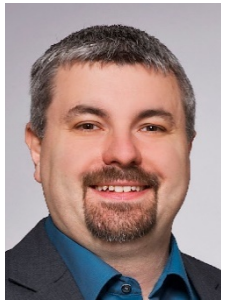
Programming OpenMP

Christian Terboven

Michael Klemm



Agenda (in total 7 Sessions)

- Session 1: OpenMP Introduction
- Session 2: Tasking
- Session 3: Optimization for NUMA and SIMD
- Session 4: What Could Possibly Go Wrong Using OpenMP
- Session 5: Introduction to Offloading with OpenMP
- Session 6: Advanced Offloading Topics
- **Session 7: Miscellaneous Topics**
  - → Review of Session 6, Q&A
  - → Review of Homework Assignments
  - → SIMD, Part 2
  - → Task Affinity
  - → Real World Applications Case Study: NWChem
  - → Hybrid Programming: MPI + OpenMP

Programming OpenMP

SIMD, Part 2

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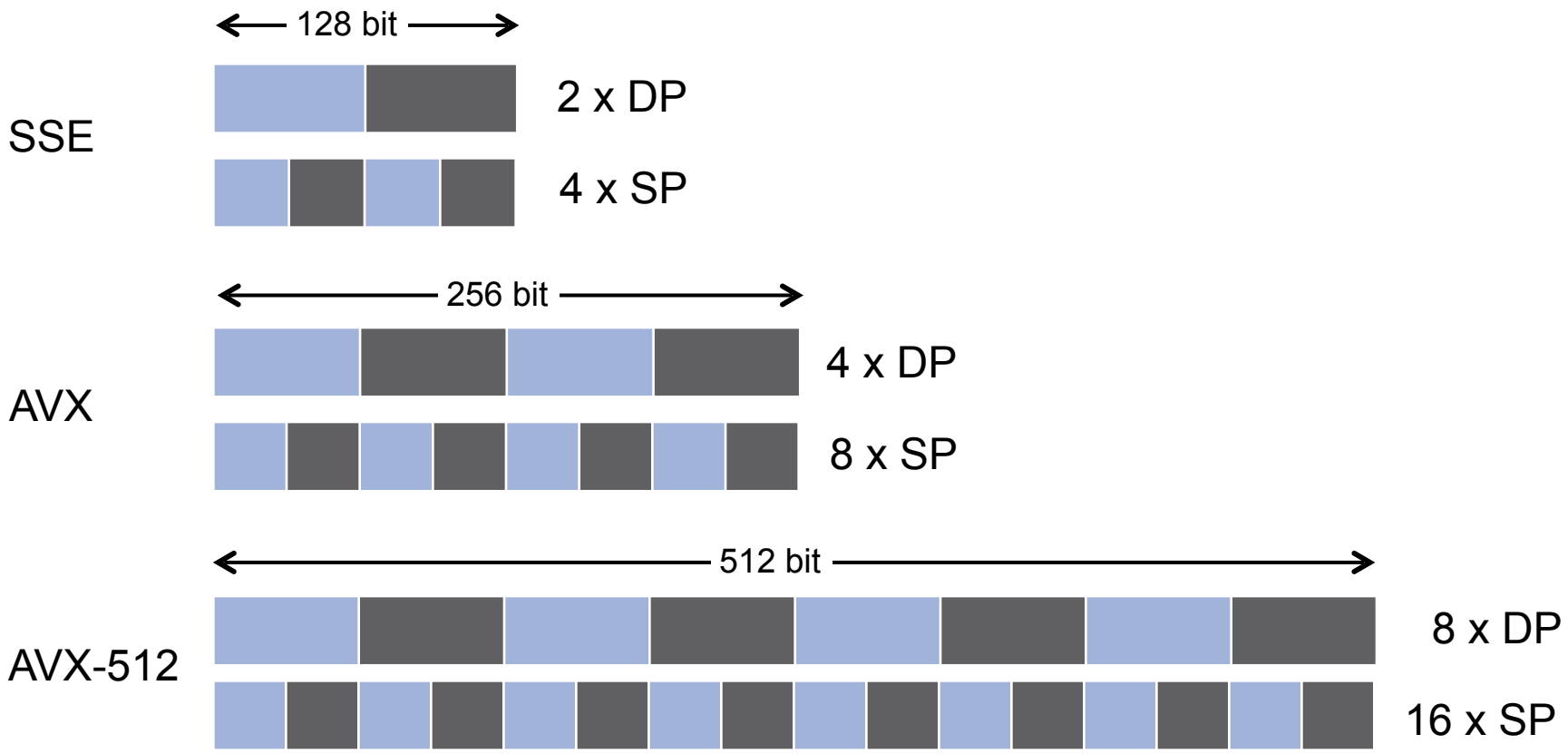
SIMD on x86 Architectures (Recap)

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



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Example: clang/LLVM	GCC	Intel Compiler
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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++) {
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}
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```
#pragma omp parallel for
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for (int i = 0; i < N; i++) {
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}
```

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
```

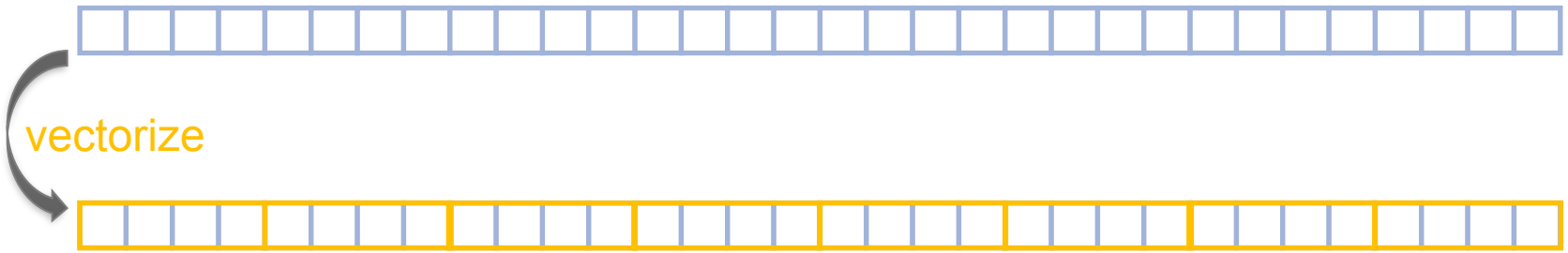
- Syntax (Fortran)

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

Example

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

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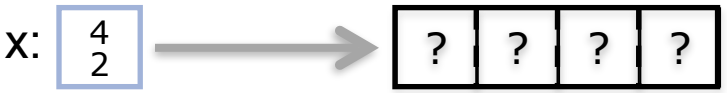
- `private(var-list)`:
  Uninitialized vectors for variables in *var-list*



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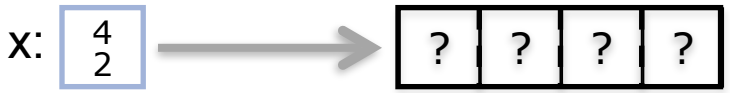

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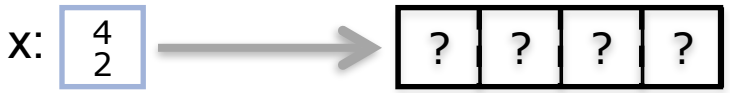

- `firstprivate(var-list):`
  Initialized vectors for variables in *var-list*

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

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  - → Maximum number of iterations that can run concurrently without breaking a dependence
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- `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]]
```

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  float sum = 0.0f;
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  for (int k=0; k<n; k++)
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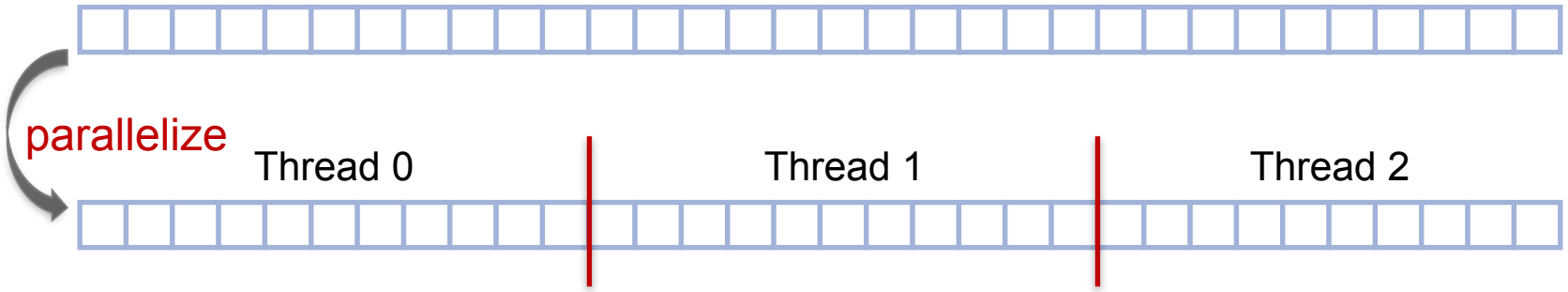

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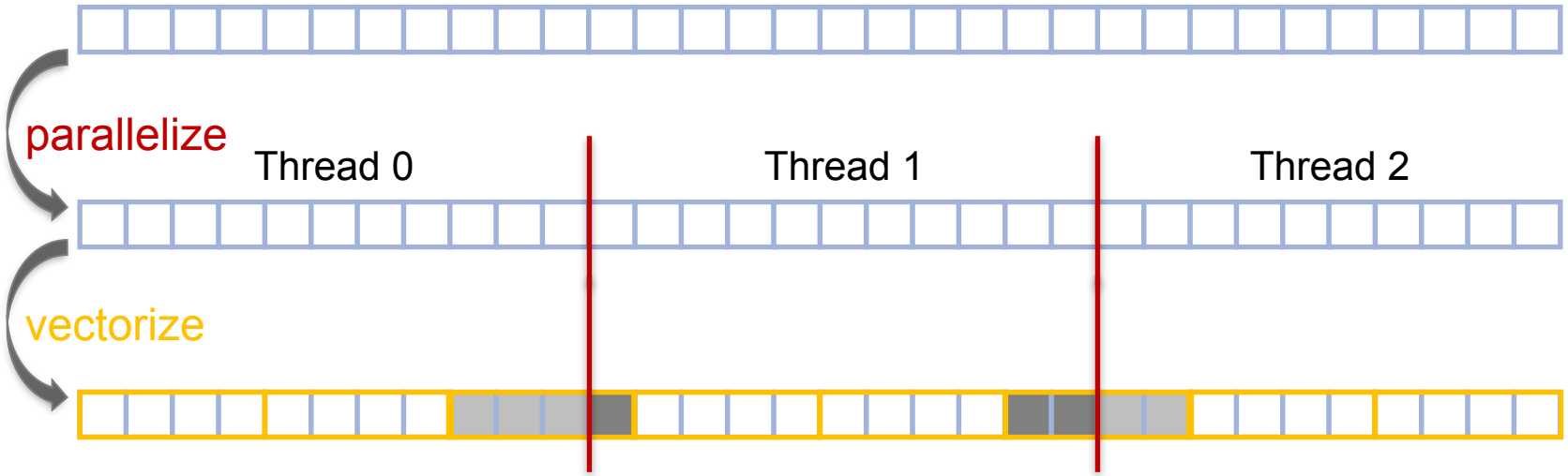

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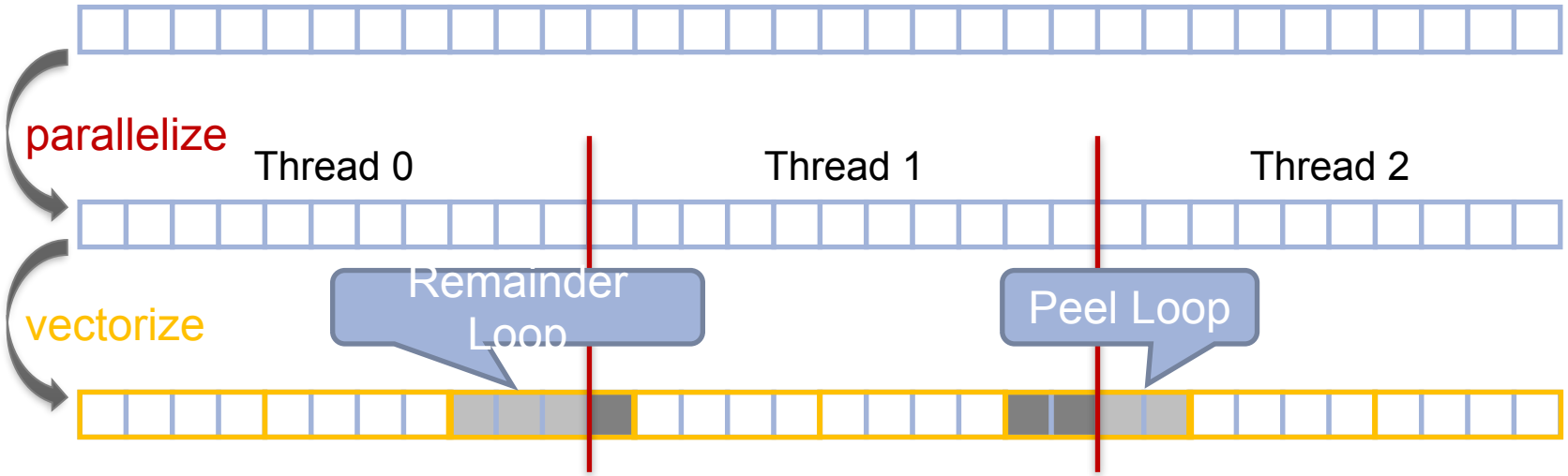

Be Careful What You Wish For…

- You should choose chunk sizes that are multiples of the SIMD length
  - → Remainder loops are not triggered
  - → Likely better performance

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```
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;
}
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```

- You should choose chunk sizes that are multiples of the SIMD length
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- 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

- 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
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SIMD Function Vectorization

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)
```

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    for (i=0; i<N; i++) {
        d[i] = min(distsq(a[i], b[i]), c[i]);
}   }
```

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

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

```
vmovups (%r14,%r12,4), %zmm0
vmovups (%r13,%r12,4), %zmm1
call _ZGVZN16vv_distsq
vmovups (%rbx,%r12,4), %zmm1
call _ZGVZN16vv_min
```

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- `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]);
}
```

inbranch & notinbranch

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}
```

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

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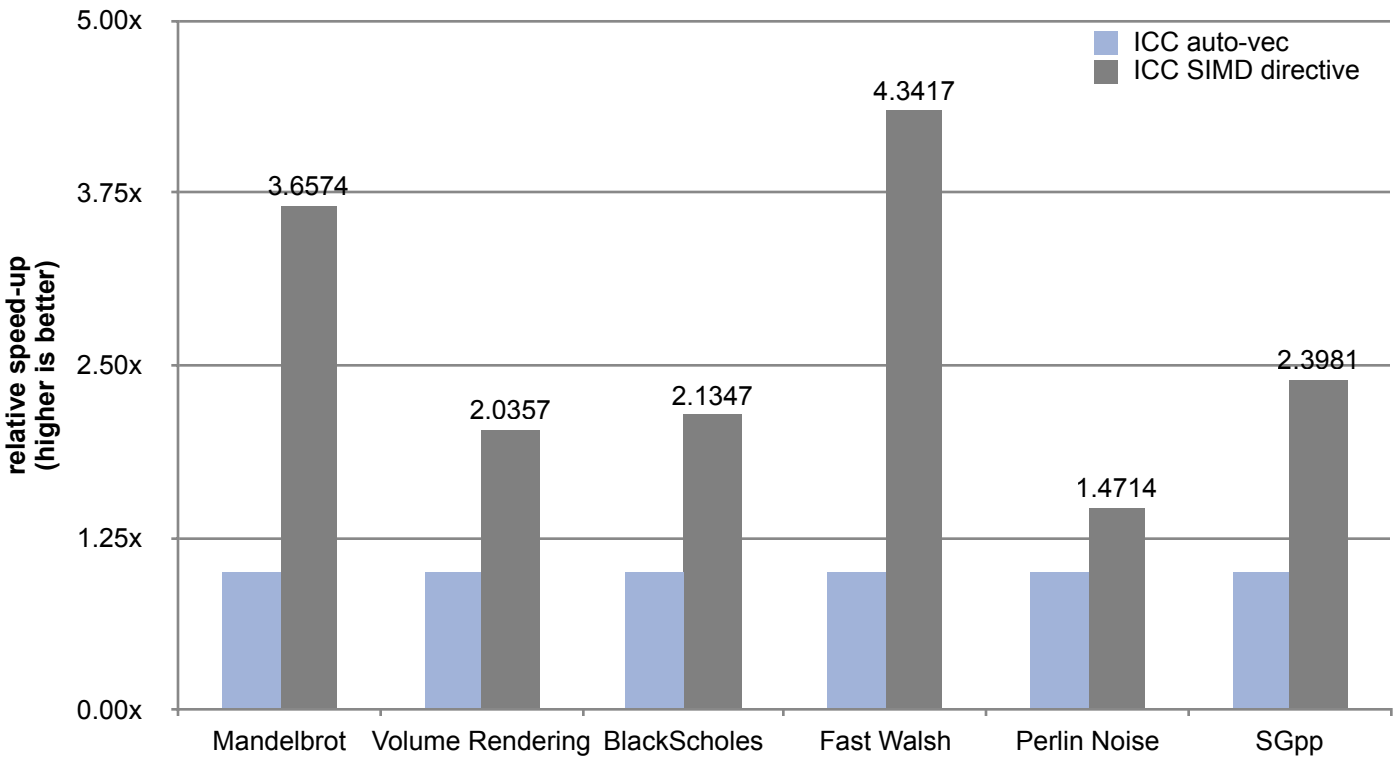
    return tmp;
}
```

```
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

NUMA

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RWTH AACHEN UNIVERSITY

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`

<u>OpenMP Tasking:</u>

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

<u>OpenMP 5.0:</u>

- `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

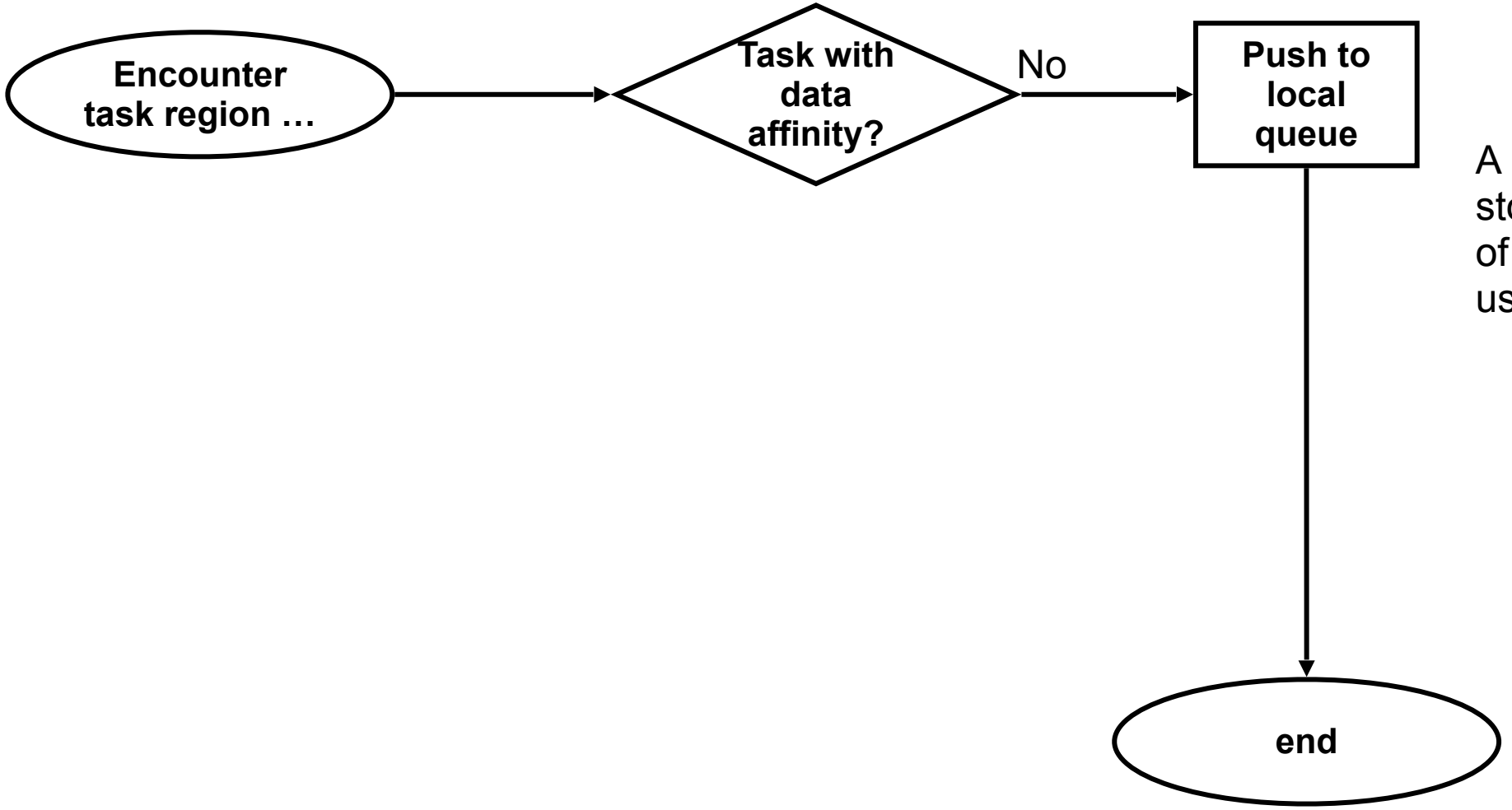
- Excerpt from task-parallel STREAM

```
#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`)

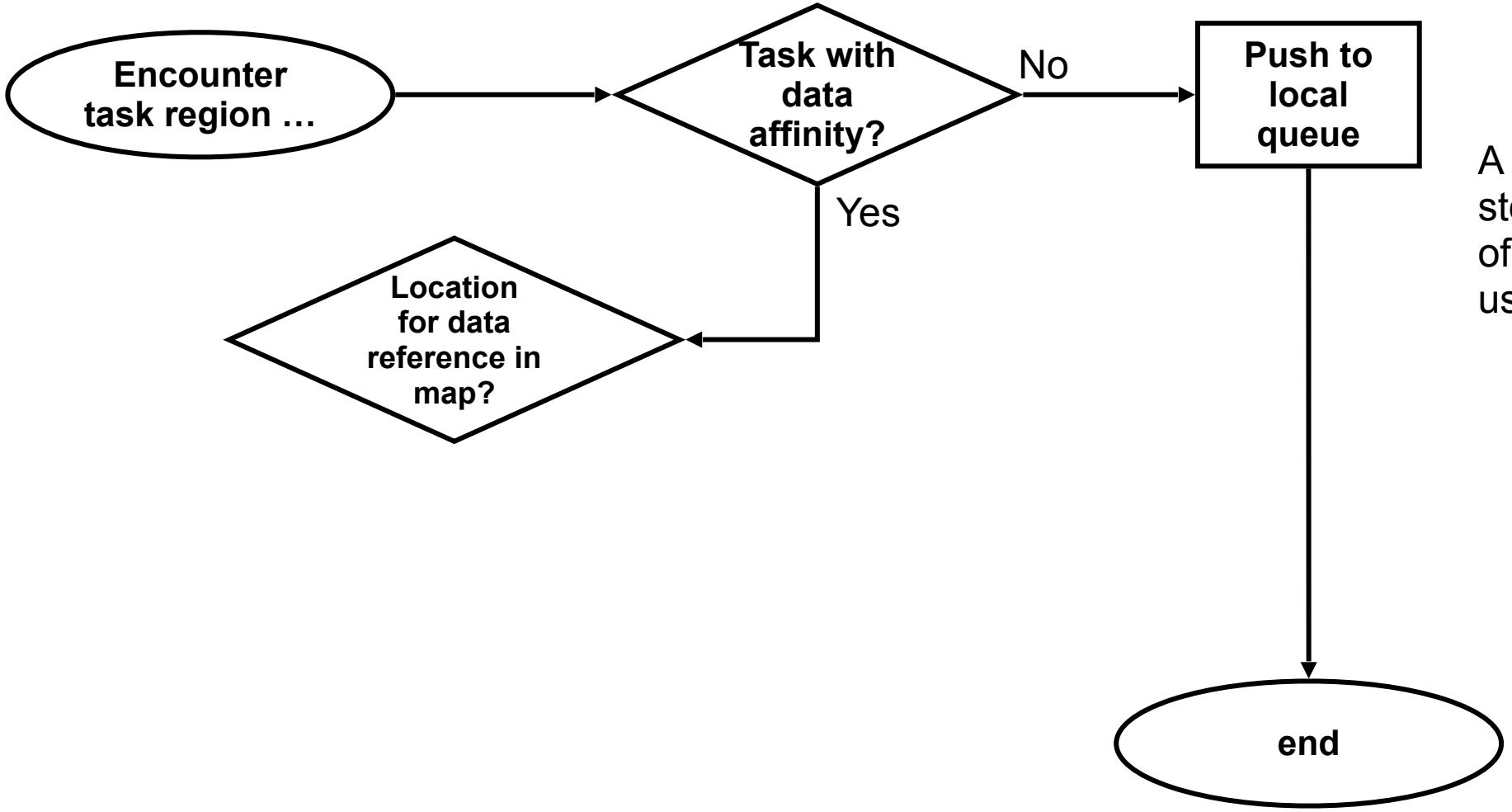
→Assumption: initialization and computation have same blocking and same affinity

Selected LLVM implementation details



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

Selected LLVM implementation details



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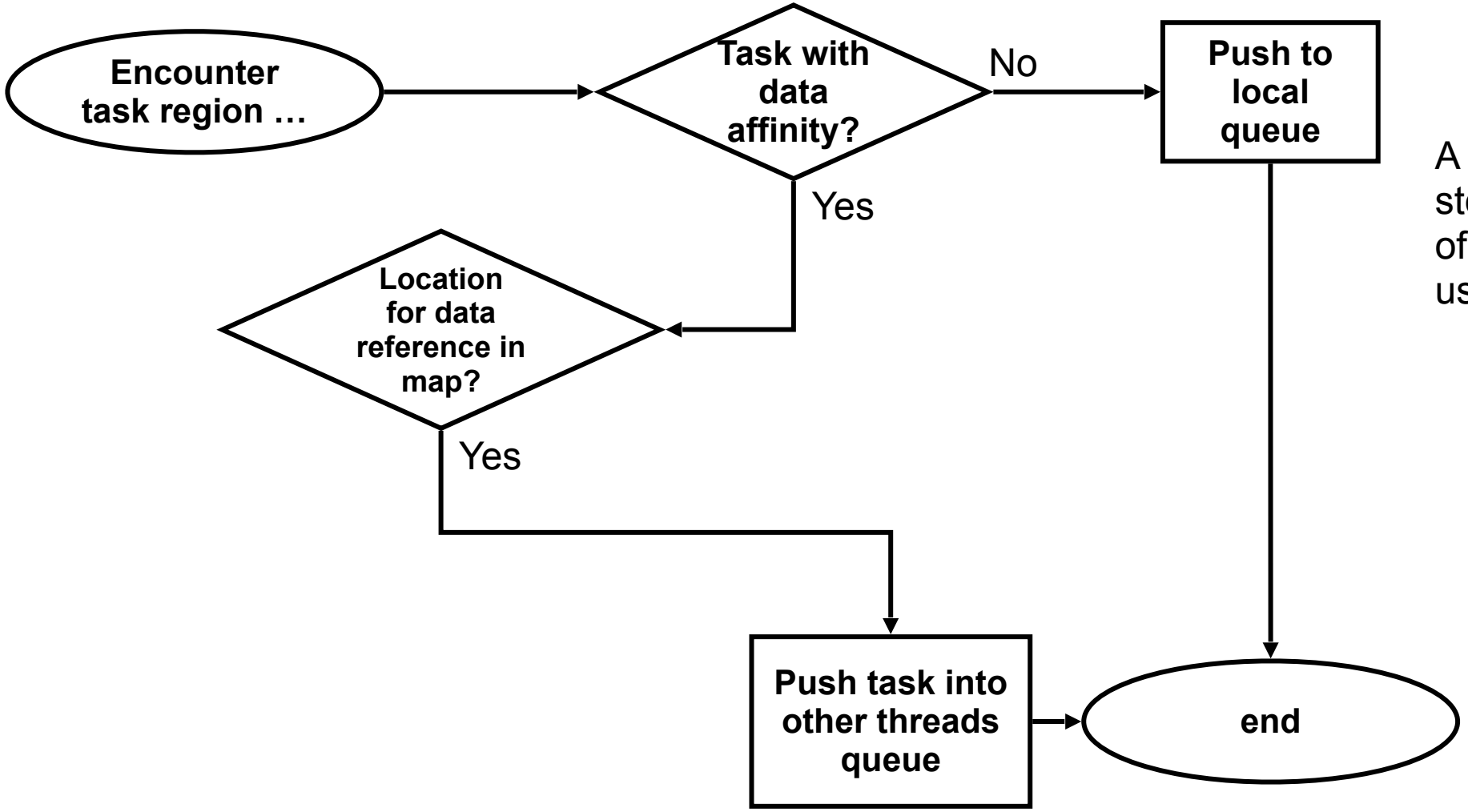

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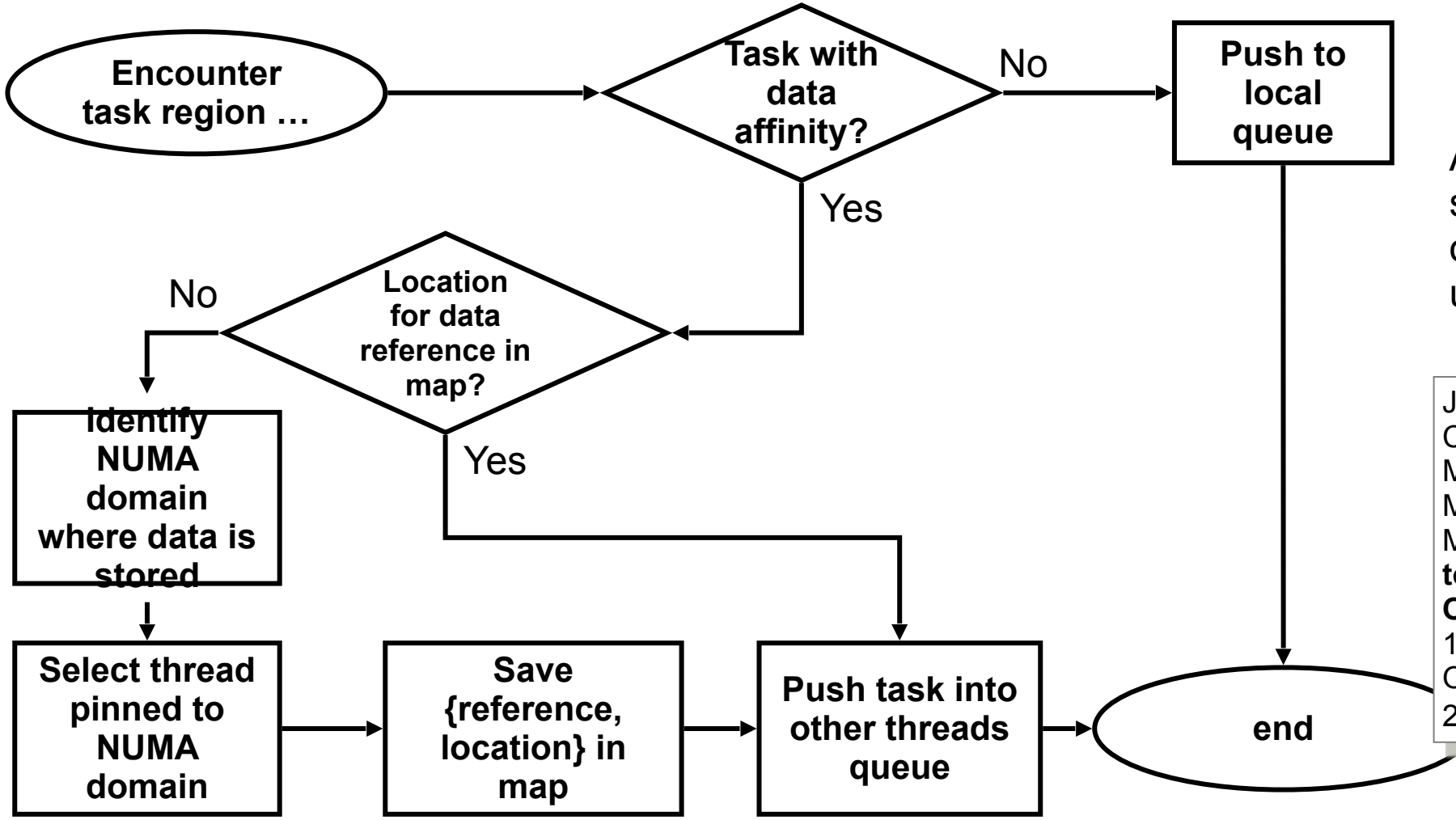

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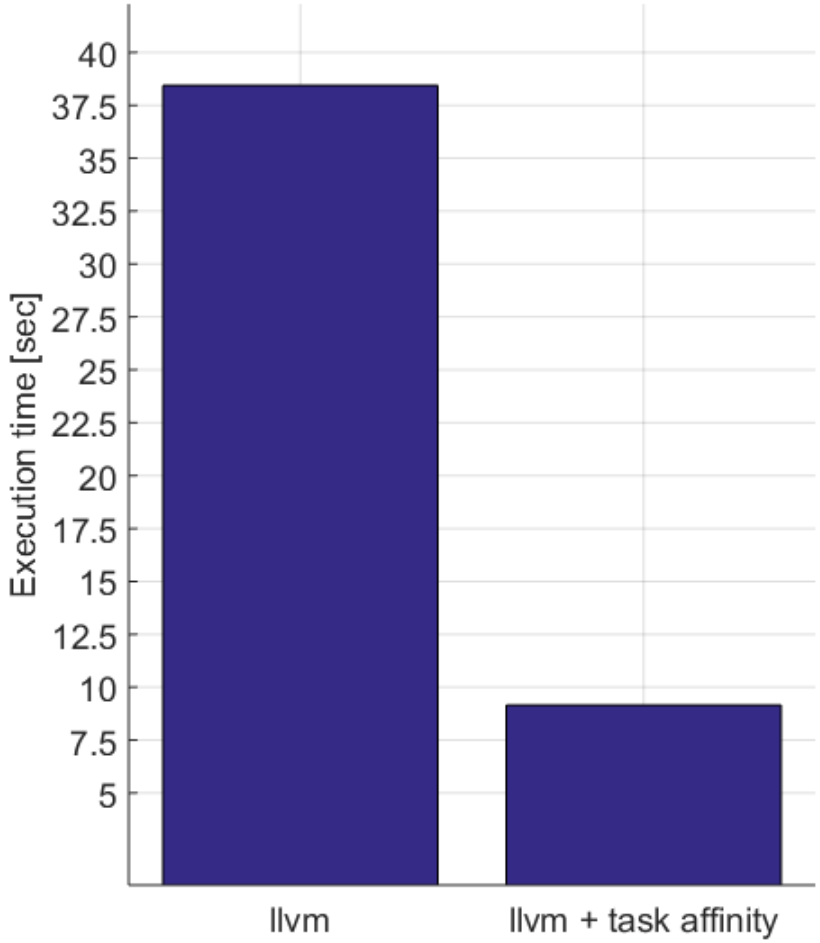
Jannis Klinkenberg, Philipp Samfass, Christian Terboven, Alejandro Duran, Michael Klemm, Xavier Teruel, Sergi Mateo, Stephen L. Olivier, and Matthias S. Müller. **Assessing Task-to-Data Affinity in the LLVM OpenMP Runtime**. Proceedings of the 14th International Workshop on OpenMP, IWOMP 2018. September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

Evaluation

Program runtime
Median of 10 runs



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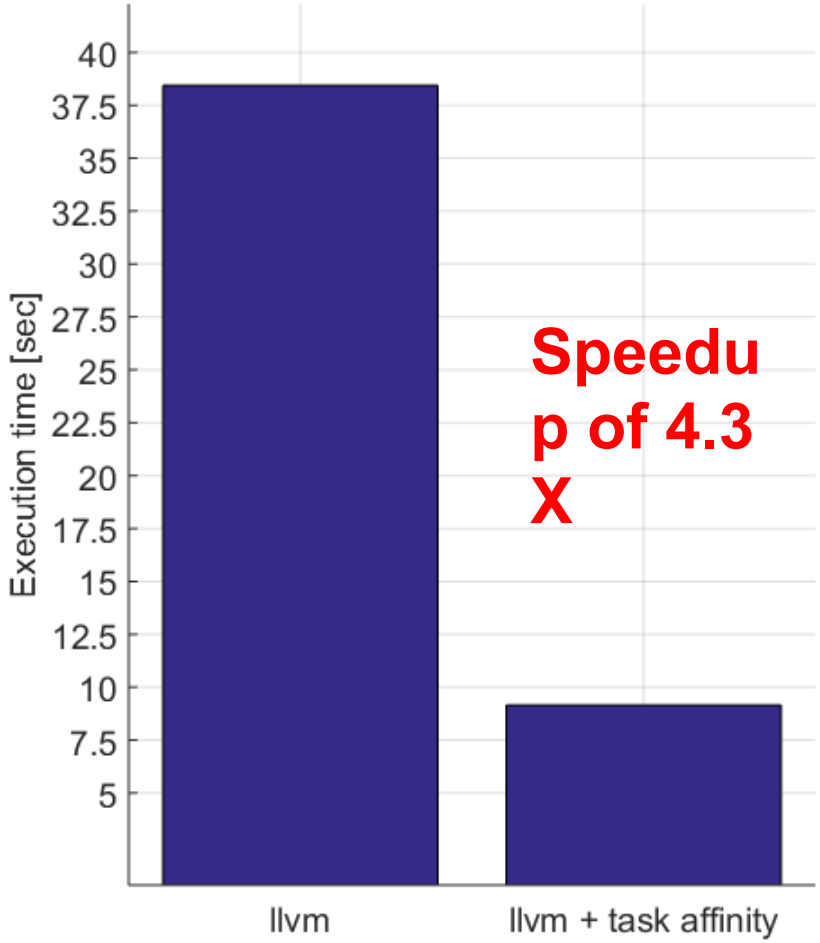

Speedup of 4.3X

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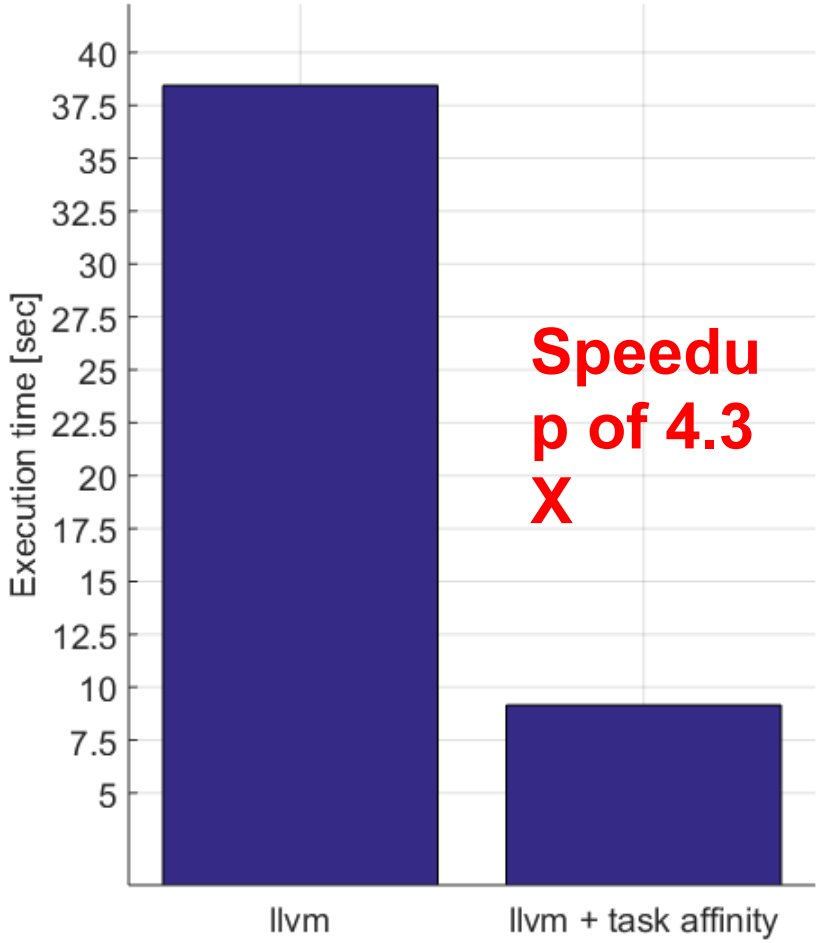

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LIKWID: reduction of remote data volume from 69% to 13%

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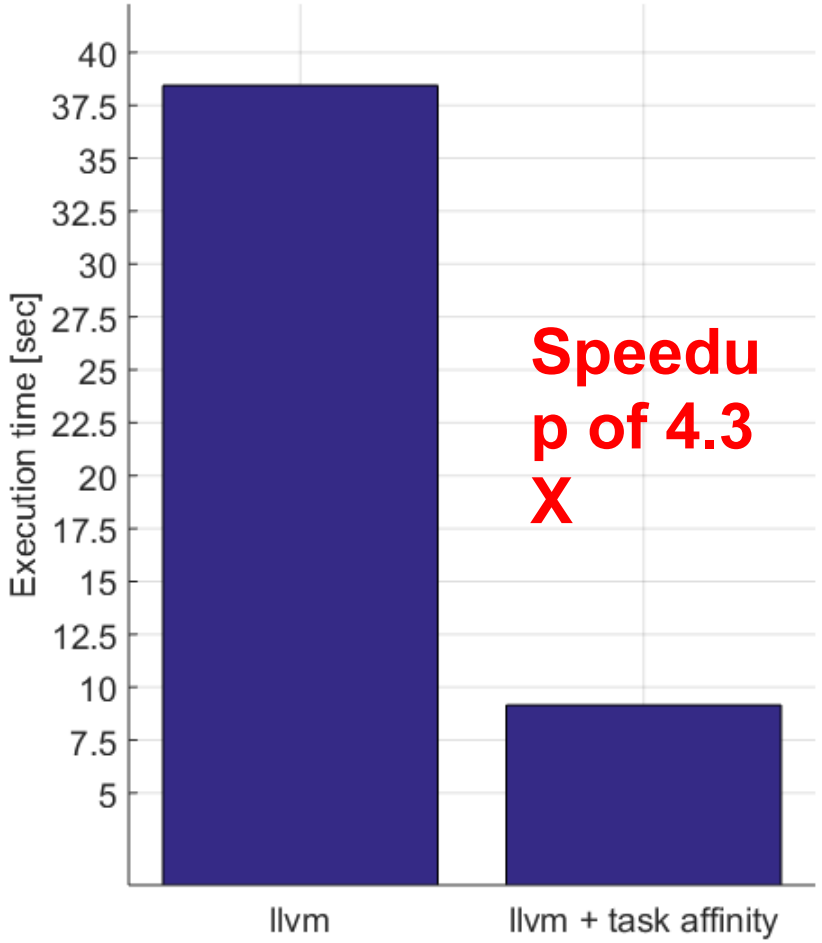
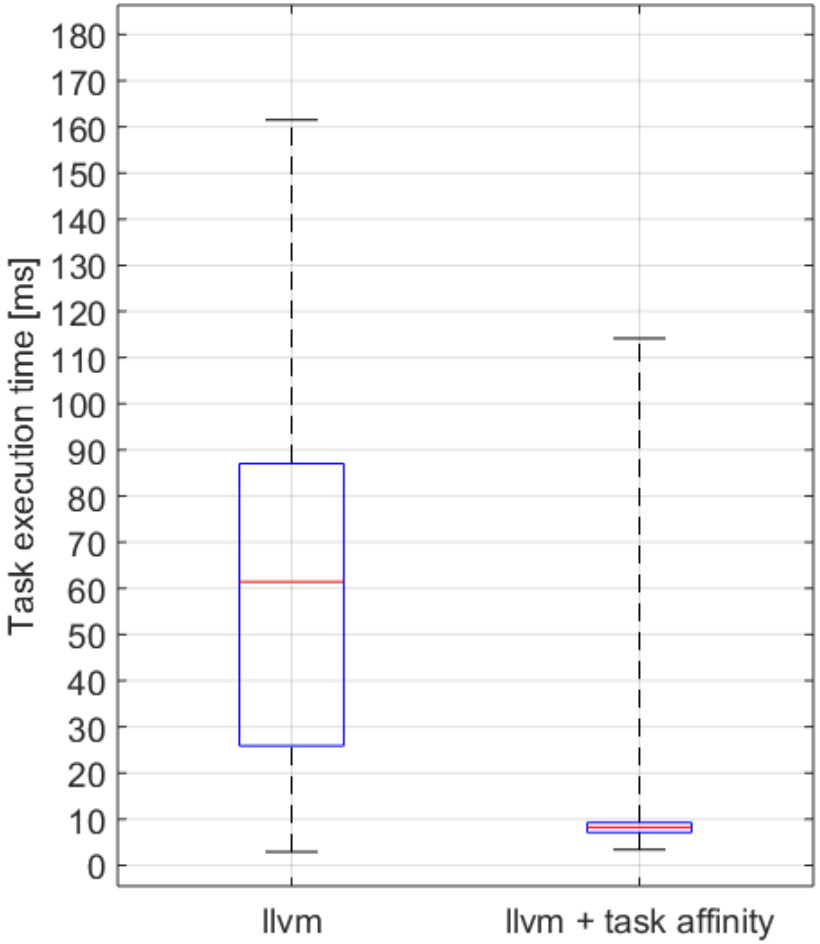


Speedup of 4.3 X

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

Case Study: NWChem TCE CCSD(T)

TCE: Tensor Contraction Engine
CCSD(T): Coupled-Cluster with Single, Double, and perturbative Triple replacements

NWChem

- Computational chemistry software package
  - Quantum chemistry
  - Molecular dynamics
- Designed for large-scale supercomputers
- Developed at the EMSL at PNNL
  - EMSL: Environmental Molecular Sciences Laboratory
  - PNNL: Pacific Northwest National Lab
- URL: http://www.nwchem-sw.org

Finding Offload Candidates

- Requirements for offload candidates
  - Compute-intensive code regions (kernels)
  - Highly parallel
  - Compute scaling stronger than data transfer, e.g., compute $O(n^3)$ vs. data size $O(n^2)$

Example Kernel (1 of 27 in total)

```
      subroutine sd_t_d1_1(h3d,h2d,h1d,p6d,p5d,p4d,
     1                 h7d,triplesx,t2sub,v2sub)
c     Declarations omitted.
      double precision triplesx(h3d*h2d,h1d,p6d,p5d,p4d)
      double precision t2sub(h7d,p4d,p5d,h1d)
      double precision v2sub(h3d*h2d,p6d,h7d)
!$omp target „presence?(triplesx,t2sub,v2sub)"
!$omp teams distribute parallel do
private(p4,p5,p6,h2,h3,h1,h7)
      do p4=1,p4d
      do p5=1,p5d
      do p6=1,p6d
      do h1=1,h1d
      do h7=1,h7d
      do h2h3=1,h3d*h2d
       triplesx(h2h3,h1,p6,p5,p4)=triplesx(h2h3,h1,p6,p5,p4)
     1   - t2sub(h7,p4,p5,h1)*v2sub(h2h3,p6,h7)
      end do
      end do
      end do
      end do
      end do
      end do
!$omp end teams distribute parallel do
!$omp end target
      end subroutine
```

- All kernels have the same structure
- 7 perfectly nested loops
- Some kernels contain inner product loop (then, 6 perfectly nested loops)
- Trip count per loop is equal to “tile size” (20-30 in production)

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- Trip count per loop is equal to “tile size” (20-30 in production)
- Naïve data allocation (tile size 24)
  - Per-array transfer for each `target` construct
  - triplesx: 1458 MB
  - t2sub, v2sub: 2.5 MB each

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      do h7=1,h7d
      do h2h3=1,h3d*h2d
       triplesx(h2h3,h1,p6,p5,p4)=triplesx(h2h3,h1,p6,p5,p4)
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1.5GB data transferred (host to device)

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  - triplesx: 1458 MB
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Invoking the Kernels / Data Management

- Simplified pseudo-code

```
!$omp target enter data map(alloc:triplesx(1:tr_size))
c     for all tiles
      do ...
        call zero_triplesx(triplesx)
        do ...
          call comm_and_sort(t2sub, v2sub)
!$omp target data map(to:t2sub(t2_size)) map(to:v2sub(v2_size))
          if (...)
            call
sd_t_d1_1(h3d,h2d,h1d,p6d,p5d,p4d,h7,triplesx,t2sub,v2sub)
          end if
c         same for sd_t_d1_2 until sd_t_d1_9
!$omp target end data
        end do
        do ...
c         Similar structure for sd_t_d2_1 until sd_t_d2_9, incl. target
data
        end do
        call sum_energy(energy, triplesx)
      end do
!$omp target exit data map(release:triplesx(1:size))
```

- Reduced data transfers:

Invoking the Kernels / Data Management

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Allocate 1.5GB data once, stays on device.

- Reduced data transfers:
  - triplesx:
    - allocated once
    - always kept on the target

Invoking the Kernels / Data Management

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          if (...)
            call
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          end if
c         same for sd_t_d1_2 until sd_t_d1
!$omp target end data
        end do
        do ...
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      end do
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```

Allocate 1.5GB data once, stays on device.

Update 2x2.5MB of data for (potentially) multiple kernels.

- Reduced data transfers:
  - triplesx:
    - allocated once
    - always kept on the target
  - t2sub, v2sub:
    - allocated after comm.
    - kept for (multiple) kernel invocations

Invoking the Kernels / Data Management

- Simplified pseudo-code

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!$omp target enter data map(alloc:triplesx(1:tr_size))
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        do ...
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          end do
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          end do
          call sum_energy(energy, triplesx)
        end do
!$omp target exit data map(release:triplesx(1:size))
```

Allocate 1.5G
stays on

Update 2x2.5
(potentially) r

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      do h1=1,h1d
      do h7=1,h7d
      do h2h3=1,h3

triplesx(h2h3,h1,
     1   - t2sub(h7,p4,p5,h1)*v2sub(h2h3,p6,h7)
      end do
      end do
      end do
      end do
      end do
      end do
!$omp end teams distribute parallel do
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      end subroutine
```

Presence check determines that arrays have been allocated in the device data environment already.

Programming OpenMP

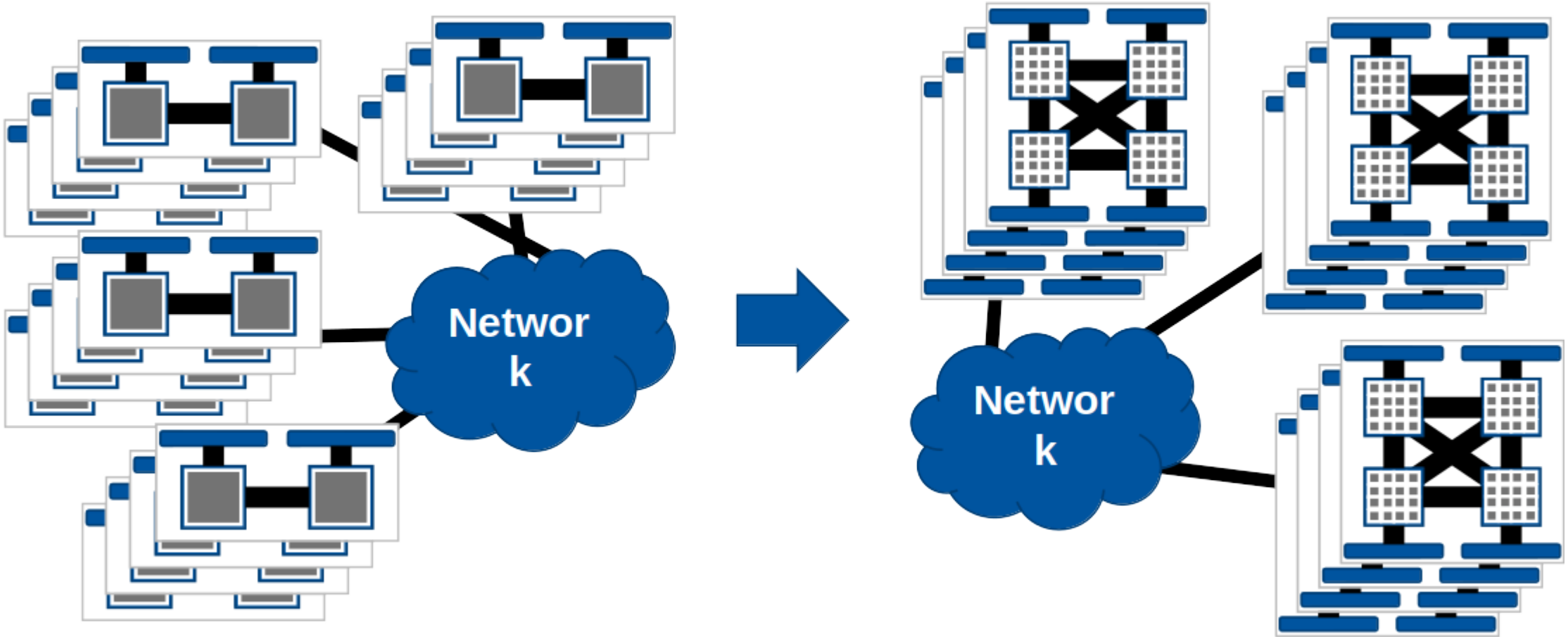
OpenMP and MPI

Christian Terboven
Michael Klemm

Motivation

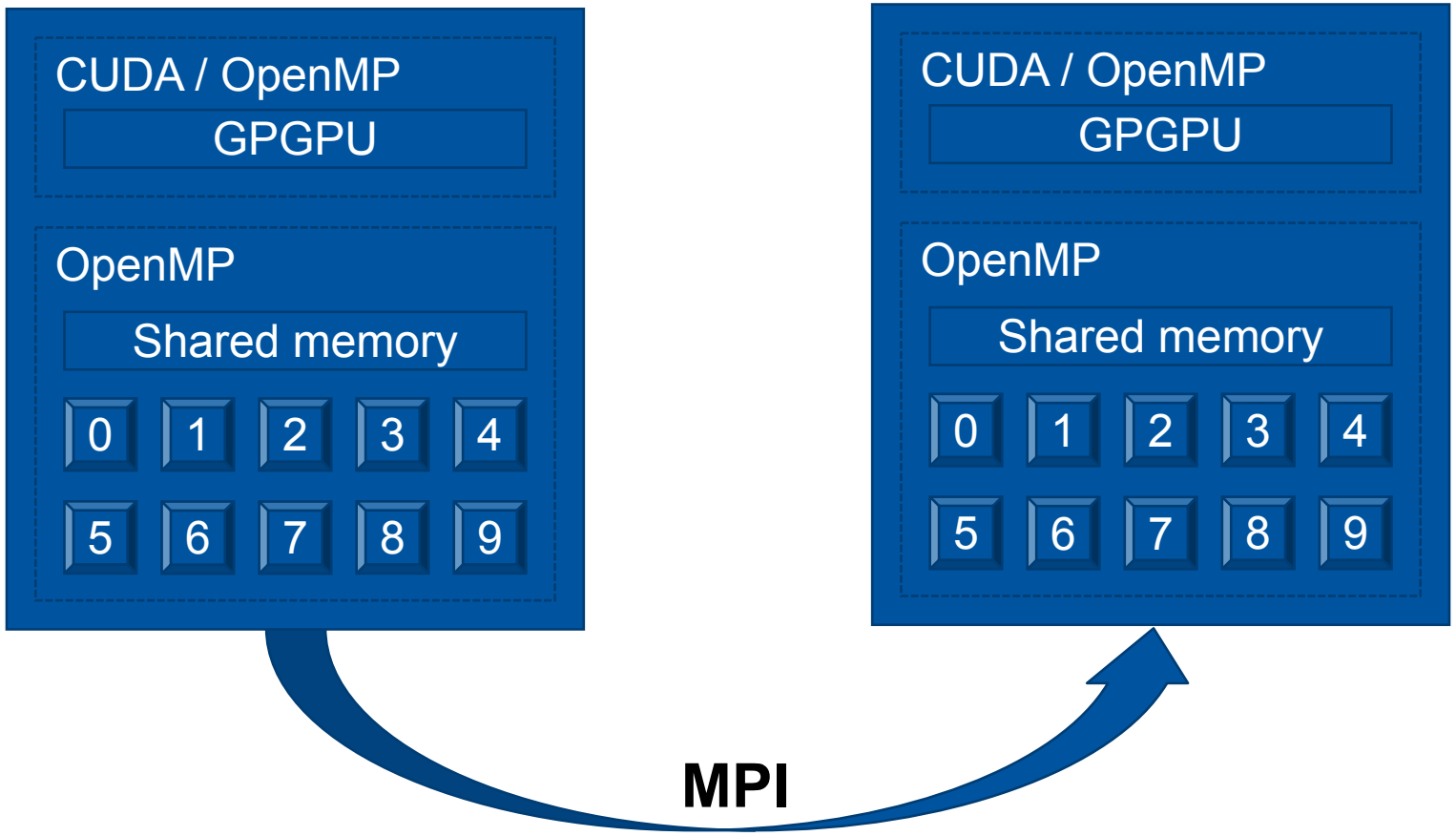
Motivation for hybrid programming

- 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

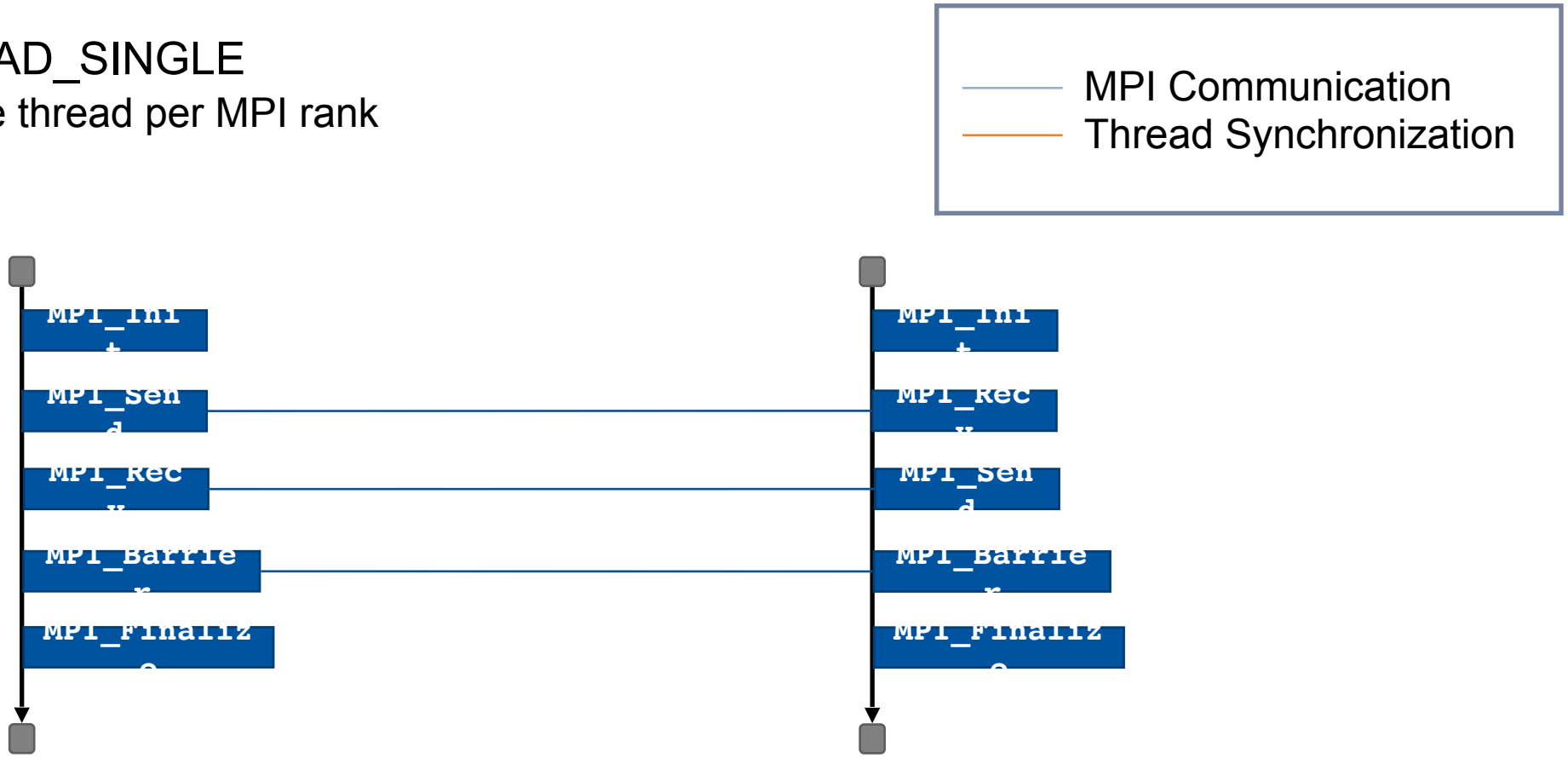
Higher levels

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

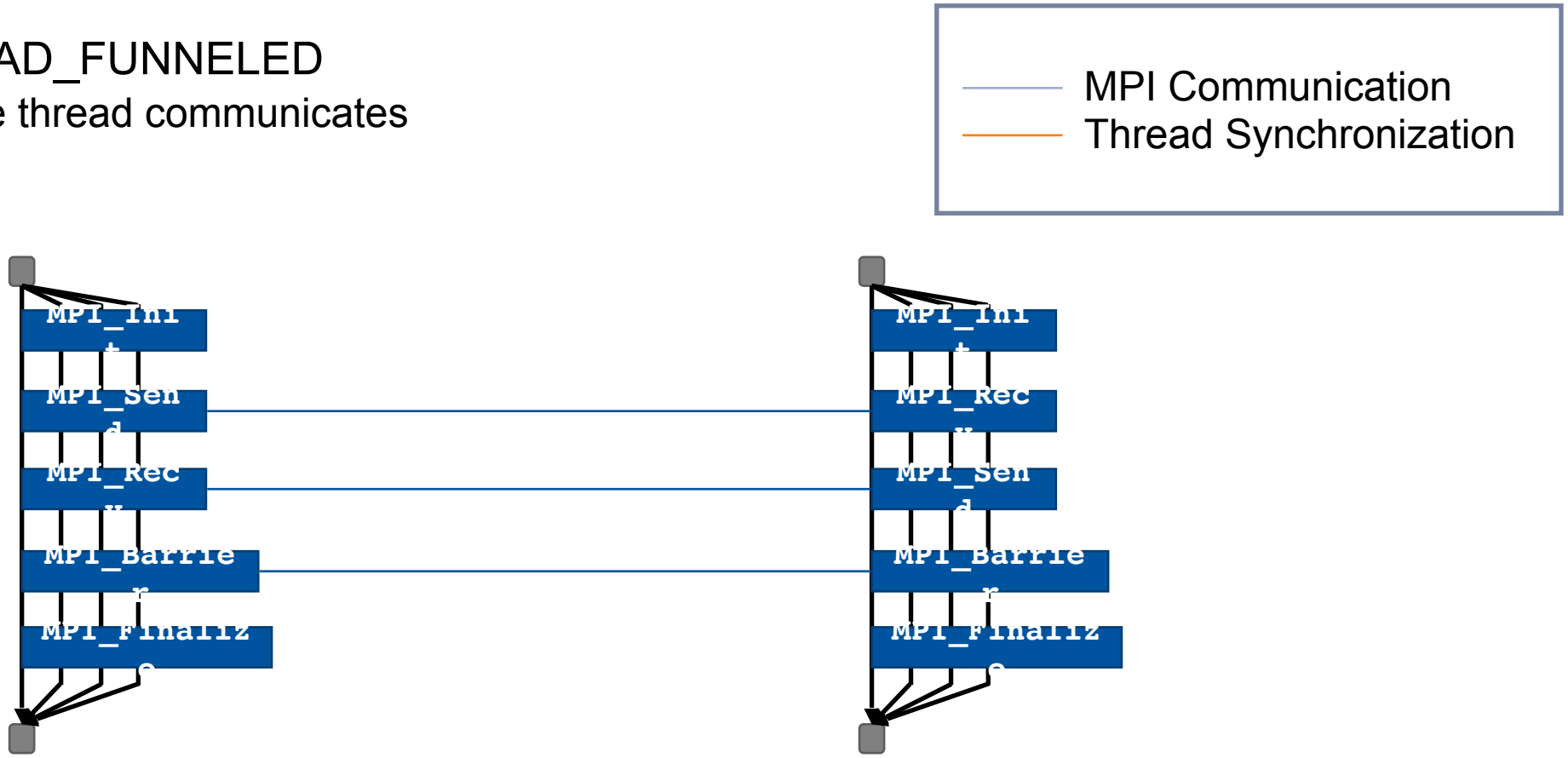
MPI – Threading support levels

- MPI_THREAD_SINGLE
  - Only one thread per MPI rank



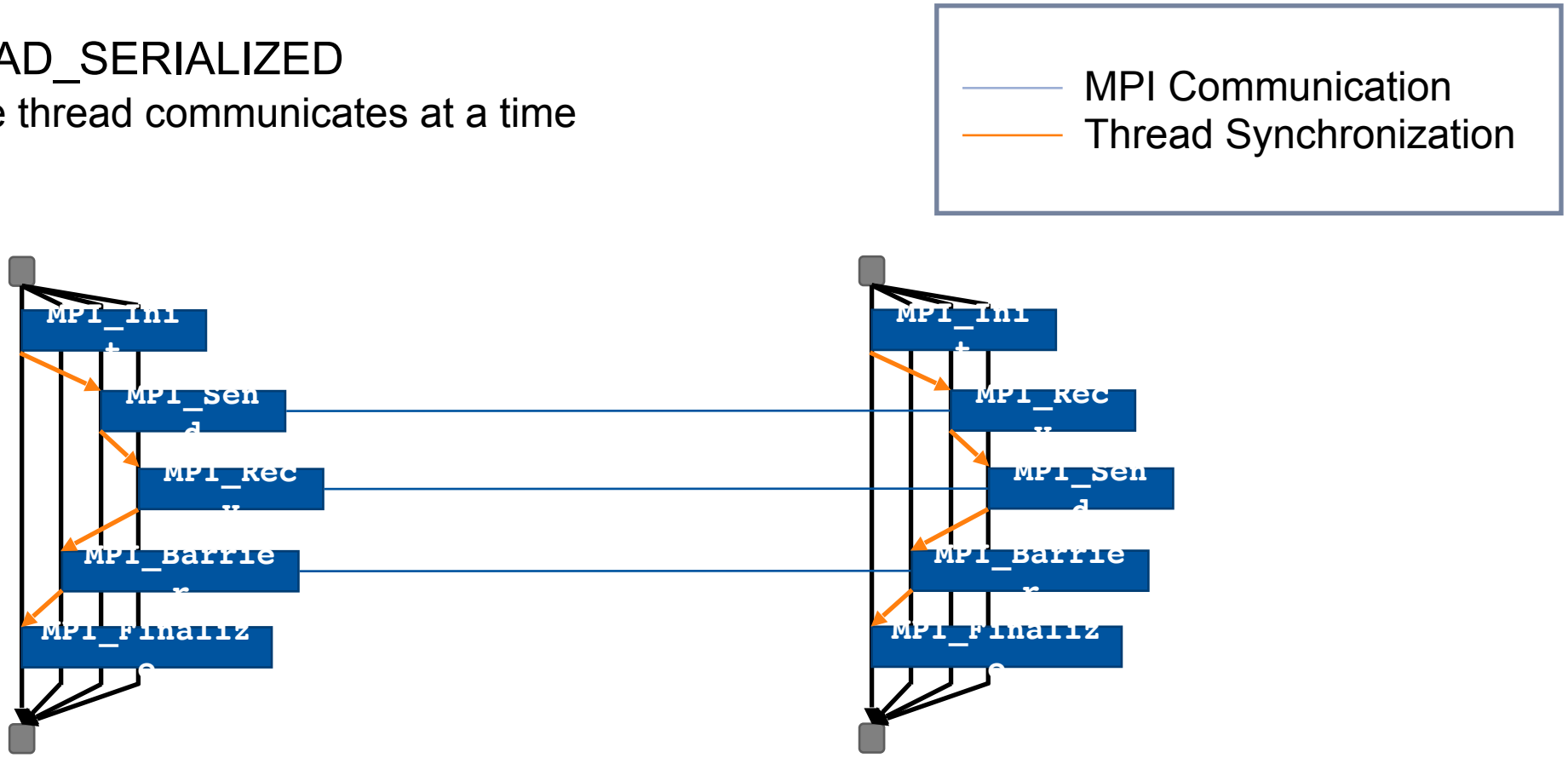
MPI – Threading support levels

- MPI_THREAD_FUNNELED
  - Only one thread communicates



MPI – Threading support levels

- MPI_THREAD_SERIALIZED
  - Only one thread communicates at a time



MPI – Threading support levels

- MPI_THREAD_MULTIPLE
  - All threads communicate concurrently without synchronizatio