 1, N
         D(I) = A(I) * B(I)
      ENDDO
!SOMP END SECTIONS NOWAIT
!SOMP END PARALLEL
      END
```

Functional parallelism (MPMD)

Enclosed sections of code are computed in parallel, one section per thread (unless more sections than threads, then some threads have multiple sections executed serially)

Implicit barrier at end of SECTIONS unless NOWAIT

Cannot orphan SECTION i.e. have it physically outside a SECTIONS extent (see later)

No conditional branching out of sections

OpenMP – Directives: WORKSHARE

```
PROGRAM WORKSHARE
     INTEGER N, I, J
     PARAMETER (N=100)
     REAL AA(N,N), BB(N,N), CC(N,N), DD(N,N), FIRST, LAST
      Some initializations
     DO I = 1, N
       DO J = 1, N
         AA(J,I) = I * 1.0
         BB(J,I) = J + 1.0
        ENDDO
      ENDDO
!$OMP PARALLEL SHARED(AA, BB, CC, DD, FIRST, LAS
!$OMP WORKSHARE
     CC = AA * BB
      DD = AA + BB
     FIRST = CC(1,1) + DD(1,1)
     LAST = CC(N,N) + DD(N,N)
!SOMP END WORKSHARE NOWAIT
!$OMP END PARALLEL
      END
```

e.g.

```
!$OMP DO

Do i=2,1000

B(i)=10*(i+1)

A(i)=A(i)+B(i)

End Do

!$OMP END DO
```

Bad (RAW)

```
!$OMP WORKSHARE
Forall (i=1:999)
  B(i)=10*(i+1)
End Forall
A=A+B
!$OMP END WORKSHARE
```

FORTRAN ONLY!

Parallelizes Fortran commands that have hidden implicit DO loops (like full array operations, FORALL, WHERE, array intrinsics like MATMUL, etc)

ONLY CERTAIN ACTIONS CAN BE CONTAINED UNDER THE DIRECTIVE!

- ✓ array assignments
- ✓ MUTMUL, DOT_PRODUCT, SUM, PRODUCT. MAXVAL, MINVAL, MAXLOC, MINLOC, RESHAPE, TRANSPOSE, PACK, CSHIFT, ...
- ✓ scalar assignments
- ✓ FORALL statements
- ✓ FORALL constructs
- ✓ WHERE statements and constructs
- ✓ ATOMIC constructs
- ✓ CRITICAL constructs

Block of code is parallelized sequentially (!), parallelizing each unit of work (line) one at a time (note: incurs overhead, syncronizing)

Variables which are referenced or modified within construct MUST be shared variables

Good!

OpenMP – Directives: Composites

PARALLEL DO

PARALLEL SECTIONS

PARALLEL WORKSHARE

Same as PARALLEL followed by DO etc

Just for convenience

Note: PARALLEL incurs significant overhead so do not do multiple PARALLEL DO's in a row; rather do one PARALLEL and multiple DO's.

```
PROGRAM VECTOR ADD
      INTEGER N, I, CHUNKSIZE, CHUNK
     PARAMETER (N=1000)
     PARAMETER (CHUNKSIZE=100)
     REAL A(N), B(N), C(N)
     Some initializations
     DO I = 1, N
       A(I) = I * 1.0
       B(I) = A(I)
      ENDDO
     CHUNK = CHUNKSIZE
!SOMP PARALLEL DO
!$OMP& SHARED(A,B,C,CHUNK) PRIVATE(I)
!$OMP& SCHEDULE(STATIC, CHUNK)
     DO I = 1, N
        C(I) = A(I) + B(I)
     ENDDO
!$OMP END PARALLEL DO
     END
```

OpenMP – Directives: Single

Code only operates on one thread of the team (first to arrive)

Important for parts of the code that are not thread-safe

Other threads wait at the end of the block unless NOWAIT

Fortran	!\$OMP SINGLE [clause] PRIVATE (list) FIRSTPRIVATE (list)
	block !\$OMP END SINGLE [NOWAIT]
C/C++	#pragma omp single [clause] newline private (list) firstprivate (list) nowait
	structured_block

OpenMP – Directives: Task

NEW OpenMP 3.0!!

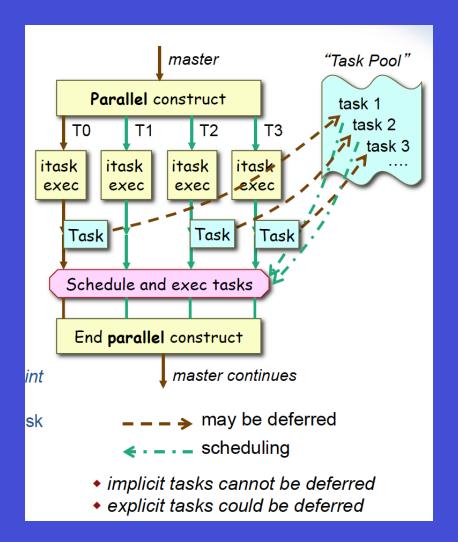
Task specifies a block of code for task scheduling

Like section but scheduled

(Note: synchronize with TASKWAIT)

Parallel region is an implicit task; TASK is explicit

```
!$OMP TASK [clause ...]
                      IF (scalar logical expression)
                      FINAL (scalar logical expression)
                      UNTIED
                      DEFAULT (PRIVATE | FIRSTPRIVATE | SHARED | NONE)
                      MERGEABLE
                      PRIVATE (list)
Fortran
                      FIRSTPRIVATE (list)
                      SHARED (list)
           block
         !SOMP END TASK
        #pragma omp task [clause ...] newline
                            if (scalar expression)
                            final (scalar expression)
                            default (shared | none)
                            mergeable
C/C++
                            private (list)
                            firstprivate (list)
                            shared (list)
             structured block
```



Two models now: threading and tasking

Threading: thread and work go together

Tasking: task generation and task execution separate. Thread is execution engine but no direct control of when task executed. More dynamic environment.

OpenMP – Directives: Synchronization

!SOMP MASTER

<block>

!\$OMP END MASTER

Only executed by the master

(no barrier for other threads)

Same as single except thread is master not first to arrive.

!\$OMP CRITICAL [name]

<block>

!\$OMP END CRITICAL [name]

Must be executed by one thread at a time

Threads BLOCK until executing thread in critical region has completed

All critical sections with no name are treated as SAME critical section (names are global entities in Fortran). Recommendation: always give them names!

!\$OMP BARRIER

Synchronizes all threads in the team. All threads must hit the same BARRIER! Do not call in a SECTION for example

!\$OMP ATOMIC

Mini (one line) critical region. Must be updated atomically (i.e. only one thread can access at a time). Good for writing to shared variables, for example doing a global sum a=a+i.

!\$OMP FLUSH (list)

Point at which consistent view of memory demanded. Thread variables written out of register and cache into main memory. Important EVEN IF shared memory is CACHE COHERENT! Confusing! Flush is implied at end of some directives (e.g. BARRIER, PARALLEL, CRITICAL, DO, SECTION, ...)

!\$OMP DO ORDERED

<...>

!\$OMP ORDERED

<block>

!\$OMP END ORDERED

<...>

!\$OMP END DO

Fine tuning of loops: specifies which iterations of a loop are executed in the same order as if in serial. (e.g. writing to a file)

Must be in dynamic extent of DO (or PARALLEL DO) (see later ... soon!)

Threads may have to wait if previous iteration not completed

```
!$omp parallel do private(myval) ordered
do i = 1, n
  myval = do_lots_of_work(i)
  !$omp ordered
  print*, i, myval
  !$omp end ordered
```

OpenMP – Directives: Synchronization

ATOMIC -- quick example:

Trying to avoid race/overwrite of shared variable A using ATOMIC

```
!$OMP DO
do i = 1, 10000
!$OMP ATOMIC
A = A + i
enddo
!$OMP END DO
```

Not efficient!

Better:

```
Atmp = 0

!$OMP DO
do i = 1, 1000
Atmp = Atmp + i
enddo
!$OMP END DO

!$OMP ATOMIC
A = A + Atmp
```

OpenMP – Directives: Synchronization

IMPLICIT DATA SYNCHRONIZATIONS:

YES!

- !\$OMP BARRIER
- !\$OMP CRITICAL and !\$OMP END CRITICAL
- !\$OMP END DO
- !\$OMP END SECTIONS
- !\$OMP END SINGLE
- !\$OMP END WORKSHARE
- !\$OMP ORDERED and !\$OMP END ORDERED
- | SOMP PARALLEL and SOMP END PARALLEL
- !\$OMP PARALLEL DO and !\$OMP END PARALLEL DO
- !SOMP PARALLEL SECTIONS and !SOMP END PARALLEL SECTIONS
- !\$OMP PARALLEL WORKSHARE and !\$OMP END PARALLEL WORKSHARE

NO!

- !\$OMP DO
- !\$OMP MASTER and !\$OMP END MASTER
- !\$OMP SECTIONS
- !\$OMP SINGLE
- !\$OMP WORKSHARE

Obviously NOWAIT overrides, if you use it.

Recap from Tues

OpenMP – Directives: Data environment

One separate directive (now)

+ data scoping associated with existing directives (see next)

```
!$OMP THREADPRIVATE (list)
```

- -- variable is local to each thread but global in extent to the thread
- equivalent to SAVE'd declared variables in FORTRAN (or COMMON variables)

```
integer, save :: a
!$OMP THREADPRIVATE(a)

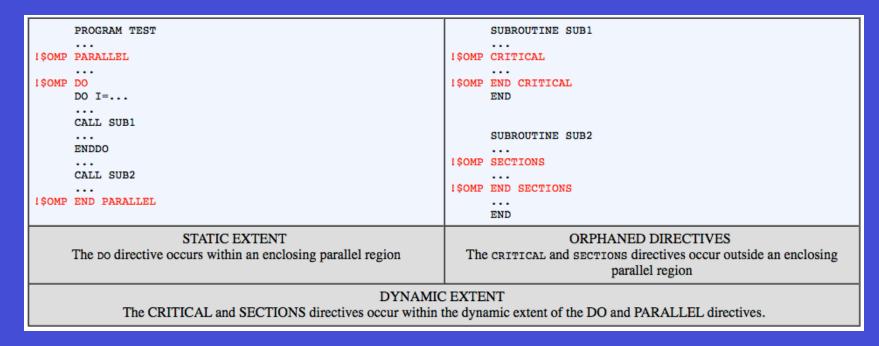
!$OMP PARALLEL
    a = OMP_get_thread_num()
!$OMP END PARALLEL

!$OMP PARALLEL
...
!$OMP END PARALLEL
```

Keeps thread id in a as allocated from first parallel region

OpenMP – Directives: Extents

<u>DIRECTIVE SCOPING: EXTENTS</u>



Static (lexical): textually enclosed, not spanning multiple routines or code files

Orphaned: Appears independently from enclosing directive i.e. OUTSIDE the static extent of the other

Dynamic: the composition of the two

Sooo ...?

OpenMP has a bunch of rules about binding and nesting depending on the extent (see later)

OpenMP – Directives: Extents

e.g.

```
PROGRAM ORPHAN
     COMMON /DOTDATA/ A, B, SUM
     INTEGER I, VECLEN
     PARAMETER (VECLEN = 100)
     REAL*8 A(VECLEN), B(VECLEN), SUM
     DO I=1, VECLEN
        A(I) = 1.0 * I
        B(I) = A(I)
     ENDDO
     SUM = 0.0
!$OMP PARALLEL
     CALL DOTPROD
                        static extent
!$OMP END PARALLEL
     WRITE(*,*) "Sum = ", SUM
     SUBROUTINE DOTPROD
     COMMON /DOTDATA/ A, B, SUM
     INTEGER I, TID, OMP GET THREAD NUM, VECLEN
     PARAMETER (VECLEN = 100)
     REAL*8 A(VECLEN), B(VECLEN), SUM
     TID = OMP GET THREAD NUM()
!$OMP DO REDUCTION(+:SUM) ← orphaned
     DO I=1, VECLEN
        SUM = SUM + (A(I)*B(I))
        PRINT *, ' TID= ',TID, 'I= ',I
     ENDDO
     RETURN
     END
```

dynamic extent

OpenMP – Directives: Data scope clauses

Shared memory => most data shared by default

Default GLOBAL variables include:

FORTRAN – COMMON blocks (!), SAVE variables, MODULE variables

C – file scope variables, static

Default PRIVATE variables include:

Stack variables in subroutines called from parallel regions

Explicit scoping via Data Scope Attribute Clauses:

Fortran

x = x operator expr

 $x = expr \ operator \ x \ (except \ subtraction)$

x = intrinsic(x, expr)

x = intrinsic(expr, x)

x is a scalar variable in the list expr is a scalar expression that does not reference xintrinsic is one of MAX, MIN, IAND, IOR, IEOR operator is one of +, *, -, .AND., .OR., .EQV., .NEQV.

PRIVATE (list)

Variables in list are private to each thread

New object of same type created for each thread.

Uninitialised? Final value? (see: FIRSTPRIVATE, LASTPRIVATE, etc)

SHARED (list)

Variables in list are shared amongst team

Only one memory location and all threads can write to it

REDUCTION (op | intrinsic: list)

Performs a reduction operation on variables in list

Private copy created for each thread; reduction applied to all private copies and applied to global shared variable

OpenMP – Directives: Data scope clauses

```
DEFAULT(DEFSCOPE) — sets default scope SHARED (the default DEFAULT!) | PRIVATE | NONE

FIRSTPRIVATE(VAR) — sets first value of private var to value it had coming into region (otherwise is undefined)

LASTPRIVATE(VAR) — sets exit value of var to last value it would have had in sequential code (Note: takes place at time of synchronization, so watch out for NOWAIT!)

COPYIN(VAR) — sets first value of a THREADPRIVATE var to the value supplied from the MASTER thread

COPYPRIVATE(VAR) — broadcasts the result of a SINGLE region to the other threads
```

!\$OMP SINGLE
 read(1,*) a
!\$OMP END SINGLE COPYPRIVATE(a)

OpenMP – Directives: Data scope clauses

e.g.

```
PROGRAM DOT PRODUCT
       INTEGER N, CHUNKSIZE, CHUNK, I
       PARAMETER (N=100)
       PARAMETER (CHUNKSIZE=10)
       REAL A(N), B(N), RESULT
      Some initializations
      DO I = 1, N
        A(I) = I * 1.0
        B(I) = I * 2.0
       ENDDO
       RESULT= 0.0
       CHUNK = CHUNKSIZE
ISOMP PARALLEL DO
!$OMP& DEFAULT(SHARED) PRIVATE(I)
ISOMP& SCHEP THE SUPPLIE
!$OMP& (REDUCTION(+:RESULT)
       DO I = 1, N
         RESULT = RESULT + (A(I) * B(I))
       ENDDO
!$OMP END PARALLEL DO
       PRINT *, 'Final Result= ', RESULT
       END
```

OpenMP – Directives: Synchronization

REMEMBER FROM EARLIER??? ATOMIC -- quick example:

Trying to avoid race/overwrite of shared variable A using ATOMIC

```
!$OMP DO
    do i = 1, 10000
        !$OMP ATOMIC
        A = A + i
    enddo
!$OMP END DO
```

NOTE: REDUCTION solves this (earlier) problem too!

Not efficient!

Better:

```
Atmp = 0
!$OMP DO
   do i = 1, 1000
       Atmp = Atmp + i
   enddo
!$OMP END DO

!$OMP ATOMIC
A = A + Atmp
```

```
!$OMP DO REDUCTION(+:a)
  do i = 1, 1000
    a = a + i
  enddo
!$OMP END DO
```

(Note again: shared variable only updated at time of synch)

OpenMP – Directives: Data scope clauses

Other clauses:

```
IF (scalar_logical_expr) — only do parallel op if expr evaluates true e.g. if n_iters in loop is big enough

NUM_THREADS (scalar_integer_expr) — number of threads to use. Overrrides other settings such as those
from GET_NUM_THREADS

NOWAIT — threads do not have to finish at same time

SCHEDULE(TYPE, CHUNK) — sets the way DO loops iterations are scheduled:

Static — loop divided into pieces of size chunk (default: evenly) then statically assigned to threads

Dynamic — default chunk =1. Threads assigned dynamically i.e. start one chunk, and grab another when finished

Guided — dynamic but in blocks that decrease in size, since blocksize = n_iter_remaining/n_threads

Runtime — schedule determined at runtime by env variable OMP_SCHEDULE

AUTO — compiler decides!

ORDERED — sets loops to sequential
```

OpenMP – Directives: Clauses: Summary

• The table below summarizes which clauses are accepted by which OpenMP directives.

	Directive					
Clause	PARALLEL	DO/for	SECTIONS	SINGLE	PARALLEL DO/for	PARALLEL SECTIONS
IF	•				•	•
PRIVATE	•	•	•	•	•	•
SHARED	•	•			•	•
DEFAULT	•				•	•
FIRSTPRIVATE	•	•	•	•	•	•
LASTPRIVATE		•	•		•	•
REDUCTION	•	•	•		•	•
COPYIN	•				•	•
COPYPRIVATE				•		
SCHEDULE		•			•	
ORDERED		•			•	
NOWAIT		•	•	•		

- The following OpenMP directives do not accept clauses:
 - MASTER
 - o CRITICAL
 - BARRIER
 - ATOMIC
 - FLUSH
 - o ORDERED
 - o THREADPRIVATE
- Implementations may (and do) differ from the standard in which clauses are supported by each directive.

OpenMP – Directives: Binding/nesting

Urgh!

Directive Binding:

- The DO/for, SECTIONS, SINGLE, MASTER and BARRIER directives bind to the dynamically enclosing PARALLEL, if one exists. If no parallel region is currently being executed, the directives have no effect.
- The ORDERED directive binds to the dynamically enclosing DO/for.
- The ATOMIC directive enforces exclusive access with respect to ATOMIC directives in all threads, not just the current team.
- The CRITICAL directive enforces exclusive access with respect to CRITICAL directives in all threads, not just the current team.
- A directive can never bind to any directive outside the closest enclosing PARALLEL.

Directive Nesting:

- A worksharing region may not be closely nested inside a worksharing, explicit task, critical, ordered, atomic, or master region.
- · A barrier region may not be closely nested inside a worksharing, explicit task, critical, ordered, atomic, or master region.
- A master region may not be closely nested inside a worksharing, atomic, or explicit task region.
- · An ordered region may not be closely nested inside a critical, atomic, or explicit task region.
- An ordered region must be closely nested inside a loop region (or parallel loop region) with an ordered clause.
- A critical region may not be nested (closely or otherwise) inside a critical region with the same name. Note that this restriction is not sufficient to prevent deadlock.
- · parallel, flush, critical, atomic, taskyield, and explicit task regions may not be closely nested inside an atomic region.

The term "closely nested region" means a region that is dynamically nested inside another region with no parallel region nested between them.

OpenMP – Runtime Library Routines

Routine	Purpose			
OMP_SET_NUM_THREADS	Sets the number of threads that will be used in the next parallel region			
OMP_GET_NUM_THREADS	Returns the number of threads that are currently in the team executing the parallel region from which it is called			
OMP_GET_MAX_THREADS	Returns the maximum value that can be returned by a call to the OMP_GET_NUM_THREADS function			
OMP_GET_THREAD_NUM	Returns the thread number of the thread, within the team, making this call.			
OMP_GET_THREAD_LIMIT	Returns the maximum number of OpenMP threads available to a program			
OMP_GET_NUM_PROCS	Returns the number of processors that are available to the program			
OMP_IN_PARALLEL	Used to determine if the section of code which is executing is parallel or not			
OMP_SET_DYNAMIC	Enables or disables dynamic adjustment (by the run time system) of the number of threads available for execution of parallel regions $\frac{1}{2}$			
OMP_GET_DYNAMIC	Used to determine if dynamic thread adjustment is enabled or not			
OMP_SET_NESTED	Used to enable or disable nested parallelism			
OMP_GET_NESTED	Used to determine if nested parallelism is enabled or not			
OMP_SET_SCHEDULE	Sets the loop scheduling policy when "runtime" is used as the schedule kind in the OpenMP directive			
OMP GET SCHEDULE	Returns the loop scheduling policy when "runtime" is used as the schedule kind in the OpenMP directive			
OMP_SET_MAX_ACTIVE_LEVELS	Sets the maximum number of nested parallel regions			
OMP_GET_MAX_ACTIVE_LEVELS	Returns the maximum number of nested parallel regions			
OMP_GET_LEVEL	Returns the current level of nested parallel regions			
OMP GET ANCESTOR THREAD NUM	Returns, for a given nested level of the current thread, the thread number of ancestor thread			
OMP GET TEAM SIZE	Returns, for a given nested level of the current thread, the size of the thread team			
OMP_GET_ACTIVE_LEVEL	Returns the number of nested, active parallel regions enclosing the task that contains the call			
OMP_IN_FINAL	Returns true if the routine is executed in the final task region; otherwise it returns false			
OMP_INIT_LOCK	Initializes a lock associated with the lock variable			
OMP_DESTROY_LOCK	Disassociates the given lock variable from any locks			
OMP_SET_LOCK	Acquires ownership of a lock			
OMP_UNSET_LOCK	Releases a lock			
OMP_TEST_LOCK	Attempts to set a lock, but does not block if the lock is unavailable			
OMP_INIT_NEST_LOCK	Initializes a nested lock associated with the lock variable			
OMP DESTROY NEST LOCK	Disassociates the given nested lock variable from any locks			
OMP_SET_NEST_LOCK	Acquires ownership of a nested lock			
OMP_UNSET_NEST_LOCK	Releases a nested lock			
OMP_TEST_NEST_LOCK	Attempts to set a nested lock, but does not block if the lock is unavailable			
OMP_GET_WTIME	Provides a portable wall clock timing routine			
OMP GET WTICK	Returns a double-precision floating point value equal to the number of seconds between successive clock ticks			

In Fortran, some are functions and some are subroutines ©

e.g.

Call OMP SET NUM THREADS(8)

e.g.

Integer nt

nt=OMP_GET_NUM_THREADS()

Locks are for blocking:

Init lock -- initiates var

Set_lock – wait until lock available

Unset lock – releases lock

Test_lock – like set but does not block if lock not available

Destroy lock – removes lock variable

LOCKS = INTEGER*8 (to hold an address)

OpenMP – Lock example

```
program Main
use omp_lib
implicit none
integer(kind = OMP_lock_kind) :: lck
integer(kind = OMP_integer_kind) :: ID
call OMP_init_lock(lck)
!$OMP PARALLEL SHARED(LCK) PRIVATE(ID)
  ID = OMP_get_thread_num()
 call OMP_set_lock(lck)
  write(*,*) "My thread is ", ID
 call OMP_unset_lock(lck)
!$OMP END PARALLEL
call OMP_destroy_lock(lck)
end program Main
```

This dumb example is equivalent to:

```
program Main
use omp_lib
implicit none
integer(kind = OMP_integer_kind) :: ID
!$OMP PARALLEL SHARED(LCK) PRIVATE(ID)
  ID = OMP_get_thread_num()
!$OMP CRITICAL
  write(*,*) "My thread is ", ID
!$OMP END CRITICAL
!$OMP END PARALLEL
end program Main
```

OpenMP – Lock example

```
PROGRAM BUG5
      INTEGER*8 LOCKA, LOCKB
      INTEGER NTHREADS, TID, I,
              OMP GET NUM THREADS, OMP GET THREAD NUM
     PARAMETER (N=1000000)
      REAL A(N), B(N), PI, DELTA
      PARAMETER (PI=3.1415926535)
     PARAMETER (DELTA=.01415926535)
     Initialize the locks
      CALL OMP INIT LOCK(LOCKA)
      CALL OMP INIT LOCK(LOCKB)
      Fork a team of threads giving them their own copies of variables
!SOMP PARALLEL SHARED(A, B, NTHREADS, LOCKA, LOCKB) PRIVATE(TID)
      Obtain thread number and number of threads
      TID = OMP GET THREAD NUM()
ISOMP MASTER
     NTHREADS = OMP GET NUM THREADS()
     PRINT *, 'Number of threads = ', NTHREADS
!$OMP END MASTER
      PRINT *, 'Thread', TID, 'starting...'
!SOMP BARRIER
ISOMP SECTIONS
!$OMP SECTION
     PRINT *, 'Thread', TID, initializing A()'
      CALL OMP SET LOCK(LOCKA)
     DO I = 1, N
        A(I) = I * DELTA
     ENDDO
     CALL OMP SET LOCK(LOCKB)
     PRINT *, 'Thread', TID, ' adding A() to B()'
     DO I = 1, N
        B(I) = B(I) + A(I)
      ENDDO
      CALL OMP UNSET LOCK(LOCKB)
     CALL OMP_UNSET_LOCK(LOCKA)
ISOMP SECTION
     PRINT *, 'Thread', TID, 'initializing B()'
      CALL OMP_SET_LOCK(LOCKB)
     DO I = 1, N
        B(I) = I * PI
      CALL OMP SET LOCK(LOCKA)
     PRINT *, 'Thread', TID, ' adding B() to A()'
     DO I = 1, N
        A(I) = A(I) + B(I)
      CALL OMP UNSET LOCK(LOCKA)
      CALL OMP UNSET LOCK (LOCKB)
ISOMP END SECTIONS NOWAIT
     PRINT *, 'Thread', TID, ' done.'
ISOMP END PARALLEL
      END
```

```
PROGRAM BUG5
      INTEGER*8 LOCKA, LOCKB
      INTEGER NTHREADS, TID, I,
              OMP GET NUM THREADS, OMP GET THREAD NUM
      PARAMETER (N=1000000)
      REAL A(N), B(N), PI, DELTA
      PARAMETER (PI=3.1415926535)
      PARAMETER (DELTA=.01415926535)
     Initialize the locks
      CALL OMP INIT LOCK(LOCKA)
      CALL OMP INIT LOCK(LOCKB)
      Fork a team of threads giving them their own copies of variables
!$OMP PARALLEL SHARED(A, B, NTHREADS, LOCKA, LOCKB) PRIVATE(TID)
      Obtain thread number and number of threads
      TID = OMP GET THREAD NUM()
ISOMP MASTER
      NTHREADS = OMP GET NUM THREADS()
      PRINT *, 'Number of threads = ', NTHREADS
! $OMP END MASTER
      PRINT *, 'Thread', TID, 'starting...'
!SOMP BARRIER
!SOMP SECTIONS
!$OMP SECTION
      PRINT *, 'Thread', TID, ' initializing A()'
      CALL OMP SET LOCK(LOCKA)
      DO I = 1, N
        A(I) = I * DELTA
      CALL OMP UNSET LOCK(LOCKA)
      CALL OMP SET LOCK(LOCKB)
      PRINT *, 'Thread', TID, adding A() to B()'
      DO I = 1, N
         B(I) = B(I) + A(I)
      CALL OMP UNSET LOCK(LOCKB)
      PRINT *, 'Thread', TID, ' initializing B()'
      CALL OMP SET LOCK(LOCKB)
      DO I = 1. N
         B(I) = I * PI
      CALL OMP_UNSET_LOCK(LOCKB)
      CALL OMP SET LOCK(LOCKA)
      PRINT *, 'Thread', TID, 'adding B() to A()'
      DO I = 1, N
         A(I) = A(I) + B(I)
      CALL OMP_UNSET_LOCK(LOCKA)
!SOMP END SECTIONS NOWAIT
      PRINT *, 'Thread', TID, ' done.'
!$OMP END PARALLEL
      END
```

OpenMP – Environment Variables

OMP_SCHEDULE

Applies only to DO, PARALLEL DO (Fortran) and for, parallel for (C/C++) directives which have their schedule clause set to RUNTIME. The value of this variable determines how iterations of the loop are scheduled on processors. For example:

```
setenv OMP_SCHEDULE "guided, 4"
setenv OMP_SCHEDULE "dynamic"
```

OMP NUM THREADS

Sets the maximum number of threads to use during execution. For example:

```
setenv OMP_NUM_THREADS 8
```

OMP_DYNAMIC

Enables or disables dynamic adjustment of the number of threads available for execution of parallel regions. Valid values are TRUE or FALSE. For example:

```
setenv OMP_DYNAMIC TRUE
```

OMP_PROC_BIND

Enables or disables threads binding to processors. Valid values are TRUE or FALSE. For example:

```
setenv OMP PROC BIND TRUE
```

OMP NESTED

Enables or disables nested parallelism. Valid values are TRUE or FALSE. For example:

```
setenv OMP NESTED TRUE
```

If nested parallelism is supported, it is often only nominal, in that a nested parallel region may only have one thread.

OpenMP – Environment Variables

OMP STACKSIZE

Controls the size of the stack for created (non-Master) threads. Examples:

```
setenv OMP_STACKSIZE 2000500B
setenv OMP_STACKSIZE "3000 k "
setenv OMP_STACKSIZE 10M
setenv OMP_STACKSIZE " 10 M "
setenv OMP_STACKSIZE "20 m "
setenv OMP_STACKSIZE "1G"
setenv OMP_STACKSIZE 20000
```

OMP_WAIT_POLICY

Provides a hint to an OpenMP implementation about the desired behavior of waiting threads. A compliant OpenMP implementation may or may not abide by the setting of the environment variable. Valid values are ACTIVE and PASSIVE. ACTIVE specifies that waiting threads should mostly be active, i.e., consume processor cycles, while waiting. PASSIVE specifies that waiting threads should mostly be passive, i.e., not consume processor cycles, while waiting. The details of the ACTIVE and PASSIVE behaviors are implementation defined. Examples:

```
setenv OMP_WAIT_POLICY ACTIVE
setenv OMP_WAIT_POLICY active
setenv OMP_WAIT_POLICY PASSIVE
setenv OMP_WAIT_POLICY passive
```

OMP_MAX_ACTIVE_LEVELS

Controls the maximum number of nested active parallel regions. The value of this environment variable must be a non-negative integer. The behavior of the program is implementation defined if the requested value of OMP_MAX_ACTIVE_LEVELS is greater than the maximum number of nested active parallel levels an implementation can support, or if the value is not a non-negative integer. Example:

```
setenv OMP MAX ACTIVE LEVELS 2
```

OMP THREAD LIMIT

Sets the number of OpenMP threads to use for the whole OpenMP program. The value of this environment variable must be a positive integer. The behavior of the program is implementation defined if the requested value of OMP_THREAD_LIMIT is greater than the number of threads an implementation can support, or if the value is not a positive integer. Example:

```
setenv OMP_THREAD_LIMIT 8
```

Final tips

Thread stack size

```
Implementation specific and can be small!
```

```
e.g. gfortran \sim 2MB (\sim 500x500 double values)
```

OpenMP 3.0:

```
setenv OMP STACKSIZE 10M
```

Linux:

```
setenv KMP_STACKSIZE 12000000
limit stacksize unlimited
```

Thread binding

Performance may be better if threads bound to processors (thread affinity) due to cache re-use

OpenMP 3.1:

```
setenv OMP_PROC_BIN TRUE
```

Things we didn't talk about much

OpenMP 3.0-5.0

(Task parallelism)

Dynamics creation of threads

Nested parallelism

Support for co-processors/accelerators

Support for NUMA systems

OpenMP 5.0 press release:

- Full support for accelerator devices. OpenMP now has full support for accelerator devices, including mechanisms to require unified shared memory between the host system and coprocessor devices, the ability to use device-specific function implementations, better control of implicit data mappings, and the ability to override device offload at runtime. In addition, it supports reverse offload, implicit function generation, and the ability to copy object-oriented data structures easily.
- Improved debugging and performance analysis. Two new tool interfaces enable the development of third party tools to support intuitive debugging and deep performance analysis.
- Support for the latest versions of C, C++, and Fortran. OpenMP now supports important features of Fortran 2008, C11, and C++17.
- Support for a fully descriptive loop construct. The loop construct lets the compiler optimize a loop while not forcing any specific implementation. This construct allows the compiler more freedom to choose a good implementation for a specific target than do other OpenMP directives.
- Multilevel memory systems. Memory allocation mechanisms are available that place data in different kinds of memories, such as high-bandwidth memory. New OpenMP features also make it easier to deal with the NUMA-ness of modern HPC systems.
- Enhanced portability. The declare variant directive and a new meta-directive allow programmers to improve performance portability by adapting OpenMP pragmas and user code at compile time.

THE END

OPENMP: Homework 6

Write, in parallel, using OpenMP

- A "hello world"
- 2. A program that initializes two matrices A and B with some values, calculates the product C = AB and finds the minimum value in the C matrix and where it is in the matrix. Make two versions:
 - (a) Use do loops to do the matrix multiply and OpenMP PARALLEL DO
 - (b) Use Fortran MATMUL and OpenMP workshare

Run some tests for large matrices to see which one works best.

Submit a tar file *named with your name < name.tar>* that contains

- the .f90 files for your program
- A README of instructions on how to compile and run
- Sample output that shows that the programs work
- An analysis which shows which one works best for question 2