Programming OpenMP

Christian Terboven

Michael Klemm

Agenda (tentative – tell us what else you need)

	Day 1	Day 2	Day 3
09:00-10:30 CET	**Introduction to OpenMP 1**	**Tasking 1** • Tasking Intro • Lab 1	**GPUs** • OpenMP for Compute Accelerators
10:45-12:15 CET	**Hands-on: Introduction to OpenMP**	**Tasking 2** • Taskloop • Dependencies • Cancellation • Lab 2	**Tools for Perf. and Correctness** • VI-HPS Tools for Performance • VI-HPS Tools for Correctness
13:00-14:45 CET	**Introduction to OpenMP 2**	**Host Perf.: SIMD** • Vectorisation • Lab 3	**Misc. OpenMP 5.1 Features** • DOACROSS Loops
15:00-16:00 CET	**Hands-on: Introduction to OpenMP** If requested	**Host Perf.: NUMA** • Memory Access • Task Affinity • Memory Management • Lab 4	**Roadmap / Outlook** • Open Discussion • OpenMP 5.1 and beyond

Lab: hands-on time

Material

- You can find all on github.com:
  - Slide decks
  - Exercise tasks
  - Solutions

- https://github.com/cterboven/OpenMP-tutorial-PRACE-2022

GitHub

Programming OpenMP

An Overview Of OpenMP

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History

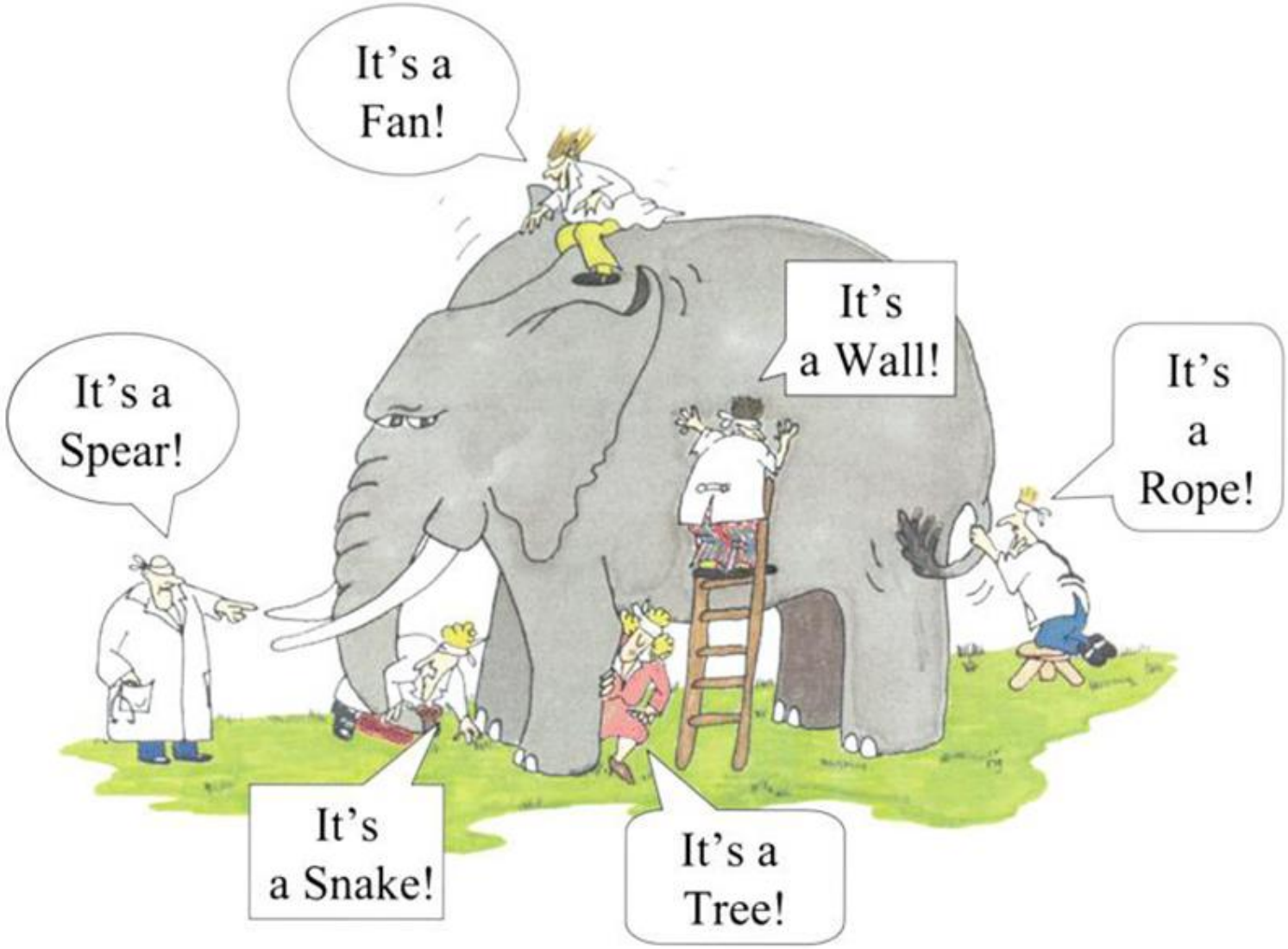
- De-facto standard for Shared-Memory Parallelization.
- 1997: OpenMP 1.0 for FORTRAN
- 1998: OpenMP 1.0 for C and C++
- 1999: OpenMP 1.1 for FORTRAN
- 2000: OpenMP 2.0 for FORTRAN
- 2002: OpenMP 2.0 for C and C++
- 2005: OpenMP 2.5 now includes both programming languages.
- 05/2008: OpenMP 3.0
- 07/2011: 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

OpenMP™

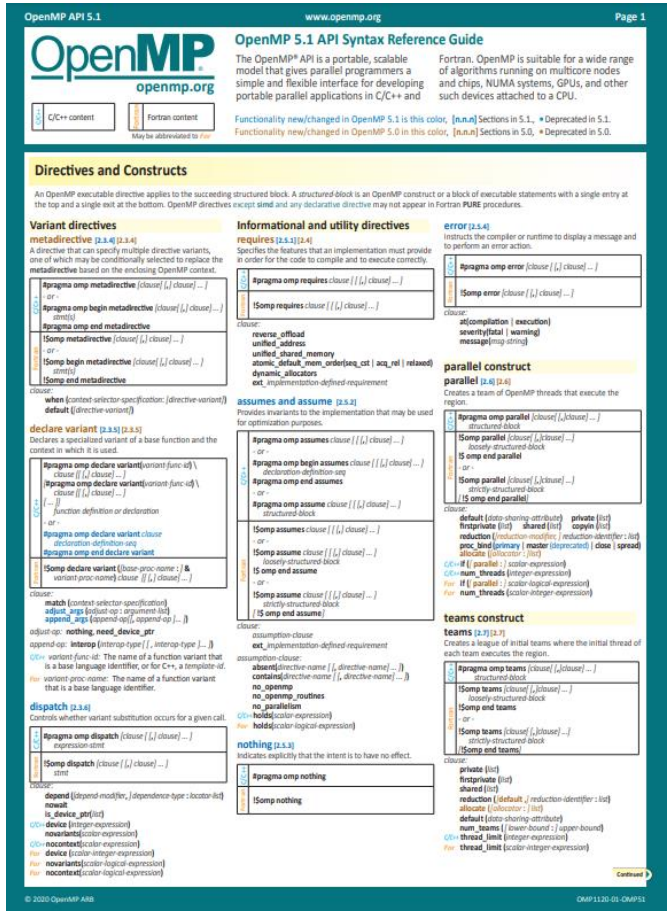
http://www.OpenMP.org

What is 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!



OpenMP API 5.1 www.openmp.org Page 1

OpenMP 5.1 API Syntax Reference Guide

The OpenMP® API is a portable, scalable model that gives parallel programmers a simple and flexible interface for developing portable parallel applications in C/C++ and Fortran. OpenMP is suitable for a wide range of algorithms running on multicore nodes and chips, NUMA systems, GPUs, and other such devices attached to a CPU.

Directives and Constructs

Variant directives

metadirective [2.3.4] [2.3.4]

declare variant [2.3.5] [2.3.5]

dispatch [2.3.6]

Informational and utility directives

requires [2.5.1] [2.4]

assumes and assume [2.5.2]

nothing [2.3.3]

error [2.5.4]

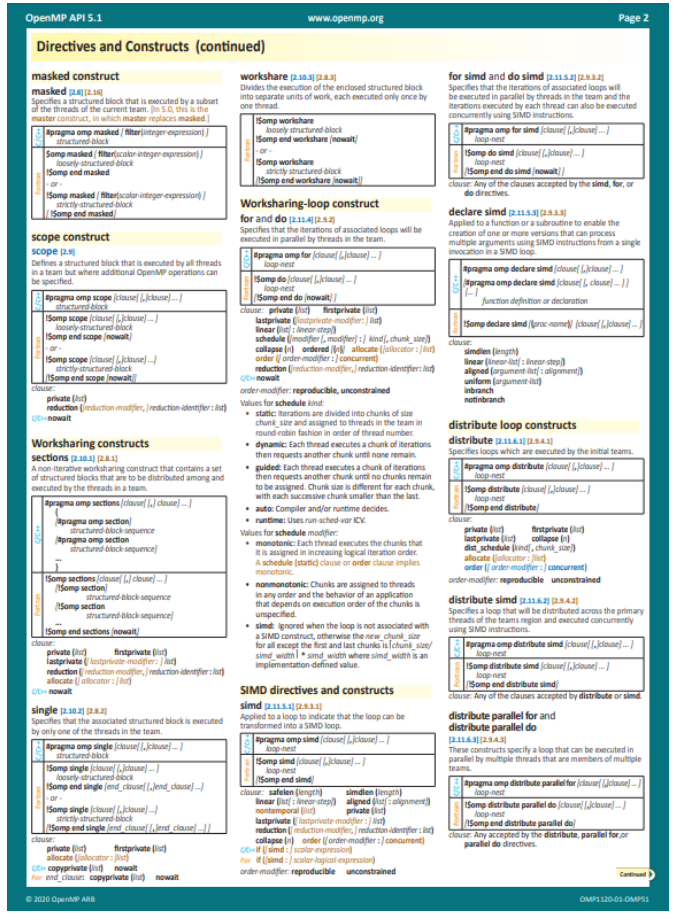
parallel construct

parallel [2.6] [2.6]

teams construct

teams [2.7] [2.7]

single [2.10.2] [2.8.2]



OpenMP API 5.1 www.openmp.org Page 2

Directives and Constructs (continued)

masked construct

masked [2.8] [2.16]

scope construct

scope [2.9]

Worksharing constructs

sections [2.10.1] [2.8.1]

workshare [2.10.3] [2.8.3]

Worksharing-loop construct

for and do [2.11.4] [2.9.2]

SIMD directives and constructs

simd [2.11.5.1] [2.9.3.1]

for simd and do simd [2.11.5.2] [2.9.3.2]

declare simd [2.11.5.3] [2.9.3.3]

distribute loop constructs

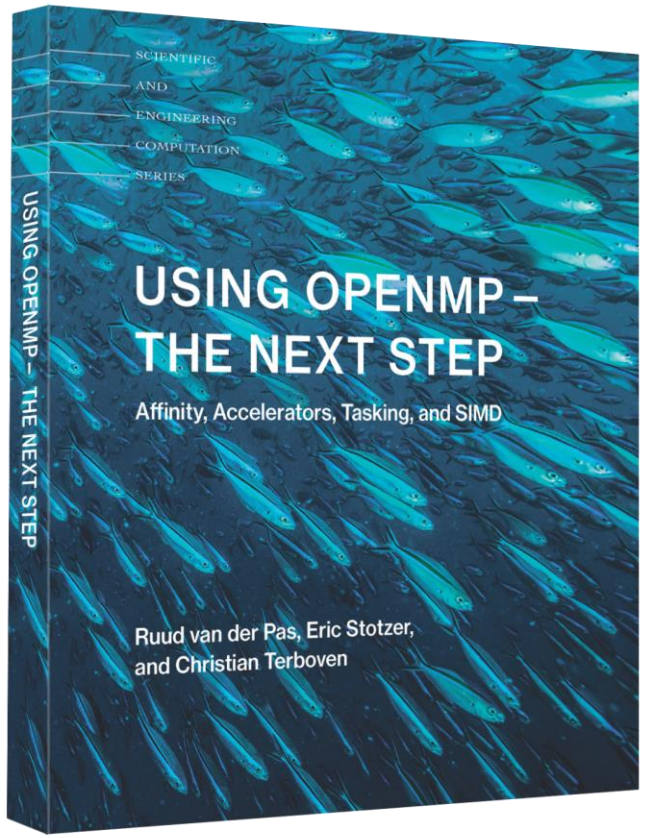
distribute [2.11.6.1] [2.9.4.1]

distribute simd [2.11.6.2] [2.9.4.2]

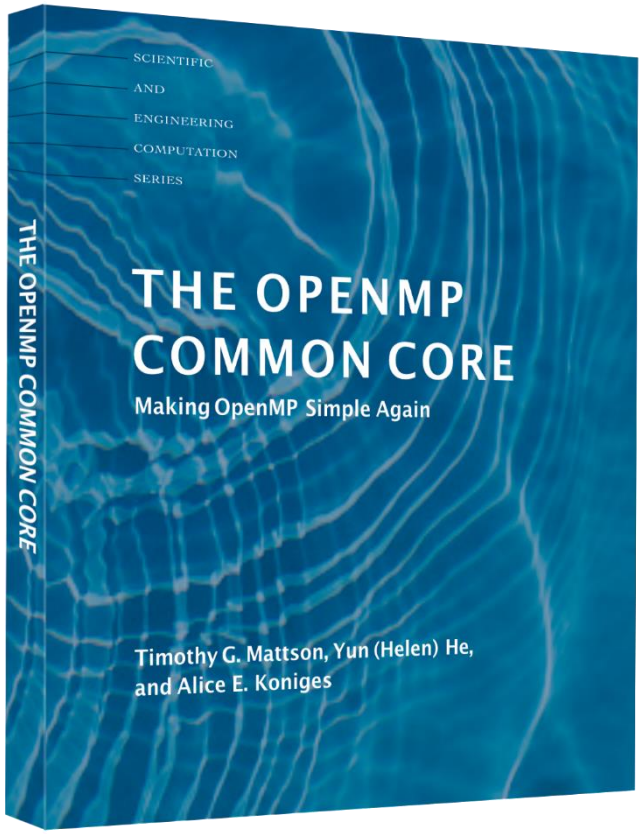
distribute parallel for and distribute parallel do [2.11.6.3] [2.9.4.3]

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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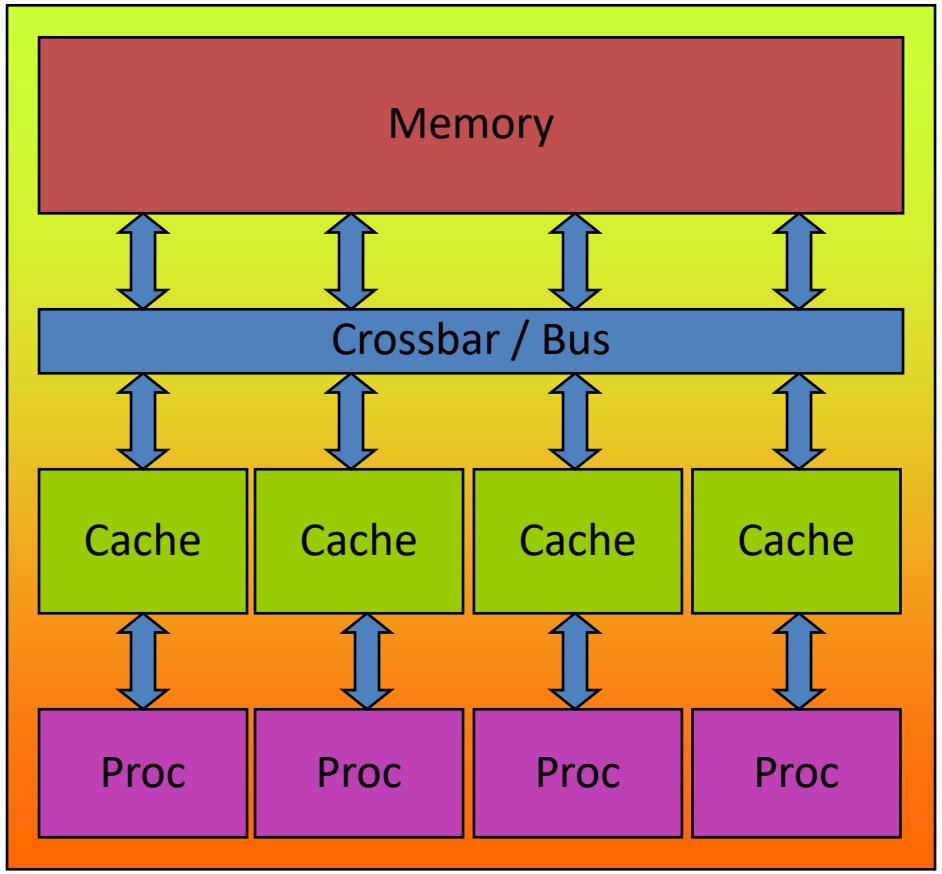
OpenMP‘s machine model

- OpenMP: Shared-Memory Parallel Programming Model.



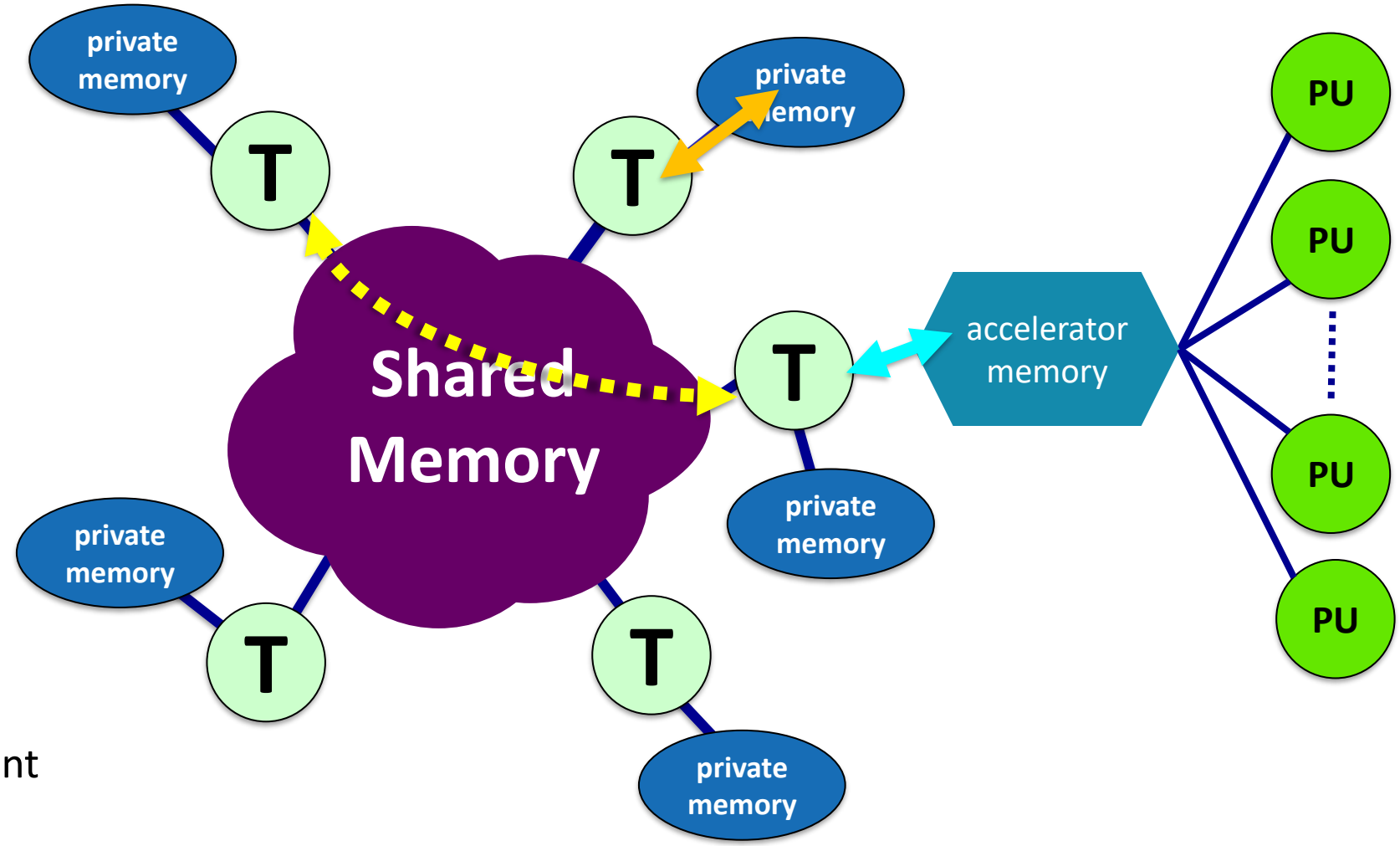
All processors/cores access a shared main memory.

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

Parallelization in OpenMP employs multiple threads.

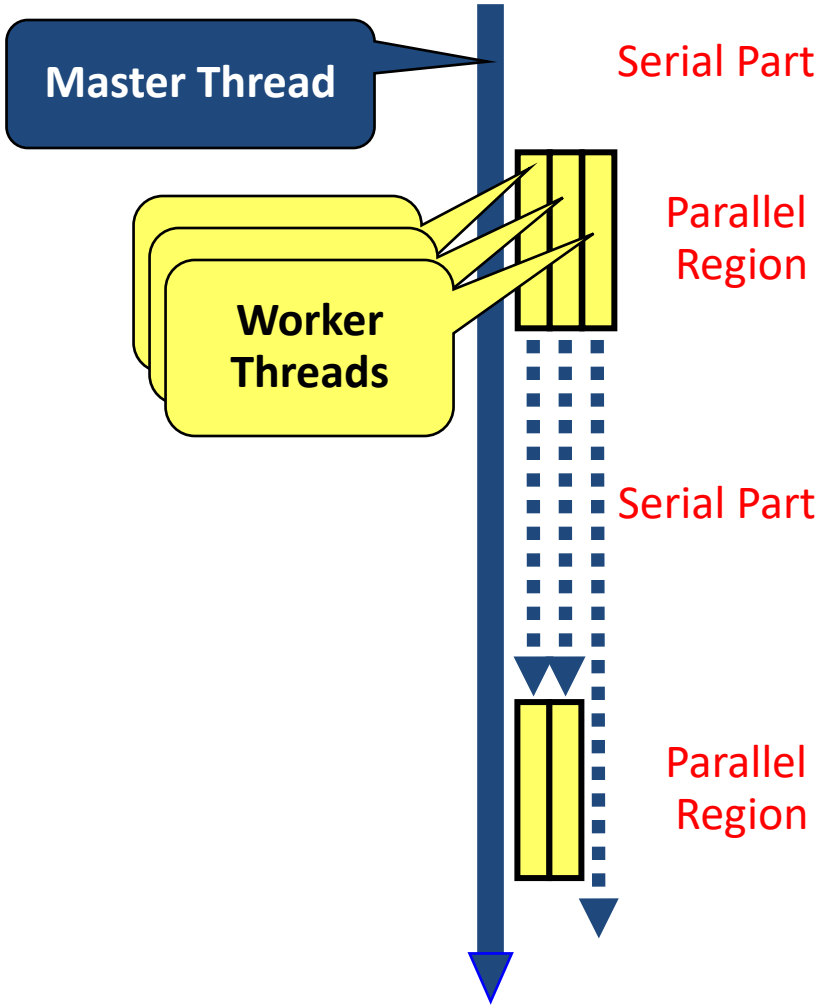
The OpenMP Memory Model

- 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 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!



Parallel Region and Structured Blocks

- 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

Starting OpenMP Programs on Linux

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

```
export OMP_NUM_THREADS=4
./program
```

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

```
OMP_NUM_THREADS=4    ./program
```

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];
}
```

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

Pseudo-Code
Here: 4 Threads

Serial

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

Thread 1

```
do i = 0, 24
    a(i) = b(i) + c(i)
end do
```

Thread 2

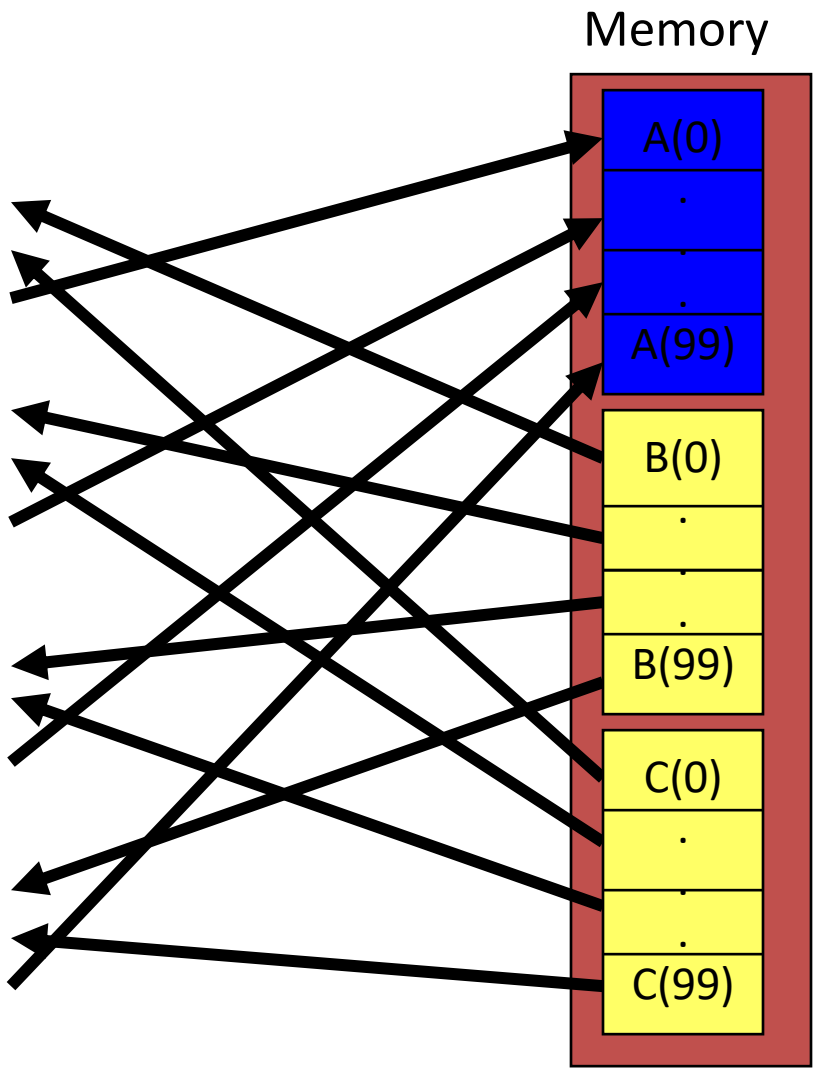
```
do i = 25, 49
    a(i) = b(i) + c(i)
end do
```

Thread 3

```
do i = 50, 74
    a(i) = b(i) + c(i)
end do
```

Thread 4

```
do i = 75, 99
    a(i) = b(i) + c(i)
end do
```



The Barrier Construct

- 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

The Single Construct

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…

The Master Construct

C/C++

```
#pragma omp master[clause]
... structured block ...
```

Fortran

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

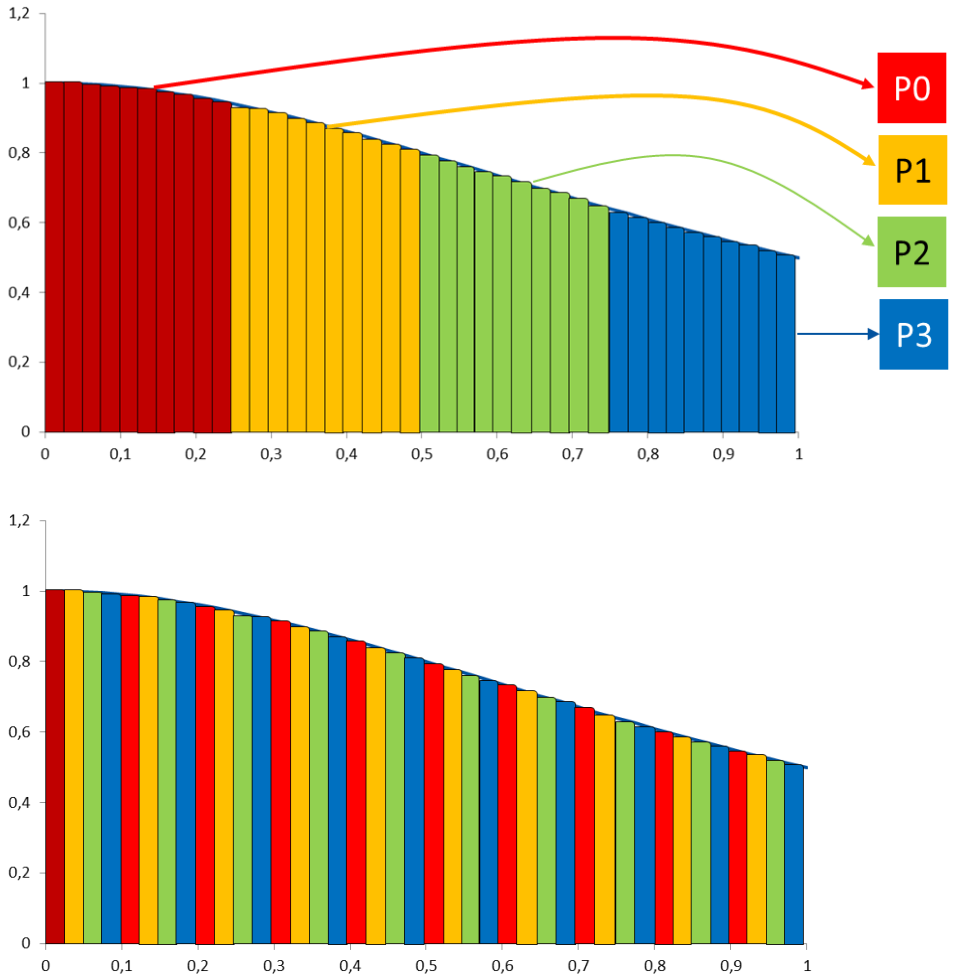
Vector Addition

Influencing the For Loop Scheduling / 1

- *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])`
  - → Decomposition depending on chunksize
  - → Equal parts of size ‘chunksize’ distributed in round-robin fashion
- **Pros?**
  - → No/low runtime overhead
- **Cons?**
  - → No dynamic workload balancing



Influencing the For Loop Scheduling / 3

- 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

Synchronization Overview

- 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];
}
```

- *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).

Synchronization: Critical Region

- 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?

C/C++

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

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

Privatization of Global/Static Variables

- 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

- 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)

Really: try to avoid the use of threadprivate and static variables!

C/C++

```
static int i;
#pragma omp threadprivate(i)
```

Fortran

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

Back to our example

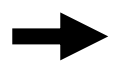
C/C++

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

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
```

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



```
do i = 0, 24
    s = s + a(i)
end do
```

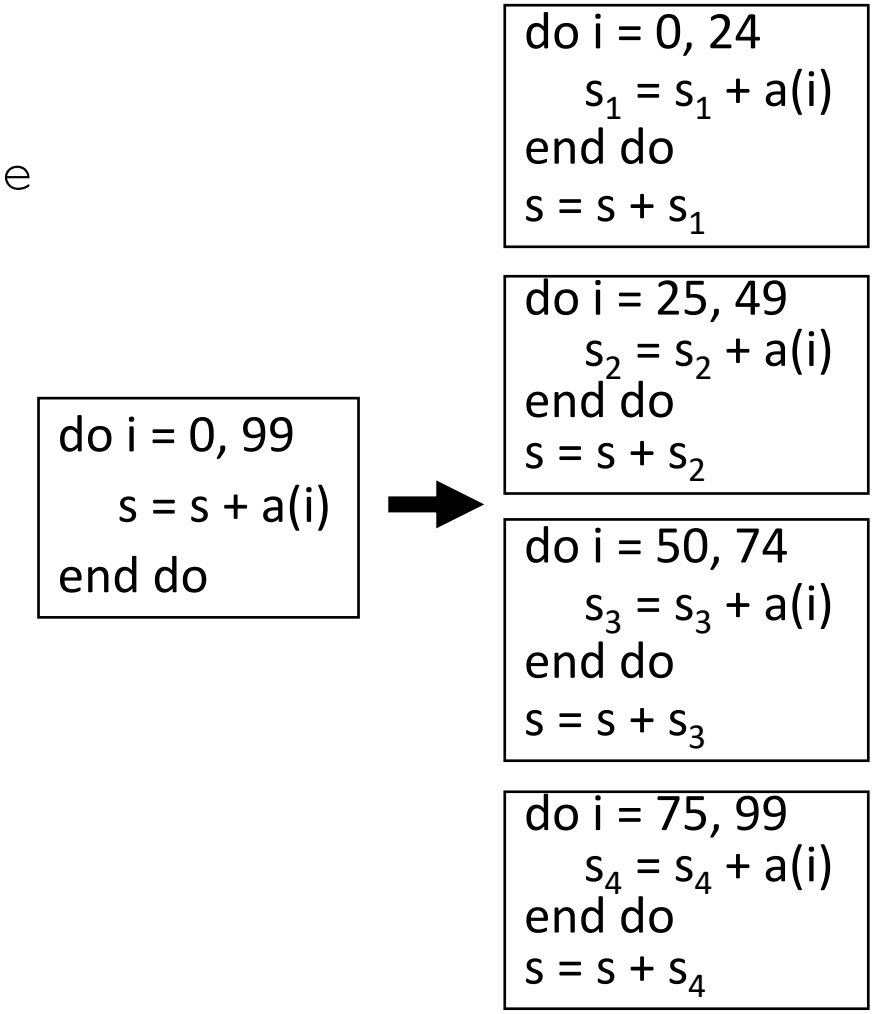
```
do i = 25, 49
    s = s + a(i)
end do
```

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

```
do i = 75, 99
    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
```



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];
}
```

  - 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)

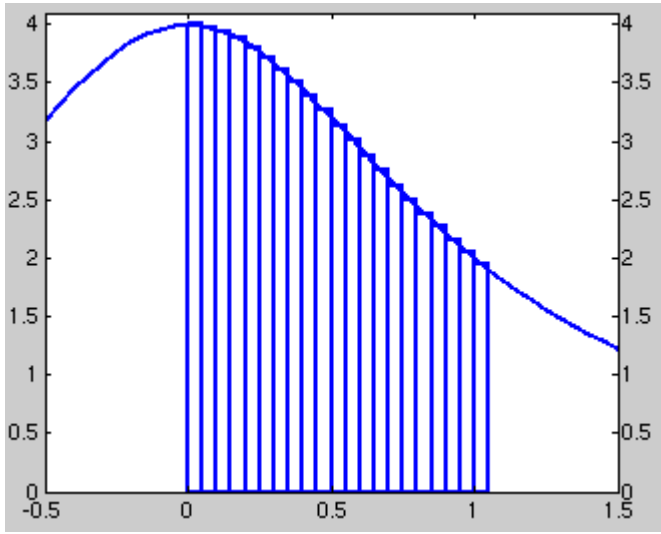
Example

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;
}
```

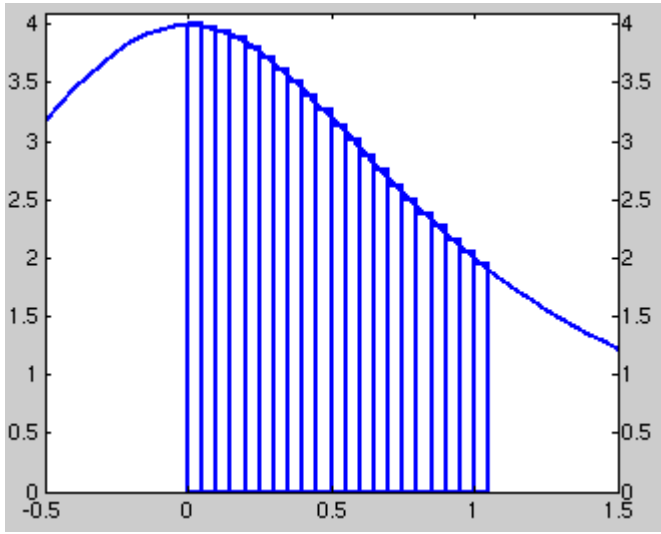
$$\pi = \int_0^1 \frac{4}{1+x^2}$$



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

Programming OpenMP

Using OpenMP Compilers

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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
```

Programming OpenMP

Hands-on Exercises

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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`
  - → 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

Programming OpenMP

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 → implicit tasks are created (per thread)
  - … when encountering a task construct → explicit task is created
  - … when encountering a taskloop construct → explicit tasks per chunk are created
  - … when encountering a target construct → target task is created

Tasking Execution Model

- Supports unstructured parallelism
  - → unbounded loops

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

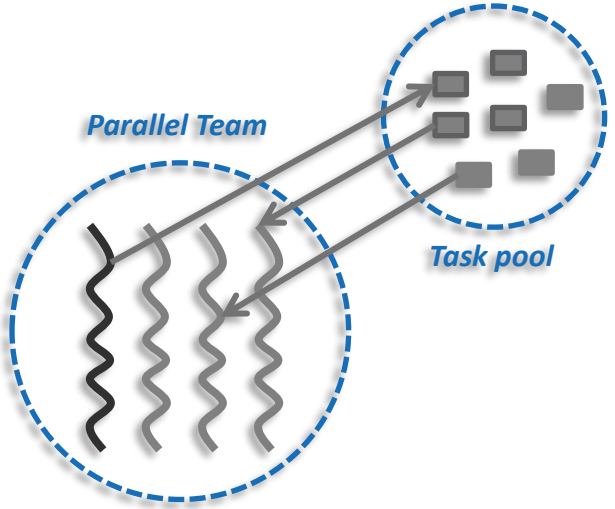
  - → recursive functions

```
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`

```
 1  int main(int argc, char* argv[])
 2  {
 3      [...]
 4      #pragma omp parallel
 5      {
 6          #pragma omp master
 7          {
 9              start_task_parallel_execution();
 9          }
10      }
11      [...]
12 }
```

```
 1  int main(int argc, char* argv[])
 2  {
 3      [...]
 4      #pragma omp parallel
 5      {
 6          #pragma omp single
 7          {
 9              start_task_parallel_execution();
 9          }
10      }
11      [...]
12 }
```

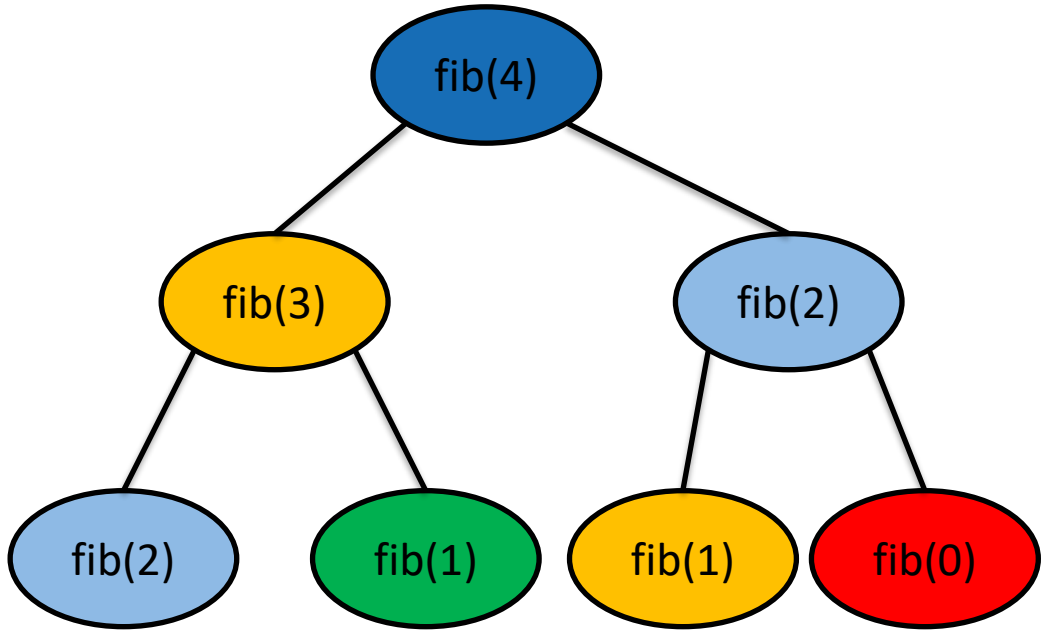
Fibonacci Numbers (in a Stupid Way ☺)

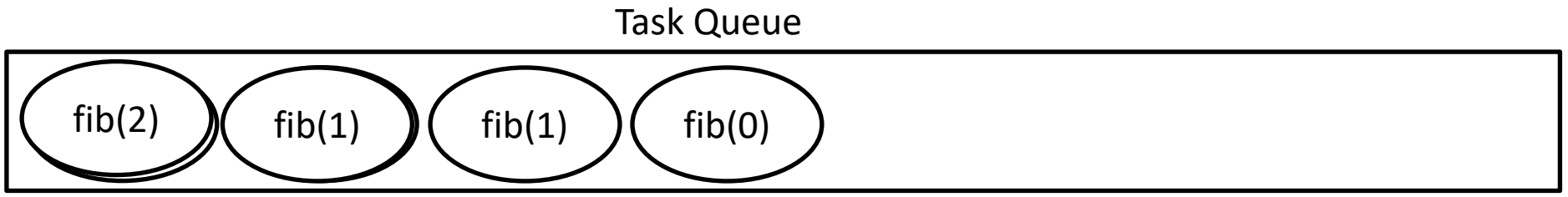
```
 1  int main(int argc,
 2           char* argv[])
 3  {
 4      [...]
 5      #pragma omp parallel
 6      {
 7          #pragma omp master
 8          {
 9              fib(input);
10          }
11      }
12      [...]
13  }
```

```
14  int fib(int n)   {
15      if (n < 2) return n;
16      int x, y;
17      #pragma omp task shared(x)
18      {
19          x = fib(n - 1);
20      }
21      #pragma omp task shared(y)
22      {
23          y = fib(n - 2);
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





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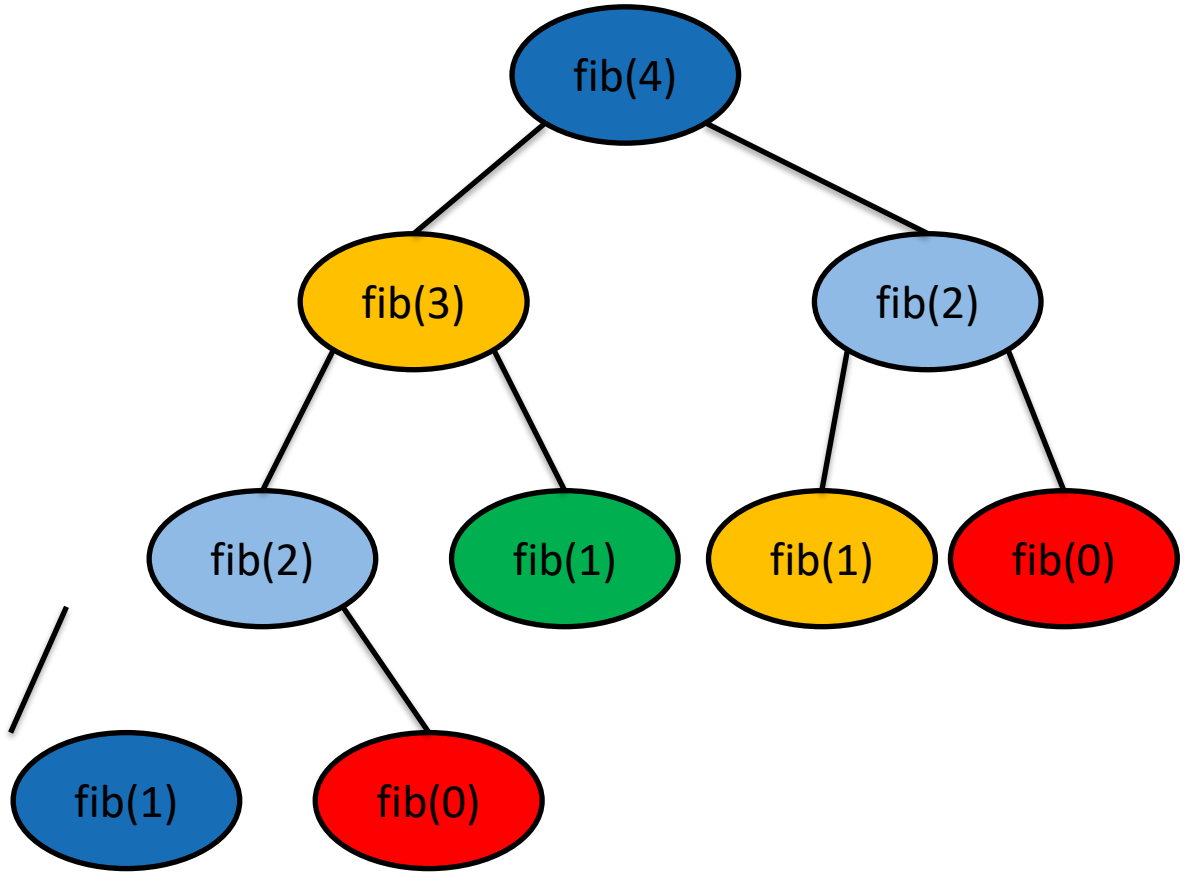
- …



Programming OpenMP

Hands-on Exercises

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Solution of Homework Assignments

Example: sin-cos

```
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 %.3lf seconds.\n", t2 - t1);
    printf("Result is %.3lf.\n", result);
    return 0;
}
```

Example: matmul

```
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[]) { ... }
```

Example: cholesky

```
void cholesky(int ts, int nt, double* Ah[nt][nt]) {
   for (int k = 0; k < nt; k++) {
      LAPACKE_dpotrf(LAPACK_COL_MAJOR, 'L', ts, Ah[k][k], 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);
}     }  }
```

Blocked matrix w/ block size *ts*