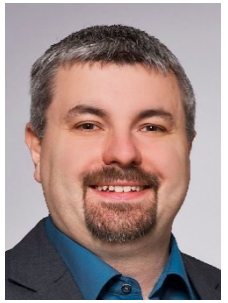
# Programming OpenMP

**Christian Terboven**

**Michael Klemm**

RWTH AACHEN UNIVERSITY

OpenMP



# 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**
  - à Review of Session 6, Q&A
  - à Review of Homework Assignments
  - à SIMD, Part 2
  - à Task Affinity
  - à Real World Applications Case Study: NWChem
  - à Hybrid Programming: MPI + OpenMP

# Programming OpenMP

## *Review*

**Christian Terboven**
Michael Klemm

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# *Questions?*

# *Jacobi*

# Example solution: Jacobi basic

```
  while ( err > tol && iter < iter_max ) {
        err = 0.0;

#pragma omp target teams distribute parallel for reduction(max:err)\
          schedule(nonmonotonic:static,1) map(to:A[0:n*m]) map(from:Anew[0:n*m], err)
        for( j = 1; j < n-1; j++) {
          for( i = 1; i < m-1; i++ ) {
            Anew[j *m+ i] = 0.25 * ( A[j     *m+ (i+1)] + A[j     *m+ (i-1)]
                                   +   A[(j-1) *m+ i]     + A[(j+1) *m+ i]);
            err = fmax(err,fabs(Anew[j*m+i]-A[j*m+i]));
          }
        }
        for( j = 1; j < n-1; j++) {
          for( i = 1; i < m-1; i++ ) {
            A[j *m+ i] = Anew[j *m+ i];
          }
        }
        …
        iter++;
    } // end while
```

# Example solution: Jacobi data

```
#pragma omp target data map(to:A[0:n*m]) map(alloc:Anew[0:n*m])
    while ( err > tol && iter < iter_max ) {
        err = 0.0;

#pragma omp target teams distribute parallel for reduction(max:err)  \
            schedule(nonmonotonic:static,1)
        for( j = 1; j < n-1; j++) {
            for( i = 1; i < m-1; i++ ) {
                Anew[j *m+ i] = 0.25 * ( A[j     *m+ (i+1)] + A[j     *m+ (i-1)]
                                       +   A[(j-1) *m+ i]     + A[(j+1) *m+ i]);
                err = fmax(err,fabs(Anew[j*m+i]-A[j*m+i]));
            }
        }

#pragma omp target teams distribute parallel for schedule(nonmonotonic:static,1)
        for( j = 1; j < n-1; j++) {
            for( i = 1; i < m-1; i++ ) {
                A[j *m+ i] = Anew[j *m+ i];
            }
        }
        …
        iter++;
    } // end while
```

# Example solution: Jacobi unstructure data

```
int main(int argc, char** argv)
{
    …

    initialize(A, Anew, m, n);

    …

    while ( error > tol && iter < iter_max )
    {
        error = calcNext(A, Anew, m, n);
        swap(A, Anew, m, n);

        if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);

        iter++;

    }

    deallocate(A, Anew, m, n);
    return 0;
}
```

# Example solution: Jacobi unstructure data

```
void initialize(double *restrict A, double *restrict Anew, int m, int n)
{
    for(int i = 0; i < m; i++){
        A[i] = 1.0; Anew[i] = 1.0;
    }

    #pragma omp target enter data map(to:A[:m*n],Anew[:m*n])
}

double calcNext(double *restrict A, double *restrict Anew, int m, int n)
{
    double error = 0.0;
    #pragma omp target teams distribute parallel for simd collapse(2) \
    map(to:A[:m*n]) map(from:Anew[:m*n]) map(tofrom:error) reduction(max:error)
    for( int j = 1; j < n-1; j++)
    {
        for( int i = 1; i < m-1; i++ )
        {
            Anew[OFFSET(j, i, m)] = 0.25 * ( A[OFFSET(j, i+1, m)] + A[OFFSET(j, i-1, m)]
                                           + A[OFFSET(j-1, i, m)] + A[OFFSET(j+1, i, m)]);
            error = fmax( error, fabs(Anew[OFFSET(j, i, m)] - A[OFFSET(j, i , m)]));
        }
    }
    return error;
}
```

# Example solution: Jacobi unstructure data

```
void swap(double *restrict A, double *restrict Anew, int m, int n)
{
    #pragma omp target teams distribute parallel for simd collapse(2) \
    map(to:A[:m*n]) map(from:Anew[:m*n])
    for( int j = 1; j < n-1; j++)
    {
        for( int i = 1; i < m-1; i++ )
        {
            A[OFFSET(j, i, m)] = Anew[OFFSET(j, i, m)];
        }
    }
}

void deallocate(double *restrict A, double *restrict Anew, int m, int n)
{
    #pragma omp target exit data map(from:A[:m*n],Anew[:m*n])
    free(A);
    free(Anew);
}
```

# Programming OpenMP

***SIMD, Part 2***

Christian Terboven

**Michael Klemm**

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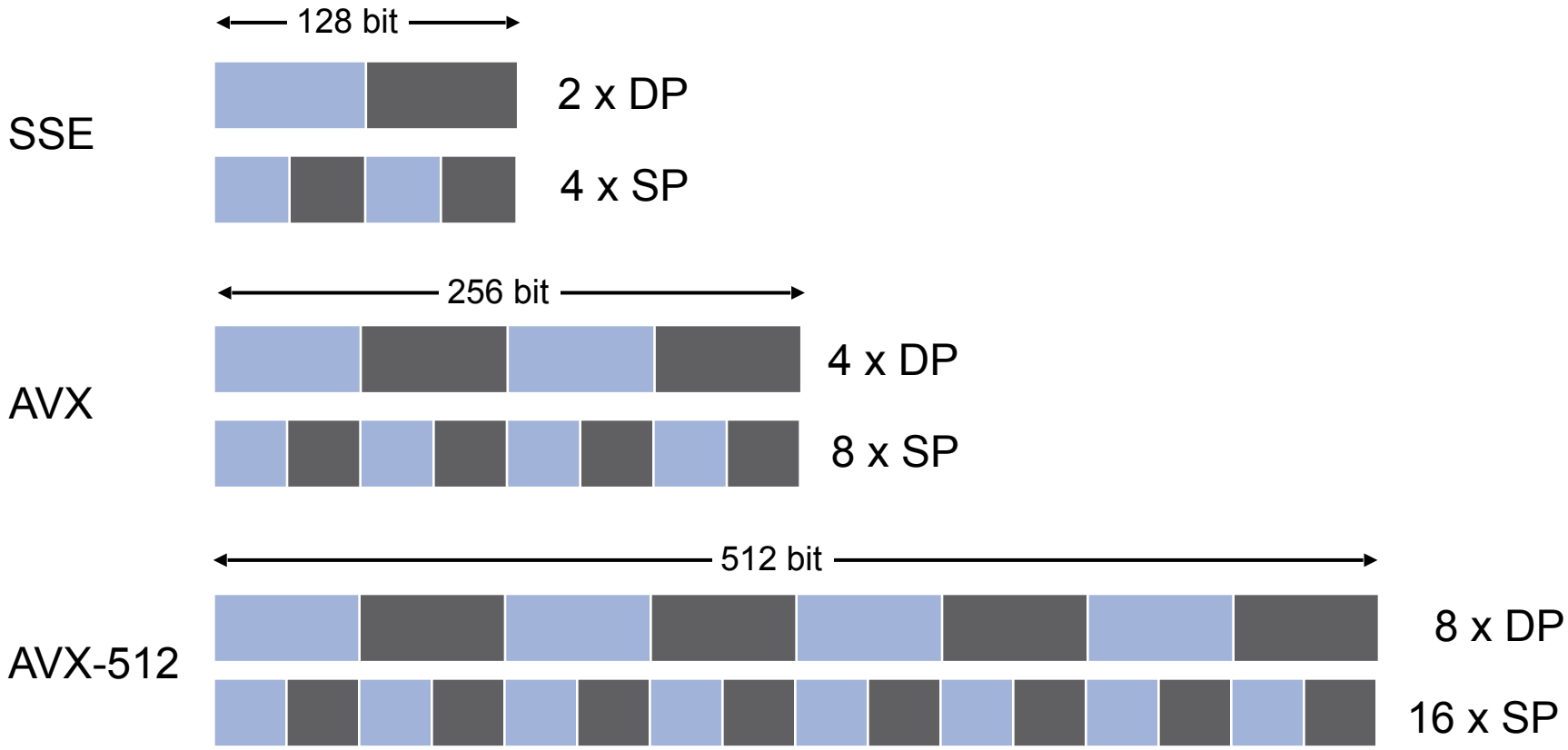
# SIMD on x86 Architectures (Recap)

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



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| Example: clang/LLVM | GCC | Intel Compiler |
|---|---|---|
| à -fvectorize | -ftree-vectorize | -vec (enabled w/ -O2) |
| à -Rpass=loop-.* | -ftree-loop-vectorize | -qopt-report=vec |
| à -mprefer-vector-width=<*width*> | -fopt-info-vec-all | |

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Intel Compiler
- -vec (enabled w/ -O2)
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# In a Time Before OpenMP 4.0

- Support required vendor-specific extensions
  - à Programming models (e.g., Intel® Cilk Plus)
  - à Compiler pragmas (e.g., `#pragma vector`)
  - à 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] + ...;
   }
```

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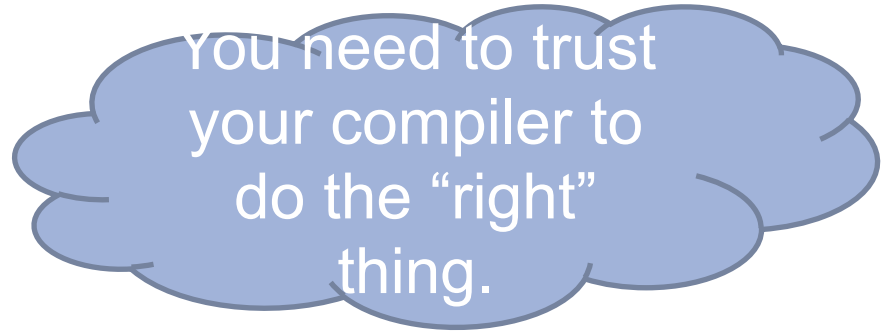


# SIMD Loop Construct

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

- Syntax (C/C++)

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

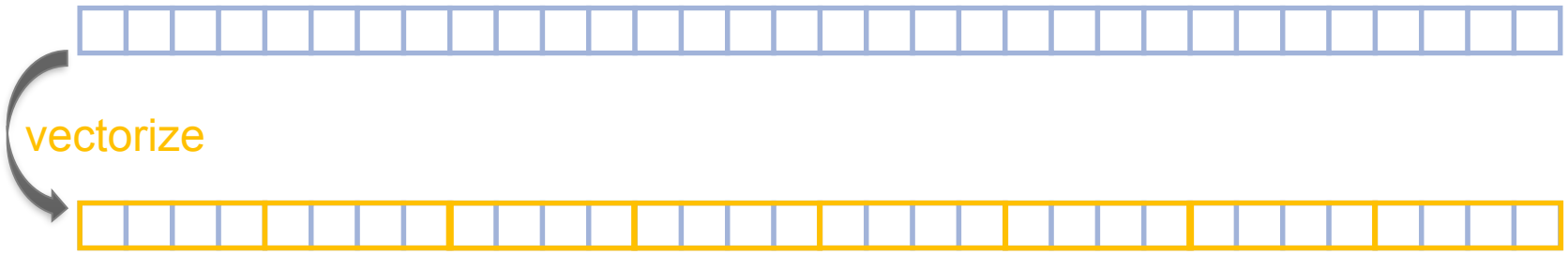
- Syntax (Fortran)

```
!$omp simd [clause[[,] clause],…]
do-loops
[!$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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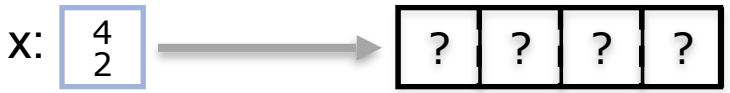
- `private(var-list)`:
  Uninitialized vectors for variables in *var-list*

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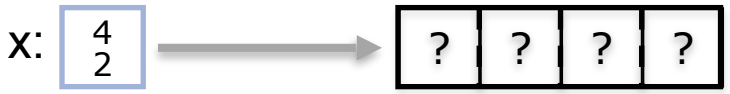


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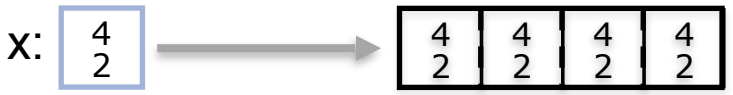


- `reduction(op:var-list):`
  Create private variables for *var-list* and apply reduction operator *op* at the end of the construct

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    - à $x_i = x_{orig} + i * \text{linear-step}$

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- `collapse (n)`

# SIMD Worksharing Construct

- Parallelize and vectorize a loop nest
  - à Distribute a loop's iteration space across a thread team
  - à 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

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float sprod(float *a, float *b, int n) {
  float sum = 0.0f;
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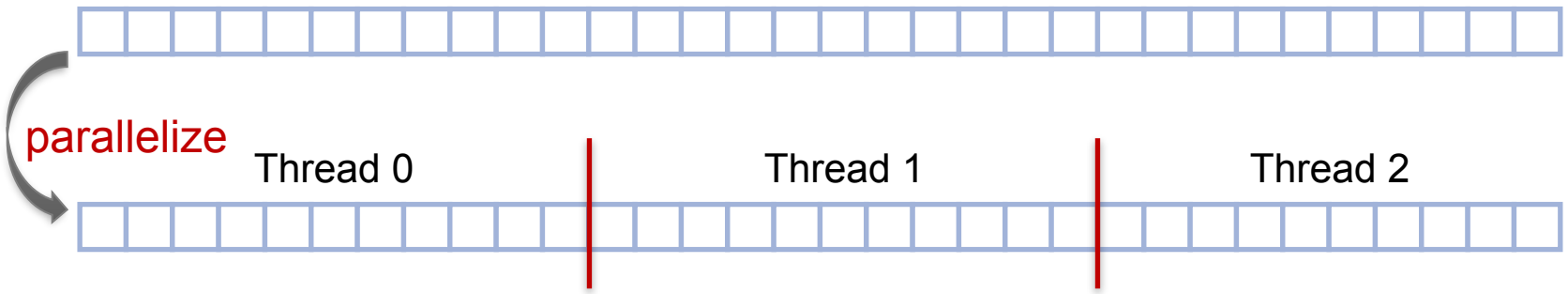
  for (int k=0; k<n; k++)
    sum += a[k] * b[k];
  return sum;
}
```



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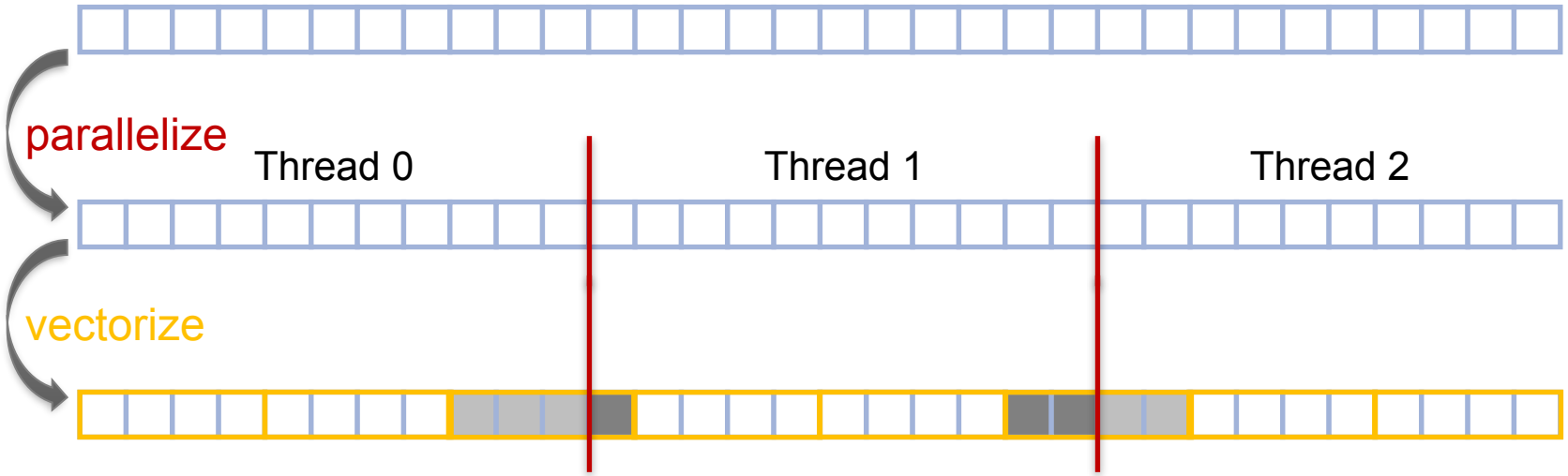

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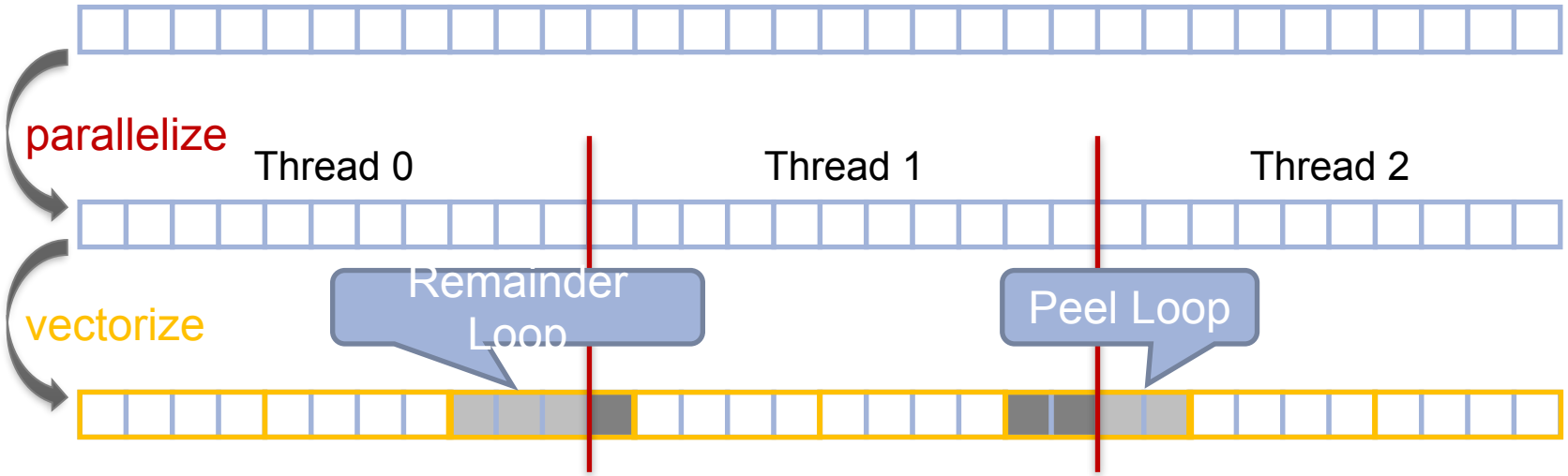

# Be Careful What You Wish For…

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

# 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;
}
```

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  return sum;
}
```

- You should choose chunk sizes that are multiples of the SIMD length
  - à Remainder loops are not triggered
  - à Likely better performance
- In the above example …
  - à and AVX2, the code will only execute the remainder loop!
  - à 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
  - à 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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# OpenMP 4.5 Simplifies SIMD Chunks

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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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#pragma omp declare simd
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void example() {
#pragma omp parallel for simd
    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
```

# SIMD Function Vectorization

- `simdlen (`*`length`*`)`
  - à generate function to support a given vector length

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  - à function always called from inside an if statement
- `notinbranch`
  - à function never called from inside an if statement

# SIMD Function Vectorization

- `simdlen (length)`
  - à generate function to support a given vector length
- `uniform (argument-list)`
  - à argument has a constant value between the iterations of a given loop
- `inbranch`
  - à function always called from inside an if statement
- `notinbranch`
  - à 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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#pragma omp declare simd inbranch
float do_stuff(float x) {
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}

void example() {
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    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;
}
```

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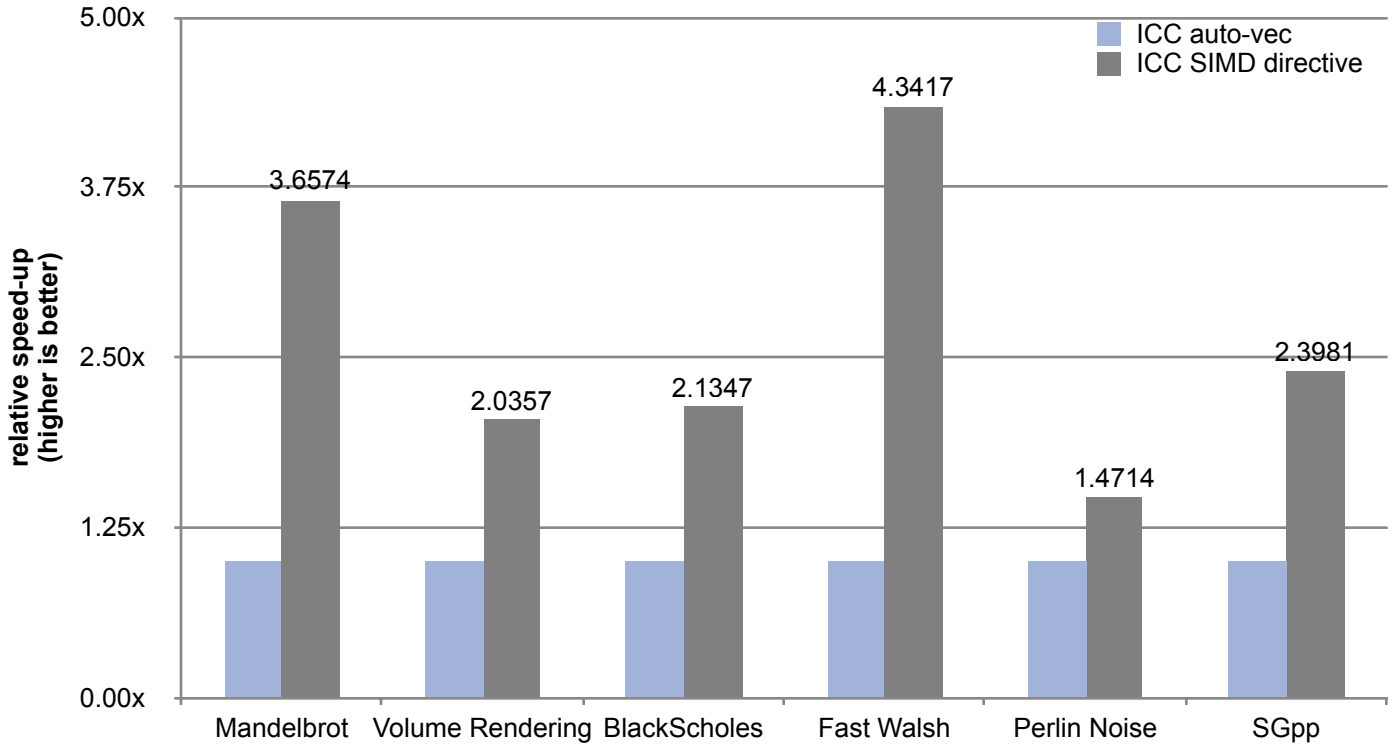
            b[i] = do_stuff(a[i]);
}
```

```
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

***NUMA***

**Christian Terboven**
Michael Klemm

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OpenMP

# Improving Tasking Performance: Task Affinity

# Motivation

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

OpenMP Tasking:

- In general: Tasks may be executed by any thread in the team
  - à 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)`
  - à Hint to the runtime to execute task closely to physical data location
  - à Clear separation between dependencies and affinity

- Expectations:
  - à Improve data locality / reduce remote memory accesses
  - à Decrease runtime variability

- Still expect task stealing
  - à In particular, if a thread is under-utilized

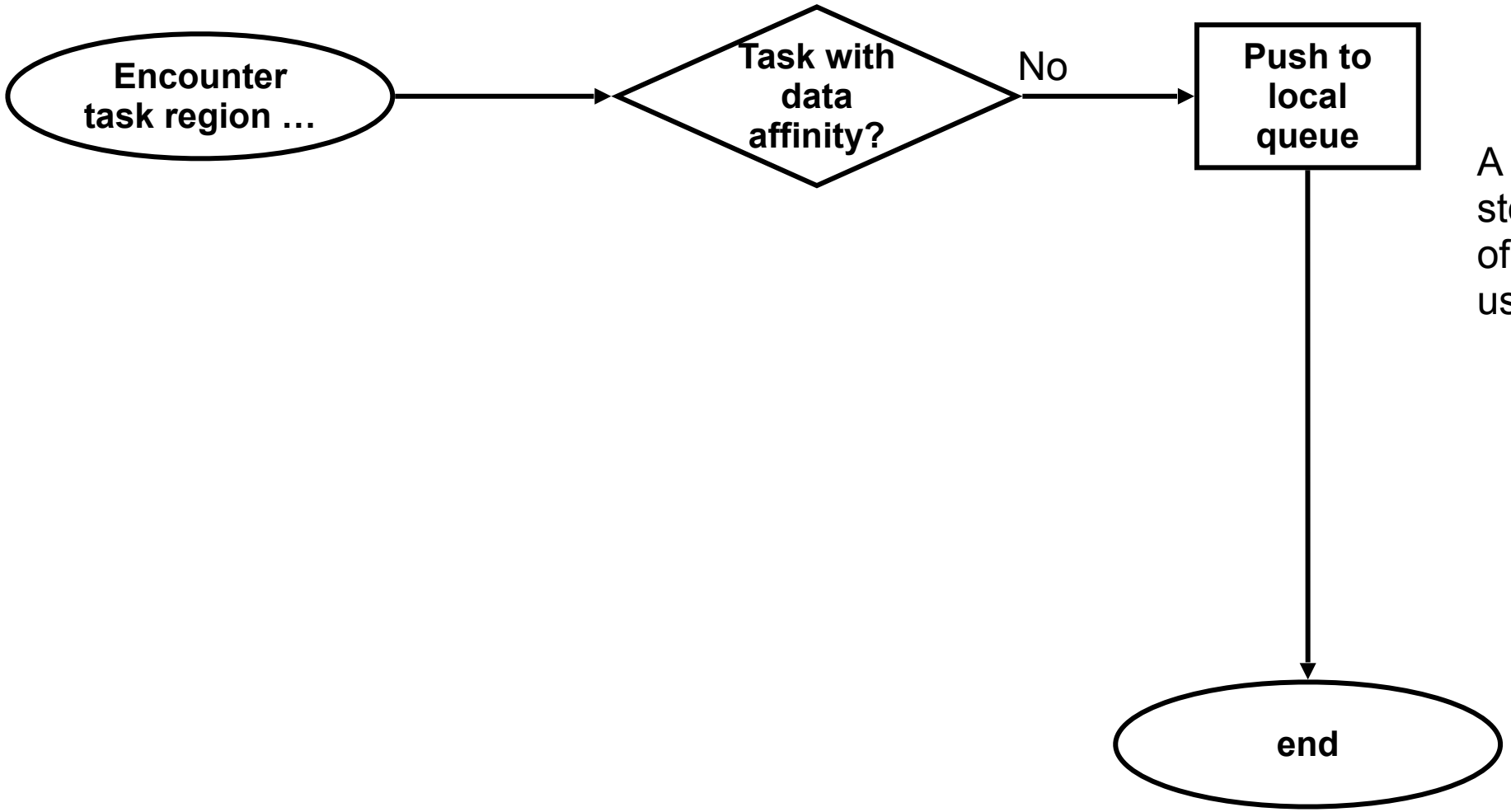
# Code Example

- Excerpt from task-parallel STREAM

```
1  #pragma omp task \
2      shared(a, b, c, scalar) \
3      firstprivate(tmp_idx_start, tmp_idx_end) \
4      affinity( a[tmp_idx_start] )
5  {
6    int i;
7    for(i = tmp_idx_start; i <= tmp_idx_end; i++)
8      a[i] = b[i] + scalar * c[i];
9  }
```

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

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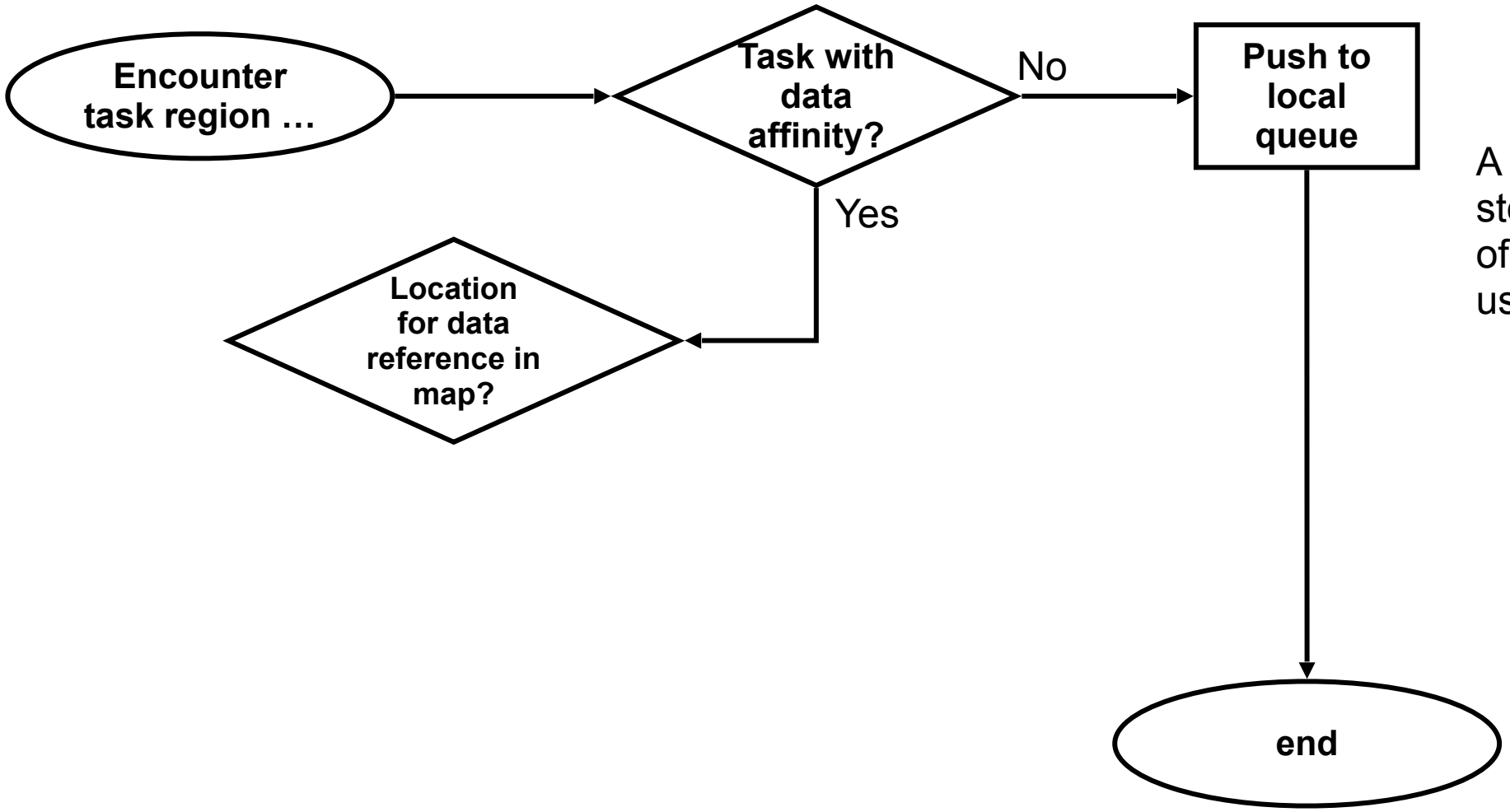


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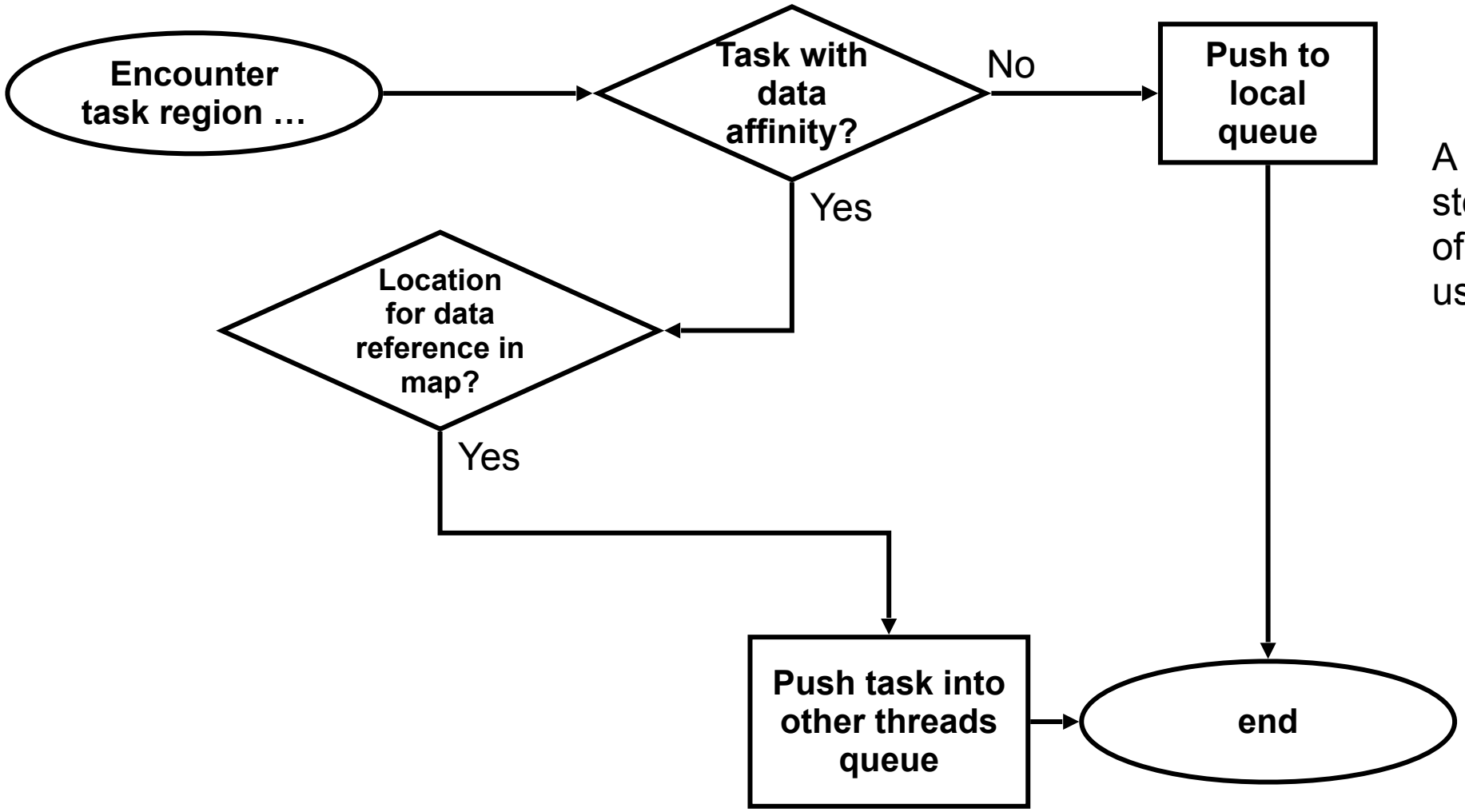


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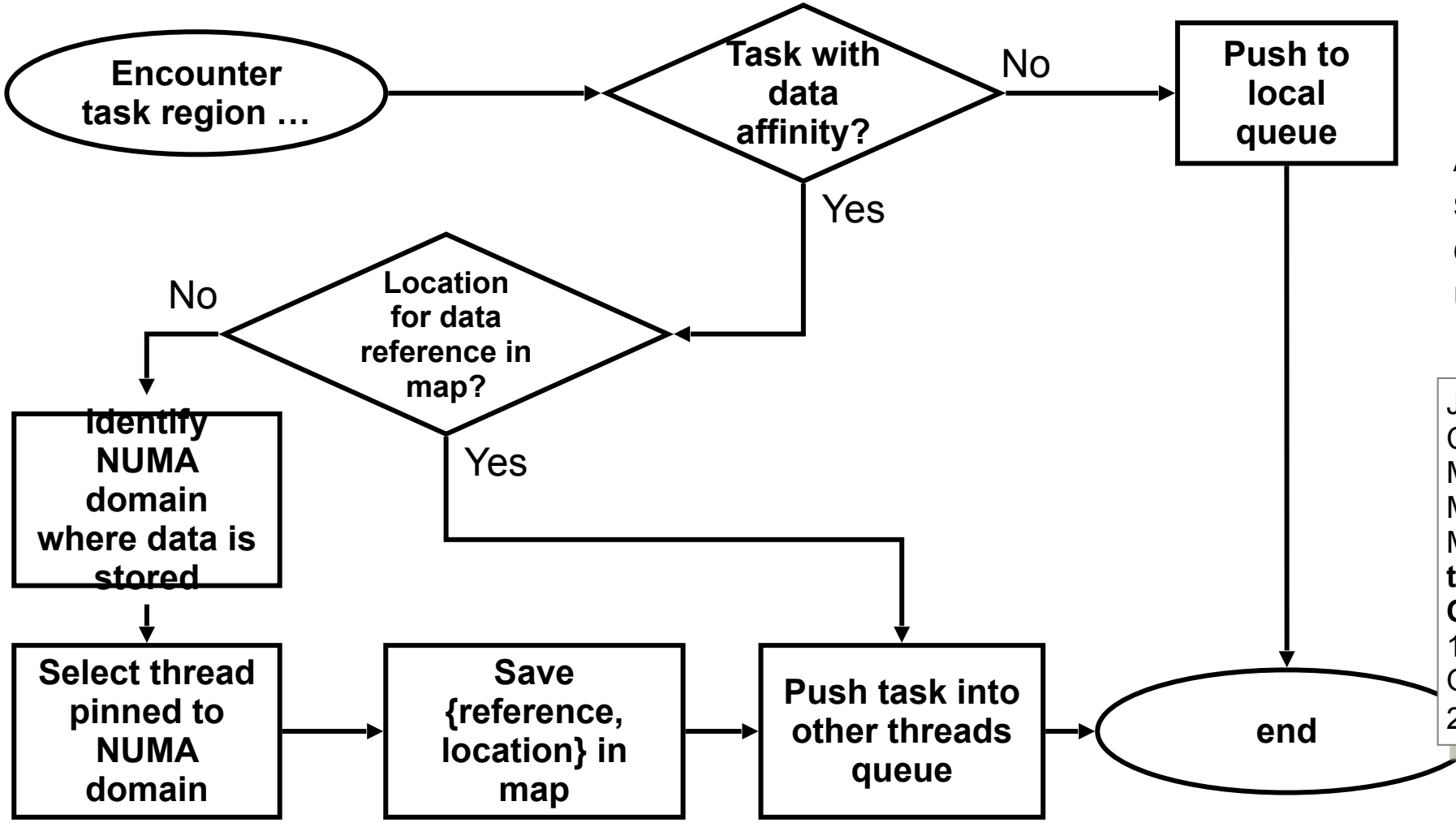


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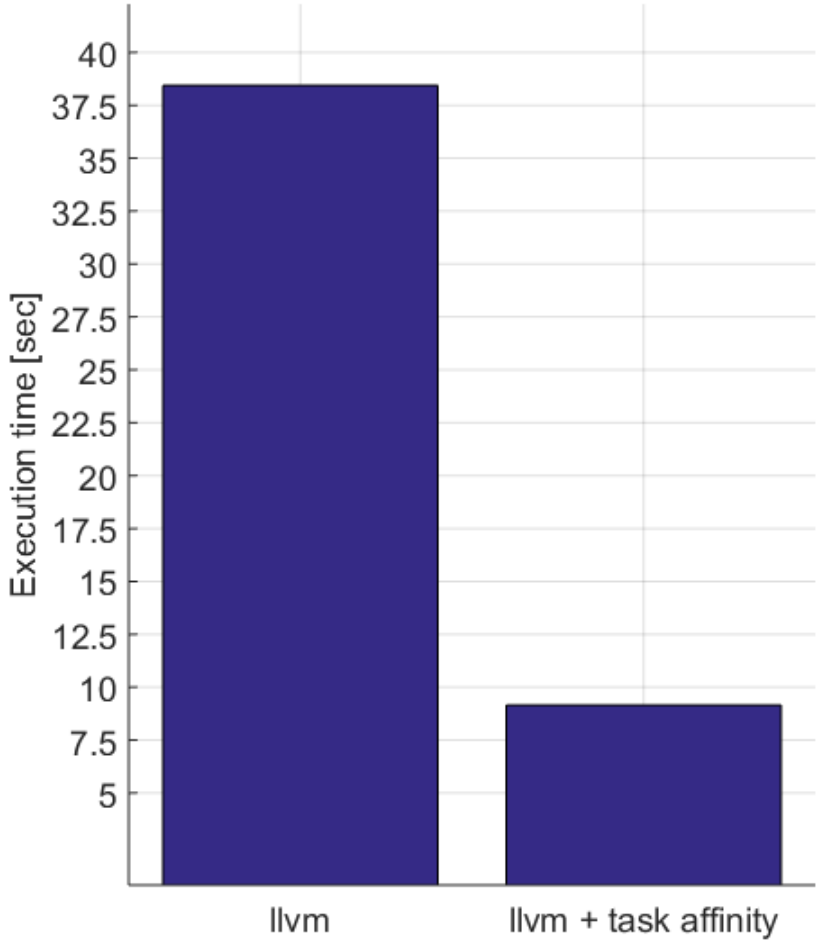
Jannis Klinkenberg, Philipp Samfass, Christian Terboven, Alejandro Duran, Michael Klemm, Xavier Teruel, Sergi Mateo, Stephen L. Olivier, and Matthias S. Müller. **Assessing Task-to-Data Affinity in the LLVM OpenMP Runtime**. Proceedings of the 14th International Workshop on OpenMP, IWOMP 2018. September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

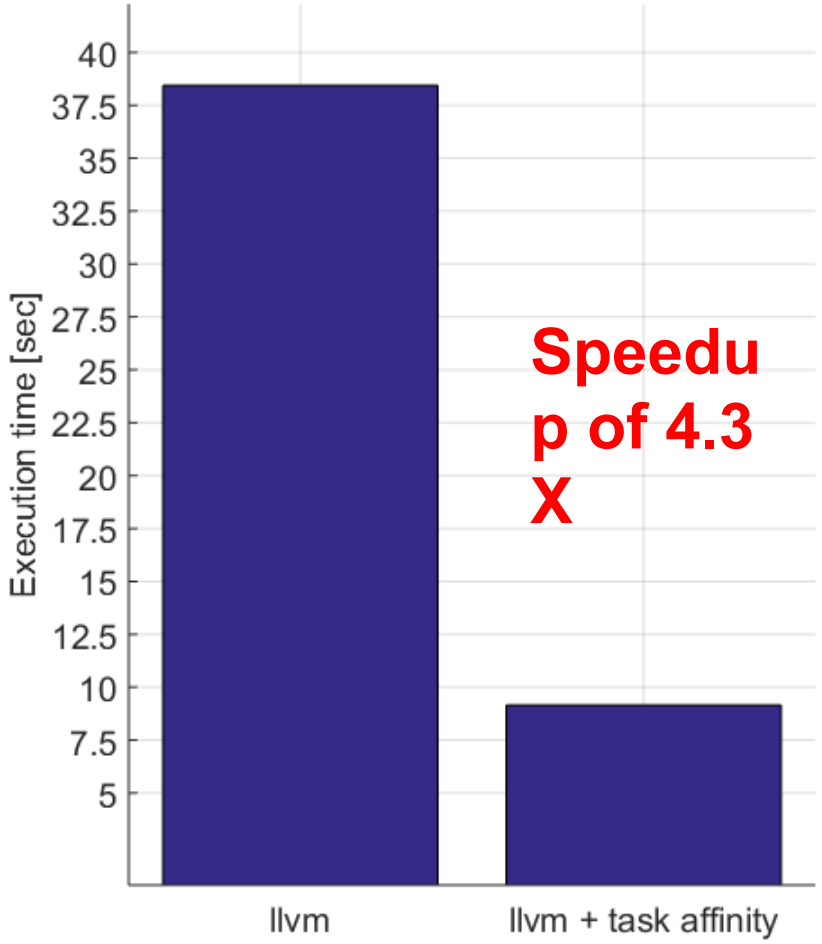
# Evaluation

## Program runtime
## Median of 10 runs



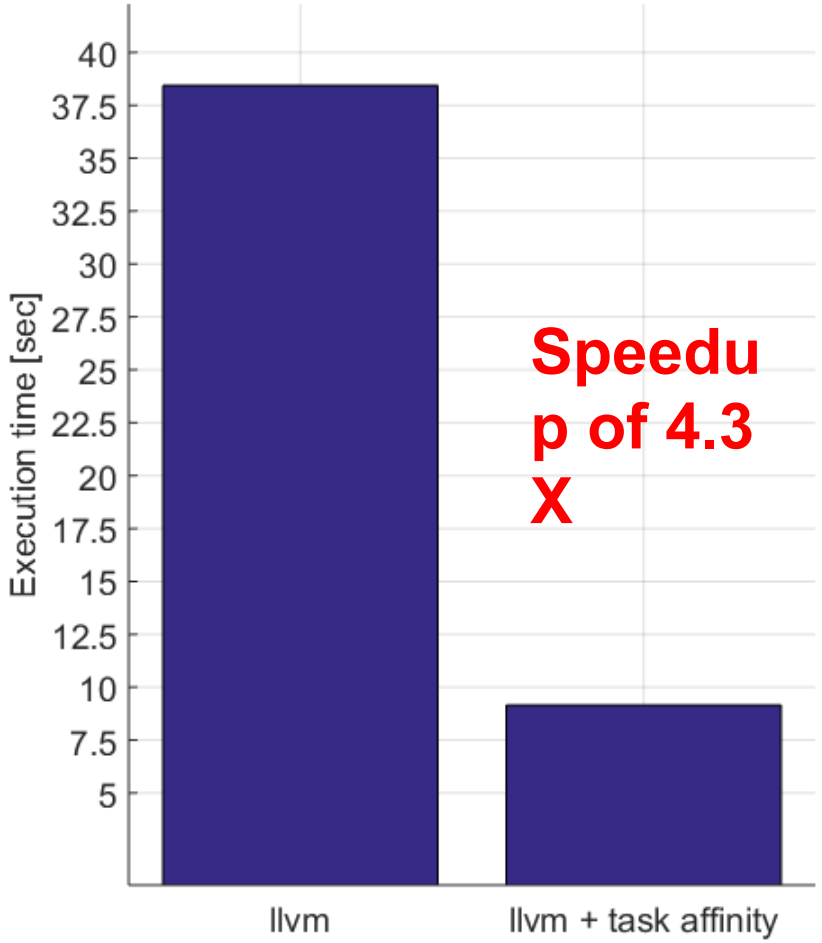
# Evaluation

**Program runtime**
**Median of 10 runs**



# Evaluation

**Program runtime**
**Median of 10 runs**




**Speedup of 4.3X**

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

# Evaluation

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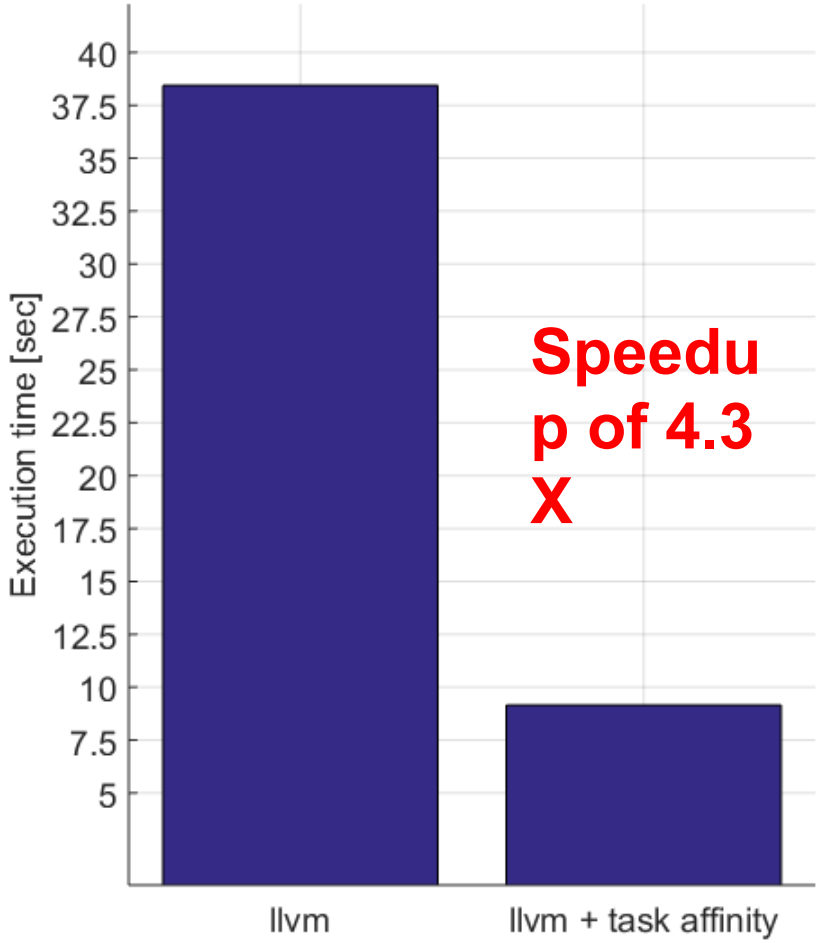
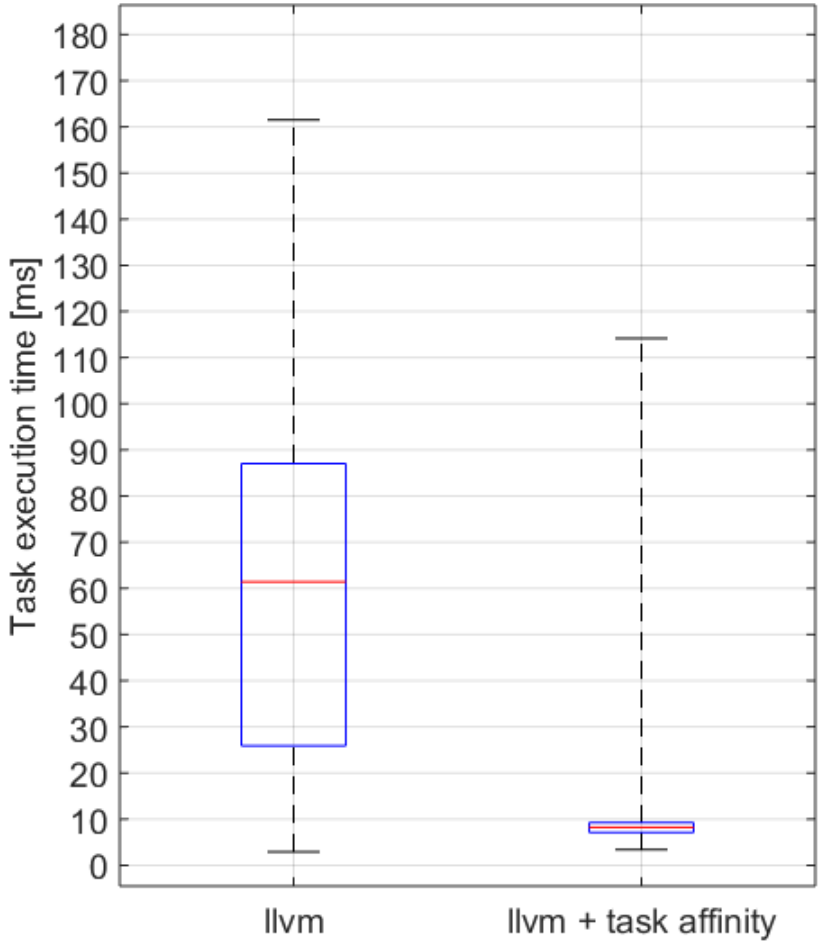



**Speedup of 4.3X**

## 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
  - à tasks access data heavily
  - à single task creator scenario, or task not created with data affinity
  - à high load imbalance among the tasks

- Different from thread binding: task stealing is absolutely allowed

OpenMP

# 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
      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)

# Example Kernel (1 of 27 in total)

```
      subroutine sd_t_d1_1(h3d,h2d,h1d,p6d,p5d,p4d,
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      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)
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      end do
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```

- All kernels have the same structure
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- Some kernels contain inner product loop (then, 6 perfectly nested loops)
- 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

# Example Kernel (1 of 27 in total)

```
      subroutine sd_t_d1_1(h3d,h2d,h1d,p6d,p5d,p4d,
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      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)
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```

1.5GB data transferred (host to device)

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- Naïve data allocation (tile size 24)
  - Per-array transfer for each target construct
  - triplesx: 1458 MB
  - t2sub, v2sub: 2.5 MB each

# 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

- Simplified pseudo-code

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```

Allocate 1.5GB data once, stays on device.

- Reduced data transfers:
  - triplesx:
    - allocated once
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# Invoking the Kernels / Data Management

- Simplified pseudo-code

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!$omp target enter data map(alloc:triplesx(1:tr_size))
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       do ...
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         if (...)
          call sd_t_d1_1(h3d,h2d,h1d,p6d,p5d,p4d,h7,triplesx,t2su
         end if
c         same for sd_t_d1_2 until sd_t_d1_9
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       end do
       do ...
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       end do
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      end do
!$omp target exit data map(release:triplesx(1:size))
```

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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```

Allocate 1.5G
stays on

Update 2x2.5
(potentially) r

```
      subroutine sd_t_d1_1(h3d,h2d,h1d,p6d,p5d,p4d,
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```

Allocate 1.5G
stays on

Update 2x2.5
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      do p6=1,p6d
      do h1=1,h1d
      do h7=1,h7d
      do h2h3=1,h3d*h2d
       triplesx(h2h3,h1,p6,p
     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
```

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

# Programming OpenMP

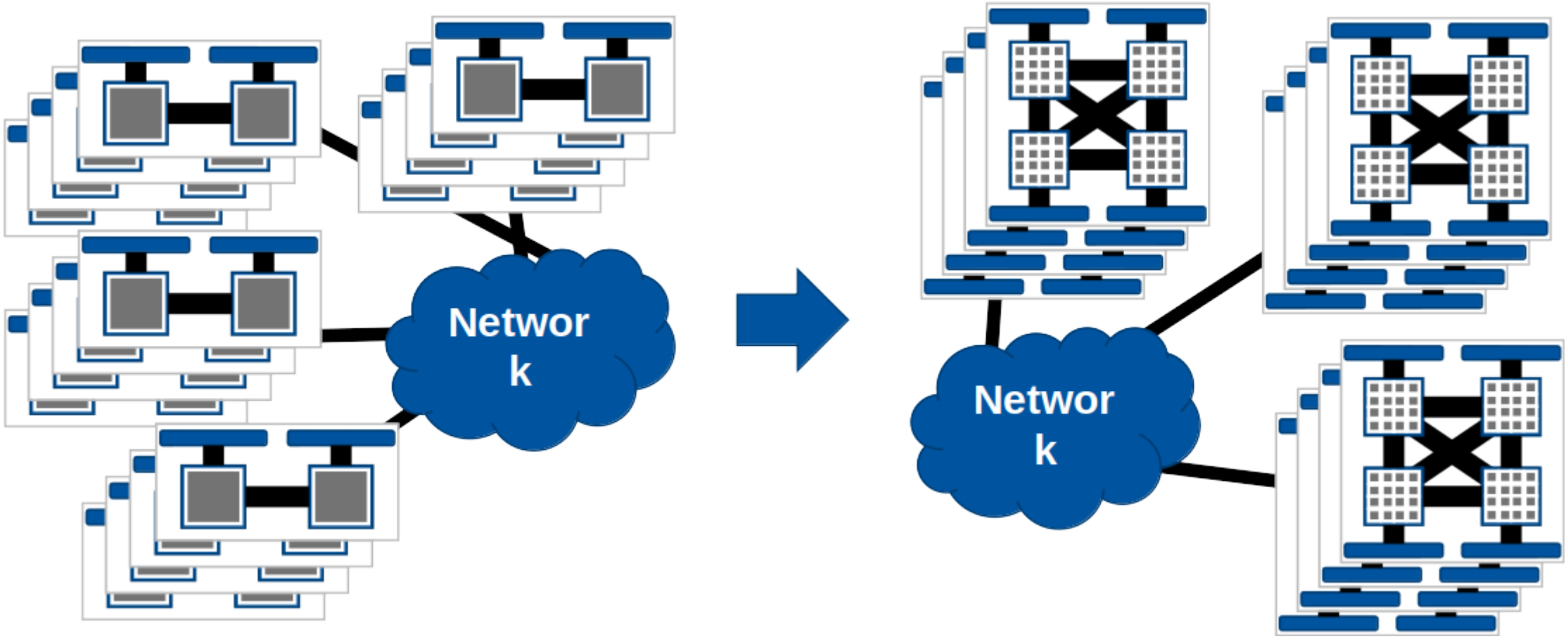
## *OpenMP and MPI*

**Christian Terboven**
Michael Klemm

# Motivation

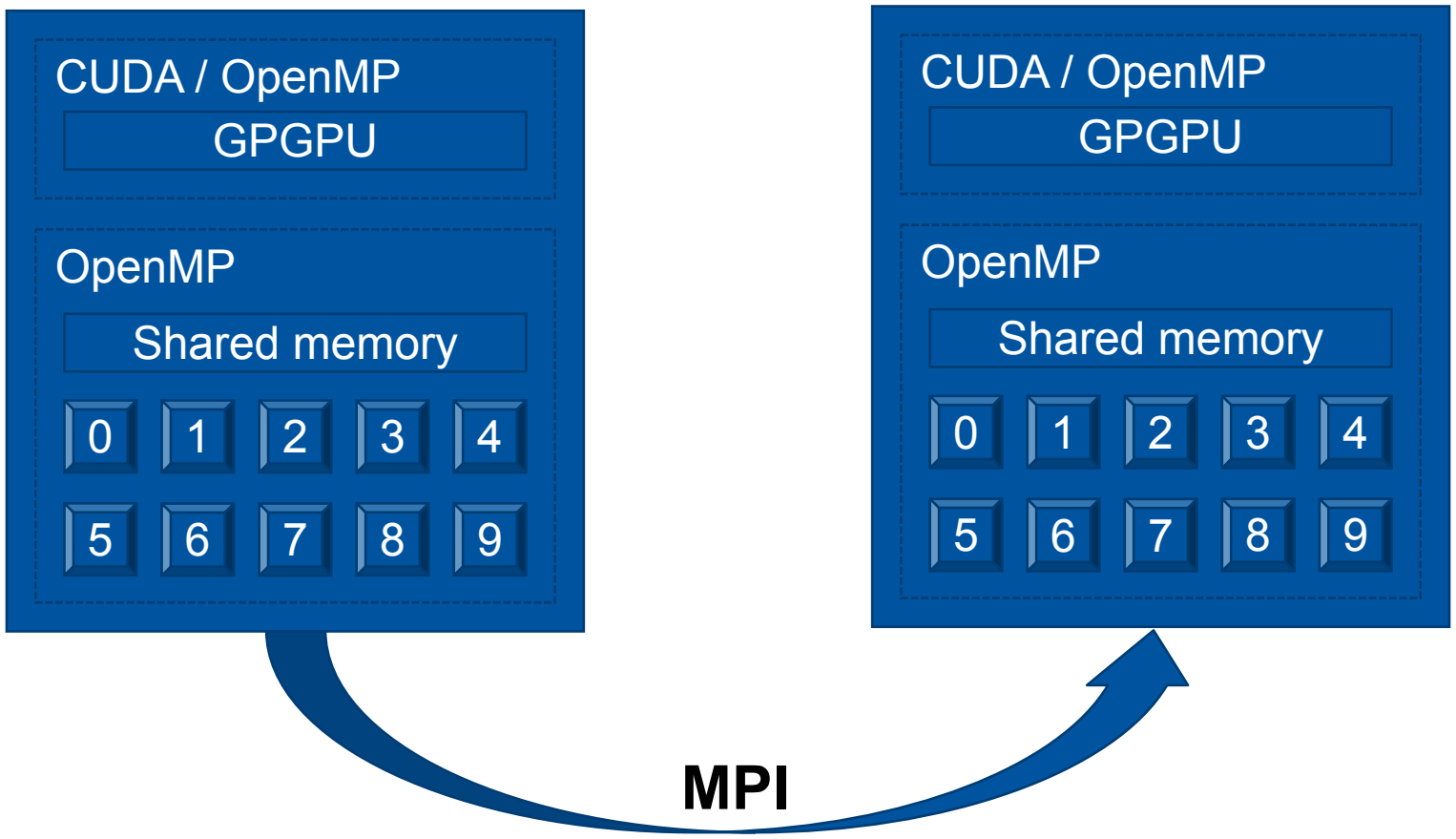
# Motivation for hybrid programming

- 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

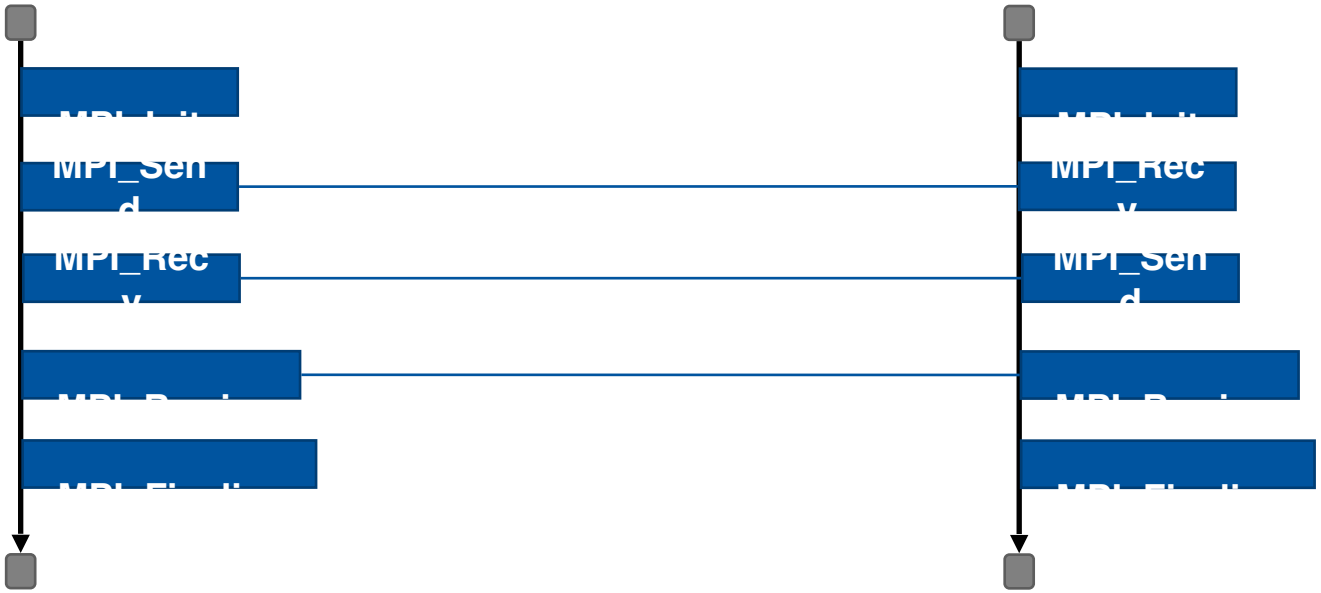
- Four levels of threading support


| 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

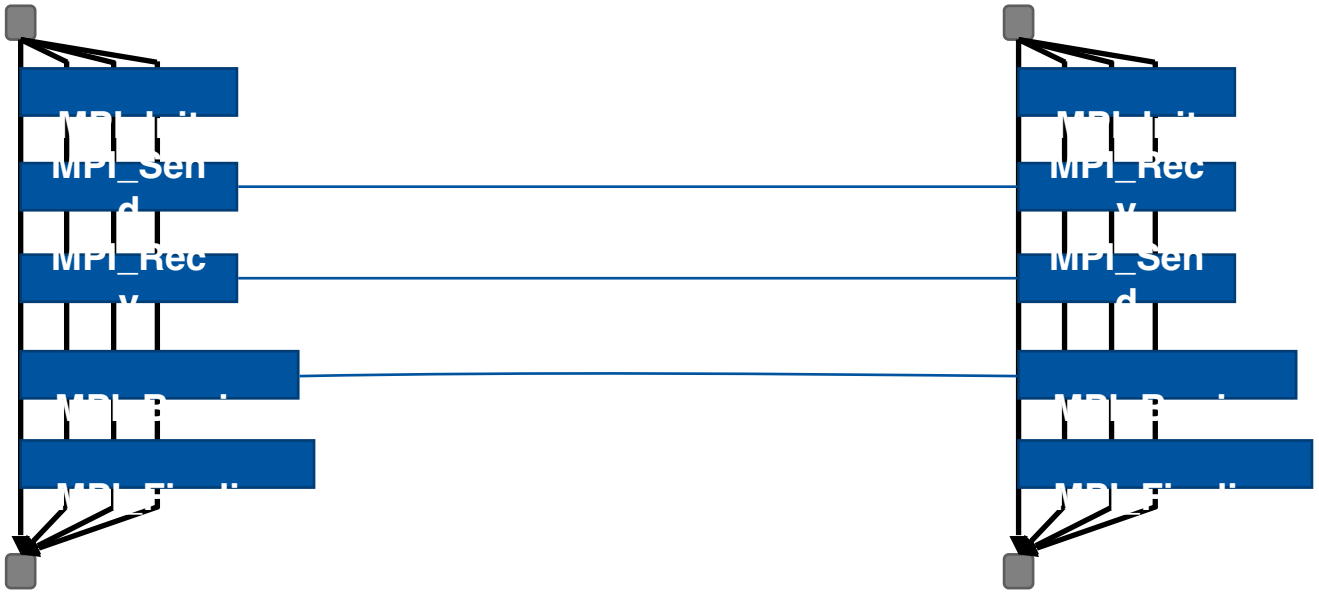
# MPI – Threading support levels

- MPI_THREAD_SINGLE
  - Only one thread per MPI rank

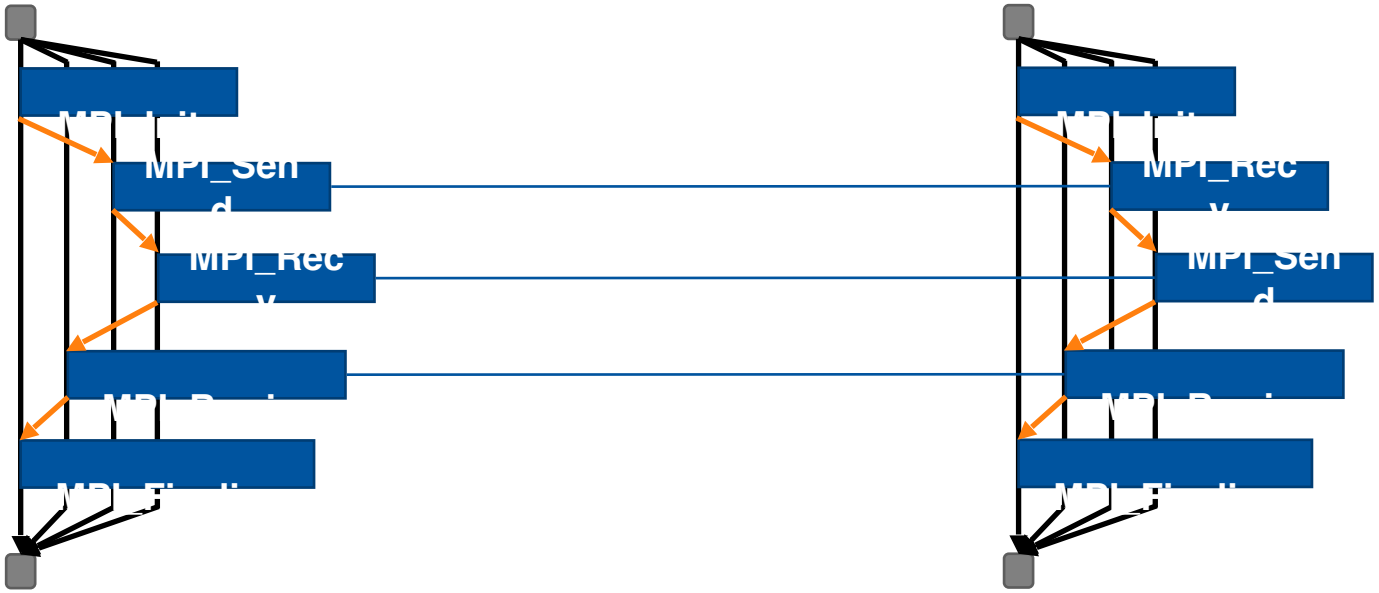
# MPI – Threading support levels

- 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

MPI Communication
Thread Synchronization