Distributed Computing and Introduction to High Performance Computing

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Introduction

- OpenMP is a parallel programming model which initially only targeted shared memory architectures. Today, it also targets accelerators, integrated systems and real-time systems.
- The calculation tasks can access a common memory space. This limits data redundancy and simplifies information exchanges between tasks.
- In practice, parallelization is based on the use of light-weight processes (threads). We are speaking, therefore, of a multithreaded program.

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History

- Multithreaded parallelization has existed for a long time at certain manufacturers (e.g. CRAY, NEC, IBM, ...) but each one had its own set of directives.
- The resurgence of shared memory multiprocessors made it compelling to define a standard
- The standardization attempt of the PCF (Parallel Computing Forum) was never adopted by the official standardization authorities.
- On the 28th October 1997, a large majority of industry researchers and manufacturers adopted OpenMP (Open Multi-Processing) as an "industrial standard".
- Today, the OpenMP specifications belong to the ARB (Architecture Review Board), the only organization responsible for its development.

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OpenMP Specifications

- The OpenMP 2 version was finalized in November 2000. Most importantly, it provided parallelization extensions to certain Fortran 95 constructions.
- The OpenMP 3 version of May 2008 primarily introduced the concept of tasks.
- The version OpenMP 4 of July 2013 followed by version 4.5 of November 2015 brought numerous innovations, notably accelerator support, dependencies between tasks, SIMD (vectorization) programming and management of thread placement.
- The version **OpenMP 5** of November 2018 followed by version 5.1 of November 2020 focused mainly on improving accelerator support. It also brought improvements for task programming, handling of non-uniform memory and support for the latest versions of C (11), C++ (17) and Fortran (2008) languages.

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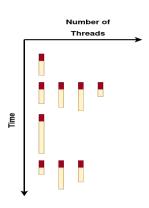
Terminology and definitions

- Thread: An execution entity with a local memory (stack).
- Team: A set of one or several threads which participate in the execution of a parallel region.
- Task: An instance of executable code and its associated data. These are generated by the PARALLEL or TASK constructs.
- Shared variable: A variable for which the name provides access to the same block of storage shared by the tasks inside a parallel region.
- Private variable: A variable for which the name provides access to a different block of storage for each task inside a parallel region.
- Host device: Hardware (usually an SMP node) on which OpenMP begins its execution.
- Target device: Hardware (accelerator card such as GPU or Xeon Phi) on which a
 portion of code and the associated data can be transferred and then executed.

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General concepts: Execution model

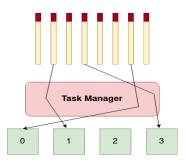
- When it begins, an OpenMP program is sequential. It has only one process, the master thread with rank 0, which executes the initial implicit task.
- OpenMP allows defining parallel regions which are code portions destined to be executed in parallel.
- At the entry of a parallel region, new threads and new implicit tasks are created. Each thread executes its implicit task concurrently with the others in order to share the work
- An OpenMP program consists of an alternation between sequential regions and parallel regions.



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General concepts: Threads (light-weight processes)

- Each thread executes its own sequence of instructions corresponding to its task.
- The operating system chooses the execution order of the processes (light-weight or not). It assigns them to the available computing units (processor cores).
- There is no guarantee of the overall order in which the parallel program instructions will be executed

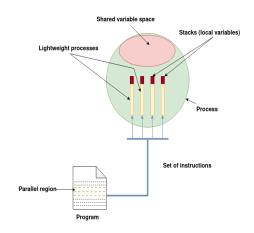


Processors

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General concepts: Threads (light-weight processes)

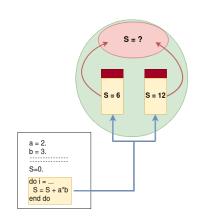
- Tasks of the same program share the memory space of the initial task (shared memory) but also dispose of a local memory space: the stack.
- Therefore, it is possible to define the shared variables (stored in the shared memory) or the private variables (stored in the stack of each one of the tasks).



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General concepts: Threads (light-weight processes)

- In shared memory, it is sometimes necessary to introduce synchronization between concurrent tasks.
- Synchronization ensures that 2 threads do not modify the value of the same shared variable in a random order (reduction operations).



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General concepts: Threads (light-weight processes)

- OpenMP facilitates the writing of parallel algorithms in shared memory by proposing mechanisms to:
 - Share the work between tasks. For example, it is possible to distribute the iterations of a loop between the tasks. Then, when the loop acts on arrays, it can easily distribute the data processing between the threads.
 - Share or privatize the variables.
 - Synchronize the threads.
- Starting with the 3.0 version, OpenMP has also allowed expressing parallelism in the form of a group of explicit tasks to be performed. OpenMP 4.0 allows offloading a part of the work to an accelerator.

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OpenMP versus MPI

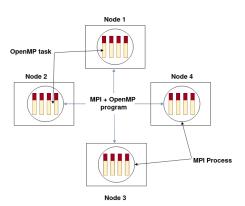
These two programming models are adapted to two different parallel architectures:

- MPI is a distributed memory programming model: Communication between the processes is explicit and the user is responsible for its management.
- OpenMP is a shared memory programming model: Each thread has a global scope of the memory.

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OpenMP versus MPI

On a cluster of independent shared memory multiprocessor machines (compute nodes), the implementation of parallelization at two levels (MPI and OpenMP) in the same program can be a major advantage for the parallel performance or the memory footprint of the code.



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programming interface: Format of a directive

An OpenMP directive has the following general form :

```
1 sentinelle directive [clause [ clause] ...]
```

- It is a comment line which is ignored by the compiler if the option that allows the interpretation of OpenMP directives is not specified.
- The sentinel is a character string whose value depends on the language used.
- There is an OMP_LIB Fortran 95 module and an 'omp.h' C/C++ include file which define the prototype of all the OpenMP functions. It is mandatory to include them in any OpenMP program unit which uses these functions.

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programming interface: Format of a directive

For Fortran, in free format

```
1 | $ use OMP_LIB
2 ...
3 ! $OMP PARALLEL PRIVATE(a,b) &
4 ! $OMP FIRSTPRIVATE(c,d,e)
5 ...
6 ! $OMP END PARALLEL ! This is a comment
```

For Fortran, in fixed format:

```
1 !$ use OMP_LIB
2 ...
3 C$OMP PARALLEL PRIVATE(a,b)
4 C$OMP! FIRSTPRIVATE(c,d,e)
5 ...
6 C$OMP END PARALLEL
```

■ For C and C++:

```
1 #ifdef _OPENMP
2 #include <omp.h>
3 #endif
4 ...
5 #pragma omp parallel private(a,b) firstprivate(c,d,e)
6 { ... }
```

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Compilation

Compilation options for activating the interpretation of OpenMP directives by some compilers are as follows:

■ The GNU compiler: -fopenmp

```
1 gfortran -fopenmp prog.f90 # Fortran compiler
```

■ The Intel compiler: -fopenmp or -qopenmp

```
1 ifort -fopenmp prog.f90 # Fortran compiler
```

■ The PGI/NVIDIA compiler : -mp

```
1 pgfortran/nvfortran -mp prog.f90 # Fortran compiler
```

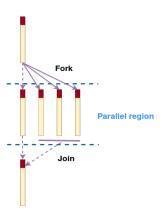
Execution example:

```
1 export OMP_NUM_THREADS = 3 # Number of desired threads
2 ./a.out # Execution
```

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Parallel construct

- An OpenMP program is an alternation of sequential and parallel regions ("fork and join" model)
- At the entry of a parallel region, the master thread (rank 0) creates/activates (forks) the "child" processes (light-weight processes or threads) and an equal number of implicit tasks. Each child thread executes its implicit task, then disappears or hibernates at the end of the parallel region (joins).
- There is an implicit synchronization barrier at the end of the parallel region.



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Compilation

- Within the same parallel region, each thread executes a separate implicit task but the tasks are composed of the same duplicated code.
- The data-sharing attribute (DSA) of the variables are shared, by default.
- There is an implicit synchronization barrier at the end of the parallel region.

```
1 program parallel
     IS use OMP LIB
     implicit none
     real · · a
    logical :: p
    a = 92290; p=.false.
     ISOMP PARALLEL
10
    !$ p = OMP_IN_PARALLEL()
11
     print * "A = " ,a
12
     ISOMP FND PARALLEL
13
     print*," Parallel ?:", p
14
15 end program parallel
```

```
1 ifort -fopenmp example2.f90
2 export OMP_NUM_THREADS =3
3 a.out
```

```
1 A = 92290.0000
2 A = 92290.0000
3 A = 92290.0000
4 Parallel ?: T
```

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Compilation: Python implementation

```
if __name__ == "_-main_-":
    from pyccel.stdlib.internal.openmp import omp_in_parallel
    a = 92290
    p = True

#$omp parallel
    p = omp_in_parallel()
    print("A =", a)
#$omp end parallel

print("Parallel ?:", p)
```

```
1 pyccel --language=c example2.py --openmp
2 export OMP_NUM_THREADS=3
3 ./example2

1 A = 92290
2 A = 92290
3 A = 92290
4 Parallel ?: True
```

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Data-sharing attribute of variables: Private variables

- The PRIVATE clause allows changing the DSA of a variable to private.
- If a variable has a private DSA, it is allocated in the stack of each task.
- The private variables are not initialized on en- try to the parallel region.



```
1 program parallel
    !$ use OMP_LIB
    implicit none
    real · · a
    logical :: p
    integer :: rank
    a = 92000
10
11
    !$OMP PARALLEL private(rank, a)
12
    !$ rank = OMP_GET_THREAD_NUM()
13
    a = a + 290
    print *."Rank : ". rank. &
14
15
          "; A = ", a
16
     !SOMP END PARALLEL
17
    print * . " Out of region . A = " .a
18
19 end program parallel
```

```
1 Rank: 0; A = 290.000000
2 Rank: 2; A = 290.000000
3 Rank: 1; A = 290.000000
4 Out of region, A = 92000.0000
```

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Private variables: Python implementation

```
if __name__ = "__main__":
    from pyccel.stdlib.internal.openmp import omp_get_thread_num
    a = 92000

#$ omp parallel private(rank, a)
    rank = omp_get_thread_num()
    a = a + 290
    print("Rank:", rank, "a = ", a)

#$ omp end parallel
print("Out of the region, A will be", a)
```

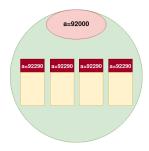
```
1 pyccel --language=c example3.py --openmp
2 export OMP_NUM_THREADS=3
3 ./example3

1 Rank: 0 a = 290
2 Rank: 2 a = 290
3 Rank: 1 a = 290
4 Out of the region, A will be 92000
```

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Data-sharing attribute of variables: Private variables

- With the FIRSTPRIVATE clause, however, it is possible to force the initialization of a private variable to the last value it had before entry to the parallel region.
- After exiting the parallel region, the private variables are lost.



```
1 program parallel
2 !$ use OMP_LIB
3
4 implicit none
5 real :: a
6 a = 92000.
7
8 !$OMP PARALLEL FIRSTPRIVATE(a)
9 a = a + 290
10 print * "A vaut : ", a
1 !$OMP END PARALLEL
12 print*,"Out of region , A = ", a
13
14 end program parallel
```

```
1 A = 92290.0000

2 A = 92290.0000

3 A = 92290.0000

4 Out of region, A = 92000.0000
```

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Private variables: Python implementation

```
if __name__ == "__main__":
    from pyccel.stdlib.internal.openmp import omp_in_parallel
    a = 92000

#$omp parallel firstprivate(a)
    a = a + 290
    print("A =", a)

#$omp end parallel

print("Out of the region, a =", a)
```

```
1 pyccel --language=c example4.py --openmp
2 export OMP_NUM_THREADS=3
3 ./example4

1 A = 92290
2 A = 92290
3 A = 92290
4 Out of the region, a = 92000
```

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Data-sharing attribute of variables: The DEFAULT clause

- The variables are shared by default but to avoid errors, it is recommended to define the DSA of each variable explicitly.
- Using the DEFAULT(NONE) clause requires the programmer to specify the status of each vari- able.
- In Fortran, it is also possible to change the implicit DSA of variables by using the DEFAULT(PRIVATE) clause.

```
1 program parallel
    !$ use OMP_LIB
    implicit none
    logical :: p
    p=.false.
     !$OMP PARALLEL DEFAULT(NONE) &
9
     !$OMP SHARED(p)
    !$ p = OMP_IN_PARALLEL ()
10
11
     ISOMP FND PARALLEL
12
13
    print*," Parallel ?:", p
14
15 end program parallel
```

```
1 Parallel ?: T
```

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Private variables: Python implementation

```
if __name__ == "...main...":
    from pyccel.stdlib.internal.openmp import omp_in_parallel

    p = False
#$omp parallel default(none) shared(p)
    p = omp_in_parallel()
#$omp end parallel
print("Parallel ?:", p)
```

```
1 pyccel --language=c example5.py --openmp
2 export OMP_NUM_THREADS=3
./example5
```

1 Parallel ?: True

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Data-sharing attribute of variables: Dynamic allocation

The dynamic memory allocation/deallocation operation can be done inside the parallel region.

- If the operation concerns a private variable, this local variable will be created/destroyed on each task.
- If the operation concerns a shared variable, it would be more prudent if only one thread (for example, the master thread) does this operation. Because of the data locality, it is recommended to initialize the variables inside the parallel region ("first touch").

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Data-sharing attribute of variables

```
1 program parallel
2 !$ use OMP LIB
3 implicit none
 4 integer::n,start,end,rank,nb_tasks,i
 5 real, allocatable, dimension(:)::a
6 n = 1024
7 allocate(a(n))
8 !$OMP PARALLEL DEFAULT(NONE) PRIVATE(start ,end , nb_tasks ,rank ,i) &
9 !$OMP SHARED(a,n) IF(n .gt. 512)
10
11
    nb_tasks= OMP_GET_NUM_THREADS () ; rank=OMP_GET_THREAD_NUM ()
12
    start=1+(rank*n)/nb_tasks
13
    end = ((rank+1)*n)/nb tasks
14
15
    do i = start, end
      a(i) = 92290. + real(i)
16
17
    end do
18
    print *,"Rank : ",rank,"; A(",start,"),...,A(",end,") : ",a(start),"←
          ,...,",a(end)
19
20
    !SOMP END PARALLEL
21
    deallocate(a)
22 end program parallel
```

```
1 Rank: 0; A(1),...,A(341): 92291.0000,..., 92631.0000
2 Rank: 1; A(342),...,A(682): 92632.0000,..., 92972.0000
3 Rank: 2; A(683),...,A(1024): 92973.0000,..., 93314.0000
```

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Data-sharing attribute of variables: IF is not supported on Pyccel

```
if name = "__main__":
1
        from pyccel.stdlib.internal.openmp import omp_get_thread_num. ←
             omp_get_num_threads
3
        import numpy as np
        n = 1024; a = np.empty(n)
        #$omp parallel default(none) private(start, end, nb_tasks, i, rank) shared(a, ↔
              n)
        nb_tasks = omp_get_num_threads()
        rank=omp_get_thread_num()
        start = int(1 + (rank * n) / nb tasks)
        end = int(((rank + 1) * n) / nb_tasks)
10
        for i in range(start, end+1):
11
            a[i] = 92290 + float(i)
        print ("Rank:", rank, ", A[", start, "],..., A[", end, "]:", a[start], a[end↔
12
             1. "...")
13
        #$omp end parallel
```

```
1 pyccel --language=c example6.py --openmp
2 export OMP_NUM_THREADS=3
3 ./example6
```

```
1 Rank: 2, A[ 683 ]..., A[ 1024 ]: 92973.00000000000 93314.00000000000 ...
2 Rank: 0, A[ 1 ]..., A[ 341 ]: 92291.00000000000 92631.00000000000 ...
3 Rank: 1, A[ 342 ]..., A[ 682 ]: 92632.00000000000 92972.000000000000 ...
```

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Extent of a parallel region

- The extent of an OpenMP construct represents its scope in the program.
- The influence (or scope) of a parallel region includes the code lexically contained in this region (the static extent) as well as the code of the called routines. The union of these two rep- resents the "dynamic extent".

```
1 program parallel
    implicit none
    ISOMP PARALLEL
    call sub()
     !SOMP END PARALLEL
  end program parallel
  subroutine sub()
    IS use OMP LIB
    implicit none
10
11
    logical :: p
12
    !$ p = OMP_IN_PARALLEL ()
13
    !$ print *." Parallel ?:". p
14 end subroutine sub
```

```
1 Parallel ?: T
2 Parallel ?: T
3 Parallel ?: T
```

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Extent of a parallel region

```
from pyccel.stdlib.internal.openmp import omp_in_parallel

def sub():
    p = omp_in_parallel()
    print("Parallel ?:", p)

if __name__ = "__main__":
    #$ omp parallel
    sub()
    #$ omp end parallel
```

```
pyccel --language=c example7.py --openmp
export OMP_NUM_THREADS=3

./example7

1 Parallel ?: True
2 Parallel ?: True
3 Parallel ?: True
```

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Extent of a parallel region

- In a routine called in a parallel region, the local variables and automatic arrays are implicitly private for each task. (They are defined in the stack.)
- In C/C++, the variables declared inside a parallel region are private.

```
1 program parallel
    implicit none
    !$OMP PARALLEL DEFAULT(SHARED)
    call sub()
    ISOMP FND PARALLEL
  end program parallel
8 subroutine sub()
    IS use OMP LIB
  implicit none
11 integer :: a
12
    a = 92290
1.3
    a = a + OMP_GET_THREAD_NUM ()
14
    print *, "A = ",a
15 end subroutine sub
```

```
1 A = 92290
2 A = 92292
3 A = 92291
```

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Extent of a parallel region

```
from pyccel.stdlib.internal.openmp import omp_get_thread_num

def sub():
    a = 92290
    a += omp_get_thread_num()
    print("A will be:", a)

if __name__ = "__main__":
    #$ omp parallel default(shared)
    sub()
    #$ omp end parallel
```

```
1 pyccel --language=c example8.py --openmp
2 export OMP_NUM_THREADS=3
3 ./example8
```

```
1 A will be: 92290
2 A will be: 92291
3 A will be: 92292
```

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Transmission by arguments

In a subroutine or function, all the variables transmitted by argument (dummy parameters) inherit the DSA defined in the lexical (static) extent of the region.

```
1 program parallel
    implicit none
  integer :: a, b
    a = 92000
  !$OMP PARALLEL SHARED(a) PRIVATE(b)
    call sub(a, b)
    print *,"B = ",b
    !$OMP END PARALLEL
9 end program parallel
10
11 subroutine sub(x, y)
12 Is use OMP LIB
13 implicit none
14 integer :: x, y
    y = x + OMP_GET_THREAD_NUM ()
16 end subroutine sub
```

```
1 B = 92000
2 B = 92002
3 B = 92001
```

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2

10

11

12 13

14

Extent of a parallel region

```
from pyccel.stdlib.internal.openmp import omp_get_thread_num

def sub(x:int, y:int):
    y = x + omp_get_thread_num()
    return y

if __name__ == "__main__":
    b = 0
    a = 92000
    #$ omp parallel shared(a) private(b)
    b = sub(a, b)
    print("B will be:", b)
    #$ omp end parallel
```

```
1 pyccel — language=c example9.py — openmp
2 export OMP_NUM_THREADS=3
3 ./example9

1 B will be: 92000
2 B will be: 92001
3 B will be: 92002
```

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Static variables

- A static variable is accessible during the entire lifespan of a program.
 - In Fortran, this is the case with variables appearing in COMMON, in a MODULE, declared SAVE, or initialized in the declaration (instruction DATA or symbol =).
 - In C/C++, these are variables declared with the keyword static.
- In an OpenMP parallel region, a static variable is shared by default.

```
1 module var_stat
2 real::c
3 end module var_stat
```

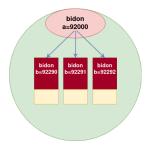
```
1 gfortran -fopenmp var_stat.f90 ↔ example9.f90
```

```
1 program parallel
    use var stat
    implicit none
    real :: a
    common /bidon/a
  ISOMP PARALLEL
    call sub()
     !SOMP END PARALLEL
9 end program parallel
10
11 subroutine sub()
12
    use var stat
13
    use OMP LIB
14
     implicit none
     real::a. b=10.
15
16
    integer :: rang
17
    common /bidon/a
18
    rang = OMP_GET_THREAD_NUM ()
19
    a=rang; b=rang; c=rang
20
    !SOMP BARRIER
21
    print *,"A, B and C: ",a,b,c
22 end subroutine sub
```

```
1 A, B and C: 2.00000000 2.00000000 2.00000000 2 A, B and C: 2.00000000 2.00000000 2.00000000 3 A, B and C: 2.00000000 2.00000000 2.00000000
```

Static variables

- The THREADPRIVATE directive allows privatizing a static instance (for the threads and not the tasks) and makes this persistent from one parallel region to another.
- If the COPYIN clause is specified, the initial value of the static instance is transmitted to all the threads.



```
1 program parallel
    IS use OMP LIB
    implicit none
    integer :: a
    common/bidon/a
  !$OMP THREADPRIVATE(/bidon/)
    a = 92000
    !$OMP PARALLEL COPYIN(/bidon/)
    a = a + OMP GET THREAD NUM ()
10
    call sub()
11
    !SOMP END PARALLEL
12
    print * . " Out of region . A = " .a
13 end program parallel
14
15 subroutine sub()
    implicit none
    integer :: a, b
    common/bidon/a
19 !$OMP THREADPRIVATE(/bidon/)
20
    b = a + 290
    print *,"B = ",b
22 end subroutine sub
```

```
1 B = 92290

2 B = 92292

3 B = 92291

4 Out of region, A = 92000
```

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Complementary information

- A parallel region construct accepts two other clauses:
 - REDUCTION: with implicit synchronization between the threads.
 - NUM_THREADS: Allows specifying the number of desired threads at the entry of a parallel region in the same way as the OMP_SET_NUM_THREADS routine would do this.
- The number of concurrent threads can vary, if desired, from one parallel region to another.

```
1 program parallel
2 implicit none
3 !SOMP PARALLEL NUM_THREADS(2)
4 print *,"Good Morning !"
5 !SOMP END PARALLEL
6 !SOMP PARALLEL NUM_THREADS(3)
7 print *,"Hello !"
8 !SOMP END PARALLEL
9 end program parallel
```

```
Good Morning!
2 Good Morning!
3 Hello!
4 Hello!
5 Hello!
```

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Complementary information

```
from pyccel.stdlib.internal.openmp import omp_get_thread_num

if __name__ = "_-main_-":
    #$ omp paralle! num_threads(2)
    print("Hello !")
    #$ omp end paralle!
    #$ omp paralle! num_threads(3)
    print("Ahoy !")
    #$ omp end paralle!
```

```
1 pyccel --language=c example10.py --openmp
2 ./example10

1 Hello!
2 Hello!
3 Ahoy!
4 Ahoy!
5 Ahoy!
```

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Complementary information

It is possible to nest parallel regions but this will have no effect if it isn't activated by a call to the OMP_SET_NESTED routine or by setting the OMP_NESTED environment variable at true.

```
1 gfortran -fopenmp prog.f90
2 export OMP_NESTED=true
3 ./a.out
```

```
1 program parallel
    IS use OMP LIB
    implicit none
    integer::rank
    !$OMP PARALLEL NUM_THREADS(3) &
    !$OMP PRIVATE(rank)
    rank=OMP_GET_THREAD_NUM ()
    print * "My rank in region 1:" rank
9
    !$OMP PARALLEL NUM_THREADS(2) &
10
    !$OMP PRIVATE(rank)
11
    rank=OMP_GET_THREAD_NUM ()
12
    print *." My rank in region 2 :".↔
          rank
13
    !SOMP END PARALLEL
    ISOMP FND PARALLEL
14
15 end program parallel
```

```
1 My rank in region 1:0
2 My rank in region 1:2
3 My rank in region 2:0
4 My rank in region 2:1
5 My rank in region 1:1
6 My rank in region 2:0
7 My rank in region 2:1
8 My rank in region 2:0
9 My rank in region 2:1
```

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```
1
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```

```
from pyccel.stdlib.internal.openmp import omp_get_thread_num

if __name__ == "__main__":
    #$ omp parallel num_threads(3) private(rank)
    rank = omp_get_thread_num()
    print("My rank in region 1:", rank)
    #$ omp parallel num_threads(2) private(rank)
    rank = omp_get_thread_num()
    print(" My rank in region 2:", rank)
    #$ omp end parallel
    #$ omp end parallel
```

```
1 pyccel --language=c example11.py --openmp
2 export OMP_NESTED=true
3 ./example11

1 My rank in region 1: 0
2 My rank in region 2: 0
4 My rank in region 2: 1
5 My rank in region 1: 2
6 My rank in region 2: 0
7 My rank in region 2: 1
8 My rank in region 2: 1
9 My rank in region 2: 1
```

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