THE LAPW METHOD WITH EIGENDECOMPOSITION BASED ON THE HARI–ZIMMERMANN GENERALIZED HYPERBOLIC SVD

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Abstract. In this paper we propose an accurate, highly parallel algorithm for the generalized eigendecomposition of a matrix pair \((H, S)\), given in a factored form \((F^∗JF, G^∗G)\). Matrices \(H\) and \(S\) are generally complex and Hermitian, and \(S\) is positive definite. These type of matrices emerge from the representation of the Hamiltonian of a quantum mechanical system in terms of an overcomplete set of basis functions. This expansion is part of a class of models within the broad field of Density Functional Theory, which is considered the golden standard in Condensed Matter Physics. The overall algorithm consists of four phases, the second and the fourth being optional, where the two last phases are computation of the generalized hyperbolic SVD of a complex matrix pair \((F, G)\), according to a given matrix \(J\) defining the hyperbolic scalar product. If \(J = I\), then these two phases compute the GSVD in parallel very accurately and efficiently.

Key words. FLAPW methods, generalized eigendecomposition, generalized (hyperbolic) singular value decomposition, hyperbolic QR factorization

AMS subject classifications. 65F15, 65F25, 65Y05, 65Z05

1. Introduction. Density Functional Theory (DFT) is the Standard Model at the base of simulations in Condensed Matter Physics. At the center of most DFT simulations lays the initialization of the Hamiltonian matrix \(H\) and its diagonalization. In many DFT methods the form and size of the Hamiltonian depends on the choice of the set of basis functions used to expand the atomic orbitals. When such a basis set is not orthonormal, a positive definite and Hermitian Overlap matrix \(S\) has to be computed and diagonalized simultaneously with \(H\); this pair of matrices \((H, S)\) define a generalized Hermitian eigenproblem (or eigenpencil, in short). In a subset of all DFT methods labeled as LAPW, the entries of both \(H\) and \(S\) are represented as multiple sums and products of smaller matrices with specific properties. It this paper, we show how one can exploit this peculiar representation and solve the generalized eigenvalue problem without explicitly assembling the \(H\) and \(S\) matrices. Our alternative method solves the eigenpencil using a cascade of phases ending with the Hari–Zimmermann algorithm for a generalized SVD. We implemented a shared memory version of this method and demonstrate its scalability on a number of test cases extracted from concrete DFT simulations. In those cases where the matrix \(S\) is ill-conditioned, our eigendecomposition has the additional benefit of providing enhanced accuracy and avoid altogether the need of the failure-prone Cholesky decomposition.

The birth of DFT is marked by two fundamental articles authored in the mid-

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60s by the Nobel prize winner Walter Kohn and his collaborator Lu J. Sham and Pierre Hohenberg [14, 16]. DFT provides an approach to the theory of electronic structure that is alternative to the solution of the Schrödinger equation. While in the latter the emphasis is on a many-electron wave function describing the dynamics of electrons in a multi-atomic system, in DFT the electron density distribution $n(r)$ plays a central role. Besides providing a complementary perspective by focusing on quantities depending mainly on the three-dimensional coordinate space $r$, DFT has made possible the simulation of much larger systems than the conventional multi-particle wave function methods. Depending on the specific DFT method, computing complexity scales at most with the cube of the number of atoms, with ongoing progress towards bringing it down to linear scaling.

Despite being a general theory, DFT can be realized in as many flavors as are the sets of basis functions one can choose from. Two widely spread classes of basis functions build on the simplicity of plane waves to build more complex and rich sets of basis functions, namely Projected Plane Waves (PAW) [23] and Linearized Augmented Plane Waves (LAPW) [26]. The complexity of these sets lays in that they are made up of non-orthogonal basis functions. In the case of LAPW, the set of functions is also overcomplete. The consequence of non-orthogonality is that the matrix $S$, whose entries are the scalar products among all the basis functions of any given finite size set, is usually dense. In the particular case of LAPW methods such matrix is positive definite but could have few singular values quite close to zero. This potential problem is due to the overcompleteness of the basis set and tends to worsen as the number of atoms increases since the number of basis functions grows linearly with the number of atoms.

In DFT methods the dynamics of the quantum systems is described by a Hamiltonian operator. In practice, the Hamiltonian is translated into a Hermitian matrix $H$ whose size and structure depends on the specific DFT method. This is because the matrix $H$ is the result of the projection of the Hamiltonian operator over the finite set of basis functions of the given method. In the LAPW method, the mathematical form of the functions leads to an expression for both $H$ and $S$ in terms of a sum of smaller matrices over all possible atoms,

$$
H = \sum_{a=1}^{N_A} (A_a^*T_a^{[AA]}A_a + A_a^*T_a^{[AB]}B_a + B_a^*T_a^{[BA]}A_a + B_a^*T_a^{[BB]}B_a)
$$

and

$$
S = \sum_{a=1}^{N_A} (A_a^*A_a + B_a^*U_a^*U_a B_a),
$$

where $A_a, B_a \in \mathbb{C}^{N_L \times N_G}$, $N_G \geq N_L$, while the remaining matrices in (1.1) are complex, square, and of order $N_L$, with some additional properties. Matrices $U_a$ are real and diagonal, $T_a^{[AA]}$ and $T_a^{[BB]}$ are Hermitian, and for all $T_a^{[AB]}$ holds

$$
(T_a^{[AB]})^* = T_a^{[BA]}.
$$

Except for $U_a$, the other matrices are in general dense, and can have a range of sizes dictated by the constants $N_A, N_G,$ and $N_L$ (see section 2 for some their typical range). Despite the formulation above could lend itself to computation through specialized middleware libraries such as the Basic Linear Algebra Subprograms (BLAS), the standard approach followed by most code developers was one based on minimizing memory footprint and FLOP count [8, 17].
Recently, an alternative method for the assembly of the matrices $H$ and $S$ was presented in [11] and further developed in [9]. In their work [11], Di Napoli et al. consolidate the underlying matrix structure of the operations and proceed to encapsulate them in terms of the level 3 kernels of the BLAS library. For instance, in order to maximize the arithmetic intensity of the computation, matrix $H$ is written as

$$H = H_{AA} + H_{AB+BA+BB},$$

with

$$H_{AA} = \sum_{a=1}^{N_A} A_{a}^* T_{a}^{[AA]} A_{a}, \quad H_{AB+BA+BB} = \sum_{a=1}^{N_A} (B_{a}^* Z_{a} + Z_{a}^* B_{a}),$$

where

$$Z_{a} = T_{a}^{[BA]} A_{a} + \frac{1}{2} T_{a}^{[BB]} B_{a}.$$  

Each of the $Z_{a}$s and $B_{a}$s matrices is then packed in memory in two consecutive 2-dimensional arrays $Z_{a}$ and $B_{a}$, respectively. In the end, the sum $H_{AB+BA+BB}$ is computed by just two ZHER2K BLAS subroutines. A similar procedure holds for the matrix $S$. Once assembled the algebraic dense generalized eigenproblem is solved by standard methods. A Cholesky decomposition $LL^T = S$ is used to reduce the problem to standard form $A \leftarrow L^{-1} A L^{-T}$. In turn, the standard problem is solved by a dense direct algorithm such as MRRR [10] provided by the LAPACK library [1], or an iterative eigensolver specialized for DFT computation (e.g., the ChASE library [30]). When the assembled $S$ matrix is ill-conditioned, as it may happen for quantum systems with a large number of atoms ($>100$), the Cholesky decomposition may fail and makes it practically impossible to solve the corresponding generalized eigenproblem.

In this work, we propose an alternative numerical method for solving the eigenproblem generated by the matrix pair $(H, S)$ from (1.1), without forming the matrices explicitly. The core of the method is based on the generalized hyperbolic singular value decomposition (GHSVD) [2]. Not only such a method solves for the eigenproblem directly without assembling $H$ and $S$, but also could give more accurate results when $S$ is nearly singular. This is possible since the GHSVD decomposition acts directly on the multiplying factors making up $S$, conceivably reducing the singularity down to the square root of the condition number of $S$. As a surplus, if $J$, the matrix of the hyperbolic scalar product, is equal to the identity, the GHSVD reduces to the generalized SVD (GSVD), which is computed very efficiently in parallel.

The four phases of the algorithm are:

1. The problem is expressed as $H = F_0^* \text{diag}(T_1, \ldots, T_{N_A}) F_0$, $S = \tilde{G}^* \tilde{G}$, the (tall-and-skinny) matrices $F_0$ and $G$ are assembled, and the matrices $T_a$, formed from $T_{a}^{[AA]}$, $T_{a}^{[AB]}$, $T_{a}^{[BA]}$, and $T_{a}^{[BB]}$, are simultaneously factored by the Hermitian indefinite factorization with complete pivoting, reformulating $H$ as $H = \tilde{F}* J \tilde{F}$, with $J = \text{diag}(\pm 1)$.

2. Optionally, the matrix $\tilde{F}$ is shortened by the indefinite, $J$-QR factorization to obtain the square factor $\tilde{F}$ and a new signature matrix $J$; also, $\tilde{G}$ is shortened by the QR factorization to obtain the square factor $\tilde{G}$.

3. The GEVD of $(H, S)$ is obtained by computing the $J$-GHSVD of $(F, G)$ (or $J$-GHSVD of $(\tilde{F}, \tilde{G})$, if the second phase is skipped) by the implicit Hari–Zimmermann method.

4. Optionally, the GHSVD process is formally completed by explicitly computing the right generalized singular vectors $X$ from the generalized eigenvector matrix $Z$. 

All the phases are implemented in Fortran (with some C) code and parallelized using OpenMP threading, but the non-optional ones are carefully designed to facilitate an easy conversion into a distributed-memory algorithm, should the problem sizes so require. The Hermitian indefinite factorization with complete pivoting, the indefinite QR factorization, and the complex GHSVD of the Hari–Zimmermann type constitute an efficient (due to heavy vectorization efforts) shared memory software contribution in their own right, with an intent for them to be reusable in other problems as well.

The paper is subdivided into eight sections. In section 2, we present in more detail the physics of the problem and the mathematical model leading to the expression (1.1) for $H$ and $S$. Section 3 is devoted to formulating the problem in precise algebraic terms. The next four sections deal with the four phases of the algorithm, where the first three of them belong to the algorithm proper, and the fourth one completes the computation of the GHSVD and is unrelated to the underlying mathematical physics origin of the problem. Since each phase is an algorithm on its own, at the end of each section we present the numerical results and the parallelization techniques applied. The paper concludes with a discussion of the possible future work.

2. The $H$ and $S$ matrices in LAPW methods. Density Functional Theory is based on the seminal work of Hohenberg [14], and the follow up landmark paper by Kohn and Sham [16]. At the core of DFT are a set of equations, called Kohn–Sham equations, that have to be solved for each of the single particle wave function $\psi_i$:

$$\hat{H}_\text{KS} \psi_i(r) = \left[ -\frac{\hbar^2}{2m_e} \nabla_r^2 + V[n(r)](r) \right] \psi_i(r) = \epsilon_i \psi_i(r), \quad i = 1, \ldots, N_e.$$  

The peculiarity of these equations is that the Hamiltonian operator $\hat{H}_\text{KS}$ depends implicitly on all the $\psi_i$s through the charge density function $n(r)$, which makes the entire set of Kohn–Sham equation strongly coupled and non-linear. In particular the function $n(r)$ is the sum of the squares of all $\psi_i$s up to the total number of electrons $N_e$ in any given quantum system:

$$n(r) = \sum_{i=1}^{N_e} |\psi_i(r)|^2.$$  

Because the equations (2.1) are non-linearly coupled, they can be solved only self-consistently: one starts from a reasonable guess for the charge density $n(r)_{\text{start}}$, computes the potential $V[n(r)]$, and solves (2.1). The resulting functions $\psi_i$s and values $\epsilon_i$s are then used to compute a new density as in (2.2), which is compared to the starting one. If the two densities do not match, the self-consistent loop is repeated with a new mixed charge density. The loop stops only when the new and the old density agree up to some defined constant.

So far we have described the general setup. There are many methods that translate this setup into a computable algorithm, and this is where the various “flavors” of DFT differ. The first element of difference is in the choice of the set of functions $\varphi_t$s used to expand every one particle wave function $\psi_i$:

$$\psi_i(r) = \sum_{t=1}^{N_G} c_{t,i} \varphi_t(r).$$  

In the LAPW method [29, 15], the configuration space where the atomic cells are defined is divided in two disjoint areas where the wave functions have distinct symmetries: close to the atomic nuclei, solutions tend to be spherically symmetric and
integrals between the radial basis functions $T$. Then the new matrices $(2.6)$
and each of the $\phi$ being piece-wise functions, one ends up with the following expressions for
By substituting explicitly the functions $(2.4)$ of the Hamiltonian and Overlap matrices, respectively
The complexity of the LAPW basis set is transferred to the definition of the entries
and each atomic index $t$ sphere defined by $r$ and so depends solely on the MT spherical angles. Despite
being piece-wise functions, $\phi$ must be continuous and differentiable for each index $t$ and each atomic index $a$. The coefficients $A_{t,m,a}, B_{t,m,a} \in \mathbb{C}$ are set to guarantee that $\psi_t \in C^1$ for each of the values of the indices $L \equiv (l, m)$ and $a$. The variable $t$ ranges over the size of the plane wave functions set in INT, and is used to label the vector $k_t$ living in the space reciprocal to $r$. As such, the momentum $k_t$ characterizes the specific wave function entering in the basis set. The total size of the basis set is determined by setting a cutoff value $K_{max} \geq k_t$.

When one substitutes the expansion of $\psi_t$ (2.3) in (2.1), the Kohn–Sham equations become an algebraic generalized eigenvalue problem that needs to be solved for the $N_G$-tuples of coefficients $c_t = (c_{1,t}, \ldots, c_{N_G,t})^T$
$$\sum_{t=1}^{N_G} (H)_{t',t} c_{t,i} = \epsilon_i \sum_{t=1}^{N_G} (S)_{t',t} c_{t,i}$$
The complexity of the LAPW basis set is transferred to the definition of the entries
of the Hamiltonian and Overlap matrices, respectively $H$ and $S$, given by
$$(H)_{t',t} = \sum_a \iint \phi_t^* (r) \hat{H}_{KS} \phi_t (r) \, dr, \quad (S)_{t',t} = \sum_a \iint \phi_t^* (r) \phi_t (r) \, dr.$$ By substituting explicitly the functions $\phi_t$ of equation (2.4) and computing the integrals, one ends up with the following expressions for $H$ and $S$:
$$\begin{align*}
(H)_{t',t} &= \sum_a \sum_{L' \leq L} A_{L',a,t}^* T_{L',L,a}^{[AA]} A_{L,a,t} + \left( A_{L',a,t}^* T_{L',L,a}^{[AB]} B_{L,a,t} \right) \\
&\quad + \left( B_{L,a,t}^* T_{L',L,a}^{[BA]} A_{L,a,t} \right) + \left( B_{L,a,t}^* T_{L',L,a}^{[BB]} B_{L,a,t} \right),
\end{align*}$$
and
$$\begin{align*}
(S)_{t',t} &= \sum_a \sum_{L=(l,m)} A_{L,a,t}^* A_{L,a,t} + B_{L,a,t}^* B_{L,a,t} \| \hat{u}_{t,a} \|^2.
\end{align*}$$
The new matrices $T_{L',L,a}^{[*]} \in \mathbb{C}^{N_L \times N_L}$ are dense and their computation involves multiple integrals between the radial basis functions $u_{t,a}$ and the non-spherical part of the
potential $V$ multiplied by Gaunt coefficients*. As can be seen by simple inspection, equations (2.5)–(2.6) are equivalent to equations (1.1): while the former are written with all indices explicit, the latter have a subset of them implicit which highlights their matrix form.

We conclude with a small excursus on the structure of the self-consistent loop and its computational cost. In the first step, a starting charge density $n(r)_{\text{start}}$ is used to compute the Kohn–Sham Hamiltonian $H_{\text{KS}}$. In a second step the set of basis functions is set up and the set of $A,B$ coefficients are derived. Then, the Hamiltonian $H$ and Overlap $S$ matrices are initialized, followed by the fourth step when the generalized eigenvalue problems $Hc = \epsilon Sc$ is solved numerically to return the eigenpairs $(C, \text{diag}(\epsilon))$. Finally a new charge density $n(r)$ is computed and convergence is checked before starting a new loop. Out of all the steps above, initializing $H$ and $S$ and solving the eigenproblem accounts for more than 80% of CPU time. Having cubic complexity $O(N_A^3)$, the eigenproblem solution is usually considered the most expensive of the two. It turns out that generating the matrices may be as expensive. If $N_A$ and $N_G$ are the range of the summations $\Sigma_a$ and $\Sigma_L$, then a simple evaluation shows that equations (2.6) and (2.5) have complexity equal to $O(N_A \cdot N_L \cdot N_G^2)$ and $O(N_A \cdot N_L \cdot N_G \cdot (N_L + N_G))$, respectively. A typical simulation uses approximately $N_G$ basis functions, with $N_G$ ranging from about $50 \cdot N_A$ to about $80 \cdot N_A$, and an angular momentum $l_{\text{max}} \leq 10$, which results in $N_L = (l_{\text{max}} + 1)^2 \leq 121$. It follows that the factor $N_A \cdot N_L$ is roughly of the same order of magnitude as $N_G$, so that the generation of $H$ and $S$ also displays cubic complexity $O(N_G^3)$. In practice, the constants above have values in the following order of magnitude: $N_A = O(100)$, $N_G = O(1000)$–$O(10000)$, and $N_L = O(100)$.

3. Problem formulation. Our intention is to keep the matrices $H$ and $S$ from (1.1), given in a factored form, factored during the whole diagonalization process. The core of the algorithm (its third phase) uses a one-sided Jacobi-like method for the implicit diagonalization. More precisely, it computes a hyperbolic analog of the generalized SVD.

**Definition 3.1.** For the given matrices $F \in \mathbb{C}^{m \times n}$, $m \geq n$, $J \in \mathbb{R}^{m \times m}$, $J = \text{diag}(\pm 1)$, and $G \in \mathbb{C}^{p \times n}$, where $G$ is of full column rank, there exist a $J$-unitary matrix $U \in \mathbb{C}^{m \times m}$ (i.e., $U^*JU = J$), a unitary matrix $V \in \mathbb{C}^{p \times p}$, and a nonsingular matrix $X \in \mathbb{C}^{m \times n}$, such that

$$
F = U\Sigma_F X, \quad G = V\Sigma_G X, \quad \Sigma_F \in \mathbb{R}^{m \times n}, \quad \Sigma_G \in \mathbb{R}^{p \times n}.
$$

The elements of $\Sigma_F$ and $\Sigma_G$ are zeroes, except for the diagonal entries, which are real and nonnegative. Furthermore, $\Sigma_F$ and $\Sigma_G$ satisfy

$$
\Sigma_F^T \Sigma_F + \Sigma_G^T \Sigma_G = I.
$$

The ratios $\Sigma_{ii} := (\Sigma_F)_{ii}/(\Sigma_G)_{ii}$ are called the generalized hyperbolic singular values of the pair $(F,G)$. If the pair $(F,G)$ is real, then all matrices in (3.1) are real.

We choose to define the generalized hyperbolic SVD (GHSVD) only if the matrix $G$ is of full column rank. This implies $p \geq n$, and there is no need to mention this in the definition. In the case of full column rank $G$, the matrix $S := G^*G$ is positive definite, and the matrix pair $(H,S)$, where $H := F^*JF$, is Hermitian and definite, so it can be simultaneously diagonalized by congruences (see, for example, [22]).

*For details see [17].
If the GHSVD is computed as in (3.1), then the generalized eigenvalues and eigenvectors of $(H, S)$ are easily retrieved, since

$$H = F^* J F = X^* \Sigma_F U J U^* \Sigma_F X = X^* \Sigma_F J \Sigma_F X := X^* \Lambda_F X,$$

$$S = G^* G = X^* \Sigma_G V^* \Sigma_G X = X^* \Sigma_G \Sigma_G X := X^* \Lambda_G X.$$ 

Substituting $X^* = S X^{-1} \Lambda_G^{-1}$ in the expression for $H$ above, we get

$$(3.2) \quad H Z = S Z \Lambda; \quad Z := X^{-1}, \quad \Lambda := \Lambda_G^{-1} \Lambda_F. $$

Thus, from (3.2), the generalized eigenvalues $\text{diag}(\Lambda)$ of the matrix pair are the squared generalized hyperbolic singular values, with the signs taken from the corresponding diagonal elements in $J$, i.e., $\text{diag}(\Sigma^2 J)$, and the matrix of the generalized eigenvectors $Z$ is the inverse of the matrix $X$ of the right generalized singular vectors. For theoretical purposes it can be assumed that $\text{diag}(\Lambda)$ is sorted descendingly, though for simplicity it is not the case in our implementation.

An approach that uses the SVD on a matrix factor, instead of the eigendecomposition on the multiplied factors, usually computes small eigenvalues more accurately.

The idea of our algorithm is to transform the initial problem by using the properties of matrices $T_a^{[AA]}$, $T_a^{[AB]}$, $T_a^{[BA]}$, and $T_a^{[BB]}$. In the first phase of the algorithm, matrices $T_a$,

$$T_a = \begin{bmatrix} T_a^{[AA]} & T_a^{[AB]} \\ T_a^{[BA]} & T_a^{[BB]} \end{bmatrix}$$

are assembled from the already mentioned matrices and factored, to bring them in a suitable form for the GHSVD computation.

After that, we are left with two tall matrices, which have, in our test examples, between 2 and 22 times more rows than columns. It is widely known that the Jacobi-like SVD algorithms are more efficient if the factors are square, so in the second (optional) phase we could preprocess the factors — $F$ by the hyperbolic QR factorization (see [24]), and $G$ by the ordinary tall and skinny QR factorization ($ZGEQR$ routine from LAPACK), into square ones.

The third phase, optionally augmented by the fourth phase, is a complex version of the implicit Hari–Zimmermann method. This method is a slight modification (at least from the mathematical point of view) of the real method presented in [21]. The complex transformations, for the two-sided method, have been derived in the PhD thesis of Vjeran Hari [12].

3.1. Testing environment. The testing environment consists of an Intel Xeon Phi 7210 CPU, running at 1.30 GHz with Turbo Boost turned off, in Quadrant cluster mode with 96 GiB of RAM and 16 GiB of flat-mode MCDRAM, under 64-bit CentOS Linux 7.6.1810 with the Intel Fortran and C compilers and Math Kernel Library (MKL), version 19.0.3.199. For the Intel 80-bit extended floating-point type support, required by the error-checking code, GNU Fortran 8.2.1 (and KIND=10) was used.

The software distribution† of all phases presented in this paper is written mostly in Fortran, with some auxiliary parts in C, while the parallelization relies on the OpenMP constructs. The phases are meant to be run in a sequence, where each phase is executed as a separate process with a number of OpenMP threads. Since the testing machine has enough memory to hold all required data, as the modern

†Available in https://github.com/venovako/FLAPWxHZ repository.
compute nodes in general do, the algorithms are implemented for the shared memory, but at least the algorithms for Phases 1, 3, and 4 can be easily transformed into distributed-memory ones, should the volume of data so require.

After extensive testing, it was established that each thread should be bound to its own physical CPU core, with `OMP_PROC_BIND=SPREAD` placement policy and the upper limit on the number of threads set to 64 (the number of cores of the CPU). The MKL library, which provided the double precision and the double-complex BLAS and LAPACK routines, was used in its threaded variant, but in all tests (except for the ZSWAP, ZROT, and ZGEQR routines in Phase 2 and ZGETC2 routine in Phase 4, where the MKL library was allowed to use either 32 or 64 threads) with only one thread (i.e., the calling thread) allowed per call. The nested parallelism it therefore not required (but remains possible) within our code. Hyper Threading was, though enabled, not explicitly utilized. However, nothing precludes a possibility that on a different architecture the BLAS and/or LAPACK calls could benefit from some form of intra-core symmetric multi-threading, and then the thread placement policy `OMP_PROC_BIND=SPREAD,CLOSE` might help better reuse of data in the cache levels shared among the threads of a core.

Apart from the maximal number of threads as described above (64), the tests were also performed with 32 threads, to assess the effects on the computational time of the larger block sizes and the availability of the whole L2 data cache (1 MiB, shared among two cores) to a thread. The algorithms do not require any particular number of threads in principle, but are not intended to be used single-threadedly.

Another hardware feature targeted is the SIMD vectorization: each core has a private L1 data cache of 32 kiB with a line size of 64 B, and equally wide (e.g., for 8 double precision floating-point numbers) vector registers upon which a subset of AVX-512 instructions is capable to operate in the SIMD fashion. The vectorization was employed both implicitly, by aligning the data to the cache line size whenever possible and instructing the compiler to vectorize the loops, and (semi-)explicitly, as will be described in the following sections. The code is parametrized by the maximal SIMD length (i.e., the number of 8 B lanes in the widest vector register type) $v$, and it vectorizes successfully on other architectures (e.g., on AVX2, with $v = 4$).

Under an assumption that the compiler-generated floating-point reductions (e.g., those of the SUM Fortran intrinsic) obey the same order of operations in each run, and due to the alignment enforced as above, the algorithms should be considered conditionally reproducible, in a sense that the multiple runs of the executables on the same data in the same environment should produce bitwise-identical results.

### 3.2. Datasets

Each dataset under test contained all matrix inputs ($A_a$, $B_a$, $U_a$, $T_a^{[AA]}$, $T_a^{[BA]}$, and $T_a^{[BB]}$) for a single problem instance. With 8 datasets, summarized in Table 3.1, we believe to have a representative coverage of the small-to-medium size problems from practice. As already mentioned in section 2, the maximum value of the momentum $K_{\text{max}}$ which appears as an index to the dataset label (e.g., $AuAg_2.5$) determines the size of the basis functions set $N_G$. This is why datasets with same label (e.g., $AuAg$) but different index (e.g., 2.5 vs. 3.0) have differing values for $N_G$. In the following, the datasets are referred to by their IDs.

### 4. Phase 1 – simultaneous factorizations of $T_a$ matrices

The goal of this section is to rewrite the problem (1.1) in a form suitable for GHSVD computation.
Table 3.1  
The datasets under test.

| ID | dataset     | $N_L$ | $N_A$ | $m = 2N_LN_A$ | $n = N_G$ |
|----|-------------|-------|-------|---------------|-----------|
| A1 | AuAg_2.5    | 121   | 108   | 26136         | 3275      |
| A2 | AuAg_3.0    | 121   | 108   | 26136         | 5638      |
| A3 | AuAg_3.5    | 121   | 108   | 26136         | 8970      |
| A4 | AuAg_4.0    | 121   | 108   | 26136         | 13379     |
| B1 | NaCl_2.5    | 49    | 512   | 50176         | 2256      |
| B2 | NaCl_3.0    | 49    | 512   | 50176         | 3893      |
| B3 | NaCl_3.5    | 49    | 512   | 50176         | 6217      |
| B4 | NaCl_4.0    | 49    | 512   | 50176         | 9273      |

4.1. Problem reformulation. The first step is to write (1.1) as

\[
H = \sum_{a=1}^{N_A} H_a^* T_a H_a, \quad S = \sum_{a=1}^{N_A} S_a^* S_a,
\]

where

\[
T_a = \begin{bmatrix} T_a^{[AA]} & T_a^{[AB]} \\ (T_a^{[AB]})^* & T_a^{[BB]} \end{bmatrix}, \quad H_a = \begin{bmatrix} A_a \\ B_a \end{bmatrix}, \quad S_a = \begin{bmatrix} A_a \\ U_a B_a \end{bmatrix}.
\]

Furthermore, matrices in (4.1) can be expressed as

\[
H = \begin{bmatrix} H_1^* & \cdots & H_{N_A}^* \end{bmatrix} \text{diag}(T_1, \ldots, T_{N_A}) \begin{bmatrix} H_1 \\ \vdots \\ H_{N_A} \end{bmatrix} := F_0^* T F_0
\]

\[
S = \begin{bmatrix} S_1^* & \cdots & S_{N_A}^* \end{bmatrix} \begin{bmatrix} S_1 \\ \vdots \\ S_{N_A} \end{bmatrix} := \tilde{G}^* \tilde{G}.
\]

In (4.2), \(\text{diag}(T_1, \ldots, T_{N_A})\) stands for a block-diagonal matrix with the prescribed diagonal blocks \(T_a, a = 1, \ldots, N_A\). Newly defined matrices have the following dimensions: \(H_a, S_a \in \mathbb{C}^{(2N_L) \times N_G}, T_a \in \mathbb{C}^{(2N_L) \times (2N_L)}, F_0, \tilde{G} \in \mathbb{C}^{(2N_A N_L) \times N_G}, \) and \(T \in \mathbb{C}^{(2N_A N_L) \times (2N_A N_L)}\). From now on, let \(m := 2N_A N_L\), and \(n := N_G\).

To efficiently exploit the structure of the problem, the matrix \(T\) needs to be diagonal, with its diagonal elements equal to either 1 or \(-1\) (possibly with some zeroes in the case of singular \(T\)). There is no mathematical obstacle to apply the simultaneous (Jordan-)orthogonalization in the computation of the GHSVD on the already described matrices \(F_0, \tilde{G}, \) and \(T\) implicitly, but the repeated multiplication (in each reduction step) by \(T\) is slow. Therefore, \(T\) should be either factored concurrently, by using a somewhat modified version of the Hermitian indefinite factorization of all \(T_a\) blocks, or diagonalized concurrently: the factorizations (or diagonalizations) are completely independent of each other and can proceed in parallel. Since the diagonalization, compared to the Hermitian indefinite factorization, is a slower process, our choice is to factor all the diagonal blocks \(T_a\).
4.2. Hermitian indefinite factorization. Each $T_a$ is factored by the algorithm described in [27]. The algorithm for each $T_a$ consists of the Hermitian indefinite factorization with a suitable pivoting [3, 4, 5, 6, 7], followed by the transformation of the block-diagonal matrix. Such factorization has the following form

\[ T_a = P_a^T M_a^* D_a M_a P_a, \]

where $P_a$ is a permutation (in the LAPACK sense), $M_a$ is upper triangular, and $D_a$ is block-diagonal, with diagonal blocks of order 1 or 2.

Then, $D_a$ is transformed into $\tilde{J}_a = \text{diag}(\pm 1)$. If $D_a$ has a diagonal block of order 1 at position $k$, then $\tilde{J}_a$ stores the sign of this block in its $k$th diagonal element, and the $k$th row of $M_a$ is scaled by $\sqrt{|(D_a)_{kk}|}$. In the case of a (Hermitian) pivot block of order 2, this block is diagonalized by a single Jacobi rotation, and the corresponding two rows of $M_a$ in (4.3) are multiplied by that rotation. After that, two transformations of the new diagonal elements of $D_a$ are performed, as above. To speed-up the process, the rotation and the scaling of two rows of $M_a$ are combined and then applied as a single transformation.

The outer permutations $P_a$ are generated starting from the identity, and stored as the partial permutations of the principal submatrices, as in LAPACK, according to the pivoting of choice. Since the matrices $T_a$ are of a relatively small order, our choice is the complete pivoting from [7].

4.3. Postprocessing. After the factorization, a postprocessing step is applied to obtain

\[ T_a = \tilde{M}_a^* \tilde{J}_a \tilde{M}_a, \]

where $\tilde{M}_a = M_a P_a$. Note that $\tilde{M}_a$ does not need to remain triangular.

Finally, by applying an inner permutation $\tilde{P}_a$, $\tilde{J}_a$ can be rearranged into a diagonal matrix $\tilde{J}_a$, where the positive signs precede the negative ones on the diagonal. This property of $\tilde{J}_a$ matrices can be exploited to speed-up computation of the hyperbolic scalar products $x^* J x$ in the subsequent phases. Let the whole factorization routine described thus far be called \texttt{ZHEBPJ}$. Then,

\[ T_a = \tilde{M}_a^* \tilde{J}_a \tilde{M}_a, \quad \tilde{M}_a = \tilde{P}_a \tilde{M}_a, \]

and $H_a$ is multiplied by $\tilde{M}_a$ from the left, i.e., $\tilde{H}_a = \tilde{M}_a H_a$.

After such preprocessing, $H$ from (4.2) is written as

\[ H = \tilde{F}^* \tilde{J} \tilde{F}, \quad \tilde{F} = \begin{bmatrix} \tilde{H}_1 \\ \vdots \\ \tilde{H}_{N_A} \end{bmatrix}, \quad \tilde{J} = \text{diag}(\tilde{J}_1, \cdots, \tilde{J}_{N_A}). \]

For datasets A1–A4, each $\tilde{J}_a$ has 3 positive and 239 negative signs, for a total of 324 positive and 25812 negative signs in $\tilde{J}$. For datasets B1–B4, a (non-consecutive) half of $\tilde{J}_a$ matrices has 0 positive and 98 negative signs in each matrix, and the other half has 98 positive and 0 negative signs in each matrix (i.e., $T_a$ matrices are definite), for a total of 25088 positive and the same number of negative signs in $\tilde{J}$.

\[ \text{‡In the software distribution, ZHEBPJ corresponds to HIF_ZHEBPC routine, followed by HIF_JPART.} \]


4.4. Implementation. The computational task for an index $a$ is essentially sequential, up to a possible usage of a parallel BLAS. On the other hand, for different indices $a$, the tasks are embarrassingly parallel. Therefore, it seems reasonable to parallelize the algorithm such that each thread is responsible for one or more indices $a$, as indicated in the pseudocode of Algorithm 4.1.

Algorithm 4.1 A pseudocode for the Phase 1.

\begin{verbatim}
for all atoms $a$, $1 \leq a \leq N_A$ do  \{an OpenMP parallel do\}
    factorize $T_a = M_a^* J_a M_a$;  \{ZHEBPJ with BLAS level 1 and 2 routines\}
    multiply $H_a = M_a H_a$;  \{1 ZGEMM, of a $2N_L \times 2N_L$ and a $2N_L \times N_G$ matrix\}
    scale the rows of $B_a$ as $U_a B_a$;  \{$N_L$ ZDSCALs, each on a row of $N_G$ elements\}
end for
\end{verbatim}

Computing $U_a B_a$ to assemble $\tilde{G}$ is in itself a loop with completely independent iterations, and could also be done in parallel, using the nested parallelism within each thread, should $N_G$ be large enough and should also the newly spawned threads for that loop have enough computational resources available to warrant the overhead of the thread management.

In our implementation, MCDRAM is not explicitly used. Each thread is solely responsible for allocating and accessing the memory for the data it processes. Thus, the NUMA data locality is achievable whenever each NUMA node has enough storage, what makes the algorithm viable in the heavily non-uniform memory access settings (e.g., SNC-4 mode of the Intel Xeon Phi CPUs).

In a distributed memory setting (e.g., using the MPI processes), the assembling of $\tilde{F}, \tilde{J},$ and $\tilde{G}$ can be done by assigning to each process a (not necessarily contiguous) subrange of the iteration range of the for-all loop from Algorithm 4.1, while inside the process all atoms assigned to it are processed exactly as above, within an OpenMP parallel-do loop. The matrices $\tilde{F}, \tilde{J},$ and $\tilde{G}$ would then end up being distributed in the chunks corresponding to the chosen subranges among the processes.

4.5. Testing. In Table 4.1 the average per-atom wall execution time of Phase 1 is shown. The results suggest that it is beneficial to have more L2 data cache available per thread, as is the case with 32 threads overall. In the breakdown of the weights (i.e., percentages of time taken) of each computational step it is confirmed that ZGEMM starts to dominate the other computational steps of Algorithm 4.1 as the ratio $n/m$ increases. It is a strong indication that even a procedure more expensive than ZHEBPJ, such as a diagonalization of $T_a$, may be applied on the datasets having a square-like shape, without considerably degrading the relative performance of Phase 1.

4.6. An alternative way forward. After this phase has completed, one can proceed as described in the rest of the paper, should the condition numbers of (the yet unformed) matrices $H$ and $S$ be large enough to severely affect the accuracy of a direct solution of the generalized Hermitian eigenproblem with the pair $(H, S)$.

An alternative and more time-efficient way to proceed would be to explicitly form $H$ and $S$. For $S = \tilde{G}^* \tilde{G}$, one ZHERK call would suffice. For $H = \tilde{F}^* \tilde{J} \tilde{F}$, a copy of $\tilde{F}$ should be made, and that copy’s rows should be scaled in parallel by the diagonal elements of $\tilde{J}$. One ZGEMM call on $\tilde{F}^*$ and $\tilde{J} \tilde{F}$ then completes the formation of $H$. After that, an efficient solver for the generalized Hermitian eigenproblem can be employed on $(H, S)$, such as ZHEGV or ZHEGVD from LAPACK.
The average per-atom wall execution time (wtime) of Phase 1 with 32 and 64 threads. Since the routine weights are rounded to the nearest per mil, their sum may not yield 100%. The first weight corresponds to ZHEBPJ, the second one to ZGERM, and the third one to ZSCALs step of Algorithm 4.1.

| ID | average wtime [s] per atom | routine weights % | 32 threads | 64 threads | 32 threads | 64 threads |
|----|---------------------------|-------------------|------------|------------|------------|------------|
| A1 | 0.242376                  | 0.276322          | 72.2 : 26.0 : 1.9 | 65.2 : 32.1 : 2.7 |
| A2 | 0.277639                  | 0.322397          | 59.9 : 36.3 : 3.8 | 52.9 : 41.2 : 5.9 |
| A3 | 0.343664                  | 0.427566          | 48.1 : 46.0 : 5.8 | 39.8 : 45.9 : 14.3 |
| A4 | 0.437396                  | 0.558827          | 37.7 : 53.5 : 8.8 | 30.5 : 49.2 : 20.3 |
| B1 | 0.022895                  | 0.026992          | 56.2 : 38.5 : 5.3 | 42.2 : 48.3 : 9.5 |
| B2 | 0.031303                  | 0.038163          | 38.9 : 53.9 : 7.2 | 29.5 : 51.4 : 19.0 |
| B3 | 0.048914                  | 0.090977          | 23.9 : 66.8 : 9.2 | 12.7 : 72.6 : 14.7 |
| B4 | 0.071882                  | 0.108011          | 15.9 : 71.7 : 12.4 | 11.1 : 71.7 : 17.2 |

4.6.1. Row scaling. A cache-friendly implementation\(^6\) of the row scaling by \(\tilde{J}\) is to iterate sequentially over the rows of a fixed column \(j\), and change the sign of each element \(\tilde{F}_{ij}\) for which \(\tilde{J}_{ii} = -1\), while the outer parallel-do loop iterates over all column indices \(j\). However, that implementation can be optimized further.

If \(\tilde{J}\) has its diagonal partitioned into (regularly or irregularly sized) blocks of the same sign, then \(\tilde{J}\) can be compactly encoded as a sequence of pairs \((i, l)\), one for each block of negative signs, where \(i\) is the first index belonging to a block \(k\), and \(l \geq 1\) is the block’s length. The iteration over all rows and the conditional sign changes as above can be replaced by iteration over all such blocks. For each block, iterate sequentially in the range of indices \(i\) from \(i\) to \(i + l - 1\), and change the signs unconditionally, thus eliminating the conditional branching based on the sign of \(\tilde{J}_{ii}\).

Such run-length-like encoding is employed in Phase 3, where it also accelerates the hyperbolic dot products in the case where the positive signs precede the negative ones on the diagonal of a sign matrix (i.e., at most one negative block exists) given by ZHEBPJ when forming the square factors for the inner Hari–Zimmermann method.

5. Phase 2 – optional (\(J, I\)) URV factorization. It is a well-established fact that the one-sided Jacobi-type algorithms are fastest if they work on square matrices, since the column dot-products and updates are the shortest possible.

Therefore, if we find the square factors \(F, G\), and the corresponding \(J\) of the matrix pair \((\tilde{F}^*, J\tilde{F}, \tilde{G}^*\tilde{G})\), instead of the rectangular factors \(\tilde{F}, \tilde{G}\), and the corresponding \(\tilde{J}\), then we expect that the overhead of such a shortening will be less than the computational time saved by avoiding the rectangular factors. To this end, matrix \(\tilde{F}\) is shortened by using the hyperbolic QR factorization (also called the JQR factorization), according to the given \(\tilde{J}\):

\[
P_1 \tilde{F} P_2 = Q F; \quad Q_F \tilde{J} Q_F = J, \quad Q_F := P_F^T Q_F,
\]

where \(F \in \mathbb{C}^{n \times n}\) is block upper triangular with diagonal blocks of order 1 or 2, \(J = \text{diag}(\pm 1) \in \mathbb{R}^{n \times n}\) is the shortened signature matrix, \(P_2 \in \mathbb{R}^{n \times n}\) and \(P_1 \in \mathbb{R}^{m \times m}\) are the column and the row permutation matrix, respectively. Our application does

\(^6\)See src/test/zhegvt.F90 in FLAPWxH2 repository for an example of such an approach.
not use $Q_F \in \mathbb{C}^{m \times n}$, so it is not explicitly formed. From (5.1) holds
\[ P_2^T \tilde{F}^* \tilde{J} \tilde{F} P_2 = F^* Q_F^* P_1 \tilde{J} P_1^T Q_F F = F^* \tilde{Q}_F^* \tilde{J} \tilde{Q}_F F = F^* J F. \]

Since the JQR requires both row and column pivoting (see [24]), matrix $\tilde{G}$, with its columns prepermutated according to $P_2$, the column pivoting of the JQR, will then be factored by the ordinary (tall and skinny) QR factorization (e.g., by the LAPACK routine ZGEQR). The latter QR factorization does not employ column pivoting, but in principle the row pivoting or presorting may be used:
\[ P_3(\tilde{G} P_2) = Q_G G; \quad \tilde{Q}_G^* Q_G = I_n, \quad \tilde{Q}_G := P_3^T Q_G, \]
where $G \in \mathbb{C}^{n \times n}$ is upper triangular, and $Q_G \in \mathbb{C}^{m \times n}$, which is not needed in our application. We also do not depend on the special forms of $F$ and $G$ later on.

From (3.1) it follows that the $\tilde{J}$-GHSVD of $\tilde{F}$ and $\tilde{G}$, and that of $FP_2$ and $\tilde{G} P_2$, differ only in the column permutation of the right singular vectors, i.e., $\tilde{X} = XP_2^T$, or, from (3.2), the row permutation of the eigenvectors, i.e., $\tilde{Z} = P_2 Z$, while $\Sigma$, and thus $\Lambda$, stay the same. Therefore, the square factors $F$, $G$, and $J$ can be used in place of $\tilde{F}$, $\tilde{G}$, and $\tilde{J}$ throughout the rest of the computation, and then the results could be easily converted back to the ones of the original problem.

If we expect $\tilde{G}$ to be badly conditioned, this optional phase could be skipped, or we should resort to a slower but more stable QR factorization of $GP_2$ with the column (and maybe row) pivoting,
\[ P_4(\tilde{G} P_2)P_5 = Q_{G'} G'; \quad \tilde{Q}_{G'}^* \tilde{Q}_{G'} = I_n, \quad \tilde{Q}_{G'} := P_4^T Q_{G'}, \]
where $P_5$ has to be applied back to $F$. The blocked, column-pivoted QR factorization is provided by the LAPACK routine ZGEQP3.

Then, $F' := FP_5$ and $G'$ could be substituted for $F$ and $G$ in the rest of the computation. For $X$ (or $Z$) thus obtained it holds $\tilde{X} P' = X$ (or, $P' Z = \tilde{Z}$), where $P' := P_2 P_5$. Such an approach has not been tested, since it was not required for our datasets, but it is not hard to be implemented should a need for it arise.

5.1. $\tilde{J}$-dot products and norms. Since $\tilde{J}$ can in principle contain the positive and the negative signs in any order, and vectorization is strongly desired, a $\tilde{J}$-dot product of two vectors, $f^* \tilde{J} g$, is computed as $v$ piecewise sums $\Sigma_j$, $1 \leq j \leq v$,
\[
\text{Re}(\Sigma_j) = \text{Re}(\Sigma_j) + \tilde{J}_i(\text{Re}(f_i) \text{Re}(g_i) + \text{Im}(f_i) \text{Im}(g_i)),
\]
\[
\text{Im}(\Sigma_j) = \text{Im}(\Sigma_j) + \tilde{J}_i(\text{Re}(f_i) \text{Im}(g_i) - \text{Im}(f_i) \text{Re}(g_i)),
\]
where $i$ starts with a value of $j$ and increments in steps of $v$ up to $m$. The real and the imaginary component of the resulting $\Sigma$ are obtained by sum-reducing Re($\Sigma_j$) and Im($\Sigma_j$), respectively. Similarly, $f^* \tilde{J} f$ is computed by sum-reducing $\Sigma'_j$, where
\[
\Sigma'_j = \Sigma_j + \tilde{J}_i(\text{Re}(f_i)^2 + \text{Im}(f_i)^2).
\]

The “square” of the $\tilde{J}$-norm of a vector thus obtained can be positive or negative, with a possibility of cancellations inadvertently occurring in the summations. It remains an open question how to compute the $\tilde{J}$-norms both efficiently and accurately, though one possible speed improvement might be to encode $\tilde{J}$ as described in subsection 4.6.1 and simplify the above three piecewise summations accordingly.
5.2. Pivoting. To achieve the maximal numerical stability, the JQR factorization is usually performed with the complete pivoting. In the first step the pivot column(s) are chosen from the \( \tilde{J} \)-Grammian matrix \( H = \tilde{F}^* \tilde{J} \tilde{F} \), and later on, in the \( k \)th step, from the \( \tilde{J}_k \)-Grammian matrix \( H_k = \tilde{F}_k^* \tilde{J}_k \tilde{F}_k \), where \( \tilde{F}_k \) is a part of the matrix yet to be reduced, and \( \tilde{J}_k \) is the matrix of signs that corresponds to the unreduced matrix \( \tilde{F}_k \) (see Fig. 5.1). The complete pivoting in the first step needs formation of the whole \( H \), i.e., \( \mathcal{O}(mn^2) \) floating-point operations. Such an approach, consistently implemented throughout the algorithm, leads to \( \mathcal{O}(m^2 n^2) \) operations solely for the choice of pivots. Therefore, we relaxed the pivoting strategy to the diagonal pivoting supplemented with the partial pivoting [5, Algorithm C].

![Diagram](image)

**Fig. 5.1.** Choosing a single pivot column or two pivot columns. Matrices \( \tilde{J}_k \) and \( \tilde{F}_k \) are shaded.

5.2.1. Diagonal pivoting. First, \( n - k + 1 \) squares of the \( \tilde{J}_k \)-norms \( h_{i1}^{[k]} := \tilde{f}_i^* \tilde{J}_k \tilde{f}_i \), where \( \tilde{f}_i \) is the \( i \)th column of \( \tilde{F}_k \) and \( i \geq 1 \), are computed in a parallel-do loop over \( i \) and stored in a work array. Since all columns have the length of \( m - k + 1 \), each parallel loop iteration executes (sequentially) in approximately the same time and the work is therefore well balanced among the threads.

Let \( j \geq 1 \) be the smallest index such that \( |h_{jj}^{[k]}| \geq |h_{i1}^{[k]}| \) for all \( i \). If \( j > 1 \), the \( k \)th and the \( (j + k - 1) \)th column of \( \tilde{F} \) (and thus also the first and the \( j \)th column of \( \tilde{F}_k \)) are swapped. If \( k = n \), the column pivoting is completed.

5.2.2. Partial pivoting. Otherwise, \( n - k \) \( \tilde{J}_k \)-dot products \( h_{1j}^{[k]} := \tilde{f}_1^* \tilde{J}_k \tilde{f}_j \), where \( \tilde{f}_j \) is the \( j \)th column of \( \tilde{F}_k \) and \( j > 1 \), are computed in a parallel-do loop over \( j \) and stored in a complex workspace, while their magnitudes \( |h_{1j}^{[k]}| \) are placed in a real workspace. Same as above, this work is well balanced among the threads.

Let \( i > 1 \) be the smallest index such that \( |h_{1i}^{[k]}| \geq |h_{1j}^{[k]}| \) for all \( j > 1 \). As in [5], if

\[
|h_{1i}^{[k]}| \geq \alpha |h_{1j}^{[k]}|,
\]

where \( \alpha := (1 + \sqrt{7})/8 \), then the column pivoting for the step \( k \) is completed.

Otherwise, \( n - k \) \( \tilde{J}_k \)-dot products \( h_{i1}^{[k]} := \tilde{f}_i^* \tilde{J}_k \tilde{f}_1 \), where \( \tilde{f}_i \) is the \( i \)th column of \( \tilde{F}_k \) and \( i \neq l \geq 1 \), are computed in a parallel-do loop over \( l \) and their magnitudes \( |h_{i1}^{[k]}| \) are stored in a real workspace. This work is only slightly imbalanced among threads, since for \( l = i \) a thread assigned to the iteration sets \( |h_{i1}^{[k]}| = 0 \) as a way of recording
that such value (and its index) should be skipped when searching for a maximum.

Let \( j \geq 1 \) be the smallest index such that \( |h_{ij}^{[k]}| \geq |h_{il}^{[k]}| \) for all \( l \). As in [5], if

\[
|h_{11}^{[k]}||h_{ij}^{[k]}| \geq \alpha|h_{11}^{[k]}|^2,
\]

then the column pivoting for the step \( k \) is completed; else, if

\[
|h_{ii}^{[k]}| \geq \alpha|h_{ij}^{[k]}|,
\]

then the \( k \)th and the \((i + k - 1)\)th column of \( \tilde{F} \) (and thus also the first and the \( i \)th column of \( \tilde{F}_k \)) are swapped and the column pivoting for the step \( k \) is completed.

Otherwise, a \( 2 \times 2 \) pivot is chosen, by taking the first column of \( \tilde{F}_k \) and swapping the \((k + 1)\)th and \((i + k - 1)\)th column of \( \tilde{F} \) (and thus also the second and the \( i \)th column of \( \tilde{F}_k \)), if \( i \neq 2 \); else, the second pivot column is already in place.

The pivot column(s) have thus been brought to the front of the matrix \( \tilde{F}_k \) by at most two column swaps. The ensuing row pivoting is explained further below.

### 5.3. Hyperbolic Householder reflectors

If a single pivot is chosen, the first column \( f_1 \) of \( \tilde{F}_k \) is reduced by a single hyperbolic Householder reflector [25, Theorem 4.4] to a vector \( f_1 = c_1e_1 \), \( c_1 \in \mathbb{C} \), and \( e_1 \) is the first vector of the canonical base.

For the sake of completeness, a modified version of Theorem 4.4 (for the hyperbolic scalar product and a simple shape of \( f_1 \)) is included here.

**Theorem 5.1.** Let \( \tilde{J}_k \) be a hyperbolic scalar product matrix of order \( \ell \). Let \( \tilde{f}_1, f_1 \in \mathbb{C}^\ell \) be two distinct vectors. There exists a basic \( \tilde{J}_k \)-reflector \( H(w) \),

\[
H(w) = I - 2w^*(w^*\tilde{J}_k w)^+ w^* \tilde{J}_k,
\]

such that \( H(w)f_1 = f_1 \) if and only if

(a) \( \tilde{f}_1 \) and \( f_1 \) satisfy the \( \tilde{J}_k \)-isometry property

\[
\tilde{f}_1^* \tilde{J}_k \tilde{f}_1 = f_1^* \tilde{J}_k f_1,
\]

and \( \tilde{J}_k \)-symmetry property

\[
\tilde{f}_1^* \tilde{J}_k f_1 = f_1^* \tilde{J}_k \tilde{f}_1,
\]

(b) \( d = \tilde{f}_1 - f_1 \neq 0 \) is nondegenerate, i.e., \( d^* \tilde{J}_k d \neq 0 \).

Furthermore, whenever \( H(w) \) exists, it is unique. \( H(w) \) can be generated by any \( w \in \mathbb{C}^\ell \) such that \( w = \lambda d \), \( \lambda \in \mathbb{C} \), \( \lambda \neq 0 \).

Finally, the same remains valid if we replace \( f_1 \) by \(-f_1\), and \( d \) by \( s = f_1 + \tilde{f}_1 \).

If \( \tilde{f}_1 = f_1 \), there is nothing to do in this step, so we take \( H(w) = I \). Otherwise, since we want to obtain \( f_1 \) in the form \( f_1 = c_1e_1 \), equation (5.3) is equivalent to a requirement that the sign of \( \tilde{J}_{11} \), the first diagonal element of \( \tilde{J}_k \), is equal to the sign of \( \tilde{f}_1^* \tilde{J}_k \tilde{f}_1 = |c_1|^2 \tilde{J}_{11} = f_1^* \tilde{J}_k f_1 \). As \( \tilde{f}_1^* \tilde{J}_k \tilde{f}_1 \) has already been computed by the diagonal pivoting (see subsection 5.2.1), it is trivial to check if the requirement holds.

---

*Unless all other values are also 0.*
### 5.3.1. Row pivoting. If not, it can be shown that there exists at least one element with the correct sign in $\tilde{J}_k$. When there is more than one such element, our implementation sequentially finds the one that corresponds to the largest element in $\tilde{f}_1$ by magnitude (say, $1$th). By permuting the diagonal of $\tilde{J}_k$, this element can be brought to the first diagonal position. Of course, this implies a corresponding row permutation of $\tilde{F}_k$ that swaps the first and the $1$th row of $\tilde{F}_k$. For that, we employ the parallel $\texttt{ZSWAP}$ routine, but should the rows be short enough, a sequential version of the routine could be considered instead.

### 5.3.2. Computing the $\tilde{J}_k$-Householder reflector. Relation (5.3) also implies that

\[ |c_1| = \sqrt{\bar{f}_1^* \tilde{J}_k \tilde{f}_1}. \]

In general, $c_1$ is a complex number, $c_1 = re^{i\delta}$, and we have already determined $r$, the absolute value of $c_1$. It remains to find $\delta$, the argument of $c_1$.

From (5.4) it follows

\[ \tilde{f}_1 \tilde{J}_{11} c_1 = \tilde{c}_1 \tilde{J}_{11} \tilde{f}_1, \]

where $\tilde{f}_1 := r_1 e^{i\delta_1}$ is the the first element in $\tilde{f}_1$. Relation (5.5) can be divided by $\tilde{J}_{11}$ and written as

\[ r_1 r e^{i(\delta - \delta_1)} = r_1 r e^{-i(\delta - \delta_1)}. \]

Since $r_1, r \neq 0$, we may choose $\delta = \delta_1$ for the argument of $c_1$. We only need to compute $e^{i\delta}$, so

\[ e^{i\delta} = \frac{\tilde{f}_1}{|\tilde{f}_1|}. \]

Now we have satisfied conditions (5.3)–(5.4) for the construction of the reflector that maps $\tilde{f}_1$ either to $c_1 e_1$, or to $-c_1 e_1$.

We would like to compute $d$ or $s$ accurately. First we need to compute $w^* \tilde{J}_k w$, where $w = \tilde{f}_1 \pm f_1$ (with the addition for $s$ and the subtraction for $d$). We have

\[ w^* \tilde{J}_k w = (\tilde{f}_1 \pm f_1)^* \tilde{J}_k (\tilde{f}_1 \pm f_1) = \tilde{f}_1^* \tilde{J}_k \tilde{f}_1 + f_1^* \tilde{J}_k f_1 \pm (\tilde{f}_1^* \tilde{J}_k f_1 + f_1^* \tilde{J}_k f_1). \]

Since $\tilde{f}_1$ and $f_1$ satisfy (5.3)–(5.4), the previous relation can be written as

\[ w^* \tilde{J}_k w = 2(\tilde{f}_1^* \tilde{J}_k \tilde{f}_1 \pm f_1^* \tilde{J}_k f_1) = 2(\tilde{f}_1^* \tilde{J}_k \tilde{f}_1 \pm \tilde{c}_1 \tilde{J}_11 \tilde{f}_11) \]

\[ = 2 \left( \tilde{f}_1^* \tilde{J}_k \tilde{f}_1 \pm \sqrt{|\tilde{f}_1^* \tilde{J}_k \tilde{f}_1|} \tilde{J}_11 \tilde{f}_11 \right) = 2 \left( \tilde{f}_1^* \tilde{J}_k \tilde{f}_1 \pm \sqrt{|\tilde{f}_1^* \tilde{J}_k \tilde{f}_1|} |\tilde{J}_11| |\tilde{f}_11| \right). \]

Since (5.3) should be valid, we have

\[ \text{sgn}(\tilde{f}_1^* \tilde{J}_k \tilde{f}_1) = \tilde{J}_11, \]

and both terms in the previous relation have the same sign. Therefore, to avoid unnecessary cancellation, our choice is $w = s$, and $H(s)$ from (5.2) is then equal to

\[ H(s) = I + \tau ss^* \tilde{J}_k, \quad \tau = -\frac{1}{fct}, \quad fct = \tilde{f}_1^* \tilde{J}_k \tilde{f}_1 + \sqrt{|\tilde{f}_1^* \tilde{J}_k \tilde{f}_1|} |\tilde{J}_11| |\tilde{f}_11|. \]
5.3.3. **Column updates by a reflector.** The update of a column $\tilde{f}_j$, $j > 1$, is performed as

$$H(s)\tilde{f}_j = \tilde{f}_j + \tau s(\tilde{J}_k \tilde{f}_j),$$

which involves computing the $\tilde{J}_k$-dot product of $s$ and $\tilde{f}_j$, scaling it by $\tau$, and calling the ZAXPY BLAS 1 routine. We opted for a sequential ZAXPY version, but it can be argued that for the extremely long columns a parallel version would be better suited.

The column updates are mutually independent, and therefore can be performed in a parallel-do loop over $j$, with the work being well balanced among the threads.

In our application it is not required that the reflector generators ($s_k$ and $\tau_k$ in the step $k$) are preserved, but that is nevertheless done with time overhead close to none in a separate complex matrix (the vector $s_k$ is stored in its $k$th column, with the leading rows set to 0) and a real vector (the scalar $\tau_k$ is stored as its $k$th element).

5.3.4. **2 × 2 pivots.** The situation is more complicated if a pair of pivot columns is chosen. According to [25], the reduction can be performed by the block Householder matrix defined by these two columns. However, the computation of a block Householder reflector is a more difficult approach than the computation of a variant of the URV factorization with $U$ hyperbolic, not unitary. The proposed factorization is similar, but not equal to the hyperbolic (sometimes also called signed) URV factorization presented in [28, 31].

**Definition 5.2.** Let $F \in \mathbb{C}^{m \times n}$, and $J \in \mathbb{Z}^{m \times m}$, $J = \text{diag}(\pm 1)$ be given matrices, and let $J' = P^TJP$ for any permutation matrix $P$. Factorization

$$F = URV,$$

where $U \in \mathbb{C}^{m \times m}$ is $J'$-unitary, $V \in \mathbb{C}^{n \times n}$ is unitary, and $R \in \mathbb{C}^{m \times n}$

$$R = \begin{bmatrix} R_0 \\ 0 \end{bmatrix},$$

where $R_0 \in \mathbb{C}^{n \times n}$ is upper triangular, is called $(J, I)$ URV factorization according to given $J$.

Note that the $(J, I)$ URV factorization is not unique.

The Grammian matrix $A_{12}$ of the pivot block $\tilde{F}_{12} := [\tilde{f}_1 \tilde{f}_2]$ (see Fig. 5.1)

$$A_{12} = \begin{bmatrix} f^*_1 \tilde{J}_k \tilde{f}_1 & f^*_1 \tilde{J}_k \tilde{f}_2 \\ f^*_2 \tilde{J}_k \tilde{f}_1 & f^*_2 \tilde{J}_k \tilde{f}_2 \end{bmatrix}$$

is nonsingular. Since the pivot strategy has chosen this block for the pivot block, the off-diagonal elements are larger in magnitude than the diagonal elements of $A_{12}$. The matrix $A_{12}$ will be diagonalized by a single Jacobi rotation $R_k$, 

$$R_k^* A_{12} R_k = R_k^* \tilde{F}_{12} \tilde{J}_k \tilde{F}_{12} R_k = \text{diag}(d_k, d_{k+1}).$$

This shows that the columns

$$[\tilde{f}_1 \tilde{f}_2] := \tilde{F}_{12} R_k$$

are mutually $\tilde{J}_k$ orthogonal – their scalar product is zero, and the squares of their $\tilde{J}_k$ norms are $d_k$ and $d_{k+1}$, respectively. Since these columns are mutually $\tilde{J}_k$ orthogonal, the only way to handle them is applying two successive hyperbolic Householder transformations to reduce the pivot matrix $\tilde{F}_{12}$ to an upper triangular matrix $\tilde{F}_{12}$. 
The first hyperbolic transformation, by \( H(s_k) \), reduces the first column to a single element. Then, the second hyperbolic transformation, by \( H(s_{k+1}) \), reduces the elements, already transformed by \( H(s_k) \), of the shortened (the first row of \( \tilde{F}_{12} \) is not changed anymore) second column.

Finally, we should multiply \( \tilde{F}_{12} \) by \( R_k^* \) to obtain the reduced matrix \( F_{12} \) with, generally full, topmost \( 2 \times 2 \) block

\[
F_{12} := \tilde{F}_{12}R_k^* = \begin{bmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \end{bmatrix}.
\]

Then, the step counter \( k \) is incremented by 2 (instead of 1 for a single pivot), and the process continues again with the column pivoting, as in subsection 5.2.

5.3.5. Wrapping up. When present, the multiplications from right, first by the Jacobi rotation \( R_k \), and then by \( R_k^* \), cancel each other (since \( R_k R_k^* = I_2 \)), so the right matrix \( V \) in this URV-like factorization is in fact identity.

The Jacobi rotations are applied by calling the parallel \texttt{ZROT} routine, but should the columns be short enough, a sequential version of the routine could be warranted.

After the final step of the reduction (for \( k = n \)), the new \( F \) and \( J \) are square matrices of order \( n \). More precisely, \( J \) is the leading part of \( \tilde{J} \) as left after all permutations due to the row pivoting, and \( F \), unlike the standard compact representation of the LAPACK’s QR factorizations, has zeroes below the diagonal block set explicitly.

5.4. Testing. In Table 5.1 the wall execution time of both the JQR and the TSQR for 32 and 64 threads is shown. It is evident that there is still room for the JQR’s efficiency improvement, which might be achieved, e.g., by blocking and delaying the columns updates. However, that is left for future work.

| ID | JQR wtime [s] | TSQR wtime [s] | \( \tilde{G}P_2 \) wtime [s] | 2 \times 2 pivots |
|----|--------------|----------------|----------------------------|-----------------|
| A1 | 166.054482 | 186.194647 | 9.977216 | 7.008014 | 0.396921 | 11 |
| A2 | 454.877289 | 501.898283 | 14.175633 | 8.055503 | 0.673552 | 9 |
| A3 | 1068.114470 | 1125.761739 | 21.076636 | 14.741344 | 1.396966 | 7 |
| A4 | 2174.316943 | 2222.306937 | 41.335779 | 28.427826 | 2.000921 | 6 |
| B1 | 182.819958 | 182.125339 | 11.808603 | 12.103482 | 0.061961 | 16 |
| B2 | 525.235514 | 508.890242 | 15.906218 | 11.596856 | 0.626455 | 16 |
| B3 | 1292.151319 | 1199.613560 | 36.314596 | 21.722369 | 1.699456 | 20 |
| B4 | 2803.932457 | 2504.247016 | 49.387198 | 32.731226 | 3.217564 | 16 |

5.4.1. Prepermuting of \( \tilde{G} \). Table 5.1 also contains the wall time of preparing \( \tilde{G}P_2 \) in parallel. The fastest way to prepermute the columns of \( \tilde{G} \) is to copy them to
another matrix of the same size, with the column \( j \) going to \( \pi_2(j) \), where \( \pi_2 \) denotes the permutation represented by \( P_2 \). Such copying occurs in a parallel-do loop over \( j \).

6. Phase 3 – generalized hyperbolic SVD. Vjeran Hari in his PhD thesis \([12]\) has developed a method for solving the generalized eigenproblem, when at least one of the two matrices is positive definite. The method is based on the ideas from the PhD thesis of Katharina Zimmermann \([32]\), and has been revisited recently in \([13]\).

Based on the Hari–Zimmermann algorithm for the generalized eigenproblem, in \([21]\) a one-sided method for computing the real generalized SVD has been derived. The main trick, how to obtain a one-sided method for the SVD from the two-sided method for the eigenproblem is always the same: think about the transformations in the two-sided fashion, and apply them from one (right or left) side on a matrix factor.

Since the elements of the pivot submatrices \( H_{pq} \) of \( H \) and \( S_{pq} \) of \( S \) are the scalar products of the columns of \( F \) and \( G \), respectively, it is easier to write the transformations in terms of the elements of \( H_{pq} \) and \( S_{pq} \):

\[
H_{pq} = \begin{bmatrix} h_{pp} & h_{pq} \\ h_{qp} & h_{qq} \end{bmatrix} = \begin{bmatrix} f_p^* J_f p & f_p^* f_q \\ f_q J_f q & f_q^* f_q \end{bmatrix}, \quad S_{pq} = \begin{bmatrix} s_{pp} & s_{pq} \\ s_{qp} & s_{qq} \end{bmatrix} = \begin{bmatrix} g_p^* g_q & g_p g_q \\ g_p g_q & g_q g_q \end{bmatrix},
\]

instead of in terms of the columns \( f_p, f_q, g_p, \) and \( g_q \).

The original method consists of 3 active transformations, and an auxiliary transformation that helps in coupling them all together.

6.1. Pointwise algorithm. The whole pointwise algorithm (with a pair of \( 2 \times 2 \) pivot submatrices in each annihilation step) is taken from the PhD thesis of Vjeran Hari \([12]\). However, we feel that the algorithm should be presented succinctly here, to aid its implementors, and also to incorporate some minor corrections.

6.1.1. Preprocessing. In the preprocessing step, \( H \) and \( S \) are scaled by a diagonal matrix \( D \) such that \( \text{diag}(DSD) = I \), i.e.,

\[
H_0 := DH \mathcal{D}, \quad S_0 := \mathcal{D}SD, \quad D = \begin{bmatrix} 1/\sqrt{s_{11}} & 1/\sqrt{s_{22}} & \ldots & 1/\sqrt{s_{nn}} \end{bmatrix}.
\]

Such preprocessing can be done only once, at the start of the algorithm, or it can be done before each annihilation step for the pivot column pair in question. The latter might seem redundant, but in a floating-point realization of the algorithm, after enough steps, \( \text{diag}(DSD) \) could veer off the identity enough to warrant such a rescaling. In that case, form a matrix \( D_0 \) that has, for the chosen pivot indices \( (p, q) \), as its \( p \)th and \( q \)th diagonal entries \( 1/\sqrt{s_{pp}} \) and \( 1/\sqrt{s_{qq}} \), respectively, while being equal to the identity elsewhere. For the approach with a single rescaling, let \( D_0 = I \).

In both cases, let \( \tilde{D}_0 \) be a \( 2 \times 2 \) restriction of \( D_0 \) to the \( p \)th and the \( q \)th row and column. We have implemented the pivot pair rescaling in each annihilation step.

6.1.2. Diagonalization of \( \tilde{S}_0 \). In the first step the \( 2 \times 2 \) pivot submatrix \( \hat{S}_0 \) of \( S_0 \) (at the crossings of the \( p \)th and the \( q \)th rows and columns) is diagonalized by a complex Jacobi rotation

\[
\hat{R}_1 = \begin{bmatrix} \cos \varphi_1 & e^{i\beta_1} \sin \varphi_1 \\ -e^{-i\beta_1} \sin \varphi_1 & \cos \varphi_1 \end{bmatrix}.
\]

The same transformation is then applied to \( H_0 \), to keep the new pair equivalent to the original one. After that, the new pair is

\[
H_1 = R_1^* H_0 R_1, \quad S_1 = R_1^* S_0 R_1,
\]
where \( R_1 = I \), except at the pivot positions, where \( R_1 = \hat{R}_1 \). Since \( H \) and \( S \) have been preprocessed as in subsection 6.1.1, the diagonal elements of \( \hat{S}_0 \) are the same, and we may choose \( \varphi_1 = -\pi/4 \). Therefore, (6.1) could be written as

\[
\hat{R}_1 = \frac{\sqrt{2}}{2} \begin{bmatrix}
1 & -e^{i\beta_1} \\
e^{-i\beta_1} & 1
\end{bmatrix}.
\]

Now it is easy to determine that

\[
\beta_1 = \arg(s_{pq}).
\]

If \( s_{pq} \), written in the trigonometric form, was \( s_{pq} = xe^{i\beta_1} \), with \( x = |s_{pq}| \), before the transformation, then after it we obtain

(6.2)

\[
\hat{S}_1 = \text{diag}(1 + x, 1 - x).
\]

6.1.3. Rescaling of \( \hat{S}_1 \). The second step rescales the diagonal of \( S_1 \) to ones, and rescales \( \hat{H}_1 \) with the same diagonal matrix. After the transformation, similar to the preprocessing step, we obtain

\[
H_2 := D_2 H_1 D_2, \quad S_2 := D_2 S_1 D_2.
\]

From (6.2) we conclude that

\[
\hat{D}_2 = \text{diag} \left( \frac{1}{\sqrt{1 + x}}, \frac{1}{\sqrt{1 - x}} \right).
\]

Elements of \( \hat{H}_2 \) are

(6.3)

\[
\hat{H}_2 = \begin{bmatrix}
\hat{h}_{pp}^{(2)} & \hat{h}_{pq}^{(2)} \\
\hat{h}_{pq}^{(2)} & \hat{h}_{qq}^{(2)}
\end{bmatrix} = \begin{bmatrix}
\frac{1}{1 + x} \left( \frac{b_{pp} + b_{qq}}{2} + u \right) & \frac{e^{i\beta_1}}{\sqrt{1 - x}} \left( \frac{b_{pp} - b_{qq}}{2} + iv \right) \\
\frac{e^{-i\beta_1}}{\sqrt{1 - x}} \left( \frac{b_{pp} - b_{qq}}{2} - iv \right) & \frac{1}{1 - x} \left( \frac{b_{pp} + b_{qq}}{2} - u \right)
\end{bmatrix},
\]

where

(6.4)

\[
u + iv = e^{-i\beta_1} h_{pq} = e^{-i \arg(s_{pq})} h_{pq}.
\]

6.1.4. Diagonalization of \( \hat{H}_2 \). In the third step the pivot submatrix \( \hat{H}_2 \) of \( H_2 \) is diagonalized by a complex Jacobi rotation

(6.5)

\[
\hat{R}_3 = \begin{bmatrix}
\cos \varphi_3 & e^{i\alpha_3} \sin \varphi_3 \\
-e^{-i\alpha_3} \sin \varphi_3 & \cos \varphi_3
\end{bmatrix}.
\]

The third transformation can be written as

\[
H_3 = R_3^* H_2 R_3, \quad S_3 = R_3^* S_2 R_3,
\]

where \( R_3 = I \), except at the pivot positions, where \( R_3 = \hat{R}_3 \). If we express \( \varphi_3 \) as \( \varphi_3 = \vartheta + \pi/4 \), then (6.3) can be written as

\[
\hat{R}_3 = \begin{bmatrix}
\cos \left( \vartheta + \frac{\pi}{4} \right) & e^{i\alpha_3} \sin \left( \vartheta + \frac{\pi}{4} \right) \\
-e^{-i\alpha_3} \sin \left( \vartheta + \frac{\pi}{4} \right) & \cos \left( \vartheta + \frac{\pi}{4} \right)
\end{bmatrix}.
\]
The relations for the angles of a rotation that annihilates the off-diagonal element of $\hat{H}_2$ are given by

\begin{equation}
\tan\left(2\vartheta + \frac{\pi}{2}\right) = \frac{2|\hat{H}_{pq}^{(2)}|}{\hat{H}_{qq}^{(2)} - \hat{H}_{pp}^{(2)}}, \quad \alpha_3 = \beta_1 + \arg\left(\frac{\hat{H}_{pq}^{(2)}}{\hat{H}_{pp}^{(2)}}\right) + (1 - \sigma)\frac{\pi}{2},
\end{equation}

where $h = \hat{H}_{qq} - \hat{H}_{pp}$. The requirement

\begin{equation}
\gamma := \alpha_3 - \beta_1 \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)
\end{equation}

yields

\begin{equation}
\sigma = \begin{cases} 
1, & h \geq 0, \\
-1, & h < 0.
\end{cases}
\end{equation}

This choice of $\sigma$ and the constraint $\vartheta \in (-\pi/4, \pi/4]$ ensures the convergence of the algorithm (see [12]).

Since

$$
\tan\left(2\vartheta + \frac{\pi}{2}\right) = -\cot(2\vartheta) = -\frac{1}{\tan(2\vartheta)},
$$

then, from (6.3) and (6.6), we obtain

\begin{equation}
\tan(2\vartheta) = \frac{2u - (h_{pp} + h_{qq})x}{t\sqrt{h^2 + 4v^2}}, \quad t := \sqrt{1-x^2},
\end{equation}

After the first three steps, the pivot submatrix $\hat{S}_3$ is still diagonal (in fact identity), i.e., $\hat{S}_3 = \hat{R} \hat{S}_0 \hat{R} = I$, where

\begin{equation}
\hat{R} = \hat{R}_1 \hat{D}_2 \hat{R}_3
\end{equation}

This constructively shows that $\hat{R}$ diagonalizes the matrix pair $(\hat{H}_0, \hat{S}_0)$.

**6.1.5. Expressing $\hat{R}$ as a single matrix.** Hari in [12, Theorem 2.2] has proved the form of the general nonsingular matrix that diagonalizes a $2 \times 2$ Hermitian positive definite matrix. The intention of representing $\hat{R}$ as

\begin{equation}
\hat{R} = \frac{1}{t} \begin{bmatrix} \cos \varphi & e^{i\sigma} \sin \varphi \\
-e^{-i\beta} \sin \psi & \cos \psi \end{bmatrix} \text{diag}(e^{i\sigma_p}, e^{i\sigma_q})
\end{equation}
is to simplify (6.10). By a comparison of the elements of (6.10) and (6.11), after a tedious computation, we obtain

\[
\cos \varphi = \frac{1}{\sqrt{2}} \sqrt{1 + x \sin(2\theta) + t \cos \gamma \cos(2\theta)}, \quad 0 \leq \varphi < \frac{\pi}{2},
\]

\[
\cos \psi = \frac{1}{\sqrt{2}} \sqrt{1 - x \sin(2\theta) + t \cos \gamma \cos(2\theta)}, \quad 0 \leq \psi < \frac{\pi}{2},
\]

\[
e^{i\alpha} \sin \varphi = e^{i\beta}\cos \psi \frac{(\sin(2\theta) - x) + it \sin \gamma \cos(2\theta)}{1 - x \sin(2\theta) + t \cos \gamma \cos(2\theta)},
\]

\[
e^{-i\beta} \sin \psi = e^{-i\beta}\cos \varphi \frac{(\sin(2\theta) + x) - it \sin \gamma \cos(2\theta)}{1 + x \sin(2\theta) + t \cos \gamma \cos(2\theta)}.
\]

(6.12)

Since in (6.12) we need only \(\sin \gamma \cos \gamma\), from (6.6) it then follows

\[
(6.13) \quad \tan \gamma = 2 \frac{v}{h}.
\]

6.1.6. Forming \(\hat{Z}'\). The fourth step only deals with a formal simplification of \(\hat{R}\), by introducing a transformation \(\Phi_4\) such that

\[
H_4 = \Phi_4^* H_3 \Phi_4, \quad S_4 = \Phi_4^* S_3 \Phi_4.
\]

The matrix \(\Phi_4\) is a diagonal matrix equal to identity, except at pivot positions, where

\[
\hat{\Phi}_4 = \text{diag}(e^{-i\sigma_p}, e^{-i\sigma_q}).
\]

Obviously, if \(\hat{R}\) diagonalizes the pair \((\hat{H}_0, \hat{S}_0)\), then the transformation

\[
\hat{Z} = \hat{R} \hat{\Phi}_4 = \frac{1}{r} \begin{bmatrix}
\cos \varphi & e^{i\alpha} \sin \varphi \\
-e^{-i\beta} \sin \psi & \cos \psi
\end{bmatrix}
\]

will leave the final diagonal matrices intact. Then, let \(\hat{Z}' = \hat{D}_0 \hat{Z}\).

6.1.7. Exceptional cases. There can be a few exceptions in the computations of the elements of the matrix \(\hat{Z}\) which have to be accounted for in the algorithm.

If \(h_{pq} = s_{pq} = 0\), we have nothing to do, since both pivot submatrices are already diagonal. In that case the transformation is voided by formally setting \(\varphi = \psi = \alpha = \beta = 0\). We could still apply the scaling by \(\hat{D}_0\), but not count that as a transformation.

If \(h_{pq} \neq 0\), but \(s_{pq} = 0\) (i.e., \(x = 0\)), we only need to determine \(\hat{Z}\) as an ordinary Jacobi rotation that diagonalizes \(\hat{H}_0\). The computation does not need to diverge into a special case handler, though, if we set \(\beta_1 = 0\) and proceed as described above.

If \(h = v = 0\) in (6.13), i.e., when \(\arg s_{pq} = \arg h_{pq}\) and \(h_{pp} = h_{qq}\), it can be shown that \(\hat{R}_1\), the Jacobi rotation that diagonalizes \(\hat{S}_0\), also diagonalizes \(\hat{H}_0\), so \(\hat{Z} = \hat{R}_1 \hat{D}_2\).
**6.1.8. Convergence criterion.** As in [21], the convergence criterion in floating-point arithmetic has to take into account the relative magnitudes of the off-diagonal elements, compared to the diagonal ones, in the pivot pairs. Therefore, a pivot pair undergoes the transformation if, for the machine precision $\varepsilon$,

\begin{equation}
|h_{pq}| \geq \max\{|h_{pp}|, |h_{qq}|\} \cdot (\varepsilon\sqrt{n}) \cdot \min\{|h_{pp}|, |h_{qq}|\} \quad \text{or} \quad |s_{pq}| \geq \varepsilon\sqrt{n}.
\end{equation}

If $\hat{Z}'$ turns out to be identity, it is not applied. If $\cos \varphi = \cos \psi = 1$, such transformation is considered “small”, and “big” otherwise. Near the end of the process, the transformations turn out to be small, and (in a blocking variant, the last level of) the algorithm is stopped when no big transformations are encountered in a sweep, to avoid perpetually applying the transformations that spring only from the accumulation of the rounding errors. With blocking, the inner level(s) of the algorithm count all transformations (big and small) in a sweep for stopping. For details, see [21, 19].

**6.1.9. Outputs.** The algorithm stops when the columns of $F$ and $G$ are numerically mutually $J$-orthogonal, and orthogonal, respectively. Let $F'$ and $G'$ be the final, in-place transformed matrices, and let $Z'$ be the accumulated product of the applied transformations. Then,

$$
\Sigma_F' = \text{diag} \left( \sqrt{|f_{11}^* Jf_1|}, \ldots, \sqrt{|f_{n1}^* Jf_n|} \right), \quad \Sigma_G' = \text{diag} \left( \sqrt{|g_{11}^* g_1|}, \ldots, \sqrt{|g_{n1} g_n|} \right),
$$

$$
U = F' \Sigma_F'^{-1}, \quad V = G' \Sigma_G'^{-1}, \quad \Sigma_j = \sqrt{(\Sigma_F')_j^2 + (\Sigma_G')_j^2}, \quad \Sigma = \text{diag} (\Sigma_1, \ldots, \Sigma_n), \quad \Sigma_F = \Sigma_F' \Sigma^{-1}, \quad \Sigma_G = \Sigma_G' \Sigma^{-1}, \quad \text{and} \quad Z = Z' \Sigma^{-1}.
$$

For the inner levels of blocking, only the matrix $Z$ (and therefore also $\Sigma_F', \Sigma_G', \text{ and } \Sigma$) is required.

Observe that $Z'^{-1}$ could be also obtained, by accumulating $\hat{Z}'$ transformations from the right and their inverses $\hat{Z'}^{-1}$ from the left. Then, $X = Z^{-1} = Z \Sigma^{-1}$, so Phase 4 would not be needed for the full G(H)SVD. However, since our main concern is a solution of the generalized eigenproblem, that approach has not been implemented.

**6.1.10. The G(H)SVD algorithm.** After obtaining the matrix $\hat{Z}'$, the pointwise implicit Hari–Zimmermann G(H)SVD algorithm can be written similarly to [21, Algorithm 3.1]. In Algorithm 6.1 we take into account the signature matrix $J$, since $H = F^* J F$, but with $J = I$ it reduces to a generalized SVD method.

If the prescaling as described in subsection 6.1.1 is performed only once, then in Algorithm 6.1 only $g_p g_q$ is computed, since the diagonal elements of $\hat{S}$ are assumed to be unity. Otherwise, by passing once through the columns $g_p$ and $g_q$ all three dot products can be formed. Similar holds for $f_p, f_q$, and the three $J$-dot products of $\hat{H}$.

**6.2. Vectorization.** Many computational building blocks of Algorithm 6.1 provide both the challenges and the opportunities for the SIMD vectorization. The most obvious such primitives are the $J$-dot products (and norms), which are computed combining the approaches presented in subsections 5.1 (for the unstructured patterns of signs in $J$) and 4.6.1 for a compact, partitioned representation of $J$ with only a number $n_+$ of the leading positive (and therefore $n - n_+$ tailing negative) signs.

**6.2.1. Applying $\hat{Z}'$.** The column updates by $\hat{Z}'$ cannot be realized by a simple call to a LAPACK routine (e.g., ZROT), since there are two angles involved in a transformation, and the columns are meant to be transformed in-place (overwritten). For that purpose, a ZVRROT routine has been implemented as a vectorized loop, that resembles a simplified version of the BLAS routine DROT, but with the complex sines.
Algorithm 6.1 The pointwise implicit Hari–Zimmermann G(H)SVD algorithm.

\[ Z' = I; \text{optional computing of } D \text{ and prescaling } H_0 = DHD, S_0 = DSD, Z' = D; \]

\[ it = 1; \{ \text{The sweep counter. Maximal number of sweeps, maxcyc, is usually } \approx 30. \} \]

repeat
  for all pairs \((p, q), 1 \leq p < q \leq n\) do
  \[ \text{compute } \tilde{H} = \begin{bmatrix} f_p J f_p & f_p J f_q \\ f_q J f_p & f_q J f_q \end{bmatrix}; \]
  \[ \text{compute the elements of } \tilde{Z}' \text{ from } (6.4), (6.7)–(6.9), (6.12)–(6.13); \]
  \[ [f_p, f_q] = [f_p, f_q] \cdot \tilde{Z}'_0; \]
  \[ [g_p, g_q] = [g_p, g_q] \cdot \tilde{Z}'_0; \]
  \[ [z_p', z_q'] = [z_p', z_q'] \cdot \tilde{Z}'_0; \]
end for
until (no transformations in this sweep) or (it > maxcyc)
Output: Z and (optionally) U, V, Σ_F, Σ_G, and Σ;

6.2.2. Computing \(\tilde{Z}'\). The greatest challenge lies in computing the transformations in the SIMD-parallel way, where each vector lane computes \(\tilde{Z}'_l\) for its own pivot pair with indices \((p_l, q_l)\). For now, assume that \(v\) pivot pairs \((\tilde{H}_l, \tilde{S}_l)\) have been obtained, with their corresponding \(p_l\) and \(q_l\) indices all different. If in reality there are fewer than \(v\) such pairs, let \(H_l = S_l = I\) for the missing indices (i.e., lanes) \(i\).

Note that all values have to be kept in the properly aligned arrays of length \(v\), in which the \(i\)th position holds data for the \(i\)th lane. To help the compiler, we have also opted for a handwritten implementation of the complex arithmetic operations in terms of the real and the imaginary parts of the complex numbers in all “manually” vectorized parts of the code. For example, the real part of \(\tilde{S}_{12}^{[i]} = g_p, g_q\), is held in \(\text{RE}_S_{PQ}(i)\), and the imaginary part in \(\text{IM}_S_{PQ}(i)\), with the array names in capitals.

For the start, check for which lanes their pivot pair has to be transformed by evaluating the criterion (6.14) in each lane. To aid the compiler, (6.14) can be rewritten as a branch-free arithmetic expression that has a non-zero value if and only if the criterion is fulfilled. If those values constitute a zero vector, no transformation is required for any \(i\), and a fresh set of pivot pairs (if any remain) should be considered.

Then, compute \(\tilde{Z}'_i\) unconditionally (i.e., for all \(i\)). The idea is that the unneeded computation comes at no cost, while its results can be discarded afterwards. However, the exceptional cases from subsection 6.1.7 should be carefully dealt with, since a naïve branching might spoil the vectorization opportunities. The logical conditions are therefore arithmetized, while halting on the arithmetic exceptions is suppressed.

For example, when calculating the polar form of \(\tilde{S}_{12}^{[i]} = |\tilde{S}_{12}^{[i]}| e^{i \phi_i}\), a division of the real and the imaginary part by the absolute value can be undefined (yield a Not-a-Number) if \(\tilde{S}_{12}^{[i]} = 0\). If we denote \(\cos \phi_i\) by \(\text{CA}_S_{PQ}(i)\), then selecting a default of \(\cos \phi_i = 1\) can be done by presetting the variable to 1, and taking \(\text{CA}_S_{PQ}(i) = \text{MIN}(\text{value}(i), \text{CA}_S_{PQ}(i))\), where \(\text{value}\) is obtained by the vector division (or the multiplication by the reciprocal), if the compiler returns the second argument when the first argument of \(\text{MIN}\) is a NaN\(^1\). For \(\sin \phi_i\), the default value can be also set to

\(^1\)A behavior not mandated for the \text{MIN} and \text{MAX} intrinsics by the Fortran standard, but observed with the GNU 8, Intel 19, and PGI 19 compilers, at least, and required at runtime by our code.
1 (we in fact want 0), but the final value is obtained by multiplying the result by a variable that is 0 if $\hat{S}^{[i]}_{12} = 0$, and otherwise is 1 (set in the process of checking (6.14)).

The most complex case arises when, in (6.13), $v_i = 0$, so $\tan \gamma_1 = \text{NaN}$. The expression $B(i) = (1 - \text{MAX}(V(i)/V(i),0)) \times (1 - \text{MAX}(H(i)/H(i),0))$ evaluates to 1 in such a case, and also if $h_i = \pm \infty$ (due to an overflow) with $v_i = 0$; otherwise, it is 0. The computation resumes regardless of $B(i)$. However, $\hat{Z}'_i$ in those lanes where $B(i) = 1$ consists of useless data, so a new, correct $\hat{Z}'_i$ is taken according to the rules of subsection 6.1.7 at the end, sequentially for all such $i$. That is the only exception when $\hat{Z}'_i$ is not computed in one go for all $i$, but it should occur rarely in practice.

6.3. Parallelization. There are $n := n(n - 1)/2$ pairs of indices $(p_i, q_i)$ such that they belong to a strictly upper triangle (i.e., $1 \leq p_i < q_i \leq n$) of the square matrices of order $n$. Let $P := \{(p_i, q_i): 1 \leq i \leq n\}$ be a set of those index pairs. At most $[n/2]$ such pairs can be chosen from $P$ so that all their indices are distinct.

Let $S_j$, for some $j \geq 1$, be a set of at most $[n/2]$ index pairs, with all indices distinct. Then, the pivot pairs formed from the columns of $F$ and $G$ and indexed by the elements of $S_j$ can be transformed concurrently. We call $S_j$ the $j$th parallel Jacobi step, and a sequence of steps $S := \{S_1, S_2, \ldots, S_n\}$ a parallel (quasi-)cyclic Jacobi strategy if $\bigcup_j S_j = P$, and under assumption that the sequence is repeated forever in principle (or, in practice, until the convergence criteria are met). A strategy is called cyclic if its steps are mutually disjoint; else, it is called quasi-cyclic. In a cycle (also called a sweep) all pivot pairs are accessed (at least once, but maybe more under a quasi-cyclic strategy), in $\bar{n} \geq n - 1$ steps. We aim for the steps as large as possible.

6.3.1. Bordering. For an odd $n$, no more than $(n - 1)/2$ pairs fit into a step, so $\bar{n} \geq n$. We therefore consider the strategies for even $n$ only, with the steps of size $n/2$, and when necessary border the matrices by appending a zero column and a zero row, except for the new element at position $(n + 1, n + 1)$, which is set to unity.

6.3.2. Parallel strategies. There are a few classes of the parallel Jacobi strategies to choose from. We opted for testing two of them: the modified modulus strategy (MM), as described in, e.g., [21], and a generalization of the Mantharam–Eberlein strategy [18] (ME), as described in [19]. The former is a quasi-cyclic strategy with $\bar{n} = n$, but easily generated on-the-fly as the computation progresses. The latter is cyclic, attains $\bar{n} = n - 1$, has provided a faster execution (compared to MM) to the one-sided Jacobi SVD, with more accurate results, but it needs to be pretabulated, is not readily available for all even $n$, and no convergence results have yet been proven.

6.3.3. Vector-Parallel algorithm. Let a step $S_j$, with $k_1 := n/2$ index pairs, be given. Then, partition $S_j$ into $k_v := [k_1/v]$ disjoint subsets $V_k$, where each subset has at most $v$ pairs, i.e., $S_j = (V_1, V_2, \ldots, V_{k_v})$. For each subset, the requirements for the vectorized computation of $\hat{Z}'$ as described in subsection 6.2.2 are satisfied.

Now, let $t \geq 1$ be a number of available (OpenMP) threads. Then, $S_j$ is traversed with a parallel-do loop over the subsets, where a thread takes a chunk of subsets to be processed independently, while the subsets within a chunk are handled in sequence.

A sweep of such Vector-Parallel (VP) variant is shown in Algorithm 6.2. Note that each thread has to have a private set of vector variables, which is most easily done by reserving a $v \times t$ rank-2 array for each variable and making the $l$th thread access the $l$th column of such an array, where $l$ is a thread’s unique number, $1 \leq l \leq t$.

6.4. Blocking. To better exploit the memory hierarchy by keeping data in the cache(s) longer, a multilevel blocking principle can be applied, with the Level 1 being
Algorithm 6.2 A sweep of the Vector-Parallel implicit HZ algorithm.

for all steps $S_j \in S$, $1 \leq j \leq n$ do \{a sequential loop over the steps of $S$\}

for all subsets $V_k \in S_j$, $1 \leq k \leq k_j$ do \{an OpenMP parallel do with $t$ threads\}

for all $(p_i, q_i) \in V_k$, $1 \leq i \leq |V_k| \leq v$ do \{a sequential loop over $V_k$\}

get $\hat{H}_i = \begin{bmatrix} \hat{f}_{p_i} \hat{f}_{q_i} \\ \hat{f}_{p_i} \hat{f}_{q_i} \end{bmatrix}$; $\hat{S}_i = \begin{bmatrix} \hat{g}_{p_i} \hat{g}_{q_i} \end{bmatrix}$; \{vectorized $a^*(J)h$\}

end for

for all $(p_i, q_i) \in V_k$, $1 \leq i \leq |V_k| \leq v$ do \{a SIMD parallel do over $V_k$\}

check the transformation criterion (6.14);

end for

if no pivot pairs have to be transformed, cycle; \{a reduction\}

for all $(p_i, q_i) \in V_k$, $1 \leq i \leq |V_k| \leq v$ do \{a SIMD parallel do over $V_k$\}

compute the elements of $\hat{Z}_i^t$ from (6.4), (6.7)–(6.9), (6.12)–(6.13);

end for

for all $(p_i, q_i) \in V_k$, $1 \leq i \leq |V_k| \leq v$ do \{a sequential loop over $V_k$\}

check if $\hat{Z}_i^t$ has to be corrected and cycle if $\hat{Z}_i^t = I$

$[f_{p_i}, f_{q_i}] = [f_{p_i}, f_{q_i}] \cdot \hat{Z}_i^t$; \{ZVROT\}

$[g_{p_i}, g_{q_i}] = [g_{p_i}, g_{q_i}] \cdot \hat{Z}_i^t$; \{ZVROT\}

$[z^*_p, z^*_q] = [z^*_p, z^*_q] \cdot \hat{Z}_i^t$; \{ZVROT\}

end for

end for

end for



the pointwise algorithm in its VP variant. In the next, second level of the algorithm the block columns of width $w \geq 1$ take place of the single columns, and the $2 \times 2$ pivot pairs are replaced by $(2w) \times (2w)$ block pivots. The same principle can be applied recursively further (e.g., see [19]), but we consider only the Level 2 algorithms here.

6.4.1. Block-column partitioning. There are two ways a matrix can be partitioned into block columns. The first one is to prescribe $w$, and then split the matrix into at least $\lfloor n/w \rfloor$ block columns of width at most $w$, bearing in mind that the number of block columns has to be even, as explained in subsection 6.3.1, and reducing the maximal width accordingly. For $w \geq 2$, all block columns can be made to contain either $w$ or $w - 1$ (but no less) columns by redistributing their individual widths.

The second way, and the one we have chosen to implement, is to query at runtime a number $t$ of threads to be used. A thread $l$ is to be assigned one pair of block columns with the block indices $(p_{jl}, q_{jl})$ in the $j$th block step, so the maximal width $w$ is computed as $\lfloor n/(2t) \rfloor$, with exactly $2t$ block columns. The block column widths $w_i$ are non-increasing across the whole partition and are equal to either $w$ or $w - 1$.

The blocking overhead can dominate the actual computation time for the matrices small enough, so we assume that $n > 2t$, and suggest a pointwise algorithm otherwise.

Each thread allocates a contiguous storage (in its own NUMA region, but visible to the other threads) for $2w$ columns (two block columns of the maximal width) of $F$, and similarly for $G$ and $Z$. The same amount of memory, and of the same shape, is additionally allocated for the columns of the “shadow” matrices $F$, $G$, and $Z$. Let, for the $l$th thread in the $j$th step of the $s$th block sweep, the contents of that storage be named $X_{jl}^{[s]} := \begin{bmatrix} X_{p_{jl}}^{[s]} \\ X_{q_{jl}}^{[s]} \end{bmatrix}$, with $X \in \{F, G, Z, F, G, Z\}$. If $w_{p_{jl}} = w - 1$, the columns of $X_{p_{jl}}$ are placed from the second column of $X_{jl}$, while the columns of $X_{q_{jl}}$ are always
placed from the column \( w + 1 \) of \( X_j \). That way all the columns of a block column pair are stored contiguously and can be viewed by the BLAS routines as a single matrix.

The storage for the block pivots and for the workspaces, along with a copy of \( J \) and the strategy tables, is also preallocated per thread, in MCDRAM if possible. There are two strategy tables; one for the outer, Level 2 Jacobi strategy \( S^{[2]} \), and one for the inner, Level 1 strategy \( S^{[1]} \), which do not have to belong to the same class. The tables are fully initialized, with all the (block) steps, before the start of the iterations.

The initial data for \( F^{[1]}_I \) and \( G^{[1]}_I \) is loaded from the block columns \( (p_I, q_{11}) \in S^{[2]}_I \), \( Z^{[1]}_I \) is initialized to a corresponding part of \( I_n \), while \( F^{[1]}_I \), \( G^{[1]}_I \), and \( Z^{[1]}_I \) are undefined.

6.4.2. Forming the block pivots. In a step \( j \) (of a block sweep \( s \), which index we omit from the superscripts of the matrices for simplicity when it is implied by the context), the \( i \)th thread shortens its \( J \) to \( \hat{J}_I \) and its block column pairs from \( F_j \) to \( \hat{F}_I \) such that \( \hat{H}_I := \hat{F}_I^* \hat{J}_I \hat{F}_I = F_j^* J F_j \), and \( G_I \) to \( \hat{G}_I \) such that \( \hat{S}_I := \hat{G}_I^* \hat{G}_I = G_j^* G_j \), where \( \hat{F}_I \) and \( \hat{G}_I \) are both square, of order \( 2w \) or \( 2(w-1) \) (the order in between the two is necessarily odd, so the bordering from subsection 6.3.1 should then be applied).

There are two ways to shorten the block column pairs. The more efficient one is to form \( \hat{H}_I \) and \( \hat{S}_I \) explicitly. To do that, \( F_j^* \) is copied to \( \hat{F}_I \), and then the rows of \( F_j \) are scaled by \( J \). Here, it is beneficial to have \( J \) in the compact, run-length encoded form. Then, a single (parallel, or in our case, sequential) ZGEMM call computes \( \hat{H}_I = F_j^* (J F_j) \) and stores it temporarily into \( \hat{G}_I \). Then, \( \hat{F}_I \) and \( \hat{J}_I \) (partitioned to the positive and the negative sign block) are obtained by the Hermitian indefinite factorization with complete pivoting (see section 4), \( \hat{H}_I = \hat{F}_I^* \hat{J}_I \hat{F}_I \). The factorization should reveal if \( \hat{H}_I \) is rank deficient, in which case the process stops (the computation could be retried with the (J)QR approach, as below, if the input data has been preserved). Finally, \( \hat{F}_I \) is copied, with the transposition and the complex conjugation applied, to \( \hat{F}_I \).

A simpler procedure is used for \( \hat{G}_I \). It suffices to compute \( G_I^* G_I \) by a single (parallel, or in our case, sequential) ZHERK call, store \( \hat{S}_I \) temporarily to \( \hat{Z}_I \), and perform either the diagonally-pivoted Cholesky factorization, or even the Hermitian indefinite factorization with complete pivoting, to obtain \( \hat{S}_I = \hat{G}_I^* \hat{G}_I \). If \( \hat{S}_I \) is rank deficient of indefinite, the algorithm stops**. Otherwise, \( \hat{G}_I \) is copied, with the transposition and the complex conjugation applied, to \( \hat{G}_I \). A ZLASSET call finally initializes \( \hat{Z}_I \) to \( I \).

The (J)QR approach, similar to the Phase 2 (see section 5), should be more accurate and even necessary when the conditions of the matrices \( \hat{H}_I \) and/or \( \hat{S}_I \) are so prohibitively large that forming them explicitly and then factorizing them might fail. Both \( F_j \) and \( G_j \) should then be copied to \( \hat{F}_I \) and \( \hat{G}_I \), respectively, and the JQR factorization on \( F_j \), followed by the column prepermutation and the tall-and-skinny QR factorization on \( G_j \), should be performed to obtain \( \hat{F}_I \) with \( \hat{J}_I \) and \( \hat{G}_I \), respectively. Such an approach has neither been implemented nor tested, though.

6.4.3. Transforming the block pivots. The block pivots \( \hat{F}_I \) with \( \hat{J}_I \) and \( \hat{G}_I \) are handed over to the Level 1 (VP) algorithm to be transformed. We have prepared a simpler VP version, executing single-threadedly, i.e., in the contexts of the already running threads. The Level 1 algorithm can either fully (implicitly) diagonalize \( \hat{H}_I \) and \( \hat{S}_I \), or at least iterate until a reasonably high number of the inner sweeps has been attained (\( maxcyc = 30 \)), in which case we talk about the Full Block (FB) variant; or

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**A similar treatment is possible (and in fact implemented) for \( \hat{H}_I \), if \( J = I \).
pass over the block pivots only a prescribed number of times, e.g., once ($\text{maxcyc} = 1$), in the Block-Oriented (BO) variant (for more details on both, see [21]). The former variant corresponds to a full two-sided annihilation of the off-diagonal of $\hat{H}_{jl}$ and $\hat{S}_{jl}$, while the latter implicitly reduces their off-diagonal norms.

Also, the BO variant exhibits similar execution times for every call of the Level 1 routine across all threads in a block step, while those can vary significantly, due to data, among the threads in the FB variant. On some platforms (e.g., the GPUs), that does not pose a huge problem [19], but on the CPUs it can cause delays on the synchronization primitives (OpenMP barriers) required between the block steps [21].

In any case, the transformations applied in the Level 1 are accumulated in $\hat{Z}_{jl}$, while the counters of all and of “big” transformations are added atomically to the respective counters (shared among the threads) for the current block sweep.

6.4.4. Updating and exchanging the block columns. If no transformations have been applied in the Level 1, $F_{jl}$, $G_{jl}$, and $Z_{jl}$ are then copied to $\hat{F}_{jl}$, $\hat{G}_{jl}$, and $\hat{Z}_{jl}$, respectively. Otherwise, $F_{jl} = F_{jl}\hat{Z}_{jl}$, $G_{jl} = G_{jl}\hat{Z}_{jl}$, and $Z_{jl} = Z_{jl}\hat{Z}_{jl}$ (three ZGEMM calls).

Thus far, all computation (apart from the atomic operations\footnote{In the MPI (distributed memory) setting, e.g., MPI\_ALLREDUCE might serve the same purpose.}) have been local to a thread. Now, by looking to $S_{jl+1}^{[2]}$, it is easy to figure out which of the two block columns should be retained by the thread, and to which thread the other block column has to be sent (in fact, the whole communication pattern has been precomputed). Also, the block columns can swap roles: the first one in the current step can become the second one, in the presently owning or in the receiving thread, and vice versa, in the next step. A thread might even send away both its block columns (each to a different recipient), and receive two new block columns (each from a different sender).

It might seem unnecessary to perform the physical exchanges of data on the shared memory, but the reason behind them is twofold. First, most modern machines have their memory partitioned according to the speed of access by, or “proximity” to, each CPU (NUMA), and it is beneficial to bring the data close to (a thread bound to) the CPU that processes it. Second, such a design makes the algorithm convertible to a distributed memory one (e.g., by using an MPI process for what a thread does now).

To perform the block column copies, a thread has to know the memory addresses of the storage of the threads it communicates to. All such addresses are kept available to all threads, and the block columns from the “shadow” storage are copied by their present owners to the regular storage of their future ones. Before a block column pair can be copied (from or to), it has to be updated first, so there is an OpenMP barrier between the three updates above and the three copying actions (by two ZLACPY calls each, one per a block column). Also, a thread cannot continue with the next block step until it has the new data ready and its shadow storage available, which is enforced for all threads simultaneously by placing another barrier after the copying actions.

It is a legitimate question if it is worthwhile (and in what circumstances) to try hiding the communication behind the computation, maybe by relying on some tasking mechanism. For example, $F_{q_j}$ can be copied to $F_{q_{j+1}}$, and $F_{q_j}$ to $F_{q_{j+1}}$, while $G_{jl}$, $G_{jl'}$, and $G_{jl''}$ are being updated. We leave these considerations for a future work.

6.4.5. Wrapping up. At the end of a block sweep, the transformation counters are read and reset. If no “big” transformations have been applied in any of the threads in the block sweep, the process stops, and the outputs, now including $\Lambda_F$, $\Lambda_G$, and $\Lambda$, are generated, piecewise per thread, as described in subsection 6.1.9 and section 3.
6.5. Testing. The aim of testing was to establish what algorithm variant to recommend for practice, as well as should the Phase 2 be employed, and if so, when.

6.5.1. Blocked vs. pointwise algorithms. In Table 6.1 it is shown that the Level 2 (BO) algorithm is several times faster than both the Level 1 (VP) and the Level 2 (FB) algorithms, and that blocking in general gives a significant advantage over the pointwise approach. Also, having more threads, and thus the smaller block pivot orders, benefits the FB algorithm, since the speedup with 64 versus 32 threads is more than twofold. On the contrary, the speedup with twice more threads is less than twofold for the BO algorithm, since the formation of the block pivots in the BO variant takes a bigger portion of the overall time, compared to the Level 1 inner iterations. Nevertheless, the Level 2 (BO) algorithm is our choice for the Phase 3.

Table 6.1
The wall execution time (wtime), with 32 and 64 threads, of the three algorithm candidates.

| ID | Level 1 (VP) wtime [s] | Level 2 (FB) wtime [s] | Level 2 (BO) wtime [s] |
|----|------------------------|------------------------|------------------------|
|    | 32 threads              | 64 threads              | 32 threads              | 64 threads              | 32 threads              | 64 threads              |
| A1 | 825.004150             | 845.773066             | 392.857860             | 229.095431             | 125.394272             | 128.413842             |
| A2 | 4519.72931             | 4598.667799            | 2325.848994            | 951.833517             | 643.73640              | 489.192929             |
| A3 | 18998.642156           | 19669.167008           | 9665.228718            | 3815.970553            | 2419.929790            | 1482.310420            |
| A4 | 67109.302507           | 69908.726510           | 31466.466103           | 11303.601239           | 8102.409902            | 4548.486574            |
| B1 | 254.814443             | 262.025957             | 139.82196              | 91.070519              | 43.309597              | 50.132631              |
| B2 | 1370.171514            | 1480.886640            | 615.490611             | 326.671314             | 188.634394             | 174.956353             |
| B3 | 6373.764255            | 6363.678531            | 3125.098243            | 1133.191509            | 799.279404             | 531.860802             |
| B4 | 21434.266195           | 22706.329023           | 10122.305039           | 4177.217792            | 2392.928749            | 1521.403611            |

6.5.2. Square vs. tall-and-skinny inputs. Instead of $F$, $J$, and $G$, we might have run the Phase 3 on the original, tall-and-skinny $F$, $J$, and $G$. In Table 6.2 it is shown that the preprocessing of the tall-and-skinny inputs by the Phase 2 into the square ones for the Phase 3 is preferred, both time-wise and sweep-wise, but that advantage diminishes as the inputs approach a square-like form ($m \gtrsim n$).

Table 6.2
The wall execution time (wtime), the speedups, and the numbers of block sweeps, with 32 and 64 threads, of the Phase 3 on the tall-and-skinny and the square inputs (obtained by the Phase 2).

| ID | BO tall-and-skinny (•) | Phase 2 & BO square (○) | speedup (•)/○ & sweeps |
|----|------------------------|------------------------|------------------------|
|    | 32 threads              | 64 threads              | 32 threads              | 64 threads              | 32 threads              | 64 threads              |
| A1 | 564.844448             | 576.975329             | 301.804567             | 322.013424             | 1.872; 15/14           | 1.792; 15/14           |
| A2 | 1855.068758            | 1560.997590            | 1113.329358            | 999.820267             | 1.666; 17/16           | 1.561; 16/16           |
| A3 | 1637.545045            | 3408.128731            | 3510.099673            | 2624.210469            | 1.492; 19/17           | 1.299; 17/16           |
| A4 | 12691.448583           | 7576.776758            | 10319.707019           | 6801.22258             | 1.230; 19/18           | 1.114; 18/18           |
| B1 | 567.310839             | 996.114705             | 237.997719             | 244.421613             | 2.384; 12/12           | 4.075; 12/12           |
| B2 | 1351.84530             | 1693.217834            | 730.402581             | 695.959997             | 1.851; 14/13           | 2.433; 13/13           |
| B3 | 3166.640988            | 3100.428006            | 2129.208772            | 1754.896187            | 1.487; 15/15           | 1.767; 14/14           |
| B4 | 6664.735474            | 5999.403236            | 5248.877211            | 4061.599417            | 1.270; 15/15           | 1.477; 15/15           |
6.5.3. Generalized eigenvalues. In Figures 6.1 and 6.2 the generalized eigenvalues $\Lambda$, obtained by the Phase 3 with 64 threads, are plotted for the entire dataset.

Fig. 6.1. Left to right, top to bottom: the generalized eigenvalues $\Lambda(A1)$, $\Lambda(A2)$, $\Lambda(A3)$, $\Lambda(A4)$.

7. Phase 4 – optional computation of the full G(H)SVD. The Phase 4 computes $X = Z^{-1}$ by the LU factorization with complete pivoting, $Z = P^T LU Q^T$, as implemented in the LAPACK routine ZGETC2, followed by solving a linear system $ZX = I_n$ for $X$, with $Z$ factored as above, by calling the (sequential) routine ZGESV in a parallel do loop. Each of $n$ loop iterations solves for one column of $X$, and the iteration space is divided among the same number of OpenMP threads as used for the previous phases. That number of threads is also available to ZGETC2.

Phase 4 could also be made to compute $\tilde{Z} = P_Z^T Z$ and $\tilde{X} = Z^{-1}$ from it, alongside with $\tilde{U} = Q_F^{-1} U$ and $\tilde{V} = Q_G^{-1} V$, should the G(H)SVD of the tall and skinny (i.e., non-shortened) factors be required, but that has not yet been implemented.

7.1. Relative errors in the full GHSVD. To measure the accuracy of the Phase 3 algorithm, we can look at the Frobenius norm of the error in the obtained GHSVD decomposition, relative to the Frobenius norm of the original matrix, i.e.,

\[
\frac{\|F - U\Sigma_F X\|_F}{\|F\|_F} \quad \text{and} \quad \frac{\|G - V\Sigma_G X\|_F}{\|G\|_F}.
\]

Another option, to look at $\|FZ - U\Sigma_F\|_F/\|F\|_F$ and $\|GZ - V\Sigma_G\|_F/\|G\|_F$, thus avoiding the Phase 4, is also possible, but is neither general enough to be used for the other types of the G(H)SVD algorithms, nor it would account for the effects of the Phase 4, should it be employed after the execution of the algorithms described herein.

7.1.1. Computing the relative errors. The relative errors from (7.1) have to be obtained in a higher precision than the one used for the rest of the computation, to reduce the effects of the rounding errors. However, the exact (or “infinite” precision) arithmetic is prohibitively expensive with the data of all but very small dimensions.
In our case, that implies using either the 128-bit quadruple (emulated in software and thus slower) or the 80-bit Intel extended (hardware provided) floating-point types. The latter has been chosen, but it is supported only in the GNU Fortran compiler.

The data is read in double precision and promoted to extended precision. The column scalings by $\Sigma_F$ and $\Sigma_G$, the matrix multiplications, and the Frobenius norm computation are manually parallelized with OpenMP. The last operation is performed by accumulating $\bar{z} \cdot z$ per each column (followed by a reduction and a square root), but since the exponent range of the datatype is also significantly wider than what is contained in the data, no overflow or underflow should occur.

### 7.1.2. Accuracy results.

From the range of errors shown in Table 7.1 it can be concluded both that our datasets are not highly ill-conditioned, and that, at least in those cases, the Phases 3 and 4 do not behave erratically. A serious stability analysis (or the numerical testing) of the GHSVD algorithm remains open for the future work.

For experimenting with different combinations of precision of arithmetic and in-memory data, up to quadruple precision of either or both, a separate software distribution is also provided\(^\dagger\).

### 7.2. Comparison with ZGGSVD3.

The Phase 3 algorithm can also be used for the ordinary GSVD by setting $J = I$. It is therefore reasonable to compare it to the ZGGSVD3 LAPACK routine (from the parallel Intel MKL) serving the same purpose.

#### 7.2.1. Datasets under test.

For such a comparison, a set, called C, comprising five Hermitian matrix pairs, each with both matrices positive definite, has been generated using the ZLATMS LAPACK testing routine, by one call for each matrix (of the full bandwidth) with its pseudorandom eigenvalues uniformly distributed in $(0, 1)$. The matrix orders are 1000, 2000, 3000, 4000, 5000, and the full GSVD is required.

\(^\dagger\)Available in https://github.com/venovako/MPHZ repository.
The relative errors in the full GHSVD (from the Phases 3 and 4, with 32 and 64 threads), obtained in extended precision. While \( \|F\|_F \) does not vary with the number of threads used in the Phase 2, \( \|G\|_F \) varies so negligibly that the rounding to the six decimal places shown is not affected.

| ID  | \( \|F\|_F \) | \( \|G\|_F \) | \( \|F - U\Sigma F X\|_F / \|F\|_F \) | \( \|G - V\Sigma G X\|_F / \|G\|_F \) |
|-----|-----------------|-----------------|---------------------------------|---------------------------------|
|     | 32 threads      | 64 threads      | 32 threads                      | 64 threads                      |
| A1  | 197.339487      | 57.118214       | 1.250533e−13                   | 1.287069e−13                   |
| A2  | 318.701344      | 75.513862       | 1.618982e−13                   | 1.613006e−13                   |
| A3  | 317.883120      | 85.813833       | 2.721986e−13                   | 2.725099e−13                   |
| A4  | 385.297523      | 103.571436      | 3.522477e−13                   | 3.524929e−13                   |
| B1  | 148.478058      | 40.515148       | 1.107195e−13                   | 1.111215e−13                   |
| B2  | 275.148879      | 54.161577       | 2.244659e−13                   | 2.234393e−13                   |
| B3  | 423.840558      | 66.447550       | 4.175919e−13                   | 4.196549e−13                   |
| B4  | 565.824887      | 76.845006       | 7.181818e−13                   | 7.223445e−13                   |

7.2.2. Timing results. In Tables 7.2 and 7.3 the speedup of the Phase 3 followed by the Phase 4 versus ZGGSVD3 is shown, with 32 and 64 threads, respectively.

| n   | ZGGSVD3 wtime [s] (●) | Phase 3 wtime [s] & sweeps | Phase 4 wtime [s] | Phases 3 & 4 wtime [s] (○) | speedup (●)/(○) |
|-----|------------------------|-----------------------------|-------------------|-----------------------------|------------------|
| 1000| 381.917823             | 6.026115; 13                | 3.122737          | 9.488852                    | 41.744890        |
| 2000| 5870.780192            | 33.575362; 14               | 22.160818         | 55.736180                   | 105.311585       |
| 3000| 22069.080533           | 102.090203; 16              | 71.852700         | 173.942903                  | 126.875430       |
| 4000| 54065.661969           | 234.424527; 17              | 198.504696        | 432.929223                  | 124.883374       |
| 5000| 106936.074368          | 441.616918; 17              | 326.152234        | 767.769152                  | 139.281546       |

| n   | ZGGSVD3 wtime [s] (●) | Phase 3 wtime [s] & sweeps | Phase 4 wtime [s] | Phases 3 & 4 wtime [s] (○) | speedup (●)/(○) |
|-----|------------------------|-----------------------------|-------------------|-----------------------------|------------------|
| 1000| 386.915902             | 8.345257; 13                | 2.850181          | 11.195438                   | 34.560140        |
| 2000| 5891.039753            | 37.426487; 14               | 20.551169         | 57.977656                   | 101.608795       |
| 3000| 22045.476336           | 104.476443; 16              | 69.922543         | 174.398986                  | 126.408283       |
| 4000| 54337.172978           | 192.772770; 16              | 180.097083        | 372.869853                  | 145.726914       |
| 5000| 107431.980263          | 332.406350; 17              | 328.697272        | 661.103622                  | 162.503396       |
implementation of those phases, and from Table 5.1 it follows that such reshuffling would have a negligible impact on the overall speedup for the matrices large enough.

From the tests it is evident that the Phase 3 (with the Phase 4 if needed) is a very competitive, highly parallel algorithm for the ordinary GSVd as well, while being adaptable to a wide variety of the modern high performance computing hardware.

8. Conclusions and future work. In the paper we have demonstrated a successful approach to computing the generalized eigendecomposition of a Hermitian matrix pair, with one matrix positive definite, by the implicit Hari–Zimmermann algorithm for the generalized hyperbolic SVD, in the context of the FLAPW methods.

We have also provided a method of computing the hyperbolic QR factorization (JQR), shown its potential benefits, and throughout the paper suggested the various paths open to the future research, some of which are already under way.

Namely, a GPU implementation of the implicit Hari–Zimmermann algorithm for the ordinary GSVd [20], as an extension of the GPU SVD algorithm from [19], shows the promising results and complements the highly efficient CPU implementation described herein. Therefore, a GPU implementation of the GHSVD and the Phase 1 might be a practical companion to the present research.

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