Parameter-Dependent Eigencomputations and MEMS Applications

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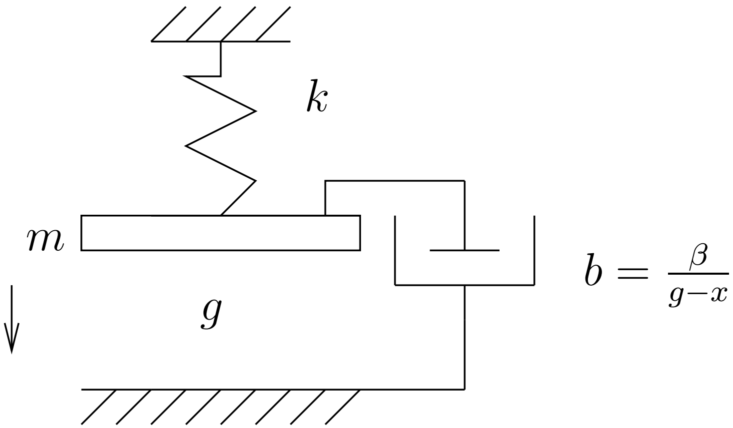
Outline

- Some applications
- Mathematical background
- Continuing invariant subspaces

Illustrative example: damped gap actuator



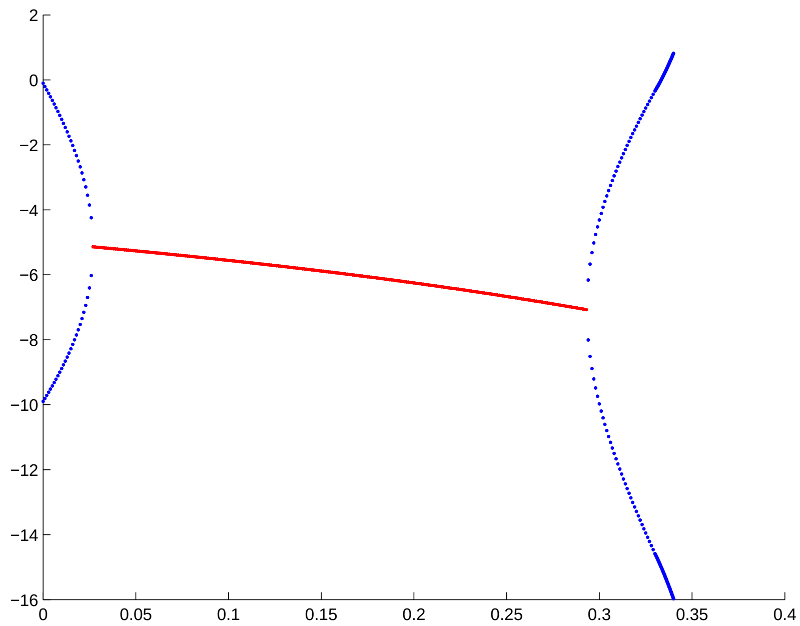
Nonlinear governing equation:

$$mx'' + \frac{\beta}{g-x}x' + kx - \frac{\alpha V^2}{2(g-x)^2} = 0 \qquad (1)$$

Linearized at equilibrium $kx - \frac{\alpha V^2}{2(g-x)^2} = 0$:

$$m(\Delta x)'' + \frac{\beta}{g-x}(\Delta x)' + k\left(1 - \frac{2x}{g-x}\right)(\Delta x) = 0 \qquad (2)$$

Illustrative example: frequency behaviors



Real parts of eigenvalues vs. displacement

- Small deflection: overdamped
- Moderate deflection: underdamped
- $x = g/3 - \mathrm{small}$: overdamped
- $x = g/3$: loss of stability (bifurcation)

Resonator design

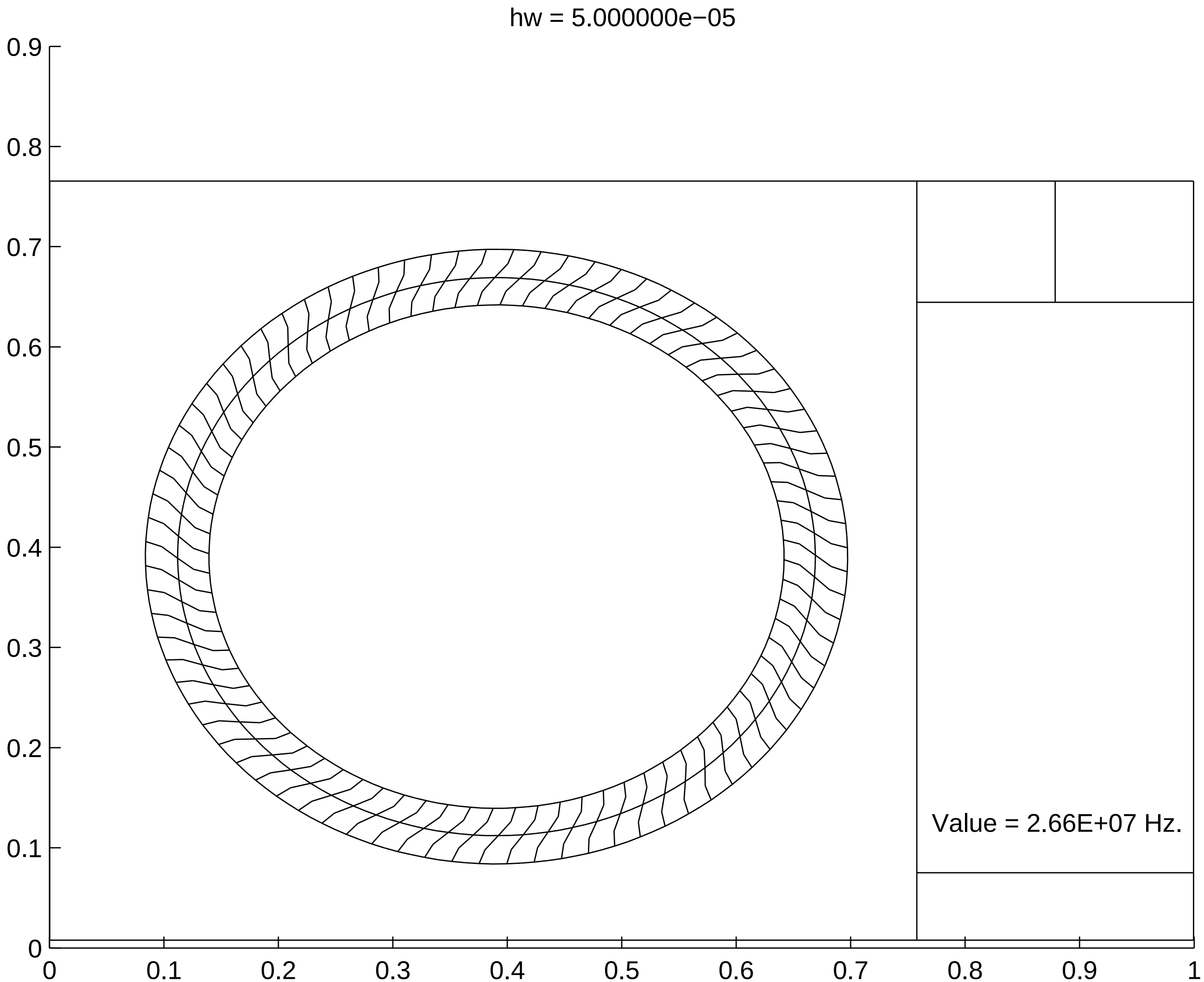
Problem domain:

- RF frequency microresonators for cell phone filters
- High frequency, low amplitude – very linear

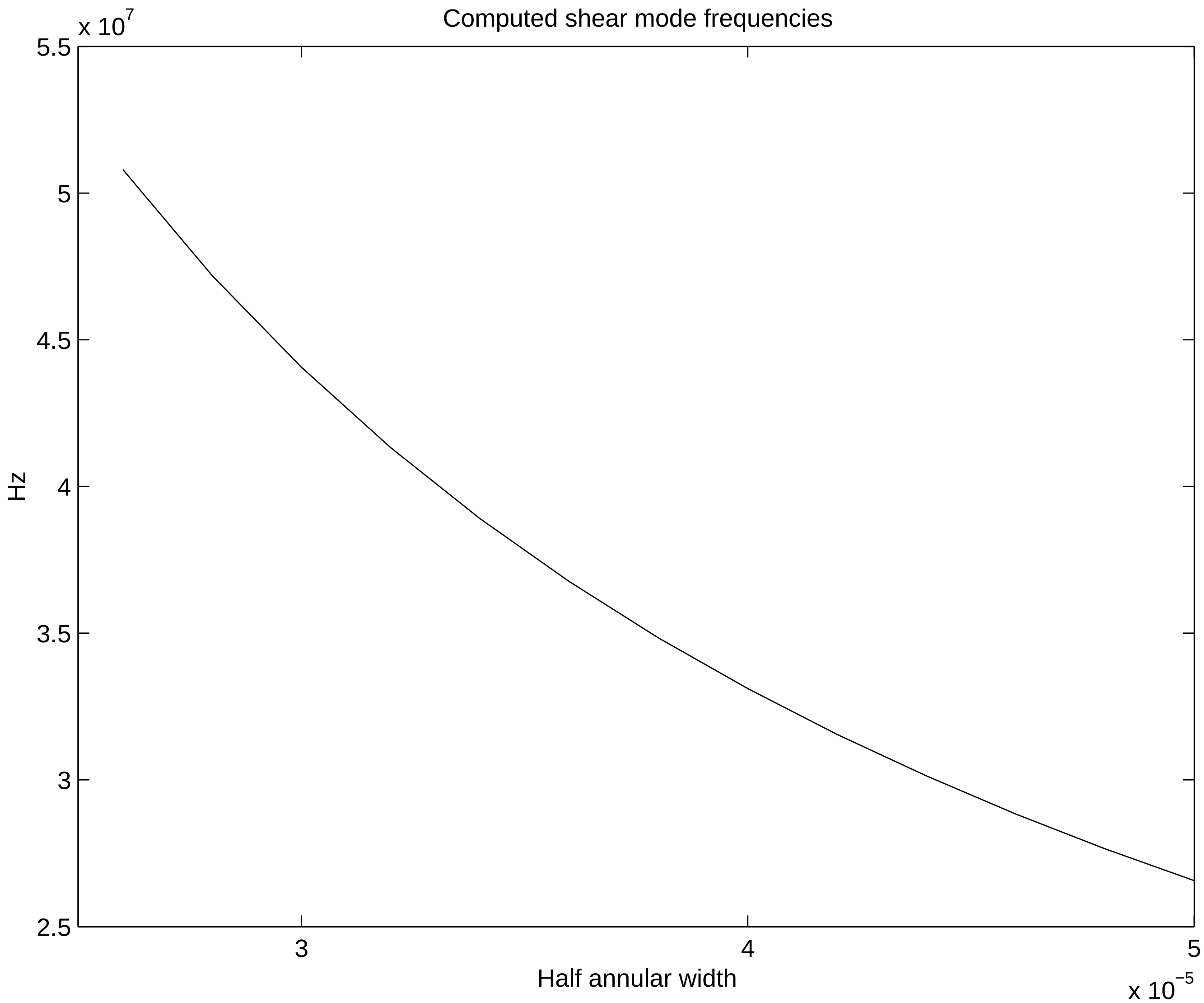
Questions:

- How does resonant behavior change with shape?
- How sensitive are modes to fabrication misalignments?

Ring resonator



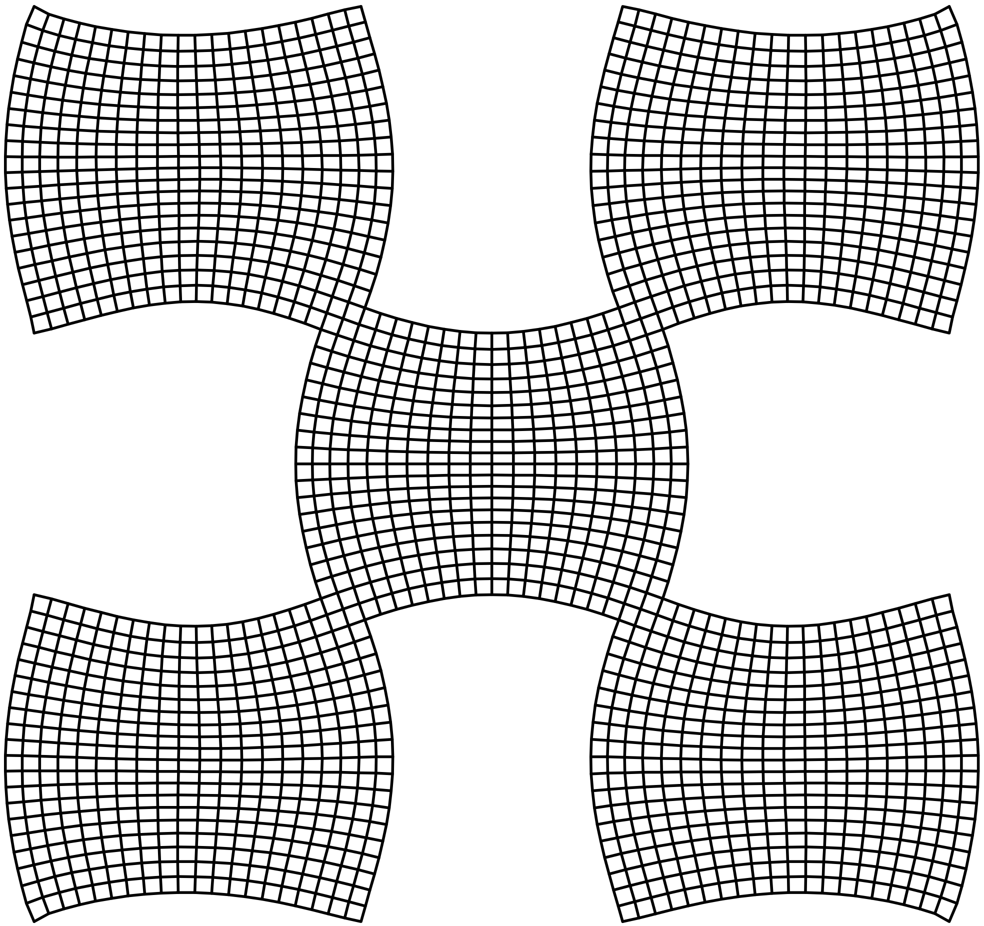
Ring resonator



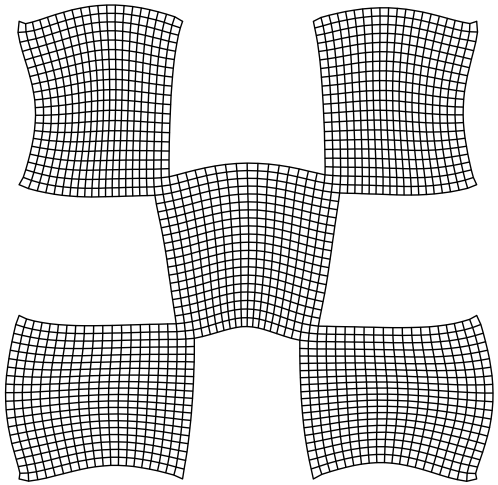
Ring resonator

- Studied shear mode vs ring radius and width
- Estimated eigenvalue by predictor
- Shifted subspace iteration to get values and vectors
- Choose vector to maximize $|q(s_k)^T q(s_{k+1})|$
- Convergence criteria, step control based on $|q(s_k)^T q(s_{k+1})|$

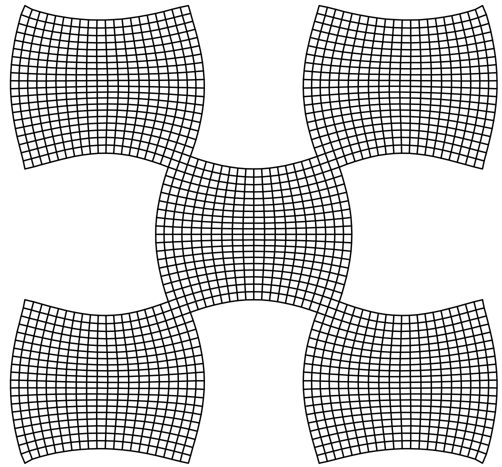
Checkerboard resonator



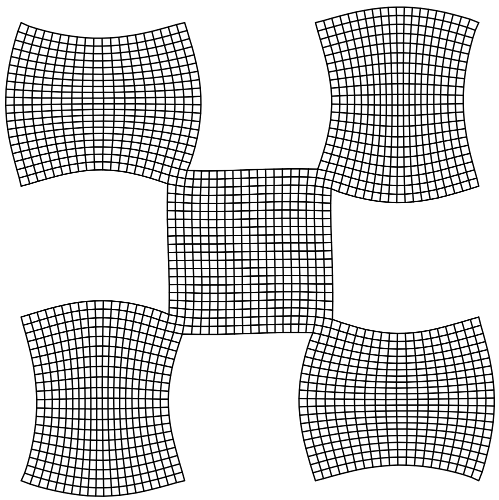
Checkerboard resonator



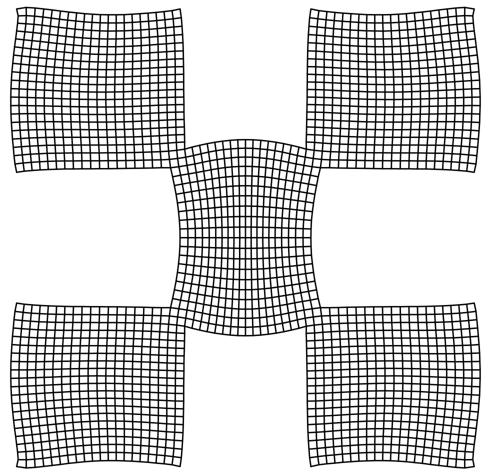
9.27 MHz.



9.31 MHz.

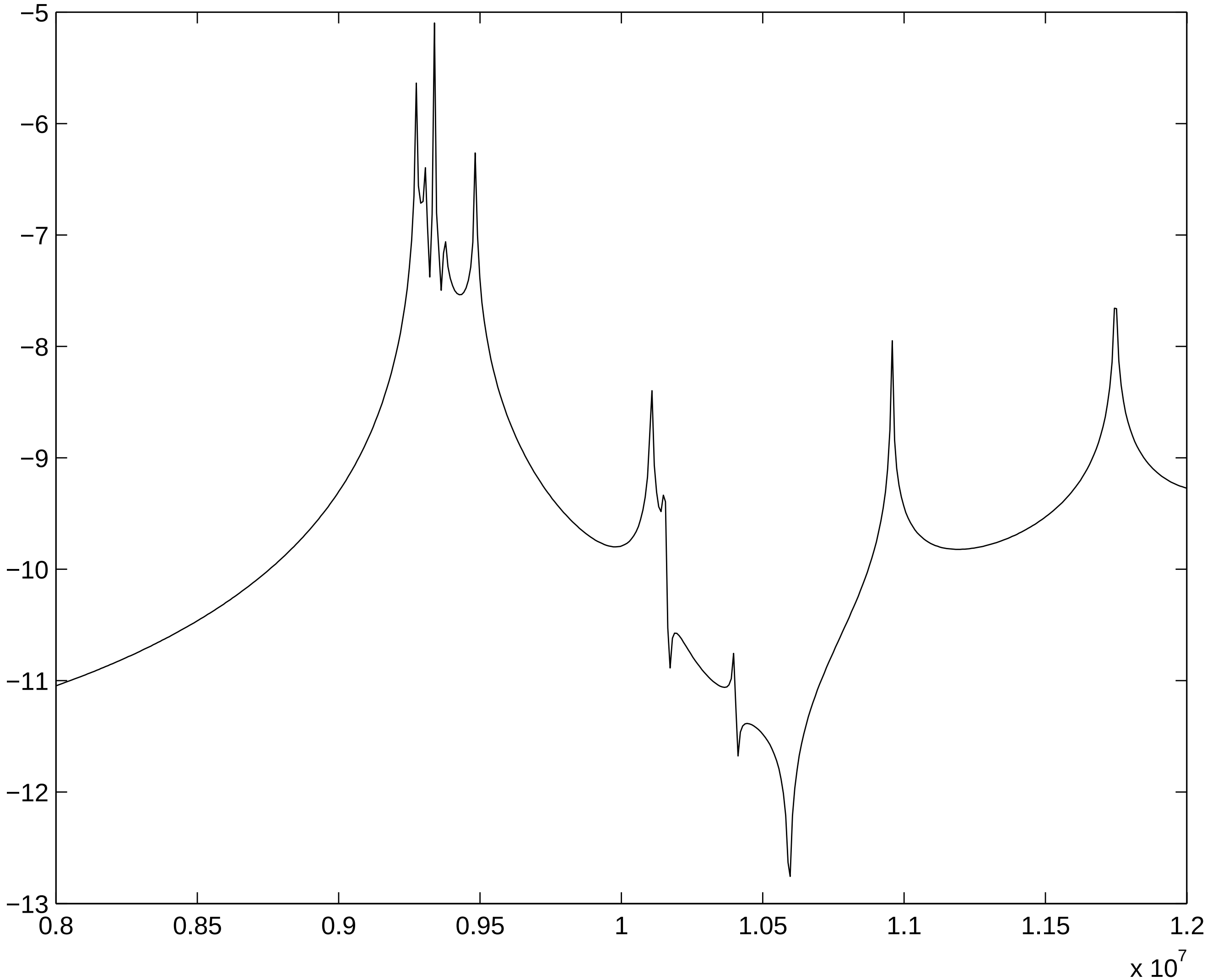


9.34 MHz.



9.37 MHz.

Checkerboard resonator



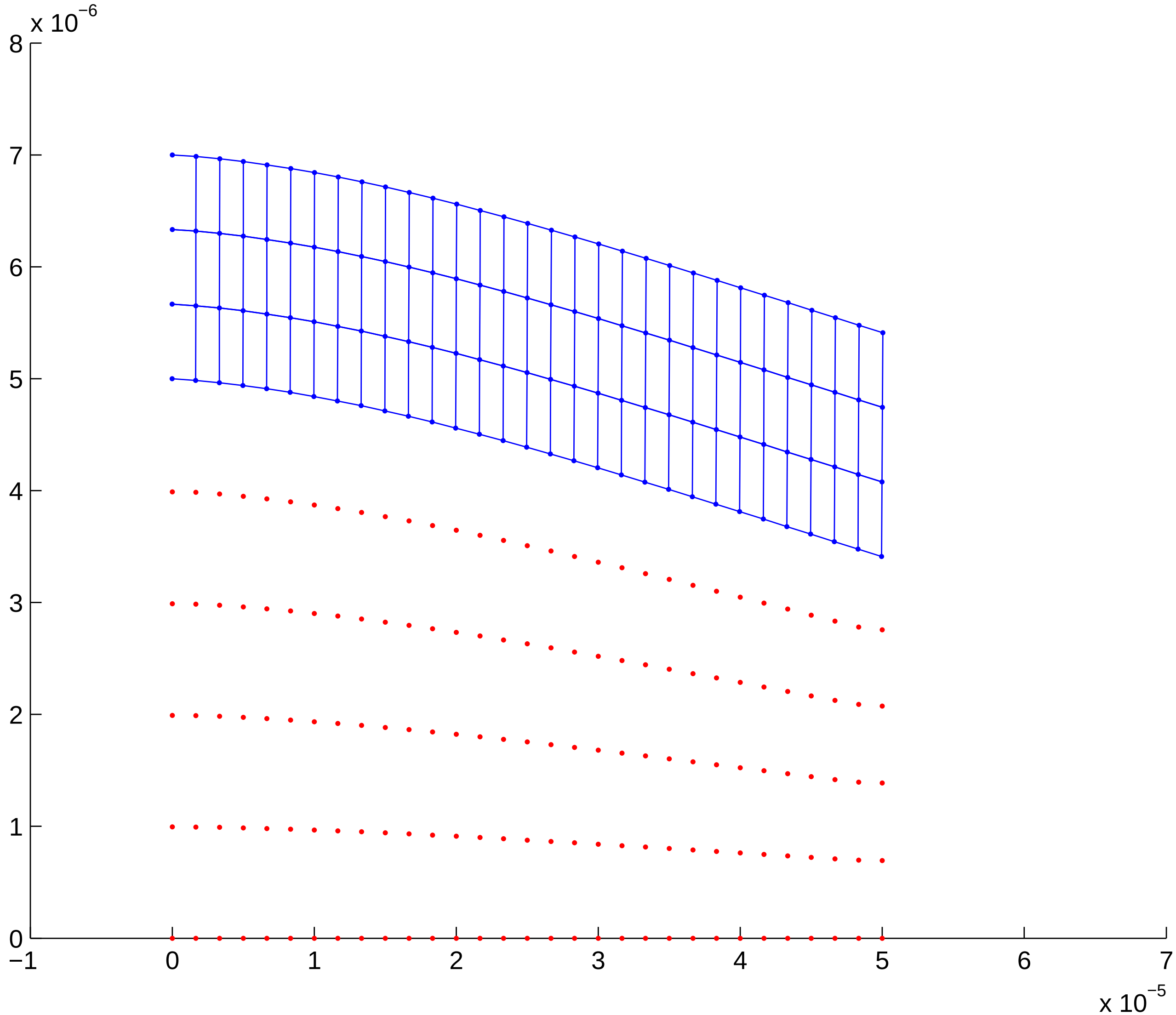
Checkerboard resonator

- Studied mode change vs amount of corner overlap
- Discretization changes between steps
- Identified modes by distance to target frequency
- Manually directed computation so far

Bifurcation analysis

- Working to integrate CIS code into the MatCont bifurcation analysis package
- Evaluate test functions using projected matrices.
- Use basis derivatives for projected versions of test functions that use higher derivatives than the Jacobian.
  - Bifurcation location equations
  - Continuation of codimension 1 bifurcations

Electrostatic actuator



Electrostatic actuator

- Large, undamped version of the 1-d example
- Usually:
  - Compute equilibrium by nonlinear Gauss-Seidel
  - Use finite differences to apply Jacobian
- We form the Jacobian for the fully coupled problem

Related work

- Moving frames on solution manifolds (Rheinboldt)
- Analytic SVD computation (Bunse-Gerstner, Byers, Mehrman, Nichols)
- Analytic null space computations and DAEs (Kunkel, Mehrmann)
- Smooth matrix decompositions (Dieci, Eirola)
- Bifurcation analysis (Thummler, Beyn, Kless; Friedman, Dieci, Demmel)
- Perturbation theory (Kato; Stewart; Demmel)

Overview of the math

For differentiable $A : [0, 1] \to \mathbb{R}^{n \times n}$:

- Eigenvalues are continuous functions.
- While eigenvalues stay inside a contour Γ, the correspondent subspace has a differentiable basis.
- There's more than one differentiable basis for a space. Pick a unique basis by not letting vectors "spin."

Spaces and bases

Define the Stiefel manifold $\text{Stief}(n, m)$ and the Grassman manifold $\text{Grass}(n, m)$ to be

$$\text{Stief}(n, m) := \{Y \in \mathbb{R}^{n \times m} : Y^T Y = I\} \quad (3)$$

$$\text{Grass}(n, m) := \text{Stief}(n, m) / [Y \sim YU, U \in O(m)] \quad (4)$$

Special cases:

- $\text{Stief}(n, n)$ is the set of orthogonal matrices $O(n)$
- $\text{Stief}(n, 1)$ is the unit sphere S_{n-1} in $\mathbb{R}^n$
- $\text{Grass}(n, 1)$ is the projective space P_{n-1}

Tangents in $\mathbb{R}^{n\times m}$

Let $Y_0 \in \mathrm{Stief}(n,m)$. Tangents satisfy:

$$\begin{aligned} 0 &= \delta(Y^T Y - I) && (5)\\ &= (\delta Y)^T Y_0 + Y_0^T \delta Y && (6)\\ &= 2\,\mathrm{sym}\left(Y_0^T \delta Y\right) && (7) \end{aligned}$$

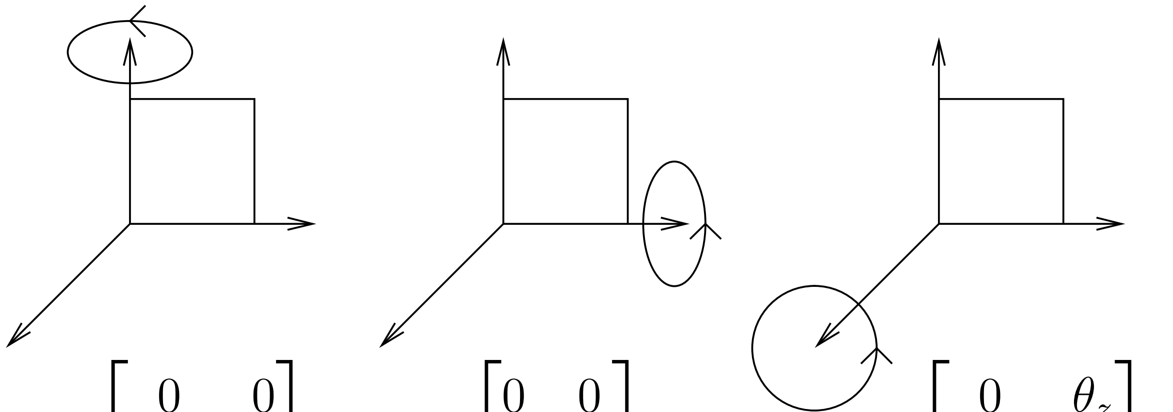
If $Y_0^\perp$ is a complementary orthonormal basis

$$\delta Y = \begin{bmatrix} Y_0 & Y_0^\perp \end{bmatrix} \begin{bmatrix} \delta Y_H \\ \delta Y_V \end{bmatrix} \tag{8}$$

where $Y_H \in \mathbb{R}^{m\times m}$ is skew, $Y_V \in \mathbb{R}^{n-m\times m}$

Horizontal and vertical motion

The tangent space is divided into *vertical* directions that change the space and *horizontal* directions that “spin” the basis.



$$\begin{bmatrix} 0 & 0 \\ 0 & 0 \\ -\theta_y & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & \theta_x \end{bmatrix} \qquad \begin{bmatrix} 0 & \theta_z \\ -\theta_z & 0 \\ 0 & 0 \end{bmatrix}$$

Basis normalization

Suppose

$$\mathcal{Y} : [0,1] \to \mathrm{Grass}(n,m) \text{ is } C^1$$
$$Y_0 \in \mathrm{Stief}(n,m)$$
$$\mathrm{span}(Y_0) = \mathcal{Y}(0)$$

Then there is a unique $Y : [0,1] \to \mathrm{Stief}(n,m)$ such that

$$Y(0) = Y_0 \quad (9)$$
$$\mathcal{Y}(s) = \mathrm{span}(Y(s)) \quad (10)$$
$$Y(s)^T \dot{Y}(s) = 0 \quad (11)$$

The basis Y minimizes the arclength $\int_0^1 \|\dot{Y}(s)\|_F \, ds$.

Continuous basis: algebraic version

Suppose $A_{21}(s_0) = 0$. Seek continuous $Y(s)$, $L(s)$

$$\begin{bmatrix} A_{11}(s) & A_{12}(s) \\ A_{21}(s) & A_{22}(s) \end{bmatrix} \begin{bmatrix} I \\ Y(s) \end{bmatrix} = \begin{bmatrix} I \\ Y(s) \end{bmatrix} L(s) \tag{12}$$

Eliminate L to get a generalized algebraic Riccati equation:

$$YA_{11} - A_{22}Y = A_{21} - YA_{12}Y \tag{13}$$

If $\lambda(A_{11}(s_0)) \cap \lambda(A_{22}(s_0)) = \emptyset$, then for s near s_0, fixed point iteration from $Y_0(s) = 0$ converges uniformly.

Can also prove this with complex analysis or by an ODE.

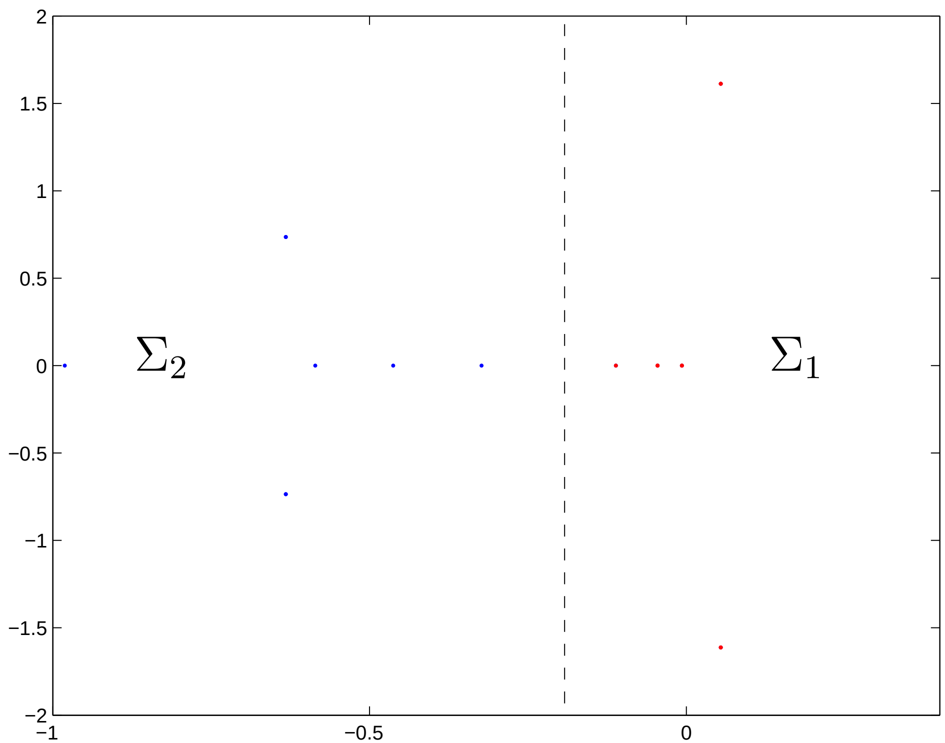
CIS algorithm

- Compute continuous invariant subspace bases
- Components:
  - Choose initial invariant subspace
  - Compute a continuation step
  - Normalize the solution
  - Adapt space and step size to improve convergence, resolve features of interest

Sparse considerations

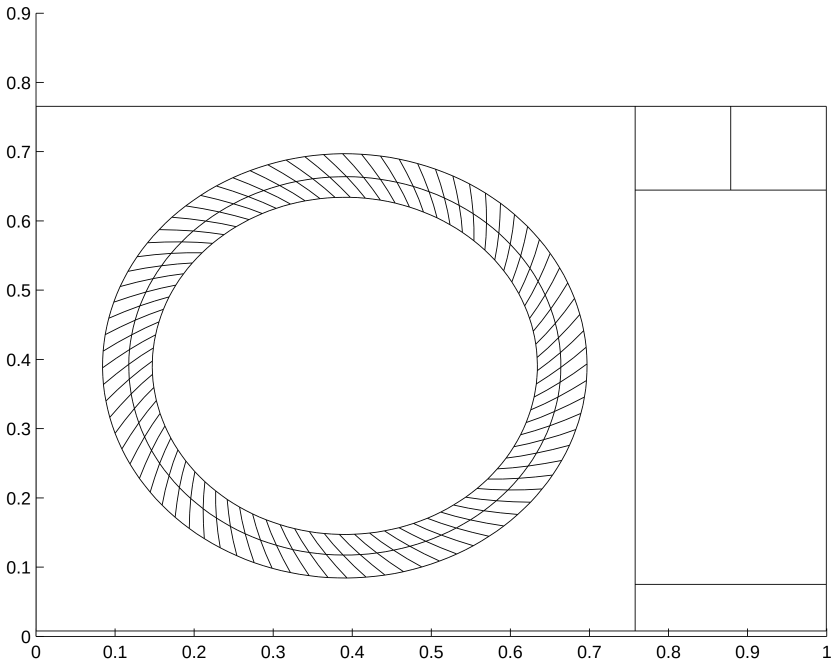
- Initialization and continuation step change in sparse case
- Need both the continued space and a few extra eigenvalues
- Use spectrally transformed IRAM to build a projection basis
- Possible better ways to build approximation basis:
  - Blocked methods
  - Re-use factorization for several steps
  - Higher-order rational spectral transformations
  - Start with bases from several previous steps

Initialization: Bifurcation case



- Compute rightmost part of the spectrum
- Include all unstable eigenvalues + a few stable ones
- Don't split clusters of eigenvalues

Initialization: Mode tracking



Reference: (3.8274×10^{15})
Computed: (2.7857×10^{16})

To initialize when spectrum interior is of interest:

- Find eigenvalues near specified λ_{target}
- Find modes near specified shape
- Compute lots of modes, let user select

Single continuation step

- Input: Partial Schur form $A(s)Q(s) = Q(s)T(s)$, $Q(s) \in \mathrm{Stief}(n, m)$ for $s = s_1, \ldots s_k$
- Output: $A(s_{k+1})Q(s_{k+1}) = Q(s_{k+1})T(s_{k+1})$
- Steps:
  - Predict $Q(s_{k+1})$
  - Correct to get a basis for space at s_{k+1}
  - Normalize the basis
  - Accept step, cut step size and retry, or quit

Note: We suppress the argument s_{k+1} when possible

Newton-based selection

Apply Newton to find $\hat{Q}$, $\hat{T}$ such that

$$R = \begin{bmatrix} A\hat{Q} - \hat{Q}\hat{T} \\ Q(s_k)^T\hat{Q} - I \end{bmatrix} = 0$$

- Start iteration at the predicted space
- Can apply Newton directly or eliminate T first
- Solve a Newton step by m linear solves with

$$\begin{bmatrix} A - \hat{T}_{ii}I & \hat{Q} \\ Q(s_k)^T & 0 \end{bmatrix}$$

Eigenvalue-based selection

- Compute (partial) Schur decomposition of $A(s_{k+1})$
- Predict eigenvalue motion (can use values at s_k)
- Find m eigenvalues of $A(s_{k+1})$ nearest predicted
- Sort those eigenvalues to the front of the Schur form

Eigenvector-based selection

- Compute (partial) Schur decomposition of $A(s_{k+1})$
- Compute unit eigenvectors that might be in space
- Choose m vectors v that maximize $\|Q(s_k)^T v\|$
- Sort Schur form accordingly

Solution normalization

- Continuous: minimize $\int_{s_k}^{s_{k+1}} \|\dot{Q}(s)\|_F \, ds$
- Discrete: minimize $\|Q(s_k) - Q(s_{k+1})\|_F$
- Discrete version approximates continuous version to $O(h)$ global error
- In case $\hat{Q}$ already has orthonormal columns, have an *orthogonal Procrustes problem*:

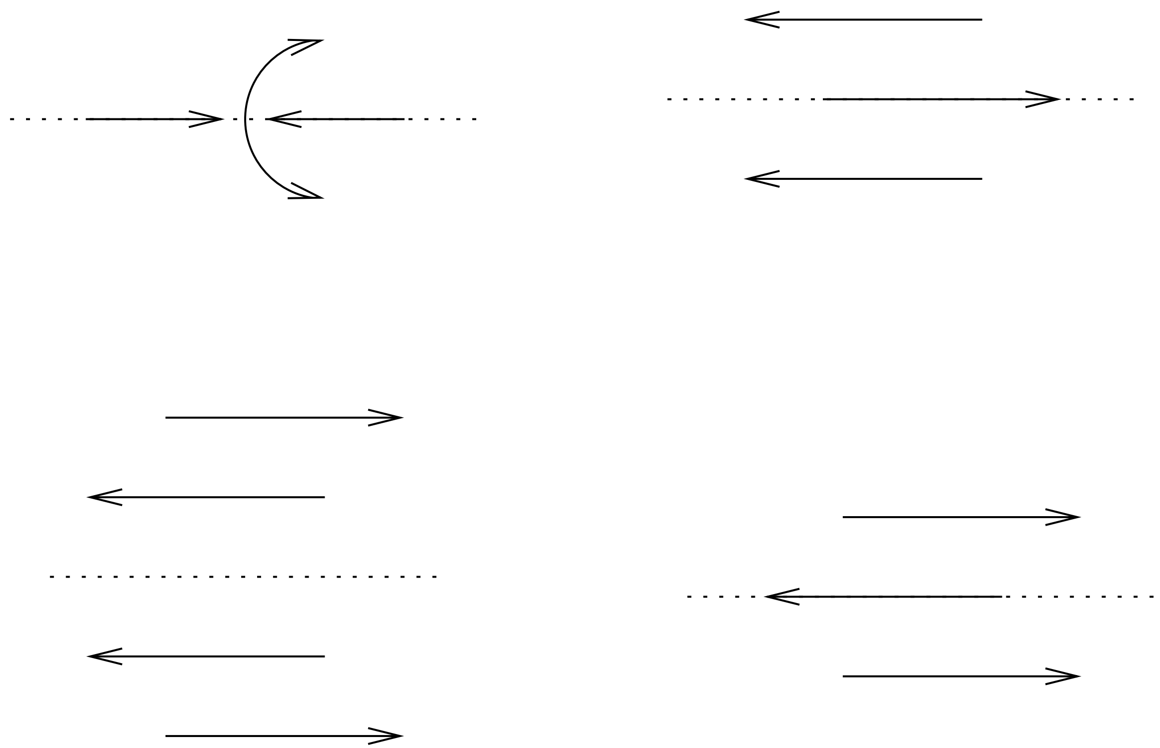
$$\text{minimize}_{B \in O(m)} \|Q(s_k) - \hat{Q}B\|^2$$

  Can solve with a small SVD. Let $Q(s_{k+1}) = \hat{Q}B$.
- The case $Q(s_k)^T \hat{Q} = I$ is similar

Acceptance criteria

- A priori step size bounds are too pessimistic
- Derived posterior bound to check if the computed $Q(s_{k+1})$ is a continuous extension of $Q(s_k)$; have not tested
- Both bounds involve bounds on the inverse of a Sylvester operator
- Use tolerances on
  - Residual error and iteration count in Newton
  - $\max_i \min_j |\lambda_i(s_k) - \lambda_j(s_{k+1})|$ for continued eigenvalues
  - $\|Q(s_{k+1}) - Q(s_k)\|$

Features



May need to adjust space if

- Real parts of continued eigenvalues overlap the rest of the spectrum (generic possibilities shown)
- Eigenvalues cross imaginary axis (bifurcation)

Global control

- Attempt a step from s_k to s_{k+1}
- If convergence failure, reinitialize at s_k and retry
- Check for interesting features (bifurcation or overlap)
- If multiple features occur, cut step to resolve them
- If one feature occurs, may choose to reinitialize space

Conclusions

- Algorithms for continuous invariant subspace computation
- Initial code base and a few examples
- Code is partly integrated into MatCont

Future work

- Numerical mathematics:
  - Study discretization effects from coarse models
  - More intelligent formation of projection spaces
  - Comparison of subspace selection methods
  - Generalized and polynomial problems
- Software:
  - Better integration with MatCont
  - Performance studies
- Models:
  - Air-damped electrostatic actuators
  - Resonator models with radiation loss
  - Models coupled to circuitry