Parallel solution of the generalized eigenvalue problem given in a factored form

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Outline of the talk:

- description of the problem,
- solution of the problem in three steps
  - step 1 — Hermitian indefinite factorizations
  - optional step 2 — hyperbolic QR factorization (JQR)
  - step 3 — implicit HZ algorithm for the hyperbolic generalized SVD
- implementation details of the parallel algorithm,
- partial results of numerical testing.

Problem description

Density Functional Theory framework

- is used in simulation of the physical properties of complex quantum mechanical systems made of few dozens up to few hundreds of atoms
- the core of the method relies on the simultaneous solution of a set of Schrödinger–like equations also known as Kohn–Sham equations
- there exists a wide variety of approaches that can be used to "translate" the DFT mathematical layout into a computational tool.

Full-potential Linearized Augmented Plane Wave (FLAPW) method

- FLAPW method is one of the most accurate methods — particular discretization of the DFT fundamental equations
- FLAPW is all-electron method — it explicitly describes all of the (potentially large number of) electrons in the material with a much larger number of basis function
- it is a quite computationally expensive method.

FLAPW method

Full-potential Linearized Augmented Plane Wave (FLAPW) method

- the discretization in FLAPW method leads to the solution of the generalized eigenvalue problem for matrices (H, S), where

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

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

where $A_a, B_a \in \mathbb{C}^{N_L \times N_G}$, $T_a^{[\cdots]} \in \mathbb{C}^{N_L \times N_L}$, $U \in \mathbb{C}^{N_L \times N_L}$ is a diagonal matrix, while $(T^{[AA]})^* = T^{[AA]}$, $(T^{[BB]})^* = T^{[BB]}$, and $(T^{[AB]})^* = T^{[BA]}$.

Problem sizes

Typical matrix sizes

- $N_A = \mathcal{O}(100)$, $N_G = \mathcal{O}(1000)$–$\mathcal{O}(10000)$, and $N_L = \mathcal{O}(100)$
- test examples NaCl – $N_A = 512$, $N_L = 49$
  - $N_G = 2256$, $N_G = 3893$, $N_G = 6217$, $N_G = 9273$
- test examples AuAg – $N_A = 128$, $N_L = 121$
  - $N_G = 3275$, $N_G = 5638$, $N_G = 8970$, $N_G = 13379$.

Computation of H and S

Proposed by Fabregat–Traver at al.

- write H as $H = H_{AA} + H_{AB+BA+BB}$

$$H_{AA} = \sum_{a=1}^{N_A} A_a^* T^{[AA]} A_a$$

$$H_{AB+BA+BB} = \sum_{a=1}^{N_A} \left(B_a^* T^{[BA]} A_a + A_a^* T^{[AB]} B_a + B_a^* T^{[BB]} B_a \right)$$

$$= \sum_{a=1}^{N_A} (B_a^* Z_a + Z_a^* B_a)$$

(`ZHER2K`s!), where

$$Z_a = T^{[BA]} A_a + \frac{1}{2} T^{[BB]} B_a.$$

Transformation of the problem

Modification?

Why

- the algorithm proposed by Fabregat–Traver at al. computes in parallel only H and S — then use any GEVD,
- intention to keep matrices in a factored form – ideal for parallelization of the GEVD
- usage of one-sided methods — faster than the two-sided methods — columnwise action
- such approach usually computes small eigenvalues more accurately
- similar algorithm for the (real) generalized SVD is approximately 125 times faster than the LAPACK routine with threaded MKL.

Transform the problem!

Transformed problem

- by using the properties of matrices $T^{[\cdots]}$ it is obvious that the problem can be written as

$$H = \sum_{a=1}^{N_A} \begin{bmatrix} A_a^* & B_a^* \end{bmatrix} \begin{bmatrix} T^{[AA]} & T^{[AB]} \\ (T^{[AB]})^* & T^{[BB]} \end{bmatrix} \begin{bmatrix} A_a \\ B_a \end{bmatrix} := \sum_{k=1}^{n} H_k^* T_k H_k,$$

$$S = \sum_{a=1}^{N_A} \begin{bmatrix} A_a^* & B_a^* U_a^* \end{bmatrix} \begin{bmatrix} A_a \\ U_a B_a \end{bmatrix} := \sum_{k=1}^{n} S_k^* S_k.$$

Transform the problem!

... or as products of three (two) matrices

$$H = \begin{bmatrix} H_1^* & \cdots & H_n^* \end{bmatrix} \begin{bmatrix} T_1 & & \\ & \ddots & \\ & & T_n \end{bmatrix} \begin{bmatrix} H_1 \\ \vdots \\ H_n \end{bmatrix} := \widetilde{F}^* T \widetilde{F}$$

$$S = \begin{bmatrix} S_1^* & \cdots & S_n^* \end{bmatrix} \begin{bmatrix} S_1 \\ \vdots \\ S_n \end{bmatrix} := G^* G.$$

Matrix sizes

- $H_k, S_k \in \mathbb{C}^{(2N_L)\times N_G}$, $T_k \in \mathbb{C}^{(2N_L)\times(2N_L)}$,
- $F, G \in \mathbb{C}^{(2N_A N_L)\times N_G}$, $T \in \mathbb{C}^{(2N_A N_L)\times(2N_A N_L)}$.

Transform the problem!

Make T simpler

- the method can be applied even on already described matrices $\widetilde{F}$, G and T implicitly, but multiplication by T is slow
- T should be either factored by using somewhat modified Hermitian indefinite factorization (HIF) — simultaneous factorizations of all T_ks, or
- T could be diagonalized (simultaneous diagonalization of T_ks) — diagonalization is too slow
- therefore, H could be written as

$$H := F^* J F, \qquad J = \mathrm{diag}(\pm 1).$$

Step 1

Hermitian indefinite factorization

'Cholesky-like' factorization for indefinite matrices?

- Factorization exists in the following form for any indefinite A

$$A = P^T R^T D R P$$

- 2×2 blocks in D or 2×2 diagonal blocks in R are permitted
- problem: 1×1 or 2×2 block at the pivot position could be singular
- solution: two-sided pivoting (permutation matrix P). If
  - all diagonal elements are 0 and
  - all principal submatrices of order 2 are singular

  then $A = 0$.
- factorization with 2×2 blocks in D is constructed by James Bunch in his PhD thesis (1969)

Modified Hermitian indefinite factorization

From HIF to modified HIF

- modified form, with diagonal $D = \mathrm{diag}(\pm 1)$ is given by Ivan Slapničar in his PhD thesis (1992)
- if d_{ii} is 1×1 block — leave $\mathrm{sign}(d_{ii})$ on the diagonal, and multiply i-th row of R by $\sqrt{|d_{ii}|}$
- if D_{ii} is 2×2 block — diagonalize D_{ii} by a single Jacobi rotation, multiply both rows with this rotation, and repeat previous step for both rows
- now D has 1 or -1 on its diagonal, and, in the case of 2×2 blocks in the original D, R has 2×2 blocks on its diagonal

Examples and problems of HIF

Example

For nonsingular matrix

$$A = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \\ 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \end{bmatrix}$$

- there is no 1×1 pivots (diagonal is 0);
- we need symmetric pivoting since 2×2 block at the pivot position is singular
- Stability reasons – swap 'most nonsingular block' at pivot position — swap first and fourth row and column.

Examples and problems of HIF

Example

For nonsingular matrix

$$A = \begin{bmatrix} 0 & 4 & 0 \\ 4 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

- pivoting is not needed, but
- factorization is not unique, for example if $D = \mathrm{diag}(\pm 1)$, then

$$A = \begin{bmatrix} 0 & 4 & 0 \\ 4 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \alpha & \beta & 0 \\ \alpha & -\beta & 0 \\ 0 & 0 & 1 \end{bmatrix}^* \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \alpha & \beta & 0 \\ \alpha & -\beta & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

for all $\alpha \cdot \beta = 2$.

Pivoting in the Hermitian indefinite factorizations

Complete pivoting

- Described in the quite famous paper by Bunch and Parlett (1971)
- define $\mu_1 = \max_i |a_{ii}|$, $\mu_0 = \max_{i,j} |a_{ij}|$, $\alpha = (1 + \sqrt{17})/8$
- if $\mu_1 \geq \alpha \cdot \mu_0$ then choose 1×1 pivot, otherwise 2×2 pivot
- this pivoting is based on the smallest element growth
- Kahan's suggestion (in letter to R. de Meersman and L. Schotsmans, (1965)) — take pivot block as the 'most nonsingular' block, i.e., with biggest μ_c

$$\mu_c = \max_{i,j,k} \{|a_{ii}|, |a_{jj} a_{kk} - |a_{jk}|^2|\}$$

- $\mathcal{O}(n^4)$ operations needed to find pivot if A is given implicitly, by its factors

Pivoting in the Hermitian indefinite factorizations

Partial pivoting

- Described in the papers by Bunch, Kaufmann and Parlett (1976–1977)
- little bit more complicated to describe
- searches 1×1 pivots on the whole diagonal
- in the case of 2×2 pivots, searches only for the new second row (first row is fixed)
- advantage $\mathcal{O}(n^3)$ operations needed to find pivot if A is given implicitly, by its factors
- disadvantage — less stable than complete pivoting

Step 2 (optional)

Optional step

Optional step — make J, F and G square

- square matrix – faster third step — HZ algorithm
- this step is the hyperbolic QR factorization on F and the QR factorization on G – both algorithms are moderately parallel
- pivoting strategy – partial pivoting?, threshold pivoting?
- usage of (block)-reflectors, Hyperbolic URV (HURV) factorization, or (block)-rotations?
- do it or not – depends on the ratio (number of rows) / (number of columns) of F and G

Hyperbolic QR factorization

Definition

Let $F \in \mathbb{C}^{m \times n}$, $m \geq n$, and $J \in \mathbb{C}^{m \times m}$, $J = \mathrm{diag}(j_{11}, \ldots, j_{mm})$, $j_{ii} \in \{1, -1\}$, be given matrices, such that $A := F^* J F$ is nonsingular. Factorization

$$F = P_1 Q R P_2^* = P_1 Q \begin{bmatrix} R_1 \\ 0 \end{bmatrix} P_2^*, \quad Q^* J' Q = J', \quad J' = P_1^* J P_1,$$

where P_1 and P_2 are permutation matrices, matrix Q is J'-unitary, and R_1 is block upper triangular with diagonal blocks of order 1 or 2, is called the hyperbolic QR factorization of F according to J.

Reflectors

Definition

A matrix $H \in \mathbb{C}^{m\times m}$ will be called a J-reflector if it is J-unitary, J-Hermitian and a reflector, i.e.,

$$H^* J H = J, \quad JH = H^* J, \quad H^2 = I.$$

Proposition

Let $J \in \mathbb{C}^{m\times m}$ be a given nonsingular matrix. Any two equalities in the definition imply the third one.

Nondegenerate matrix

Matrix $W \in \mathbb{C}^{m \times p}$ is nondegenerate (with respect to J) if and only if range of W, $\mathcal{R}(W)$ is nondegenerate.

Proposition

The following statements are equivalent:

- W is nondegenerate,
- $\mathcal{N}(W^* J W) = \mathcal{N}(W)$,
- $\mathcal{R}(W^* J^* W) = \mathcal{R}(W^*)$,
- $\operatorname{rank}(W^* J W) = \operatorname{rank}(W)$.

Simple and block reflectors

Block J-reflector

For any given $W \in \mathbb{C}^{m \times p}$, a matrix $H \in \mathbb{C}^{m \times m}$ defined by

$$H = H(W) = I - 2W(W^*JW)^+W^*J$$

will be called a block J-reflector (generated by W).

If $p = 1$ (W is a vector), H is sometimes called a simple J-reflector (Bunse Gerstner).

Proposition

$H = H(W)$ satisfies all three reflector properties, i.e., it is a J-reflector.

Reflection properties

Theorem
Let $H = H(W)$ be a block J-reflector generated by W.
If W is nondegenerate, then

$$\begin{aligned} Hx &= -x, \quad \text{for all } x \in \mathcal{R}(W), \\ Hy &= y, \quad \text{for all } y \in \mathcal{R}(W)^{[\perp]}, \end{aligned}$$

i.e., H reflects (reverses) $\mathcal{R}(W)$ with respect to $\mathcal{R}(W)^{[\perp]}$.

If W is degenerate then

$$Z = Z(W) = W(W^*JW)^+$$

is nondegenerate and $H(Z) = H(W)$.
Moreover, $\mathcal{R}(Z) \subseteq \mathcal{R}(W)$, and $\mathcal{R}(Z) = \mathcal{R}(W)$ holds if and only if W is nondegenerate.

A few comments

- If $p = 1$ it is easy to see that $w \neq 0$ is nondegenerate if and only if w is nonisotropic, i.e., $w^* J w \neq 0$
- For $p \geq 2$, nondegeneracy becomes less restrictive than nonisotropy
- $\mathcal{R}(W)$ may contain some nonzero isotropic vectors
- As long as none of these vectors are J-perpendicular to the whole subspace, W is nondegenerate and $H(W)$ reflects the whole range of W.
- This fact will be used later (with $p = 2$) to obtain the hyperbolic QR factorization.

The mapping problem

For given matrices $F, R \in \mathbb{C}^{m\times q}$, $q \geq 1$, we seek a block J-reflector $H = H(W)$ such that

$$HF = R.$$

If H exists, F and R satisfy

(i) J-isometry property:

$$F^*JF = R^*JR, \tag{1}$$

(ii) J-symmetry property (symmetry with respect to J):

$$R^*JF = F^*JR. \tag{2}$$

Obviously, if R satisfies these conditions, so does $-R$.

An example

Note, if $J = I$ requirements (1) and (2) are necessary and sufficient (Schreiber–Parlett). If $J \neq I$:

- (1) and (2) are necessary for the existence of H, but may not be sufficient.

Example

Let $J = \text{diag}(1, -1, 1, -1)$ be the hyperbolic scalar product and

$$F = \begin{bmatrix} 1 & 1 \\ 0 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}, \quad R = \begin{bmatrix} 1 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

Obviously, $\text{rank}(F) = 2$, $\text{rank}(R) = 1$, and it is easy to verify that both (1) and (2) are satisfied by F and R.

Sum S and difference D

Let D (for "difference") and S (for "sum") be the matrices defined by

$$D = R - F, \quad S = R + F.$$

Lemma

If $F, R \in \mathbb{C}^{m \times q}$ satisfy (1) and (2), then D and S satisfy

$$D^* JS = 0.$$

Mapping theorem 1

J-reflector partial mapping theorem

Let F and R be two matrices in $\mathbb{C}^{m \times q}$ which satisfy (1) and (2). Then $H(D)F = R$ if and only if D is nondegenerate, i.e., D satisfies the rank condition

$$\text{rank}(D^* JD) = \text{rank}(D).$$

Furthermore, $H(S)F = -R$ if and only if S is nondegenerate, i.e., S satisfies the rank condition

$$\text{rank}(S^* JS) = \text{rank}(S).$$

When $J \neq I$, this Theorem gives only sufficient conditions for the existence of a mapping reflector H.

An example

Example

Let $J = \mathrm{diag}(1, -1, 1, -1)$ and

$$F = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad R = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

$\mathrm{rank}(F) = \mathrm{rank}(R) = 1$, (1)–(2) are satisfied, but $D^* J D = S^* J S = 0$, and we cannot construct H by using either D or S. On the other hand, $H(W)F = R$ with

$$W = \begin{bmatrix} 0 & 1/4 \\ 0 & -3/4 \\ -1 & -2 \\ -1 & 0 \end{bmatrix}.$$

Mapping theorem 2

J-reflector full mapping theorem

Let F and R be two matrices in $\mathbb{C}^{m\times q}$ which satisfy (1) and (2). There exists a J-reflector H such that

$$H(W)F = R,$$

if and only if

$$\mathcal{R}(D) \cap \mathcal{R}(S) = \{0\}.$$

Single column reduction

- If a single pivot column f_1 is chosen then

$$e_k^* J e_k = \mathrm{sign}(f_1^* J f_1) \neq 0.$$

- In the case of two pivot columns

$$F = [f_1, f_2] = \begin{bmatrix} F_1 \\ F_2 \end{bmatrix},$$

where F_1 is 2×2 matrix,

$$M := F^* J F$$

is nonsingular, indefinite, with nonzero offdiagonal elements.

Reduction of two columns

We seek a hyperbolic block reflector H such that $HF = R$. R should be determined such that:

- R and J have the special structures,

$$R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}, \quad J = \mathrm{diag}(J_1, J_2),$$

  R_1 is 2×2 matrix, $J_1 = \mathrm{diag}(j_{11}, -j_{11})$,

- R and F satisfy (1)–(2).

We hope that this system of equations can be solved for R_1, and H follows from the partial mapping theorem.

Reduction of two columns

$M = F^*JF$ is indefinite $\Longrightarrow$ we can find a row permutation P_1 such that

- F_1 is nonsingular and
- $J_1 = \mathrm{diag}(j_{11}, -j_{11})$.

Now

$$HF = H \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$$

implies

$$R_1^* J_1 R_1 = F^* JF = M, \qquad R_1^* J_1 F_1 = F_1^* J_1 R_1.$$

Note that R_1 is nonsingular, so we define

$$K := F_1 R_1^{-1}.$$

Reduction of two columns

In terms of K we have

$$KJ_1K^* = F_1M^{-1}F_1^*, \qquad J_1K = K^*J_1,$$

so K is J-Hermitian, and the first equation can be written as

$$K^2 = F_1M^{-1}F_1^*J_1.$$

Since all matrices are nonsingular square root K always exists, but it not need to be primary square root.

It is difficult to show that either D or S is nondegenerate. Possible solution: swap rows and/or columns of F to make K primary square root.

Alternative reduction of two columns

Since M is Hermitian and indefinite

- it can be diagonalized by a singe Jacobi rotation, U i.e., columns of J are orthogonalized,
- therefore, after the application of this rotation

$$\widehat{F} = FU$$

- we can proceed with two simple J-reflectors that annihilates f_1, and f_2
- these Jacobi rotations U^* are either stored, so we obtain HURV factorization, or can be applied back to the columns r_1 and r_2.

Step 3

One-sided vs. two-sided method

- the original Hari–Zimmerman method works from both sides on the Hermitian matrix pair
- the modified method works from one side on the factors of the Hermitian matrix pair
- idea: think two-sided, act one-sided
- transformations will be computed from the pivot submatrices H_{pq} of H and S_{pq} of S

$$H_{pq} = \begin{bmatrix} F_p^* J F_p & F_p^* J F_q \\ & F_q^* J F_q \end{bmatrix}, \quad S_{pq} = \begin{bmatrix} G_p^* G_p & G_p^* G_q \\ & G_q^* G_q \end{bmatrix}.$$

The complex Hari–Zimmermann method for the GEP

The method consists of 3 transformations (Hari)

- as a preprocessing step H and S can be scaled by the diagonal matrix D such that $\operatorname{diag}(DSD) = I$

$$H_0 := DHD, \quad S_0 := DSD,$$
$$D = \operatorname{diag}\left(\frac{1}{\sqrt{s_{11}}}, \frac{1}{\sqrt{s_{22}}}, \ldots, \frac{1}{\sqrt{s_{nn}}}\right)$$

- in the first step the pivot submatrix $\widehat{S}_0$ of S_0 is diagonalized by the complex rotation

$$\widehat{R}_1 = \begin{bmatrix} \cos\varphi_1 & e^{i\beta_1}\sin\varphi_1 \\ -e^{-i\beta_1}\sin\varphi_1 & \cos\varphi_1 \end{bmatrix},$$

The complex Hari–Zimmermann method for the GEP

The transformations

- the first transformation is

$$H_1 = R_1^* H_0 R_1, \quad S_1 = R_1^* S_0 R_1,$$

  $R_1 = I$ except at the pivot positions, where $R_1 = \widehat{R}_1$.
- if H and S are preprocessed, then $\varphi_1 = -\frac{\pi}{4}$
- in the second step – the diagonal of S_1 is rescaled to I
- this transformation is similar to the preprocessing step

$$H_2 := D_2 H_1 D_2, \quad S_2 := D_2 S_1 D_2.$$

The transformations

- in the third step the pivot submatrix $\widehat{H}_2$ of H_2 is diagonalized by the complex rotation

$$\widehat{R}_3 = \begin{bmatrix} \cos\varphi_3 & e^{i\alpha_3}\sin\varphi_3 \\ -e^{-i\alpha_3}\sin\varphi_3 & \cos\varphi_3 \end{bmatrix},$$

- the third transformation is

$$H_3 = R_3^* H_2 R_3, \quad S_3 = R_3^* S_2 R_3,$$

  $R_3 = I$ except at the pivot positions, where $R_3 = \widehat{R}_3$.
- if H and S are preprocessed, then $\varphi_3 = \vartheta + \frac{\pi}{4}$.

The transformations

- note that after the first three steps, the pivot submatrix $\widehat{S}_3$ is still diagonal (in fact identity)

$$\widehat{S}_3 = \widehat{Z}^* \widehat{S} \widehat{Z}, \quad \widehat{Z} = \widehat{R}_1 \widehat{D}_2 \widehat{R}_3$$

- if H and S are preprocessed, the fourth step is only formal — it helps in coupling together all the transformations

$$H_4 = \Phi_4^* H_3 \Phi_4, \quad S_4 = \Phi_4^* S_3 \Phi_4, \quad \widehat{\Phi}_4 = \mathrm{diag}(e^{-i\sigma_p}, e^{-i\sigma_q}).$$

HZ transformations

$$
\begin{array}{|c|c|}
\hline
* & * \\
\hline
* & * \\
\hline
\end{array}
\qquad\qquad
\begin{array}{|c|c|}
\hline
1 & * \\
\hline
* & 1 \\
\hline
\end{array}
$$

HZ transformations

$$\begin{bmatrix} * & * \\ * & * \end{bmatrix} \qquad \begin{bmatrix} * & 0 \\ 0 & * \end{bmatrix}$$

HZ transformations

$*$	$*$
$*$	$*$

1	0
0	1

HZ transformations

$*$	0
0	$*$

1	0
0	1

The complex Hari–Zimmermann method for the GEP

The coupled transformation Z ...

- looks similar to an ordinary plane rotation: it is the identity matrix, except for its (p,q)-restriction $\widehat{Z}$, where

$$\widehat{Z} = \frac{1}{\sqrt{1-\left(|s_{pq}|\right)^2}} \begin{bmatrix} \cos\varphi & e^{i\alpha}\sin\varphi \\ -e^{-i\beta}\sin\psi & \cos\psi \end{bmatrix},$$

- φ and ψ are determined so that the transformations diagonalize the pivot submatrices $\widehat{H}$ and $\widehat{S}$
- the transformation keeps the diagonal elements of S intact
- if $S = I$ then Z is the ordinary rotation, the method is the ordinary Jacobi method for a single matrix.

The Hari–Zimmermann method for the GEP

Computation of the elements of $\widehat{Z}$

- let

$$s = |s_{pq}|, \quad t = \sqrt{1 - s^2}, \quad r = s_{qq} - s_{pp},$$

$$\sigma = \begin{cases} 1 & e \geq 0 \\ -1 & e < 0, \end{cases}, \quad u + iv = e^{-i\arg(s_{pq})} h_{pq},$$

- then if $\gamma = \alpha - \beta$

$$\tan(\gamma) = 2\frac{v}{r}, \qquad -\frac{\pi}{2} \leq \gamma \leq \frac{\pi}{2}$$

$$\tan(2\vartheta) = \sigma \frac{2u - (h_{pp} + h_{qq})s}{\sqrt{e^2 + 4v^2} \cdot t}, \qquad -\frac{\pi}{4} < \vartheta \leq \frac{\pi}{4}$$

Computation of the elements of $\widehat{Z}$

- and

$$2\cos^2\varphi = 1 + s\sin(2\vartheta) + t\cos(2\vartheta)\cos(\gamma), \quad 0 \le \varphi < \frac{\pi}{2}$$

$$2\cos^2\psi = 1 - s\sin(2\vartheta) + t\cos(2\vartheta)\cos(\gamma), \quad 0 \le \psi < \frac{\pi}{2}$$

$$e^{i\alpha}\sin(\varphi) = \frac{(\sin(2\vartheta) - s) + i\sqrt{1-s^2}\sin(\gamma)\cos(2\vartheta)}{1 - s\sin(2\vartheta) + \sqrt{1-s^2}\cos(\gamma)\cos(2\vartheta)}$$

$$e^{-i\beta}\sin(\psi) = \frac{(\sin(2\vartheta) + s) - i\sqrt{1-s^2}\sin(\gamma)\cos(2\vartheta)}{1 + s\sin(2\vartheta) + \sqrt{1-s^2}\cos(\gamma)\cos(2\vartheta)}.$$

The implicit HZ algorithm

$Z = I$; $\qquad it = 0$

`repeat` // sweep loop

$\quad it = it + 1$

$\quad$ `for` all pairs (p, q), $1 \le p < q \le k$

$\qquad$ compute

$$\widehat{H} = \begin{bmatrix} f_p^* J f_p & f_p^* J f_q \\ & f_q^* J f_q \end{bmatrix}; \qquad \widehat{S} = \begin{bmatrix} g_p^* g_p & g_p^* g_q \\ & g_q^* g_q \end{bmatrix}$$

$\qquad$ compute the elements of $\widehat{Z}$

$\qquad\quad$ // transform F, G and Z

$\qquad [f_p, f_q] = [f_p, f_q] \cdot \widehat{Z}$

$\qquad [g_p, g_q] = [g_p, g_q] \cdot \widehat{Z}$

$\qquad [z_p, z_q] = [z_p, z_q] \cdot \widehat{Z}$

`until` (no transf. in this sweep) `or` $(it \ge maxcyc)$

Parallelization and numerical testing

Hardware platform

Developer Edition of the Intel Xeon Phi 7210 (KNL) processor

- 96 GB of RAM per node,
- 64 cores per node,
- clock 1.30 GHz (Turbo Boost off),
- Intel AVX-512 (Advanced Vector Extensions) instruction set
- presence of two vector processing units (VPUs) per core — each VPU operates independently on 512-bit vector registers – suitable for simultaneous processing of 16 `single precision` or 8 `double precision` numbers.

The first step

Hermitian indefinite factorization of all T_k's

- `for all` T_k`'s do in parallel`

$$T_k = P_k^T R_k^* D_k R_k P_k,$$

P_k is a permutation matrix – formed as in LAPACK
(as a sequence of partial permutations),
D_k is block diagonal, with 1×1 or 2×2 diagonal blocks,
R_k is upper triangular

- pivoting — complete pivoting used (numerical stability)

- `diagonalize all` D_k`'s in parallel`

$$D_k = U_k^* \Delta_k U_k = U_k^* \sqrt{|\Delta_k|} J_k \sqrt{|\Delta_k|} U_k,$$

Δ_k diagonal, U_k block-diagonal, unitary, $J_k = \mathrm{diag}(\pm 1)$,

The first step (cnt'd)

- `for all` J_k `repermute them in parallel`

$$J_k := \widetilde{P}_k^T \operatorname{diag}(I, -I)\widetilde{P}_k$$

  $\widetilde{P}_k$ is a permutation,

- `multiply rows of all` R_k `and repermute them`

$$R_k = \widetilde{P}_k \sqrt{|\Delta_k|} U_k$$

- `repermute columns of all` R_k `according to permutations stored in` P_k

$$R_k := R_k P_k.$$

The first step (cnt'd)

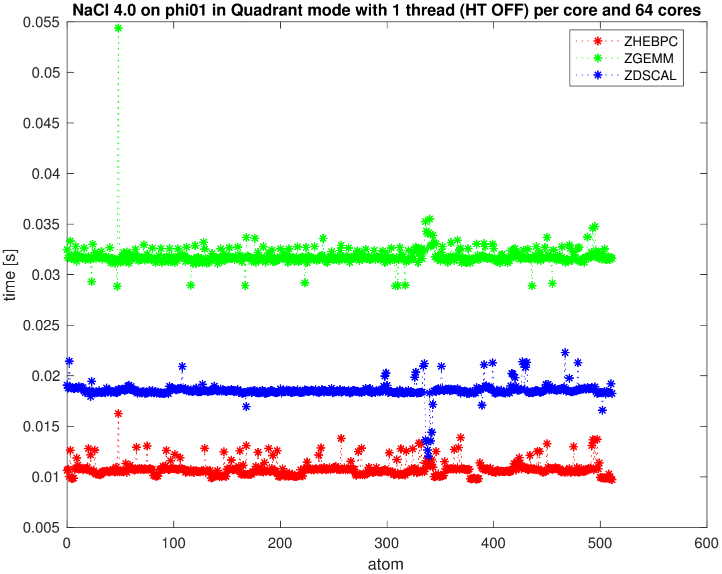
Final state

$$T_k = R_k^* \operatorname{diag}(I, -I) R_k, \quad k = 1, \ldots, n.$$

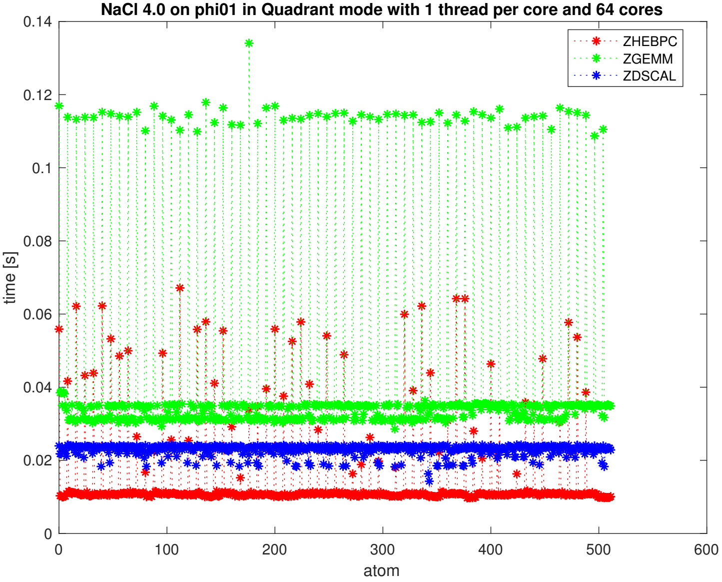
Comments

- in the first step, the factorization is sequential for each T_k
- each physical core of the Xeon Phi deals with one or more T_k in turn (OpenMP `parallel do` over all T_k)
- each core can use its own 1–4 hyperthreads in a call of the threaded BLAS routines – therefore even per core algorithm is somewhat parallel – but do not use hyperthreading, since...

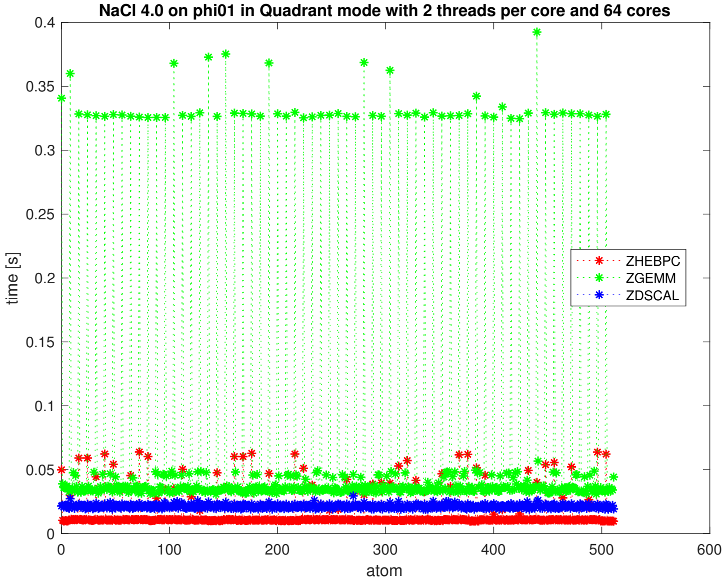
1 thread, HT off, NaCl, $N_L = 49$, $N_A = 512$, $N_G = 9273$



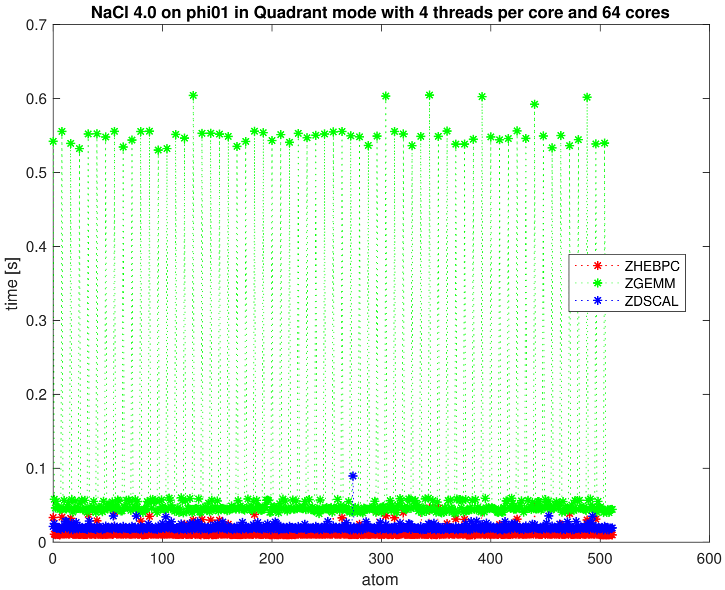
1 thread, NaCl, $N_L = 49$, $N_A = 512$, $N_G = 9273$



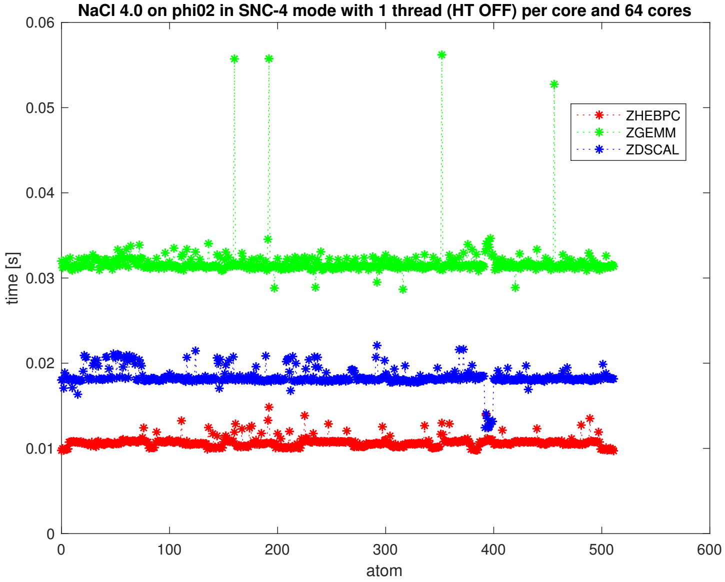
2 threads, NaCl, $N_L = 49$, $N_A = 512$, $N_G = 9273$



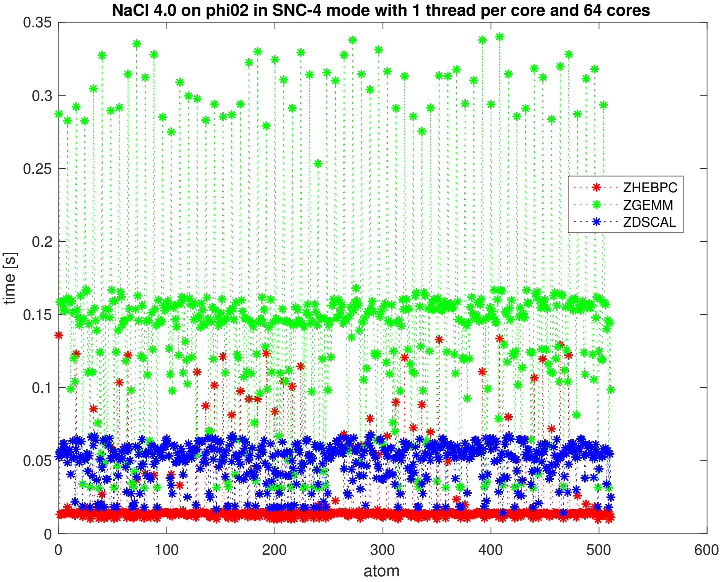
4 threads, NaCl, $N_L = 49$, $N_A = 512$, $N_G = 9273$



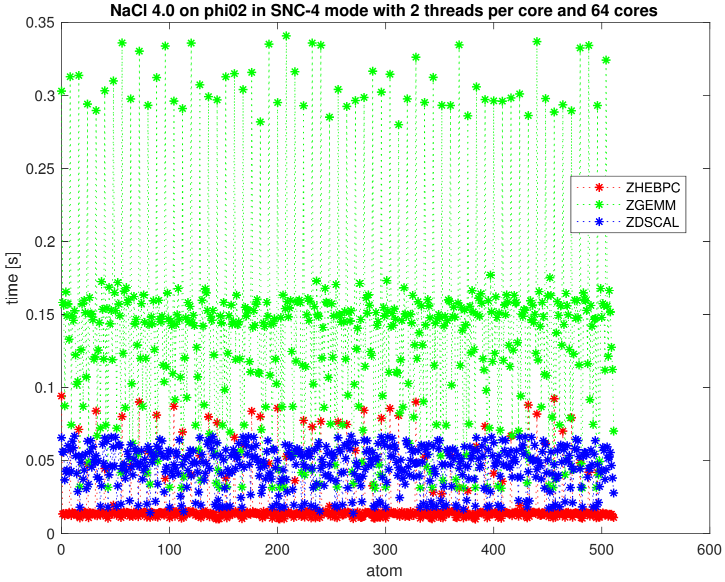
1 thread, HT off, NaCl, $N_L = 49$, $N_A = 512$, $N_G = 9273$



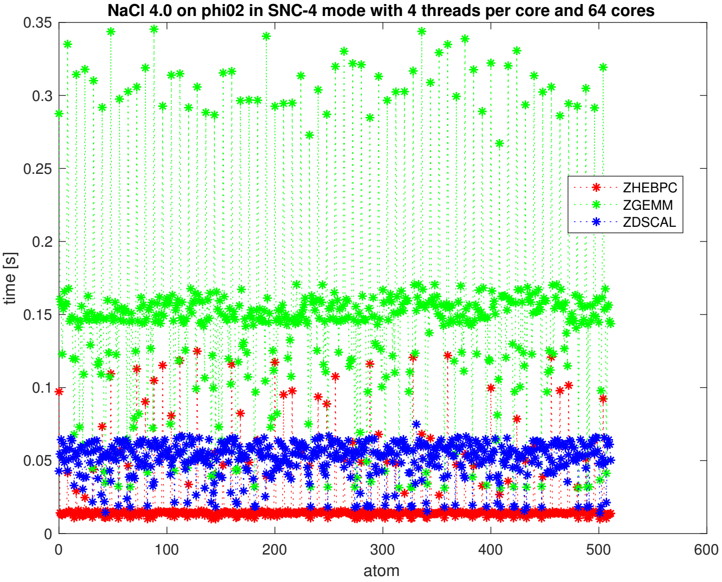
1 thread, NaCl, $N_L = 49$, $N_A = 512$, $N_G = 9273$



2 threads, NaCl, $N_L = 49$, $N_A = 512$, $N_G = 9273$



4 threads, NaCl, $N_L = 49$, $N_A = 512$, $N_G = 9273$



The second and the optional step

Form J, F and G

- `store` $J = \mathrm{diag}(J_1, \ldots, J_n)$,
- `multiply` $F = \mathrm{diag}(R_1, \ldots, R_n)F$, `each` R_k `in parallel`
- `scale` B_k `by` U_k `in parallel and store` G

Optional step — make J, F and G square

- what is the efficient way to compute the JQR?
- note that the second matrix G should shortened by the ordinary QR factorization with the same pivoting as in the JQR
- this factorization should be done by prepermutation (first), and the by the tall-and-skinny QR
- we hope that there is a crossing when JQR + QR + HZ algorithm is faster than the HZ on the rectangular matrices.

Driver level of the implicit HZ algorithm

Details of the level-2 algorithm

- algorithm is Generalized Hyperbolic SVD of (F, G) with respect to J
- matrices F and G are divided in even number of block-columns

$$F = [F_1, \ldots, F_{2b}], \quad G = [G_1, \ldots, G_{2b}]$$

- number of block-columns depend on the number of physical cores of the processor (our case: 64 cores = maximum 128 blocks, no hyperthreading)
- each thread is connected to one physical core.

Driver level of the implicit HZ algorithm

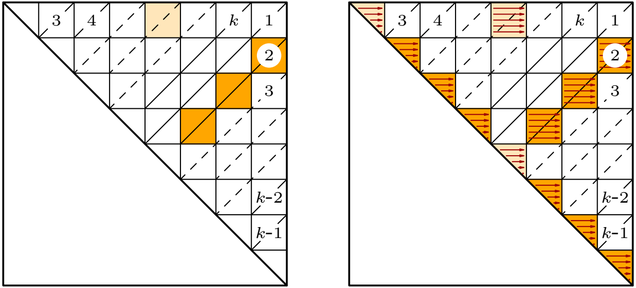
Each thread . . .

- works on a pair of block-columns of each matrix given by some parallel pivot strategy
- allocates storage for $[F_p, F_q]$, $[G_p, G_q]$, their "shadow" counterparts, and for the part of the transformation matrix
- "shadow" memory — used for scaling by J_k and data exchange
- since architecture is NUMA (Non Uniform Memory Access), columns are also physically copied to "shadow" memory (alternative: reassignment of pointers)
- allocates square space in fast MCDRAM for computation of the transformation Z_{pq} and the pivot block submatrices H_{pq} and S_{pq}.

Pivoting strategy

Parallel pivoting strategy

- Choose pivot blocks independently in each step, for example, by using (block)-modulus strategy (not optimal!)



- stopping criterion
  - skip a transformation if cosines are 1
  - final stop — all transformations are skipped.

Driver level of the implicit HZ algorithm

Each thread . . .

- actually computes H_{pq} and S_{pq} (ZGEMM and ZHERK)
- factorizes H_{pq} and S_{pq} by the Hermitian indefinite factorization (test of definiteness of S_{pq})

  $$H_{pq} = F_{pq}^* J_{pq} F_{pq}, \quad S_{pq} = G_{pq}^* G_{pq},$$

  where F_{pq}, G_{pq}, and J_{pq} are square
- calls level-1 (non-blocked routine) on the triplet (F_{pq}, G_{pq}, J_{pq})
- applies transformation matrix to original F_{pq}, G_{pq}, and Z_{pq} (ZGEMMs)
- transfers one triplet of (F_ℓ, G_ℓ, Z_ℓ), $\ell \in \{p, q\}$ to the next "owner" (thread) into its "shadow" memory.

Computational level of the implicit HZ algorithm

Details of the level-1 algorithm

- single-threaded (including BLAS calls) SIMD-parallel code,
- the main loop — `sweep` iterations (1, m, until convergence)
- parallel pivot strategy determines maximal number of independent pivot pairs — stage of the algorithm
- in each stage — pairs are divided into groups of 8 pairs (AVX-512 instructions)
- compute 6 dot products (vectorized + reductions) with only 4 accesses of f_p, f_q, g_p, and g_q:

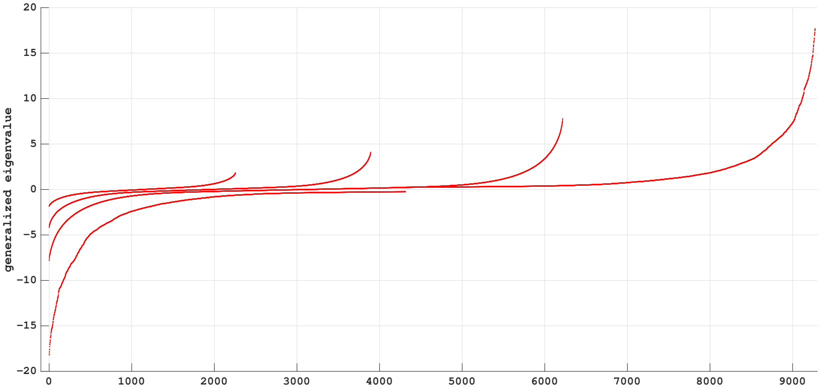
$$\widehat{H}_{pq} = \begin{bmatrix} f_p^* J_p f_p & f_p^* J_q f_q \\ & f_q^* J_q f_q \end{bmatrix}, \qquad \widehat{S}_{pq} = \begin{bmatrix} g_p^* g_p & g_p^* g_q \\ & g_q^* g_q \end{bmatrix},$$

Computational level of the implicit HZ algorithm

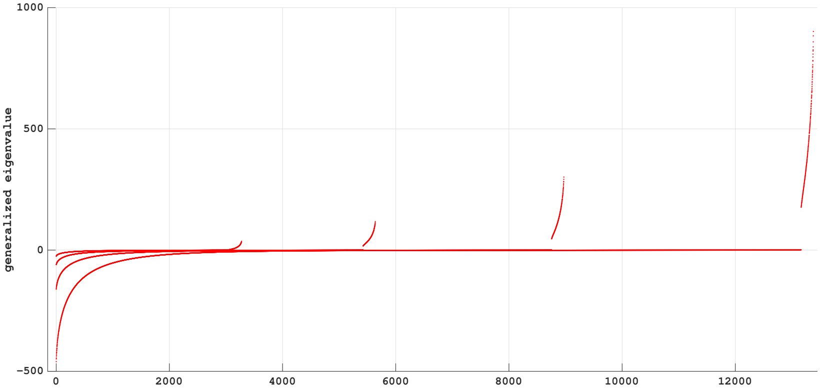
Details of the level-1 algorithm

- an example: the dot products are computed without BLAS to avoid function calls (slow!)
- computing transformation matrices for 8 pairs simultaneously
- transformations to 8 column pairs (f_p, f_q), (g_p, g_q), (z_p, z_q) are applied sequentially for each pair (cache!)

Distribution of eigenvalues – NaCl



Distribution of eigenvalues – AuAg



Timings

Example	Problem size	Number of cores 64	32
NaCl 2.5	50176 × 2256	800.70	556.95
NaCl 3.0	50176 × 3893	1973.64	1465.68
NaCl 3.5	50176 × 6217	2810.50	3660.44
NaCl 4.0	50176 × 9273	4846.98	7028.50
AuAg 2.5	26136 × 3275	724.20	587.23
AuAg 3.0	26136 × 5638	1549.92	1715.60
AuAg 3.5	26136 × 8970	3152.78	4711.65
AuAg 4.0	26136 × 13379	6544.16	11955.74

Conclusion

On a particular hardware testing space is enormous

- use Quadrant or SNC-4 clustering mode?
- in a single step — transform columns only once (block-oriented algorithm) or fully diagonalize them (full block algorithm)
- best pivoting strategy?
- is there need to shorten the columns by the hyperbolic QR factorization, and is there a switching point (use them or not)

  ...

Work in progress

- only lower 20% of the eigenvalues are needed
- is there any sufficiently parallel algorithm to compute them (without multiplication of the factors)?