AMath 483/583 — Lecture 14 — April 27, 2011

Today:

- OpenMP

Friday:

- More OpenMP

Read: Class notes and references

Homework 4 is posted, due next Thursday.

Notes:

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Memory stack

Note: Parallel threads use stack and you may need to increase the limit (e.g. on the VM):

```
$ gfortran -fopenmp yeval.f90
$ ./a.out
Segmentation fault

$ ulimit -s
8192

$ ulimit -s unlimited

$ ./a.out
Using OpenMP with   2 threads
 Filled vector y of length   100000000
```

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Memory: Heap and Stack

Memory devoted to data for a program is generally split up:

Heap: Dynamically allocated memory — memory allocator looks for free block of memory, keeps track of free list, does garbage collection, etc.

Stack: Block of memory where space is allocated on "top" of the stack as needed and "popped" off the stack when no longer needed. Last in – first out (LIFO).

Fast relative to heap allocation.

Natural way to allocate storage for nested subroutine or function calls: If A calls B calls C, then when the variables used by C are popped off the stack, we're back to the variables of B.

Private variables for threads also put on stack, popped off when parallel block ends.

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OpenMP compiler directives

Uses compiler directives that start with `!$` (pragmas in C.)

These look like comments to standard Fortran but are recognized when compiled with the flag `-fopenmp`.

OpenMP statements:

Ordinary Fortran statements conditionally compiled:

```
!$ print *, "Compiled with -fopenmp"
```

OpenMP compiler directives, e.g.

```
!$omp parallel do
```

Calls to OpenMP library routines:

```
use omp_lib    ! need this module
!$ call omp_set_num_threads(2)
```


Notes:

OpenMP test code

```
program test
   use omp_lib
   integer :: thread_num

   ! Specify number of threads to use:
   !$ call omp_set_num_threads(2)

   print *, "Testing openmp ..."

   !$omp parallel
   !$omp critical
   !$ thread_num = omp_get_thread_num()
   !$ print *, "This thread = ",thread_num
   !$omp end critical
   !$omp end parallel
end program test
```


Notes:

OpenMP test code

Could change to add a private clause:

```
!$omp parallel private(thread_num)

!$ thread_num = omp_get_thread_num()

!$omp critical
!$ print *, "This thread = ",thread_num
!$omp end critical
!$omp end parallel
```

Then each thread has it's own version of the `thread_num` variable.

Notes:

OpenMP parallel do loops

```
!$omp parallel do
do i=1,n
   ! do stuff for each i
   enddo
!$omp end parallel do    ! OPTIONAL
```

indicates that the do loop can be done in parallel.

Requires:

what's done for each value of i is independent of others
Different values of i can be done in any order.

The iteration variable `i` is private to the thread: each thread has its own version.

By default, all other variables are shared between threads unless specified otherwise.

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OpenMP parallel do loops

This code fills a vector `y` with function values that take a bit of time to compute:

```
! fragment of $CLASSHG/codes/openmp/yeval.f90

dx = 1.d0 / (n+1.d0)

!$omp parallel do private(x)
do i=1,n
   x = i*dx
   y(i) = exp(x)*cos(x)*sin(x)*sqrt(5*x+6.d0)
enddo
```

Elapsed time for $n = 10^8$, without OpenMP: about 9.3 sec.

Elapsed time using OpenMP on 2 processors: about 5.0 sec.

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OpenMP parallel do loops

This code is not correct:

```
!$omp parallel do
do i=1,n
   x = i*dx
   y(i) = exp(x)*cos(x)*sin(x)*sqrt(5*x+6.d0)
enddo
```

By default, `x` is a shared variable.

Might happen that:

Processor 0 sets `x` properly for one value of `i`,
Processor 1 sets `x` properly for another value of `i`,
Processor 0 uses `x` but is now incorrect.

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OpenMP parallel do loops

Correct version:

```
!$omp parallel do private(x)
do i=1,n
   x = i*dx
   y(i) = exp(x)*cos(x)*sin(x)*sqrt(5*x+6.d0)
enddo
```

Now each thread has its own version of `x`.

Iteration counter `i` is private by default.

Note that `dx, n, y` are shared by default.

`dx, n` are used but not changed,
`y` is changed, but independently for each `i`

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OpenMP parallel do loops

Incorrect code:

```
dx = 1.d0 / (n+1.d0)
!$omp parallel do private(x,dx)
do i=1,n
   x = i*dx
   y(i) = exp(x)*cos(x)*sin(x)*sqrt(5*x+6.d0)
enddo
```

Specifying `dx` private won't work here.

This will create a private variable `dx` for each thread but it will be uninitialized.

Will run but give garbage.

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OpenMP parallel do loops

Could fix with:

```
dx = 1.d0 / (n+1.d0)
!$omp parallel do firstprivate(dx)
do i=1,n
   x = i*dx
   y(i) = exp(x)*cos(x)*sin(x)*sqrt(5*x+6.d0)
enddo
```

The firstprivate clause creates private variables and initializes to the value from the master thread prior to the loop.

There is also a lastprivate clause to indicate that the last value computed by a thread (for $i = n$) should be copied to the master thread's copy for continued execution.

Notes:

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OpenMP parallel do loops

```
! from $CLASSHG/codes/openmp/private1.f90

   n = 7
   y = 2.d0
   !$omp parallel do firstprivate(y) lastprivate(y)
   do i=1,n
      y = y + 10.d0
      x(i) = y
      !omp critical
      print *, "i = ",i,"  x(i) = ",x(i)
      !omp end critical
   enddo
   print *, "At end, y = ",y
```

might produce:

```
     i =            1   x(i) =    12.0000000000000
     i =            5   x(i) =    12.0000000000000
     i =            2   x(i) =    22.0000000000000
     i =            6   x(i) =    22.0000000000000
     i =            3   x(i) =    32.0000000000000
     i =            7   x(i) =    32.0000000000000
     i =            4   x(i) =    42.0000000000000
    At end, y =    32.0000000000000
```

Order might be different but final y will be from $i = 7$.

Notes:

OpenMP parallel do loops — changing default

Default is that loop iterator is private, other variables shared.

Can change this, e.g.

```
!$omp parallel do default(private) shared(x,z) &
!$omp firstprivate(y) lastprivate(y)
do i=1,n
   etc.
```

With this change, only `x` and `z` are shared.

Note continuation character `&` and continuation line.

Notes:

OpenMP synchronization

```
!$omp parallel do
do i=1,n
   ! do stuff for each i
enddo
!$omp end parallel do  ! OPTIONAL

! master thread continues execution
```

There is an implicit barrier at the end of the loop.

The master thread will not continue until all threads have finished with their subset of `1, 2, ..., n`.

Except if ended by:

```
!$omp end parallel do nowait
```


Notes:

Conditional clause

Loop overhead may not be worthwhile for short loops.
(Multi-thread version may run slower than sequential)

Can use conditional clause:

```
$omp parallel do if (n > 1000)
do i=1,n
    ! do stuff
    enddo
```

If $n \leq 1000$ then no threads are created,
master thread executes loop sequentially.

Notes:

Nested loops

```
!$omp parallel do private(i)
do j=1,m
   do i=1,n
      a(i,j) = 0.d0
   enddo
enddo
```

The loop on `j` is split up between threads.

The thread handling `j=1` does the entire loop on `i`,
sets `a(1,1), a(2,1), ..., a(n,1).`

Note: The loop iterator `i` must be declared private!

`j` is private by default, `i` is shared by default.

Notes:

Nested loops

Which is better? (assume $m \approx n$)

```
!$omp parallel do private(i)
do j=1,m
   do i=1,n
      a(i,j) = 0.d0
   enddo
enddo
```

or

```
do j=1,m
   !$omp parallel do
   do i=1,n
      a(i,j) = 0.d0
   enddo
enddo
```

The first has less overhead: Threads created only once.
The second has more overhead: Threads created m times.

Notes:

Nested loops

But have to make sure loop can be parallelized!

Incorrect code for replicating first column:

```
!$omp parallel do private(j)
do i=2,n
   do j=1,m
      a(i,j) = a(i-1,j)
   enddo
enddo
```

Corrected: (j's can be done in any order, i's cannot)

```
!$omp parallel do private(i)
do j=1,m
   do i=2,n
      a(i,j) = a(i-1,j)
   enddo
enddo
```


Notes:

Reductions

Incorrect code for computing $\|x\|_1 = \sum_i |x_i|$:

```
norm = 0.d0
!$omp parallel do
do i=1,n
    norm = norm + abs(x(i))
    enddo
```

There is a race condition: each thread is updating same shared variable `norm`.

Correct code:

```
!$omp parallel do reduction(+ : norm)
do i=1,n
    norm = norm + abs(x(i))
    enddo
```

A reduction reduces an array of numbers to a single value.

Notes:

Reductions

A more complicated way to do this:

```
norm = 0.d0
!$omp parallel private(mysum) shared(norm)
mysum = 0
!$omp do
do i=1,n
    mysum = mysum + abs(x(i))
    enddo

!$omp critical
norm = norm + mysum
!$omp end critical
!$omp end parallel
```


Notes:

Some other reductions

Can do reductions using $+, -, *$, min, max, .and., .or., some others

General form:

```
!$omp parallel do reduction(operator : list)
```

Example with max:

```
y = -1.d300  ! very negative value
!$omp parallel do reduction(max: y)
do i=1,n
   y = max(y,x(i))
enddo
print *, 'max of x = ',y
```


Notes:

Some other reductions

General form:

```
!$omp parallel do reduction(operator : list)
```

Example with .or.:

```
logical anyzero

! set x...
anyzero = .false.

!$omp parallel do reduction(.or.: anyzero)
do i=1,n
   anyzero = anyzero .or. (x(i) == 0.d0)
   enddo
print *, 'anyzero = ',anyzero
```

Prints `T` if any `x(i)` is zero, `F` otherwise.

Notes: