

Programming OpenMP

Christian Terboven







Michael Klemm





Agenda (tentative – tell us what else you need) OpenMP



	Day 1	Day 2	Day 3
09:00- 10:30 CET	Introduction to OpenMP 1	Tasking 1 Tasking Intro Lab 1	OpenMP for Compute Accelerators
10:45- 12:15 CET	Hands-on: Introduction to OpenMP	Tasking 2TaskloopDependenciesCancellationLab 2	VI-HPS Tools for Performance VI-HPS Tools for Correctness
13:00- 14:45 CET	Introduction to OpenMP 2	Vectorisation Lab 3	Misc. OpenMP 5.1 Features DOACROSS Loops
15:00- 16:00 CET	Hands-on: Introduction to OpenMP If requested	Memory Access Task Affinity Memory Management Lab 4	Open Discussion OpenMP 5.1 and beyond

Material



- You can find all on github.com:
 - Slide decks
 - Exercise tasks
 - Solutions
- https://github.com/cterboven/OpenMP-tutorial-PRACE-2022







Programming OpenMP

An Overview Of OpenMP

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History

OpenMP

- De-facto standard for Shared-Memory Parallelization.
- 1997: OpenMP 1.0 for FORTRAN
- 1998: OpenMP 1.0 for C and C++
- 1999: OpenMP 1.1 for FORTRAN
- 2000: OpenMP 2.0 for FORTRAN
- 2002: OpenMP 2.0 for C and C++
- 2005: OpenMP 2.5 now includes both programming languages.
- 05/2008: OpenMP 3.0
- 07/2011: OpenMP 3.1
- 07/2013: OpenMP 4.0
- 11/2015: OpenMP 4.5
- 11/2018: OpenMP 5.0
- 11/2020: OpenMP 5.1
- 11/2021: OpenMP 5.2

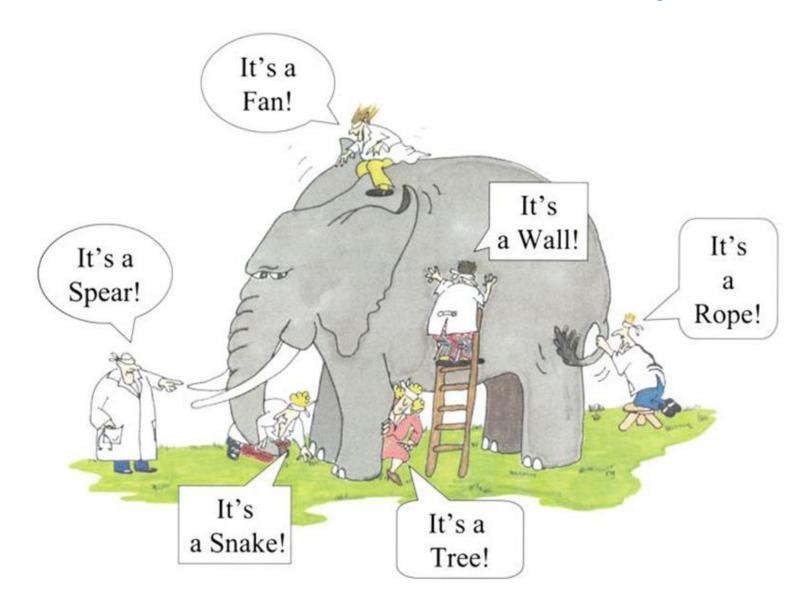


What is OpenMP?

OpenMP

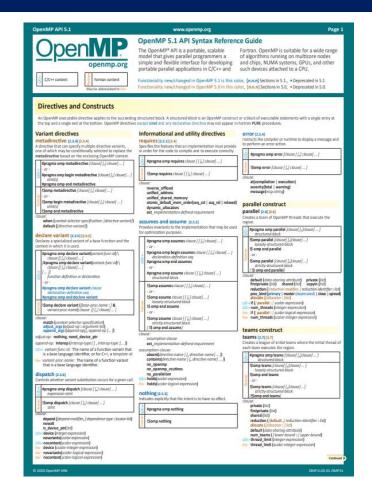
- Parallel Region & Worksharing
- Tasking
- SIMD / Vectorization
- Accelerator Programming

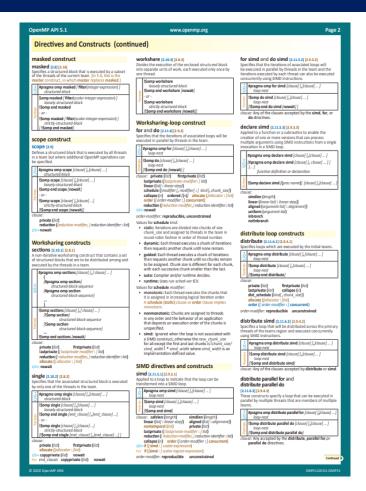
• ...





Get your C/C++ and Fortran Reference Guide! Covers all of OpenMP 5.1/5.2!



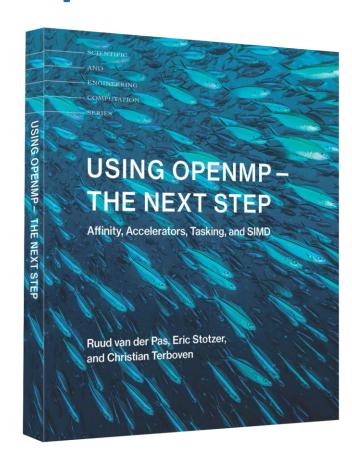


Recent Books About OpenMP

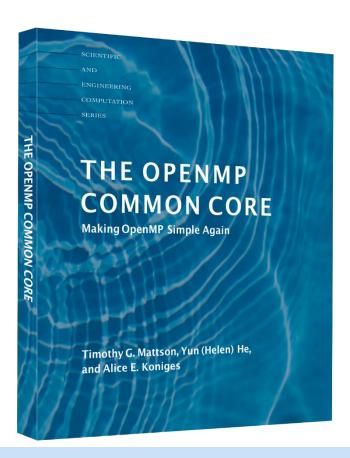




A printed copy of the 5.1 specifications, 2020



A book that covers all of the OpenMP 4.5 features, 2017



A new book about the OpenMP Common Core, 2019



Programming OpenMP

Parallel Region

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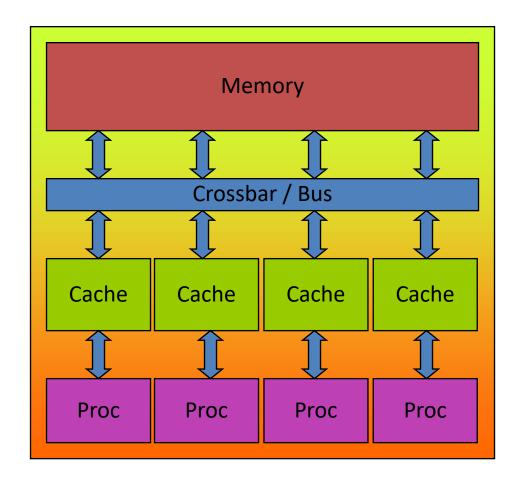
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OpenMP's machine model



OpenMP: Shared-Memory Parallel Programming Model.



All processors/cores access a shared main memory.

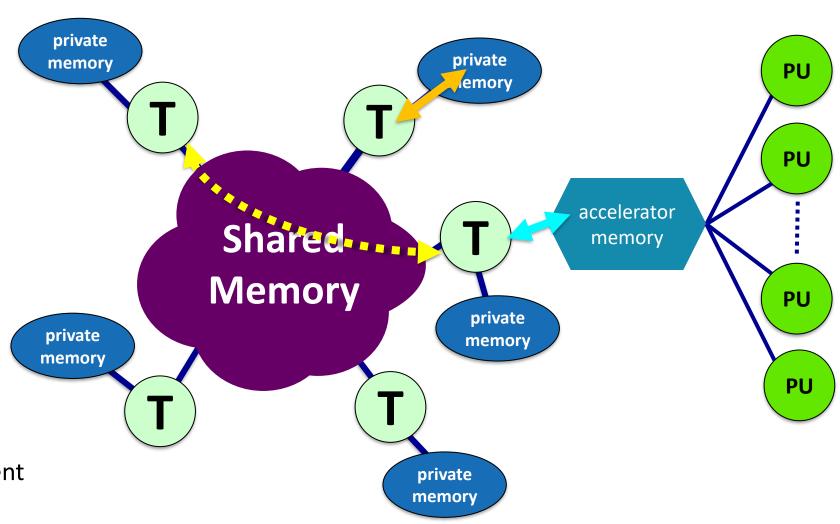
Real architectures are more complex, as we will see later / as we

Parallelization in OpenMP employs multiple threads.

The OpenMP Memory Model



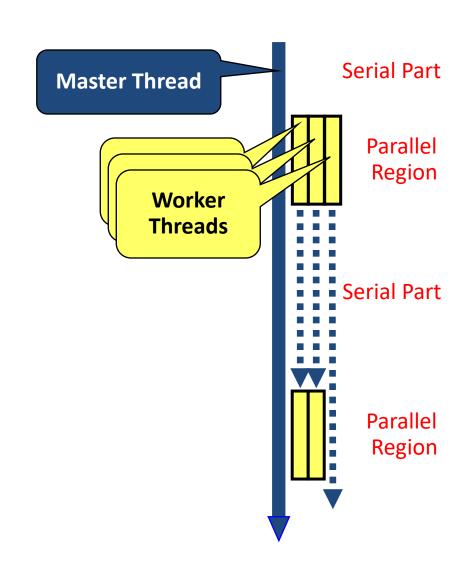
- All threads have access to the same, globally shared memory
- Data in private memory is only accessible by the thread owning this memory
- No other thread sees the change(s) in private memory
- Data transfer is through shared memory and is 100% transparent to the application



The OpenMP Execution Model

OpenMP

- OpenMP programs start with just one thread: The Master.
- Worker threads are spawned at Parallel Regions, together with the Master they form the Team of threads.
- In between Parallel Regions the Worker threads are put to sleep.
 The OpenMP Runtime takes care of all thread management work.
- Concept: Fork-Join.
- Allows for an incremental parallelization!







The parallelism has to be expressed explicitly.

```
C/C++
#pragma omp parallel
{
    ...
    structured block
    ...
}
```

```
Fortran
!$omp parallel
...
structured block
...
!$omp end parallel
```

- Structured Block
 - Exactly one entry point at the top
 - Exactly one exit point at the bottom
 - Branching in or out is not allowed
 - Terminating the program is allowed (abort / exit)

- Specification of number of threads:
 - Environment variable: OMP NUM THREADS=...
 - Or: Via num_threads clause:
 add num_threads (num) to the
 parallel construct





• From within a shell, global setting of the number of threads:

From within a shell, one-time setting of the number of threads:

Demo



Hello OpenMP World



Programming OpenMP

Worksharing

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For Worksharing



- If only the parallel construct is used, each thread executes the Structured Block.
- Program Speedup: Worksharing
- OpenMP's most common Worksharing construct: for

```
C/C++
int i;
#pragma omp for
for (i = 0; i < 100; i++)
{
   a[i] = b[i] + c[i];
}</pre>
```

```
Fortran

INTEGER :: i
!$omp do

DO i = 0, 99

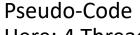
a[i] = b[i] + c[i]

END DO
```

- Distribution of loop iterations over all threads in a Team.
- Scheduling of the distribution can be influenced.
- Loops often account for most of a program's runtime!

Worksharing illustrated





Here: 4 Threads

Thread 1

Thread 2

do i = 0, 24

$$a(i) = b(i) + c(i)$$

end do

Serial

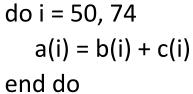
do
$$i = 0, 99$$

 $a(i) = b(i) + c(i)$
end do



a(i) = b(i) + c(i)end do

do i = 25, 49



Thread 3

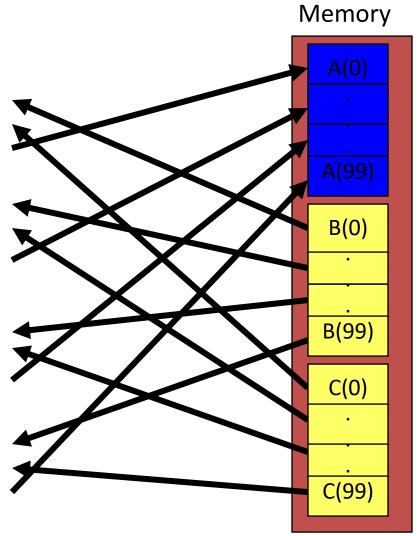
Thread 4

do i = 75, 99

$$a(i) = b(i) + c(i)$$

end do









- OpenMP barrier (implicit or explicit)
 - Threads wait until all threads of the current *Team* have reached the barrier

```
C/C++
#pragma omp barrier
```

All worksharing constructs contain an implicit barrier at the end





```
C/C++
#pragma omp single [clause]
... structured block ...
```

```
Fortran
!$omp single [clause]
... structured block ...
!$omp end single
```

- The single construct specifies that the enclosed structured block is executed by only on thread of the team.
 - It is up to the runtime which thread that is.
- Useful for:
 - I/O
 - Memory allocation and deallocation, etc. (in general: setup work)
 - Implementation of the single-creator parallel-executor pattern as we will see later...





```
C/C++
#pragma omp master[clause]
... structured block ...
```

```
!$omp master[clause]
... structured block ...
!$omp end master
```

- The master construct specifies that the enclosed structured block is executed only by the master thread of a team.
- Note: The master construct is no worksharing construct and does not contain an implicit barrier at the end.

Demo



Vector Addition





- for-construct: OpenMP allows to influence how the iterations are scheduled among the threads of the team, via the schedule clause:
 - schedule(static [, chunk]): Iteration space divided into blocks of chunk size, blocks are assigned to threads in a round-robin fashion. If chunk is not specified: #threads blocks.
 - schedule (dynamic [, chunk]): Iteration space divided into blocks of chunk (not specified: 1) size,
 blocks are scheduled to threads in the order in which threads finish previous blocks.
 - schedule(guided [, chunk]): Similar to dynamic, but block size starts with implementation-defined value, then is decreased exponentially down to chunk.
- Default is schedule (static).

Influencing the For Loop Scheduling / 2



Static Schedule

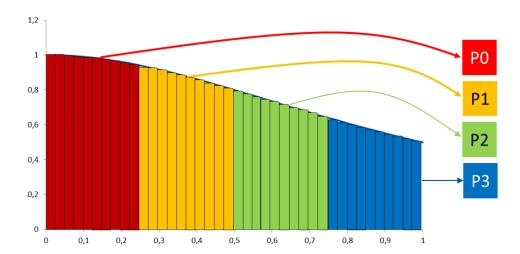
- → schedule(static [, chunk])
- Decompositiondepending on chunksize
- → Equal parts of size 'chunksize' distributed in round-robin fashion

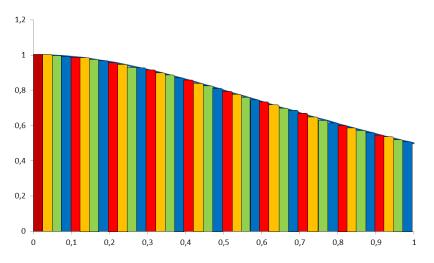
Pros?

→ No/low runtime overhead

Cons?

→ No dynamic workload balancing









- Dynamic schedule
 - schedule(dynamic [, chunk])
 - Iteration space divided into blocks of chunk size
 - Threads request a new block after finishing the previous one
 - Default chunk size is 1
- Pros ?
 - Workload distribution
- Cons?
 - Runtime Overhead
 - Chunk size essential for performance
 - No NUMA optimizations possible





- Can all loops be parallelized with for-constructs? No!
 - Simple test: If the results differ when the code is executed backwards, the loop iterations are not independent.
 BUT: This test alone is not sufficient:

```
C/C++
int i, int s = 0;
#pragma omp parallel for
for (i = 0; i < 100; i++)
{
    s = s + a[i];
}</pre>
```

• Data Race: If between two synchronization points at least one thread writes to a memory location from which at least one other thread reads, the result is not deterministic (race condition).





• A Critical Region is executed by all threads, but by only one thread simultaneously (Mutual Exclusion).

```
C/C++
#pragma omp critical (name)
{
    ... structured block ...
}
```

Do you think this solution scales well?



Programming OpenMP

Scoping

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Scoping Rules



- Managing the Data Environment is the challenge of OpenMP.
- Scoping in OpenMP: Dividing variables in shared and private:
 - private-list and shared-list on Parallel Region
 - private-list and shared-list on Worksharing constructs
 - General default is shared for Parallel Region, firstprivate for Tasks.
 - Loop control variables on for-constructs are private
 - Non-static variables local to Parallel Regions are private
 - private: A new uninitialized instance is created for the task or each thread executing the construct
 - *firstprivate*: Initialization with the value before encountering the construct
 - *lastprivate*: Value of last loop iteration is written back to Master
 - Static variables are shared

Tasks are introduced later





- Global / static variables can be privatized with the threadprivate directive
 - One instance is created for each thread
 - Before the first parallel region is encountered
 - Instance exists until the program ends
 - Does not work (well) with nested Parallel Region
 - Based on thread-local storage (TLS)
 - TlsAlloc (Win32-Threads), pthread_key_create (Posix-Threads), keyword thread (GNU extension)

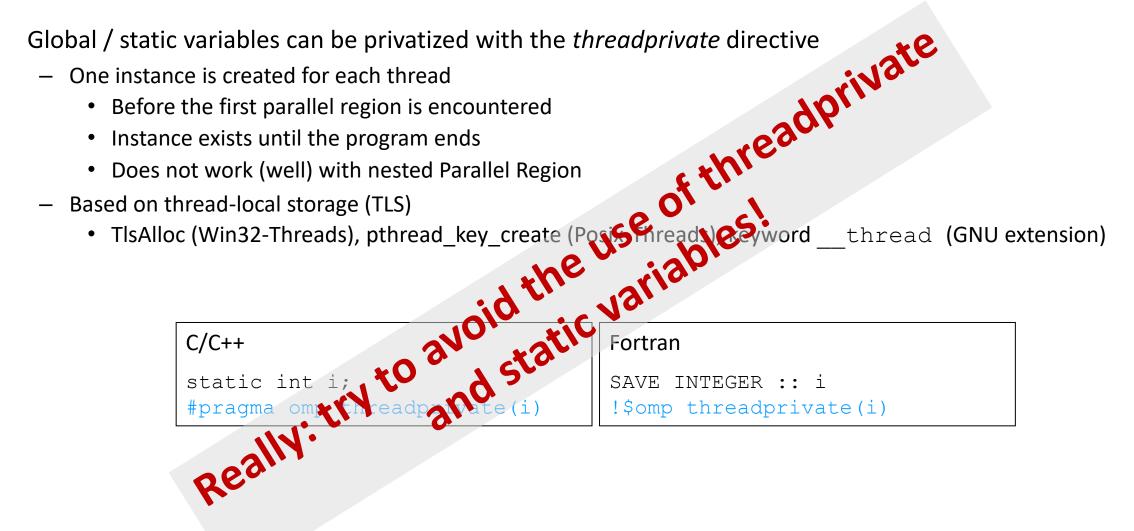
```
C/C++
static int i;
#pragma omp threadprivate(i)
```

```
Fortran
```

```
SAVE INTEGER :: i
!$omp threadprivate(i)
```

Privatization of Global/Static Variables







Back to our example

It's your turn: Make It Scale!



```
#pragma omp parallel
#pragma omp for
  for (i = 0; i < 99; i++)
        s = s + a[i];
} // end parallel
```

s = s + a(i)

end do

do i = 50, 74 s = s + a(i) end do

(done)



```
#pragma omp parallel
  double ps = 0.0; // private variable
#pragma omp for
  for (i = 0; i < 99; i++)
        ps = ps + a[i];
#pragma omp critical
   s += ps;
 // end parallel
```

```
do i = 0, 99
  s = s + a(i)
end do
```

do i = 0, 24

$$s_1 = s_1 + a(i)$$

end do
 $s = s + s_1$

do i = 25, 49

$$s_2 = s_2 + a(i)$$

end do
 $s = s + s_2$

do i = 50, 74

$$s_3 = s_3 + a(i)$$

end do
 $s = s + s_3$

do i = 75, 99

$$s_4 = s_4 + a(i)$$

end do
 $s = s + s_4$

The Reduction Clause



- In a reduction-operation the operator is applied to all variables in the list. The variables have to be shared.
 - reduction(operator:list)
 - The result is provided in the associated reduction variable

```
C/C++
int i, s = 0;
#pragma omp parallel for reduction(+:s)
for(i = 0; i < 99; i++)
{
    s = s + a[i];
}</pre>
```

Possible reduction operators with initialization value:

```
+ (0), * (1), - (0), & (~0), | (0), && (1), || (0), ^ (0), min (largest number), max (least number)
```

Remark: OpenMP also supports user-defined reductions (not covered here)

Example



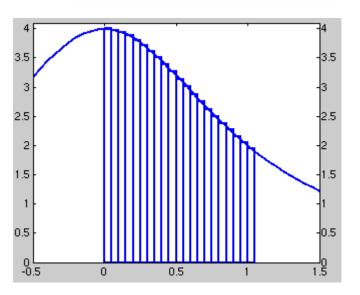
PI

Example: Pi (1/2)



```
double f(double x)
  return (4.0 / (1.0 + x*x));
double CalcPi (int n)
  const double fH = 1.0 / (double) n;
  double fSum = 0.0;
  double fX;
  int i;
#pragma omp parallel for
  for (i = 0; i < n; i++)
    fX = fH * ((double)i + 0.5);
    fSum += f(fX);
  return fH * fSum;
```

$$\pi = \int_{0}^{1} \frac{4}{1 + x^2}$$

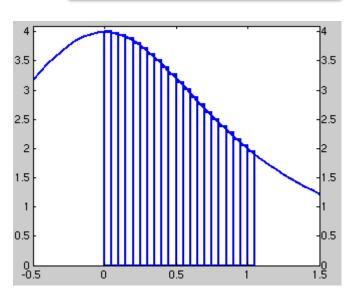


Example: Pi (2/2)



```
double f(double x)
  return (4.0 / (1.0 + x*x));
double CalcPi (int n)
  const double fH = 1.0 / (double) n;
  double fSum = 0.0;
  double fX;
  int i;
#pragma omp parallel for private(fX,i) reduction(+:fSum)
  for (i = 0; i < n; i++)
    fX = fH * ((double)i + 0.5);
    fSum += f(fX);
  return fH * fSum;
```

$$\pi = \int_{0}^{1} \frac{4}{1 + x^2}$$



Demo



PI



Using OpenMP Compilers

Christian Terboven



Production Compilers w/ OpenMP Support



- GCC
- clang/LLVM
- Intel Classic and Next-gen Compilers
- AOCC, AOMP, ROCmCC
- IBM XL
- ... and many more
- See https://www.openmp.org/resources/openmp-compilers-tools/ for a list

Compiling OpenMP



- Enable OpenMP via the compiler's command-line switches
 - → GCC: -fopenmp
 - → clang: -fopenmp
 - → Intel: -fopenmp or -qopenmp (classic) or -fiopenmp (next-gen)
 - → AOCC, AOCL, ROCmCC: -fopenmp
 - → IBM XL: -qsmp=omp
- Switches have to be passed to both compiler and linker:

```
$ gcc [...] -fopenmp -o matmul.o -c matmul.c
$ gcc [...] -fopenmp -o matmul matmul.o
$./matmul 1024
Sum of matrix (serial): 134217728.000000, wall time 0.413975, speed-up 1.00
Sum of matrix (parallel): 134217728.000000, wall time 0.092162, speed-up 4.49
```



Hands-on Exercises

Christian Terboven



Webinar Exercises



- We have implemented a series of small hands-on examples that you can use and play with.
 - → Download: git clone https://github.com/cterboven/OpenMP-tutorial-PRACE-2022.git
 - → Build: make (in the corresponding subdirectories)
 - → You can then find the compiled code in the "bin" folder to run it
 - → We use the GCC compiler mostly, some examples require Intel's Math Kernel Library
- Each hands-on exercise has a folder "solution"
 - → It shows the OpenMP directive that we have added
 - → You can use it to cheat ©, or to check if you came up with the same solution
- Also provided: basic exercises in the openmp-simple-exercises.tar archive
 - → Instructions contained in the archive: Exercises_OMP_2021.pdf



OpenMP Tasking Introduction

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What is a Task in OpenMP?



- Tasks are work units whose execution
 - → may be deferred or...
 - → ... can be executed immediately
- Tasks are composed of
 - → code to execute, a data environment (initialized at creation time), internal control variables (ICVs)
- Tasks are created...
 - ... when reaching a parallel region \rightarrow implicit tasks are created (per thread)
 - ... when encountering a task construct \rightarrow explicit task is created
 - ... when encountering a taskloop construct \rightarrow explicit tasks per chunk are created
 - ... when encountering a target construct \rightarrow target task is created

Tasking Execution Model



- Supports unstructured parallelism
 - → unbounded loops

```
while ( <expr> ) {
    ...
}
```

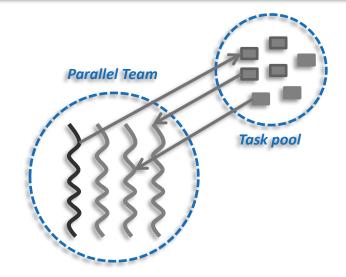
recursive functions

```
void myfunc( <args> )
{
    ...; myfunc( <newargs> ); ...;
}
```

- Several scenarios are possible:
 - → single creator, multiple creators, nested tasks (tasks & WS)
- All threads in the team are candidates to execute tasks

Example (unstructured parallelism)

```
#pragma omp parallel
#pragma omp master
while (elem != NULL) {
    #pragma omp task
        compute(elem);
    elem = elem->next;
}
```



OpenMP Tasking Idiom



- OpenMP programmers need a specific idiom to kick off task-parallel execution: parallel master
 - → OpenMP version 5.0 introduced the parallel master construct
 - → With OpenMP version 5.1 this becomes parallel masked

```
int main(int argc, char* argv[])
 2
 3
         [\ldots]
        #pragma omp parallel
 4
 5
 6
            #pragma omp master
                start task parallel execution();
 9
 9
10
         [\ldots]
11
12 }
```





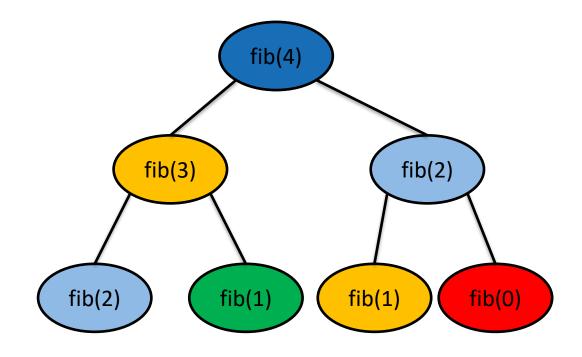
```
int main(int argc,
              char* argv[])
        [\ldots]
        #pragma omp parallel
            #pragma omp master
                fib(input);
10
11
12
         [\ldots]
13 }
```

```
int fib(int n)
        if (n < 2) return n;</pre>
16
        int x, y;
        #pragma omp task shared(x)
17
18
             x = fib(n - 1);
19
20
21
        #pragma omp task shared(y)
22
             y = fib(n - 2);
23
24
25
        #pragma omp taskwait
26
             return x+y;
27 }
```

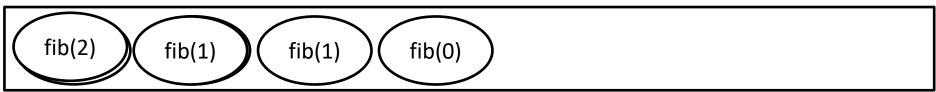
- Only one thread enters fib() from main().
- That thread creates the two initial work tasks and starts the parallel recursion.
- The taskwait construct is required to wait for the result for x and y before the task can sum up.



- T1 enters fib(4)
- T1 creates tasks for fib(3) and fib(2)
- T1 and T2 execute tasks from the queue
- T1 and T2 create 4 new tasks
- T1 T4 execute tasks

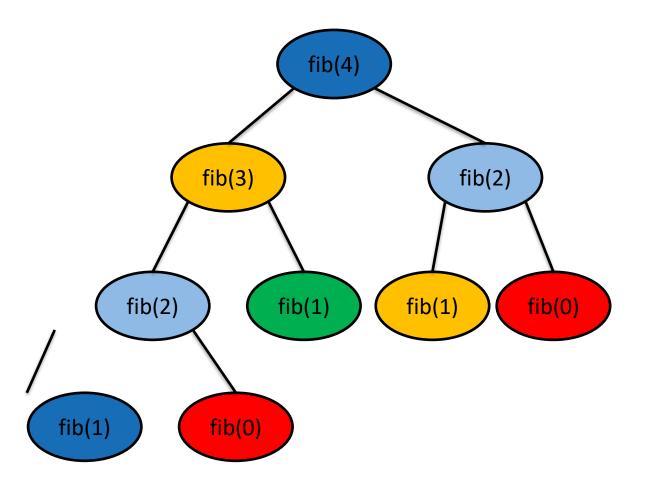








- T1 enters fib(4)
- T1 creates tasks for fib(3) and fib(2)
- T1 and T2 execute tasks from the queue
- T1 and T2 create 4 new tasks
- T1 T4 execute tasks
- ...





Hands-on Exercises

Christian Terboven





Solution of Homework Assignments





```
double do some computation(int i) {
   double t = 0.0; int j;
    for (j = 0; j < i*i; j++) {
        t += sin((double)j) * cos((double)j);
    return t;
int main(int argc, char* argv[]) {
    const int dimension = 500;
    int i;
    double result = 0.0;
    double t1 = omp get wtime();
    #pragma omp parallel for schedule(dynamic) reduction(+:result)
    for (i = 0; i < dimension; i++) {
        result += do some computation(i);
   double t2 = omp_get_wtime();
   printf("Computation took %.31f seconds.\n", t2 - t1);
    printf("Result is %.31f.\n", result);
    return 0;
```





```
void matmul seq(double * C, double * A, double * B, size t n) { ... }
void matmul par(double * C, double * A, double * B, size t n) {
#pragma omp parallel for shared(A,B,C) firstprivate(n) \
                         schedule(static) // collapse(2)
  for (size t i = 0; i < n; ++i) {
    for (size t k = 0; k < n; ++k) {
      for (size t j = 0; j < n; ++j) {
        C[i * n + j] += A[i * n + k] * B[k * n + j];
void init mat(double * C, double * A, double * B, size t n) { ... }
void dump mat(double * mtx, size t n) { ... }
double sum mat(double * mtx, size t n) { ... }
int main(int argc, char *argv[]) { ... }
```





```
void cholesky(int ts, int nt, double* Ah[nt][nt]) {
   for (int k = 0; k < nt; k++) {
                                                                      Blocked matrix
      LAPACKE dpotrf(LAPACK COL MAJOR, 'L', ts, Ah[k][k], ts);
                                                                      w/ block size ts
      #pragma omp parallel for
      for (int i = k + 1; i < nt; i++) {
         cblas dtrsm(CblasColMajor, CblasRight, CblasLower, CblasTrans,
                     CblasNonUnit, ts, ts, 1.0, Ah[k][k], ts, Ah[k][i], ts);
      #pragma omp parallel for
      for (int i = k + 1; i < nt; i++) {
         for (int j = k + 1; j < i; j++) {
            cblas dgemm (CblasColMajor, CblasNoTrans, CblasTrans, ts, ts, ts, -1.0,
            Ah[k][i], ts, Ah[k][j], ts, 1.0, Ah[j][i], ts);
         cblas dsyrk (CblasColMajor, CblasLower, CblasNoTrans, ts, ts, -1.0,
                     Ah[k][i], ts, 1.0, Ah[i][i], ts);
```