MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC

COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Efficient Implementation of BLAS Level-3 solvers for Sylvester-type Matrix Equations

Martin Köhler

February 14, 2017

7th Workshop on Matrix Equations and Tensor Techniques

Introduction

Generalized Sylvester Equation (GSYLV)

$$AXB \pm CXD = Y$$

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Standard Sylvester Equation (SYLV)

$$AX \pm XB = Y$$

Standard Lyapunov Equation (LYAP)

$$AX + AX^T = Y$$

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Equation	Software Packages				
	RECSY[1]	SLICOT[2]	LAPACK	Alg. 432[3]	Alg. 705[4]
SYLV	RECSYCT	SB04PD	xTRSYL	AXPXB	-
SYLV2	RECSYDT	SB04PD	-	-	-
LYAP	RECLYCT	SB03TD	-	ATXPXA	-
STEIN	RECLYDT	SB03UD	-	-	-
GSYLV	RECGSYL	-	-	-	SYLG
CSYLV	RECGCSY	SB04OD	xTGSYL	-	-
GLYAP	RECGLYCT	SG03AD	-	-	SYLGC
GSTEIN	RECGLYDT	SG03AD	-	-	SYLGD

[1] http://www8.cs.umu.se/~isak/recsy/

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→ **SLICOT** implementations only use Level-2 BLAS.

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All packages are not feature complete and mostly old.

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General Workflow in Direct Solvers:

Compute real Schur forms:

$$A = QA_sQ^T \text{ and } B = ZB_sZ^T.$$

Transform the right hand side:

$$\tilde{Y} = Q^TYZ.$$

Solve the (quasi-) triangular equation:

$$A_s\tilde{X} \pm \tilde{X}B_s = \tilde{Y}.$$

Transform the solution:

$$X = Q\tilde{X}Z^T.$$

Compute generalized real Schur forms:

$$(A, C) = (Q_1A_sZ_1^T, Q_1C_sZ_1^T)$$

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Transform the solution:

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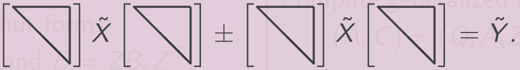
Introduction

Our focus:

Fast solution of (quasi-) triangular Sylvester-type Matrix Equations:



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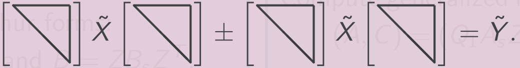

We use the Generalized Sylvester Equation as most complex variant for the optimizations.

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Block-Algorithm

The real Generalized Schur Decomposition of (A, C) and (B, D) yields:

$$A_s = \begin{bmatrix} A_{11} & \cdots & A_{1p} \\ & \ddots & \vdots \\ 0 & & A_{pp} \end{bmatrix}, \quad C_s = \begin{bmatrix} C_{11} & \cdots & C_{1p} \\ & \ddots & \vdots \\ 0 & & C_{pp} \end{bmatrix}, \quad \tilde{X} = \begin{bmatrix} \tilde{X}_{11} & \cdots & \tilde{X}_{1q} \\ \vdots & \ddots & \vdots \\ \tilde{X}_{p1} & \cdots & \tilde{X}_{pq} \end{bmatrix},$$

$$B_s = \begin{bmatrix} B_{11} & \cdots & B_{1q} \\ & \ddots & \vdots \\ 0 & & B_{qq} \end{bmatrix}, \quad D_s = \begin{bmatrix} D_{11} & \cdots & C_{1q} \\ & \ddots & \vdots \\ 0 & & D_{qq} \end{bmatrix}, \quad \tilde{Y} = \begin{bmatrix} \tilde{Y}_{11} & \cdots & \tilde{Y}_{1q} \\ \vdots & \ddots & \vdots \\ \tilde{Y}_{p1} & \cdots & \tilde{Y}_{qq} \end{bmatrix},$$

where (A_{ii}, C_{ii}) and (B_{ii}, D_{ii}) are 1×1 or 2×2 according to the eigenvalues of (A, C), or (B, D) respectively.

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where (A_{ii}, C_{ii}) and (B_{ii}, D_{ii}) are 1×1 or 2×2 according to the eigenvalues of (A, C), or (B, D) respectively.

We need to solve $p \cdot q$ small Sylvester equations:

$$A_{kk}\tilde{X}_{kl}B_{ll} + C_{kk}\tilde{X}_{k\ell}D_{ll} = \tilde{Y}_{kl} - \sum_{\substack{i=k,\dots,p \\ j=1,\dots,l \\ (i,j)\neq(k,l)}} \left(A_{ki}\tilde{X}_{ij}B_{jl} \pm C_{ki}\tilde{X}_{ij}D_{jl} \right).$$

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Special cases: $(A_s,\ C_s \in \mathbb{R}^{m \times m},\ B_s,\ D_s \in \mathbb{R}^{n \times n}$ and $\tilde{X},\ \tilde{Y} \in \mathbb{R}^{m \times n})$

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$\rightarrow$ Why are m_b and n_b not chosen such that $A_{kk},\ B_{ll},\ C_{kk},\ D_{ll},\ \tilde{X}_{kl}$ and $\tilde{Y}_{kl}$ fit into the CPU's cache(s)?

Efficient Implementation

General Aspects:

- The updates on the right hand sides $\tilde{Y}_{kl}$

$$\tilde{Y}_{kl} - \sum_{\substack{i=k,\dots,p\\ j=1,\dots,l\\ (i,j)\neq(k,l)}} \left(A_{ki}\tilde{X}_{ij}B_{jl} \pm C_{ki}\tilde{X}_{ij}D_{jl} \right)$$

can be rewritten and unified into few GEMM/TRMM operations.
→ Assumed to be as efficient as possible for sufficiently large matrices.

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- Block sizes m_b and n_b are a freely selectable parameter.
- The solution $\tilde{X}$ overwrites the right hand side $\tilde{Y}$.
- All matrices are stored in the Fortran Column-Major-Scheme.

Efficient Implementation

Algorithm 1 Block Bartels-Stewart Algorithm for Generalized Sylvester Equations

```
Input: $A_s,\ C_s \in \mathbb{R}^{m\times m},\ B_s,\ D_s \in \mathbb{R}^{n\times n}$ and $\tilde{Y} \in \mathbb{R}^{m\times n},\ m_b,\ n_b \in \mathbb{N}$
Output: $\tilde{X} \in \mathbb{R}^{m\times n}$ overwriting $\tilde{Y}$
if  $m \leq m_b$ and $n \leq n_b$ then
    Solve $A_s\tilde{X}B_s \pm C_s\tilde{X}D_s = \tilde{Y}$.
else
    for $k = m, \ldots, 1$ step by $m_b$ do
        for $l = 1, \ldots, n$ step by $n_b$ do
            Solve $A_{kk}\tilde{X}_{kl}B_{ll} \pm C_{kk}\tilde{X}_{kl}D_{ll} = \tilde{Y}_{kl}$.
            $\tilde{Y}_{k,l+1:n} = \tilde{Y}_{k,l+1:n} - A_{kk}\tilde{X}_{kl}B_{kl} \mp C_{kk}\tilde{X}_{kl}D_{kl}$
        end for
        $\tilde{Y}_{1:k-1,1:n} = \tilde{Y}_{1:k-1,1:n} - A_{1:k-1,k:k+m_b-1}\tilde{X}_{k:k+m_b-1,1:l}B_s$
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Critical operation for a fast solution scheme.

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Critical operation for a fast solution scheme.

Goal: Develop an efficient solver for small Sylvester Equations.

Efficient Inner Solvers

Hardware and Software Setup

We use a test driven development scheme for the kernels on random matrices.

Hardware

- Intel Xeon E5-2640v3 (Haswell), 2x8 Cores, 16x256kB L2 Cache, 2x20MB L3 Cache, AVX vector unit
- 64GB DDR3 RAM

Software

- CentOS 7.3 – x86_64
- Intel Parallel Studio XE 2017 C/Fortran Compiler + Intel MKL 2017.0.1
- Compiler-Flags: `-O3 -xHost -qopenmp`
- Computational routines are written in Fortran 90/95.
- Reference results with Algorithm 705 and RECSY, double precision.
- Residual and Forward error of all results are comparable.

Efficient Inner Solvers

Naive Approach

- Sylvester equations with $m \leq 2$ and $n \leq 2$ are trivial to solve via their Kronecker representation:

$$AXB \pm CXD = Y \quad \Longleftrightarrow \quad (B^T \otimes A \pm D^T \otimes C) \operatorname{vec} X = \operatorname{vec} Y$$

- Larger problems are solved using Algorithm 1 with $m_b = 1$ and $n_b = 1$.

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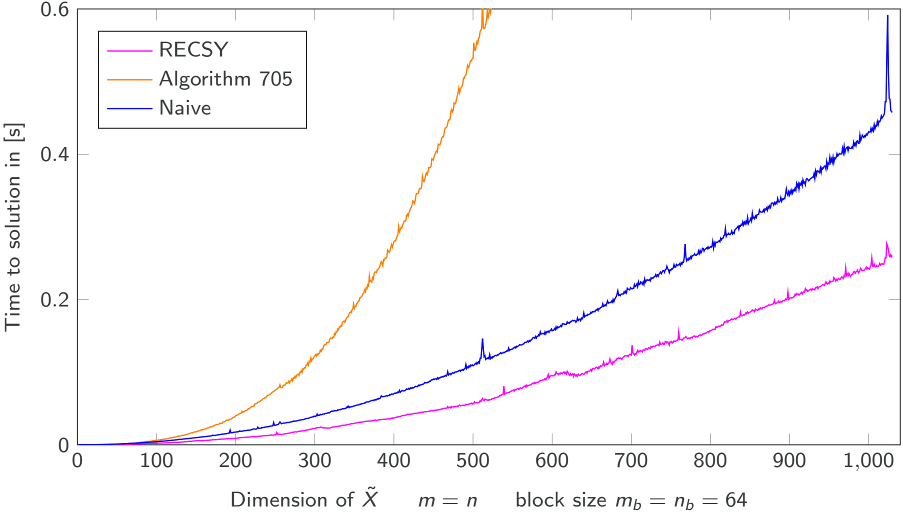
Test Procedure

- Algorithm 1 with random matrices $A, B, C, D \in \mathbb{R}^{m \times m}$, $m = 1, \ldots, 1030$.
- Eigenvalues sorted such that $A_{64k+1,64k} = 0$ and $B_{64k+1,64k} = 0$, $\forall k \in \mathbb{N}$.
- Only inner solver exchanged/optimized.
- 16 threads for multi-threaded BLAS calls.

Efficient Inner Solvers

Naive Approach



Efficient Inner Solvers

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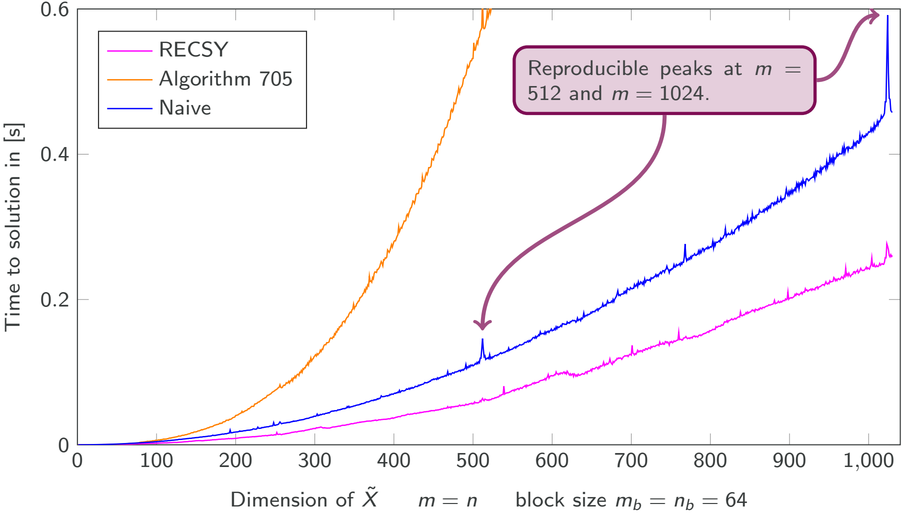

Reproducible peaks at $m = 512$ and $m = 1024$.

Efficient Inner Solvers

Level-2 BLAS Calls

- Replace Level-3 BLAS calls with the corresponding Level-2 operations:
  - xGEMM → xGEMV, xGER, and xAXPY,
  - xTRMM → xTRMV.

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  - xTRMM → xTRMV.
- GEMM operations up to 2×2 are directly computed.
- Appearing xAXPY operations, caused by the GEMM replacement, are performed by Fortran intrinsics:

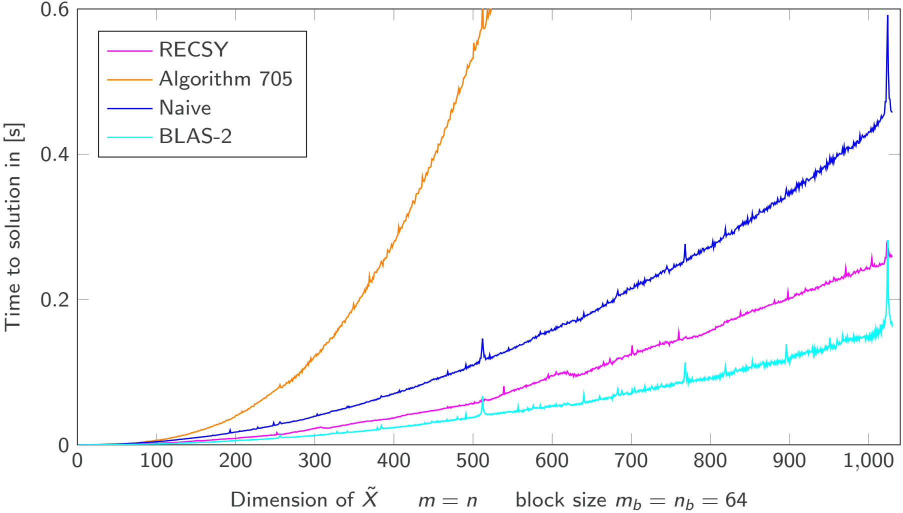
```
CALL DAXPY(N-LH, -MAT(1,1), B(L,LH+1), LDB, X(K,LH+1), LDX)
CALL DAXPY(N-LH, -MAT(3,1), B(LH,LH+1), LDB,X(K,LH+1), LDX)
CALL DAXPY(N-LH, -MAT(2,1), B(L,LH+1), LDB, X(KH,LH+1), LDX)
CALL DAXPY(N-LH, -MAT(4,1), B(LH,LH+1), LDB,X(KH,LH+1), LDX)
```

  is transformed into

```
X(K,LH+1:N) = X(K,LH+1:N) - MAT(1,1) * B(L,LH+1:N) -
  MAT(3,1) * B(LH,LH+1:N) - SGN * MAT(1,2) * D(L,LH+1:N)
  - SGN * MAT(3,2) * D(LH, LH+1:N)
```

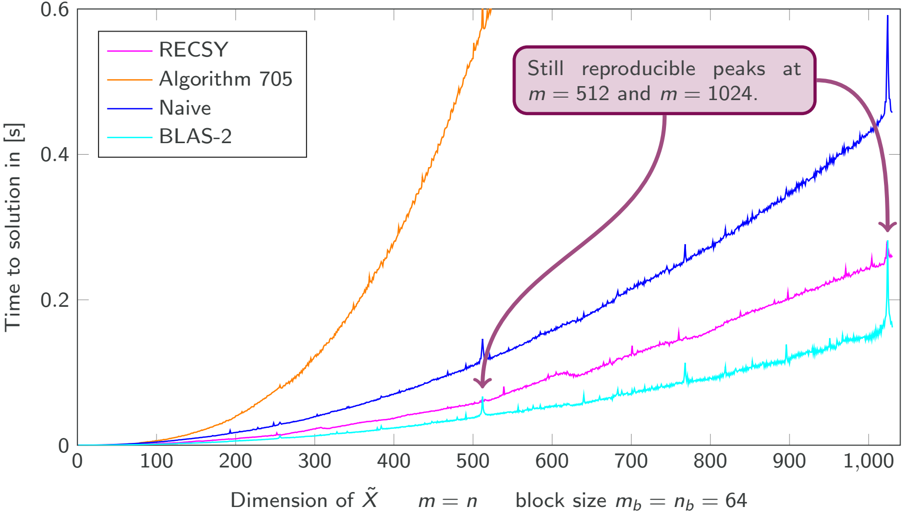
Efficient Inner Solvers

Level-2 BLAS Calls



Efficient Inner Solvers

Level-2 BLAS Calls



Still reproducible peaks at $m = 512$ and $m = 1024$.

Efficient Inner Solvers

Reorder the data access

The peaks at $m = 512$ and $m = 1024$ (and the next ones at 1536 and 2048) are caused by cache-misses/unused prefetching.
Reason: The leading dimension of the matrix (times 8 Byte per value) is a multiple of the pagesize (4096 Bytes).

The access to `X(K,LH+1:N)`, `B(L,LH+1:N)`, and `D(L,LH+1:N)` is not well suited for the matrix storage. (column-major-storage vs. row-wise access).

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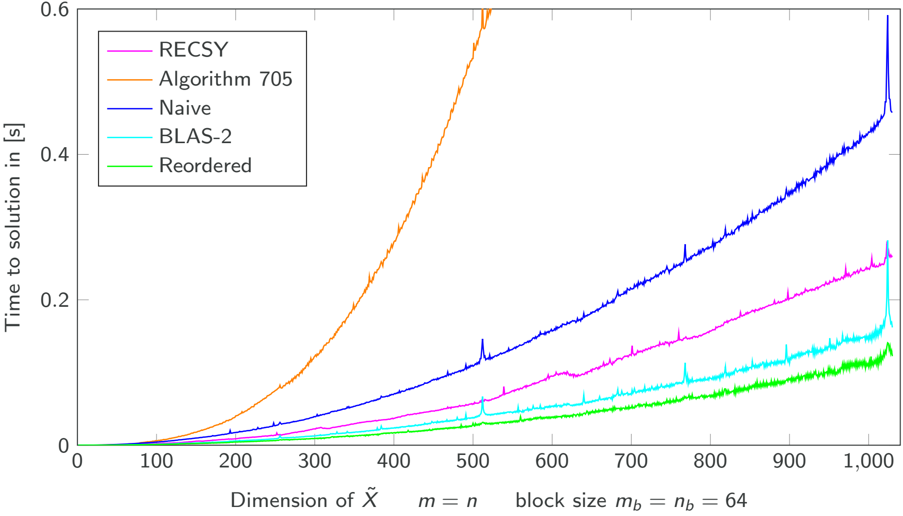
- Same optimizations as before but…
- solve the small equation column-wise instead of row-wise.
  The crucial operations change to:

```
X(1:K-1,L) = X(1:K-1,L) - MAT(1,1) * A(1:K-1,K)
   - MAT(2,1) * A(1:K-1,KH) - SGN * MAT(1,2) * C(1:K-1,K)
   - SGN * MAT(2,2) * C(1:K-1,KH)
```

→ Access on X_{kl}, A_{kk} and C_{kk} fits the storage scheme.

Efficient Inner Solvers

Reorder the data access



Efficient Inner Solvers

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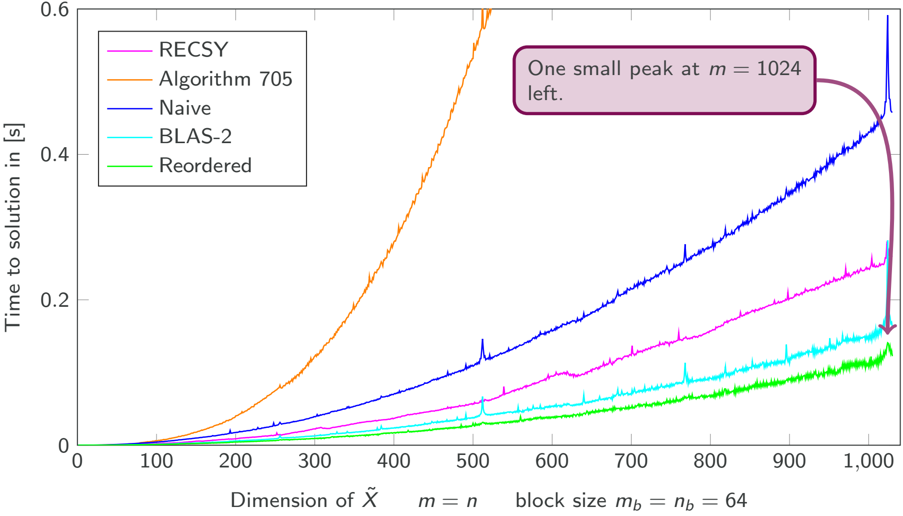

One small peak at $m = 1024$ left.

Efficient Inner Solvers

Use local copies of A_{kk}, B_{ll}, C_{kk}, D_{ll}, and X_{kl}

The leading dimension of A_s, B_s, C_s and D_s still yields cache misses and unnecessary prefetching.

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All data can be copied to the (L2) cache before the solution of the inner Sylvester equation starts.

Efficient Inner Solvers

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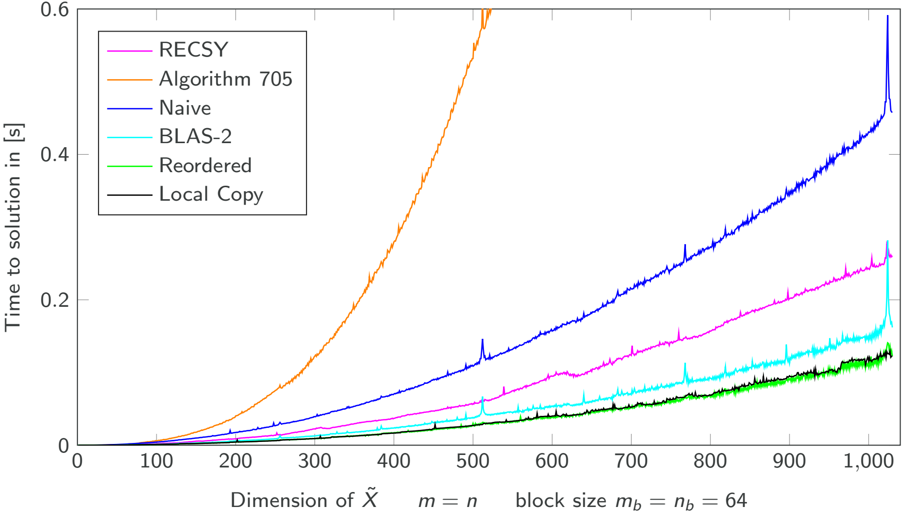

Efficient Inner Solvers

Alignment of the local copies

Vector units (AVX, VSX,. . .) of modern CPUs need a special data alignment to work really fast.
→ Without additional help compilers cannot produce efficient code for them.

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- Keep all previous optimizations, especially the local copies.
- Annotate the declaration of the local data such that they are 64-byte aligned:

  ```
  !dir$ attributes align: 64:: AL, BL, CL, DL, XL
  ```

  or

  ```
  !IBM* ALIGN(64,AL,BL,CL,DL,XL)
  ```

  depending on the Fortran compiler.

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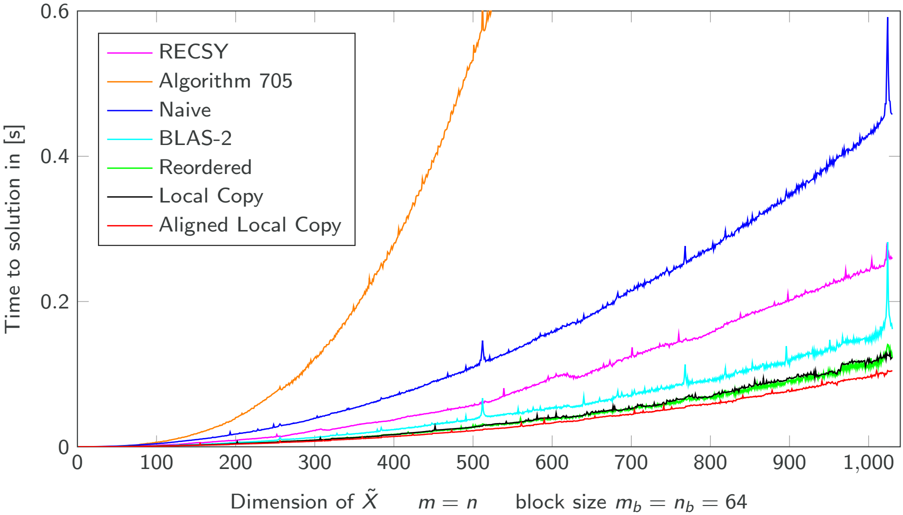
→ The compiler should be able to optimize our code.

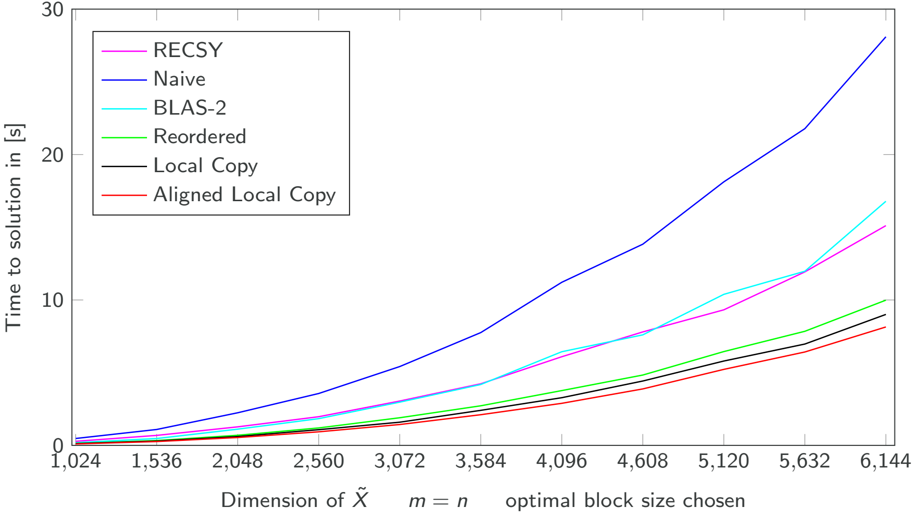
Efficient Inner Solvers

Alignment of the local copies



Efficient Inner Solvers

Large Scale Test



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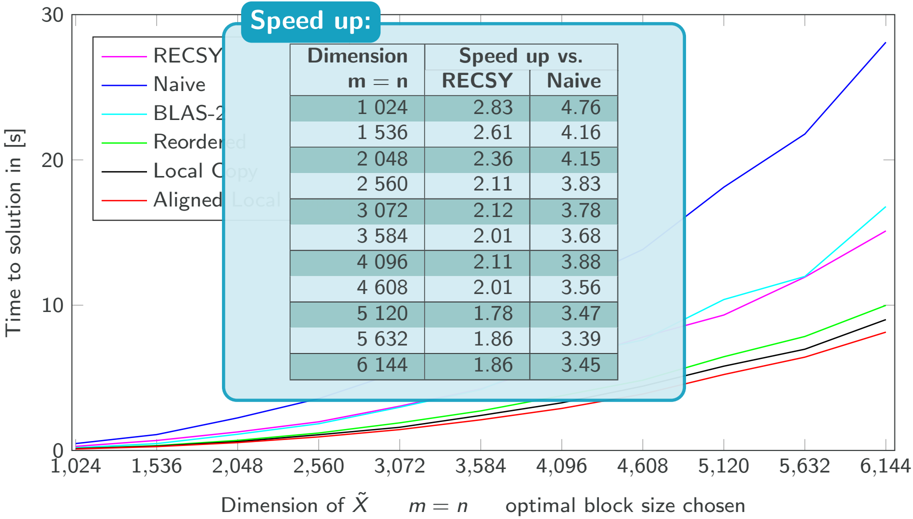

Speed up:

Dimension	Speed up vs.	
m = n	RECSY	Naive
1 024	2.83	4.76
1 536	2.61	4.16
2 048	2.36	4.15
2 560	2.11	3.83
3 072	2.12	3.78
3 584	2.01	3.68
4 096	2.11	3.88
4 608	2.01	3.56
5 120	1.78	3.47
5 632	1.86	3.39
6 144	1.86	3.45

Further Optimization

Optimal Block Sizes m_b and n_b

The optimal block sizes m_b and n_b must be chosen such that:

- small enough that the inner solvers working nearly inside the (L2) CPU cache
- and large enough that the matrix-matrix products in Algorithm 1 are making use of the multi-threading capabilities of the BLAS library.

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For large m and n and increasing number of CPU cores it is no longer possible to satisfy both conditions properly.

Idea

Move the parallelization from the BLAS library to the Algorithm.
Use the data dependencies between the $p \cdot q$ blocks of the solution matrix $\tilde{X}$:

- $\tilde{X}_{p1}$ depends on nothing.
- $\tilde{X}_{pj}$, $j = 2 \dots q$ depend on $\tilde{X}_{p,j-1}$.
- $\tilde{X}_{i1}$, $i = p - 1 \dots 1$ depend on $\tilde{X}_{i+1,1}$.
- $\tilde{X}_{ij}$, $i = p - 1 \dots 1$, $j = 2 \dots q$ depend on $\tilde{X}_{i,j-1}$ and $\tilde{X}_{i+1,j}$.

Further Optimization

Direct-Acyclic-Graph (DAG) Scheduling

The data dependencies in the solution lead to the following DAG:

$$\begin{bmatrix}
\vdots & \dots & \vdots & \dots & \vdots & \dots \\
\uparrow & & \uparrow & & \uparrow & \\
\tilde{X}_{p-2,1} & \rightarrow & \tilde{X}_{p-2,2} & \rightarrow & \tilde{X}_{p-2,3} & \dots \\
\uparrow & & \uparrow & & \uparrow & \\
\tilde{X}_{p-1,1} & \rightarrow & \tilde{X}_{p-1,2} & \rightarrow & \tilde{X}_{p-1,3} & \dots \\
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The blocks $\tilde{X}_{ij}$ on the same anti-diagonal can be solved independently from each other (in parallel).

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OpenMP 4.0 – `task depend`

Since OpenMP 4.0 such data dependencies can be attached to the `omp task` directive and the OpenMP runtime system does the scheduling with respect to the DAG.

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$$\begin{tikzcd}
\vdots & \vdots & \vdots & \\
\tilde{X}_{p-2,1} \arrow[u] \arrow[r] & \tilde{X}_{p-2,2} \arrow[u] \arrow[r] & \tilde{X}_{p-2,3} \arrow[u] & \cdots \\
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Sketch of the Implementation:

OpenMP parallelization is done using annotations in the source code:

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 & A,LDA,B,LDB,C,LDC,D,LDD,X,LDX,SGN,SCAL,WORK,INFO1,ARCH )
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!$omp& default(shared)
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→ Annotations are ignored by non OpenMP compatible compilers.

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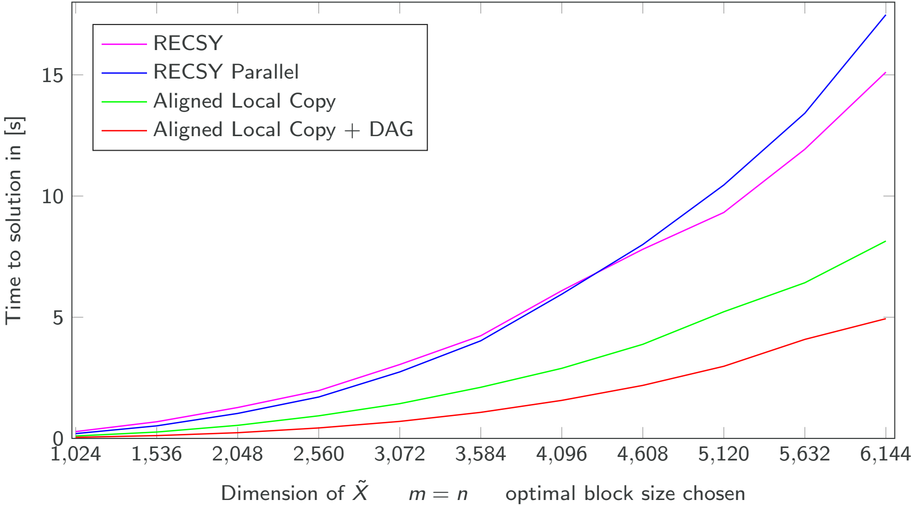

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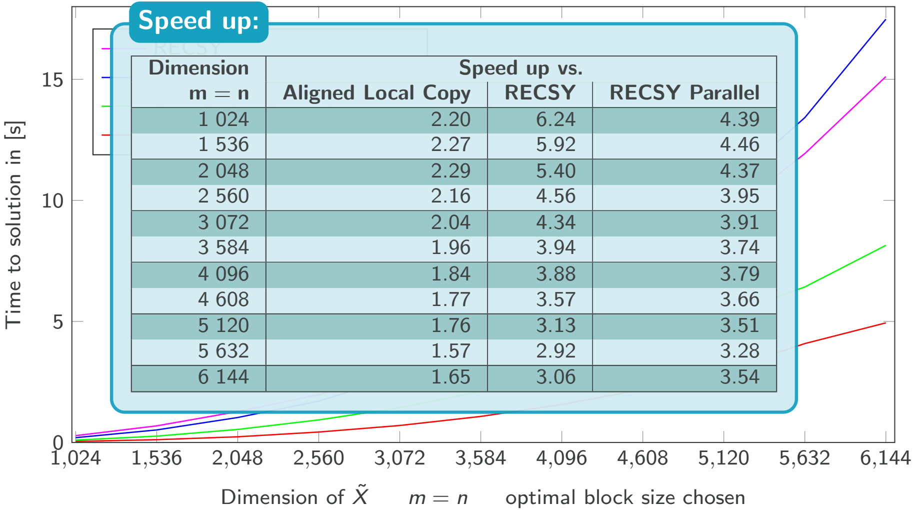

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Conclusions

- Block Bartels-Stewart algorithms can beat the RECSY approach by a factor of 2.8 or 6.2.
- Performance gain of a factor 4.7 if the code is written in a way such that the compiler can optimize the code properly.
- DAG-Scheduling in OpenMP 4 allows easy high level parallelization on top of the data dependencies. (GCC since 4.9.1, Intel since 15.0, LLVM since 3.9)
- Same ideas work for LYAP, STEIN, SYLV, SYLV2, GLYAP, GSTEIN and CSYLV.

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- Compile-time tuning by benchmarks of xGEMM and xTRMM.
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Thank you for your attention.

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