Programming OpenMP

Christian Terboven

Michael Klemm

Agenda (in total 5 webinars)

- Webinar 1: OpenMP Introduction
- Webinar 2: Tasking
- **Webinar 3: Optimization for NUMA and SIMD**
  - →Review of webinar 2 / homework assignments
  - →OpenMP and NUMA architectures
  - →Task Affinity
  - →SIMD
  - →User-defined reductions
  - →Misc. optimizations
  - →MPI and multi-threading
  - →Homework assignments ☺
- Webinar 4: Introduction to Offloading with OpenMP
- Webinar 5: Advanced Offloading Topics

Programming OpenMP

Review

Christian Terboven

Michael Klemm

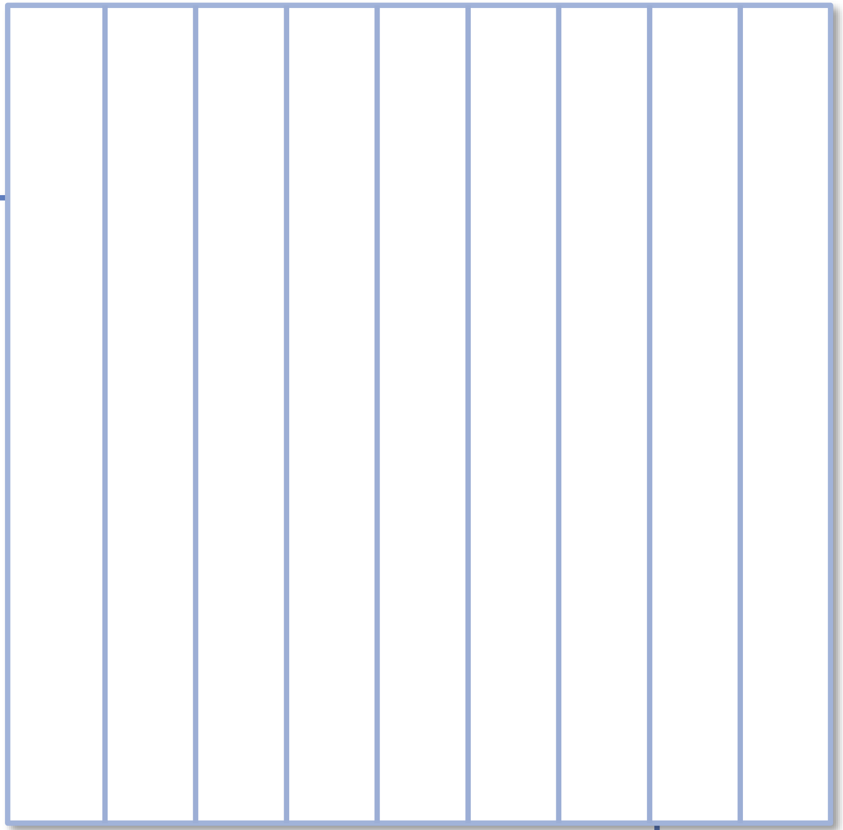
Questions?

Example: Quick Sort

```
void quicksort(int * array, int first, int last){
        int pivotElement;
        if((last - first + 1) < 10000) {
                serial_quicksort(array, first, last);
        } else {
                pivotElement = pivot(array,first,last);
                #pragma omp task default(shared)
                {
                        quicksort(array,first,pivotElement-1);
                }
                #pragma omp task default(shared)
                {
                        quicksort(array,pivotElement+1,last);
                }
                #pragma omp taskwait
        }
}
```

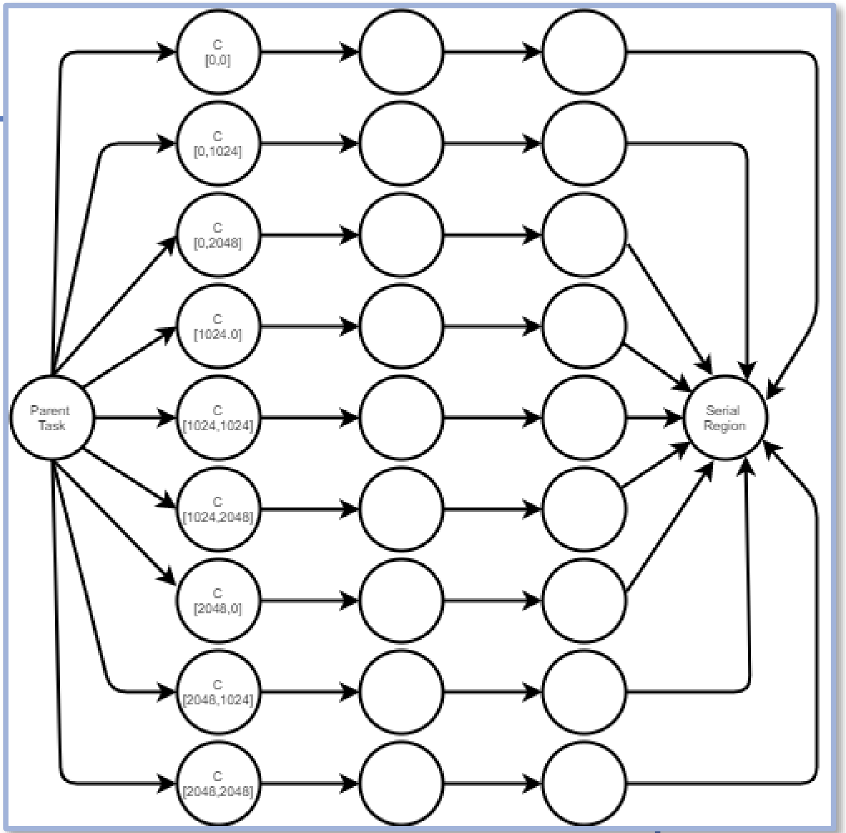
Example: matmul – `taskloop` Version

```
void matmul_tloop(float * C, float * A, float * B,
                  size_t n) {
#pragma omp parallel firstprivate(n)
#pragma omp single nowait
#pragma omp taskloop
    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];
            }
        }
    }
}
```



Example: matmul – task Version

```
void matmul_task(float * C, float * A, float * B, size_t n
#pragma omp parallel firstprivate(n, bf)
#pragma omp master // masked w/ OpenMP API 5.1
    {
        // work on the blocks of the matrix
        for (size_t ib = 0; ib < n; ib += bf)
            for (size_t kb = 0; kb < n; kb += bf)
                for (size_t jb = 0; jb < n; jb += bf) {
#pragma omp task firstprivate(ib, kb, jb) \
                 firstprivate(n, bf) \
                 depend(inout:C[ib * n + jb:bf]) \
                 depend(in:A[ib * n + kb:bf]) \
                 depend(in:B[kb * n + jb:bf])
                    {
                        // work on a single block
                        for (size_t i = ib; i < (ib + bf); ++i)
                            for (size_t k = kb; k < (kb + bf); ++k)
                                for (size_t j = jb; j < (jb + bf); ++j)
                                    C[i * n + j] += A[i * n + k] * B[k * n + j];
}   }           }   }
```



Programming OpenMP

NUMA

Christian Terboven

Michael Klemm

OpenMP: Memory Access

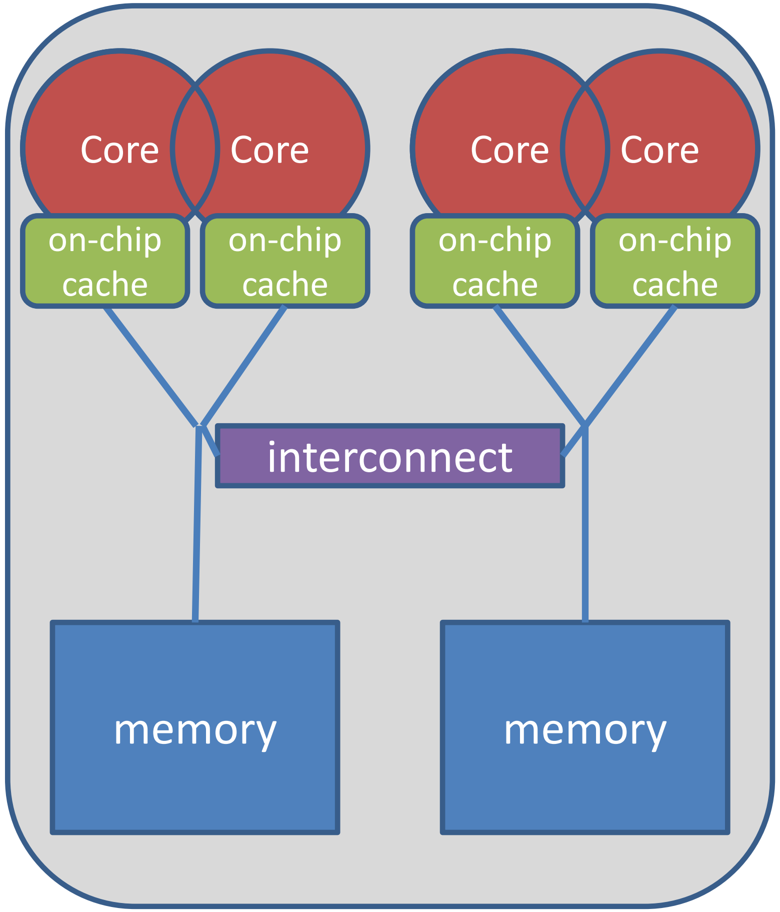
Non-uniform Memory

How To Distribute The Data ?

```
double* A;
A = (double*)
    malloc(N * sizeof(double));



for (int i = 0; i < N; i++) {
   A[i] = 0.0;
}
```



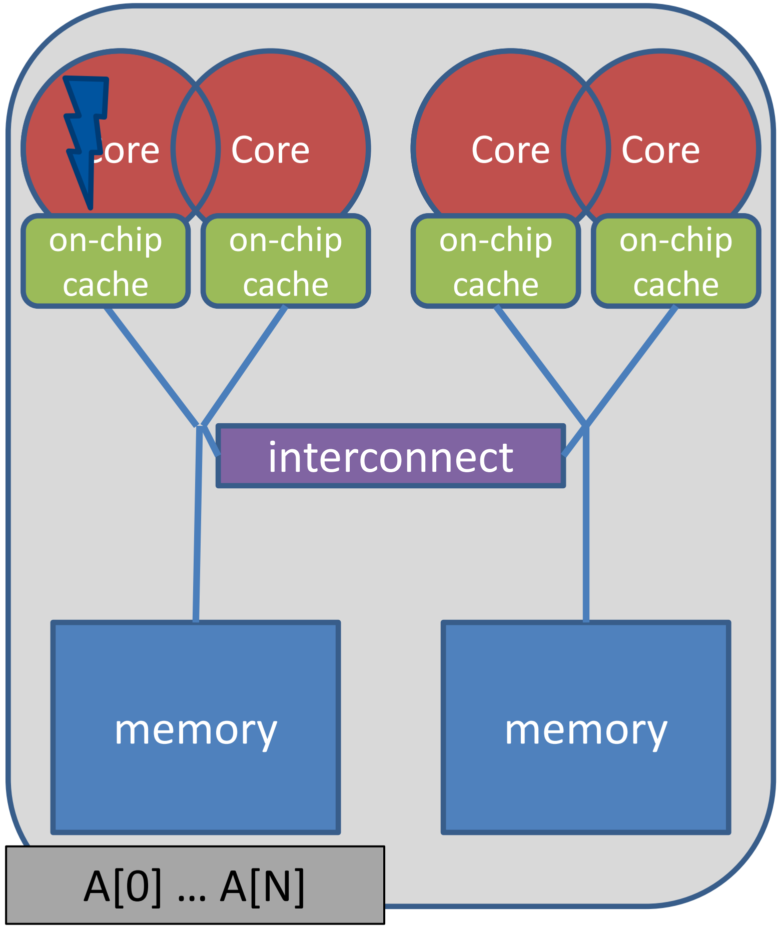
Non-uniform Memory

- **Serial code: all array elements are allocated in the memory of the NUMA node closest to the core executing the initializer thread (first touch)**

```
double* A;
A = (double*)
    malloc(N * sizeof(double));



for (int i = 0; i < N; i++) {
   A[i] = 0.0;
}
```



About Data Distribution

- Important aspect on cc-NUMA systems
  - → If not optimal, longer memory access times and hotspots
- Placement comes from the Operating System
  - → This is therefore Operating System dependent
- Windows, Linux and Solaris all use the “First Touch” placement policy by default
  - → May be possible to override default (check the docs)

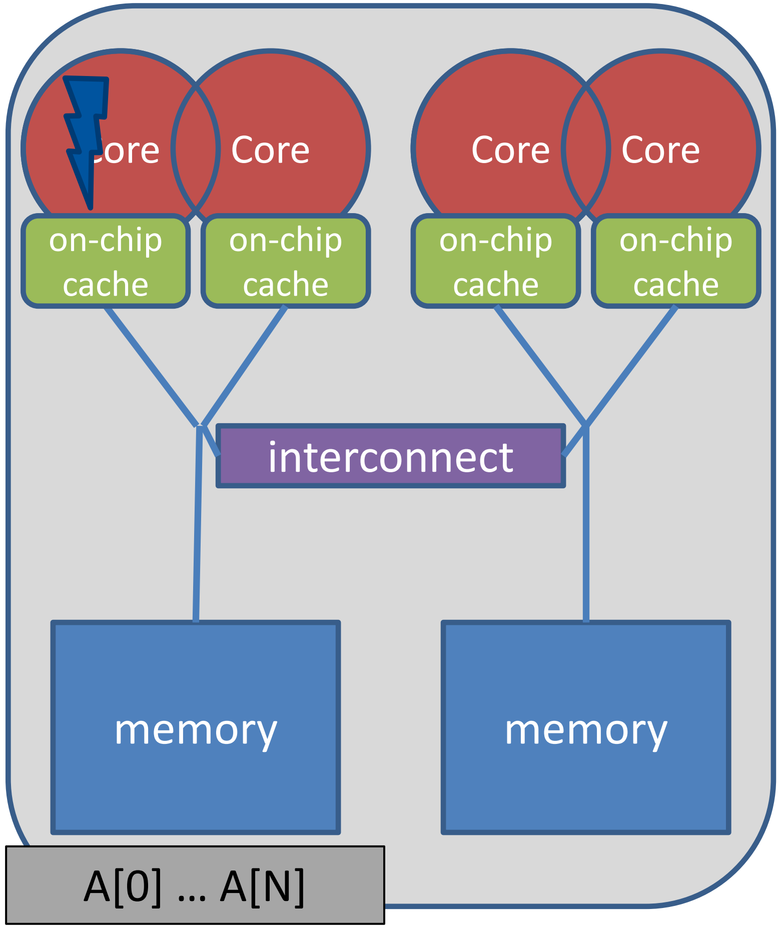
Non-uniform Memory

- **Serial code: all array elements are allocated in the memory of the NUMA node closest to the core executing the initializer thread (first touch)**

```
double* A;
A = (double*)
    malloc(N * sizeof(double));




for (int i = 0; i < N; i++) {
   A[i] = 0.0;
}
```



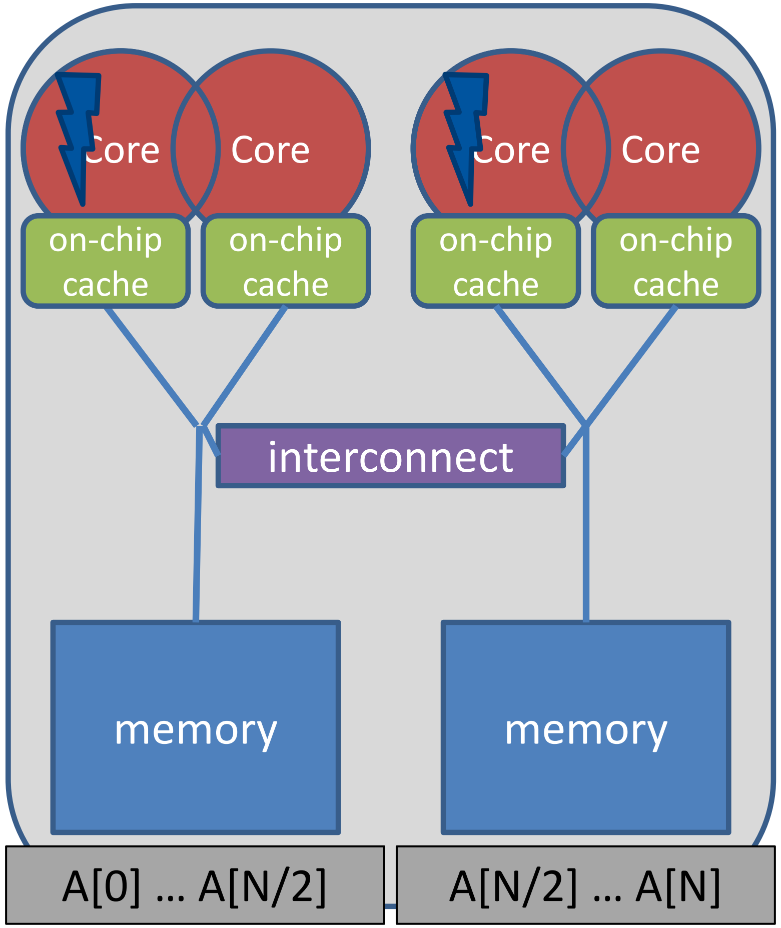
First Touch Memory Placement

- **First Touch w/ parallel code: all array elements are allocated in the memory of the NUMA node that contains the core that executes the thread that initializes the partition**

```
double* A;
A = (double*)
     malloc(N * sizeof(double));

omp_set_num_threads(2);

#pragma omp parallel for
for (int i = 0; i < N; i++) {
   A[i] = 0.0;
}
```

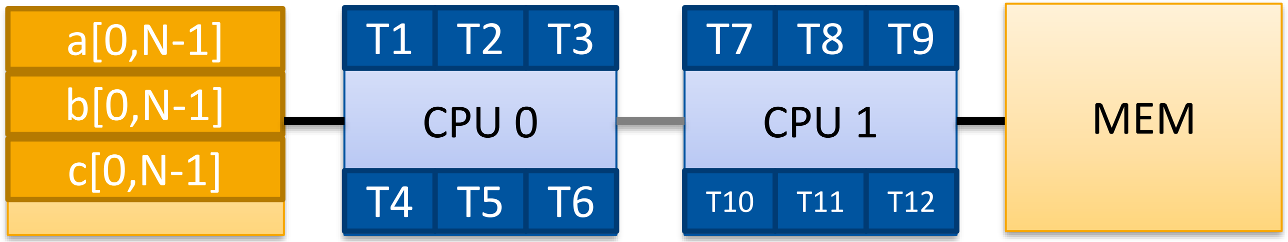


Serial vs. Parallel Initialization

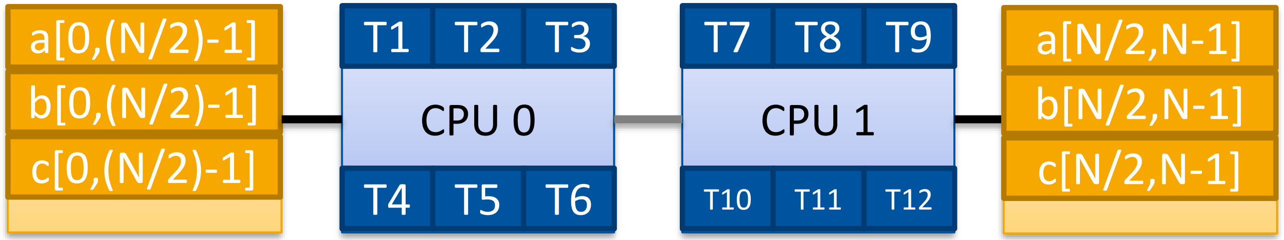
- Stream example on 2 socket sytem with Xeon X5675 processors, 12 OpenMP threads:

	copy	scale	add	triad
ser_init	18.8 GB/s	18.5 GB/s	18.1 GB/s	18.2 GB/s
par_init	41.3 GB/s	39.3 GB/s	40.3 GB/s	40.4 GB/s

ser_init:



par_init:



Get Info on the System Topology

- Before you design a strategy for thread binding, you should have a basic understanding of the system topology. Please use one of the following options on a target machine:
  - Intel MPI‘s `cpuinfo` tool
    - `cpuinfo`
    - Delivers information about the number of sockets (= packages) and the mapping of processor ids to cpu cores that the OS uses.
  - hwlocs‘ `hwloc-ls` tool
    - `hwloc-ls`
    - Displays a graphical representation of the system topology, separated into NUMA nodes, along with the mapping of processor ids to cpu cores that the OS uses and additional info on caches.

Decide for Binding Strategy

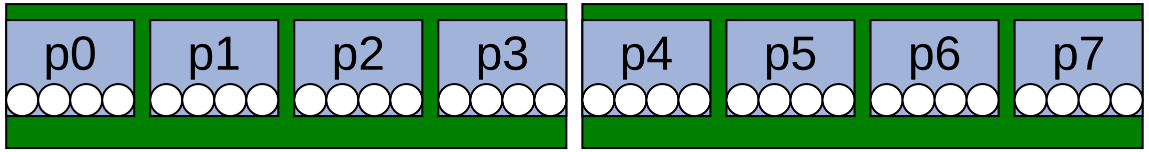
- Selecting the „right“ binding strategy depends not only on the topology, but also on application characteristics.
  - → Putting threads far apart, i.e., on different sockets
    - → May improve aggregated memory bandwidth available to application
    - → May improve the combined cache size available to your application
    - → May decrease performance of synchronization constructs
  - → Putting threads close together, i.e., on two adjacent cores that possibly share some caches
    - → May improve performance of synchronization constructs
    - → May decrease the available memory bandwidth and cache size

Places + Binding Policies (1/2)

- Define OpenMP Places
  - → set of OpenMP threads running on one or more processors
  - → can be defined by the user, i.e. `OMP_PLACES=cores`
- Define a set of OpenMP Thread Affinity Policies
  - → SPREAD: spread OpenMP threads evenly among the places, partition the place list
  - → CLOSE: pack OpenMP threads near master thread
  - → MASTER: collocate OpenMP thread with master thread
- Goals
  - → user has a way to specify where to execute OpenMP threads
  - → locality between OpenMP threads / less false sharing / memory bandwidth

Places

- Assume the following machine:



→ 2 sockets, 4 cores per socket, 4 hyper-threads per core

- Abstract names for OMP_PLACES:

→ threads: Each place corresponds to a single hardware thread on the target machine.

→ cores: Each place corresponds to a single core (having one or more hardware threads) on the target machine.

→ sockets: Each place corresponds to a single socket (consisting of one or more cores) on the target machine.

→ ll_caches: Each place corresponds to a set of cores that share the last level cache.

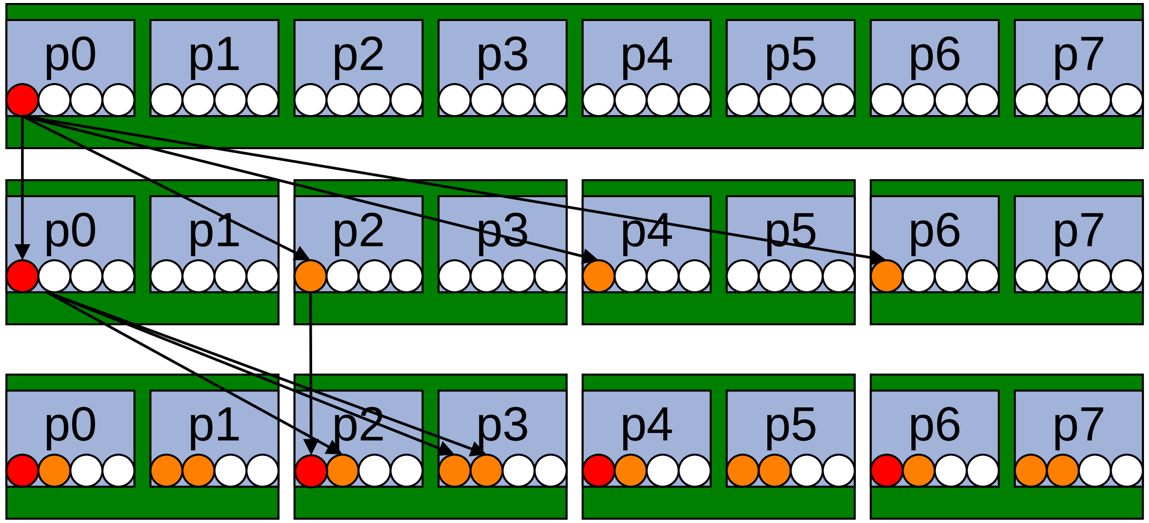
→ numa_domains: Each place corresponds to a set of cores for which their closest memory is: the same memory; and at a similar distance from the cores.

Places + Binding Policies (2/2)

- Example‘s Objective:
  - → separate cores for outer loop and near cores for inner loop
- Outer Parallel Region: proc_bind(spread) num_threads(4)
  Inner Parallel Region: proc_bind(close) num_threads(4)
  - → spread creates partition, compact binds threads within respective partition

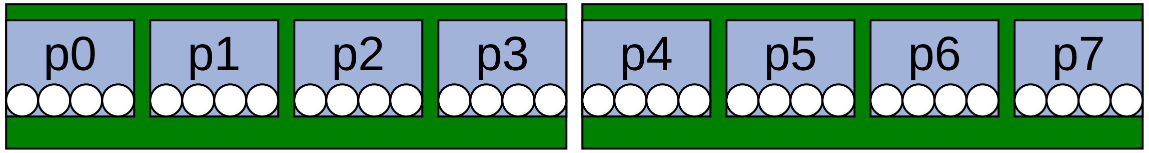
```
OMP_PLACES=(0,1,2,3), (4,5,6,7), ... = (0-3):8:4   = cores
#pragma omp parallel proc_bind(spread) num_threads(4)
#pragma omp parallel proc_bind(close) num_threads(4)
```

- Example
  - → initial
  - → spread 4
  - → close 4



More Examples (1/3)

- Assume the following machine:



→2 sockets, 4 cores per socket, 4 hyper-threads per core

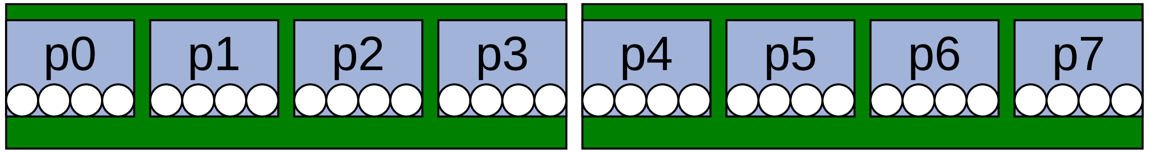
- Parallel Region with two threads, one per socket

→`OMP_PLACES=sockets`

→`#pragma omp parallel num_threads(2) proc_bind(spread)`

More Examples (2/3)

- Assume the following machine:



- Parallel Region with four threads, one per core, but only on the first socket
  - →`OMP_PLACES=cores`
  - →`#pragma omp parallel num_threads(4) proc_bind(close)`

More Examples (3/3)

- Spread a nested loop first across two sockets, then among the cores within each socket, only one thread per core
  - →`OMP_PLACES=cores`
  - →`#pragma omp parallel num_threads(2) proc_bind(spread)`
  - →`#pragma omp parallel num_threads(4) proc_bind(close)`

Working with OpenMP Places

Places API (1/2) (just for reference)

- 1: Query information about binding and a single place of all places with ids 0 … `omp_get_num_places()`:

- `omp_proc_bind_t omp_get_proc_bind()`: returns the thread affinity policy (omp_proc_bind_false, true, master, …)

- `int omp_get_num_places()`: returns the number of places

- `int omp_get_place_num_procs(int place_num)`: returns the number of processors in the given place

- `void omp_get_place_proc_ids(int place_num, int* ids)`: returns the ids of the processors in the given place

Places API (2/2) (just for reference)

- 2: Query information about the place partition:
- `int omp_get_place_num()`: returns the place number of the place to which the current thread is bound
- `int omp_get_partition_num_places()`: returns the number of places in the current partition
- `void omp_get_partition_place_nums(int* pns)`: returns the list of place numbers corresponding to the places in the current partition

Places API: Example (just for reference)

- Simple routine printing the processor ids of the place the calling thread is bound to:

```
void print_binding_info() {
     int my_place = omp_get_place_num();
     int place_num_procs = omp_get_place_num_procs(my_place);

     printf("Place consists of %d processors: ", place_num_procs);

     int *place_processors = malloc(sizeof(int) * place_num_procs);
     omp_get_place_proc_ids(my_place, place_processors)

     for (int i = 0; i < place_num_procs - 1; i++) {
             printf("%d ", place_processors[i]);
     }
     printf("\n");

     free(place_processors);
}
```

OpenMP 5.0 way to do this

- Set `OMP_DISPLAY_AFFINITY=TRUE`
  - →Instructs the runtime to display formatted affinity information
  - →Example output for two threads on two physical cores:

```
nesting_level=   1,   thread_num=   0,   thread_affinity=   0,1
nesting_level=   1,   thread_num=   1,   thread_affinity=   2,3
```

  - →Output can be formatted with `OMP_AFFINITY_FORMAT` env var or corresponding routine
  - →Formatted affinity information can be printed with `omp_display_affinity(const char* format)`

Affinity format specification

t	omp_get_team_num()
T	omp_get_num_teams()
L	omp_get_level()
n	omp_get_thread_num()
N	omp_get_num_threads()

a	omp_get_ancestor_thread_num() at level-1
H	hostname
P	process identifier
i	native thread identifier
A	thread affinity: list of processors (cores)

- Example:

```
OMP_AFFINITY_FORMAT=“Affinity: %0.3L %.8n %.15{A} %.12H“
```

→Possible output:

```
Affinity: 001        0      0-1,16-17      host003
Affinity: 001        1      2-3,18-19      host003
```

A first summary

A first summary

- Everything under control?
- In principle Yes, but only if
  - →threads can be bound explicitly,
  - →data can be placed well by first-touch, or can be migrated,
  - →you focus on a specific platform (= OS + arch) → no portability

- What if the data access pattern changes over time?

- What if you use more than one level of parallelism?

NUMA Strategies: Overview

- First Touch: Modern operating systems (i.e., Linux >= 2.4) decide for a physical location of a memory page during the first page fault, when the page is first „touched“, and put it close to the CPU causing the page fault.

- Explicit Migration: Selected regions of memory (pages) are moved from one NUMA node to another via explicit OS syscall.

- Automatic Migration: Limited support in current Linux systems.

  → Not made for HPC and disabled on most HPC systems.

User Control of Memory Affinity

- Explicit NUMA-aware memory allocation:
  - → By carefully touching data by the thread which later uses it
  - → By changing the default memory allocation strategy
    - → Linux: `numactl` command
    - → Windows: `VirtualAllocExNuma()` (limited functionality)
  - → By explicit migration of memory pages
    - → Linux: `move_pages()`
    - → Windows: no option

- Example: using numactl to distribute pages round-robin:
  - → `numactl –interleave=all ./a.out`

Managing Memory Spaces

Memory Management

- Allocator := an OpenMP object that fulfills requests to allocate and deallocate storage for program variables

- OpenMP allocators are of type `omp_allocator_handle_t`

- Default allocator for Host
  - →via `OMP_ALLOCATOR` env. var. or corresponding API

- OpenMP 5.0 supports a set of memory allocators

OpenMP Allocators

- Selection of a certain kind of memory

Allocator name	Storage selection intent
omp_default_mem_alloc	use default storage
omp_large_cap_mem_alloc	use storage with large capacity
omp_const_mem_alloc	use storage optimized for read-only variables
omp_high_bw_mem_alloc	use storage with high bandwidth
omp_low_lat_mem_alloc	use storage with low latency
omp_cgroup_mem_alloc	use storage close to all threads in the contention group of the thread requesting the allocation
omp_pteam_mem_alloc	use storage that is close to all threads in the same parallel region of the thread requesting the allocation
omp_thread_local_mem_alloc	use storage that is close to the thread requesting the allocation

Using OpenMP Allocators

- New clause on all constructs with data sharing clauses:
  - → `allocate( [allocator:] list )`
- Allocation:
  - → `omp_alloc(size_t size, omp_allocator_handle_t allocator)`
- Deallocation:
  - → `omp_free(void *ptr, const omp_allocator_handle_t allocator)`
  - → `allocator` argument is optional
- `allocate` directive: standalone directive for allocation, or declaration of allocation stmt.

OpenMP Allocator Traits / 1

- Allocator traits control the behavior of the allocator

sync_hint	contended, uncontended, serialized, private default: contended
alignment	positive integer value that is a power of two default: 1 byte
access	all, cgroup, pteam, thread default: all
pool_size	positive integer value
fallback	default_mem_fb, null_fb, abort_fb, allocator_fb default: default_mem_fb
fb_data	an allocator handle
pinned	true, false default: false
partition	environment, nearest, blocked, interleaved default: environment

OpenMP Allocator Traits / 2

- `fallback`: describes the behavior if the allocation cannot be fulfilled
  - →`default_mem_fb`: return system's default memory
  - →Other options: null, abort, or use different allocator

- `pinned`: request pinned memory, i.e. for GPUs

OpenMP Allocator Traits / 3

- `partition`: partitioning of allocated memory of physical storage resources (think of NUMA)
  - → `environment`: use system’s default behavior
  - → `nearest`: most closest memory
  - → `blocked`: partitioning into approx. same size with at most one block per storage resource
  - → `interleaved`: partitioning in a round-robin fashion across the storage resources

OpenMP Allocator Traits / 4

- Construction of allocators with traits via
  - → `omp_allocator_handle_t   omp_init_allocator(`

    `omp_memspace_handle_t memspace,`

    `int ntraits, const omp_alloctrait_t traits[]);`
  - → Selection of memory space mandatory
  - → Empty traits set: use defaults
- Allocators have to be destroyed with `*_destroy_*`
- Custom allocator can be made default with `omp_set_default_allocator(omp_allocator_handle_t allocator)`

OpenMP Memory Spaces

- Storage resources with explicit support in OpenMP:

omp_default_mem_space	System's default memory resource
omp_large_cap_mem_space	Storage with larg(er) capacity
omp_const_mem_space	Storage optimized for variables with constant value
omp_high_bw_mem_space	Storage with high bandwidth
omp_low_lat_mem_space	Storage with low latency

→Exact selection of memory space is implementation-def.

→Pre-defined allocators available to work with these

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NUMA

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Improving Tasking Performance:

Task Affinity

Motivation

- Techniques for process binding & thread pinning available
  - →OpenMP thread level: `OMP_PLACES & OMP_PROC_BIND`
  - →OS functionality: `taskset -c`

OpenMP Tasking:

- In general: Tasks may be executed by any thread in the team
  - →Missing task-to-data affinity may have detrimental effect on performance

OpenMP 5.0:

- `affinity` clause to express affinity to data

`affinity` clause

- New clause: `#pragma omp task affinity (list)`
  - →Hint to the runtime to execute task closely to physical data location
  - →Clear separation between dependencies and affinity
- Expectations:
  - →Improve data locality / reduce remote memory accesses
  - →Decrease runtime variability
- Still expect task stealing
  - →In particular, if a thread is under-utilized

Code Example

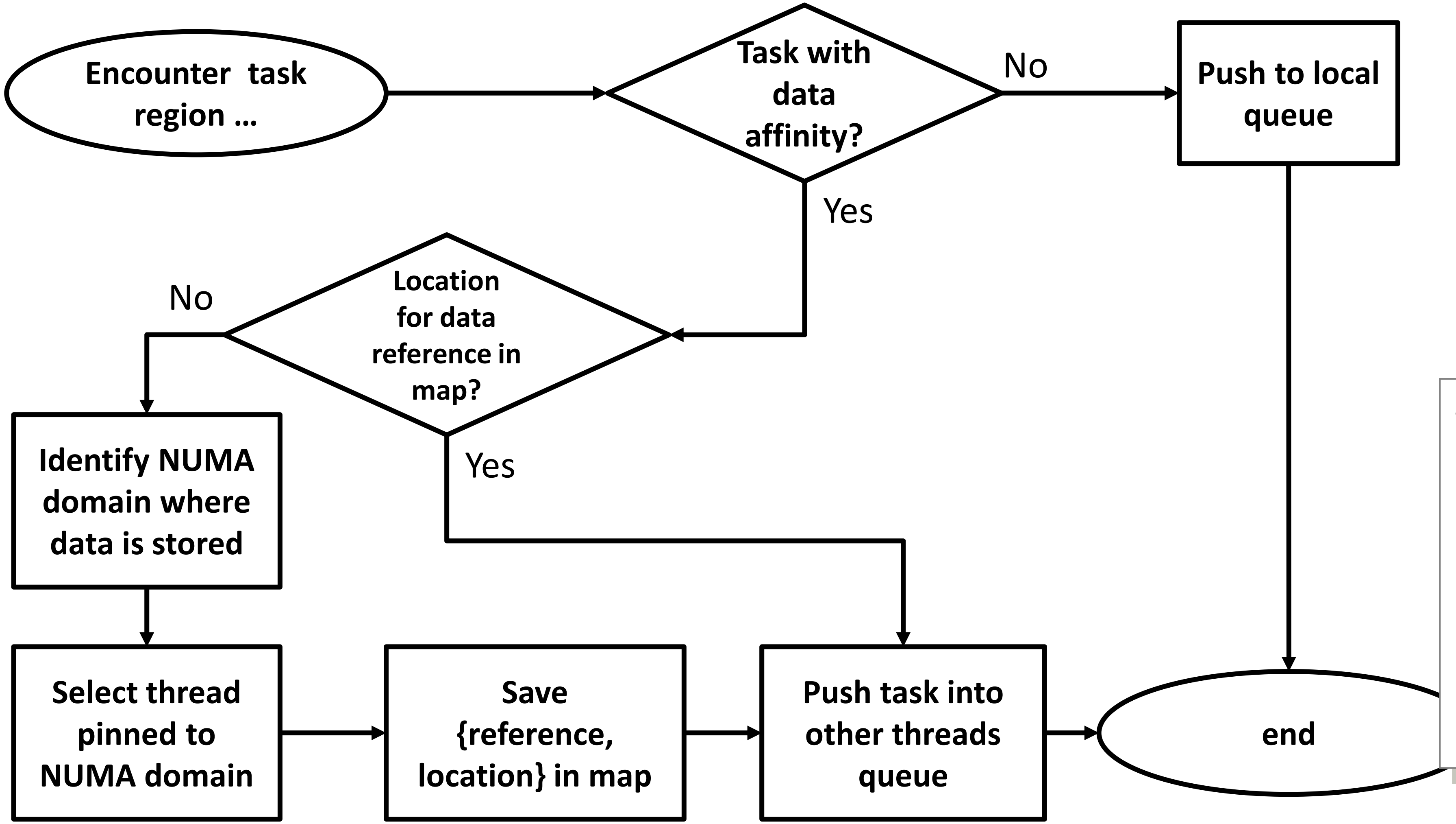
- Excerpt from task-parallel STREAM

```
#pragma omp task \
    shared(a, b, c, scalar) \
    firstprivate(tmp_idx_start, tmp_idx_end) \
    affinity( a[tmp_idx_start] )
{
   int i;
   for(i = tmp_idx_start; i <= tmp_idx_end; i++)
        a[i] = b[i] + scalar * c[i];
}
```

→Loops have been blocked manually (see `tmp_idx_start/end`)

→Assumption: initialization and computation have same blocking and same affinity

Selected LLVM implementation details



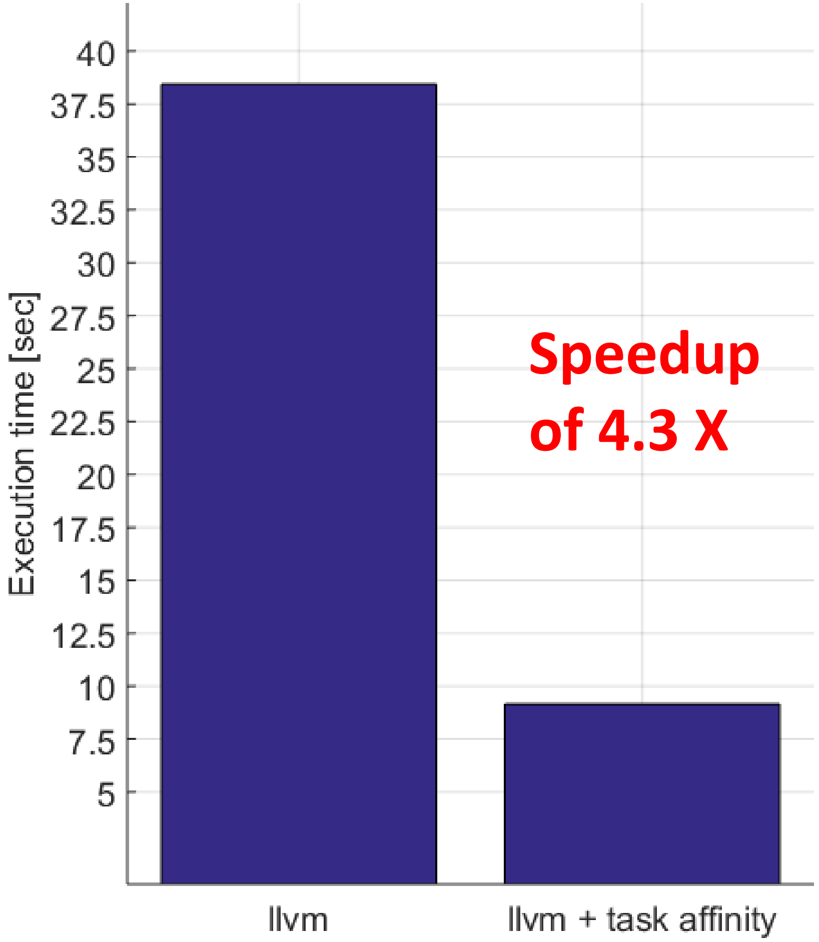
Encounter task region …
Task with data affinity?
No
Push to local queue
Yes
Location for data reference in map?
No
Identify NUMA domain where data is stored
Yes
Select thread pinned to NUMA domain
Save {reference, location} in map
Push task into other threads queue
end

A map is introduced to store location information of data that was previously used

Jannis Klinkenberg, Philipp Samfass, Christian Terboven, Alejandro Duran, Michael Klemm, Xavier Teruel, Sergi Mateo, Stephen L. Olivier, and Matthias S. Müller. **Assessing Task-to-Data Affinity in the LLVM OpenMP Runtime**. Proceedings of the 14th International Workshop on OpenMP, IWOMP 2018. September 26-28, 2018, Barcelona, Spain.

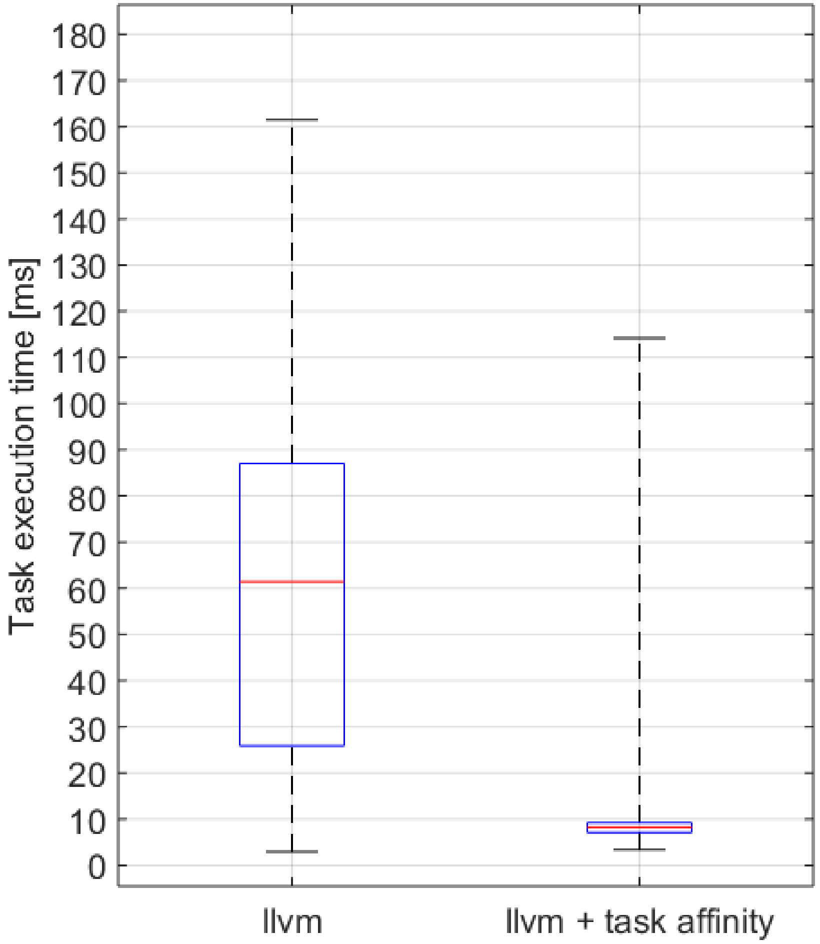
Evaluation

Program runtime
Median of 10 runs



Speedup of 4.3 X

Distribution of single task execution times



LIKWID: reduction of remote data volume from 69% to 13%

Summary

- Requirement for this feature: thread affinity enabled

- The `affinity` clause helps, if
  - →tasks access data heavily
  - →single task creator scenario, or task not created with data affinity
  - →high load imbalance among the tasks

- Different from thread binding: task stealing is absolutely allowed

Programming OpenMP

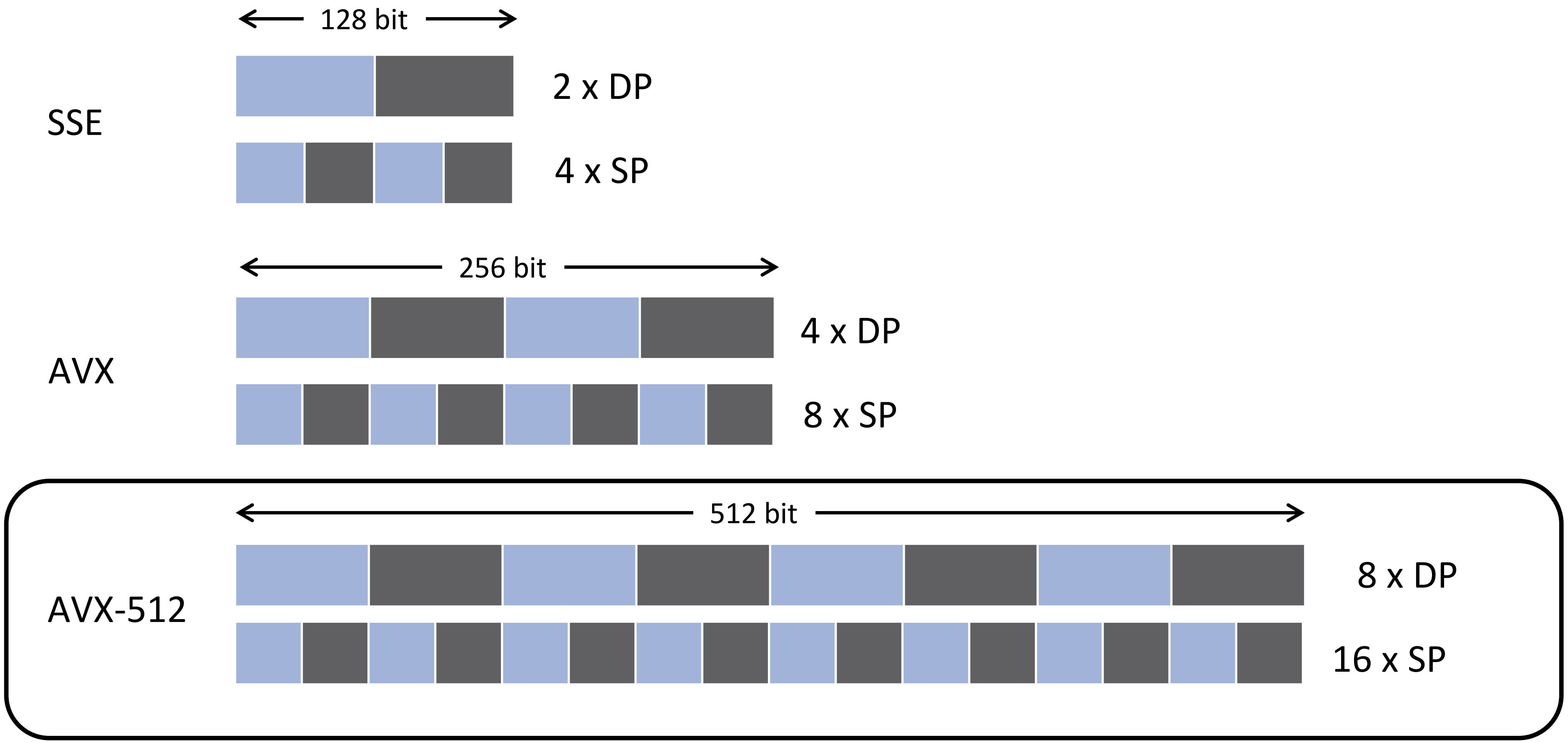
SIMD

Christian Terboven

Michael Klemm

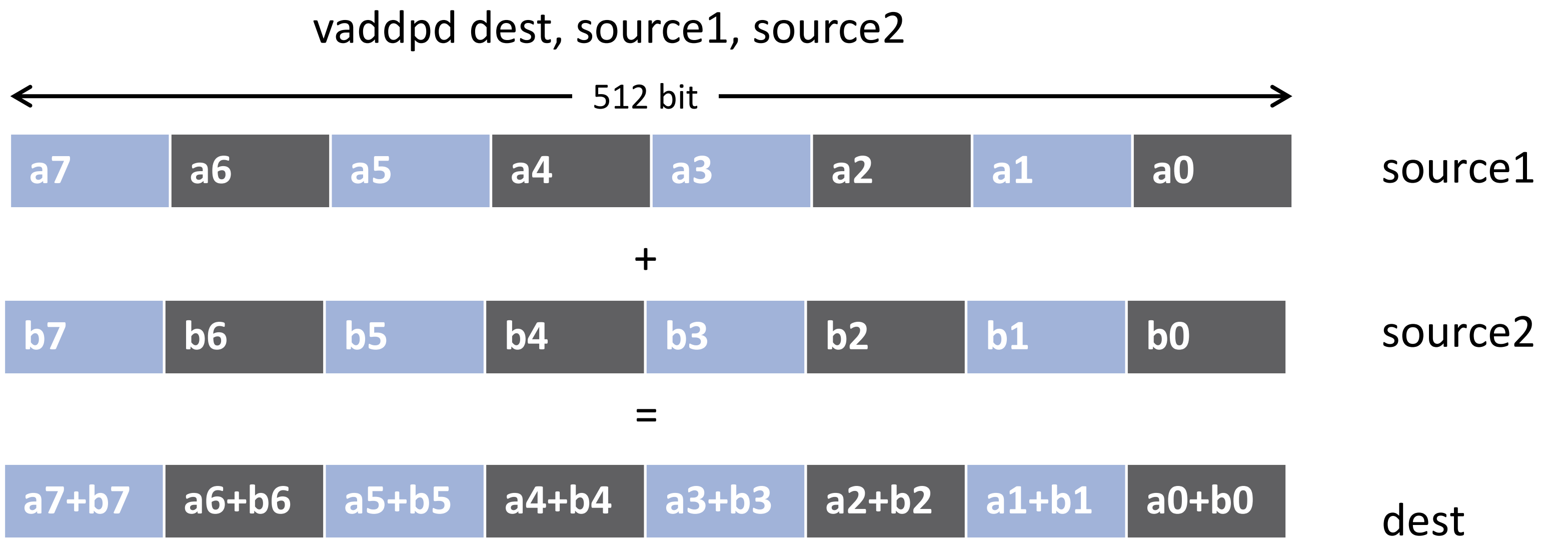
SIMD on x86_64

- Width of SIMD registers has been growing in the past:



More Powerful SIMD Units

- SIMD instructions become more powerful
- One example are the Intel® Advanced Vector Extensions 512



vaddpd dest, source1, source2

512 bit

a7	a6	a5	a4	a3	a2	a1	a0	source1

+

b7	b6	b5	b4	b3	b2	b1	b0	source2

=

a7+b7	a6+b6	a5+b5	a4+b4	a3+b3	a2+b2	a1+b1	a0+b0	dest

More Powerful SIMD Units

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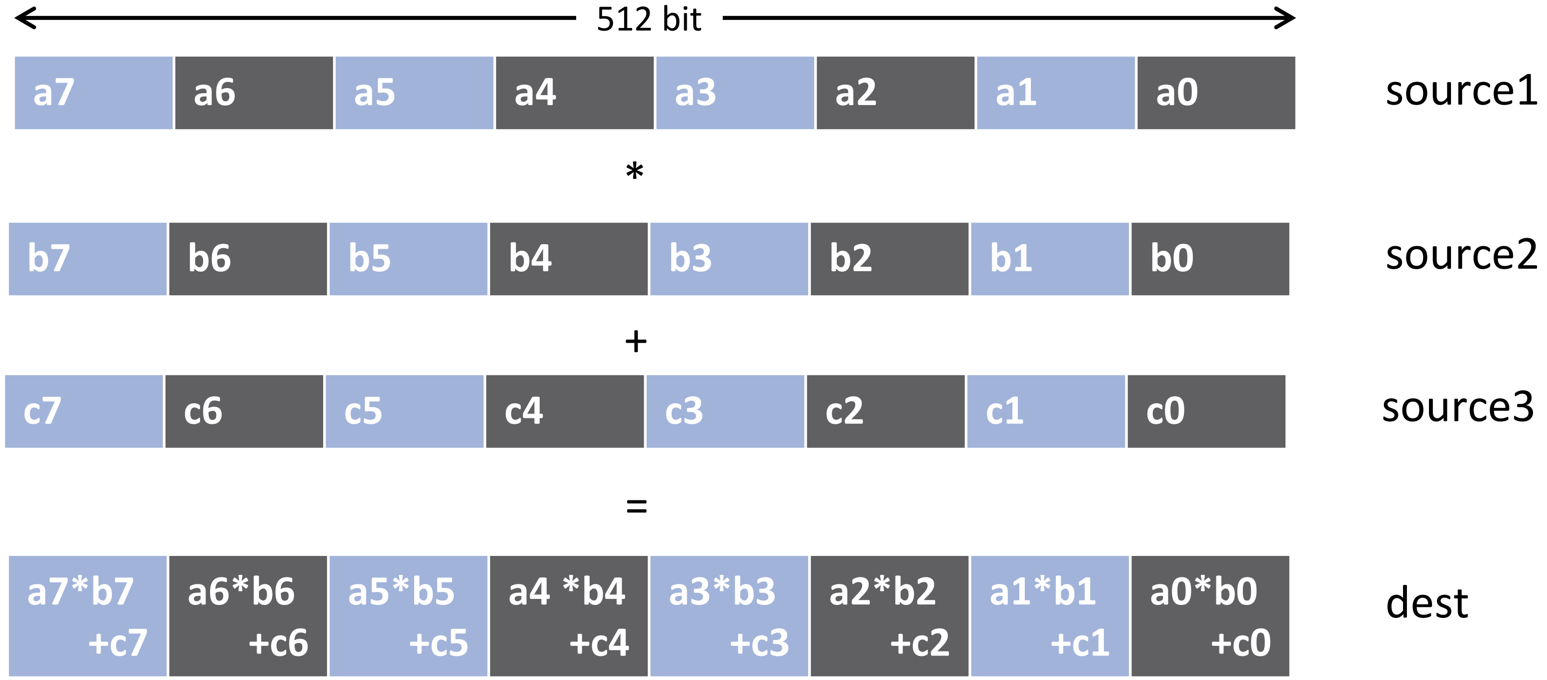
vfmadd213pd source1, source2, source3



512 bit

a7	a6	a5	a4	a3	a2	a1	a0	source1
*								
b7	b6	b5	b4	b3	b2	b1	b0	source2
+								
c7	c6	c5	c4	c3	c2	c1	c0	source3
=								
a7*b7 +c7	a6*b6 +c6	a5*b5 +c5	a4 *b4 +c4	a3*b3 +c3	a2*b2 +c2	a1*b1 +c1	a0*b0 +c0	dest

More Powerful SIMD Units

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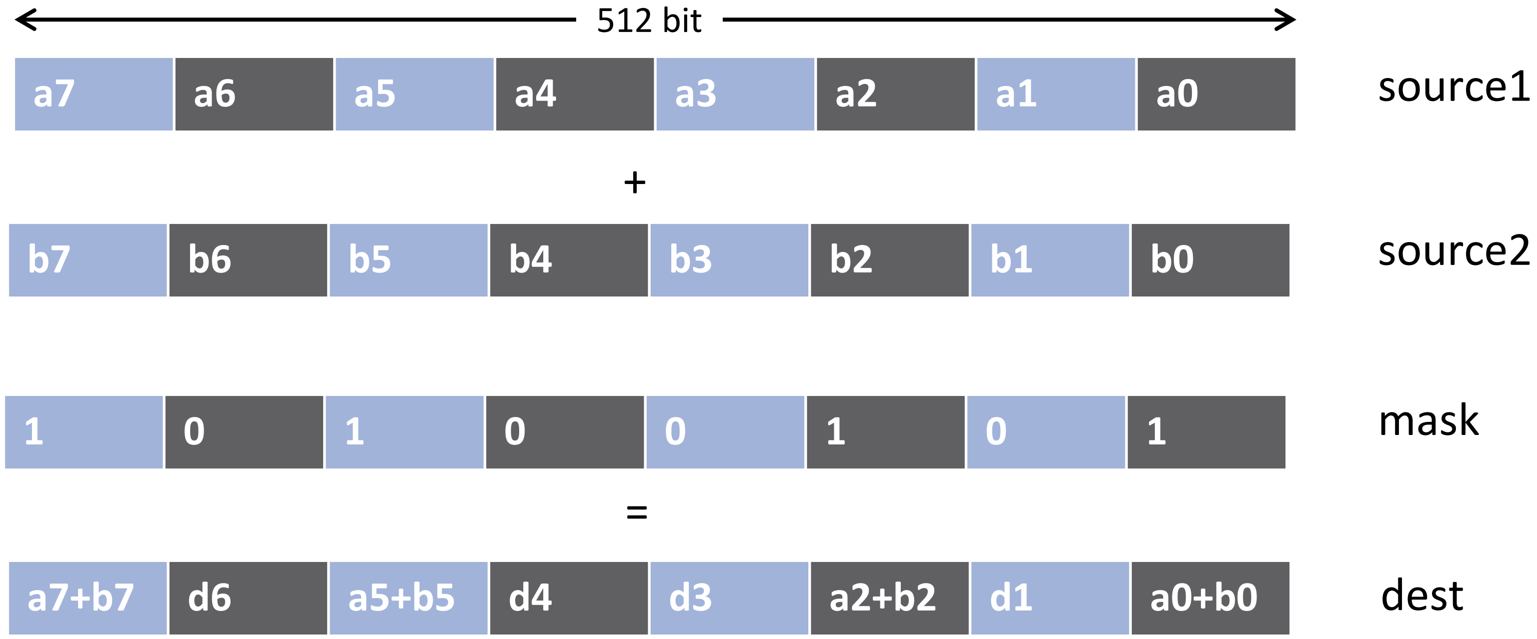
vaddpd dest{k1}, source2, source3

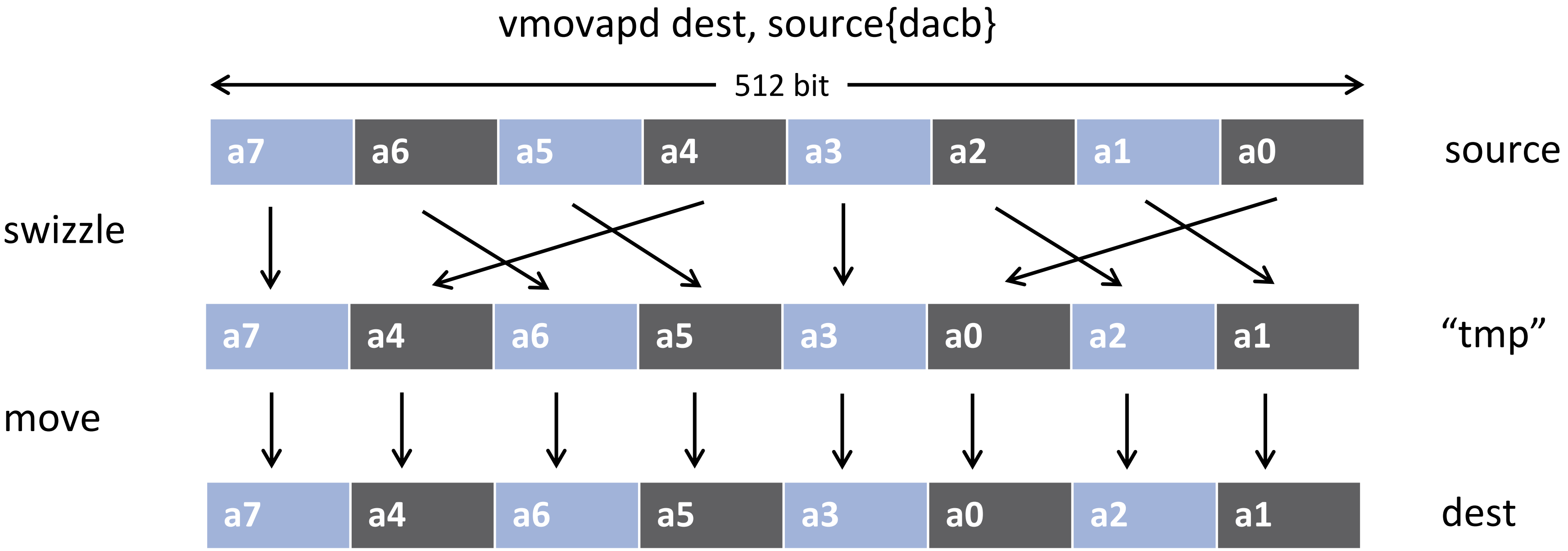


512 bit

a7	a6	a5	a4	a3	a2	a1	a0	source1
+								
b7	b6	b5	b4	b3	b2	b1	b0	source2
1	0	1	0	0	1	0	1	mask
=								
a7+b7	d6	a5+b5	d4	d3	a2+b2	d1	a0+b0	dest

More Powerful SIMD Units

- SIMD instructions become more powerful
- One example are the Intel® Advanced Vector Extensions 512



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
  - →-fvectorize
  - →-mprefer-vector-width=<*width*>

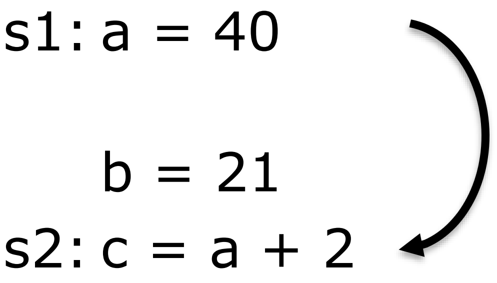
Why Auto-vectorizers Fail

- 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

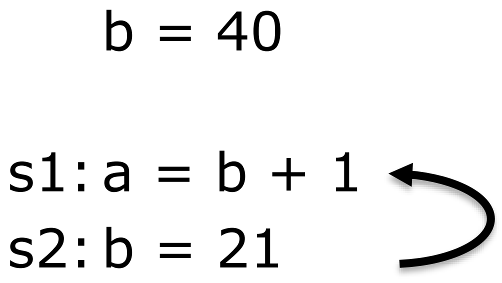
FLOW



```
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];
    }
}
```

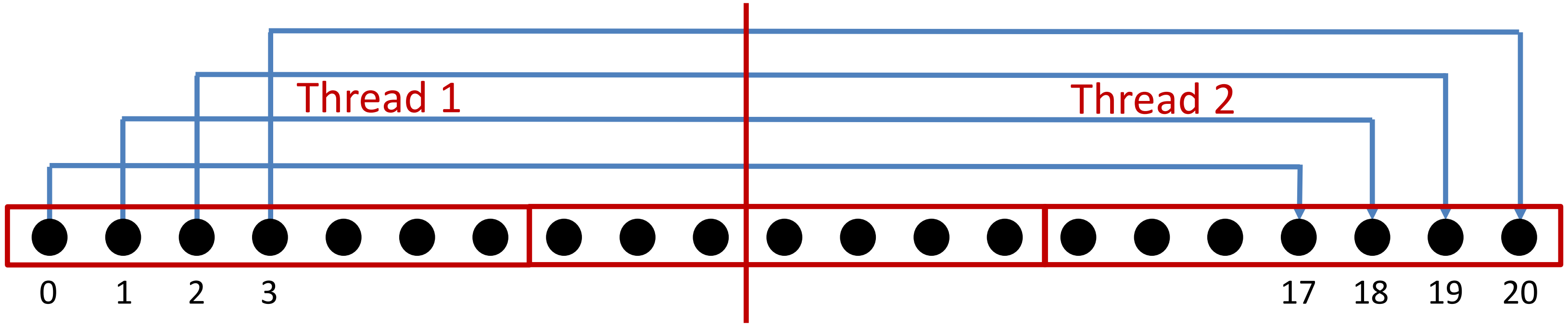
Loop-carried dependency for a[i] and a[i+17]; distance is 17.

- 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?

Loop-carried Dependencies

- 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];
}   }
```



→ Parallelization: no
(except for very specific loop schedules)

→ Vectorization: yes
(iff vector length is shorter than any distance of any dependency)

Example: Loop not Countable

- “Loop not Countable” plus “Assumed Dependencies”

```
typedef struct {
    float* data;
    size_t size;
} vec_t;

void vec_eltwise_product(vec_t* a, vec_t* b, vec_t* c) {
    size_t i;
    for (i = 0; i < a->size; i++) {
        c->data[i] = a->data[i] * b->data[i];
    }
}
```

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] + ...;
}
```

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++)

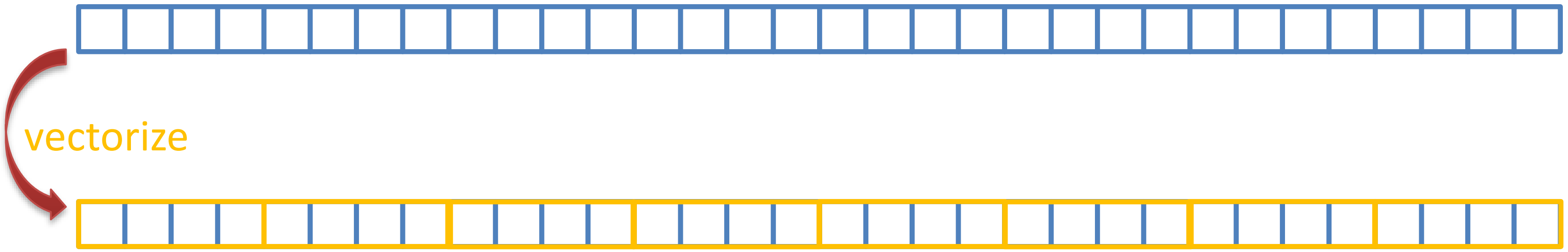
```
#pragma omp simd [clause[[,] clause],…]
for-loops
```

- Syntax (Fortran)

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

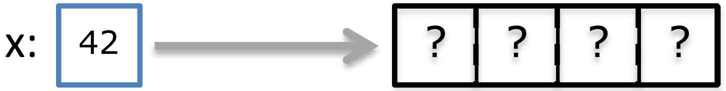
Example

```
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;
}
```



Data Sharing Clauses

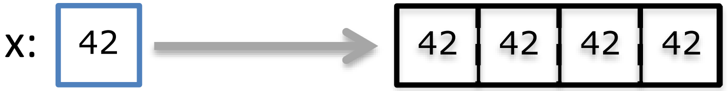
- `private(`*`var-list`*`):`
  Uninitialized vectors for variables in *var-list*



x: 42

? ? ? ?

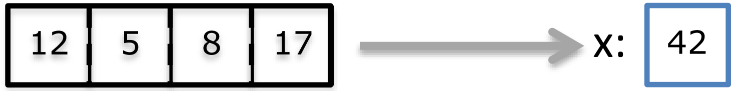
- `firstprivate(`*`var-list`*`):`
  Initialized vectors for variables in *var-list*



x: 42

42 42 42 42

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



12 5 8 17

x: 42

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
    - →$x_i = x_{orig} + i * \text{linear-step}$
- `aligned (`*`list`*`[:`*`alignment`*`])`
  - →Specifies that the list items have a given alignment
  - →Default is alignment for the architecture
- `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++)

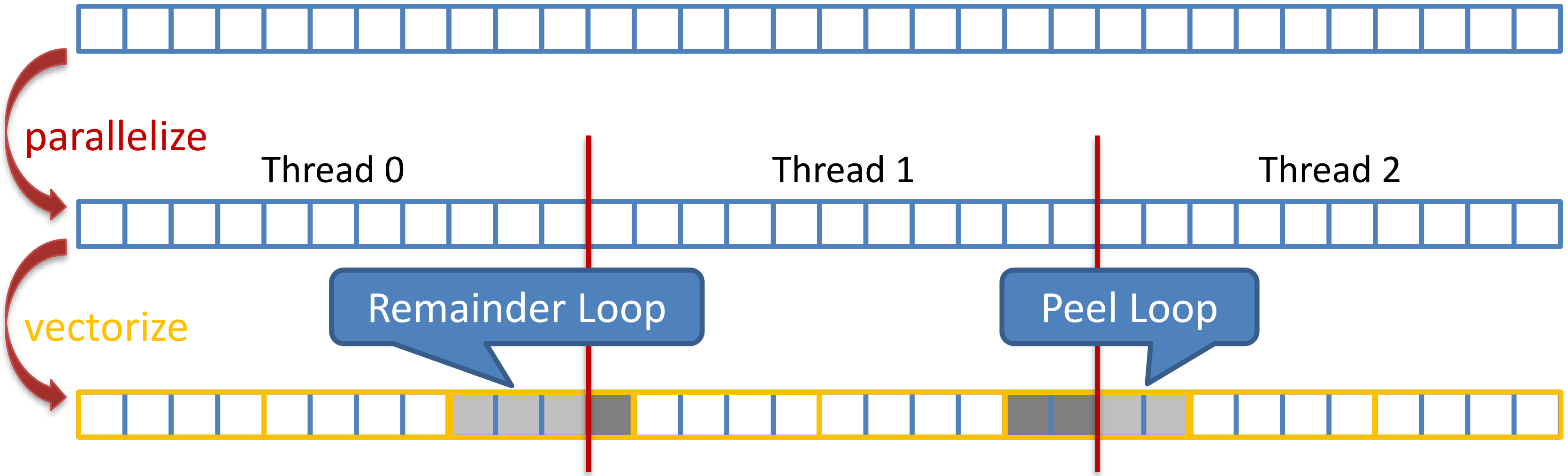
```
#pragma omp for simd [clause[[,] clause],…]
for-loops
```

- 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;
}
```



Be Careful What You Wish For…

```
float sprod(float *a, float *b, int n) {
  float sum = 0.0f;
#pragma omp for simd reduction(+:sum) \
                     schedule(static, 5)
  for (int k=0; k<n; k++)
    sum += a[k] * b[k];
  return sum;
}
```

- 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!

OpenMP 4.5 Simplifies SIMD Chunks

```
float sprod(float *a, float *b, int n) {
  float sum = 0.0f;
#pragma omp for simd reduction(+:sum) \
                     schedule(simd: static, 5)
  for (int k=0; k<n; k++)
    sum += a[k] * b[k];
  return sum;
}
```

- 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

SIMD Function Vectorization

```
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 SIMD-parallel 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)
```

SIMD Function Vectorization

```
#pragma omp declare simd
float min(float a, float b) {
    return a < b ? a : b;
}
```

```
_ZGVZN16vv_min(%zmm0, %zmm1):
    vminps %zmm1, %zmm0, %zmm0
    ret
```

```
#pragma omp declare simd
float distsq(float x, float y) {
    return (x - y) * (x - y);
}
```

```
_ZGVZN16vv_distsq(%zmm0, %zmm1):
    vsubps %zmm0, %zmm1, %zmm2
    vmulps %zmm2, %zmm2, %zmm0
    ret
```

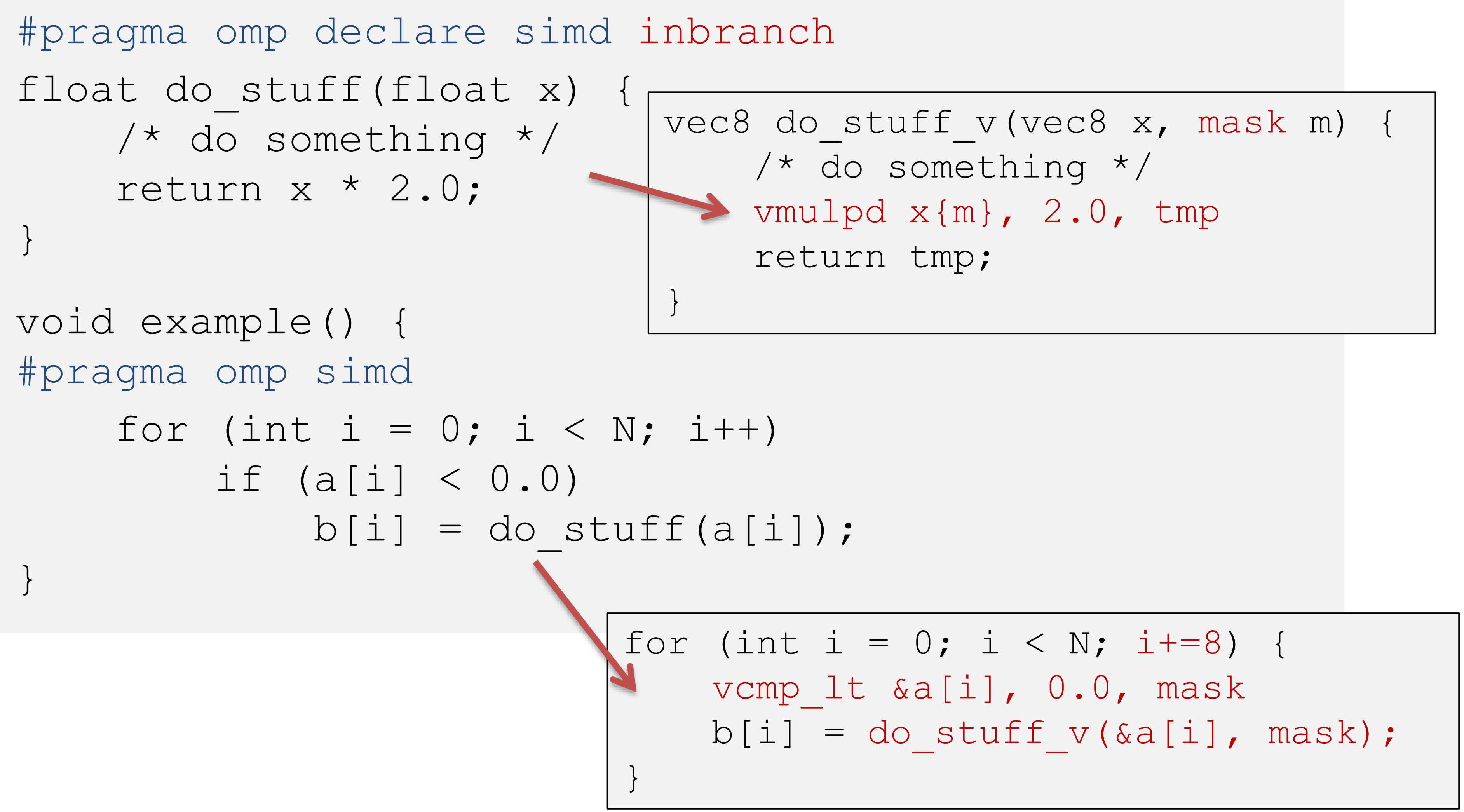
```
void example() {
#pragma omp parallel for simd
    for (i=0; i<N; i++) {
        d[i] = min(distsq(a[i], b[i]), c[i]);
}   }
```

```
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]`*`)`

inbranch & notinbranch



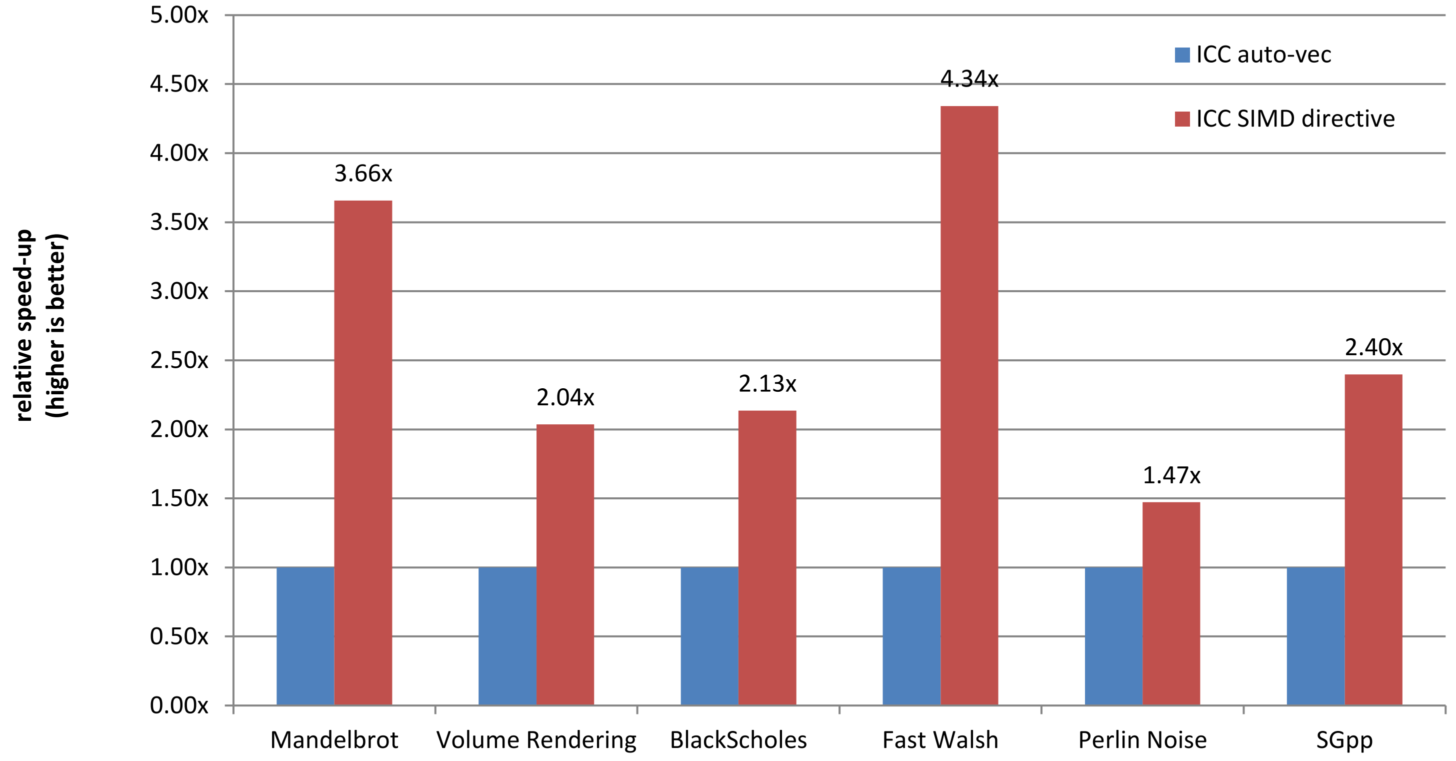
```
#pragma omp declare simd inbranch
float do_stuff(float x) {
    /* do something */
    return x * 2.0;
}

void example() {
#pragma omp simd
    for (int i = 0; i < N; i++)
        if (a[i] < 0.0)
            b[i] = do_stuff(a[i]);
}
```

```
vec8 do_stuff_v(vec8 x, mask m) {
    /* do something */
    vmulpd x{m}, 2.0, tmp
    return tmp;
}
```

```
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

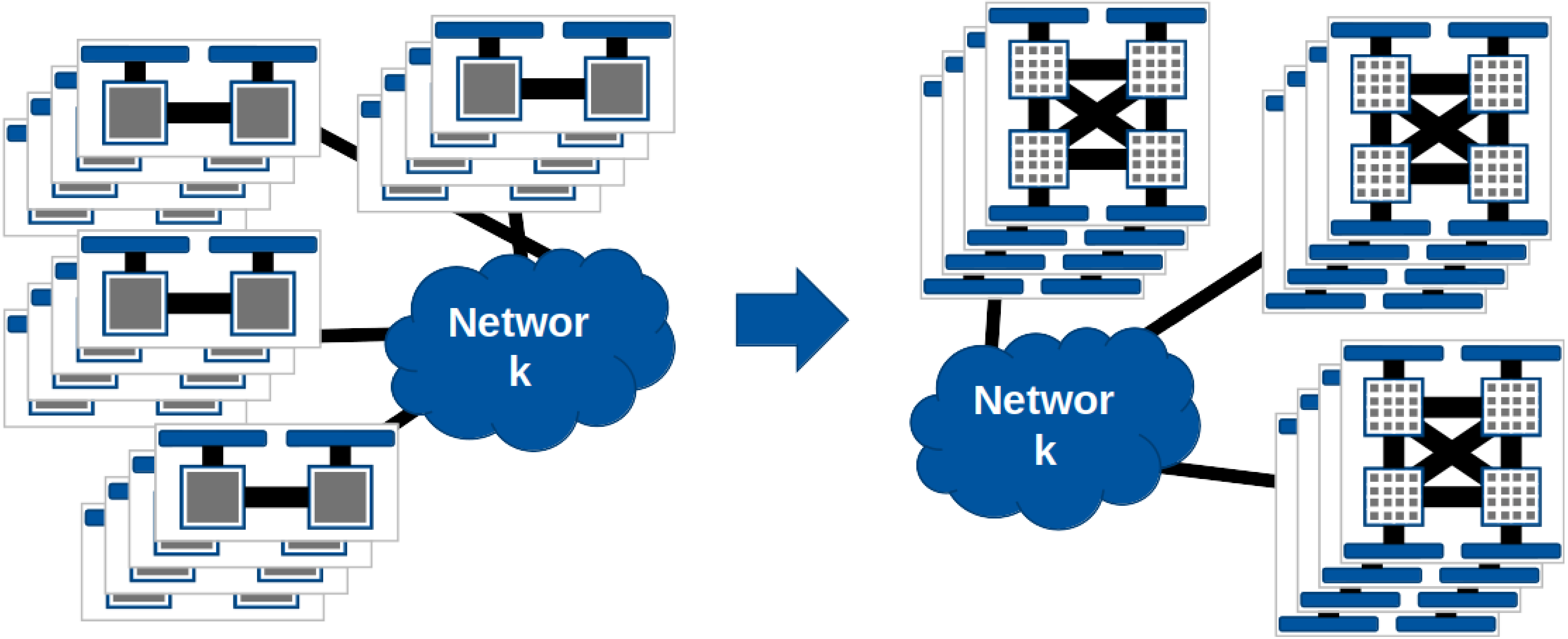
OpenMP and MPI

Christian Terboven
Michael Klemm

Motivation

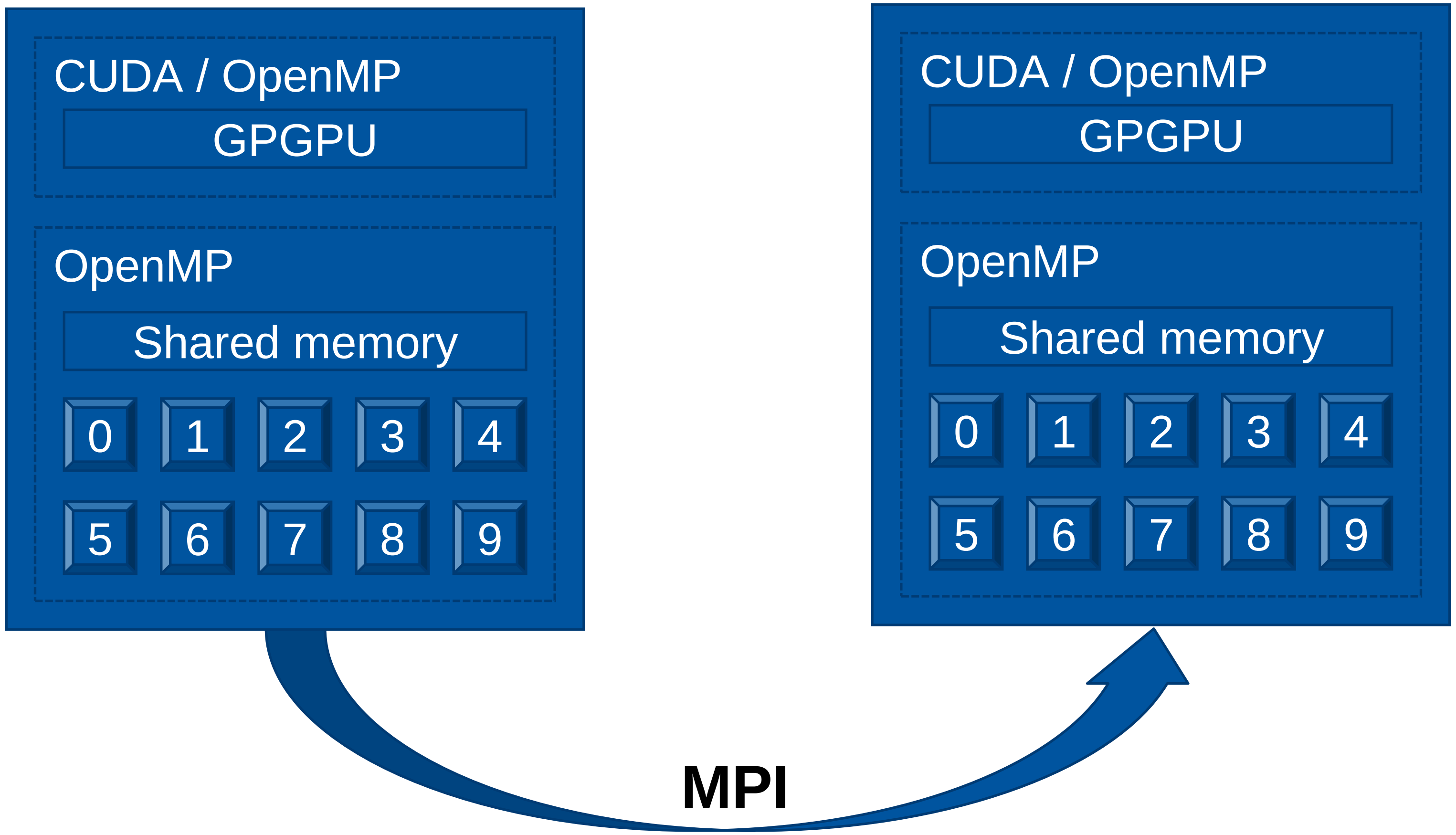
Motivation for hybrid programming

- Increasing number of cores per node



Hybrid programming

- (Hierarchical) mixing of different programming paradigms

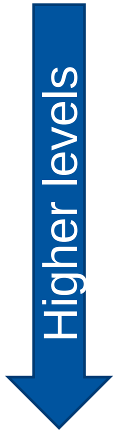


MPI and OpenMP

MPI – threads interaction

- MPI needs special initialization in a threaded environment
  - Use `MPI_Init_thread` to communicate thread support level

- Four levels of threading support


Higher levels

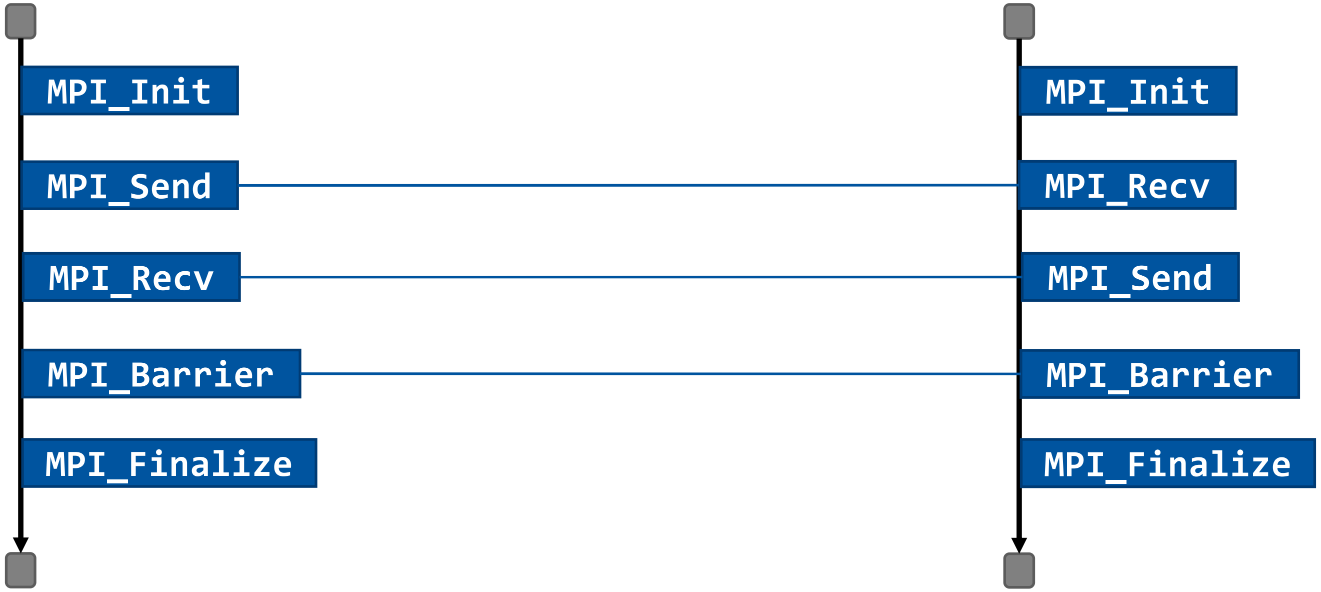
Level identifier	Description
`MPI_THREAD_SINGLE`	Only one thread may execute
`MPI_THREAD_FUNNELED`	Only the main thread may make MPI calls
`MPI_THREAD_SERIALIZED`	Any one thread may make MPI calls at a time
`MPI_THREAD_MULTIPLE`	Multiple threads may call MPI concurrently with no restrictions

- `MPI_THREAD_MULTIPLE` may incur significant overhead inside an MPI implementation

MPI – Threading support levels

- MPI_THREAD_SINGLE
  - Only one thread per MPI rank

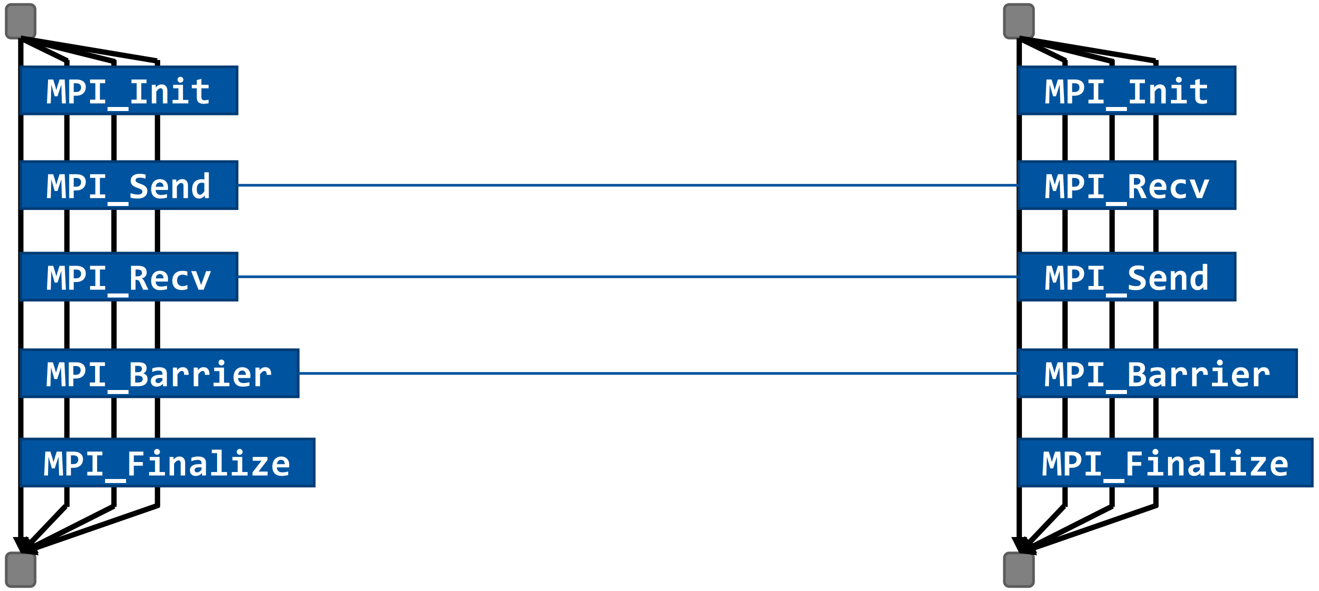
MPI Communication
Thread Synchronization



MPI – Threading support levels

- MPI_THREAD_FUNNELED
  - Only one thread communicates

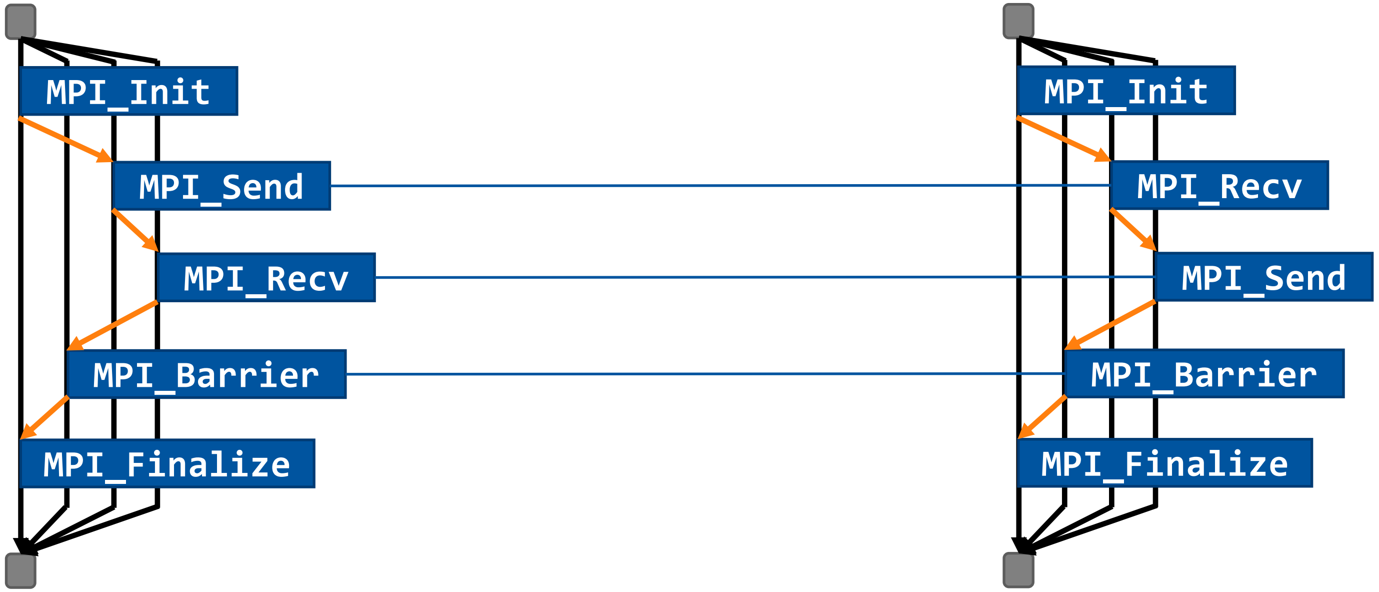
MPI Communication
Thread Synchronization



MPI – Threading support levels

- MPI_THREAD_SERIALIZED
  - Only one thread communicates at a time

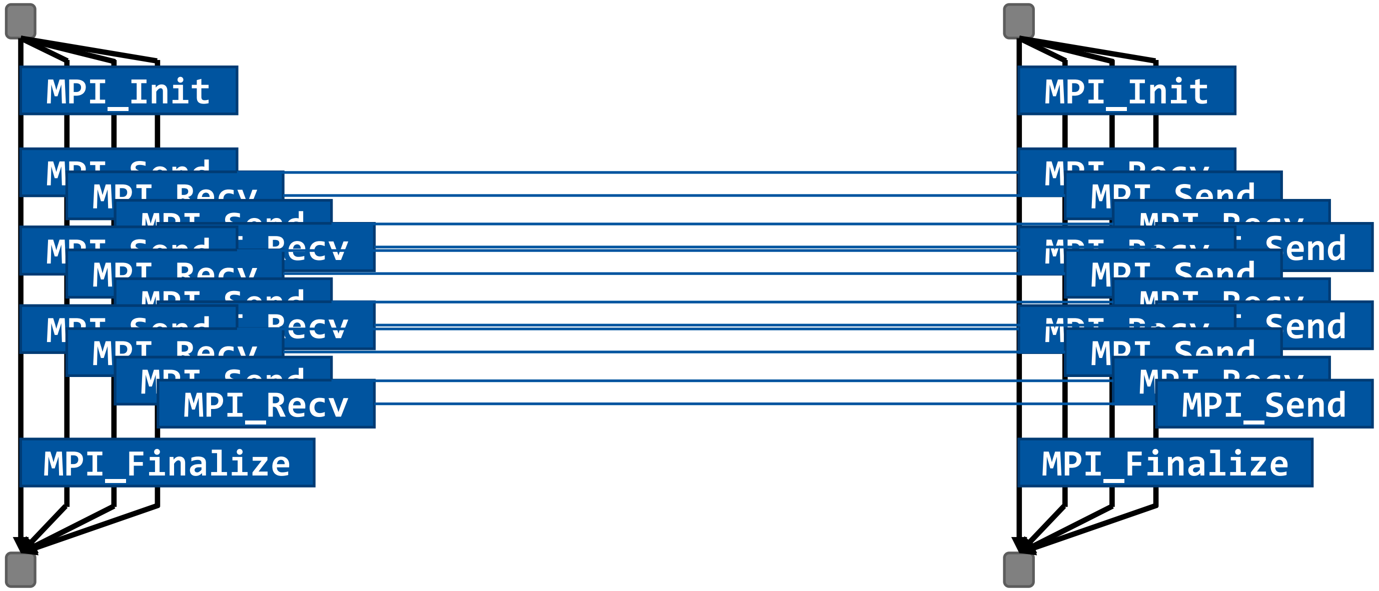
— MPI Communication
— Thread Synchronization



MPI – Threading support levels

- MPI_THREAD_MULTIPLE
  - All threads communicate concurrently without synchronizatio

— MPI Communication
— Thread Synchronization


MPI_Init
MPI_Send
MPI_Recv
MPI_Send
MPI_Recv
MPI_Finalize
MPI_Init
MPI_Recv
MPI_Send
MPI_Recv
MPI_Send
MPI_Finalize