Parallelization of Object-oriented Codes

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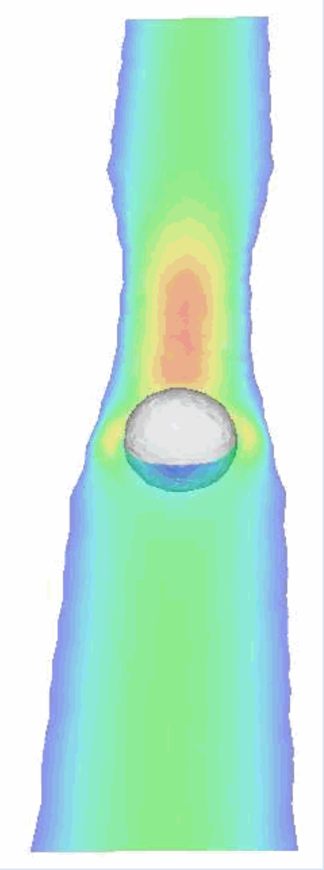
Agenda

- Motivation and Computational Task
- Overview of Parallelization Paradigms
- Programmability Evaluation
- Performance and Scalability Evaluation
- Conclusion and Future Work

DROPS: A Navier-Stokes Solver in C++

- Numerical Simulation of two-phase flow
- Modeled by instationary and non-linear Navier-Stokes equation
- Level Set function is used to describe the interface between the two phases
- Written in C++: is object-oriented, uses nested templates, uses STL types, uses compile-time polymorphism, …
- (Adaptive) Tetrahedral Grid Hierarchy
- Finite Element Method (FEM)

Example:
Silicon oil drop in D_2O (fluid/fluid)



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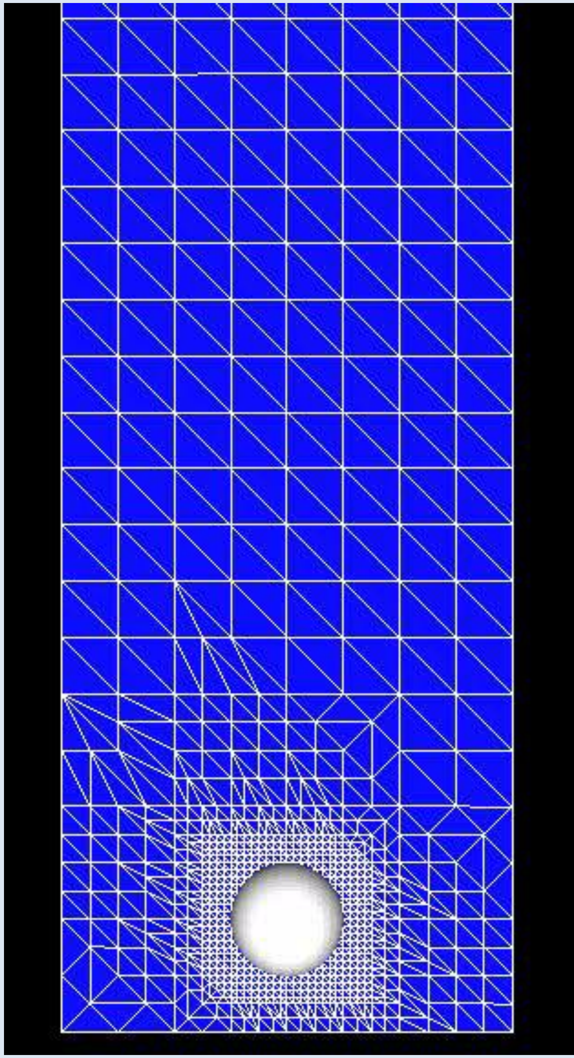
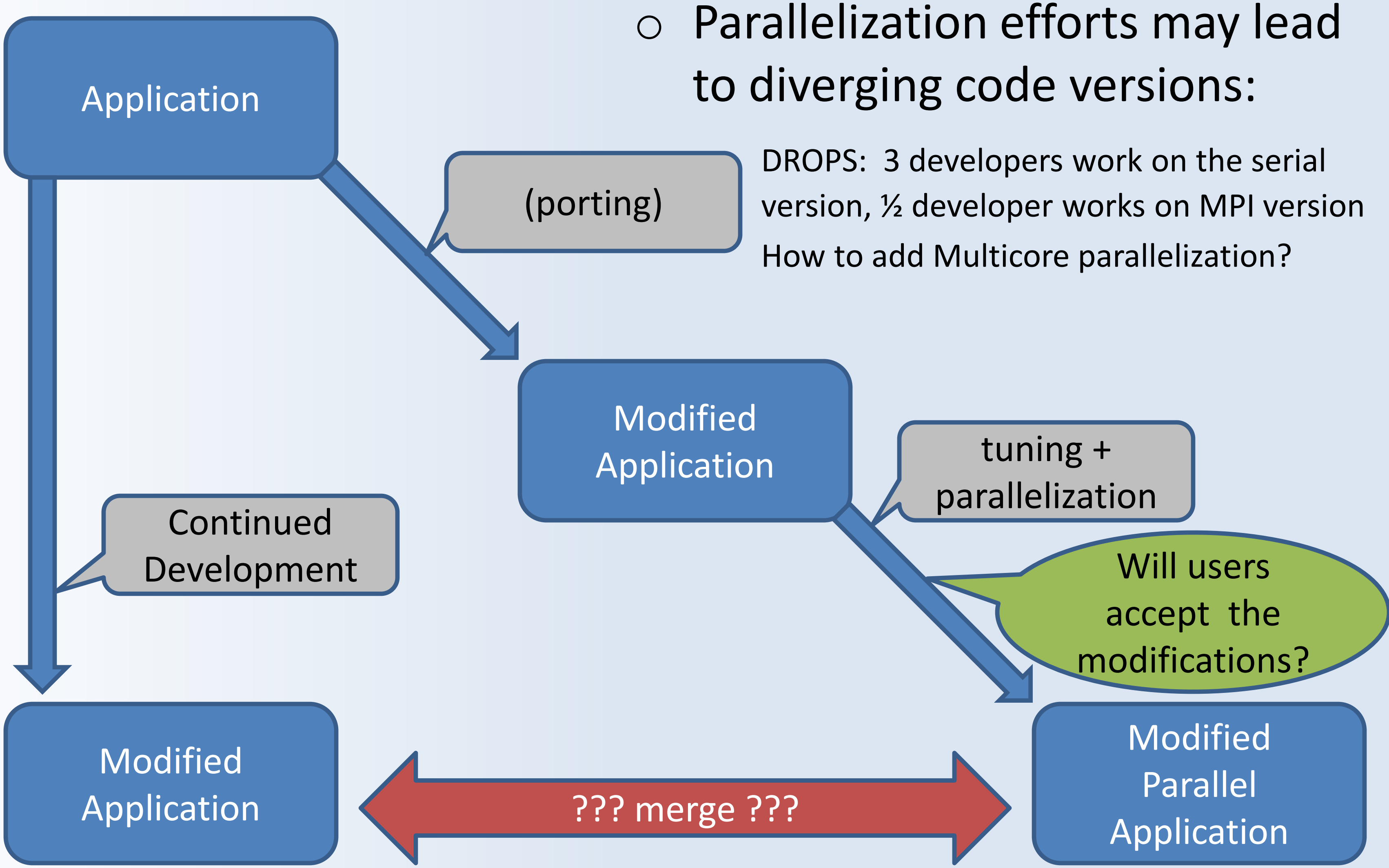


Parallelization may lead to Dead Ends

- Parallelization efforts may lead to diverging code versions:

DROPS: 3 developers work on the serial version, ½ developer works on MPI version

How to add Multicore parallelization?



DROPS: Iteration Loop of CG-type solver

- Our targets:
  - Efficient parallelization not hindering development
  - Maintain the object-oriented programming style

```
PCG(const MatrixCL& A, VectorCL& x, const VectorCL& b,
    const PreCon& M, int& max_iter, double& tol)
{
  VectorCL q(n), p(n), r(n);
  […]
  for (int i=1; i<=max_iter; ++i) {
    […]
    q = A * p;
    double alpha = rho / (p*q);
    x += alpha * p;
    r -= alpha * q;
    […]
```

Evaluation of:

- OpenMP (2.5 and 3.0)
- Threading Building Blocks
- Native Threading

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Multicore Parallelization Paradigms

- OpenMP: fork-join parallelism
  - Fortran, C and C++
  - Parallel Region: pragma + structured block
  - Worksharing and Task-based parallelization
- (Intel) Threading Building Blocks: library-based parallelism
  - C++ template library, global Task scheduler
  - Worksharing-like expressions and parallel STL-type algorithms
  - Everything is a Task concept (implicit or explicit Tasks)
- Posix-Threads / Win32-Threads: native threading
  - API to create and manage OS-level threads
  - Worksharing has to be implemented manually
- Other: Hardly portable / supportable

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Parallelization: Naive Approach w/ OpenMP

```
PCG(const MatrixCL& A, VectorCL& x, const VectorCL& b,
    const PreCon& M, int& max_iter,
    double& tol)
{
  VectorCL p(n), z(n), q(n), r(n);
  […]
  for (int i=1; i<=max_iter; ++i) {
    […]
    q = A * p;
    double alpha = rho / (p*q);
    x += alpha * p;
    r -= alpha * q;
    […]
```

Option 1: Replace operator calls

```
y_Ax_par(&q.raw()[0],
    A.num_rows(), A.raw_val(),
    A.raw_row(), A.raw_col(),
    Addr( p.raw()));
```

Option 2: Place parallelization inside operator calls

- Problems of both options:
  - Code Changes
  - Parallelization not applicable to complex expressions
  - Parallelization may introduce additional overhead

Parallelization: New Approach via Library

- Extend existing abstractions to introduce parallelism!

- For the DROPS code, just replace

```
typedef VectorBaseCL<double>     VectorCL;
typedef SparseMatBaseCL<double> MatrixCL;
```

- with

```
typedef laperf::vector<double,
                       OpenMPInternalParallelization>
                       VectorCL;
typedef laperf::matrix_crs<double> MatrixCL;
```

element data type

parallelization type

- Specification of parallelization type by the user allows to
  1. Experiment with several parallelization strategies
  2. Mix and match parallel and sequential code

Implementation History

- V1: Using C++ operator overloading and giant switch statements to differentiate between different parallelization paradigms ➔ difficult to maintain and extend, performance problems because of temporary copies
- V2: Using inheritance to improve maintainability
  ➔ still problems with temporary copies
- Current: V3: No inheritance; using C++ Template Expressions to avoid unnecessary temporary copies
- Future: V4: Policy-based design („Mix-In“); using C++0x lambda functions and move semantics

Problem: Temporaries

Users' Code

```
laperf::vector<double> x(dim),a(dim),b(dim);
x = (a * 2.0) + b;
```

ideal code for this vector operation:

```
for( int i = 0; i < dim; ++i )
  x[i] = a[i] * 2.0 + b[i];
```

but in C++ it translates to:

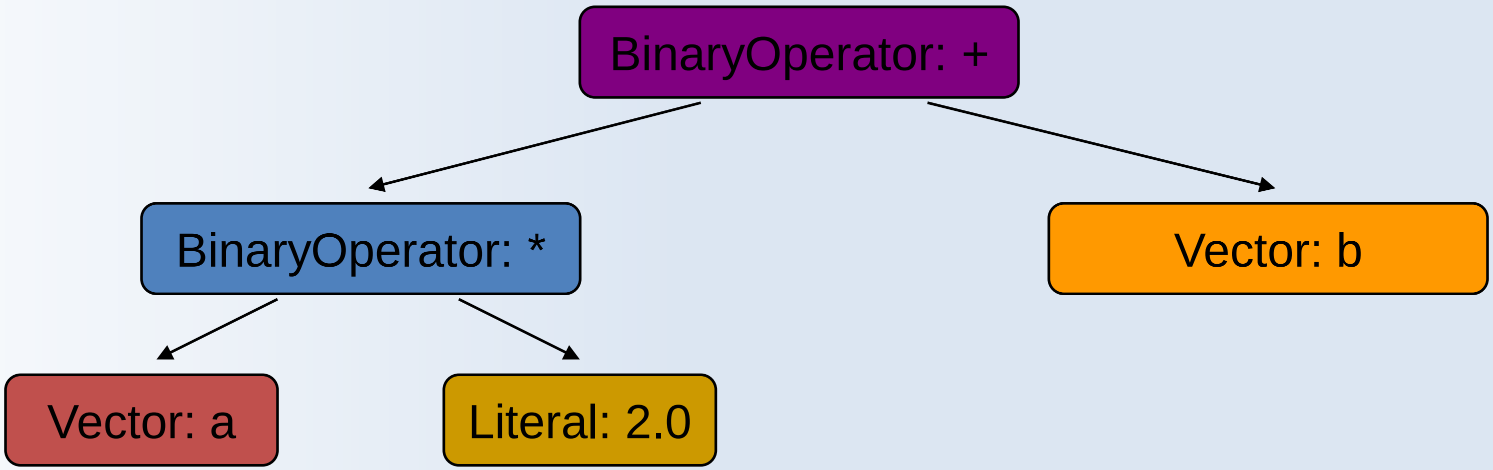
```
laperf::vector<double> _t1 = operator*(a,2.0);
laperf::vector<double> _t2 = operator+(_t1,b);
x.operator=(_t2);
```

➔ two temporary vector copies and unnecessary overhead
➔ impossible to implement efficient parallelization
➔ bad placement of temporaries on cc-NUMA architectures

Operator evaluation with Template Expressions

During compile time the compiler builds a template expression resembling the syntax tree:

```
x = (a * 2.0) + b;
```




```
LB<OpAdd, LB<OpMul,vector,double>, vector>
expr( LB<OpAdd,LB<OpMul, vector, double>, vector>(
    LB<OpMul, vector, double>(a,2.0), b
  )
);
```

Achieves 95-99.5% efficiency of hand- coded C while still having all benefits of C++'s object orientation

Parallelization of Template Expressions

```
LB<OpAdd, LB<OpMul,vector,double>, vector>
expr( LB<OpAdd,LB<OpMul, vector,double>,vector>(
    LB<OpMul, vector, double>(a,2.0), b
  )
);
```

This expression can then be applied to the `operator=` of `x`:

```
template<typename TExpr>
vector::operator=( TExpr expr ) {
  for( size_t i = 0; i < dim; ++i )
    this[i] = expr[i];
}
```

Library Code: parallelizable!

and with inlining it will be resolved to:

```
for( size_t i = 0; i < dim; ++i )
  x[i] = a[i] * 2.0 + b[i];
```

This is done by the Compiler

which can then be **parallelized efficiently!**

Handling of cc-NUMA architectures

- All x86-based multi-socket system will be cc-NUMA!
  - Current Operating Systems apply first-touch placement
  - If cc-NUMA is ignored, the speedup will be zero, typically
- STL provides the concept of an allocator to encapsulate memory management

  → build on the same concept to optimize for cc-NUMA
- We created two allocators:
  - Can optionally be plugged into our data types
  - `dist_allocator`: Distribute data according to OpenMP schedule type (same scheduling as in computation)
  - `chunked_allocator`: Distribute data according to explicitly precalculated scheme to improve load balacing

Data Type Design

- We extended the data types by adding
  - Two (optional) template parameters:
    - `Parallelization`: parallelization strategy
    - `Alloc`: STL-type allocator (cc-NUMA optimization)
  - One (optional) constructor argument:
    - `Scheduling`: Specify how work is distributed to the threads
- Abstract data type for vector + CRS-matrix implementation to
  - Evaluate Parallelization Paradigms
  - Hide Parallelization from the User
- Our approach is easy to use and delivers full performance
  - while hiding the parallelization from the user
  - and hiding cc-NUMA tuning from the user.

DROPS: Parallel Iteration Loop of CG-type solver

```
typedef VectorBaseCL<double, OpenMPInternalPar> VectorCL;

PCG(const MatrixCL& A, VectorCL& x, const VectorCL& b,
    const PreCon& M, int& max_iter, double& tol)
{
  VectorCL q(n), p(n), r(n);
  […]
  for (int i=1; i<=max_iter; ++i) {
    […]
    q = A * p;
    double alpha = rho / (p*q);
    x += alpha * p;
    r -= alpha * q;
    […]
```

Expression Templates allow parallelization of whole line. Here: Complete Parallel Region inside operator calls.

Evaluation Result (1/2)

1. Library use of parallel data types (really hide parallelization):
   - OpenMP with Internal Parallelization
     - Each operator contains a distinct parallel region

     → Safe to use and completely invisible
   - TBB with Algorithms
     - Algorithmic skeletons create implicit Tasks inside operator call
     - Synchronization done by skeleton constructs

     → Safe to use and completely invisible
   - TBB with Tasks
     - Task-based Worksharing inside operator call
     - Synchronization has to be done by the library

     → Safe to use and completely invisible

Evaluation Result (2/2)

2. Usage to provide algorithms via libary:
   - OpenMP with External Parallelization
     - Worksharing inside operator call, Parallel Region outside
     - Barriers can be eliminated by using *nowait* on Worksharing

     → Performance improvement over Internal version, but unsafe
   - OpenMP with Tasks
     - Task-based Worksharing inside operator call, Par. Reg. Outside

     → Safe, but no compiler was able to compile our code yet

- Our approach:
  - Use *safe* version during development and for algorithmic experiments
  - Carefully use possibly *unsafe* but *faster* version for production

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Sequential Performance Measurements

- UMA: 2-socket quad-core Intel Xeon E5450 (3.0 GHz)
- cc-NUMA: 4-socket dual-core AMD Opteron 875 (2.2 GHz)

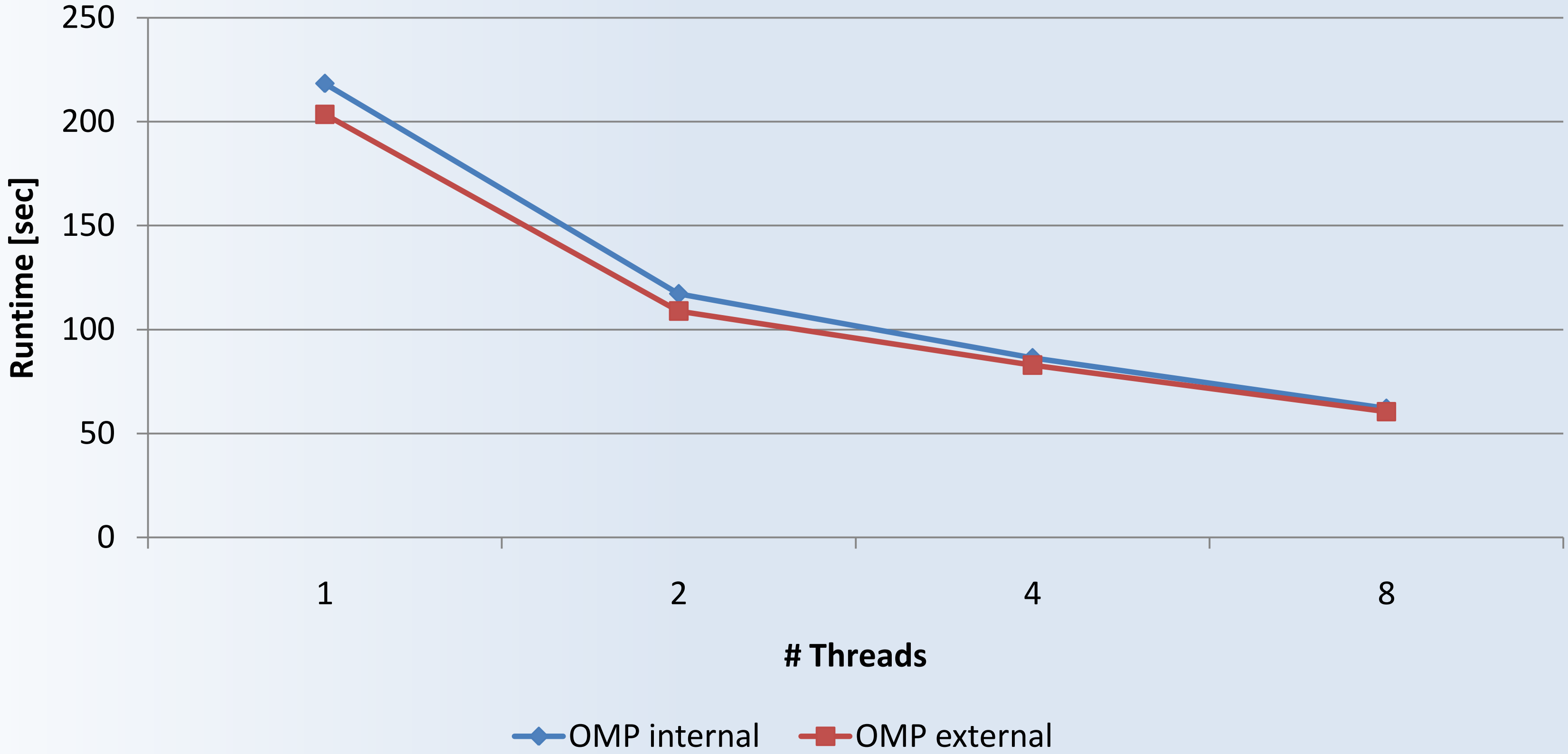
- Sparse Matrix-Vector-Multiplication performance [MFLOP/s]
  - Each results is measured with two threads!

Machine	Dataset	laperf (OMP) std Allocator	laperf (OMP) dist Allocator	laperf (OMP) chunked Allocator	Intel MKL
UMA	medium	406	-	-	397
UMA	large	390	-	-	383
cc-NUMA	medium	-	310	389	177
cc-NUMA	large	-	329	428	182

- Same performance as Intel MKL: Performance costs of abstractions and OpenMP parallelization are negligible
- Intel MKL has no notion / support for cc-NUMA architectures

Parallel Performance Measurements (1/2)

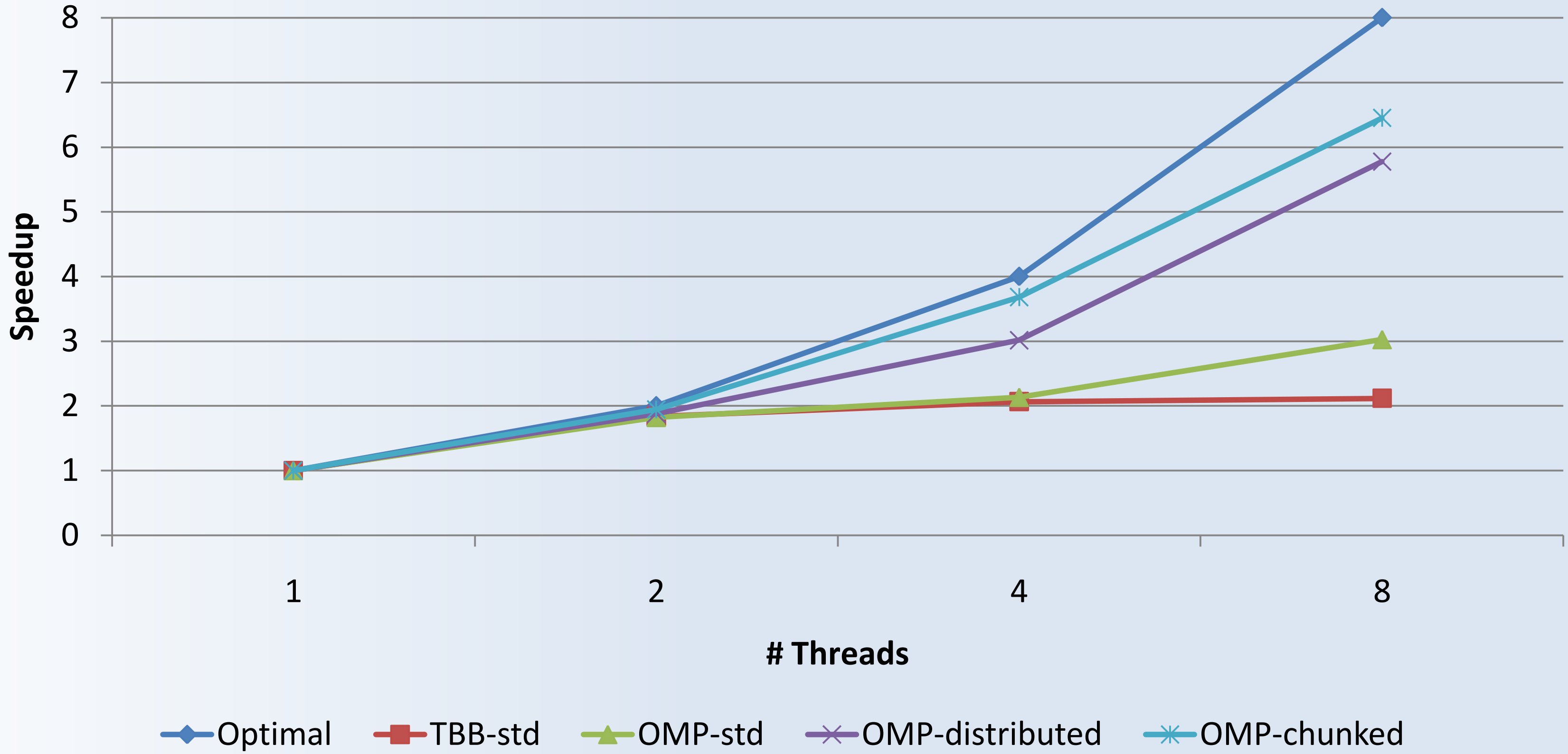
- Library-parallelized GMRES solver on UMA machine:



- Scalability on UMA architecture is limited
- External Parallelization is faster (but irrelevant with 8 threads)

Parallel Performance Measurements (2/2)

- Library-parallelized GMRES solver on cc-NUMA machine:



- cc-NUMA architecture provides good memory bandwidth
- Allocator concept successfull, TBB Tasks have no affinity

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Conclusion

- Object-oriented abstractions can be exploited to hide parallelization from the user (as much as wanted)
- Expression Templates can be used to implement parallelization efficiently
- Todays best compromise: Use OpenMP in operator functions
- Architecture abstractions proved to be easy and successfull
- Future Work:
  - Apply concepts to other programming languages (FORTRAN)
  - Further exploit enhanced application knowlegde
    - Provide insight for compiler / Apply optimization under the hood
  - Find a way to include aspects of Parallelization in interface descriptions of software components

The End

Thank you for

your attention!