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

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Joint work with Heike Faßbender and Martin Stoll

Dedicated to Ralph Byers (1955–2007)

Overview

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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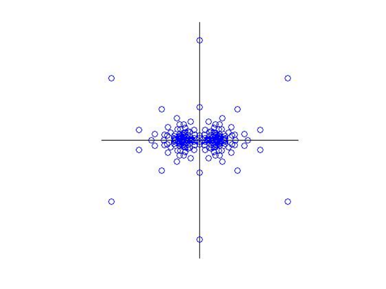
Typical Hamiltonian spectrum:



Hamiltonian Eigenproblems

Goal

Structure-preserving algorithm, i.e., if $\tilde{\lambda}$ is a computed eigenvalue of $H - \lambda N$, then $\bar{\tilde{\lambda}}, -\tilde{\lambda}, -\bar{\tilde{\lambda}}$ 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 $\quad S^T J S = J, \quad$ i.e., $S^{-1} = J^T S^T J$.

Lemma

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

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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

$$Q(\lambda)x := (\lambda^2 M + \lambda G + K)x = 0,$$
$$\text{where } M = M^T,\ K = K^T,\ G = -G^T,$$

These QEPs arise in

linear elasticity

gyroscopic systems

vibro-acoustics

opto-electronics

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: computation of corner singularities in 3D anisotropic elastic structures [Apel/Mehrmann/Watkins '01];

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: 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];

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optical waveguide design, using Maxwell eigenproblems [Schmidt et al '03].

The Symplectic Lanczos Algorithm

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

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

- 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

$$HV_k = V_k T_k + \zeta_{k+1} v_{k+1} e_{2k}^T, \qquad V_k = [S(:,1:k),\ S(:,k+1:2k)].$$

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

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

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 $(S := [v_1, \ldots, v_n, w_1, \ldots, w_n])$

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

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

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

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

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

The Symplectic Lanczos Algorithm

Derivation using Partial J-Tridiagonalization

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$$\begin{aligned} Hv_k &= \delta_k v_k + \nu_k w_k \quad \Longleftrightarrow \quad \nu_k w_k = Hv_k - \delta_k v_k =: \widetilde{w}_k, \\ Hw_m &= \zeta_m v_{k-1} + \beta_k v_k - \delta_k w_k + \zeta_{k+1} v_{k+1} \\ &\Longleftrightarrow \quad \zeta_{k+1} v_{k+1} = Hw_k - \zeta_k v_{k-1} - \beta_k v_k + \delta_k w_k =: \widetilde{v}_{k+1}. \end{aligned}$$

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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 $k = 1, 2, \ldots, m$
   (a) $t = Hv_m, \; u = Hw_m$
   (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) $w_m = \frac{1}{\nu_m} \tilde{w}_m$
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   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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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,

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

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}.

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

The Symplectic Lanczos Algorithm

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

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The SR Algorithm

Key Ingredients

- 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. [Fassbender '07]

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- 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 ⇝ parametric SR algorithm. [Fassbender '07]

The SR Algorithm

Key Ingredients

- 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 × "psychologically" upper triangular) decomposition, using orthosymplectic Givens and Householder as well as symplectic Gaussian eliminations. [Bunse-Gerstner/Mehrmann '86]
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The SR Algorithm

Hamiltonian Schur-like form obtained from SR algorithm

SR iterates converge to

$$
\left[\begin{array}{cccccc|cccccc}
A_1 & & & & & & G_1 & & & & & \\
& \ddots & & & & & & \ddots & & & & \\
& & A_k & & & & & & G_k & & & \\
& & & 0 & & & & & & G_{k+1} & & \\
& & & & \ddots & & & & & & \ddots & \\
& & & & & 0 & & & & & & G_m \\
\hline
0 & & & & & & -A_1^T & & & & & \\
& \ddots & & & & & & \ddots & & & & \\
& & 0 & & & & & & -A_k^T & & & \\
& & & Q_{k+1} & & & & & & 0 & & \\
& & & & \ddots & & & & & & \ddots & \\
& & & & & Q_m & & & & & & 0
\end{array}\right],
$$

- the 1×1 blocks A_j represent real eigenvalues with $\lambda_j < 0$,
- the 2×2 blocks A_j represent complex eigenvalues with $\mathrm{Re}(\lambda_j) < 0$,
- the blocks $\begin{bmatrix} A_j & G_j \\ Q_j & -A_j^T \end{bmatrix}$ represent purely imaginary eigenvalues.
- Re-ordering of eigenvalues requires (block-)permutation only!

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 & & & & \ddots & & & & & & \ddots & \\
 & & & & & 0 & & & & & & G_m \\
\hline
0 & & & & & & -A_1^T & & & & & \\
 & \ddots & & & & & & \ddots & & & & \\
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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

- $\operatorname{rank}\left([\hat{V}_m, v_{m+1}]\right) = 2m+1$,
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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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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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A Hamiltonian Krylov-Schur-Type Algorithm

Symplectic Lanczos decomposition ⇒ Hamiltonian Krylov-Schur-type decomposition

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

A Hamiltonian Krylov-Schur-Type Algorithm

Hamiltonian Krylov-Schur-type decomposition $\Rightarrow$ symplectic Lanczos decomposition

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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2. Compute orthogonal symplectic matrix W such that $W^T \hat{s} = \hat{\zeta} e_{2k}^T \Rightarrow$
$$HUW = UW(W^T BW) + \hat{u}\hat{s}^T W =: UW\tilde{B} + \hat{\zeta}\hat{u}e_{2k}^T.$$

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$$HUW = UW\tilde{B} + \hat{\zeta}\hat{u}e_{2k}^T.$$
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) $\Rightarrow$
$$H\underbrace{UWS}_{=:V} = \underbrace{UWS}_{=:V}\underbrace{S^{-1}\tilde{B}S}_{=\hat{T}} + \hat{\zeta}\hat{u}e_{2k}^T$$
is an equivalent symplectic Lanczos decomposition.

Algorithm HKS

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

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

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.

Shift-and-invert

- 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]

$$\begin{aligned} R_2(\tau) &:= (H-\tau I)^{-1}(H+\tau I)^{-1}, & \tau \in \mathbb{R}, \imath\mathbb{C}, \\ R_4(\tau) &:= R_2(\tau)R_2(\overline{\tau}), & \tau \in \mathbb{C}, \end{aligned}$$

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

- [Watkins '04]

$$\begin{aligned} H_1(\tau) &= H^{-1}(H-\tau I)^{-1}(H+\tau I)^{-1}, & \tau \in \mathbb{R}, \imath\mathbb{C}, \\ H_2(\tau) &= H(H-\tau I)^{-1}(H+\tau I)^{-1}, & \tau \in \mathbb{R}, \imath\mathbb{C}, \\ H_3(\tau) &= H_1(\tau)R_2(\overline{\tau}), & \tau \in \mathbb{C}, \\ H_4(\tau) &= H_2(\tau)R_2(\overline{\tau}), & \tau \in \mathbb{C}, \end{aligned}$$

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

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A Hamiltonian Krylov-Schur-Type Algorithm

Optimal control: cooling of steel profiles

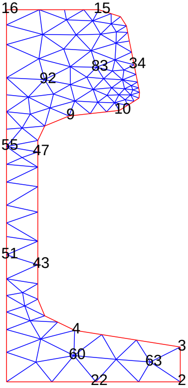
- Mathematical model: boundary control for linearized 2D heat equation.

$$\begin{aligned} c \cdot \rho \frac{\partial}{\partial t} x &= \lambda \Delta x, & \xi \in \Omega \\ \lambda \frac{\partial}{\partial n} x &= \kappa(u_k - x), & \xi \in \Gamma_k,\ 1 \le k \le 7, \\ \frac{\partial}{\partial n} x &= 0, & \xi \in \Gamma_7. \end{aligned}$$

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

- 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.

- 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: $\max(\mathrm{cond}\,(SR)) = 573$.
- Eigenvalues scaled by 0.001.

`eigs`		HKS	
Eigenvalue	Residual	Eigenvalue	Residual
$-0.018075916001 54$	$8 \cdot 10^{-17}$	$-0.018075916001 55$	$1 \cdot 10^{-13}$
$-0.030878370320 49$	$2 \cdot 10^{-16}$	$-0.030878370320 47$	$4 \cdot 10^{-13}$
$-0.0881449471 6419$	$1 \cdot 10^{-16}$	$-0.0881449471 6421$	$5 \cdot 10^{-14}$
$-0.1925846092 6304$	$3 \cdot 10^{-16}$	$-0.1925846092 6318$	$1 \cdot 10^{-14}$
$-0.2638859529 9811$	$4 \cdot 10^{-16}$	$-0.2638859529 9809$	$8 \cdot 10^{-13}$
$-0.3366874293 9988$	$2 \cdot 10^{-15}$	$-0.3366874293 9977$	$1 \cdot 10^{-11}$

Quadratic Eigenproblems with Hamiltonian Symmetry

$$Q(\lambda)x := (\lambda^2 M + \lambda G + K)x = 0,$$
$$\text{where } M = M^T,\ K = K^T,\ G = -G^T,$$

can be solved using linearization

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

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

Quadratic Eigenvalue Problems

Quadratic Eigenproblems with Hamiltonian Symmetry

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

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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!

Quadratic Eigenvalue Problems

Quadratic Eigenproblems with Hamiltonian Symmetry

$$Q(\lambda)x := (\lambda^2 M + \lambda G + K)x = 0,$$
$$\text{where } M = M^T,\ K = K^T,\ G = -G^T,$$

can be solved using linearization

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

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

Skew-Hamiltonian/Hamiltonian eigenproblem is equivalent to Hamiltonian eigenproblem $Hz = \lambda z$ with

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

Quadratic Eigenvalue Problems
Shift-and-invert

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}!

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 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 $R_2(\tau)$!

For eigenvalues of largest magnitude apply HKS to

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

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

For interior complex eigenvalues apply HKS to

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

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.

- 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 $m(.,.), k(.,.)$ are Hermitian positive definite sesquilinear forms and $g(.,.)$ 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.

Quadratic Eigenvalue Problems

Corner singularities

- 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: $\max(\mathrm{cond}\,(SR)) = 3.35 \cdot 10^5$.

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SHIRA		HKS	
Eigenvalue	Residual	Eigenvalue	Residual
0.90510929898162	$2 \cdot 10^{-14}$	0.90510929894951	$6 \cdot 10^{-16}$
0.90529568786502	$2 \cdot 10^{-14}$	0.90529568784944	$5 \cdot 10^{-16}$
1.07480595544983	$5 \cdot 10^{-15}$	1.07480595544985	$4 \cdot 10^{-16}$
1.60117345104537	$1 \cdot 10^{-13}$	1.60117345101134	$6 \cdot 10^{-16}$
1.65765608689959	$4 \cdot 10^{-14}$	1.65765608679830	$3 \cdot 10^{-15}$
1.65914529725492	$1 \cdot 10^{-14}$	1.65914529702482	$7 \cdot 10^{-15}$

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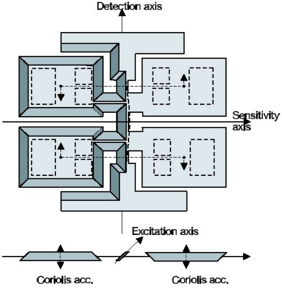
`eigs`		HKS	
Eigenvalue	Residual	Eigenvalue	Residual
0.9051092989**8127**	$4 \cdot 10^{-16}$	0.9051092989**4951**	$6 \cdot 10^{-16}$
0.9052956878**6417**	$4 \cdot 10^{-16}$	0.9052956878**4944**	$5 \cdot 10^{-16}$
1.0748059554**5002**	$4 \cdot 10^{-16}$	1.0748059554**4985**	$4 \cdot 10^{-16}$
1.6011734510**2312**	$2 \cdot 10^{-16}$	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**	$7 \cdot 10^{-15}$

- 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.imtek.de/simulation/benchmark

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

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

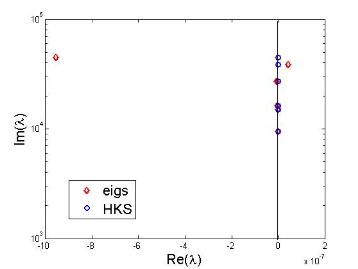
Quadratic Eigenvalue Problems

Gyroscopic systems: micro-gyroscope

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

H^{-1}

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



Quadratic Eigenvalue Problems

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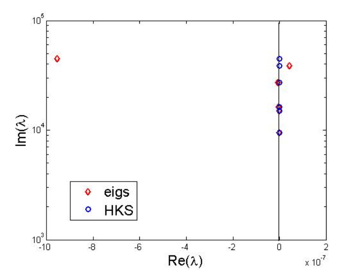
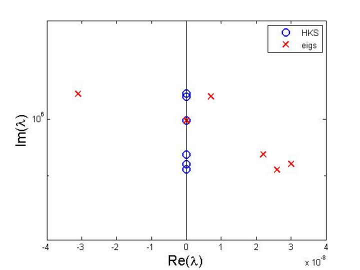


$H_2(\tau) = H(H - \tau I)^{-1}(H + \tau I)^{-1}$

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

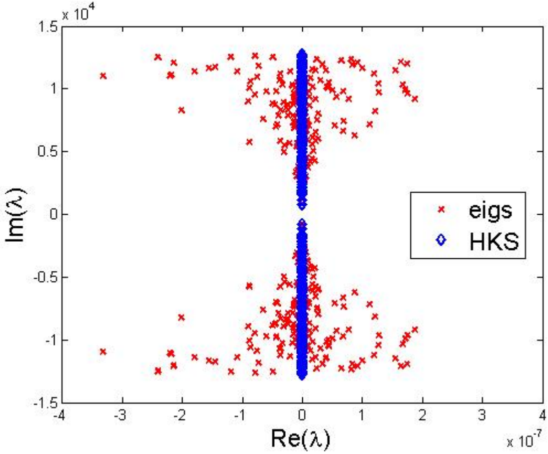


- Modeling the noise of rolling tires requires to determine the transient vibrations, [Nackenhorst/von Estorff '01].
- FEM model of a deformable wheel rolling on a rigid plane surface results in a gyroscopic system of order $n = 124,992$ [Nackenhorst '04].
- Sparse LU factorization of $Q(\tau)$ requires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

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

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

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



Conclusions and Outlook

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.

Conclusions and Outlook

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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