

INAF HPC School 2025 Catania, Sep. 22nd - 26th





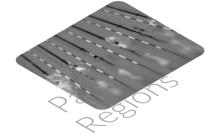


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OpenMP Outline











NUMA **AWARENESS**







OpenMP parallel loops



Loops are one of the most common work structure in HPC, and it is quite common that a vast amount of compute-intensive code resides in loops.

In fact, OpenMP, up to version 2.x, was essentially about quickly and effectively parallelizing loops without much effort. Hence, OpenMP standard presents a broad amount of features dedicated to parallel for loops.







Building up a parallel loop



```
int N = some workload;
#pragma omp parallel
  int myid = omp get thread num();
  int team = omp get num threads();
  int size = N / team;
  int rem = N % team;
  int mystart = size*mid + ((me < rem)? myid : rem);</pre>
  int myend = size + (rem > 0)*(myid < rem);</pre>
  for ( int i = mystart; i < myend; i++ )</pre>
      do something(i);
```

Splitting the work of a for loop among the threads could easily be achieved by directly assigning the boundaries of the loop to each thread.

In this example, we statically assign an equal share N/nthreads of iterations per thread, while distributing the remaining N%nthreads iteration to the first N%nthreads threads.

However, OpenMP has dedicated constructs that offer easier and more flexible mechanisms to share the work within a for loop.









Let's start with a classical and very common problem in order to understand the appropriate OpenMP work-sharing construct relative to loops.

```
double *a;
double sum = 0
int N;
...
for ( int i = 0; i < N; i++ )
        sum += a[i];</pre>
```









```
#include <omp.h>
double *a, sum = 0;
int i, N;
```

declares what variables are private: despite their name is the same within the parallel region, they have different memory locations and die with the parallel region

This is a **work-sharing** construct; workload is subdivided among threads (the default choice is implementation-dependent)

no implicit assumptions about variables scope declares what variables are shared; all threads can access and modify those memory locations







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However, variables defined (outside) within the parallel region are automatically (shared)private, and so are the integer indexes used as loop counter.

```
#include <omp.h>
double *a, sum = 0;
int
        N;
#pragma omp parallel for
for ( int i = 0; i < N; i++ )
   #pragma omp atomic
    sum += a[i];
```



What happens if you drop the atomic directive? You obtain a result that is smaller than the correct one: why?

How is the work assigned to the single threads?









How the work is assigned to the single threads?

```
#pragma omp parallel for schedule(scheduling-type)
for ( int i = 0; i < N, i++ )
```

schedule(**static**, chunk-size)

The iteration is divided in chunks of size chunk-size (or in ~equal size) distributed to threads in circular order

schedule(**dynamic**, chunk-size)

The iteration is divided in chunks of size chunk-size (or size 1) distributed to threads in no given order (a thread requests the first available chunks on a first-arrived-first-served basis)

schedule(**guided**, chunk-size)

The iteration is divided in chunks of minimum size chunk-size (or size 1) distributed to threads in no given order like dynamic. The chunk size is proportional to the number of still unassigned iterations divided by the number of threads.

runtime default The policy is set at runtime via the env. var. OMP SCHEDULE or, if that is not defined, to a default implementation-dependent value.

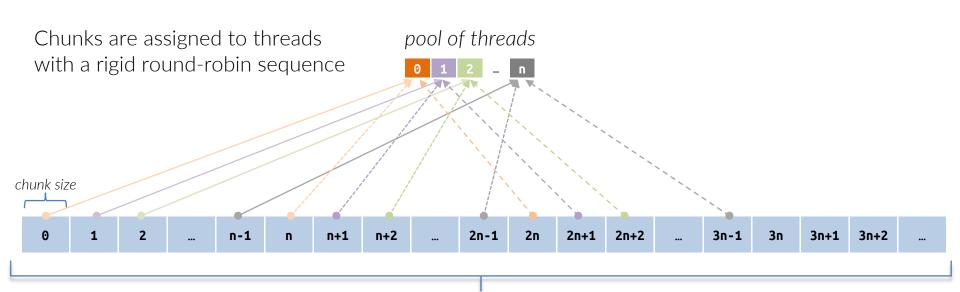






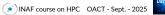


STATIC work assignment



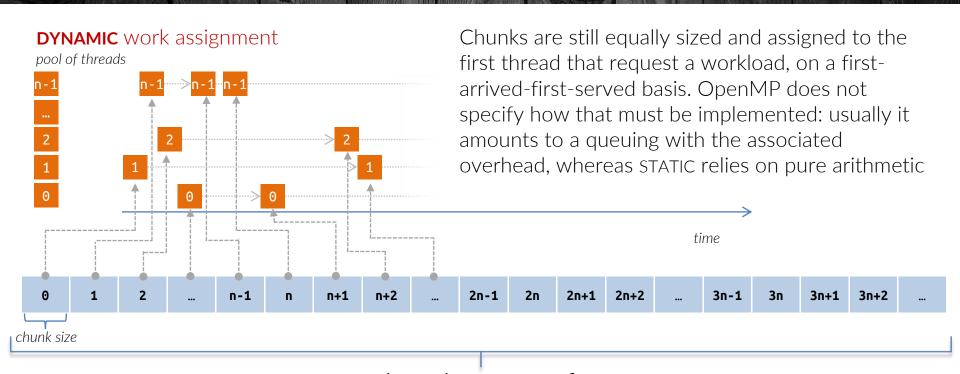
iteration space of the target for loop





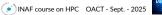






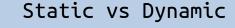
iteration space of the target for loop











end of loop with dynamic

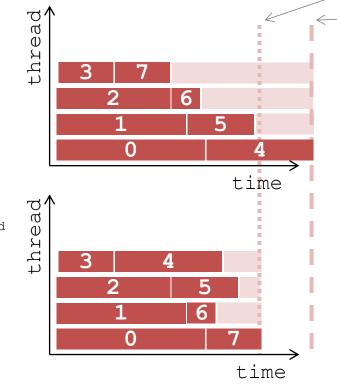
Static assignment

th 0 ← chunk 0
th 1 ← chunk 1
th 2 ← chunk 2
th 3 ← chunk 3
th 4 ← chunk 4
th 5 ← chunk 5
th 6 ← chunk 6

Dynamic assignment

← chunk 7

Chunks are assigned to the first free thread



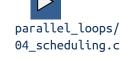
Note: in this figure, the length of each chunk on the time-line is "proportional" to its computational load; the lighter-coloured area represent the idle time of each thread (i.e. the time during which a thread is not processing any chunk).

end of loop with static

Rule-of-thumb:

the static assignment is (supposed to be) most effective when each iteration brings the same computational work, because the direct and predictable assignment has a smaller overhead:

the dynamic assignment is (supposed to be) most effective in the opposite case, i.e. when the computational load of each iteration is unpredictable.





th 7

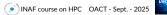






```
#pragma omp for
      schedule( policy [,chunk])
      ordered
      private ( var list )
      firstprivate ( var list )
      lastprivate (var list )
      shared ( var list )
      reduction ( op: var list )
      collapse (n)
      nowait
```









private (var list)

vars in the list will be private to each thread; despite their name is the same out of the parallel region, they have different memory locations and die with the parallel region.

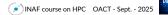
firstprivate (var list)

the variables in the list are private (in the same sense than in *private*) and are initialized at the value that shared variables have at the begin of the parallel region.

lastprivate (var list)

the shared variables will have the value of the private var in the last thread that ends the work in the parallel region.









firstprivate & lastprivate

```
double PI
                       = 3.1415blablabla;
int
       morning coffees = MAX INTEGER;
char
       password[]
                       = "dont ask dont tell"
       final mark;
int
#pragma omp parallel firstprivate( PI, morning_coffees)\
                     private(password)
    drink mycoffees( morning coffees );
    use pi( PI );
    password = setup_mypassword();
    int exam passed = 0;
    while (!exam_passed) { exam_passed = try() }
   #pragma omp for lastprivate( final mark)
    for( int i; i < nthreads; i++ )</pre>
      final mark = exam passed;
```

```
parallel_loops/
05_first_and_last_private.c
```

PI and morning_coffees are private copies of the homonym variables outside the parallel region;

password is just a different variable that has nothing to do with the outer password;

final_mark, which arrives at the last for cycle as
a shared variable, at the end will contain the last
final mark assigned







reduction (op: var list)

Possible operators are: +, \times , -, max, min, &, &&, |, | The initial value of vars is taken into account *at the end* of the parallel for; at the begin of the for, initialization values are what you logically expect: 0 for add, 1 for mul, min and max of the result type for max and min.

collapse (n)

Enable the parallelization of multiple loops level (must be perfectly nested)

nowait

```
Ignore the implicit barrier at the end of parallel region or work-sharing construct
```









```
#include <omp.h>
double *a, sum = 0;
int N;

#pragma omp parallel for
for ( int i = 0; i < N; i++ )
    sum += a[i];</pre>
```

Without the atomic directive, the assignment

determines a **data race**: between two synchronization points at least one thread writes to a data location from which another threads reads.









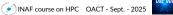
A data race happens when at least two memory accesses

- point the same location
- are performed concurrently by different threads
- are not sync ops
- at least one is a write.

A race condition is a semantic error in the code. Due to the random ordering of events, it leads the fact that its behaviour is non-deterministic and the result is not correct.

You find here a very nice discussion on these two concepts https://blog.regehr.org/archives/490









```
#pragma omp parallel for
                          Let's get back to our example to examine what may happen in reality.
for ( int i = 0; i < N; i++ )
   sum += a[i];
Let's suppose that we are using 2 threads and that array a has the following 10 entries:
 a[] = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\};
If we use schedule static, thread 0 will process a [0:4] and thread 1 will process a [5:9]
Remember that the single-line instruction
 sum += a[i];
actually requires in the following simplified (pseudo)intructions:
                          fetch sum from memory register A;
  mov sum → reqA
  add a[i], reqa
  mov regA → sum
```









| | 1 1/2 | | | | | |
|---|-------|-------------------|--------------------|--|--------------------|-----------------|
| Then, the following is one among many possible erratic combinations of execution. | Cycle | S value in memory | Thread 0 operation | note | Thread 1 operation | note |
| | | | | | | |
| | 0 | 0 | _ | let's suppose thread 0 is 1 cycle late | fetch S → regA | now regA = 0 |
| Not protecting the access to S, leads to an incorrect access. | 1 | 0 | fetch S → regA | now rega = 0 | add regA, a[i] | a[i=5] = 5 |
| | 2 | 0 | add regA, a[i] | a[i=1] = 1 | fetch regA → S | rega = 5 |
| | 3 | 5 | fetch regA → S | rega = 1 | inc i | i = 6 |
| | 4 | 1 | inc i | i = 2 | fetch S → regA | now rega = 1 |
| | 5 | 1 | fetch S → rega | now rega = 1 | add regA, a[i=6] | a[i=6] = 6 |
| | 6 | 1 | add regA, a[i] | a[i=2] = 2 | fetch regA → S | rega = 7 |
| | 7 | 7 | fetch regA → S | regA = 3 | inc i | <i>i</i> = 7 |
| ▼ICS C | | | | | | USCVIII |







After having solved the data race



Let's say that we solve the data race introducing the critical region local_sum, or an atomic directive. Does it scale? Of course no! why?

```
parallel_loops/
00_array_sum_with_race.c
```

Try to run it with a fixed, large enough, N on an increasing number of cores, and take note about the speedup. Then, measure the Parallel overhead









Why the code in the previous slide does not scale?

Because this solution makes the threads to wait for each other too frequently.

A critical region has **synchronization points** at the start and the end of critical regions, meaning that threads have to communicate with each other and decide who's waiting and who's not.

Other **sync points** are implicit and explicit barriers, locks and flush directives.









However, that is so important that the OpenMP standard offers a simple solution:

```
parallel_loops/
01_array_sum.c
```

```
#include <omp.h>
double *a, sum = 0;
int N;
```

```
#pragma omp parallel for reduction(+: sum)
for ( int i = 0; i < N; i++ )
   sum += a[i];</pre>
```

Note that *shared* clause has disappeared; implicit assumptions are ok for us.. in this simple case.









There is another way in which we can solve the conflicts on the sum

```
#include <omp.h>
double *a:
int
        N;
int
       nthreads;
#pragma omp master
nthreads = omp get num threads();
double sum[nthreads];
#pragma omp parallel
   int me = omp_get_thread_num();
   #pragma omp for
   for ( int i = 0; i < N; i++ )
     sum[me] += a[i];
```

Does this scale?









There is another way in which we can solve the conflicts on the sum

```
#include <omp.h>
               double *a:
               int
                       N;
                       nthreads:
               int
parallel_loops/
               #pragma omp master
02 falsesharing.c
               nthreads = omp get num threads();
               double sum[nthreads];
               #pragma omp parallel
                  int me = omp_get_thread_num();
                  #pragma omp for
                  for ( int i = 0; i < N; i++ )
                     sum[me] += a[i];
```

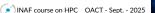
Does this scale?

Hardly

Because the values of sum[nthreads] reside in the same cache line(s); hence, when a thread access and modify its location, to maintain the coherence the cache must write-back and reflush Every time.

That is called **false sharing**







False sharing



The memory sharing is when you explicitly and purposely share some memory region among the threads; that is intentional and at the very ground of "shared-memory paradigm". You have to face all the issues about memory synchronization and caches and so on, but that is the tool to pay.

False sharing happens when each thread explicitly accesses a memory location that is different than any other thread in the parallel pool BUT at least some of those memory locations are mapped on the same cache line.

The effect of this is a very poor efficiency when te threads run on different cores.

NOTE: the false sharing is an issue when it happens a large amount of times, like in the previous example. Having an array that stores values peculiar for each threads so that they are exposed to all the other threads that access them only once a while, is something very common and not an issue (it actually is what shared memory is about..).





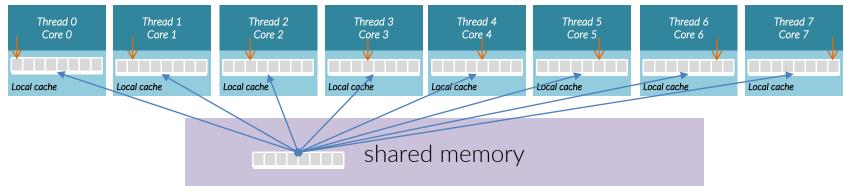




```
double sum[nthreads];
...
#pragma omp parallel
{ modify sum[me]; }
```

Each thread is modifying a memory location that is not accessed by other threads, but that is contiguous to the memory locations modified by the other threads. When we described the MESI protocol for the cache coherence, we referred to abstract "data"; however, remember that the caches *always* work by *lines* and not by single bytes and, consequently, that some bytes are modified in a cache line the whole line is flagged as modified/invalid.

Let's suppose then that 8 threads are running on 8 different cores and that each of them is writing in an array's element array[thread_id]; we also suppose this array be aligned to a cache line.









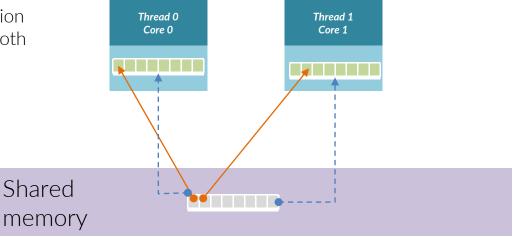
Let's concentrate on only 2 threads in order to understand in details how false sharing works.

[0] both threads read their target memory location

[1] the entire line is loaded up in the cache of both cores

[2] the line is flagged as "S" (shared)







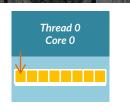


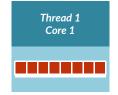




- [3] th 0 writes its target location
- [4] the line is flagged as "M" for thread 0 and "I" for all the others threads
- [5] th 0 could write again on its target location (or any other one in the line) w/o modifying the situation

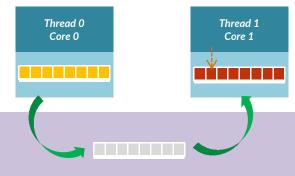
 Shared





[5] thread 1 wants to write its target location

[6] the entire cash line must be re-flushed to enforce cache-coherence because it is flagged as "I" for thread 1



Shared memory

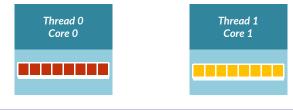
memory





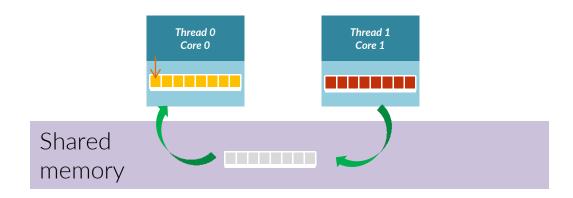


[7] once th 1 has written its target location, the entire cache line is flagged "M" for th 1 and "I" for all the other threads



Shared memory

... and so on...









There is another way in which we can solve the conflicts on the sum

```
double *a:
               int
                       N;
               int
                       nthreads:
parallel loops/
               #pragma omp master
03 falsesharing
fixed.c
               nthreads = omp get num threads();
               double sum[nthreads*8];
               #pragma omp parallel
                  int me = omp_get_thread_num();
                  #pragma omp for
                  for ( int i = 0; i < N; i++ )
                     sum[me*8] += a[i];
```

#include <omp.h>

Does this scale?

Better.

However, we are using much more memory than needed.

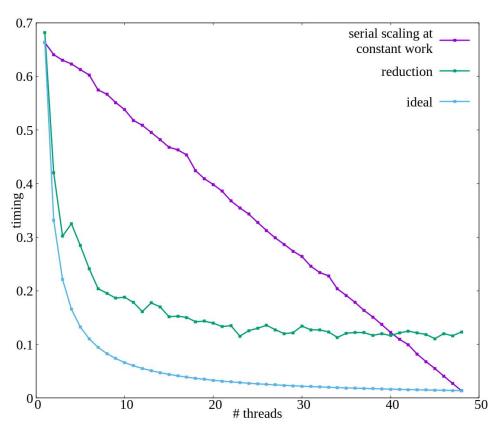
And, above all, we hard-coded a magic number (which is not a good move, in general, since it is not portable).

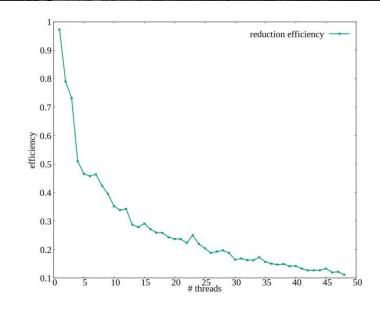












It seems that, after all, our reduction efficiency is very poor. Although one could conclude that OpenMP is somehow a bad affair, hidden in these plots there is a very important issue in multi-threading that we inquire in the next lectures.













When you declare a omp for inside an existing parallel region, there is a fundamental difference between the two codes here below. In the snippet A on the left, the for is declared without the parallel, whereas on the right, in snippet B, it has the parallel.

In A the for is shared among the threads that form the pool of the outer parallel region.

In B every thread of the pool is creating a new parallel region and inside each of the new parallel regions the new pools of threads will execute the for. So, in case B, if there are n threads in the outer parallel you will have n for cycle executed.

```
#pragma omp parallel
{
   int me = omp_get_thread_num();
   #pragma omp for
   for ( int i = 0; i < N; i++ )
      sum[me] += a[i];
}</pre>
```

```
B
#pragma omp parallel
{
   int me = omp_get_thread_num();
   #pragma omp parallel for
   for ( int i = 0; i < N; i++ )
      sum[me] += a[i];
}</pre>
```

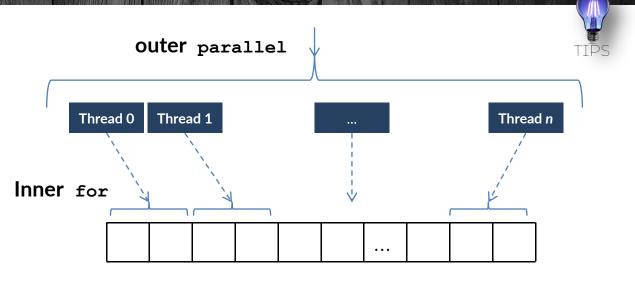








```
#pragma omp parallel
   int me = omp_get_thread_num();
   #pragma omp for
   for ( int i = 0; i < N; i++ )</pre>
      sum[me] += a[i];
```

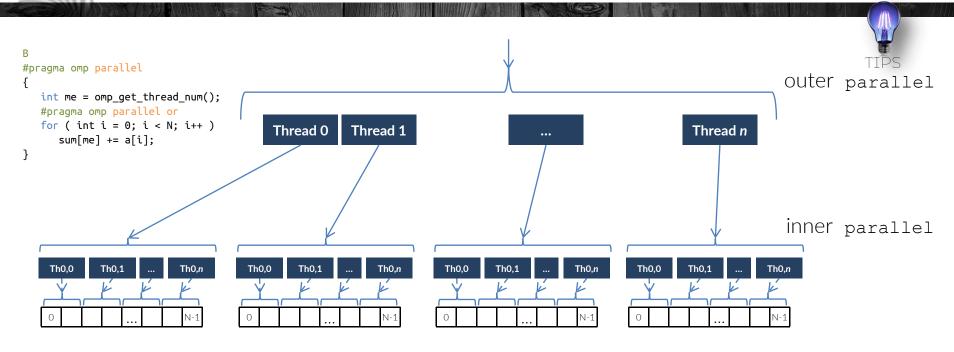


A unique foris subdivided among the threads that are in the pool



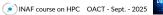






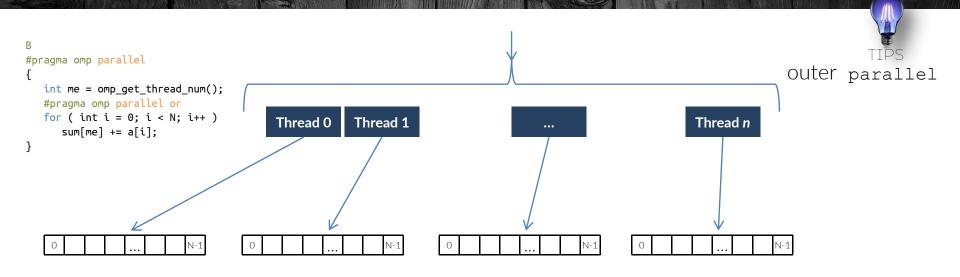
Here every thread hat participates in the outer parallel region spawns a new parallel region whose participating threads will share the for cycle. Then, we have *n* nested parallel regions each of which performs the entire for loop.











If the parallel nesting was not active at this level, each thread will enter alone in the inner parallel region executing it sequentially.

Then, each thread will execute the entire for loop.







A subtlety to note



These two "i"s are two different variables. although both are thread-private.

```
#include <omp.h>
#pragma omp parallel
   for ( i = 0; i < N; i++ )
                                                      ~/work/TEACHING/CODES/OpenMP/parallel loops$ ./01b array sum
                                             omp summation with 4 threads
                                             thread 0 : &i is 0x7ffc27c4b954
       };
                                                     thread 0 : &loopcounter is 0x7ffc27c4b958
                                             thread 1 : &i is 0x7f59f56c3ae4
                                                     thread 1: &loopcounter is 0x7f59f56c3ae8
                                             thread 2 : &i is 0x7f59f52c1b64
                                                     thread 2: &loopcounter is 0x7f59f52c1b68
                                             thread 3 : &i is 0x7f59f4ebfb64
                            parallel_loops/
                                                     thread 3: &loopcounter is 0x7f59f4ebfb68
                            01b array sum.c
                                             Sum is 4950, process took 0.000830412 of wall-clock time
```





that's all, have fun

