

Programming OpenMP

Christian Terboven
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Agenda (in total 4 days)



- Day 1: OpenMP Introduction
 - → Welcome
 - → OpenMP Overview
 - → Parallel Region
 - → Worksharing
 - → Scoping
 - → Tasking (short introduction)
 - → Vectorization / SIMD
 - → Executing OpenMP programs
 - → Hands-On
- Day 2: Tasking & Optimizations for NUMA
- Day 3: Introduction to Offloading with OpenMP
- Day 4: Advanced Offloading Topics

Material





https://github.com/cterboven/OpenMP-tutorial-CSC





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

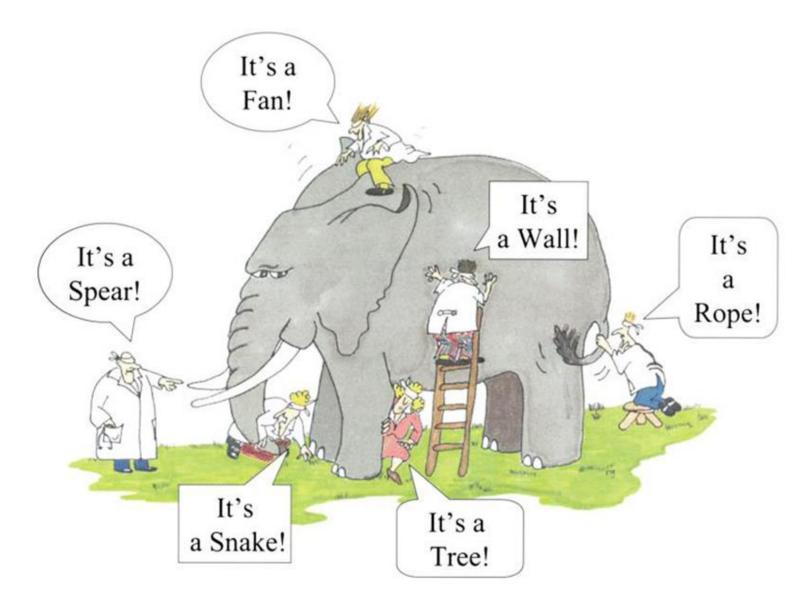


What is OpenMP?

OpenMP

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

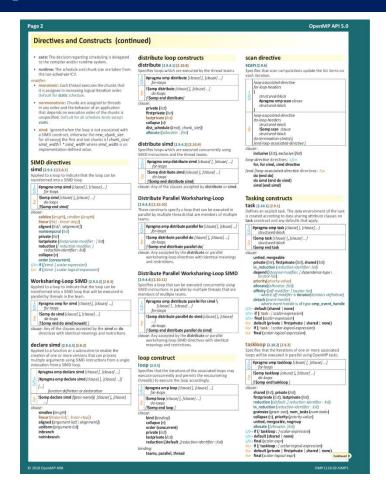
• ...





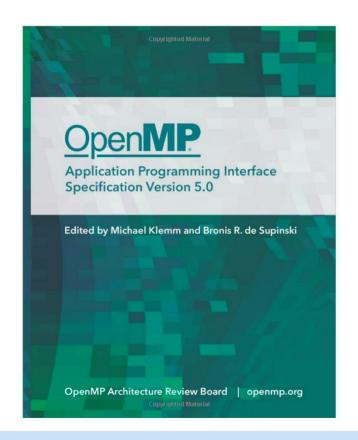
Get your C/C++ and Fortran Reference Guide! Covers all of OpenMP 5.0!



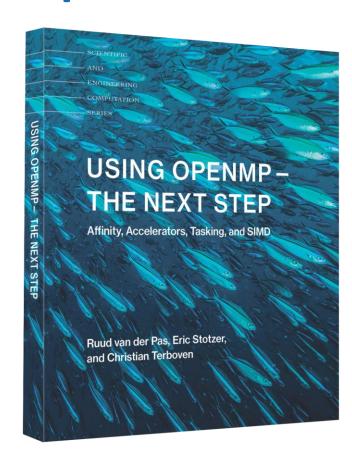


Recent Books About OpenMP

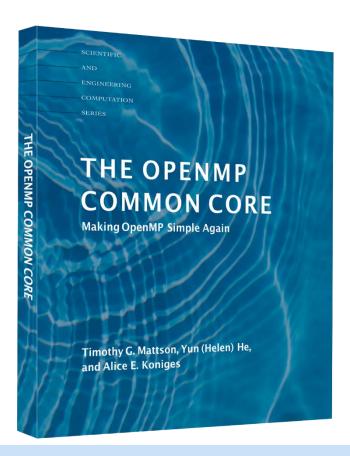




A printed copy of the 5.0 specifications, 2019



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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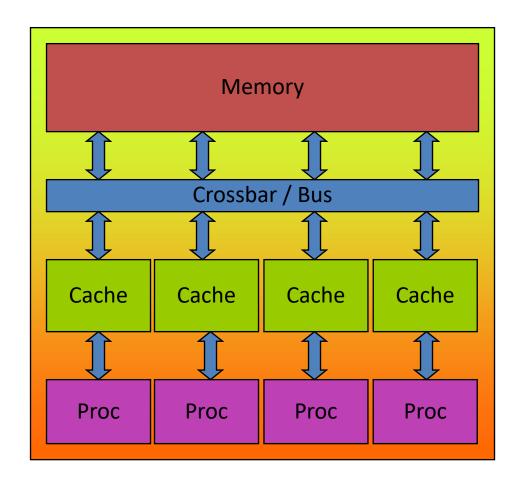
Michael Klemm



OpenMP's machine model



OpenMP: Shared-Memory Parallel Programming Model.



All processors/cores access a shared main memory.

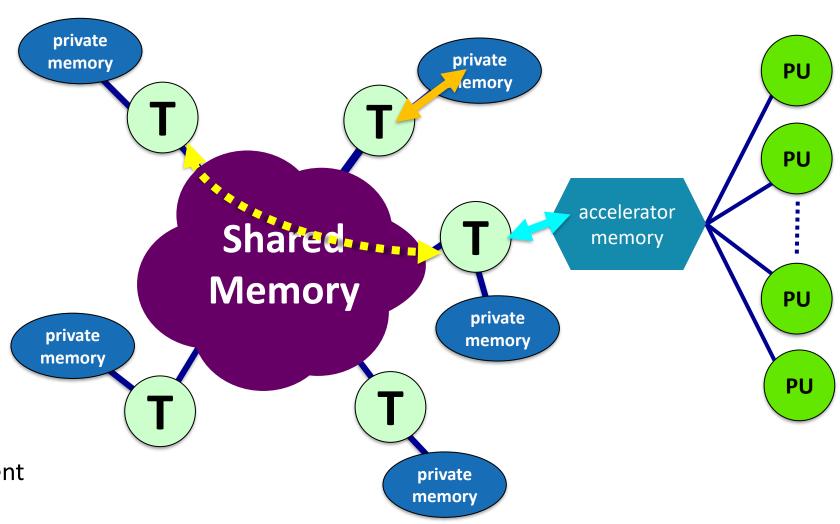
Real architectures are more complex, as we will see later / as we

Parallelization in OpenMP employs multiple threads.

The OpenMP Memory Model



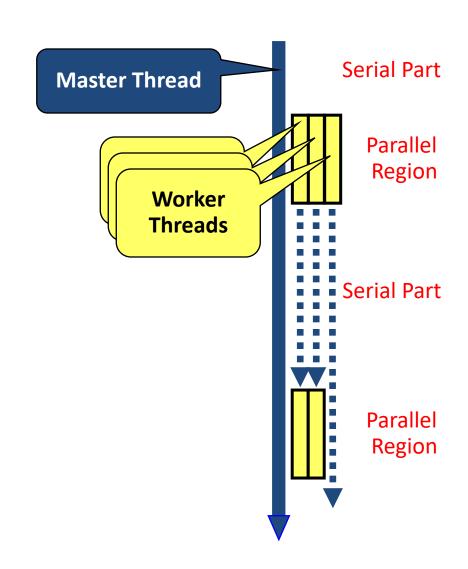
- All threads have access to the same, globally shared memory
- Data in private memory is only accessible by the thread owning this memory
- No other thread sees the change(s) in private memory
- Data transfer is through shared memory and is 100% transparent to the application



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
    ...
}
```

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

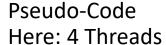
a[i] = b[i] + c[i]

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





Thread 1

Thread 2

do i = 0, 24

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

end do



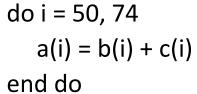
Serial

do i = 0, 99

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

end do

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



end do

do i = 75, 99

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

end do

B(0) B(99) C(0) C(99)

Thread 4

Thread 3





- 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 ...
```

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

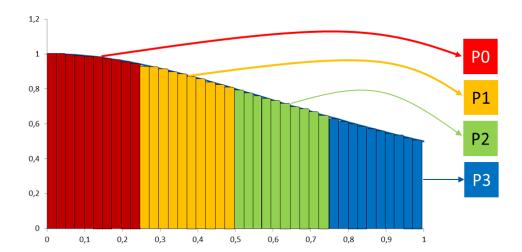
- → schedule(static [, chunk])
- Decompositiondepending on chunksize
- → Equal parts of size 'chunksize' distributed in round-robin fashion

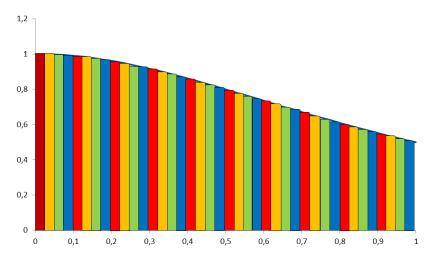
Pros?

→ 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)

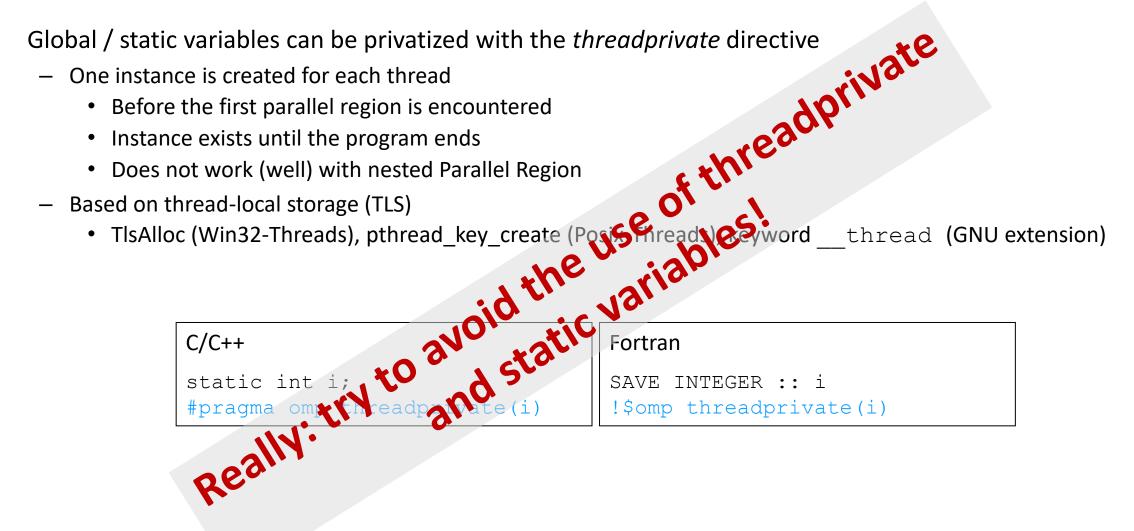
```
C/C++
static int i;
#pragma omp threadprivate(i)
```

```
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, 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



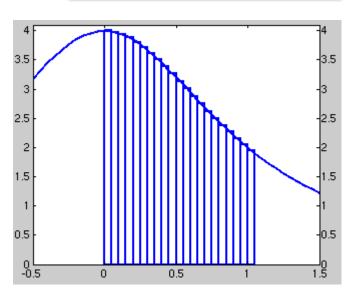
PI

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;
```

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

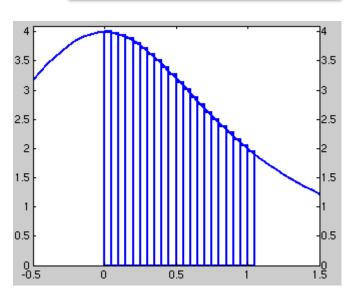


Example: Pi (2/2)



```
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;
```

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





Programming OpenMP

OpenMP Tasking Introduction

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Michael Klemm



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

OpenMP

- Supports unstructured parallelism
 - → unbounded loops

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

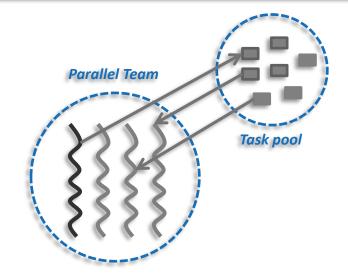
recursive functions

```
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 masked
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 masked
                start task parallel execution();
 9
 9
10
         [\ldots]
11
12 }
```





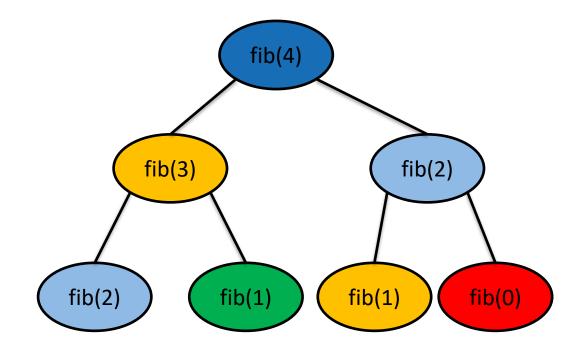
```
int main(int argc,
              char* argv[])
        [\ldots]
        #pragma omp parallel
            #pragma omp masked
                fib(input);
10
11
12
         [\ldots]
13 }
```

```
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 }
```

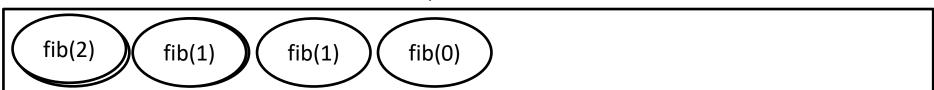
- Only one thread enters fib() from main().
- That thread creates the two initial work tasks and starts the parallel recursion.
- The taskwait construct is required to wait for the result for x and y before the task can sum up.



- 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

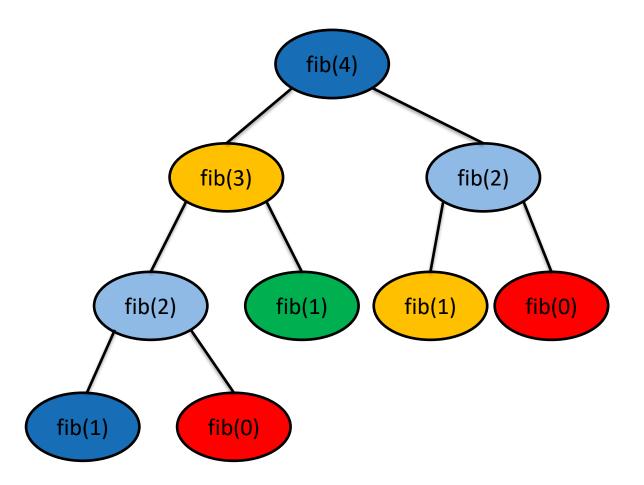








- T1 enters fib(4)
- T1 creates tasks for fib(3) and fib(2)
- T1 and T2 execute tasks from the queue
- T1 and T2 create 4 new tasks
- T1 T4 execute tasks
- _ ...





OpenMP Programming

Vectorization/SIMD

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Topics

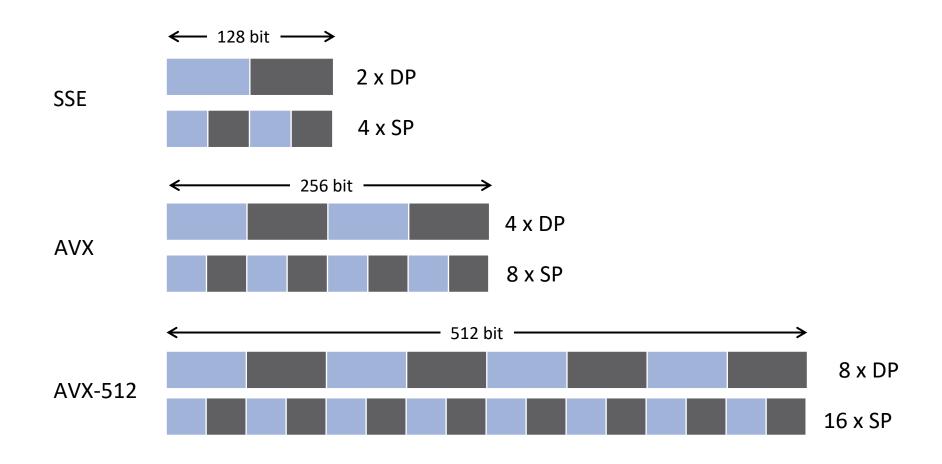


- Exploiting SIMD parallelism with OpenMP
- Using SIMD directives with loops
- Creating SIMD functions

SIMD on x86 Architectures



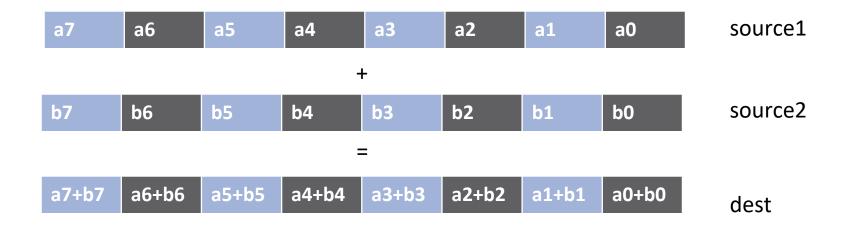
Width of SIMD registers has been growing in the past:





SIMD instructions become more powerful

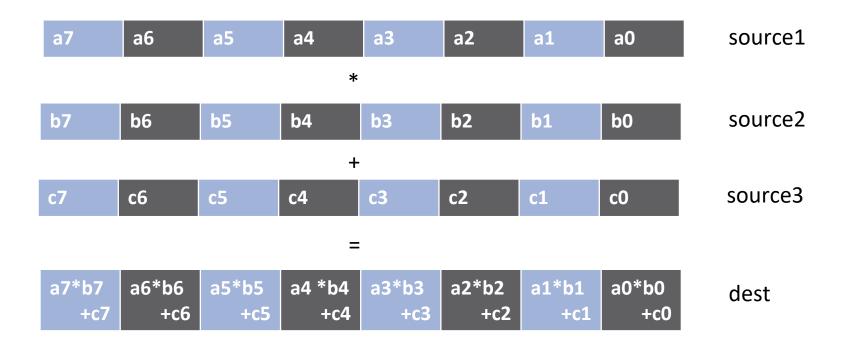
vadd dest, source1, source2





SIMD instructions become more powerful

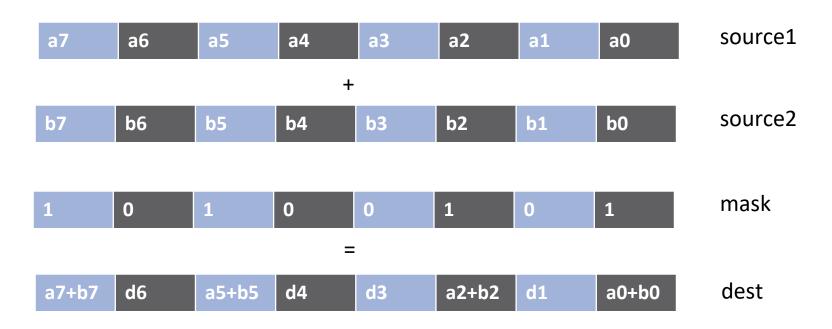
vfma source1, source2, source3





SIMD instructions become more powerful

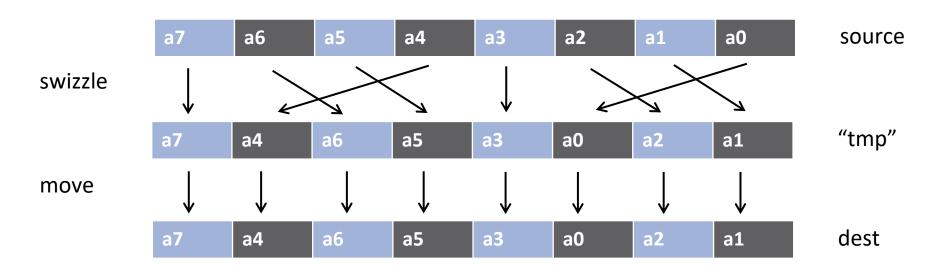






SIMD instructions become more powerful

vload dest, source{dacb}



Auto-vectorization



- Compilers offer auto-vectorization as an optimization pass
 - → Usually, part of the general loop optimization passes
 - → Code analysis detects code properties that inhibit SIMD vectorization



- → Heuristics determine if SIMD execution might be beneficial
- → If all goes well, the compiler will generate SIMD instructions
- Example: clang/LLVM GCC Intel Compiler
 - →-fvectorize -ftree-vectorize -vec (enabled w/ -O2)
 - →-Rpass=loop-.* -ftree-loop-vectorize -qopt-report=vec
 - →-mprefer-vector-width=<width> -fopt-info-vec-all

Why Auto-vectorizers Fail



- Data dependencies
- Other potential reasons
 - →Alignment
 - → Function calls in loop block
 - → Complex control flow / conditional branches
 - → Loop not "countable"
 - →e.g., upper bound not a runtime constant
 - → Mixed data types
 - → Non-unit stride between elements
 - → Loop body too complex (register pressure)
 - → Vectorization seems inefficient
- Many more ... but less likely to occur

Data Dependencies



- Suppose two statements S1 and S2
- S2 depends on S1, iff S1 must execute before S2
 - → Control-flow dependence
 - → Data dependence
 - → Dependencies can be carried over between loop iterations
- Important flavors of data dependencies

FLOW s1: a = 40 b = 21 s2: c = a + 2

ANTI
$$b = 40$$

s1: $a = b + 1$
s2: $b = 21$

Loop-Carried Dependencies



- Dependencies may occur across loop iterations
 - → Loop-carried dependency
- The following code contains such a dependency:

```
void lcd_ex(float* a, float* b, size_t n, float c1, float c2)
{
    size_t i;
    for (i = 0; i < n; i++) {
        a[i] = c1 * a[i + 17] + c2 * b[i];
    }
}</pre>
```

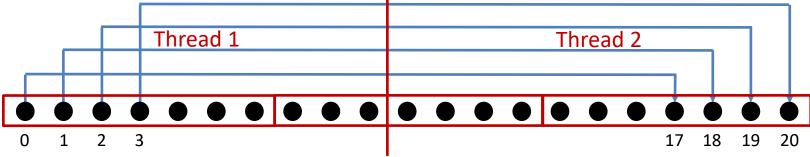
- Some iterations of the loop have to complete before the next iteration can run
 - → Simple trick: Can you reverse the loop w/o getting wrong results?





Can we parallelize or vectorize the loop?

```
void lcd_ex(float* a, float* b, size_t n, float c1, float c2) {
   for (int i = 0; i < n; i++) {
      a[i] = c1 * a[i + 17] + c2 * b[i];
}
</pre>
```



- Parallelization: no (except for very specific loop schedules)
- → Vectorization: yes (iff vector length is shorter than any distance of any dependency)

In a Time Before OpenMP 4.0



- Support required vendor-specific extensions
 - → Programming models (e.g., Intel® Cilk Plus)
 - → Compiler pragmas (e.g., #pragma vector)
 - → Low-level constructs (e.g., _mm_add_pd())

```
#pragma omp parallel for
#pragma vector always
#pragma ivdep

for (int i = 0; i < N; i++) {
    a[i] = b[i] + ...;
}</pre>
```

You need to trust your compiler to do the "right" thing.

SIMD Loop Construct



- Vectorize a loop nest
 - → Cut loop into chunks that fit a SIMD vector register
 - →No parallelization of the loop body

■ Syntax (C/C++)

```
#pragma omp simd [clause[[,] clause],...]
for-loops
```

Syntax (Fortran)

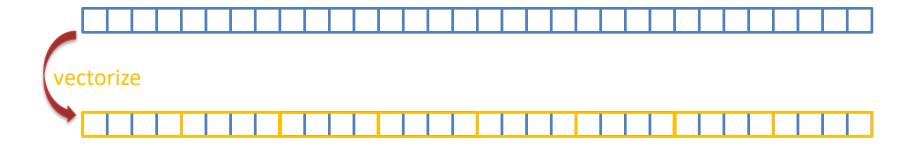
```
!$omp simd [clause[[,] clause],...]
do-loops
[!$omp end simd]
```

Example



```
float sprod(float *a, float *b, int n) {
  float sum = 0.0f;

#pragma omp simd reduction(+:sum)
  for (int k=0; k<n; k++)
    sum += a[k] * b[k];
  return sum;
}</pre>
```



Data Sharing Clauses



private(var-list):

Uninitialized vectors for variables in *var-list*



firstprivate(var-list):
Initialized vectors for variables in var-list

reduction(op:var-list):

Create private variables for *var-list* and apply reduction operator *op* at the end of the construct



SIMD Loop Clauses



- safelen (length)
 - Maximum number of iterations that can run concurrently without breaking a dependence
 - →In practice, maximum vector length
- linear (list[:linear-step])
 - The variable's value is in relationship with the iteration number $\rightarrow x_i = x_{orig} + i$ * linear-step
- aligned (list[:alignment])
 - → Specifies that the list items have a given alignment
 - → Default is alignment for the architecture
- \blacksquare collapse (n)

SIMD Worksharing Construct



- Parallelize and vectorize a loop nest
 - → Distribute a loop's iteration space across a thread team
 - → Subdivide loop chunks to fit a SIMD vector register

Syntax (C/C++)

```
#pragma omp for simd [clause[[,] clause],...]
for-loops
```

Syntax (Fortran)

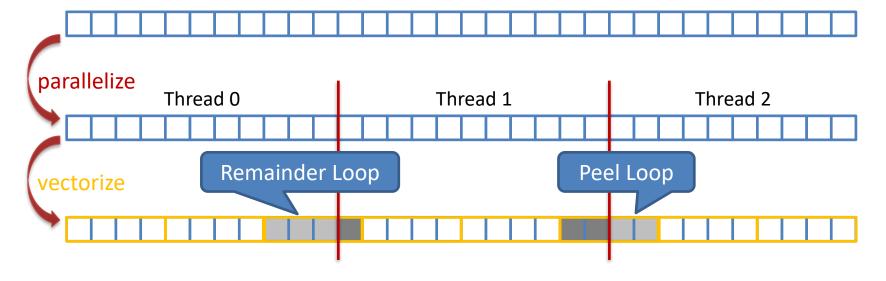
```
!$omp do simd [clause[[,] clause],...]
do-loops
[!$omp end do simd [nowait]]
```

Example



```
float sprod(float *a, float *b, int n) {
  float sum = 0.0f;

#pragma omp for simd reduction(+:sum)
  for (int k=0; k<n; k++)
    sum += a[k] * b[k];
  return sum;
}</pre>
```







- You should choose chunk sizes that are multiples of the SIMD length
 - → Remainder loops are not triggered
 - → Likely better performance
- In the above example ...
 - → and AVX2, the code will only execute the remainder loop!
 - → and SSE, the code will have one iteration in the SIMD loop plus one in the remainder loop!





- Chooses chunk sizes that are multiples of the SIMD length
 - → First and last chunk may be slightly different to fix alignment and to handle loops that are not exact multiples of SIMD width
 - → Remainder loops are not triggered
 - → Likely better performance





```
float min(float a, float b) {
    return a < b ? a : b;
float distsq(float x, float y) {
    return (x - y) * (x - y);
void example() {
#pragma omp parallel for simd
    for (i=0; i< N; i++) {
        d[i] = min(distsq(a[i], b[i]), c[i]);
```

SIMD Function Vectorization



Declare one or more functions to be compiled for calls from a SIMDparallel loop

■ Syntax (C/C++):

```
#pragma omp declare simd [clause[[,] clause],...]
[#pragma omp declare simd [clause[[,] clause],...]]
[...]
function-definition-or-declaration
```

Syntax (Fortran):

```
!$omp declare simd (proc-name-list)
```





```
#pragma omp declare simd
                                 ZGVZN16vv min(%zmm0, %zmm1):
float min(float a, float b)
                                    vminps %zmm1, %zmm0, %zmm0
    return a < b ? a : b;
                                    ret
#pragma omp declare simd
                                 ZGVZN16vv distsq(%zmm0, %zmm1):
float distsq(float x, float y)
                                    vsubps %zmm0, %zmm1, %zmm2
    return (x - y) * (x - y);
                                    vmulps %zmm2, %zmm2, %zmm0
                                    ret
void example() {
#pragma omp parallel for simd
    for (i=0; i< N; i++) {
        d[i] = min(distsq(a[i], b[i]), c[i]);
                              vmovups (%r14,%r12,4), %zmm0
                              vmovups (%r13,%r12,4), %zmm1
                              call ZGVZN16vv distsq
                              vmovups (%rbx, %r12, 4), %zmm1
                               call ZGVZN16vv min
```

SIMD Function Vectorization



- simdlen (length)
 - → generate function to support a given vector length
- uniform (argument-list)
 - → argument has a constant value between the iterations of a given loop
- inbranch
 - → function always called from inside an if statement
- notinbranch
 - → function never called from inside an if statement
- linear (argument-list[:linear-step])
- aligned (argument-list[:alignment])

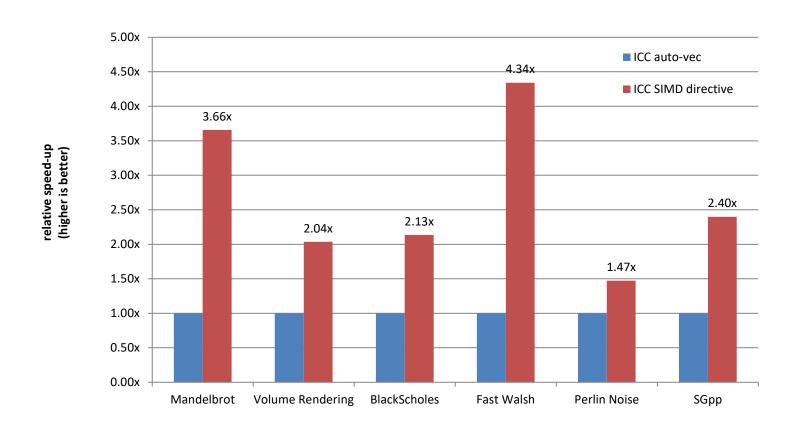




```
#pragma omp declare simd inbranch
float do stuff(float x)
                            vec8 do stuff v(vec8 x, mask m) {
    /* do something */
                                /* do something */
    return x * 2.0;
                               vmulpd x\{m\}, 2.0, tmp
                                return tmp;
void example() {
#pragma omp simd
    for (int i = 0; i < N; i++)
        if (a[i] < 0.0)
            b[i] = do stuff(a[i]);
                          for (int i = 0; i < N; i+=8) {
                              vcmp lt &a[i], 0.0, mask
                              b[i] = do stuff v(&a[i], mask);
```

SIMD Constructs & Performance





M.Klemm, A.Duran, X.Tian, H.Saito, D.Caballero, and X.Martorell. Extending OpenMP with Vector Constructs for Modern Multicore SIMD Architectures. In Proc. of the Intl. Workshop on OpenMP, pages 59-72, Rome, Italy, June 2012. LNCS 7312.



Programming OpenMP

Using OpenMP Compilers

Christian Terboven

Michael Klemm



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
 - → AOCC, AOCL, ROCmCC: -fopenmp
 - → GCC: -fopenmp
 - → clang: -fopenmp
 - → Intel: -fopenmp or -qopenmp (classic) or -fiopenmp (next-gen)
 - → 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

Christian Terboven

Michael Klemm



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-CSC.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 BLIS/LIBFLAME module load amdblis/2.2-omp amdlibflame/2.2-omp
- Each hands-on exercise has a folder "solution" or a source file "XXXXX-solved".
 - → 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.
- Please, feel free to also work on your own code; this is your change to talk with us via the chat to
 discuss your OpenMP needs, findings, problems, and everything else.