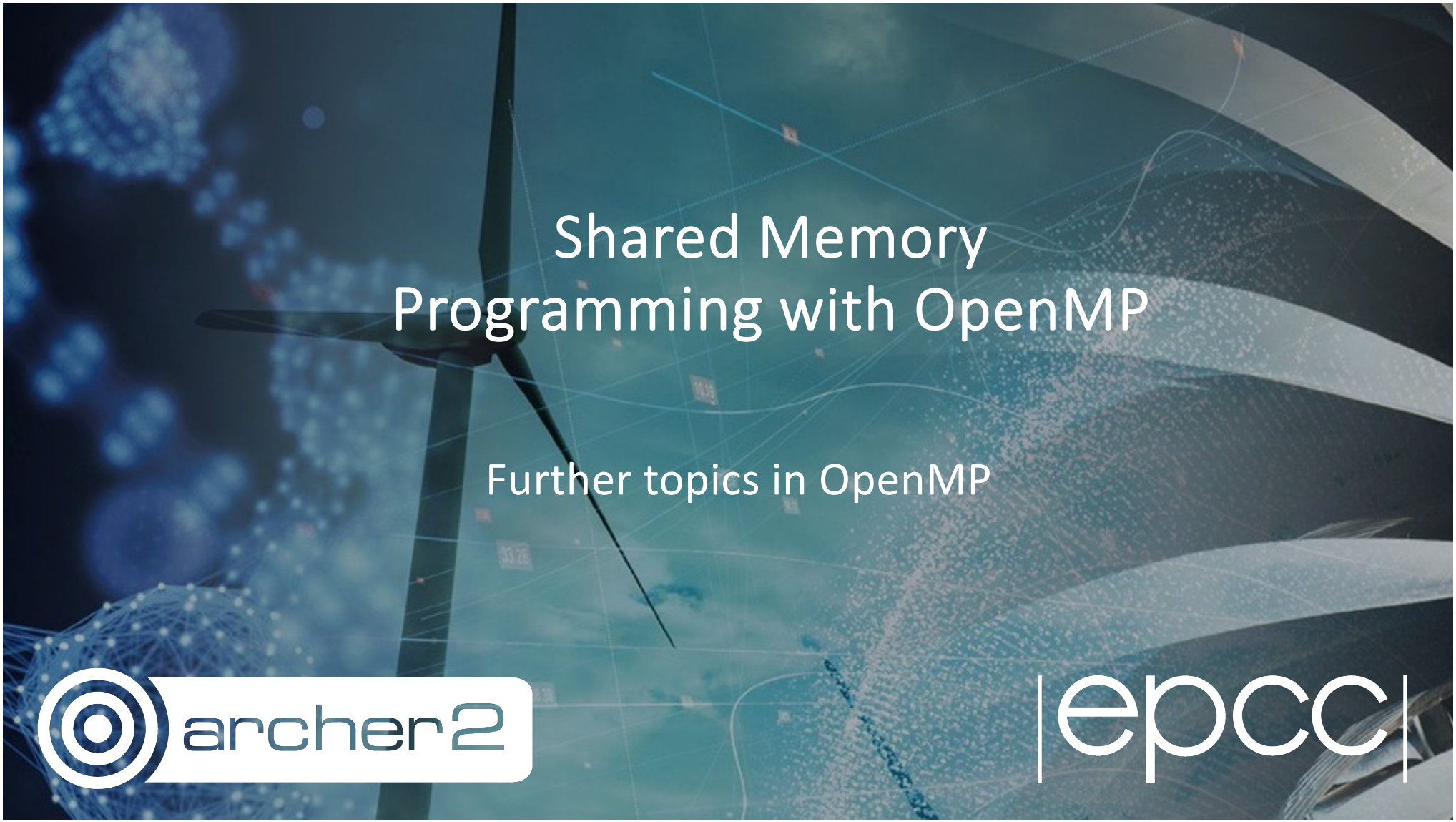

Shared Memory
Programming with OpenMP
Further topics in OpenMP
archer2
epcc

Overview

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

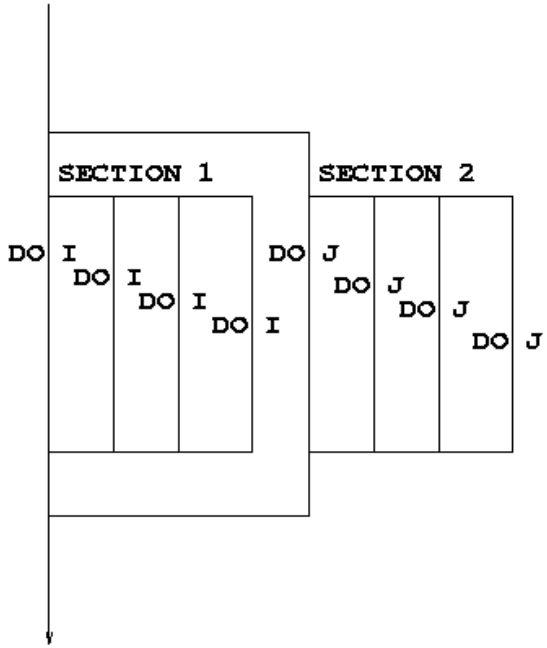
Nested parallelism

- Not often needed, but can be useful if the outer level does not contain enough parallelism, or if you want subsets of threads doing different things.
- If a PARALLEL construct is encountered within another PARALLEL construct, a new team of threads will be created.
- This is enabled with the `OMP_NESTED` environment variable or the `omp_set_nested()` routine.
- Usually disabled by default as it has some overheads
  - don't enable nested parallelism unless you are using it!
- If nested parallelism is disabled, code with nested parallel regions will still execute, 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
```



Controlling the number of threads

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- 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()

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

```
omp_set_num_threads(2);
#pragma omp parallel for
  for (int i=0; i<4; i++) {
    omp_set_num_threads(innerthreads[i]);
#pragma omp parallel for
     for (int j=0; j<N; j++) {
         a[j][i] = b[j][i] * 17;
     }
  }
```

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

`num_threads` clause

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- Another way to control the number of threads used at each level is with the `num_threads` clause:

```
#pragma omp parallel for num_threads(2)
  for (int i=0; i<4; i++) {
#pragma omp parallel for num_threads(innerthreads[i])
     for (int j=0; j<N; j++) {
         a[j][i] = b[j][i] * 17;
     }
  }
```

- 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

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- `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

Synchronisation in nested parallelism

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- Note that barriers (explicit or implicit) only affect the innermost enclosing parallel region.
- No way to have a barrier across multiple teams
- In contrast, critical regions, atomics and locks affect all the threads in the program
- If you want mutual exclusion within teams but not between them, need to use locks (or atomics).

Orphaned directives

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- Directives can be present in functions called from inside parallel regions

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
```

```
#pragma omp parallel
{
   fred();
}

void fred() {
#pragma omp for
   for (int i=0; i<N; i++) {
      a[i] += 23.5;
   }
}
```

Orphaned directives (cont)

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- 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? - the worksharing loop is all executed by the master thread)
- There are some extra rules about data scope attributes….

Data scoping rules

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When we call a subroutine from inside a parallel region:

- Variables passed by reference/address 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.

- A necessary evil to avoid extensive refactoring of codes that use global variables which are not read-only inside parallel regions.
  - Don't design them into new code!

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 possibly local to a thread: should make both calls on the same thread.

Also note: no guarantees about resolution, but you can query it!

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.
- Don't expect this to change the performance much: the idea is to see how it affects data-attribute scoping
- Be careful about harmless-looking race conditions!

Reusing this material