Shared Memory Programming with OpenMP

Lecture 7: Further topics

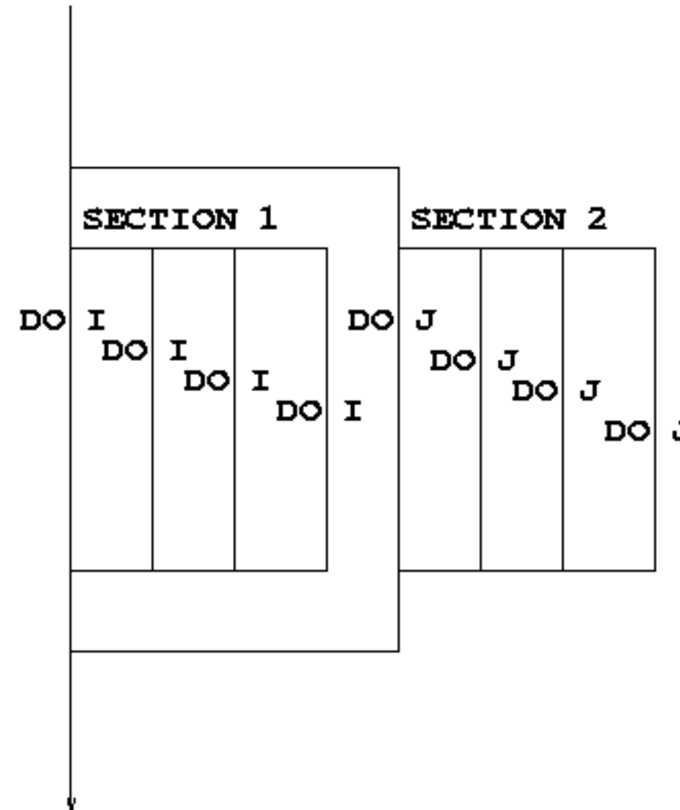
Nested parallelism

- Unlike most previous directive systems, nested parallelism is permitted in OpenMP.
- This is enabled with the **`OMP_NESTED`** environment variable or the **`OMP_SET_NESTED`** routine.
- If a PARALLEL directive is encountered within another PARALLEL directive, a new team of threads will be created.
- The new team will contain only one thread unless nested parallelism is enabled.

Nested parallelism (cont)

Example:

```
!$OMP PARALLEL
!$OMP SECTIONS
!$OMP SECTION
!$OMP PARALLEL DO
      do i = 1,n
         x(i) = 1.0
      end do
!$OMP SECTION
!$OMP PARALLEL DO
      do j = 1,n
         y(j) = 2.0
      end do
!$OMP END SECTIONS
!$OMP END PARALLEL
```



Nested parallelism (cont)

- Not often needed, but can be useful to exploit non-scalable parallelism (SECTIONS).

- Note: nested parallelism isn’t supported in some implementations (the code will execute, but as if OMP_NESTED is set to FALSE).
  - turns out to be hard to do correctly without impacting performance significantly.

Controlling the number of threads

- Can use the environment variable

```
export OMP_NUM_THREADS=2,4
```

- Will use 2 threads at the outer level and 4 threads for each of the inner teams.

- Can use **omp_set_num_threads()** or the **num_threads** clause on the parallel region.

omp_set_num_threads()

- Useful if you want inner regions to use different numbers of threads:

```
CALL OMP_SET_NUM_THREADS(2)
!$OMP PARALLEL DO
      DO I = 1,4
CALL OMP_SET_NUM_THREADS(innerthreads(i))
!$OMP PARALLEL DO
         DO J = 1,N
            A(I,J) = B(I,J)
         END DO
      END DO
```

- The value set overrides the value(s) in the environment variable OMP_NUM_THREADS

omp_get_max_threads()

- Often useful to know (an upper bound on) the number of threads which could be used in the *next* parallel region.
- This is what `omp_get_max_threads()` returns.
- Can use this to safely allocate enogh storage for each thread in the next parallel region.

Orphaned directives

- Directives are active in the *dynamic* scope of a parallel region, not just its *lexical* scope.
- Example:

```
!$OMP PARALLEL
      call fred()
!$OMP END PARALLEL


      subroutine fred()
!$OMP DO
      do i = 1,n
         a(i) = a(i) + 23.5
      end do
      return
      end
```

Orphaned directives (cont)

- This is very useful, as it allows a modular programming style….
- But it can also be rather confusing if the call tree is complicated (what happens if **`fred`** is also called from outside a parallel region?)
- There are some extra rules about data scope attributes….

Data scoping rules

When we call a subroutine from inside a parallel region:

- Variables in the argument list inherit their data scope attribute from the calling routine.
- Global variables in C++ and COMMON blocks or module variables in Fortran are shared, unless declared THREADPRIVATE (see later).
- `static` local variables in C/C++ and `SAVE` variables in Fortran are shared.
- All other local variables are private.

Thread private global variables

- It can be convenient for each thread to have its own copy of variables with global scope (e.g. COMMON blocks and module data in Fortran, or file-scope and namespace-scope variables in C/C++).

- Outside parallel regions and in MASTER directives, accesses to these variables refer to the master thread's copy.

Thread private globals (cont)

Syntax:

Fortran: **!$OMP THREADPRIVATE (*list*)**

where list contains named common blocks (enclosed in slashes), module variables and SAVEd variables..

This directive must come after all the declarations for the common blocks or variables.

C/C++: **#pragma omp threadprivate (*list*)**

This directive must be at file or namespace scope, after all declarations of variables in *list* and before any references to variables in *list*. See standard document for other restrictions.

The **COPYIN** clause allows the values of the master thread's THREADPRIVATE data to be copied to all other threads at the start of a parallel region.

Timing routines

OpenMP supports a portable timer:

- return current wall clock time (relative to arbitrary origin) with:

```
DOUBLE PRECISION FUNCTION OMP_GET_WTIME()
```

```
double omp_get_wtime(void);
```

- return clock precision with

```
DOUBLE PRECISION FUNCTION OMP_GET_WTICK()
```

```
double omp_get_wtick(void);
```

Using timers

```
DOUBLE PRECISION STARTTIME, TIME

STARTTIME = OMP_GET_WTIME()
......(work to be timed)
TIME = OMP_GET_WTIME()- STARTTIME
```

Note: timers are local to a thread: must make both calls on the same thread.

Also note: no guarantees about resolution!

Exercise

Molecular dynamics again

- Aim: use of orphaned directives.
- Modify the molecular dynamics code so by placing a parallel region directive around the iteration loop in the main program, and making all code within this sequential except for the forces loop.
- Modify the code further so that each thread accumulates the forces into a local copy of the force array, and reduce these copies into the main array at the end of the loop.