Exploiting Object-Oriented Abstractions to parallelize Sparse Linear Algebra Codes

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Agenda

- Motivation and Computational Task
- Implementation in C++
- Implementation in FORTRAN
- Comparison: C++ versus FORTRAN
- Conclusion and Future Work

Object-Oriented and Parallel Programming

- Compute intense core of many PDE solvers consists of Krylov subspace methods. Variations exist among different programs and throughout the development process.

- Object-Oriented Programming is mainstream since the 90s, Parallel Programming is just about to enter mainstream.
  - Reasons for OO: Encapsulation and Modularity → Reusability

- Parallelization is often decoupled from ongoing development.
  → Use of OO techniques to introduce and optimize parallelization
  → Use of OO techniques to investigate parallelization approaches
  → Use of OO techniques to hide complex architecture details from application / algorithm developer

C++: Iteration Loop of CG-style solver

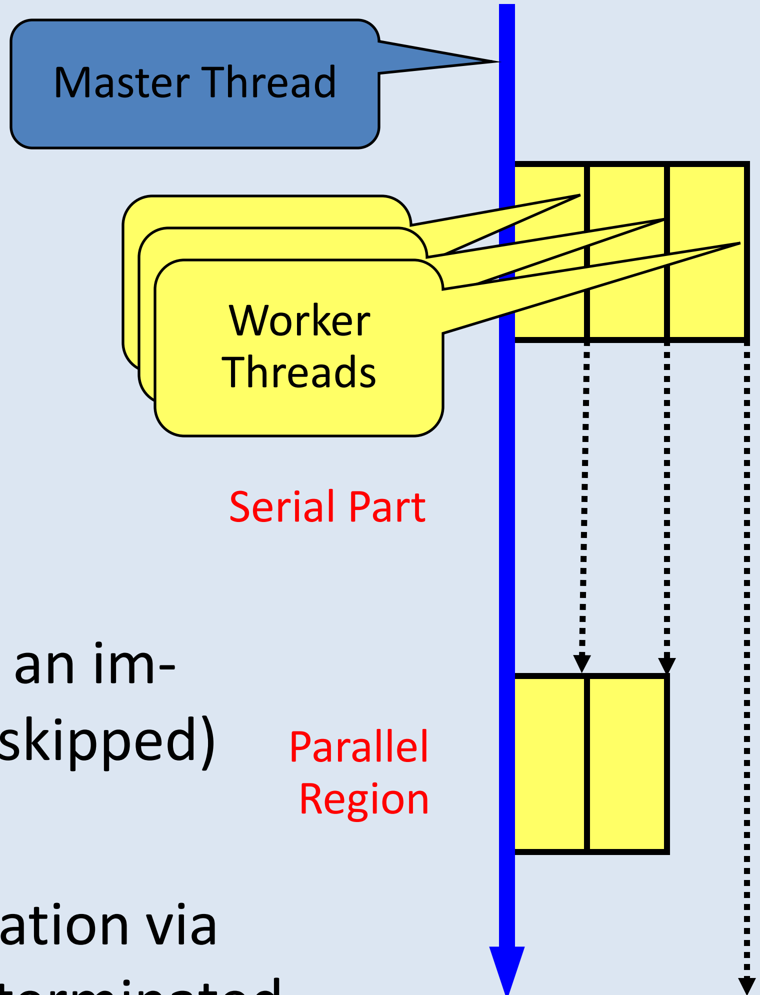
```
MatrixCL A(rows, cols, nonzeros);
VectorCL q(n), p(n), r(n);
[…]
for (int i = 1; i <= max_iter; ++i)
{
   […]
   q = A * p;
   double alpha = rho / (p*q);
   x += alpha * p;
   r -= alpha * q;
   […]
```

- Matrix data type: `MatrixCL A(rows, cols, nonzeros);`
- Vector data type: `VectorCL q(n), p(n), r(n);`
- Sparse Matrix-Vector-Multiplication (SMXV): `q = A * p;`
- Dot-Product: `double alpha = rho / (p*q);`
- Vector Operations: `x += alpha * p;` and `r -= alpha * q;`

- Code excerpt from C++ Navier-Stokes solver DROPS pretty much resembles notation found in math text books.
- Goals: Hide the parallelization as much as possible with as little overhead as possible to not hinder development.

Aspects of OpenMP

- OpenMP
  - Supports Fortran, C and C++
  - Explicit Parallelization via Parallel Regions:
    - pragma + structured block
  - Worksharing
  - Task-based parallelization



- Each Worksharing construct has an implicit Barrier associated (can be skipped)

- Intel + Sun + Others: Implementation via Thread Pool → Threads are not terminated

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C++: Naive Approach to Parallelization (Loops)

```
MatrixCL A(rows, cols, nonzeros);
VectorCL q(n), p(n), r(n);
[…]
for (int i = 1; i <= max_iter; ++i)
{
  […]
  q = A * p;
  double alpha = rho / …
  x += alpha * p;
  r -= alpha * q;
  […]
```

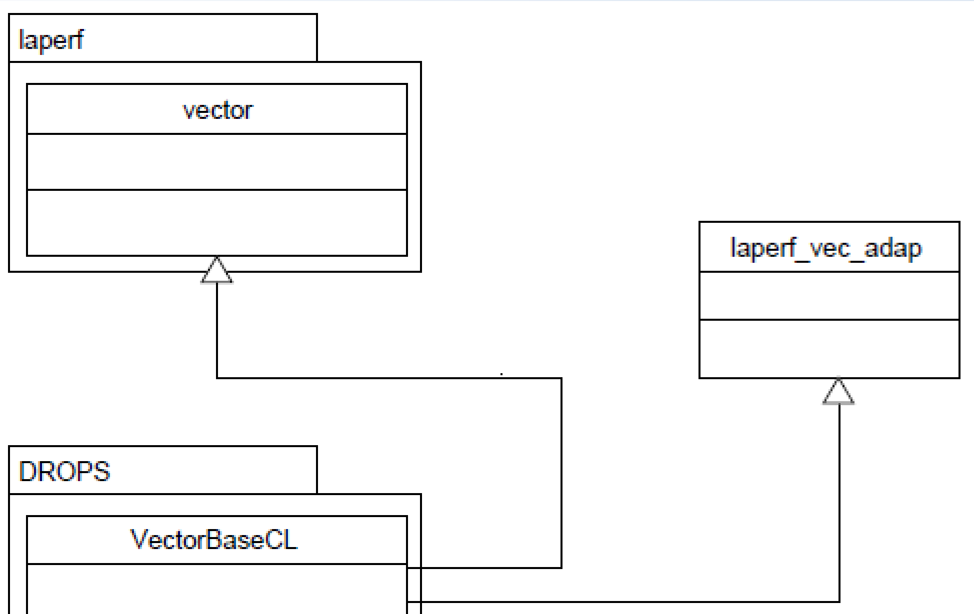
Option 1: Replace operator calls by loops:

```
#pragma omp parallel for
for (int r = 0; r < numRows, r++)
{
   double sum = 0.0; size_t nz;
   size_t rb = Arow[r];
   size_t re = Arow[r + 1];
   for (nz = rb, nz < re, nz++)
      sum += Aval[nz] * x[Acol[nz]];
   y[r] =sum;
}
```

- Refactoring code into OpenMP loops breaks OO paradigm.
- Code changes can easily break the parallelization! (races)

C++: Parallel Matrix & Vector class

- Extend existing abstractions to introduce parallelism!
- DROPS: Numerical parts are implemented via `Matrix` (CRS) and `Vector` class, or descendents of those.
  - Use *Adapter* design pattern to replace those with parallel ones



Scheme showing integration of parallel classes into DROPS.

- Problems:
  - Temporaries in complex expressions.
  - Overhead introduced by the Parallel Region in every operator call.

C++: Matrix & Vector class with Template Expressions

- Problem: The compiler translates the user code

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

into the following code

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

- Solution: Use Expression Templates to transform this into

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

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

... OpenMP ...

- which can be efficiently parallelized with OpenMP.

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Handling of cc-NUMA architectures

- All x86-based multi-socket systems will be cc-NUMA!
  - Current Operating Systems apply first-touch placement
- Thread binding is a necessity on cc-NUMA system: Hardware is examined automatically at application startup (*Singleton* design pattern).
- Policy-based approach: Apply the *Strategy* design pattern to influence the internal workings of a target class.
- Provide simple-to-choose-from options for the user:
  - `DistributedPolicy`: Distribute data according to OpenMP schedule type (same scheduling as in computation, default)
  - `ChunkedPolicy`: Distribute data according to explicitly precalculated scheme to improve load balacing (special cases)

C++: Parallel Iteration Loop of CG-style solver

```
MatrixCL A(rows, cols, nonzeros);
VectorCL<OpenMPParallelization> 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;
   […]
```

Enable Parallelization

Only one Parallel Region

- Expression Templates allow the parallelization of whole lines.
- Parallelization is completely invisible, algorithmic modifications do not break the parallelization!
- Incremental approach: (i) Go Parallel, (ii) cc-NUMA, (iii) ...

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FORTRAN: Loop-level and WORKSHARE Parallelization

- Sparse Matrix-Vector-Multiplication (SMXV) with loops:

```
!$omp parallel do private(i,j)
do i = 1, n
   q(i) = 0.0d0
   do j=irow(i),irow(i+1)-1; q(i)=q(i)+a(j)*p(icol(j)); end do
end do
!$omp end parallel do
```

- Code changes can easily break the parallelization! (races)

- Dot-Product with WORKSHARE:

```
!$omp parallel workshare
   alpha = alpha / dot_product(p,q)
!$omp end parallel workshare
```

- Array-syntax makes code much more readable, but compiler support for WORKSHARE is still weak (see performance).

FORTRAN: Parallel Matrix & Vector class (1/2)

- Matrix & Vector class in FORTRAN:

```
MODULE matvect
 TYPE :: vector ! Vector type
   DOUBLE PRECISION, ALLOCATABLE :: v(:)
 END TYPE vector
 TYPE :: matcrs ! Matrix type
   INTEGER :: n, nz_num
   INTEGER,ALLOCATABLE :: irow(:),icol(:)
   DOUBLE PRECISION, ALLOCATABLE :: a(:)
 END TYPE matcrs
 INTERFACE ASSIGNMENT (=)
   MODULE PROCEDURE assign_VV  ! vector assignment
 END INTERFACE ASSIGNMENT (=)
```

Wrapper around native vector

Implemented via allocatables

- Using Pointers *would* be more flexible, but slower. Fortran 2003 *would* bring more comfort, but is not yet supported by OpenMP. Compiler *would* provide slow, serial assignment.

FORTRAN: Parallel Matrix & Vector class (2/2)

- Similar approach as used in C++ library implementation: Complete Parallel Region inside the operators:

```
SUBROUTINE assign_VV (left, right)
  TYPE(vector),INTENT(OUT) :: left
  TYPE(vector),INTENT(IN)  :: right
  INTEGER :: i
  IF(.NOT.ALLOCATED(left%v))
     ALLOCATE(left%v(SIZE(right%v)))
!$omp parallel do schedule(runtime)
  do i = 1, SIZE(right%v); left%v(i)=right%v(i); end do
!$omp end parallel do
END SUBROUTINE assign_VV
```

- Problem of temporaries in complex expressions cannot be solved in FORTRAN. We did not see any compiler aggressive enough to optimize these temporaries away.

FORTRAN: Parallel Iteration Loop of CG-style solver

```
USE matvect
  TYPE(matcrs) :: a
  TYPE(vector) :: x, r, p, q
  DOUBLE PRECISION :: alpha
  […]
  do iter=1, max_iter
    […]
    q = a * p

    alpha = norm_2(p,q)

    x = x + alpha * p
    r = r - alpha * q
    […]
```

Use parallel data types

3 separate Parallel Regions

- Parallelization is completely invisible, algorithmic modifi-cations do not break the parallelization!
- More Overhead than in C++ implementation.

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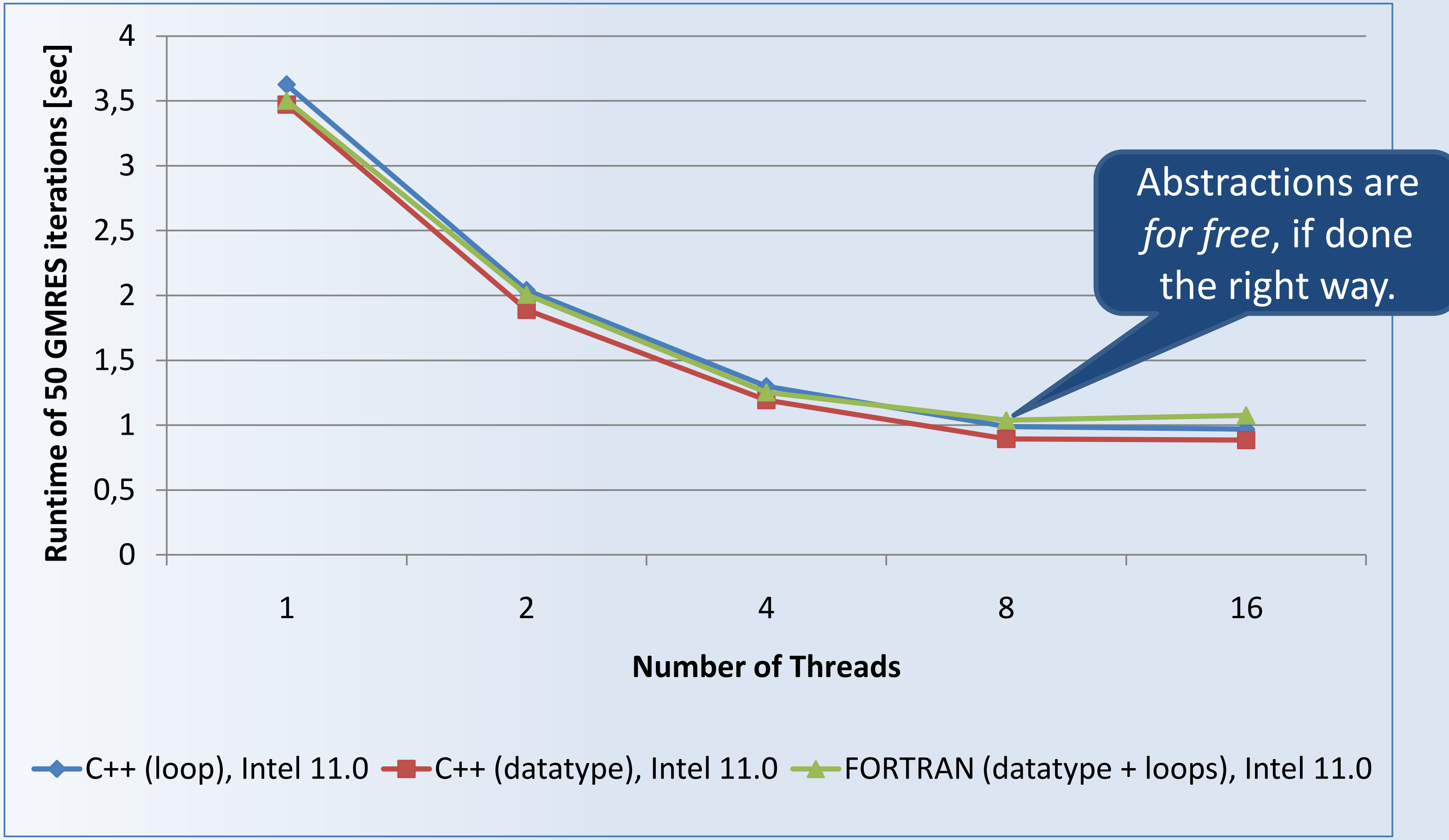
Comparison: Programmability

- OpenMP with Internal Parallelization (self-contained Parallel Region per operator): Completely invisible and safe to use.
  - External Parallelization - employ orphaned Worksharing constructs in operator, Parallel Region is outside – could be faster but can easily lead to data races.
- C++: Object-oriented design allows to write parallel code that still resembles math text book notation, parallel data types can easily be integrated into existing application → minimal changes to user application.
- FORTRAN: Array-syntax clearly improves readability, but full object-oriented design is achievable as well.

Comparison: Performance (Big Picture)

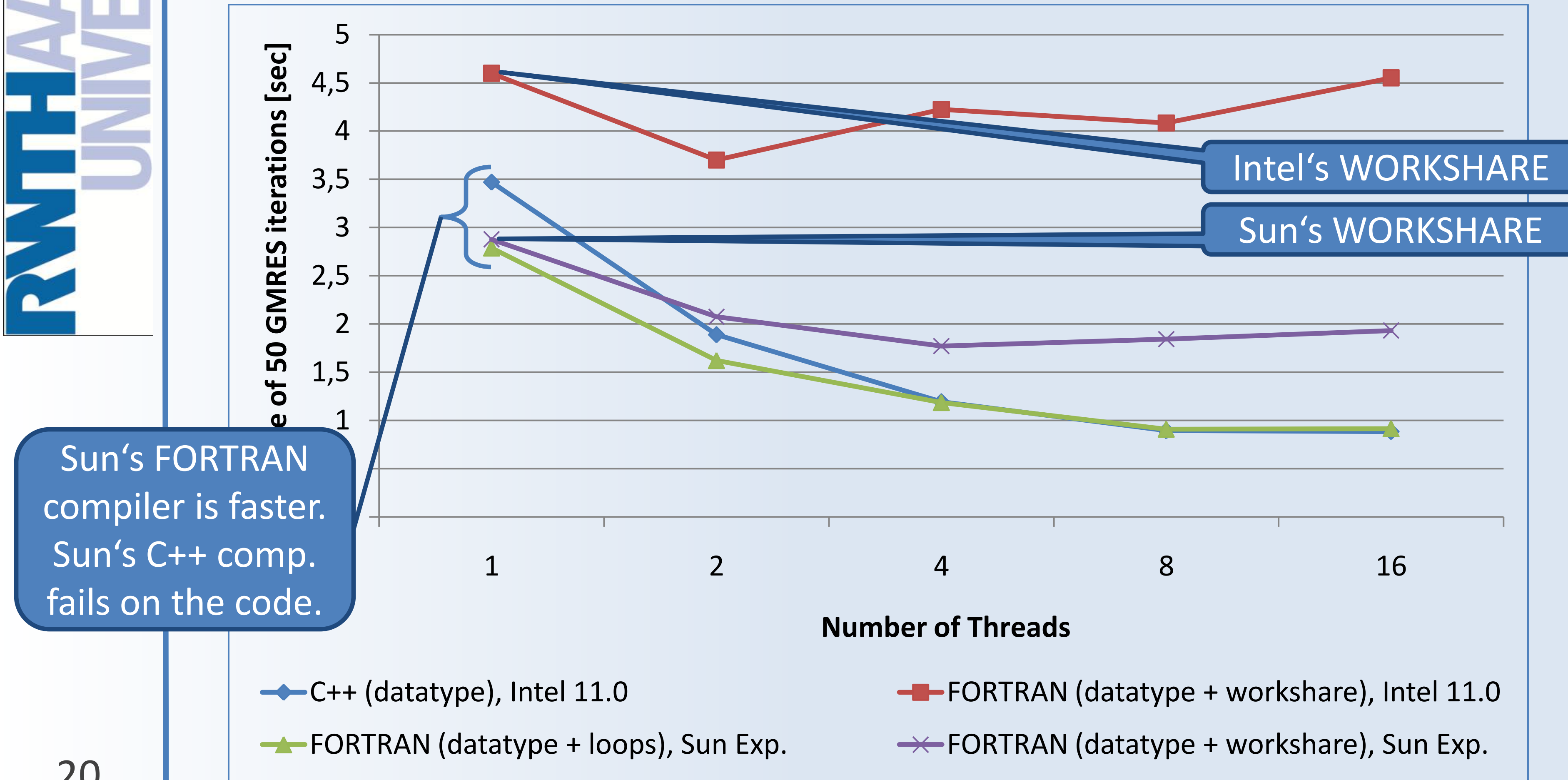
- Intel Compiler: hardly any difference in the programming language.



Two-socket Intel Nehalem (X5570) @ 2.93 GHz, Intel 11.0 compiler.

Comparison: Performance (Details 1)

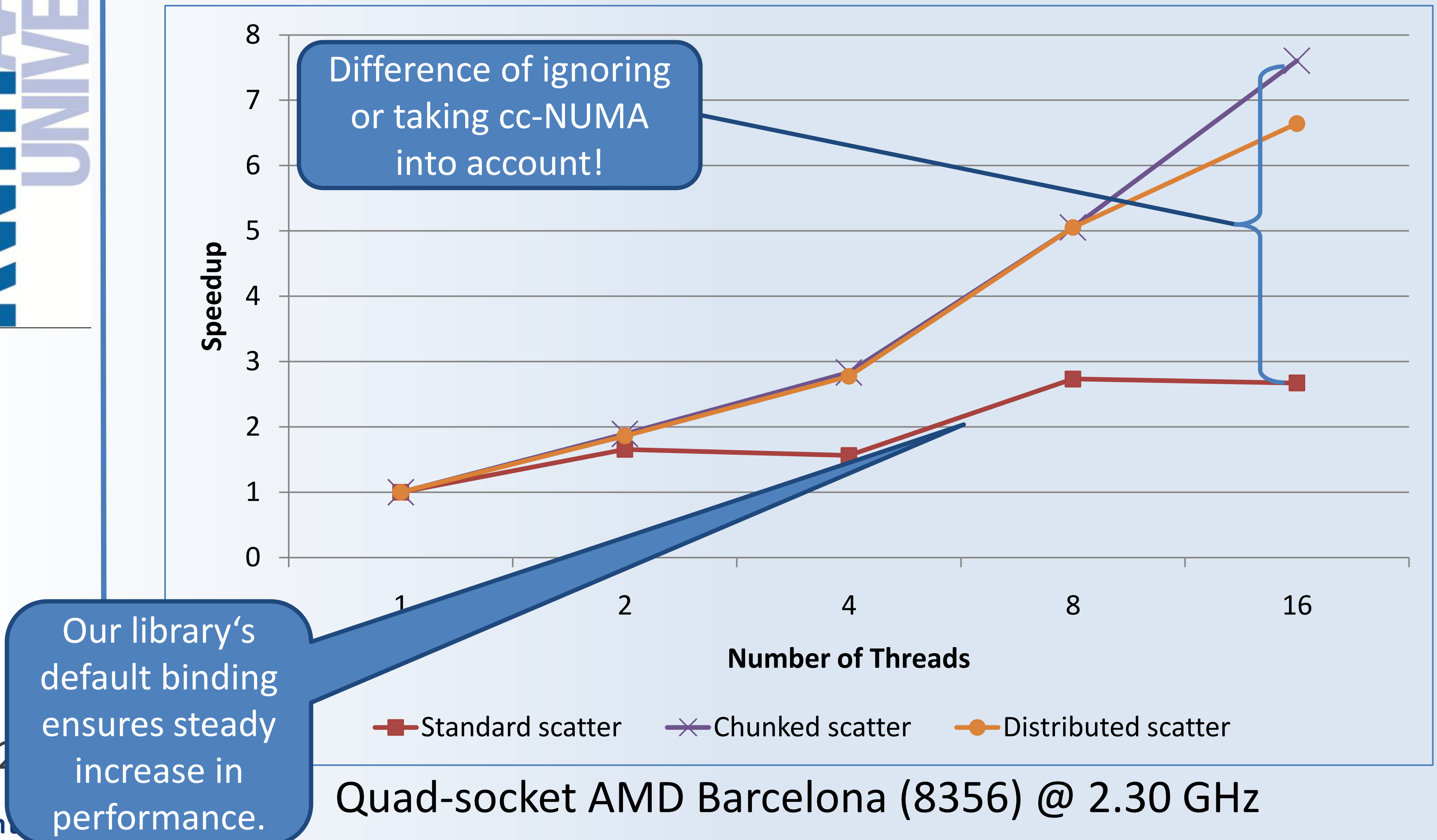
- Quality of FORTRAN implementations varies.



Two-socket Intel Nehalem (X5570) @ 2.93 GHz

Comparison: Performance (Details 2)

- cc-NUMA optimization became simple, but is very important!



Quad-socket AMD Barcelona (8356) @ 2.30 GHz

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Conclusion

- Object-oriented abstractions can be exploited to hide parallelization from the user (as much as wanted), lowering the burden of parallelization and optimization.
- C++: Expression Templates can be used to implement parallelization very efficiently, but with some coding work. FORTRAN works as well.
- Best compromise: Use OpenMP inside operators.
- Future Work:
  - Further leverage abstractions in other domains (i.e. Mesh)
  - Identify FORTRAN 2003 features which need to be (better) supported by OpenMP
  - Composability: Include details of the parallelization in interface descriptions of software components

The End

Thank you for

your attention!