HIGH-PERFORMANCE SOLVERS FOR DENSE HERMITIAN EIGENPROBLEMS*

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Abstract.
We introduce a new collection of solvers – subsequently called EleMRRR – for large-scale dense Hermitian eigenproblems. EleMRRR solves various types of problems: generalized, standard, and tridiagonal eigenproblems. Among these, the last is of particular importance as it is a solver on its own right, as well as the computational kernel for the first two; we present a fast and scalable tridiagonal solver based on the algorithm of Multiple Relatively Robust Representations – referred to as PMRRR. Like the other EleMRRR solvers, PMRRR is part of the freely available Elemental library, and is designed to fully support both message-passing (MPI) and multithreading parallelism (SMP). As a result, the solvers are equally effective in message-passing environments with and without SMP parallelism. We conducted a thorough performance study of EleMRRR and ScaLAPACK’s solvers on two supercomputers. Such a study, performed with up to 8,192 cores, provides precise guidelines to assemble the fastest solver within the ScaLAPACK framework; it also indicates that EleMRRR outperforms even the fastest solvers built from ScaLAPACK’s components.

Key words. generalized eigenproblem, eigenvalue, eigenvector, hermitian, symmetric, tridiagonal, parallel algorithms

AMS subject classifications. 65F15, 65Y05, 68W10

1. Introduction. In this section we briefly state the considered eigenproblems, give a short description of our high-level approach, and list the main contributions of this paper.

1.1. The Problem. A generalized Hermitian eigenproblem (GHEP) is identified by the equation

\[ Ax = \lambda B x, \]  

where \( A, B \in \mathbb{C}^{n \times n} \) are known matrices; the sought after scalars \( \lambda \) and associated vectors \( x \in \mathbb{C}^n, x \neq 0 \), are called eigenvalues and eigenvectors, respectively. We say that \( (\lambda, x) \) is an eigenpair of the pencil \( (A, B) \). In the following, we make the additional assumption that either \( A \) or \( B \) is positive or negative definite, which implies that all the eigenvalues are real. Without loss of generality, we assume that \( B \) is positive definite. Thus, when referring to the GHEP of Eq. (1.1), the restriction to Hermitian-definite pencils \( (A, B) \) is subsequently implied. If \( B \) is the identity matrix \( I \), Eq. (1.1) reduces to the standard Hermitian eigenproblem (HEP) \( Ax = \lambda x \); if \( A \) is also real and tridiagonal, the problem is referred to as a symmetric tridiagonal eigenproblem (STEP).

Different numerical methods were devised to solve instances of the GHEP, HEP, and STEP in accordance to the amount of eigenpairs requested and additional properties of the involved matrices (e.g., sparsity). In this paper, we concentrate on the efficient solution of dense generalized eigenproblems on modern distributed-memory

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‡That is \( A = A^* \) and \( B = B^* \). If both Hermitian matrices \( A \) and \( B \) are real valued, then the following discussion also holds with the words 'Hermitian' and 'unitary' respectively replaced by 'symmetric' and 'orthogonal'.

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platforms composed of shared-memory multiprocessor nodes; as a by-product, we also obtain results for standard and tridiagonal problems.

1.2. Three Nested Eigensolvers. Common methods to the dense generalized eigenproblems make use of the following fact: given non-singular matrices \( G \) and \( F \), the eigenvalues of the pencil \((A, B)\) are invariant under the equivalence transformation \((GAF, GBF)\); furthermore, \( x \) is an eigenvector of \((A, B)\) if and only if \( F^{-1}x \) is an eigenvector of \((GAF, GBF)\) \[34\].

The most versatile tool for the generalized eigenproblem, the QZ algorithm \[33\], uses a sequence of unitary equivalence transformations to reduce the original pencil to generalized (real) Schur form. By design, the QZ algorithm is numerically backward stable and imposes no restrictions on the input matrices; unfortunately, the algorithm does not respect the symmetry of the Hermitian pencil \((A, B)\) and is computationally rather costly.

To preserve the symmetry of the problem while reducing the pencil \((A, B)\) to simpler form, methods are limited to sequences of congruence transformations – that is, using \( G = F^* \), where \( G \) and \( F \) are no longer required to be unitary. The traditional approach for computing all or a significant fraction of the eigenpairs of \((A, B)\) relies on a reduction-backtransformation procedure, corresponding to three nested eigensolvers: generalized, standard, and tridiagonal. Since \( B \) is positive definite, the Cholesky factor can be used to transform the GHEP to a HEP \[32\], which in turn is reduced to a STEP; once the eigenvectors of the STEP are computed, they are mapped back to those of the original problem via two successive backtransformations. Overall, the process for solving a generalized eigenproblem – also known as the Cholesky-Wilkinson method – consists of six stages:

1. **Cholesky factorization:** \( B \) is factored into \( LL^* \), where \( L \) is lower triangular.
2. **Reduction to standard form:** From \( B = LL^* \), the original pencil \((A, B)\) is transformed to \((L^{-1}AL^{-*}, I)\) and Eq. \((1.1)\) takes the form of a standard Hermitian eigenproblem \( My = \lambda y \). The eigenvectors \( x \) of the GHEP and the eigenvectors of the HEP are related by \( y = L^*x \).
3. **Reduction to tridiagonal form:** A unitary matrix \( Q \) is computed such that \( T = Q^*MQ \) is real symmetric tridiagonal. The pencil \((M, I)\) is transformed to \((Q^*MQ, I)\), corresponding to the tridiagonal eigenproblem \( Tz = \lambda z \), where \( z = Q^*y \).
4. **Solution of the tridiagonal eigenproblem:** A set of eigenpairs \((\lambda, z)\) is computed such that \( Tz = \lambda z \); the existence of \( n \) such eigenpairs \((\lambda, z)\) for which the set of eigenvectors forms an orthonormal basis for \( \mathbb{C}^n \) is ensured by the Spectral Theorem \[34\].
5. **First backtransformation:** In accordance to Stage 3, the eigenvectors of the standard eigenproblem are obtained by computing \( y = Qz \).
6. **Second backtransformation:** In accordance to Stage 2, the eigenvectors of the original pencil are obtained by computing \( x = L^{-*}y \).

The above discussion shows that when the \( k \) computed eigenvalues are the entries of a diagonal matrix \( \Lambda \in \mathbb{R}^{k \times k} \), and the associated eigenvectors are the columns of a matrix \( X \in \mathbb{C}^{n \times k} \), then \( X^*AX = \Lambda \), \( X^*BX = I \), and \( AX = BXA \).

With slight modifications of Stages 2 and 6, the same six-stage procedure also applies to eigenproblems in the form \( ABx = \lambda x \) and \( BAx = \lambda x \). In the first case, the reduction and the backtransformation become \( M = L^*AL \) and \( x = L^{-*}y \), respectively; in the second case, they become \( M = L^*AL \) and \( x = Ly \).

The six-stage procedure should only be used if \( B \) is sufficiently well-conditioned.
with respect to inversion. For a detailed discussion of the properties of the GHEP, especially regarding perturbation theory and the problems arising for ill-conditioned $B$, we refer to the standard literature, including [11] [19] [34] [45].

1.3. The Impact and Contributions of this Paper. The solution of the aforementioned types of large-scale eigenproblems is integral to a number of scientific disciplines, particularly vibration analysis [4] and quantum chemistry [22] [37] [24] [46]. An example of an application where the solution of the eigenproblem is the most time consuming operation is Density Functional Theory [26, 46, 48]. There, as part of a simulation, one has to solve a set of equations in a self-consistent fashion; this is accomplished by an iterative process in which each iteration involves the solution of dozens or even hundreds of generalized eigenproblems. In many cases, the application requires 5-25% of the eigenpairs associated with the smallest eigenvalues, and the size of such problems is usually in the tens of thousands of degrees of freedom. In other applications, in which the simulations do not follow an iterative process, it is instead common to encounter only one single eigenproblem - potentially of very large size (50k–100k or more) [24] [29]. In both scenarios, the problem size is not limited by the physics of the problem, but only by memory requirements and time-to-solution.

When the execution time and/or the memory requirement of a simulation become limiting factors, scientists place their hopes on massively parallel supercomputers. With respect to execution time, the use of more processors would ideally result in faster solutions. When memory is the limiting factor, additional resources from large distributed-memory environments should enable the solution of larger problems. We study the performance of eigensolvers for both situations: increasing the number of processors while keeping the problem size constant (strong scaling), and increasing the number of processors while keeping the memory per node constant (weak scaling).

In this paper we make the following contributions:

- Given the nested nature of the generalized, standard and tridiagonal eigen-solvers, the last is both a solver in its own right and the computational kernel for the HEP and the GHEP. We present a novel tridiagonal solver, PMRRR, based on the algorithm of Multiple Relatively Robust Representations (MRRR) [13] [14], which merges the distributed and multithreaded approaches first introduced in [5] and [35]. PMRRR is well suited for both single node and large scale massively parallel computations. Experimental results indicate that PMRRR is currently the fastest tridiagonal solver available, outperforming all the solvers included in LAPACK [2], ScaLAPACK [7] and Intel’s Math Kernel Library (MKL).

- We introduce EleMRRR (from Elemental and PMRRR), a set of distributed-memory eigensolvers for generalized and standard Hermitian eigenproblems. EleMRRR provides full support for hybrid message-passing and multithreading parallelism. If multithreading is not desired, EleMRRR can be used in purely message-passing mode.

- The five stages of reduction and backtransformation in EleMRRR are based on Elemental, a library for the development of distributed-memory dense linear algebra routines [39]. Elemental embraces a two-dimensional cyclic element-wise matrix distribution, and attains performance comparable or even superior to the well established ScaLAPACK, PeiGS and PLAPACK parallel libraries [7, 7, 49]. For the reduction to standard form, an algorithm-

\[ \text{PMRRR should not be confused with the distributed-memory solver introduced in [5].} \]
A thorough performance study on two high-end computing platforms is provided. This study accomplishes two objectives. On the one hand it contributes guidelines on how to build – within the ScaLAPACK framework – an eigensolver faster than the existing ones. This is of particular interest to computational scientists and engineers as each of the commonly used routines (PZHEGVX, PDSYGVX, PZHEEVD, PDSYEVD) present performance penalties that can be avoided by calling a different sequence of subroutines and choosing suitable settings. On the other hand, the study indicates that EleMRRR is scalable – both strongly and weakly – to a large number of processors, and outperforms the standard ScaLAPACK solvers.

The paper is organized as follows: In Section 2 we discuss related work and give experimental evidence that some widely used routines fail to deliver the desired performance. In Section 3 we concentrate on EleMRRR, with emphasis on the tridiagonal stage – PMRRR. We present a thorough performance study on two state-of-the-art high-performance computer systems in Section 4. We show that ScaLAPACK contains a set of fast routines that can be combined to avoid the aforementioned performance problems, and we compare the resulting routines to our solver EleMRRR. We summarize our findings in Section 5.

2. A Study of Existing Solvers. In this section we give a brief overview of existing methods and study well-known issues of widely used routines available in the current version 4 of the ScaLAPACK library. We discuss the generalized, standard and symmetric tridiagonal eigenproblems in succession.

2.1. The Generalized Eigenproblem. In some cases, even if $A$ and $B$ do not satisfy the assumptions of Section 1.1 the problem can still be transformed into one that exhibits the desired properties [11]. In general, if $A$ and $B$ are dense but non-Hermitian or if $B$ has poor conditioning with respect to inversion [5] instead of the aforementioned six-stage approach, the QZ algorithm can be used. A parallel distributed-memory implementation is discussed in [1].

The ScaLAPACK library contains routines for the three classes of eigenproblems we consider in this paper. A complete list of routine names for both the solvers and the individual stages is given in Table 2.1. In particular, PZHEGVX and PDSYGVX are ScaLAPACK’s double precision drivers for complex Hermitian and real symmetric generalized eigenproblems, respectively.

In Fig. 2.1 we report the weak scalability of PZHEGVX for computing 15% of the eigenpairs of $Ax = \lambda Bx$ associated with the smallest eigenvalues [6]. The left graph indicates that, as the problem size and the number of processors increase, PZHEGVX does not scale as well as the EleMRRR solver presented in Section 3. In the right
graph we show the breakdown of the execution time for each of the six stages.

Independently of the input data, all the considered solvers perform a similar number of floating point operations in each of the Stages 1, 2, 3, 5, and 6; on the contrary, the complexity of Stage 4 depends on the input data, and varies from one method to another. With the exception of this stage, a comparison purely based on operation counts would be misleading; differences in execution time are mainly due to different use of the memory hierarchy and exploitation of parallelism. Throughout the paper, we rely on the execution time as the performance metric.

In Fig. 2.1, it is evident that the routines PDSTEBZ and PZSTEIN, which implement the Bisection and Inverse Iteration (BI) tridiagonal eigensolver, are the main cause for the poor performance of PZHEGVX. For the problem of size 20,000, these routines are responsible for almost 90% of the compute time. BI’s poor performance is a well understood phenomenon, e.g. [8], directly related to the effort necessary to re-orthogonalize eigenvectors corresponding to clustered eigenvalues. This issue led to the development of an improved version of Inverse Iteration, the MRRR algorithm, that avoids re-orthogonalization even when the eigenvalues are clustered. In addition to the performance issue, PZHEGVX also suffers from memory imbalances, as all the eigenvalues belonging to a cluster are computed on a single processor.

**Guideline 1.** In light of the above considerations, the use of ScaLAPACK’s routines based on Bisection and Inverse Iteration (BI) is not recommended.

We do not provide further comparisons between EleMRRR and PZHEGVX or PDSYGVX. Instead, in Section 4 we illustrate how the performance of these drivers changes when the BI algorithm for the tridiagonal eigensolver is replaced with other – faster – methods available in ScaLAPACK, namely the Divide and Conquer algorithm (DC) and the MRRR algorithm [47, 50].

### 2.2. The Standard Eigenproblem.

We restrict the discussion to dense Hermitian problems. Such problems arise in a variety of applications, ranging from electrodynamics to macro-economics [41]; they are also often solved as part of a GHEP, as discussed in Section 4.
Fig. 2.1. Weak scalability for the computation of 15% of the eigenpairs associated with the smallest eigenvalues. As done commonly in practice [46], the eigenvectors are requested to be numerically orthogonal. Left: Total execution time of PZHEGVX and EleMRRR. Right: Fraction of the execution time spent in the six stages of PZHEGVX, from bottom to top (see Table 2.1).

The standard approach to solve a standard eigenproblem consists of three stages, corresponding to Stages 3–5 in the solution of the generalized problem: (a) Reduction to a real symmetric tridiagonal form; (b) Solution of the tridiagonal eigenproblem; (c) Backtransformation of the eigenvectors. A detailed analysis of the three-stage approach, concentrating on the first and third stage, can be found in [44].

An alternative approach is Successive Band Reduction (SBR) [6]. The idea is to split the reduction to tridiagonal form in two (or more) stages. In all but the last stage, the matrix is reduced to banded form with strictly decreasing bandwidths. Unlike the direct reduction to tridiagonal form, these stages can take full advantage of highly efficient kernels from the Basic Linear Algebra Subprograms (BLAS) library [17], thus attaining high-performance. The reduction is then completed with a final band-to-tridiagonal reduction. The downside of such a strategy lies in the accumulation of the orthogonal transforms. Thus, when a significant portion of the eigenvectors is requested, the SBR routines are not competitive. For this reason, SBR is normally used for computing only the eigenvalues or a small fraction of the eigenvectors. However, a recent publication suggests that, on highly parallel systems, SBR might be faster than direct reduction to tridiagonal form even when a significant fraction of eigenvectors is computed [3].

ScaLAPACK offers a number of routines for the standard Hermitian eigenproblem, each of which differs in its algorithm of choice for the tridiagonal eigenvalue problem. The four routines PZHEEVX, PZHEEV, PZHEEVD, and the recently added PZHEEVR, implement BI [51], the QR algorithm [28, 18], the DC algorithm [9, 20], and the MRRR algorithm [14], respectively.

Among the solvers presently available in ScaLAPACK, only PZHEEVX (BI) and PZHEEVR (MRRR) offer the possibility of computing a subset of eigenpairs. PZHEEVX is widely used, even though, as highlighted in the previous section, it is highly non-scalable. Similarly, if eigenvectors are computed, the QR algorithm is known to be slower than DC for large problems [5] and thus the use of ScaLAPACK’s routines

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7 Each of these routines has the usual counterpart for the real symmetric case: PDSYEVX, PDSYEV, PDSYEVD, and PDSYEVR.
based on QR is not recommended; in the future experiments, we omit comparisons with routines that are based on the QR algorithm or BI.

We now focus on the weak scalability of the widely used routine, PZHEEVD, which uses DC for the tridiagonal eigenproblem. In Fig. 2.2 we show the results for PZHEEVD and EleMRRR from an experiment similar to that of Fig. 2.1. Note that all eigenpairs were computed, since PZHEEVD does not allow for subset computation. In the previous section, the example indicated that BI might dominate the runtime of the entire dense eigenproblem, while the DC method required less than 10% of the total execution time. Instead, as the matrix size increases, the reduction to tridiagonal form (PZHETRD) becomes the computational bottleneck, requiring up to 70% of the total time for the largest problem shown. A comparison of the left and right sides of Fig. 2.2 reveals that, for large problems, using PZHETRD for the reduction to tridiagonal form requires more time than the complete solution with EleMRRR.

ScaLAPACK also includes PZHENTRD, a routine for the reduction to STEP especially optimized for square processor grids. The performance improvement with respect to PZHETRD can be so dramatic that, for this stage, it is preferable to limit the computation to a square number of processors and redistribute the matrix accordingly. It is important to note that the performance benefit of PZHENTRD can only be exploited if the lower triangle of the input matrix is stored, otherwise the slower routine, PZHETRD, is invoked.

![Fig. 2.2. Weak scalability for the computation of all eigenpairs using DC. Left: Total execution time of PZHEEVD and EleMRRR. Right: Execution time for ScaLAPACK’s routines PZHETRD and PZHENTRD, which are responsible for the reduction to tridiagonal form. The former, used within the routine PZHEEVD, causes a performance penalty and accounts for much of the time difference compared with EleMRRR.](image)

**Guideline 2.** ScaLAPACK’s reduction routines (PxxxNGST and PxxxNTRD) optimized for square grids of processors are to be preferred over the regular reduction routines, even when non-square process grids are used; moreover, only the lower triangle of implicitly Hermitian matrices should be referenced.

For performance and scalability reasons, in Section 4 we use the routines PxxxNTRD and PxxxNGST to build the fastest solver within the ScaLAPACK framework.

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8Similar considerations also apply for the reduction to standard form via the routines PZHEGST and PZHENGST, see [40].
2.3. The Tridiagonal Eigenproblem. At the core of the reduction-backtransformation approach for the GHEP and the HEP is the symmetric tridiagonal eigenproblem. One of the main differences – and often the only difference – among solvers for generalized and standard problems lies in the method for this stage. As seen in Section 2.1, this might account for a significant computational portion of the entire solution process. In Section 2.2, we mentioned four methods: BI, QR, DC, and MRRR, and justified not providing experimental comparisons with the BI and QR approaches.

As already mentioned, in contrast to all other stages of generalized and standard problems, the number of arithmetic operations of the tridiagonal eigensolver depends on the input data. In fact, depending on the matrix entries, either DC or MRRR may be faster. Fig. 2.3 provides an example of how performance is influenced by the input data. The algorithms are compared on two types of test matrices: “1–2–1” and “Wilkinson”. The former contains ones on the subdiagonals and twos on the diagonal; its eigenpairs are known analytically. In the latter, the subdiagonals contain ones and the diagonal equals the vector \((m, m-1, \ldots, 1, 0, 1, \ldots, m)\), with \(m = (n-1)/2\). Due to the phenomenon of deflation, this matrix is known to favor the DC algorithm \[9\].

We also include timings for our solver, PMRRR; for both matrix types it eventually becomes the fastest solver. A detailed discussion of PMRRR follows in the next section.

![Weak scalability for the computation of all eigenpairs of two different test matrix types. The left and right graphs have different scales. Left: “1–2–1” matrix; Right: “Wilkinson” matrix. In contrast to the results reported in \[50\], where a similar experiment comparing PDSTEDC and PDSTEGR is performed, even when the matrices offer an opportunity for heavy deflation, our PMRRR becomes faster than DC eventually due to its superior scalability. The scalability advantage of PMRRR compared with PDSTEGR is the result of non-blocking communications used in conjunction with a task-based algorithmic design that allows processes to continue computing while waiting for data. As an example, in the Wilkinson experiment with 1024 cores, ScaLAPACK’s MRRR spends about 30 out of 50 seconds in exposed communication.](image)

We now provide a short comparison of PMRRR with ScaLAPACK’s routines PDSTEDC and PDSTEGR, which implement the tridiagonal DC and MRRR algorithms\[9\], respectively \[47, 50\].

In the worst case, PDSTEDC computes all eigenpairs at the cost of \(O(n^3)\) floating

\[\text{PMRRR} \text{ is not part of ScaLAPACK; it corresponds to the tridiagonal eigensolver used in PxxxEVR and is not encapsulated in its own routine.}\]
point operations (flops); in practice, the flop count is lower due to deflation and the run time behavior is empirically $n^{2.5}$ [12] [17]. Furthermore, most of the computation is cast in terms of fast BLAS-3 kernels [12].

While PDSTEDC cannot compute a subset of $k < n$ eigenpairs, the MRRR routine PDSTEGR returns the eigenpairs at the reduced cost of $O(nk)$ flops.

**GUIDELINE 3.** Both of ScALAPACK’s tridiagonal eigensolver routines, PDSTEDC (DC) and PDSTEGR (MRRR), are generally fast and reasonably scalable; depending on the target architecture and specific requirements from the applications, either one may be used. Specifically, if only a small subset of the spectrum has to be computed, in terms of performance, the MRRR-based solvers are to be preferred to DC.

In terms of accuracy, all tridiagonal solvers generally obtain accurate results in the sense that they achieve small residual norms and numerical orthogonality. Specifically, with machine precision $\varepsilon$,

$$\|T\hat{z}_j - \hat{\lambda}_j \hat{z}_j\| = O(n\varepsilon\|T\|), \quad \text{and}$$

$$|\hat{z}_j^T \hat{z}_i| = O(n\varepsilon), \quad i \neq j,$$

for all computed eigenpairs $(\hat{\lambda}_j, \hat{z}_j)$ with $\|\hat{z}_j\|_2 \approx 1$. It is well-known that MRRR yields slightly worse coefficients for Eq. (2.2) than QR and DC [12]. In the rare cases where this is an issue, feasible alternatives are the DC algorithm and a mixed precision variant of MRRR [?]. On the downside, DC requires $O(n^2)$ extra memory; see [12, 5, 50, ?] for further comparisons.

In Section 4, we include experimental data on generalized eigenproblems for both DC and MRRR. One of the challenges in building a scalable solver is that every stage must be scalable. This is illustrated in Fig. 2.4, which shows the results for ScALAPACK’s DC from the experiment detailed in Section 4.1.1. While the reduction to tridiagonal form and the tridiagonal eigensolver are respectively the most and the least expensive stages on 64 cores, on 2048 cores the situation is reversed. This behavior is explained by the parallel efficiencies shown in the right panel of Fig. 2.4.

![Fig. 2.4. Scalability of the computation of all eigenpairs using ScALAPACK’s DC. The details of the experiment are discussed in Section 4.1.1.](image)

**3. Elemental’s Generalized and Standard Eigensolvers.** Elemental is a framework for dense matrix computations on distributed-memory architectures [39]. The main objective of the project is to ease the process of implementing matrix
operations without conceding performance or scalability. The code resembles a high-level description of the algorithm, and the details relative to data distribution and communication are hidden. Performance is achieved through a two-dimensional cyclic elemental (entry-wise) matrix distribution.\footnote{ScaLAPACK instead deploys a block-cyclic matrix distribution.}

Elemental supports many frequently encountered dense matrix operations; these include the Cholesky, QR and LU factorizations, as well as the solution of linear systems. Recently, routines for Hermitian and symmetric eigenvalue problems have also been added. In particular, Elemental supports Hermitian-definite generalized, standard Hermitian, as well as skew-Hermitian eigenproblems. All the eigensolvers follow the classical reduction and backtransformation approach described in Section[1].

Detailed discussions the reduction and backtransformation stages, both in general and within the Elemental environment, can be found in [44, 42, 23, 40].

In terms of accuracy, Elemental’s solvers are equivalent to their sequential counterparts. We therefore do not report accuracy results and refer to [12] instead.

In terms of memory, Elemental’s solvers are quite efficient. In Table 3.1 we report approximate total memory requirements for computing \( k \) eigenpairs of generalized and standard eigenproblems. As a reference, we provide the same numbers for the solvers built from ScaLAPACK routines. In Section 4 we define the meaning of “ScaLAPACK DC” and “ScaLAPACK MRRR” precisely. The numbers in the table are expressed in units of the size of a single complex and real floating point number, depending on the required arithmetic. The memory requirement per process can be obtained by dividing by the total number of processes.

| Complex | Real |
|---------|------|
| GHEP    | HEP  | GHEP    | HEP |
| ScaLAPACK DC | \( 4n^2 \) | \( 3n^2 \) | \( 5n^2 \) | \( 4n^2 \) |
| ScaLAPACK MRRR | \( 2n^2 + 1.5nk \) | \( n^2 + 1.5nk \) | \( 2n^2 + 2nk \) | \( n^2 + 2nk \) |
| Elemental | \( 2n^2 + nk \) | \( n^2 + nk \) | \( 2n^2 + nk \) | \( n^2 + nk \) |

Table 3.1: Approximate total memory requirements in units of complex and real floating point numbers for the computation of \( k \) eigenpairs. We assume that square process grids are used, as it is recommended for optimal performance and if memory usage is a concern. The numbers also hold when a non-square grid of processes is used in combination with the standard reduction routines.

For square process grids, Elemental requires between 0.5\( n^2 \) to 2\( n^2 \) floating point numbers less memory than ScaLAPACK based solvers. If non-square grids are used, a user concerned about memory usage can make use of the non-square reduction routes – at the cost of sub-optimal performance. The reduction routines for square process grids would otherwise need a data redistribution that adds a \( n^2 \) term to Elemental and ScaLAPACK MRRR, but not to DC. On the other hand, in this situation, ScaLAPACK MRRR can save work space to perform its redistribution of the eigenvectors from a 1d to a 2d block-cyclic data layout, reducing its terms by \( nk \) real floating point numbers. This eigenvector redistribution is performed in Elemental in-place, resulting in a smaller memory footprint than possible for ScaLAPACK’s routines.

For the solution of symmetric tridiagonal eigenproblems, Elemental incorporates PMRRR, a new parallel variant of the MRRR algorithm. PMRRR combines two
solvers: one based on message-passing parallelism [5, 50], and another based on multithreading [38]. As a consequence, the solver provides the user with multiple parallel programming models (multithreading, message-passing, a hybrid of both), so that the parallelism offered by modern distributed-memory architectures can be fully exploited. In the following two subsections we focus the attention on PMRRR, our tridiagonal eigensolver.

3.1. PMRRR as the Core of Elemental’s Eigensolver. The MRRR algorithm is a form of inverse iteration. Its salient feature is that the costly re-orthogonalization, necessary when the eigenvalues are clustered together, is entirely removed. As the experiment described in Fig. 2.1 shows, the re-orthogonalization may affect the execution time dramatically: in computing 15% of the eigenpairs associated with the smallest eigenvalues of a matrix of size 20,000 using 512 cores, ScaLAPACK’s Inverse Iteration takes about 404 seconds, while PMRRR requires less than 0.3 seconds.

To achieve this performance, the classical inverse iteration was modified significantly. The basic procedure requires the repeated solution of linear systems: given an approximate eigenvalue \( \hat{\lambda}_j \) and a starting vector \( \hat{z}^{(0)}_j \), under mild assumptions

\[
(T - \hat{\lambda}_j I)\hat{z}^{(i+1)}_j = s^{(i)} \hat{z}^{(i)}_j,
\]

with appropriate scaling factors \( s^{(i)} \), results in an eigenvector approximation \( \hat{z}^{(i)}_j \) that fulfills Eq. (2.1). Nevertheless, small residual norms do not guarantee orthogonality between independently computed eigenvectors – that is Eq. (2.2) might not hold [25].

The close connection between inverse iteration and the MRRR algorithm is discussed in a number of articles [30, 16]. Here we only mention three differences: (1) Instead of representing tridiagonal matrices by their diagonal and subdiagonal entries, MRRR uses Relatively Robust Representations (RRRs); these are representations with the property that small relative perturbations to the data result in small relative perturbations to the eigenvalues [36]; (2) the selection of a nearly optimal right-hand side vector \( \hat{z}^{(0)}_j \) for a one-step inverse iteration [35]; (3) the use of so-called twisted factorizations to solve linear systems [35].

In the following, we briefly discuss both the mathematical foundations of the MRRR algorithm, and how parallelism is organized in PMRRR.

3.1.1. The MRRR algorithm. At first, a representation \( RRR_0 \) is chosen so that it defines all the desired eigenpairs in a relatively robust way [14, 52]. For example, a factorization of the form \( L_0D_0L_0^T = T - \sigma I \) is an RRR for all of the eigenvalues [36]; here, \( D_0 \) is diagonal, \( L_0 \) is lower unit bidiagonal, and \( \sigma \) is a scalar such that \( T - \sigma I \) is definite. As a second step, bisection is used to compute approximations to each eigenvalue \( \hat{\lambda}_j \). At the cost of \( \mathcal{O}(n) \) flops, bisection guarantees that each eigenvalue is computed with high relative accuracy [31].

At this point, for all the eigenvalues \( \hat{\lambda}_j \) that have large relative gaps, i.e.,

\[
\text{relgap}(\hat{\lambda}_j) = \min_{i \neq j} |\hat{\lambda}_j - \lambda_i|/|\lambda_j| > \text{tol},
\]

it is possible to compute their corresponding

---

11 In particular, \( |\lambda_i - \hat{\lambda}_j| < \max_{i \neq j} |\lambda_i - \hat{\lambda}_j| \) is required.
12 Without loss of generality, we will assume that \( T \) is numerically irreducible: No off-diagonal element is smaller in magnitude than a certain threshold. In context of the dense eigenproblem, the threshold is usually set to \( \varepsilon \|T\| \).
13 In practice, a relative gap greater than \( 10^{-3} \) is considered sufficiently large.
eigenvectors: By using one step of inverse iteration with a twisted factorization, the acute angle \( \angle(\hat{z}_j, z_j) \) between the computed eigenvector \( \hat{z}_j \) and true eigenvector \( z_j \) satisfies

\[
|\sin \angle(\hat{z}_j, z_j)| \leq O\left(\frac{n\epsilon}{\text{relgap}(\hat{\lambda}_j)}\right).
\] (3.2)

The denominator in Eq. (3.2) is the reason for which the process can be applied only to well-separated eigenvalues – measured by its relative gap. Such well-separated eigenvalues are called singletons. Indeed, for singletons the computed eigenvectors have a small angle to the true eigenvector and consequently are numerically orthogonal.

In contrast, when a set of consecutive eigenvalues have small relative gaps – that is, they form a cluster – the current RRR cannot be used to obtain numerically orthogonal eigenvectors. Instead, one exploits the fact that the relative gap is not invariant to matrix shifts. The algorithm then proceeds by constructing a new RRR \( \{L_c, D_c\} \) in a mixed relatively stable way:

\[
L_c D_c L_c^T = L_0 D_0 L_0^T - \sigma c I.
\]

By shifting, the relative gaps are modified by a factor \( |\hat{\lambda}_j| / |\hat{\lambda}_j - \sigma c| \); thus \( \sigma c \) is chosen close to one of the eigenvalues in the cluster, so that at least one of them becomes well-separated. Once the new RRR is established, the eigenvalues in the cluster are refined to high relative accuracy with respect to the new RRR and classified as singletons and clusters. If all eigenvalues in the cluster are singletons, then the representation \( \{L_c, D_c\} \) can be used to compute a set of orthogonal eigenvectors for a slightly perturbed invariant subspace of \( \{L_0, D_0\} \). If instead some eigenvalues are still clustered, the procedure is repeated recursively until all desired eigenpairs are computed.

As a detailed discussion of the MRRR algorithm is outside the scope of this article, for further information we refer the readers to \cite{35, 13, 15, 14, 52} and the references therein.

3.1.2. PMRRR’s parallelism. Our parallelization strategy consists of two layers: a global and a local one. At the global level, the \( k \) eigenvalues and eigenvectors are statically divided into equal parts and assigned to the processes. Since the unfolding of the algorithm depends on the spectrum, it is still possible that the workload is not perfectly balanced among the processes. At the local level (within each process), the computation is decomposed into tasks that can be executed in parallel by multiple threads. The processing of these tasks leads to the dynamic generation of new tasks and might involve communication with other processes. The newly generated tasks are then likewise enqueued.

When executed with \( nproc \) processes, the algorithm starts by broadcasting the input matrix and by redundantly computing the initial representation \( RRR_0 \). Once this is available, the computation of the approximations \( \hat{\lambda}_j \) of \( k \) eigenvalues of \( L_0 D_0 L_0^T \) is embarrassingly parallel: Each process is responsible for at most \( epp = \lceil k/nproc \rceil \) eigenvalues, similarly, each of the \( nthread \) threads within a process has the task to compute at most \( ept = \lceil epp/nthread \rceil \) eigenvalues. The processes then gather all the eigenvalues, and the corresponding eigenpairs are assigned as desired.

Locally, the calculation of the eigenvectors is split into computational tasks of three types: a set of singletons, clusters that require no communication, and clusters

\footnote{PMRRR (ver. 0.6) computes approximations to all \( n \) eigenvalues at this stage, such that \( epp = \lceil n/nproc \rceil \).}

\footnote{We only refer to the calculation of the eigenvectors here, although the eigenvalues are also modified in this part of the computation.}
that require communication with other processes. The computation associated with each of the three types is detailed below.

1. A set of singletons. The corresponding eigenvectors are computed locally. No further communication among processes is necessary.

2. A cluster requiring no communication. When the cluster contains eigenvalues assigned to only one process, no cooperation among processes is needed. The four necessary steps are the same as those for the cluster task in [38]: A new RRR is computed; the eigenvalues are refined to relative accuracy with respect to the new RRR; the refined eigenvalues are classified into singletons and clusters; the corresponding tasks are enqueued into the local work queue.

3. A cluster requiring communication. When the cluster contains a set of eigenvalues which spans multiple processes, inter-process communication is needed. In this case, all the processes involved perform the following steps: a new RRR is computed redundantly, the local set of eigenvalues is refined, and the eigenvalues of the cluster are gathered and reclassified.

Multithreading support is easily obtained by having multiple threads dequeue and execute tasks. The tasks are dynamically generated: their number and size highly depends on the spectral distribution of the input matrix; for this reason, the execution time for matrices of the same size may differ noticeably. By contrast, the memory requirement is matrix independent ($O(nk/nproc)$ floating point numbers per process), and perfect memory balance is achieved [5, 50].

Our tests show that the hybrid parallelization approach is equally or slightly faster than the one purely based on MPI. This is generally true for architectures with a high degree of inter-node parallelism and limited intra-node parallelism. By contrast, on architectures with a small degree of inter-node parallelism and high degree of intra-node parallelism, we expect the hybrid execution of PMRRR to be preferable to pure MPI.

We stress that even when no multithreading is used, the task-based design of PMRRR can be advantageous: By scheduling tasks that require inter-process communication with priority and using non-blocking communication, processes can continue executing tasks while waiting to receive data. This strategy often leads to a perfect overlap of communication and computation.

4. Experiments. In the next two sections we present experimental results for the execution on two state-of-art supercomputers at the Research Center Jülich, Germany: 

4.1. Juropa. Juropa consists of 2208 nodes, each comprising two Intel Xeon X5570 Nehalem quad-core processors running at 2.93 GHz with 24 GB of memory. The nodes are connected by an Infiniband QDR network with a Fat-tree topology.

All tested routines were compiled using the Intel compilers (ver. 11.1) with the flag -O3 and linked to the ParTec’s ParaStation MPI library (ver. 5.0.23) [16]. Generally, we used a two-dimensional process grid $P_r \times P_c$ (number of rows $\times$ number of columns) with $P_r = P_c$ whenever possible, and $P_c = 2P_r$ otherwise [17]. If not stated otherwise, one process per core was employed.

The ScaLAPACK library (ver. 1.8) was used in conjunction with Intel’s MKL

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16 Version 5.0.24 was used when support for multithreading was needed.
17 As discussed in Sections 2.2 and 3, $P_c \approx P_r$ or the largest square grid possible should be preferred. These choices do not affect the qualitative behavior of our performance results.
BLAS (ver. 10.2). From extensive testing, we identified that in all cases the optimal block size was close to 32; therefore we carried out the ScaLAPACK experiments only with block size of 16, 32, 48; the best result out of this pool is then reported.

Since no driver for the generalized eigenproblem that makes use of DC is available, we refer to ScaLAPACK’s DC as the sequence of routines PZPOTRF–PZHENGST–PZHENTRD–PDSTEDC–PZUNMTR–PZTRSM, as listed in Table 2.1. Similarly, we refer to ScaLAPACK’s MRRR as the same sequence with PDSTEDC replaced by PDSTEGR.

We stress that the slow routines PZHEGST and PZHETRD, for the reduction to standard and tridiagonal form, respectively, were not used, and instead replaced by the faster PZHENGST and PZHENTRD. In order to make use of ScaLAPACK’s fast reduction routines, only the lower triangular part of the matrices is referenced and enough memory for a possible redistribution of the data is provided.

Elemental (ver. 0.6) – incorporating PMRRR (ver. 0.6) – was used for the EleMRRR timings. In general, since Elemental does not tie the algorithmic block size to the distribution block size, different block sizes could be used for each of the stages. We do not exploit this fact in the reported timings. Instead the same block size is used for all stages. A block size of around 96 was in all cases optimal, therefore experiments were carried out for block sizes of 64, 96 and 128, but only the best timings are reported.

Since the timings of the tridiagonal eigenproblem depend on the input data, so does the overall solver. In order to compare fairly different solvers, we fixed the tridiagonal input matrix by using the 1–2–1 type. The performance of every other stage is data independent. Moreover, since the output of the tridiagonal solvers has to be in a format suitable for the backtransformation, the MRRR-based routines have to undergo a data redistribution; in all the experiments, the timings for Stage 4 include the cost of the redistribution.

In the next two subsections we show results for both strong and weak scaling. In all experiments the number of nodes are increased from 8 to 256. Since each node consists of two quad-core processors, this corresponds to 64 to 2048 cores.

4.1.1. Strong Scaling. We present timings of EleMRRR for the computation of all the eigenpairs of the generalized Hermitian eigenproblem $Ax = \lambda Bx$ for fixed problem size, $n = 20,000$. The results are displayed in Fig. 4.1. As a reference, we have included timings for ScaLAPACK’s solvers. The right side of the figure shows the parallel efficiency – defined as $e_p = (t_{\text{ref}} \cdot p_{\text{ref}})/(t_p \cdot p)$ – where $t_p$ denotes the execution time on $p$ processors, and $t_{\text{ref}}$ the execution time on $p_{\text{ref}}$ processors. The reference time used 8 nodes (64 cores).

Once the proper sequence of routines is rectified, the performance of ScaLAPACK’s solvers is comparable to that of EleMRRR, up to 512 cores (see Fig. 4.1). For 64 to 512 cores DC is about 10% to 40% slower than EleMRRR, while ScaLAPACK’s MRRR is about 7% to 20% slower. The advantage of EleMRRR mainly

\footnote{At the time of writing, ScaLAPACK’s latest version was 1.8. The current version, 2.0, presents no significant changes in the tested routines.}

\footnote{As PDSTEGR is not contained in ScaLAPACK, it corresponds to the sequence PZPOTRF–PZHENGST–PZHEEVR–PZTRSM.}

\footnote{The block size for matrix vector products were fixed to 32 in all cases. For the biggest matrices in the weak scaling experiment only the block size of 32 and 96 were used for ScaLAPACK and EleMRRR, respectively.}

\footnote{We did not investigate the cause for the increased run time of ScaLAPACK using 1024 and 2048 cores. While most subroutines in the sequence are slower compared with the run time using 512 cores, PZHENTRD scales well up to the tested 2048 cores – see also Fig. 2.2.
Fig. 4.1. Strong scalability for the computation of all eigenpairs. Matrices $A$ and $B$ are of size 20,000. The dashed lines refer to ScaLAPACK’s solvers when the matrices $A$ and $B$ are stored in the upper triangular part; in this scenario, the non-square routines for the reductions are used. Left: Total execution time in a log-log scale. Right: Parallel efficiency; normalized to the execution using 64 cores.

comes from the Stages 1, 2 and 6, i.e., those related to the generalized eigenproblem. The timings for the standard problem (Stages 3–5) are nearly identical, with DC slightly slower than both MRRR-based solutions.

The story for 1024 and 2048 cores changes; the performance of ScaLAPACK’s routines for the generalized eigenproblem drop dramatically. Compared to DC, EleMRRR is about 3.3 and 6.3 times faster; with respect to ScaLAPACK’s MRRR instead, EleMRRR is 2.7 and 4.7 times faster. The same holds for the standard eigenproblem, where EleMRRR is about 2.9 and 6.2 times faster than DC and 1.9 and 3.7 times faster than MRRR.

A study on the Juropa supercomputer suggests that the run time of applications can be greatly affected by settings of the underlying MPI implementation [43]. In particular, the switch from static – the default setting – to dynamic memory allocation for MPI connections may result in improved performance. In regards to the performance degradation appearing in Fig. 4.1 (left), such a switch positively impacts some of the stages, including PDSTEDC; on the other hand it gravely worsens other stages, including PDSTEGR. Overall, ScaLAPACK’s DC would only marginally improve, while MRRR’s performance would greatly deteriorate. As a consequence, we employ the default MPI settings in all later experiments.

In Fig. 4.2 we take a closer look at the six different stages of EleMRRR. The left panel tells us that roughly one third of EleMRRR’s execution time – corresponding to Stages 4, 5 and 6 – is proportional to the fraction of computed eigenpairs. Computing a small fraction of eigenpairs would therefore require roughly about two thirds of computing the complete decomposition. On the right-hand panel of Fig. 4.2 we report the parallel efficiency for all six stages separately. When analyzed in conjunction with the left figure, this panel indicates if and when a routine becomes a bottleneck due to bad scaling.

The tridiagonal eigensolver (Stage 4) obtains the highest parallel efficiency. On the other hand, it contributes for less than 2.2% to the overall run time and is therefore negligible in all experiments.

Up to 1024 cores, ScaLAPACK’s MRRR shows a similar behavior: the tridiagonal stage makes up for less than 6% of the execution time. With 2048 cores instead, the
percentage increases up to 21%. The situation is even more severe for DC, as the fraction spent in the tridiagonal stage increases from about 4.5% with 64 cores to 41% with 2048 cores. This analysis suggests that the tridiagonal stage, unless as scalable as the other stages, will eventually account for a significant portion of the execution time.

4.1.2. Weak Scaling. Fig. 4.3 illustrates EleMRRR’s timings for the computation of all the eigenpairs of \( Ax = \lambda Bx \). In this experiment, the matrix size increases (from 14,142 to 80,000) together with the number of cores (from 64 to 2048). The right panel of the figure contains the parallel efficiency, defined as \( e_p = (t_{\text{ref}} \cdot n_{\text{ref}}^3)/(t_p \cdot n^3) \), where all the quantities are like in the previous section and \( n_{\text{ref}} \) denotes the smallest matrix size in the experiment (14,142).

In the tests using 512 cores and less, EleMRRR outperforms ScaLAPACK only by a small margin, while using 1024 cores and more, the difference becomes significant. The right graph indicates that EleMRRR scales well to large problem sizes and high number of processes, with parallel efficiency close to one. Thanks to its better scalability, for the biggest problem EleMRRR is 2.1 and 2.5 times faster than ScaLAPACK’s MRRR and DC, respectively.

The execution time is broken down into stages in Fig. 4.4 (left). Four comments follow. (a) The time spent in PMRRR (Stage 4) is in the range of 2.5% to 0.7% and it is completely negligible, especially for large problem sizes. (b) The timings corresponding to the standard eigenproblem (Stages 3–5) account for about 72% of the generalized problem’s execution time. (c) The part of the solver whose execution time is roughly proportional to the fraction of desired eigenpairs (Stages 4–6) makes up 32%–37% of the execution for both the GHEP and HEP. (d) No one stage in EleMRRR is becoming a bottleneck, as all of them scale equally well.

Fig. 4.4 (right) shows the execution of EleMRRR using one process per socket with four threads per process. The resulting execution time is roughly the same as

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\[ \text{The timings relative to only Stage 4 are detailed in Fig. 2.8} \]
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Fig. 4.3. Weak scalability for the computation of all eigenpairs. Matrices $A$ and $B$ are of varying size. The dashed lines refer to ScaLAPACK’s solvers when the matrices $A$ and $B$ are stored in the upper triangular part; in this scenario, the non-square routines for the reductions are used. Left: Total execution time. Right: Parallel efficiency relative to 64 cores. All three routines are fast and efficient up to 512 cores. For higher numbers of nodes the efficiency of the ScaLAPACK routines drops, while EleMRRR retains almost perfect scalability.

Fig. 4.4. EleMRRR’s weak scalability for the computation of all eigenpairs. Left: Fraction of the execution time spent in the six stages, from bottom to top. Right: Comparison between a pure MPI execution and a hybrid execution using one process per socket with four threads per process.

for the pure MPI execution, highlighting the potential of Elemental’s hybrid mode. Similar experiments with a higher degree of multithreading would positively affect PMRRR, but not the reduction to tridiagonal form.

4.2. Jugene. In this section, we verify the prior results obtained on Juropa for a different architecture – namely, the BlueGene/P installation Jugene. Jugene consists of 73,728 nodes, each of which is equipped with 2 GB of memory and a quad core PowerPC 450 processor running at 850 MHz.

All routines were compiled using the IBM XL compilers (ver. 9.0) in combination with the vendor tuned IBM MPI library. We used a square processor grid $P_r = P_c$.
whenever possible and $P_r = 2P_c$ otherwise. Similarly, ScaLAPACK (ver. 1.8) in conjunction with the vendor-tuned BLAS included in the ESSL library (ver. 4.3) was used throughout. In contrast to the Juropa experiments, we concentrate on the weak scalability of the symmetric-definite generalized eigenproblem. Therefore ScaLAPACK’s DC timings correspond to the sequence of routines $\text{PDPTTRF - PDSYGST - PDSTEDC - PDORMR - PDTRSM}$. Accordingly, ScaLAPACK’s MRRR corresponds to the same sequence of routines with $\text{PDSTEDC}$ replaced by $\text{PDSTEGR}$. In both cases, a block size of 48 was found to be nearly optimal and used in all experiments. As already explained in Section 4.1, we avoided the use of the routines $\text{PDSYGST}$ and $\text{PDSTYRD}$ for the reduction to standard and tridiagonal form, respectively.

For EleMRRR’s timings we used Elemental (ver. 0.66), which integrates PMR (ver. 0.6). A block size of 96 was identified as nearly optimal and used for all experiments.

### 4.2.1. Weak Scaling.

In the left panel of Fig. 4.5 we present EleMRRR’s timings for the computation of all eigenpairs of the generalized problem in the form of $Ax = \lambda Bx$. While the size of the test matrices ranges from $21,214$ to $120,000$, the number of nodes increases from 64 to 2,048 (256 to 8,192 cores). In the right panel, the execution time is broken down into the six stages of the generalized eigenproblem.

![Fig. 4.5. Weak scalability for computing all eigenpairs of $Ax = \lambda Bx$. The dashed lines refer to ScaLAPACK’s solvers when the matrices $A$ and $B$ are stored in the upper triangular part; in this scenario, the non-square routines for the reductions are used. Left: Total execution time. EleMRRR is the fastest solver across the board. Right: Fraction of the execution time spent in the six stages, from bottom to top.](image)

Both graphs show a similar behavior to the experiments performed on Juropa. In all experiments EleMRRR outperforms both the ScaLAPACK’s solvers. Most importantly, ScaLAPACK again suffers from a breakdown in scalability.

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23 As noted in Section 4.1, $P_c \approx P_r$ or the largest square grid possible should be preferred. These choices do not affect the qualitative behavior of our performance results.

24 At the time of writing, ScaLAPACK’s up-to-date version was 1.8. The current version, 2.0, presents no significant changes in the tested routines.

25 As $\text{PDSTEGR}$ is not contained in ScaLAPACK, it corresponds to the sequence $\text{PDPTTRF - PDSYGST - PDSEVR - PDTRSM}$.

26 The block size for matrix vector products, which does not have a significant influence on the performance, was fixed to 64 in all cases.
When analyzing the results of Fig. 4.5 for ScaLAPACK’s solver we the following observations. (a) The scalability issues can be attributed mainly to Stages 1, 2 and 4. In particular, for the largest experiment ScaLAPACK’s reduction to standard form (28 minutes) and MRRR (25 minutes) each exceed the time that EleMRRR spends for the entire problem. (b) Although ScaLAPACK’s tridiagonal eigen solver is usually not very time consuming, for highly parallel systems it might become the bottleneck. As an example, in our experiment on 8,192 cores the tridiagonal problem accounts for 54% (MRRR) and 33% (DC) of the total execution time of the standard eigenproblem. (c) Due to better scalability, DC becomes faster than ScaLAPACK’s MRRR.

We conclude with four comments regarding EleMRRRs behavior. (a) While stage 4 of ScaLAPACK’s MRRR and DC take up to 28% and 20% of the total execution time, respectively, PMRRR accounts for less than 4%. In particular, for the largest problem 25 minutes were spent in ScaLAPACK’s MRRR, whereas PMRRR required only 20 seconds. In all experiments PMRRR’s execution time was negligible. (b) The timings corresponding to the standard eigenproblem account for 70%–74% of the generalized problem’s execution time. (c) The part which is roughly proportional to the fraction of desired eigenpairs makes up 26%–32% of both the generalized and standard problem. (d) All the six stages scale equally well and no computational bottleneck emerges.

5. Conclusions. Our study of dense large-scale generalized and standard eigenproblems was motivated by performance problems of commonly used routines in the ScaLAPACK library. In this paper we identify such problems and provide clear guidelines on how to circumvent them: by invoking suitable routines with the right settings, the users can assemble solvers faster than those included in ScaLAPACK.

The main contribution of the paper lies in the introduction of Elemental’s dense eigensolvers and our tridiagonal eigensolver, PMRRR. Together, they provide a set of routines – labeled EleMRRR – for large-scale eigenproblems. These solvers are part of the publicly available Elemental library and make use of PMRRR, a parallel version of the MRRR algorithm for computing all or a subset of eigenpairs of tridiagonal matrices. PMRRR supports pure message-passing, pure multithreading, as well as hybrid executions, and our experiments indicate that it is among the fastest and most scalable tridiagonal eigensolvers currently available.

In a thorough performance study on two state-of-the-art supercomputers, we compared EleMRRR with the solvers built within the ScaLAPACK framework according to our guidelines. For a modest amount of parallelism, ScaLAPACK’s solvers obtain results comparable to EleMRRR, provided the fastest routines with suitable settings are invoked. In general, EleMRRR attains the best performance and obtains the best scalability of all solvers.

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