

A KRYLOV-SCHUR-TYPE ALGORITHM FOR EIGENPROBLEMS WITH HAMILTONIAN SPECTRAL SYMMETRY

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RANMEP2008

National Tsinghua University, Taiwan, January 4–8, 2008

Joint work with Heike Faßbender and Martin Stoll

Dedicated to Ralph Byers (1955–2007)



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Definition

Let $J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$, then $H \in \mathbb{R}^{2n \times 2n}$ is called

- **Hamiltonian**, if $(HJ)^T = HJ$,
- **skew-Hamiltonian**, if $(HJ)^T = -HJ$.

A matrix pencil $\lambda N - H$ is called a **Hamiltonian/skew-Hamiltonian pencil**, if H is Hamiltonian and N is skew-Hamiltonian.

Explicit block form

of Hamiltonian matrices:

$$\begin{bmatrix} A & G \\ Q & -A^T \end{bmatrix}, \text{ where } A, G, Q \in \mathbb{R}^{n \times n} \text{ and } G = G^T, Q = Q^T,$$

of skew-Hamiltonian Matrices:

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Hamiltonian Eigensymmetry

Hamiltonian matrices and Hamiltonian/skew-Hamiltonian pencils exhibit the **Hamiltonian eigensymmetry**:

if λ is a finite eigenvalue of $H - \lambda N$, then $\bar{\lambda}$, $-\lambda$, $-\bar{\lambda}$ are eigenvalues of $H - \lambda N$, too.

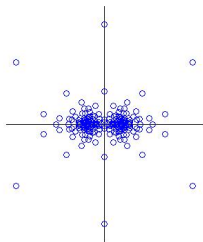
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Typical Hamiltonian spectrum:





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Goal

Structure-preserving algorithm, i.e., if $\tilde{\lambda}$ is a computed eigenvalue of $H - \lambda N$, then $\overline{\tilde{\lambda}}$, $-\tilde{\lambda}$, $-\overline{\tilde{\lambda}}$ should also be computed eigenvalues.

Goal cannot be achieved by general methods for matrices or matrix pencils like the QR/QZ, Lanczos, Arnoldi algorithms!

For an algorithm based on similarity transformations, the goal is achieved if the Hamiltonian structure is preserved.

Definition

$S \in \mathbb{R}^{2n \times 2n}$ is **symplectic** iff $S^T J S = J$, i.e., $S^{-1} = J^T S^T J$.

Lemma

If H is Hamiltonian (skew-Hamiltonian) and S is symplectic, then

$$S^{-1} H S$$

is Hamiltonian (skew-Hamiltonian), too.



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Hamiltonian eigenproblems arise in many different applications, e.g.:

- **Systems and control:**
 - Solution methods for algebraic and differential Riccati equations.
 - Design of LQR/LQG/ H_2/H_∞ controllers and filters for continuous-time linear control systems.
 - Stability radii and system norm computations; optimization of system norms.
 - Passivity-preserving model reduction based on balancing.
 - Reduced-order control for infinite-dim. systems based on inertial manifolds.
- **Computational physics:**
exponential integrators for Hamiltonian dynamics.
[EIROLA '03, LOPEZ/SIMONCINI '06]
- **Quantum chemistry:**
computing excitation energies in many-particle systems using random phase approximation (RPA).
- **Quadratic eigenvalue problems...**



Quadratic Eigenproblems with Hamiltonian Symmetry

$$Q(\lambda)x := (\lambda^2 M + \lambda G + K)x = 0,$$

where $M = M^T$, $K = K^T$, $G = -G^T$,

These QEPs arise in

- linear elasticity
- gyroscopic systems
- vibro-acoustics
- opto-electronics



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These QEPs arise in
linear elasticity

computation of corner singularities in 3D anisotropic
elastic structures [APEL/MEHRMANN/WATKINS '01];

gyroscopic systems

vibro-acoustics

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Quadratic Eigenproblems with Hamiltonian Symmetry

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linear elasticity

gyroscopic systems

used for modeling vibrations of spinning structures such as the simulation of tire noise, helicopter rotor blades, inertial navigation systems and components, or spin-stabilized satellites with appended solar panels or antennas

[LANCASTER '99, NACKENHORST '04, ELSSEL/VOSS '06, ...];

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modeling of flexible piping systems by coupling of linear wave equation with structural Lamé-Navier equations at fluid-structure interfaces; [MAESS/GAUL '05];

opto-electronics



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opto-electronics

optical waveguide design, using Maxwell eigenproblems

[SCHMIDT ET AL '03].



The Symplectic Lanczos Algorithm

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Symplectic Lanczos Algorithm for Hamiltonian operators H

- is based on transpose-free unsymmetric Lanczos process [FREUND '94];
- computes **partial J -tridiagonalization**;
- provides a symplectic (J -orthogonal) Lanczos basis $V_k \in \mathbb{R}^{2n \times 2k}$, i.e., $V_k^T J_n V_k = J_k$;
- was derived in several variants: [FREUND/MEHRMANN '94, FERNG/LIN/WANG '97, B./FASSBENDER '97, WATKINS '04];
- requires re- J -orthogonalization using, e.g., modified symplectic Gram-Schmidt;
- can be restarted implicitly using **implicit SR steps** [B./FASSBENDER '97];
- **exhibits convergence problems without locking & purging.**



The Hamiltonian J -Tridiagonal Form or Hamiltonian J -Hessenberg Form

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$$T_n = \left[\begin{array}{cccc|cccc} \delta_1 & & & & \beta_1 & \zeta_2 & & & & & & \\ & \delta_2 & & & \zeta_2 & \beta_2 & \zeta_3 & & & & & \\ & & \delta_3 & & & \zeta_3 & \ddots & \ddots & & & & \\ & & & \ddots & & & & \ddots & \ddots & & & \\ & & & & & & & & \zeta_n & \beta_n & & \\ \hline & \nu_1 & & & & & & & & & & \\ & & \nu_2 & & -\delta_1 & & & & & & & \\ & & & \nu_3 & & -\delta_2 & & & & & & \\ & & & & & & -\delta_3 & & & & & \\ & & & & & & & \ddots & & & & \\ & & & & & & & & \ddots & & & \\ & & & & & & & & & & \ddots & \\ & & & & & & & & & & & -\delta_n \end{array} \right] \in \mathbb{R}^{2n \times 2n},$$

- can be computed by symplectic similarity $T_n = S^{-1}HS$ almost always,
- is computed partially by symplectic Lanczos process, based on **symplectic Lanczos recursion**

$$HV_k = V_k T_k + \zeta_{k+1} \nu_{k+1} \mathbf{e}_{2k}^T, \quad V_k = [S(:, 1:k), S(:, k+1:2k)].$$

Theorem

If $T = S^{-1}HS$ is in Hamiltonian J -tridiagonal form, then

$$K(H, 2n - 1, v) = SR \quad \text{with} \quad s_1 = v$$

is an **SR decomposition** of the Krylov matrix

$$K(H, 2n - 1, v) := [v, Hv, \dots, H^{2n-1}v].$$

If R is nonsingular, then T is unreduced, i.e., $\zeta_j \neq 0$ for all j .

Column-wise evaluation of $HS = ST_n$ yields ($S := [v_1, \dots, v_n, w_1, \dots, w_n]$)

$$Hv_k = \delta_k v_k + \nu_k w_k \quad \iff \quad \nu_k w_k = Hv_k - \delta_k v_k =: \tilde{w}_k,$$

$$Hw_m = \zeta_m v_{k-1} + \beta_k v_k - \delta_k w_k + \zeta_{k+1} v_{k+1}$$

$$\iff \quad \zeta_{k+1} v_{k+1} = Hw_k - \zeta_k v_{k-1} - \beta_k v_k + \delta_k w_k =: \tilde{v}_{k+1}.$$

\implies Choose parameters $\delta_k, \beta_k, \nu_k, \zeta_k$ such that resulting algorithm computes symplectic (J -orthogonal) basis of Krylov subspace

$$\mathcal{K}(H, v_1, 2m) = \text{span}\{v_1, Hv_1, \dots, H^{2m-1}v_1\}.$$

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The Symplectic Lanczos Algorithm

Algorithm based on symplectic Lanczos recursion $HV_k = V_k T_k + \zeta_{k+1} v_{k+1} e_{2k}^T$

INPUT: $H \in \mathbb{R}^{2n \times 2n}$, $m \in \mathbb{N}$, and start vector $\tilde{v}_1 \neq 0 \in \mathbb{R}^{2n}$.

OUTPUT: $T_m \in \mathbb{R}^{2m \times 2m}$, $V_m \in \mathbb{R}^{2n \times 2m}$, ζ_{m+1} , and v_{m+1} .

1 $\zeta_1 = \|\tilde{v}_1\|_2$

2 $v_1 = \frac{1}{\zeta_1} \tilde{v}_1$

3 FOR $k = 1, 2, \dots, m$

(a) $t = H v_m$, $u = H w_m$

(b) $\delta_m = \langle t, v_m \rangle$

(c) $\tilde{w}_m = t - \delta_m v_m$

(d) $\nu_m = \langle t, v_m \rangle_J$

(e) $w_m = \frac{1}{\nu_m} \tilde{w}_m$

(f) $\beta_m = -\langle u, w_m \rangle_J$

(g) $\tilde{v}_{m+1} = u - \zeta_m v_{m-1} - \beta_m v_m + \delta_m w_m$

(h) $\zeta_{m+1} = \|\tilde{v}_{m+1}\|_2$

(i) $v_{m+1} = \frac{1}{\zeta_{m+1}} \tilde{v}_{m+1}$

ENDFOR

Note: 3(b) yields orthogonality of v_k, w_k [FERNG/LIN/WANG '97] and optimal conditioning of Lanczos basis [B. '03] if $\|v\|_2 = 1$ is forced.

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Implicit Restarts for given k -step Lanczos recursion $HV_k = V_k T_k + \zeta_{k+1} v_{k+1} e_{2k}^T$.

Extend Lanczos recursion by p symplectic Lanczos steps, yielding

$$HV_{k+p} = V_{k+p} T_{k+p} + \zeta_{k+p+1} v_{k+p+1} e_{2(k+p)}^T.$$

Let $S_{k+p} \in \mathbb{R}^{2(k+p) \times 2(k+p)}$ be symplectic. Then with

$$H \underbrace{(V_{k+p} S_{k+p})}_{\hat{V}_{k+p}} = \underbrace{(V_{k+p} S_{k+p})}_{\hat{V}_{k+p}} \underbrace{(S_{k+p}^{-1} T_{k+p} S_{k+p})}_{\hat{T}_{k+p}} + \zeta_{k+p+1} v_{k+p+1} e_{2(k+p)}^T S_{k+p},$$

\hat{V}_{k+p} is J -orthogonal, \hat{T}_{k+p} is Hamiltonian. Thus,

$$(*) \quad H \hat{V}_{k+p} = \hat{V}_{k+p} \hat{T}_{k+p} + \zeta_{k+p+1} v_{k+p+1} s_{k+p}^T \quad (s_{k+p}^T := S_{k+p}(2(k+p), :)).$$

Obtain new Lanczos recursion from $(*)$ by truncating back to k and choosing S_{k+p} so that

- \hat{T}_k is Hamiltonian J -tridiagonal,
- the residual term $\hat{\zeta}_{k+1} \hat{v}_{k+1} \hat{s}_k$ has the form **vector** $\times e_{2k}$.

\implies **implicit SR steps** with structure-induced shift polynomials, e.g.,
 $p_2(x) = (x - \mu)(x + \mu)$ or $p_4(x) = p_2(x) \overline{p_2(x)}$.



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\hat{V}_{k+p} is J -orthogonal, \hat{T}_{k+p} is Hamiltonian. Thus,

$$(*) \quad H \hat{V}_{k+p} = \hat{V}_{k+p} \hat{T}_{k+p} + \zeta_{k+p+1} v_{k+p+1} s_{k+p}^T \quad (s_{k+p}^T := S_{k+p}(2(k+p), :)).$$

Obtain new Lanczos recursion from $(*)$ by truncating back to k and choosing S_{k+p} so that

- \hat{T}_k is Hamiltonian J -tridiagonal,
- the residual term $\hat{\zeta}_{k+1} \hat{v}_{k+1} \hat{s}_k$ has the form **vector** $\times e_{2k}$.

\implies **implicit SR steps** with structure-induced shift polynomials, e.g.,
 $p_2(x) = (x - \mu)(x + \mu)$ or $p_4(x) = p_2(x) \overline{p_2(x)}$.

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- Bulge-chasing algorithm of GR class based on symplectic (J -orthogonal) similarity transformations. [DELLA-DORA '73]
- Algorithmic details analogous to QR algorithm, replace QR decomposition by SR (symplectic \times “psychologically” upper triangular) decomposition, using orthosymplectic Givens and Householder as well as symplectic Gaussian eliminations. [BUNSE-GERSTNER/MEHRMANN '86]
- Preserves the Hamiltonian J -tridiagonal form.
- Uses implicit double or quadruple shift SR steps which correspond to SR decomposition of $p_2(H) = (H - \mu I)(H + \mu I)$ or $p_4(H) = p_2(H)\overline{p_2(H)}$.
- Converges to Schur-like form with local cubic convergence rate. [WATKINS/ELSNER '91]
- Can be implemented using the $4n - 1$ parameters of the J -tridiagonal form only \rightsquigarrow parametric SR algorithm.

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- To enhance convergence of implicitly restarted Krylov subspace methods need deflation strategies for

- locking: deflate converged and wanted Ritz pairs,
- purging: deflate converged but unwanted Ritz pairs,

- Deflation, locking & purging technically involved and hard to realize for implicitly restarted Arnoldi/Lanczos.

[LEHOUCQ/SORENSEN '96, SORENSEN '02].

- Deflation strategies do not carry over to implicitly restarted symplectic Lanczos!
- Stewart's idea (SIMAX '01): rather than using Arnoldi decomposition (recursion), i.e.

$$AV_k = V_k H_k + r_{k+1} e_k^T \quad \text{with upper Hessenberg matrix } H_k$$

use Krylov-Schur decomposition

$$AW_k = W_k T_k + r_{k+1} t_{k+1}^T \quad \text{with } T_k \text{ in (real) Schur form}$$

for locking & purging.



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Assume we have constructed a symplectic Lanczos decomposition of length $2(k + p) = 2m$ of the form

$$HV_m = V_m T_m + \zeta_{m+1} v_{m+1} e_{2m}^T.$$

Definition

$$H\hat{V}_m = \hat{V}_m \hat{T}_m + \hat{\zeta}_{m+1} \hat{v}_{m+1} \hat{s}_m^T$$

is a **Hamiltonian Krylov-Schur-type decomposition** if

- $\text{rank}([\hat{V}_m, v_{m+1}]) = 2m + 1,$
- \hat{V}_m is J -orthogonal,
- \hat{T}_m is in Hamiltonian Schur-type form.



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Applying *SR* algorithm to T_m yields symplectic matrix S_m such that $\hat{T}_m := S_m^{-1} T_m S_m$ has Hamiltonian Schur-like form.

As noted before, \hat{T}_k can be ordered by J -orthogonal permutations so that converged and **wanted/unwanted** Ritz values appear in the **leading/trailing** blocks,

$$\hat{T}_m = \left[\begin{array}{cc|cc} A_1 & & G_1 & \\ & A_2 & & G_2 \\ \hline Q_1 & & -A_1^T & \\ & Q_2 & & -A_2^T \end{array} \right].$$



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Applying *SR* algorithm to T_m yields symplectic matrix S_m such that $\hat{T}_m := S_m^{-1} T_m S_m$ has Hamiltonian Schur-like form \rightsquigarrow

$$\begin{aligned}
 H(V_m S_m) &= (V_m S_m)(S_m^{-1} T_m S_m) + \zeta_{m+1} v_{m+1} e_{2m}^T S_m \\
 &= [V_k, V_p, W_k, W_p] \left[\begin{array}{c|cc} A_1 & & G_1 \\ & A_2 & G_2 \\ \hline Q_1 & & -A_1^T \\ & Q_2 & -A_2^T \end{array} \right] + \zeta_{m+1} v_{m+1} S_m^T
 \end{aligned}$$

Note: in case of deflation (\rightsquigarrow locking possible), $s_m^T = [0, s_{p,1}^T, 0, s_{p,2}^T]$.



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Purging: continue with Hamiltonian Krylov-Schur-type decomposition

$$H[V_k, W_k] = [V_k, W_k] T_k + \zeta_{m+1} v_{m+1} s_k^T$$

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\end{aligned}$$

Note: in case of deflation (\rightsquigarrow locking possible), $s_m^T = [0, s_{p,1}^T, 0, s_{p,2}^T]$.

Purging: continue with Hamiltonian Krylov-Schur-type decomposition

$$H[V_k, W_k] = [V_k, W_k] T_k + \zeta_{m+1} v_{m+1} s_k^T$$

Locking: continue with Hamiltonian Krylov-Schur-type decomposition

$$H[V_p, W_p] = [V_p, W_p] T_p + \zeta_{m+1} v_{m+1} s_p^T$$

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Purging: continue with Hamiltonian Krylov-Schur-type decomposition

$$H[V_k, W_k] = [V_k, W_k] T_k + \zeta_{m+1} v_{m+1} s_k^T$$

Locking: continue with Hamiltonian Krylov-Schur-type decomposition

$$H[V_p, W_p] = [V_p, W_p] T_p + \zeta_{m+1} v_{m+1} s_p^T$$

In order to expand subspace back to length m , need to return to symplectic Lanczos decomposition!

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Theorem

Every Hamiltonian Krylov-Schur-type decomposition is equivalent to a symplectic Lanczos decomposition.

Constructive proof:

Given a Hamiltonian Krylov-Schur-type decomposition of length k ,

$$HU = UT + us^T.$$

- 1 J -orthogonalize u w.r.t. U so that $U^T Ju = 0 \Rightarrow \hat{u} := \frac{1}{\gamma}(u - Ut)$,

$$HU = UT + (\gamma\hat{u} + Ut)s^T = U(T + ts^T) + \gamma\hat{u}s^T =: UB + \hat{u}\hat{s}^T.$$



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- 1 J -orthogonalize u w.r.t. U so that $U^T Ju = 0 \Rightarrow HU = UB + \hat{u}\hat{s}^T$.
- 2 Compute orthogonal symplectic matrix W such that $W^T \hat{s} = \hat{\zeta} e_{2k}^T \Rightarrow HUW = UW(W^T BW) + \hat{u}\hat{s}^T W =: UW\tilde{B} + \hat{\zeta}\hat{u}e_{2k}^T$.

Theorem

Every Hamiltonian Krylov-Schur-type decomposition is equivalent to a symplectic Lanczos decomposition.

Constructive proof:

Given a Hamiltonian Krylov-Schur-type decomposition of length k ,

$$HU = UT + us^T.$$

- 1 J -orthogonalize u w.r.t. U so that $U^T Ju = 0 \Rightarrow HU = UB + \hat{u}\hat{s}^T$.
- 2 Compute orthogonal symplectic matrix W such that $W^T \hat{s} = \hat{\zeta} e_{2k}^T \Rightarrow$

$$HUW = UW\tilde{B} + \hat{\zeta}\hat{u}e_{2k}^T.$$

- 3 Compute symplectic matrix S restoring J -tridiagonal form of \tilde{B} , i.e., $S^{-1}\tilde{B}S = \hat{T}$ is Hamiltonian J -tridiagonal and $e_{2k}^T S = e_{2k}^T$
(\rightsquigarrow row-wise bottom-to-top J -tridiagonalization) \Rightarrow

$$\underbrace{H U W S}_{=:V} = \underbrace{U W S}_{=:V} \underbrace{S^{-1} \tilde{B} S}_{=\hat{T}} + \hat{\zeta} \hat{u} e_{2k}^T$$

is an equivalent symplectic Lanczos decomposition.



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- 1 Use k steps of symplectic Lanczos process to compute symplectic Lanczos decomposition

$$HV_k = V_k T_k + \zeta_{k+1} v_{k+1} e_{2k}^T.$$

- 2 Expand Krylov subspace to length $2(k+p)$ using p steps of symplectic Lanczos process,

$$HV_{k+p} = V_{k+p} T_{k+p} + \zeta_{k+p+1} v_{k+p+1} e_{2(k+p)}^T.$$

- 3 Run (parametrized) SR algorithm on T_{k+p} to obtain Hamiltonian Krylov-Schur type decomposition

$$HU_{k+p} = U_{k+p} \tilde{T}_{k+p} + \zeta_{k+p+1} v_{k+p+1} \tilde{s}_{k+p}^T.$$

- 4 Re-order Hamiltonian Schur-type form as desired, deflate/purge, yielding new Hamiltonian Krylov-Schur type decomposition

$$H\tilde{U}_k = \tilde{U}_k \tilde{T}_k + \tilde{\zeta}_{k+1} \tilde{v}_{k+1} \tilde{s}_k^T.$$

(In case of deflation of ℓ converged Ritz values, $k \leftarrow k - \ell$.)

- 5 Compute equivalent symplectic Lanczos decomposition

$$H\hat{V}_k = \hat{V}_k \hat{T}_k + \hat{\zeta}_{k+1} \hat{v}_{k+1} e_{2k}^T.$$

- 6 IF $k > 0$, GOTO 2.



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- HKS is suitable for computing largest or smallest magnitude eigenvalues (apply to H or H^{-1}).
- For interior eigenvalues near target τ , need Hamiltonian shift-and-invert operator! But: $H - \tau I$, $(H - \tau I)^{-1}$ are not Hamiltonian!
- [MEHRMANN/WATKINS '01]

$$R_2(\tau) := (H - \tau I)^{-1}(H + \tau I)^{-1}, \quad \tau \in \mathbb{R}, i\mathbb{C},$$

$$R_4(\tau) := R_2(\tau)R_2(\bar{\tau}), \quad \tau \in \mathbb{C},$$

are skew-Hamiltonian, suitable for solution with SHIRA (skew-Hamiltonian implicitly restarted Arnoldi).

- [WATKINS '04]

$$H_1(\tau) = H^{-1}(H - \tau I)^{-1}(H + \tau I)^{-1}, \quad \tau \in \mathbb{R}, i\mathbb{C},$$

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H_2, H_4 are particularly suitable for QEPs (\rightsquigarrow later).

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are Hamiltonian and real.

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- Mathematical model: boundary control for linearized 2D heat equation.

$$c \cdot \rho \frac{\partial}{\partial t} x = \lambda \Delta x, \quad \xi \in \Omega$$

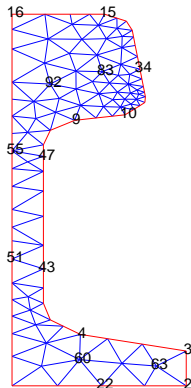
$$\lambda \frac{\partial}{\partial n} x = \kappa(u_k - x), \quad \xi \in \Gamma_k, \quad 1 \leq k \leq 7,$$

$$\frac{\partial}{\partial n} x = 0, \quad \xi \in \Gamma_7.$$

$$\implies m = 7, p = 6.$$

- FEM discretization, different models for initial mesh ($n = 371$), 3 steps of mesh refinement \Rightarrow 20209.
- Spatial semi-discretization \Rightarrow linear, time-invariant system

$$\dot{x} = Ax + Bu, \quad y = Cx.$$



Source: Physical model: courtesy of Mannesmann/Demag.

Math. model: TRÖLTZSCH/UNGER 1999/2001, PENZL 1999, SAAK 2003.



A Hamiltonian Krylov-Schur-Type Algorithm

Optimal cooling of steel profiles

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- Want 12 eigenvalues of largest magnitude ($k = 6$, choose $p = k$).
- Compare eigs and HKS applied to $H = \begin{bmatrix} A & BB^T \\ C^T C & -A^T \end{bmatrix}$.
- HKS and eigs both need 3 iterations to achieve $\frac{\|H\tilde{x} - \tilde{\lambda}\tilde{x}\|_1}{\|H\|_1 \|\tilde{x}\|_1} < 10^{-10}$, for 12 Ritz pairs $(\tilde{\lambda}, \tilde{x})$.
- Max. condition number in SR iterations: $\max(\text{cond}(SR)) = 573$.
- Eigenvalues scaled by 0.001.

eigs		HKS	
Eigenvalue	Residual	Eigenvalue	Residual
-0.01807591600154	$8 \cdot 10^{-17}$	-0.01807591600155	$1 \cdot 10^{-13}$
-0.03087837032049	$2 \cdot 10^{-16}$	-0.03087837032047	$4 \cdot 10^{-13}$
-0.08814494716419	$1 \cdot 10^{-16}$	-0.08814494716421	$5 \cdot 10^{-14}$
-0.19258460926304	$3 \cdot 10^{-16}$	-0.19258460926318	$1 \cdot 10^{-14}$
-0.26388595299811	$4 \cdot 10^{-16}$	-0.26388595299809	$8 \cdot 10^{-13}$
-0.33668742939988	$2 \cdot 10^{-15}$	-0.33668742939977	$1 \cdot 10^{-11}$



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Quadratic Eigenproblems with Hamiltonian Symmetry

$$Q(\lambda)x := (\lambda^2 M + \lambda G + K)x = 0,$$

where $M = M^T$, $K = K^T$, $G = -G^T$,

can be solved using linearization

$$\left(\lambda \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} - \begin{bmatrix} -G & -K \\ I & 0 \end{bmatrix} \right) \begin{bmatrix} y \\ x \end{bmatrix} = 0 \quad (y := \lambda x).$$

\rightsquigarrow unstructured (generalized) eigenproblem, **spectral symmetry is destroyed in finite precision computations.**



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$$(\lambda N - H)z = \left(\lambda \begin{bmatrix} I & G \\ 0 & I \end{bmatrix} - \begin{bmatrix} 0 & -K \\ M^{-1} & 0 \end{bmatrix} \right) \begin{bmatrix} y \\ x \end{bmatrix} = 0 \quad (y := \lambda Mx)$$

\rightsquigarrow skew-Hamiltonian/Hamiltonian eigenproblem as N is skew-Hamiltonian, H is Hamiltonian;



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\rightsquigarrow skew-Hamiltonian/Hamiltonian eigenproblem as N is skew-Hamiltonian, H is Hamiltonian;

\rightsquigarrow spectral symmetry can be preserved in finite precision computations if structure-preserving algorithm is used!



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\rightsquigarrow skew-Hamiltonian/Hamiltonian eigenproblem as N is skew-Hamiltonian, H is Hamiltonian;

Skew-Hamiltonian/Hamiltonian eigenproblem is equivalent to Hamiltonian eigenproblem $Hx = \lambda x$ with

$$H = \begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & -K \\ M^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix}.$$



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For eigenvalues of largest magnitude apply HKS to

$$H = \begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & -K \\ M^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix}.$$

For eigenvalues of smallest magnitude apply HKS to

$$H^{-1} = \begin{bmatrix} I & \frac{1}{2}G \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & M \\ -K^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & \frac{1}{2}G \\ 0 & I \end{bmatrix}.$$

Note: more efficient than SHIRA applied to H^{-2} !



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For interior real/purely imaginary eigenvalues apply HKS to

$$\begin{aligned} H_2(\tau) &= H(H - \tau I)^{-1}(H + \tau I)^{-1} \\ &= \begin{bmatrix} -\frac{1}{2}G & -K \\ I & 0 \end{bmatrix} \begin{bmatrix} I & \tau I \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & I \\ -Q(\tau)^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & G \\ 0 & I \end{bmatrix} \\ &\quad \times \begin{bmatrix} 0 & I \\ -Q(\tau)^{-T} & 0 \end{bmatrix} \begin{bmatrix} I & -\tau I \\ 0 & I \end{bmatrix} \begin{bmatrix} I & \frac{1}{2}G \\ 0 & M \end{bmatrix}. \end{aligned}$$

Applying $Q(\tau)^{-1}$, $Q(\tau)^{-T}$ requires only 1 LU factorization!

Note: as efficient as SHIRA applied to $R_2(\tau)$!



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For eigenvalues of largest magnitude apply HKS to

$$H = \begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & -K \\ M^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix}.$$

For eigenvalues of smallest magnitude apply HKS to

$$H^{-1} = \begin{bmatrix} I & \frac{1}{2}G \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & M \\ -K^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & \frac{1}{2}G \\ 0 & I \end{bmatrix}.$$

For interior complex eigenvalues apply HKS to

$$H_4(\tau) = H(H - \tau I)^{-1}(H + \tau I)^{-1}(H - \bar{\tau}I)^{-1}(H + \bar{\tau}I)^{-1}.$$

Note: as efficient as SHIRA applied to $R_4(\tau)$!

- We apply `eigs` and HKS (and SHIRA for nonzero shifts) to several test sets.
- Convergence is based on comparable stopping criteria: Ritz values are taken as converged if relative residuals for the shift-and-invert operators are smaller than given tolerance.
- Relative residuals in numerical examples are the residuals for the QEP, i.e.,

$$\frac{\|(\tilde{\lambda}^2 M + \tilde{\lambda} G + K)\tilde{x}\|_1}{\|\tilde{\lambda}^2 M + \tilde{\lambda} G + K\|_1 \|\tilde{x}\|_1},$$

where $(\tilde{\lambda}, \tilde{x})$ is a converged Ritz pair.



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Corner singularities

[APEL/MEHRMANN/WATKINS '02]

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- Solutions of elliptic boundary value problems like Laplace and linear elasticity (Lamé) equations in domains with polyhedral corners exhibit singularities in the neighborhood of the corners.
- Singularities can be quantified if this neighborhood is intersected with the unit ball centered at the corner and parameterized with spherical coordinates (r, ϕ, θ) .
- The singular part of the solution can be expanded in a series with terms of the form $r^\alpha u(\phi, \theta)$, where α is the singularity exponent.
- It turns out that $\alpha =: \lambda - 0.5$ and u can be computed as eigenpairs of quadratic operator eigenvalue problems of the form

$$\lambda^2 m(u, v) + \lambda g(u, v) = k(u, v),$$

where $m(\cdot, \cdot)$, $k(\cdot, \cdot)$ are Hermitian positive definite sesquilinear forms and $g(\cdot, \cdot)$ is a skew-Hermitian sesquilinear form.

- Finite-element discretization of the operator eigenvalue problem leads to a QEP, where M and $-K$ are positive definite.



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- Here: 3D elasticity problem for Fichera corner (cutting the cube $[0, 1] \times [0, 1] \times [0, 1]$ out of the cube $(-1, 1) \times (-1, 1) \times (-1, 1)$).
- $n = 12, 828$, matrix assembly with software *CoCoS* [C. PESTER '05].
- Want 12 eigenvalues closest to target shift $\tau = 1$.
- Compare SHIRA applied to $R_2(1)$, eigs and HKS applied to $H_2(1)$.
- SHIRA needs 3, eigs 6, HKS 4 iterations.
- Max. condition number in SR iterations: $\max(\text{cond}(SR)) = 3.35 \cdot 10^5$.

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SHIRA		HKS	
Eigenvalue	Residual	Eigenvalue	Residual
0.9051092989 8162	$2 \cdot 10^{-14}$	0.9051092989 4951	$6 \cdot 10^{-16}$
0.9052956878 6502	$2 \cdot 10^{-14}$	0.9052956878 4944	$5 \cdot 10^{-16}$
1.0748059554498 3	$5 \cdot 10^{-15}$	1.0748059554498 5	$4 \cdot 10^{-16}$
1.6011734510 4537	$1 \cdot 10^{-13}$	1.6011734510 1134	$6 \cdot 10^{-16}$
1.657656086 89959	$4 \cdot 10^{-14}$	1.657656086 79830	$3 \cdot 10^{-15}$
1.659145297 25492	$1 \cdot 10^{-14}$	1.659145297 02482	$7 \cdot 10^{-15}$



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eigs		HKS	
Eigenvalue	Residual	Eigenvalue	Residual
0.9051092989 8127	$4 \cdot 10^{-16}$	0.9051092989 4951	$6 \cdot 10^{-16}$
0.9052956878 6417	$4 \cdot 10^{-16}$	0.9052956878 4944	$5 \cdot 10^{-16}$
1.0748059554 5002	$4 \cdot 10^{-16}$	1.0748059554 4985	$4 \cdot 10^{-16}$
1.6011734510 2312	$2 \cdot 10^{-16}$	1.6011734510 1134	$6 \cdot 10^{-16}$
1.657656086 88689	$2 \cdot 10^{-16}$	1.657656086 79830	$3 \cdot 10^{-15}$
1.659145297 26339	$1 \cdot 10^{-16}$	1.659145297 02482	$7 \cdot 10^{-15}$

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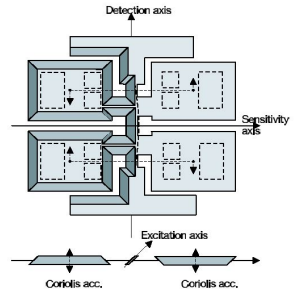
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- By applying AC voltage to electrodes, wings are forced to vibrate in anti-phase in wafer plane.
- Coriolis forces induce motion of wings out of wafer plane yielding sensor data.

- Vibrating micro-mechanical gyroscope for inertial navigation.
- Rotational position sensor.



Source: The Oberwolfach Benchmark Collection <http://www.intek.de/simulation/benchmark>

Courtesy of D. Billger (Imego Institute, Göteborg), Saab Bofors Dynamics AB.



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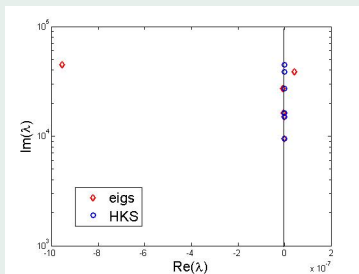
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- FEM model (ANSYS), $n = 17,361$.
- Compare eigs and HKS applied to H^{-1} and $H_2(10^6 i)$, request 12 eigenvalues.

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H^{-1}

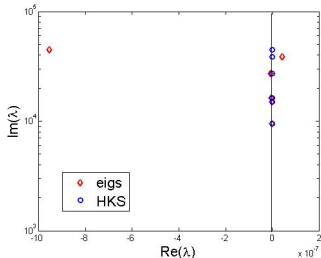
- Both need 3 iterations.
- Relative residuals $< \text{eps}$.
- $\max(\text{cond}(SR)) = 1.5 \cdot 10^3$.



- FEM model (ANSYS), $n = 17,361$.
- Compare eigs and HKS applied to H^{-1} and $H_2(10^6 i)$, request 12 eigenvalues.

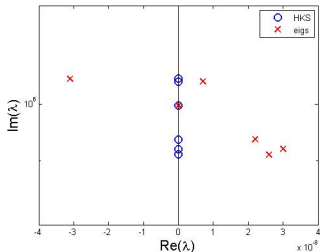
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- Both need 3 iterations.
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$H_2(\tau) = H(H - \tau I)^{-1}(H + \tau I)^{-1}$

- HKS needs 3, eigs 2 iterations.
- Relative residuals $< \text{eps}$.
- $\max(\text{cond}(SR)) = 3.15 \cdot 10^6$.





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- Modeling the noise of rolling tires requires to determine the transient vibrations, [NACKENHORST/VON ESTORFF '01].
- FEM model of a deformable wheel rolling on a rigid plane surface results in a gyroscopic system of order $n = 124,992$ [NACKENHORST '04].
- Sparse LU factorization of $Q(\tau)$ requires about 6 GByte.
- Here, use reduced-order model of size $n = 2,635$ computed by AMLS [ELSSEL/VOSS '06].



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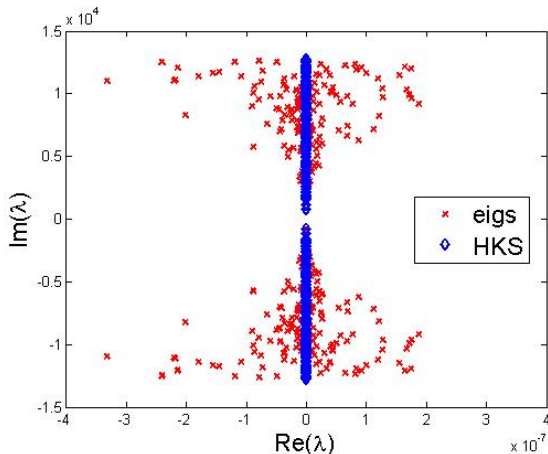
Conclusions and
Outlook

References

- Compare eigs and HKS applied to H^{-1} to compute the 12 smallest eigenvalues.
- eigs needs 8, HKS 6 iterations.
- $\max(\text{cond}(SR)) = 331$.
- Eigenvalues scaled by 1,000.

eigs		HKS	
Eigenvalue	Residual	Eigenvalue	Residual
$4 \cdot 10^{-12} + 1.73705142673i$	$2 \cdot 10^{-14}$	$1.73705142671i$	$5 \cdot 10^{-17}$
$-3 \cdot 10^{-12} + 1.66795405953i$	$8 \cdot 10^{-15}$	$1.66795405955i$	$2 \cdot 10^{-15}$
$2 \cdot 10^{-13} + 1.66552788164i$	$2 \cdot 10^{-15}$	$1.66552788164i$	$1 \cdot 10^{-16}$
$4 \cdot 10^{-14} + 1.58209209804i$	$1 \cdot 10^{-16}$	$1.58209209804i$	$5 \cdot 10^{-17}$
$-1 \cdot 10^{-14} + 1.13657108578i$	$8 \cdot 10^{-17}$	$1.13657108578i$	$7 \cdot 10^{-18}$
$1 \cdot 10^{-14} + 0.80560062107i$	$1 \cdot 10^{-16}$	$0.80560062107i$	$6 \cdot 10^{-18}$

- Compare eigs and HKS applied to H^{-1} to compute the 180 smallest eigenvalues.





Conclusions and Outlook

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Conclusions

- Solution of large-scale eigenproblems with Hamiltonian eigensymmetry in a numerically reliable way possible by combination of symplectic Lanczos process and Krylov-Schur restarting.
- Alternative to SHIRA, often with faster convergence.
- Relies on parameterized SR algorithm [FASSBENDER '07].
- Advantageous in particular in presence of eigenvalues on the imaginary axis, e.g., for stable gyroscopic systems.

Outlook

- Integration into HAPACK (\equiv better and more reliable implementation. . .)
- Comparison to SOAR [BAI/SU '05] for second-order eigenproblems.
- Solution of higher-order, structured polynomial eigenproblems.
- Version for symplectic/palindromic eigenproblems based on symplectic Lanczos process and SZ iteration.
- Two-sided symplectic (implicitly restarted) Arnoldi based on symplectic URV decomposition [B./KRESSNER/MEHRMANN/XU], soon.



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- 1** T. Apel, V. Mehrmann, and D. Watkins.
Structured eigenvalue methods for the computation of corner singularities in 3d anisotropic elastic structures.
Comput. Methods Appl. Mech. Engrg., 191:4459–4473, 2002.
- 2** P. Benner.
Structured Krylov subspace methods for eigenproblems with spectral symmetries.
Workshop Theoretical and Computational Aspects of Matrix Algorithms, Dagstuhl, October 2003.
- 3** P. Benner and H. Faßbender.
An implicitly restarted symplectic Lanczos method for the Hamiltonian eigenvalue problem.
Lin. Alg. Appl., 263:75–111, 1997.
- 4** P. Benner and H. Faßbender.
An implicitly restarted symplectic Lanczos method for the symplectic eigenvalue problem.
SIAM J. Matrix Anal. Appl., 22(3):682–713, 2000.
- 5** P. Benner, H. Faßbender, and M. Stoll.
A Krylov-Schur-type algorithm for Hamiltonian eigenproblems based on the symplectic Lanczos process.
Submitted, 2007.
- 6** P. Benner, H. Faßbender, and M. Stoll.
Solving large-scale quadratic eigenvalue problems with Hamiltonian eigenstructure using a structure-preserving Krylov subspace method.
Numerical Analysis Group Research Report NA-07/03, Oxford University, February 2007.
- 7** A. Bunse-Gerstner and V. Mehrmann.
A symplectic QR-like algorithm for the solution of the real algebraic Riccati equation.
IEEE Trans. Automat. Control, AC-31:1104–1113, 1986.
- 8** H. Faßbender.
The Parameterized SR Algorithm for Hamiltonian Matrices.
ETNA, 26:121–145, 2007.



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- 9** H. Faßbender.
A detailed derivation of the parameterized *SR* algorithm and the symplectic Lanczos method for Hamiltonian matrices.
Technical report, TU Braunschweig, Institut *Computational Mathematics*, 2006.
- 10** W. R. Ferng, W. W. Lin, and C. S. Wang.
The shift-inverted J-Lanczos algorithm for the numerical solutions of large sparse algebraic Riccati equations.
Comp. Math. Appl., 33(10):23740, 1997.
- 11** M. Stoll.
Locking und Purgung für den Hamiltonischen Lanczos-Prozess.
Diplomarbeit, Fakultät für Mathematik, TU Chemnitz, September 2005.
- 12** R.B. Lehoucq and D.C. Sorensen.
Deflation techniques for an implicitly restarted Arnoldi iteration.
SIAM J. Matrix Anal. Appl., 17:789–821, 1996.
- 13** V. Mehrmann and D. Watkins.
Structure-preserving methods for computing eigenpairs of large sparse skew-Hamiltonian/Hamiltonian pencils.
SIAM J. Sci. Comp., 22:1905–1925, 2001.
- 14** D. Sorensen.
Numerical methods for large eigenvalue problems.
Acta Numerica, 11:519–584, 2002.
- 15** G.W. Stewart.
A Krylov-Schur algorithm for large eigenproblems.
SIAM J. Matrix Anal. Appl., 23(4):601–614, 2001.
- 16** D. Watkins.
On Hamiltonian and symplectic Lanczos processes.
Linear Algebra Appl., 385:23–45, 2004.