Shared Memory Programming with OpenMP

Lecture 6: Further topics in OpenMP

Overview

- Nested parallelism
- Orphaned constructs
- Thread-private globals
- Timing routines

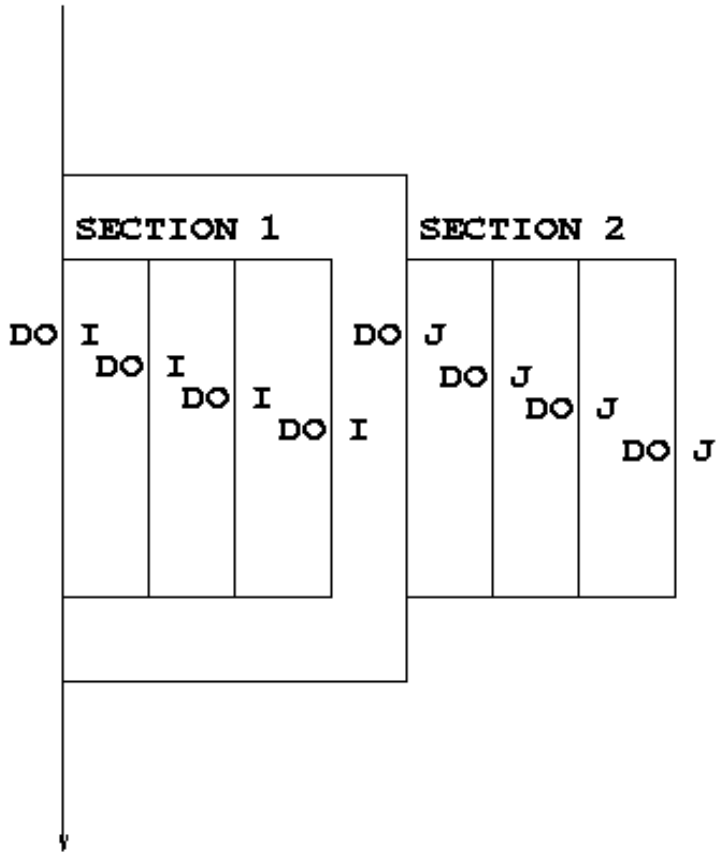
Nested parallelism

- Nested parallelism is supported in OpenMP.
- If a PARALLEL directive is encountered within another PARALLEL directive, a new team of threads will be created.
- This is enabled with the **`OMP_NESTED`** environment variable or the **`OMP_SET_NESTED`** routine.
- If nested parallelism is disabled, the code will still executed, but the inner teams will contain only one thread.

Nested parallelism (cont)

Example:

```
!$OMP PARALLEL PRIVATE(myid)
myid = omp_get_thread_num()
if (myid .eq. 0) then
!$OMP PARALLEL DO
      do i = 1,n
         x(i) = 1.0
      end do
elseif (myid .eq.1) then
!$OMP PARALLEL DO
      do j = 1,n
         y(j) = 2.0
      end do
endif
!$OMP END PARALLEL
```



Nested parallelism (cont)

- Not often needed, but can be useful if the outer level does not contain enough parallelism

- 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.
  - don't enable nested parallelism unless you are using it!

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

NUM_THREADS clause

- One way to control the number of threads used at each level is with the NUM_THREADS clause:

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

- The value set in the clause overrides the value in the environment variable OMP_NUM_THREADS and that set by `omp_set_num_threads()`

More control….

- Can also control the maximum number of threads running at any one time.

```
export OMP_THREAD_LIMIT=64
```

- …and the maximum depth of nesting

```
export OMP_MAX_ACTIVE_LEVELS=2
```

or call

```
omp_set_max_active_levels()
```

Utility routines for nested parallelism

- **`omp_get_level()`**
  - returns the level of parallelism of the calling thread
  - returns 0 in the sequential part
- **`omp_get_active_level()`**
  - returns the level of parallelism of the calling thread, ignoring levels which are inactive (teams only contain one thread)
- **`omp_get_ancestor_thread_num(level)`**
  - returns the thread ID of this thread's ancestor at a given level
  - ID of my parent:
    `omp_get_ancestor_thread_num(omp_get_level()-1)`
- **`omp_get_team_size(level)`**
  - returns the number of threads in this thread's ancestor team at a given level

Nested loops

- For perfectly nested rectangular loops we can parallelise multiple loops in the nest with the **collapse** clause:

```
#pragma omp parallel for collapse(2)
for (int i=0; i<N; i++) {
  for (int j=0; j<M; j++) {
          .....
  }
}
```

- Argument is number of loops to collapse starting from the outside
- Will form a single loop of length NxM and then parallelise and schedule that.
- Useful if N is O(no. of threads) so parallelising the outer loop may not have good load balance
- More efficient than using nested teams

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/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)

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.

Reusing this material