Recursive Algorithms for Dense Linear Algebra: The ReLAPACK Collection

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To exploit both memory locality and the full performance potential of highly tuned kernels, dense linear algebra libraries such as LAPACK commonly implement operations as blocked algorithms. However, to achieve next-to-optimal performance with such algorithms, significant tuning is required. On the other hand, recursive algorithms are virtually tuning free, and yet attain similar performance. In this paper, we first analyze and compare blocked and recursive algorithms in terms of performance, and then introduce ReLAPACK, an open-source library of recursive algorithms to seamlessly replace most of LAPACK’s blocked algorithms. In many scenarios, ReLAPACK clearly outperforms reference LAPACK, and even improves upon the performance of optimizes libraries.

CCS Concepts: ●Mathematics of computing → Mathematical software performance; Computations on matrices; ●Software and its engineering → Software performance; ●Computing methodologies → Linear algebra algorithms;

Additional Key Words and Phrases: dense linear algebra, recursion

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1. INTRODUCTION

Blocking and tiling are common concepts for increasing data locality, reducing memory stalls, and thus improving performance. In dense linear algebra, these concepts are applied to many operations through the means of blocked algorithms (detailed in Sec. 2) [Anderson et al. 1999], which organize the computation to attain an extremely favorable ratio of floating point operations per memory access. Such algorithms offer two degrees of freedom that require careful tuning: 1) for each operation, there typically exist several algorithmic variants, which although mathematically equivalent, might differ substantially in terms of both accuracy and efficiency [Du Croz and Higham 1992; Bientinesi et al. 2008]; 2) the choice of “block size” (which ultimately determines how matrices are traversed) is a critical tuning parameter to achieve nearly optimal performance [Whaley 2008]. We stress that the optimal choice for these degrees of freedom varies (sometimes wildly) with both the computing environment—the hardware, the implementation of the underlying kernels used as building blocks, the number of threads used—and the problem size. As a consequence, the selection of the algorithmic variant and a quasi-optimal block size is a tedious and time consuming process.
For many operations, recursive algorithms\(^1\) (detailed in Sec. 3) are an alternative that provides performance comparable to that of blocked algorithms\(^2\), while requiring virtually no tuning effort. Rather unexpectedly, while blocked algorithms are readily available in libraries such as the LINEAR ALGEBRA PACKAGE (LAPACK) [Anderson et al. 1999], hardly any readily available recursive counterpart exists. For this reason we introduce the RECURSIVE LAPACK COLLECTION (RELAPACK), an open-source library offering recursive implementations of many operations. By conforming to the established interfaces, these implementations (or a selected subset) can easily replace LAPACK routines in existing software. Experiments show that RELAPACK outperforms LAPACK even with optimized block sizes, as well as, in several scenarios, optimized implementations (such as MKL and OPENBLAS).

**Contributions.** Our main contribution with this paper is the RELAPACK library, which provides a total of 40 recursive algorithms. It thereby covers almost all of LAPACK’s compute routines to which recursion is efficiently applicable; through LAPACK’s hierarchical structure, RELAPACK extends the obtained performance benefits to over 100 further routines. For all but a few of the operations supported, RELAPACK is the first library offering recursive algorithms. Furthermore, we provide a detailed analysis of how both blocked and recursive algorithms use optimized BLAS to attain high performance.

**Structure of this paper.** The rest of this paper is organized as follows. Blocked and recursive algorithms and the importance of their tuning parameters are illustrated in, respectively, Sections 2 and 3; a performance comparison follows in Sec. 4. Section 5 introduces the RELAPACK collection of recursive algorithms, which are compared to high-performance LAPACK implementations in Sec. 6. Finally, Sec. 7 draws conclusions.

**2. BLOCKED ALGORITHMS**

Blocked algorithms extend the performance of the highly optimized BASIC LINEAR ALGEBRA SUBPROGRAMS (BLAS) Level 3 [Dongarra et al. 1990] kernels to more complex operations such as matrix inversions, decompositions and reductions. Each such operation can generally be implemented as several mathematically equivalent blocked algorithms, each with a potentially different performance signature. In this section, we illustrate how these algorithms operate, and which factors influence their performance. We will do so by considering an example: an algorithm for the in-place inversion of a lower triangular matrix \(A := A^{-1}\) in double precision arithmetic. This operation, known in LAPACK as dtrtri, and the selected algorithm (there are four alternative variants) are chosen deliberately simple, but are fully representative of the features and characteristics of the general class of blocked algorithms.

As shown in Fig. 1a, the algorithm traverses the lower triangular \(n \times n\) input matrix \(A\) diagonally from the top left to the bottom right in steps of a prescribed block size \(b\).

At each step of the traversal, the algorithm exposes the sub-matrices shown in Fig. 1a and makes progress by applying the three computational updates in Fig. 1b. Before the execution of these updates, the sub-matrix \(A_{00}\) (which in the very first step is of size \(0 \times 0\)) already contains a portion of the inverse; after the updates, the algorithm

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\(^1\)Algorithms that solve subproblems invoking themselves; the problem size dynamically determines the recursion depth.

\(^2\)Here, blocked algorithms are not considered recursive; they solve sub-problems using separate, unblocked routines.
For every traversal step:

1. **dtrmm**: $A_{10} := A_{10} A_{00}$
2. **dtrsm**: $A_{10} := -A_{11}^{-1} A_{10}$
3. **dtrti2**: $A_{11} := A_{11}^{-1}$

(a) Partitioning and blocked traversal of $A$

(b) Updates performed during the traversal

Fig. 1: Blocked algorithm for the inversion of a lower triangular matrix.

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(a) Execution time within the algorithm

(b) Efficiency within the algorithm

Fig. 2: Breakdown of the blocked inversion of a lower triangular matrix of size $n = 2000$ with increasing block size $b$.

progressed such that the sub-matrices $A_{10}$ and $A_{11}$ now also contain their parts of the inverse, and in the next step become part of $A_{00}$. Once the traversal reaches the bottom right corner (i.e., $A_{00}$ is now of size $n \times n$), the entire matrix is inverted.

The first two updates (dtrmm$^3$ and dtrsm$^4$) of the algorithm in Fig. 1, are calls to BLAS Level 3 kernels, while the last one (dtrti2$^5$) invokes an unblocked algorithm based on

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\[ ^3 \text{dtrmm: double precision triangular matrix times matrix (BLAS Level 3)} \]
\[ ^4 \text{dtrsm: double precision triangular linear system solve with multiple right-hand-sides (BLAS Level 3)} \]
\[ ^5 \text{dtrti2: double precision triangular matrix inversion (unblocked LAPACK)} \]
Fig. 3: Efficiency of the blocked triangular inversion algorithm for different block sizes $b$: Different block sizes are optimal for different settings.

BLAS Level 1 and 2, which is equivalent to $b = 1$. For a matrix of size $n = 2000$, Fig. 2 gives an idea (a) of how much these routines contribute to the algorithm’s total execution time and (b) what efficiency (with respect to the processors theoretical compute bound) they operate at within the algorithm. For very small values of $b$, the compute intensity\(^7\) of $dtrmm$ and $dtrsm$ is so low that they are effectively memory bound, and thus very inefficient. As $b$ increases, the size of the three kernels grows and so does their efficiency (see Fig. 2b): $dtrmm$ (—) plateaus at 85% around $b = 120$, $dtrsm$'s efficiency (—) steadily rises towards that of $dtrmm$ (—), while $dtrti2$ (—) approaches its peak of only 20% towards $b = 200$. On the other side, when increasing $b$, more and more computation is shifted from the BLAS Level 3 routines to the low performance $dtrti2$ (—); beyond $b = 150$ this low performance causes the overall runtime to increase. This trade-off between increasing BLAS Level 3 performance and shifting the computation to a less efficient unblocked kernel is a well known phenomenon inherent to all blocked algorithms.

To further illustrate the importance of this trade-off, Fig. 3 reports the performance of the presented algorithm with 1 and 10 threads, for $b = 64, 128, 256$, and increasing matrix size $n$. The performance results, which are representative for all blocked algorithms, indicate that, both for different matrix sizes and different thread counts, the ideal choice of $b$ varies. In fact, the optimal choice among the three values for single threaded BLAS and matrix size $n = 500$ is $b = 64$ (—); however, at $n = 2000$, this choice would be about 10% less efficient than $b = 256$ (—) on 1 core and only 50% as fast on 10 cores. Even though this trade-off is well known, it remains a challenging and important optimization task when implementing and tuning any blocked algorithm.

2.1. Related Work

LAPACK [Anderson et al. 1999] is a well established library that provides blocked algorithms for many higher-level operations, such as inversions, factorizations, and reductions [Anderson and Dongarra 1990]. These algorithm's block size $b$ is well un-

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\(^6\)Executed on one core of an Intel Ivy Bridge-EP E5-2680 v2 using OpenBLAS for the BLAS kernels $dtrmm$ and $dtrsm$ and reference LAPACK for the unblocked $dtrti2$.

\(^7\)The ratio of floating point operations to memory operations.
Fig. 4: Recursive algorithm for the inversion of a lower triangular matrix.

3. RECURSIVE ALGORITHMS

Blocked algorithms can be translated into recursive algorithm by setting the block size to $n/2$ and replacing the calls to the unblocked kernels with recursive algorithm invocations. Building on the same example operation used so far, this section details how such recursive algorithms operate, and what factors influence their performance.

As shown in Fig. 4a, the recursive algorithm for this operation starts off by splitting both dimensions of the lower triangular $n \times n$ input matrix $A$ in half, exposing the quadrants $A_{TL}$, $A_{BL}$, and $A_{BR}$; the updates in Fig. 4b are then applied to the quadrants: Two BLAS Level 3 invocations surrounded by two recursive applications of the inversion algorithm to $A_{TL}$ and $A_{BR}$. In principle, one could continue the recursion.

For a given operation, once the traversal direction is fixed, all blocked variants results in the same recursive algorithm.

For alignment, we ensure that, where possible, the sizes of the sub-matrice are multiples of 8, allowing the two “halves” to be of slightly different sizes.

To increase performance by 5% to 15% (depending on the matrix size), one could first invert $A_{BR}$ and replace the linear system solve ($dtrsm$) by a more efficient matrix-matrix multiplication ($dtrmm$). Since this change makes the algorithm numerically unstable [Du Croz and Higham 1992], we do not include results.

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down to the scalar matrix entries, where the operation turns into a trivial $a := 1/a$; however, in order to minimize the number of tiny BLAS Level 3 invocations, we introduce the crossover size $c$: whenever $n < c$ the algorithm switches to LAPACK’s unblocked dtrti2.

In contrast to the block size $b$ of blocked algorithms, which requires careful tuning for high performance reasons, the choice of the crossover size $c$ is entirely straightforward. Indeed, as Fig. 5a suggests, as long as $c$ is kept small, the overall performance is only moderately affected; the reason becomes clear by inspecting the recursive algorithm: Changes in $c$ have no effect whatsoever on the large BLAS calls, whose size is solely determined by $n$. In fact, considering that the inversion of a triangular $n \times n$ matrix takes $\frac{n^3}{3}$ floating point operations (FLOPs), the two BLAS Level 3 calls in the top recursion level (dtrmm and dtrsm), which together cover $2 \left( \frac{n^2}{2} \right)^3$ FLOPs, account for

$$\frac{2 \left( \frac{n^2}{2} \right)^3}{\frac{n^3}{3}} = \frac{n^3}{n^3} = \frac{3}{4} = 75\%$$

of the algorithm’s entire FLOPs. This is visualized in Fig. 5b; assuming $c < 100$, out of the total FLOPs for the inversion, the dtrmm and dtrsm account for over 99.6%; 75% of the FLOPs are covered by the two calls on the first recursion level performing at about 86% efficiency; on the second level, 18.8% perform at 79%, on the third, 4.69% at 68%, and on the fourth, 1.17% at 57%. As a result, only < 0.4% of the FLOPs attain an efficiency below 57%.

This analysis confirms that a small crossover size does not harm the performance of the BLAS Level 3 kernels. Moreover, Fig. 5a provides evidence that choosing $c$ as small as 8 does not cause any performance penalty. A comparison of recursive algorithms with LAPACK’s unblocked kernels has shown that, the unblocked kernel is slightly faster than the recursive algorithm for small matrices within the processor’s L1 cache. Hence, for the remainder of this paper, we use $c = 24$.

\[\text{In [Gustavson 1997] it is referred to as a “blocking factor”}\]
3.1. Related Work
In a series of works [Frigo et al. 1999; Brodal 2004], recursive algorithms—coined as “cache-oblivious algorithms”—were proven to be optimal in the sense that they minimize data movement independently of cache sizes. Recursion as an alternative to LAPACK’s blocked algorithms has been proposed in several publications: Starting from the description of recursive versions of the Cholesky and LU decompositions in [Gustavson 1997], FORTRAN 90 implementations for these operations are developed in [Wasniewski et al. 1998] and [Georgiev and Wasniewski 2001], specialized recursive storage schemes are proposed by [Gustavson et al. 1998] and are applied to matrix decompositions in [Andersen et al. 2001a; Andersen et al. 2001b]. Recursion is applied to the QR decomposition in [Elmroth and Gustavson 2000] and triangular matrix inversion in [Karlsson 2006]. Finally, several Sylvester-type equation solvers are implemented with recursive algorithms in the RECSY library [Jonsson and Kågström 2003].

While many of these works describe their techniques in much detail, they each only consider one or a very limited set of operations—until now, no comprehensive implementation of recursive algorithms comparable to LAPACK’s range of blocked routines is available.

LAPACK’s most recent release (version 3.6.0) introduces a recursive version of the Cholesky factorization, named dpotrf2; this routine, which is fully recursive down to the scalar level is used in LAPACK’s blocked dpotrf as a replacement for the unblocked dpotf2.

4. PERFECTLY TUNED BLOCKED VS. RECURSIVE ALGORITHMS
In this section, we compare recursive and blocked algorithms in terms of performance. For the former, we chose a reasonable crossover size at $c = 24$, and kept it constant; for the latter, we undertook an extensive tuning process, for each problem size, timing all the algorithmic variants for all reasonable block sizes. While in practice such a process is clearly infeasible, we carried it out to establish a strict upper bound to the best possible performance achievable by blocked algorithms. The comparison was performed on a 10-core INTEL IVYBRIDGE E5-2680 V2 processor running at 2.8 GHz (Turbo Boost: 3.6 GHz), using OPENBLAS (version 0.2.15) [Xianyi 2015] for the BLAS kernels, and reference LAPACK (version 3.5) for the unblocked calls. A comparison against tuned LAPACK implementations is presented in Sec. 6.

Figure 6 reports the performance of the four unblocked algorithms and the recursive algorithm for the inversion of a triangular matrix. For single-threaded OPENBLAS, the recursive algorithm (—) is on par with or slightly more efficient than the best blocked algorithm (which changes from variant 1 (—) to variant 3 (—) around $n = 3000$); when using all 10 cores of the CPU, the recursive algorithm consistently outperforms all blocked algorithms. We stress that these results come at the cost of expensive tuning for the blocked algorithms, and with no optimization at all for the recursive ones. In comparison, reference LAPACK (—) with default block size $b = 64$ is with 1 and 10 cores, respectively, about 15% and 45% slower than the recursive algorithm.

Figure 7 presents results for the following operations:

— Multiplication of a triangular matrix with its transpose from the left $A := L^T L$ (LAPACK: dlaum),

— Cholesky decomposition of a symmetric positive definite matrix $L L^T := A$ (LAPACK: dpotrf), and
Fig. 6: Blocked algorithms (optimal $b$) vs. recursive algorithm ($c = 24$) for the inversion of a lower triangular matrix (LAPACK: \texttt{dtrtri}).

— LU decomposition of a square matrix with full pivoting $\begin{bmatrix} P \\ L \ U \end{bmatrix} := A$ (LAPACK: \texttt{dgetrf})

The results are consistent across the board: the unoptimized recursive algorithm is always comparable with (or faster than) the fastest blocked algorithm with a heavily optimized block size. We performed similar comparisons on INTEL SANDY BRIDGE and HASWELL processors, linking to both MKL and OPENBLAS; in all cases, the results are in line with those reported here.

5. RELAPACK

We have established that the tedious and time-consuming tuning process, which is indispensable to attain close-to-optimal performance with blocked algorithms, can be avoided for recursive algorithms without sacrificing performance. In this section, we present \textsc{Recursive LAPACK Collection (ReLAPACK)}, an open-source library of LAPACK operations implemented in a purely recursive fashion.\footnote{ReLAPACK is available on GitHub: \url{http://github.com/HPAC/ReLAPACK}.} All operations are available in the four standard data types ($x \in \{s, d, c, z\}$) and, since LAPACK’s interface is preserved, ReLAPACK can be employed effortlessly in existing codes. Below, we list the operations currently included in ReLAPACK:

— \texttt{xlaum}: Multiplication of a triangular matrix with its (complex conjugate) transpose, resulting in a symmetric (Hermitian) matrix; example: $\begin{bmatrix} \tilde{A} \\ L \ U \end{bmatrix} := A$

— \texttt{xsygst}: Simultaneous two-sided multiplication of a symmetric (Hermitian) matrix with a triangular matrix and its (complex conjugate) transpose example: $\begin{bmatrix} \tilde{A} \\ L \ U \end{bmatrix}$

\footnote{$x \in \{ssy, dsy, che, zhe\}$, i.e., the complex variants are called \texttt{chegst} and \texttt{zhegst}.}
This routines, which also cover the case where instead of $L$ its inverse $L^{-1}$ is applied, is used to reduce symmetric (Hermitian) positive definite generalized eigenvalue problems (e.g., $Ax = \lambda Bx$) to the standard form ($A\bar{x} = \lambda \bar{x}$), for instance in \texttt{zsygv}.

\textit{User Note:} ReLAPACK’s \texttt{zsygst} performs about 30\% fewer FLOPs than LAPACK’s blocked algorithm by internally using a temporary buffer of size $\frac{n}{2} \times \frac{n}{2}$. This algorithmic improvement over LAPACK, which is inspired by the blocked algorithms for this
operation in of the LIBFLAME library [Van Zee 2009], can optionally be disabled to avoid the memory overhead.

— _ztrtri_: Inversion of a triangular matrix; example: \( L := L^{-1} \). This routine serves as a building block in the inversions of general matrices \(_{zgetri}\), and symmetric positive definite matrices \(_{zpotri}\).

— _zpotrf_: Cholesky decomposition of a symmetric (Hermitian) positive definite matrix: \( LL^H := A \). This routine is the central building block for many operations on such matrices, for instance: inversion \(_{zpotri}\), solution of linear systems \(_{zposv}\), and reduction of generalized eigenvalue problems to standard form \(_{zsygv}\).

— _zsytrf_: \(^\text{14}\) LDL decomposition of a symmetric (or Hermitian) matrix; example: \( LL^H := A \). This routine is used with symmetric indefinite matrices for inversions \(_{zsytri}\), and solutions of linear systems \(_{zsysv}\).

User Note: In contrast to LAPACK’s _zsytrf_, which requires a temporary buffer of size \( n \times b \), RELAPACK requires a buffer of size \( T = n \times \frac{n}{2} \). Conforming to the signature of LAPACK, the works-space querying mechanism (via lwork = -1) reports the required size \( T \) and the buffer is expected as the work argument. However, to avoid conflicts when plugging RELAPACK into existing codes, should the passed auxiliary buffer be too small, _zsytrf_ allocates (and frees) such a buffer on its own.

Implementation Note: Since LAPACK’s interface for _zsytrf’s_ unblocked building block _zlaszf_ is not directly suitable for recursion, RELAPACK’s _zsytrf_ comes with two auxiliary routines: An unblocked kernel, that is a slight modification of LAPACK’s _zlaszf_ and, since BLAS does not support symmetric operations of the form \( C := C - A \). \( A^{1\text{H}} \), a recursive matrix-matrix multiplication kernel that computes only a triangular part of \( C := \alpha A B + \beta C \). Note that this recursive multiplication kernel is the only update in _zsytrf_ that uses a BLAS Level 3 kernel (_gemm_).

— _zsytrf_rook_: Alternative algorithm for the LDL decomposition using the bounded Bunch-Kaufman (“rook”) diagonal pivoting method.

— _zgetrf_: LU decomposition of a general matrix with pivoting: \( PLU := A \). Among others, _zgetrf_ is used with general matrices for inversions \(_{zgetri}\) and solutions of linear systems (e.g., _zgesv_).

— _ztrsvl_: Solution of the quasi-triangular\(^\text{15}\) Sylvester equation \( A X \pm X B = C \) for \( X \). This routine is used to reorder Schur factorizations and estimate the condition number of eigenvalue problems \(_{ztrsen}\) and arises on its own in systems and control theory.

Implementation Note: LAPACK’s _ztrsvl_ is in itself unblocked; hence, since RELAPACK replaces _ztrsvl_ with a recursive algorithm requiring an unblocked version of the routine, a duplicate of the original routine is introduced under the name _ztrsv2_. Furthermore, on each recursion level, the input matrix \( C \) is only split along its larger dimension, thus maximizing the overall size of the invoked BLAS Level 3 kernel _gemm_.

\(^{14}\)In complex arithmetic, there are routines for both symmetric (cstrf and zsytrf) and Hermitian matrices (chetrf and zhetrf).

\(^{15}\)\( A \) and \( B \) are in Schur canonical form and may contain \( 2 \times 2 \) diagonal blocks.
xtgsyl: Solution of the generalized Sylvester equations \( A R - L B = C \) and \( D R - L E = F \) for \( R \) and \( L \). It is also used to reorder Schur factorizations of matrix pairs and in condition number estimations (xtgsen).

Implementation Note: Just as xtrsyl, xtgsyl splits the input matrices \( C \) and \( F \) along their larger dimension, thus maximizing the size of the generated recursive sub-problems and calls to xgemm.

At compile time, ReLAPACK allows to set the recursive-to-unblocked crossover size \( c \) either globally or individually for each routine (default: \( c = 24 \)). Furthermore, each routine can be separately excluded from the generated library librelapack.a to allow for any mixing of ReLAPACK and other LAPACK implementations.

To benefit from the nearly optimal efficiency of BLAS Level 3 kernels, several operations are implemented in LAPACK as blocked algorithms at the cost of \( O(n^2b) \) extra FLOPs with respect to the unblocked algorithm. Translated to a recursive algorithm, this overhead increases to \( O(n^3) \) extra FLOPs, hence making recursion infeasible for large \( n \) [Elmroth and Gustavson 2000]. The following routines are affected.

- xgeqrf: QR decomposition
- xormr: Multiplication with an orthogonal matrix as returned by the QR decomposition; example: \( C := Q C \).
- xorgqr: Construction of the full orthogonal matrix \( Q \) from the format returned by the QR decomposition
- xsytrd: Reduction of a symmetric (Hermitian) matrix to tridiagonal form:

\[
Q \begin{bmatrix} T \end{bmatrix} Q^H = A.
\]

- zgehrd: Reduction of a matrix to upper Hessenberg form:

\[
Q \begin{bmatrix} H \end{bmatrix} Q^H = A.
\]

- zgebrd: Reduction of a matrix to bidiagonal form:

\[
Q \begin{bmatrix} B \end{bmatrix} P^H = A.
\]

Furthermore, recursion cannot be applied efficiently to operations on banded matrices, since the bandwidths limit the traversal block size. This applies to

- xpbrtf: Banded Cholesky decomposition; example: \( L \begin{bmatrix} L^H \end{bmatrix} = A \), and
- xgbtrf: Banded LU decomposition: \( L \begin{bmatrix} U \end{bmatrix} = A \).

To the best of our knowledge, only one LAPACK operation to which recursion might be applicable is yet not covered in ReLAPACK:

- xpgstrf: Cholesky decomposition of a symmetric (Hermetian) semi-definite matrix with complete pivoting:

\[
\begin{bmatrix} P \end{bmatrix} \begin{bmatrix} L \end{bmatrix} \begin{bmatrix} L^H \end{bmatrix} \begin{bmatrix} P^H \end{bmatrix} = A.
\]

xpstrf is uses a pivoting representation different from those found in other routines such as xpgstrf and is thus incompatibl with other LAPACK operations and in fact not used anywhere throught the library.

\[16\text{The same applies to the related decompositions } RQ (xgerqt), QL (zgeqlt), LQ (zgelqt), \text{ and } RZ (ztrzrf).\]
\[17\text{xor } \in \{\text{sor, dor, cun, zun}\}, \text{ i.e., the complex routines are cunmrq and zunmrq.}\]
\[18\text{Applies respectively to the related decompositions: } RQ (zormrq), QL (zormql), LQ (zormlq), \text{ and } RZ (zormrz).\]
\[19\text{Applies respectively to the related decompositions: } RQ (zorgqr), QL (zorgql), \text{ and } LQ (zorglq).\]
To summarize, with the exception of \texttt{pstrf}, RELAPACK covers all of LAPACK’s compute routines to which recursion is applicable and promising to yield performance benefits. Due to LAPACK’s layered design, the performance benefits of these recursive routines extend to many other operations.

6. RELAPACK VS. OPTIMIZED LIBRARIES

While in Sec. 4, we compared recursive algorithms with blocked algorithms using the unblocked kernels from the reference LAPACK implementation, we conclude this study with a performance comparison between RELAPACK and two optimized LAPACK implementations. We start with a comparison of all of RELAPACK’s operations in all four data types against INTEL MKL. (Note that RELAPACK’s routines are also linked to MKL, and therefore may also benefit from optimizations of the unblocked LAPACK kernels.) We present the speedup of the RELAPACK routines over the corresponding MKL routines computed as follows:

$$\text{speedup} = \frac{\text{time(MKL)}}{\text{time(RELAPACK)}}$$

Fig. 8 presents such speedups on an INTEL HASWELL-EP E5-2680 v3 using only 1 core (left) and all of its 12 cores (right).

First off, we notice that for all data types and both in the single- and multi-threaded scenario, RELAPACK’s Sylvester solvers \texttt{ztrsyl} and \texttt{zgtsy1} (Fig. 8g and h) clearly outperform MKL’s routines: On average, the speedup for \texttt{ztrsyl} on 1 and 12 cores is, respectively, 40 and 100; for \texttt{gtsy1}, it is around 9 on 1 core, while on 12 cores, it ranges from from 6.7 (for double real) to 17 (for double complex). The numbers suggest that in MKL these routines are not optimized and are substantially equivalent to the unblocked LAPACK reference implementation.

Focusing on the single-threaded case, with only very few exceptions, the average speedup is 1.0940, i.e., using RELAPACK on top of MKL pays off, yielding a performance improvement of 9.40%: it appears that only the LDL decomposition \texttt{zsytrf} (Fig. 8e) for small matrices is slower than MKL.

With 12 threads the scenario is different; across the board the speedups are less uniform, ranging from 0.5 to above 1.5, and are considerably prone to fluctuations. For \texttt{zlaum}, \texttt{zygst} (with the exception of large matrices for double real and single complex), and \texttt{ztrtri} (Fig. 8a, b, and c), RELAPACK is overall faster than MKL, averaging a speedup of 30.53%. For \texttt{potrf} and, with large matrices (beyond \(n = 2500\)) in single precision and \(n = 4250\) in double precision, \texttt{getrf} (Fig. 8d and f), RELAPACK is clearly slower than MKL, since the latter employs alternative algorithmic schemes such as algorithms-by-blocks; these schemes are specially tailored for multi-core architectures and INTEL has put considerable effort into optimizing them. Finally, the main cause for RELAPACK’s poor multi-threaded performance for \texttt{zsytrf} (Fig. 8e) is its recursive matrix multiplication routine (see Sec. 5, \texttt{zsytrf}), which cannot match the parallelism of an optimized version close to \texttt{zgemm} likely used by MKL.

To summarize, with the exception of \texttt{potrf}, \texttt{zsytrf}, and (for large matrices) \texttt{getrf}, which are easily excluded at compile time, even when working with a highly-optimized library such as MKL, it pays off to employ RELAPACK.

This conclusion is reinforced by further experiments on different hardware/software setups: Fig. 9 presents speedups for OPENBLAS and MKL on both the HASWELL and IVYBRIDGE processors. To condense the information in this analysis, the speedup was sampled between \(n = 24\) and 6168 in steps of 128, and then averaged. While for MKL

\footnote{For all operations, we use the following flag arguments (where applicable): \texttt{uplo = L}, \texttt{trans = tranA = tranB = diag = N}, and \texttt{itype = ijob = isgn = 1}.}
| Function          | 1 thread | 12 threads |
|-------------------|----------|------------|
| Slauum            |          |            |
| Dlaum             |          |            |
| Clauum            |          |            |
| Zlaauum           |          |            |
| Ssygst            |          |            |
| Dsygst            |          |            |
| Chegst            |          |            |
| Zhegst            |          |            |
| Strtri            |          |            |
| Dtrtri            |          |            |
| Ctrtri            |          |            |
| Ztrtri            |          |            |
| Spotrf            |          |            |
| Dpotrf            |          |            |
| Cpotrf            |          |            |
| Zpotrf            |          |            |
| Ssytrf            |          |            |
| Dsytrf            |          |            |
| Chetrif           |          |            |
| Zheif             |          |            |
| Sgetrf            |          |            |
| Dgetrf            |          |            |
| Cgetrf            |          |            |
| Zgetrf            |          |            |
| Strysl            |          |            |
| Dtrysl            |          |            |
| Ctrysl            |          |            |
| Ztrysl            |          |            |
| Strysl            |          |            |
| Dtrysl            |          |            |
| Ctrysl            |          |            |
| Ztrysl            |          |            |
| Stgysl            |          |            |
| Dtgysl            |          |            |
| Ctgysl            |          |            |
| Ztgysl            |          |            |

Fig. 8: Speedup of RELAPACK over MKL on a HASWELL processor.
\( x \) (data type): \( s \) (single) \( d \) (double) \( c \) (complex) \( z \) (double complex)

Fig. 9: RELAPACK speedup averaged over matrices of size up to 6000.
Annotations for \( \text{ztrsy}l \) and \( \text{ztgsy}l \): rounded speedup \( \geq 2 \)
we observe the exact same behavior on the IVYBRIDGE (Fig. 9a) as previously on the HASWELL (Fig. 8). The speedups for OPENBLAS are slightly different, yet still predominantly larger than 1; while for the Sylvester solvers the average speedup is 11.88, for the other routines it is 8.89 %.

7. CONCLUSIONS
In this paper, we studied the performance and tuning options of both blocked and recursive algorithms for dense linear algebra operations; we showed that blocked algorithms require careful and expensive tuning to reach optimal performance, while recursive algorithms attain equivalent or better performance with virtually no tuning effort. Motivated by this observation, and in light of the surprising lack of a library providing such recursive algorithms, we developed ReLAPACK. This library offers a collection of recursive algorithms for many of LAPACK’s compute kernels. Since it preserves LAPACK’s established interfaces, it integrates effortlessly into existing LAPACK-based application codes. ReLAPACK’s routines were shown not only to outperform LAPACK but also to improve upon the performance of tuned implementations from OpenBLAS and MKL.

Software
ReLAPACK is open source (MIT license) and available on GitHub:
http://github.com/HPAC/ReLAPACK

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