Invariant Subspace Computation in Scientific Computing

D.C. Sorensen

- Collaborators: A.C. Antoulas, M. Heinkenschloss, K. Sun, H. Thornquist
- Support: NSF and AFOSR

SciDAC CScADS Summer Workshop Snowbird, July, 2007

Accelerate ARPACK - Approximate Shift Invert

Heidi Thornquist
Ph.D. Thesis
CAAM TR06-05

Linear Stability Analysis - CFD
Parameter Studies and Bifurcation Analysis

Spectral Transformations with IRA

- Accelerate convergence to the eigenvalues around σ

$$\psi(A)V_k = V_k H_k + f e_k^T, \psi(A) = \begin{cases} (A-\sigma I)^{-1} & \text{for } \psi_{SI}(A) \\ (A-\sigma I)^{-1}(A-\mu I) & \text{for } \psi_M(A) \end{cases}$$

- To build an orthogonal basis for

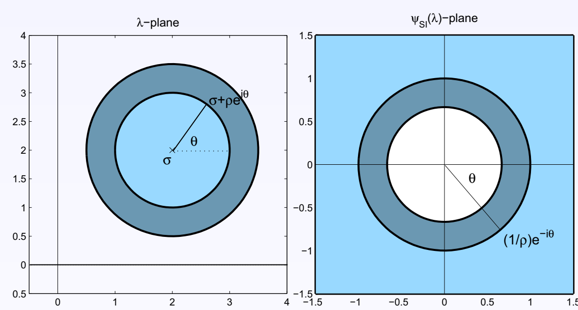
$$\mathcal{K}_k(\psi(A), v_1) = span\{v_1, \psi(A)v_1, \cdots, \psi(A)^{k-1}v_1\}$$

  $\hookrightarrow$ Need to compute $x = (A-\sigma I)^{-1}b$ for an arbitrary vector b.

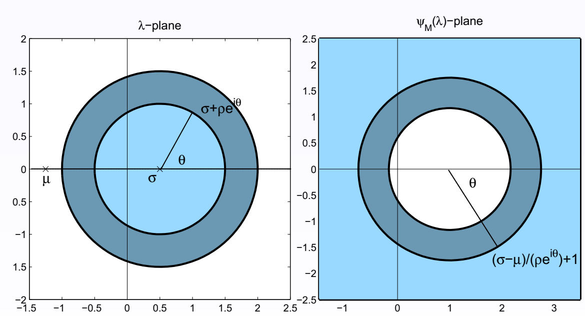
- **Classic Approach:** Exact solves using factored $(A-\sigma I)$
  - $\hookrightarrow$ Converges in very few iterations
  - $\hookrightarrow$ Typically 2-3 restarts sufficient
  - $\hookrightarrow$ Difficult to implement, may not be feasible

Spectral Transformations

Shift Invert: $\psi_{SI}(\lambda) = \frac{1}{\lambda - \sigma}$



Möbius: $\psi_M(\lambda) = \frac{\lambda - \mu}{\lambda - \sigma}$



Spectral Transformations with IRA

- **Current Approach:** Approximate solves using an iterative method.

$$\hat{x} = \phi_j(A - \sigma I)b \quad \text{where } \phi_j(z) \in \Pi_j \text{ is dependent upon } b$$

Note: Application of a different operator ϕ_j for every linear solve.

Problem: Need high accuracy solves

$\hookrightarrow$ Essentially the same operator is applied each time

$\hookrightarrow$ Retain Krylov theoretical properties

Reality: This is used in practice, ex. linear stability analysis

$\hookrightarrow$ CVD reactor simulation with 4 million variables (Lehoucq & Salinger, 2001)

$\hookrightarrow$ Buoyancy driven flows with 16 million variables (Burroughs, et al., 2002)

Spectral Transformations with IRA

- **Alternative Approach:** Approximate solves using a *fixed-polynomial operator*.

$$\hat{x} = \phi_j(A - \sigma I)b,$$

where $\phi_j(z) \in \Pi_j$ is constructed prior to any eigenvalue computation and only applied once for any linear solve.

- Equivalent to exactly working with the Krylov subspace

$$\mathcal{K}_k(\psi_{\phi,j}(A), v_1) = span\{v_1, \psi_{\phi,j}(A)v_1, \cdots, \psi_{\phi,j}(A)^{k-1}v_1\},$$

where

$$\psi_{\phi,j}(A) = \begin{cases} \phi_j(A - \sigma I) & \text{for } \psi_{SI}(A) \\ \phi_j(A - \sigma I)(A - \mu I) & \text{for } \psi_M(A) \end{cases}$$

Fixed-Polynomial Operators

Let $A_\sigma \equiv A - \sigma I$.

- Krylov subspace methods for solving non-Hermitian linear systems:

$$\hat{x}_k = \phi_{k-1}(A_\sigma)b \quad \text{and} \quad r_k = b - A_\sigma \hat{x}_k = \psi_k(A_\sigma)b,$$

  where $\psi_k(z) = 1 - z\phi_{k-1}(z) \in \Pi_k$ and $\psi_k(0) = 1$.
- Want *low degree* polynomial ψ_k such that $\|\psi_k(A_\sigma)\|$ is small.
- Use a preconditioner $M_\sigma \equiv M - \sigma I$ and modify problem, $A_\sigma M_\sigma^{-1} M_\sigma x = b$, to construct a *low degree* polynomial ψ_k such that $\|\psi_k(A_\sigma M_\sigma^{-1})\|$ is small.
- If $\|\psi_k(A_\sigma M_\sigma^{-1})\| = \|I - A_\sigma M_\sigma^{-1}\phi_{k-1}(A_\sigma M_\sigma^{-1})\|$ is small, then

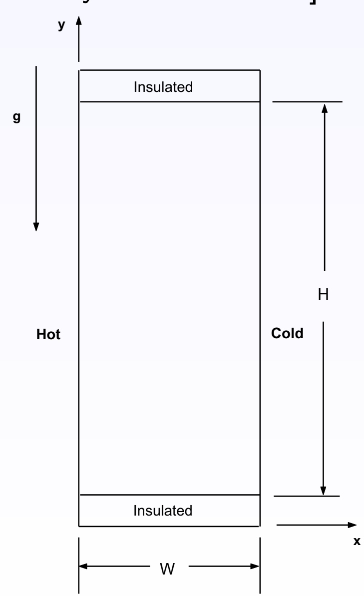
$$M_\sigma^{-1}\phi_{k-1}(A_\sigma M_\sigma^{-1}) \approx A_\sigma^{-1}.$$

Large-Scale Application:

8:1 Thermal Cavity Problem

[First MIT Conference on Computational Fluid and Solid Dynamics in 2001]

$$\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} &= -\nabla P + \sqrt{\frac{Pr}{Ra}}\nabla^2\mathbf{u} + \hat{j}\theta \\
\nabla\cdot\mathbf{u} &= 0 \\
\frac{\partial \theta}{\partial t} + \mathbf{u}\cdot\nabla\theta &= \frac{1}{\sqrt{Ra\,Pr}}\nabla^2\theta,
\end{aligned}$$



- θ - temperature, $\mathbf{u}$ - velocity
- P - deviation from hydrostatic pressure
- Pr - Prandtl number (0.71)
- Ra - Rayleigh number
- Boundary conditions:

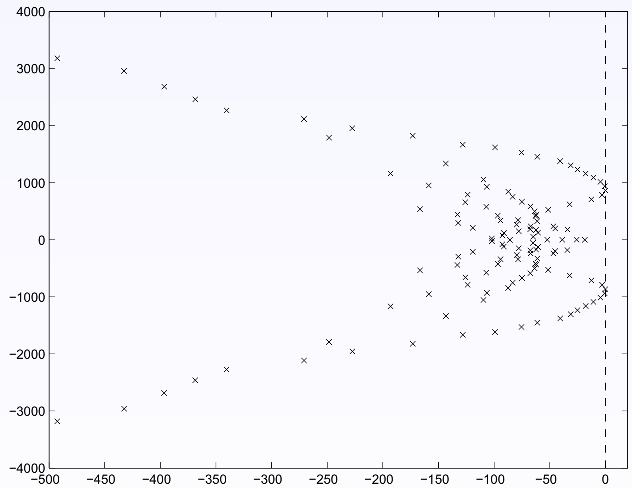
  velocity: no-slip, no-penetration
  temperature: adiabatic, $\theta = \pm 1/2$

Large-Scale Application:

8:1 Thermal Cavity Problem (3D Problem)

- Nodes: $219,373$ ($N{=}1,096,865$)
- Rayleigh number: 5.57×10^5
- Möbius transform (σ/μ): $800/-800$
- Processors: 40

Specification	Value
Processors	2
CPU	Intel® Xeon™ 2.80GHz
L2 Cache	512 KB
RAM	2GB (shared)



Conclusions

- Using fixed-polynomial operators to approximate spectral transformations is a competitive preconditioning approach.

  ↪ The GMRES fixed-polynomial operator is a more consistently effective preconditioner that those obtained by using BiCGSTAB or TFQMR.

  ↪ IRA with the GMRES fixed-polynomial operator is generally more accurate than preconditioned GMRES and less computationally expensive than either.

  ↪ It compares favorably against current eigensolvers (ex. Jacobi-Davidson) for computing select eigenvalues from a sequence of 2D scalar wave equations or the rightmost eigenvalues of a wind-driven OCM.

  ↪ Easy to construct and integrate with current eigenvalue software; extends the domain of applications for Anasazi/ARPACK/P_ARPACK.

LTI Systems and Model Reduction

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} \\ \mathbf{y} &= \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u}\end{aligned}$$

$\mathbf{A} \in \mathbb{R}^{n \times n}, \quad \mathbf{B} \in \mathbb{R}^{n \times m}, \quad \mathbf{C} \in \mathbb{R}^{p \times n}, \mathbf{D} \in \mathbb{R}^{p \times m} \quad n >> m, p$

Construct LOW dimensional system

$$\begin{aligned}\dot{\hat{\mathbf{x}}} &= \hat{\mathbf{A}}\hat{\mathbf{x}} + \hat{\mathbf{B}}\mathbf{u} \\ \hat{\mathbf{y}} &= \hat{\mathbf{C}}\hat{\mathbf{x}} + \mathbf{D}\mathbf{u}\end{aligned}$$

Goal: $\hat{\mathbf{y}}$ should approximate $\mathbf{y}$

Want the small system response to be the same as the original system response to the same input

Projection Methods : Large Scale Problems

Gramian Based Model Reduction: Balanced Reduction

Solving Large Lyapunov Equations: Approximate Balancing
1M vars now possible

Solves Linear System $\mathcal{A}\mathbf{x} = \mathbf{b}$, $N = 10^{12}$!

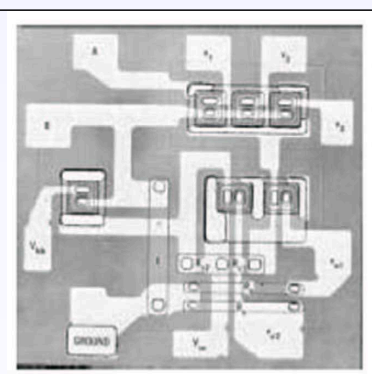
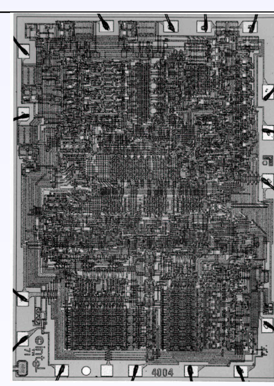
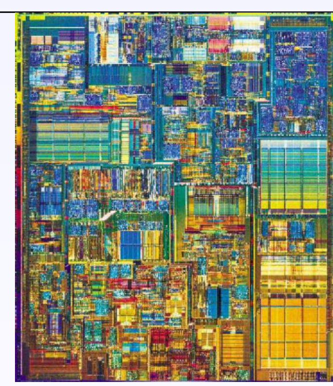
Balanced Reduction of Oseen Eqns: Extension to Descriptor System

Preserving Passivity: Structured Eigenvalue Problem

Application Examples

1. Passive devices	• VLSI circuits • Thermal issues
2. Data assimilation	• North sea forecast • Air quality forecast • Sensor placement
3. Biological/Molecular systems	• Honeycomb vibrations • MD simulations • Heat capacity
4. CVD reactor	• Bifurcations
5. Mechanical systems:	•Windscreen vibrations • Buildings
6. Optimal cooling	• Steel profile
7. MEMS: **Micro Elec-Mech Systems**	• Elf sensor

Passive Devices: VLSI circuits

		
1960's: IC	1971: Intel 4004	2001: Intel Pentium IV
	10μ details 2300 components 64KHz speed	0.18μ details 42M components 2GHz speed 2km interconnect 7 layers

Model Reduction by Projection

Approximate $\mathbf{x} \in \mathcal{S}_V = Range(\mathbf{V})$ k-diml. subspace
i.e. Put $\mathbf{x} = \mathbf{V}\hat{\mathbf{x}}$, and then force

$$\begin{aligned} \mathbf{W}^T[\mathbf{V}\dot{\hat{\mathbf{x}}} &- (\mathbf{A}\mathbf{V}\hat{\mathbf{x}} + \mathbf{B}\mathbf{u})] = 0 \\ \hat{\mathbf{y}} &= \mathbf{C}\mathbf{V}\hat{\mathbf{x}} \end{aligned}$$

If $\mathbf{W}^T\mathbf{V} = \mathbf{I}_k$, then the k dimensional reduced model is

$$\begin{aligned} \dot{\hat{\mathbf{x}}} &= \hat{\mathbf{A}}\hat{\mathbf{x}} + \hat{\mathbf{B}}\mathbf{u} \\ \hat{\mathbf{y}} &= \hat{\mathbf{C}}\hat{\mathbf{x}} \end{aligned}$$

where $\hat{\mathbf{A}} = \mathbf{W}^T\mathbf{A}\mathbf{V}$, $\hat{\mathbf{B}} = \mathbf{W}^T\mathbf{B}$, $\hat{\mathbf{C}} = \mathbf{C}\mathbf{V}$.

Balanced Reduction (Moore 81)

Lyapunov Equations for system Gramians

$$\mathbf{A}\mathcal{P} + \mathcal{P}\mathbf{A}^T + \mathbf{B}\mathbf{B}^T = 0 \quad \mathbf{A}^T\mathcal{Q} + \mathcal{Q}\mathbf{A} + \mathbf{C}^T\mathbf{C} = 0$$

With $\mathcal{P} = \mathcal{Q} = \mathbf{S}$: Want Gramians Diagonal and Equal

States Difficult to Reach are also Difficult to Observe

Reduced Model $\mathbf{A}_k = \mathbf{W}_k^T\mathbf{A}\mathbf{V}_k$, $\mathbf{B}_k = \mathbf{W}_k^T\mathbf{B}$, $\mathbf{C}_k = \mathbf{C}_k\mathbf{V}_k$

- $\mathcal{P}\mathbf{V}_k = \mathbf{W}_k\mathbf{S}_k$ $\qquad$ $\mathcal{Q}\mathbf{W}_k = \mathbf{V}_k\mathbf{S}_k$
- Reduced Model Gramians $\mathcal{P}_k = \mathbf{S}_k$ and $\mathcal{Q}_k = \mathbf{S}_k$.

Hankel Norm Error estimate (Glover 84)

Why Balanced Truncation?

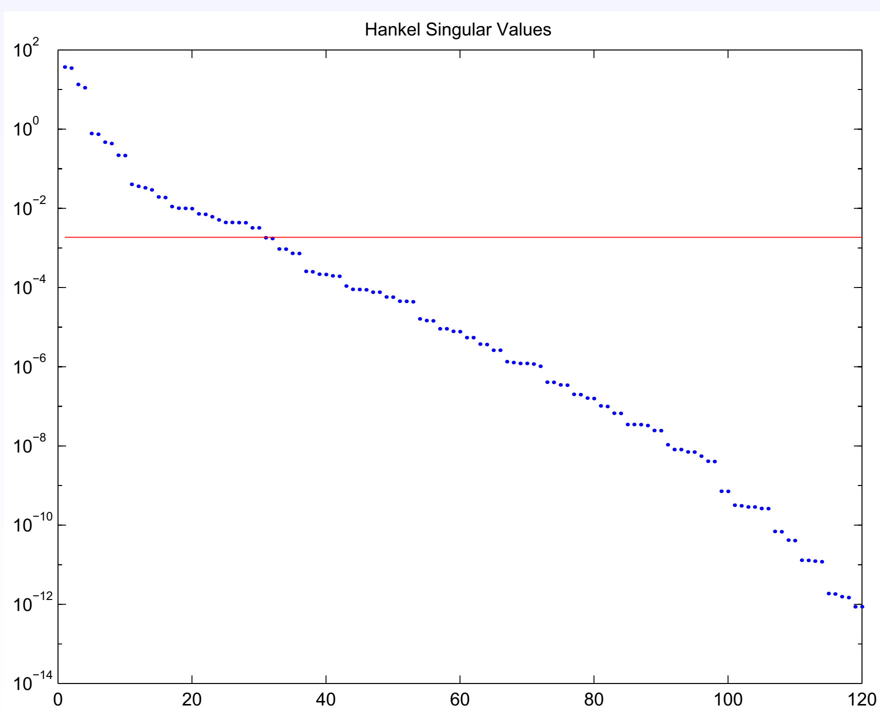
- Hankel singular values $= \sqrt{\lambda(\mathcal{P}\mathcal{Q})}$
- Model reduction $\mathcal{H}_\infty$ error (Glover)

  $\|\mathbf{y} - \hat{\mathbf{y}}\|_2 \leq 2 \times (\text{sum neglected singular values})\|u\|_2$
- Extends to MIMO
- Preserves Stability

Key Challenge

- Approximately solve large scale Lyapunov Equations in Low Rank Factored Form

CD Player - Hankel Singular Values $\sqrt{\lambda(\mathcal{P}\mathcal{Q})}$



Approximate Balancing

$$\mathbf{A}\mathcal{P} + \mathcal{P}\mathbf{A}^T + \mathbf{B}\mathbf{B}^T = 0 \quad \mathbf{A}^T\mathcal{Q} + \mathcal{Q}\mathbf{A} + \mathbf{C}^T\mathbf{C} = 0$$

- Sparse Case: Iteratively Solve in Low Rank Factored Form,

$$\mathcal{P} \approx \mathbf{U}_k\mathbf{U}_k^T, \quad \mathcal{Q} \approx \mathbf{L}_k\mathbf{L}_k^T$$

$$[\mathbf{X}, \mathbf{S}, \mathbf{Y}] = \mathrm{svd}(\mathbf{U}_k^T\mathbf{L}_k)$$

$$\mathbf{W}_k = \mathbf{L}\mathbf{Y}_k\mathbf{S}_k^{-1/2} \text{ and } \mathbf{V}_k = \mathbf{U}\mathbf{X}_k\mathbf{S}_k^{-1/2}.$$

Now: $\mathcal{P}\mathbf{W}_k \approx \mathbf{V}_k\mathbf{S}_k$ and $\mathcal{Q}\mathbf{V}_k \approx \mathbf{W}_k\mathbf{S}_k$

Balanced Reduction via Projection

Reduced model of order k:

$$\mathbf{A}_k = \mathbf{W}_k^T\mathbf{A}\mathbf{V}_k, \quad \mathbf{B}_k = \mathbf{W}_k^T\mathbf{B}, \quad \mathbf{C}_k = \mathbf{C}\mathbf{V}_k.$$

$$0 = \mathbf{W}_k^T(\mathbf{A}\mathcal{P} + \mathcal{P}\mathbf{A}^T + \mathbf{B}\mathbf{B}^T)\mathbf{W}_k = \mathbf{A}_k\mathbf{S}_k + \mathbf{S}_k\mathbf{A}_k^T + \mathbf{B}_k\mathbf{B}_k^T$$
$$0 = \mathbf{V}_k^T(\mathbf{A}^T\mathcal{Q} + \mathcal{Q}\mathbf{A} + \mathbf{C}^T\mathbf{C})\mathbf{V}_k = \mathbf{A}_k^T\mathbf{S}_k + \mathbf{S}_k\mathbf{A}_k + \mathbf{C}_k^T\mathbf{C}_k$$

Reduced model is balanced and asymptotically stable for every k.

Low Rank Smith = ADI

Convert to Stein Equation:

$$\mathbf{A}\mathcal{P} + \mathcal{P}\mathbf{A}^T + \mathbf{B}\mathbf{B}^T = 0 \quad \Longleftrightarrow \quad \mathcal{P} = \mathbf{A}_\mu \mathcal{P} \mathbf{A}_\mu^T + \mathbf{B}_\mu \mathbf{B}_\mu^T,$$

where

$$\mathbf{A}_\mu = (\mathbf{A} - \mu\mathbf{I})(\mathbf{A} + \mu\mathbf{I})^{-1}, \quad \mathbf{B}_\mu = \sqrt{2|\mu|}(\mathbf{A} + \mu\mathbf{I})^{-1}\mathbf{B}.$$

Solution:

$$\mathcal{P} = \sum_{j=0}^{\infty} \mathbf{A}_\mu^j \mathbf{B}_\mu \mathbf{B}_\mu^T (\mathbf{A}_\mu^j)^T = \mathbf{L}\mathbf{L}^T,$$

where $\mathbf{L} = [\mathbf{B}_\mu, \ \mathbf{A}_\mu\mathbf{B}_\mu, \ \mathbf{A}_\mu^2\mathbf{B}_\mu, \ \ldots]$ Factored Form

Multi-Shift (Modified) Low Rank Smith

LR - Smith: Update Factored Form $\mathcal{P}_m = L_m L_m^T$: (*Penzl*)

$$\begin{aligned} \mathbf{L}_{m+1} &= [\mathbf{A}_\mu \mathbf{L}_m, \mathbf{B}_\mu] \\ &= [\mathbf{A}_\mu^{m+1}\mathbf{B}_\mu, \mathbf{L}_m] \end{aligned}$$

Multi-Shift LR - Smith:

Update and Truncate SVD

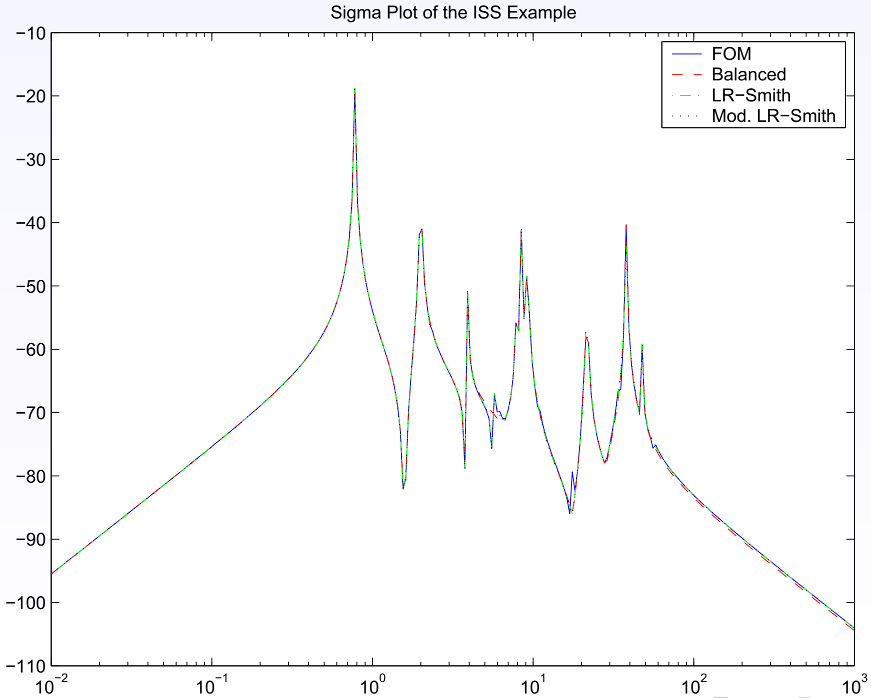
Re-Order and Aggregate Shift Applications

Much Faster and Far Less Storage

$$\begin{aligned} \mathbf{B} &\leftarrow \mathbf{A}_\mu \mathbf{B}; \\ [\mathbf{V}, \mathbf{S}, \mathbf{Q}] &= \mathrm{svd}([\mathbf{A}_\mu \mathbf{B}, \mathbf{L}_\mathrm{m}]); \\ \mathbf{L}_{m+1} &\leftarrow \mathbf{V}_k \mathbf{S}_k; \quad (\sigma_{k+1} < tol \cdot \sigma_1) \end{aligned}$$

ISS module comparison

k = 26 , n = 270



A Descriptor System

$$\begin{aligned}
\mathbf{E}_{11}\frac{d}{dt}\mathbf{v}(t) &= \mathbf{A}_{11}\mathbf{v}(t) + \mathbf{A}_{12}\mathbf{p}(t) + \mathbf{B}_1\mathbf{g}(t),\\
\mathbf{0} &= \mathbf{A}_{12}^T\mathbf{v}(t),\\
\mathbf{v}(0) &= \mathbf{v}_0,\\
\mathbf{y}(t) &= \mathbf{C}_1\mathbf{v}(t) + \mathbf{C}_2\mathbf{p}(t) + \mathbf{D}\mathbf{g}(t).
\end{aligned}$$

$$\mathcal{E}\frac{d}{dt}\mathbf{v}(t) = \mathcal{A}\mathbf{v}(t) + \mathcal{B}\mathbf{u}(t), \qquad \mathbf{y}(t) = \mathcal{C}\mathbf{v}(t) + \mathcal{D}\mathbf{u}(t)$$

Note $\mathcal{E}$ is singular   index 2

Notation

Put

$$\widetilde{\mathbf{E}} = \mathbf{\Pi}\mathbf{E}_{11}\mathbf{\Pi}^T, \quad \widetilde{\mathbf{A}} = \mathbf{\Pi}\mathbf{A}_{11}\mathbf{\Pi}^T, \quad \widetilde{\mathbf{B}} = \mathbf{\Pi}\mathbf{B}_1, \quad \widetilde{\mathbf{C}} = \mathbf{C}\mathbf{\Pi}^T.$$

With this notation,

$$\begin{aligned} \widetilde{\mathbf{A}}\,\mathbf{P}\,\widetilde{\mathbf{E}} + \widetilde{\mathbf{E}}\,\mathbf{P}\,\;\widetilde{\mathbf{A}}^T + \widetilde{\mathbf{B}}\widetilde{\mathbf{B}}^T &= \mathbf{0}, \\ \widetilde{\mathbf{A}}^T\,\mathbf{Q}\,\widetilde{\mathbf{E}} + \widetilde{\mathbf{E}}\,\mathbf{Q}\,\widetilde{\mathbf{A}} + \widetilde{\mathbf{C}}^T\widetilde{\mathbf{C}} &= \mathbf{0}. \end{aligned}$$

where

$$\begin{aligned} \mathbf{\Pi} &= \mathbf{I} - \mathbf{A}_{12}(\mathbf{A}_{12}^T\mathbf{E}_{11}^{-1}\mathbf{A}_{12})^{-1}\mathbf{A}_{12}^T\mathbf{E}_{11}^{-1} \\ &= \mathbf{\Theta}_l\mathbf{\Theta}_r^T \end{aligned}$$

$\mathbf{\Pi}^T$ Projector onto Null($\mathbf{A}_{12}^T$)

ADI Derivation Step 1

Begin with

$$\widetilde{\mathbf{A}}\mathbf{P}\left(\widetilde{\mathbf{E}} + \bar{\mu}\,\widetilde{\mathbf{A}}\right)^T = -\left[\left(\widetilde{\mathbf{E}} - \bar{\mu}\,\widetilde{\mathbf{A}}\right)\mathbf{P}\widetilde{\mathbf{A}}^T + \widetilde{\mathbf{B}}\widetilde{\mathbf{B}}^T\right].$$

and derive

$$\left(\widetilde{\mathbf{E}} + \mu\,\widetilde{\mathbf{A}}\right)\mathbf{P}\left(\widetilde{\mathbf{E}} + \bar{\mu}\,\widetilde{\mathbf{A}}\right)^T = \left(\widetilde{\mathbf{E}} - \bar{\mu}\,\widetilde{\mathbf{A}}\right)\mathbf{P}\left(\widetilde{\mathbf{E}} - \mu\,\widetilde{\mathbf{A}}\right)^T - 2\,\mathrm{Re}(\mu)\widetilde{\mathbf{B}}\widetilde{\mathbf{B}}^T.$$

Problem: $\left(\widetilde{\mathbf{E}} + \mu\,\widetilde{\mathbf{A}}\right)$ is *Singular*

Projected Stein Equation

$$\mathbf{P} = \widetilde{\mathbf{A}}_\mu \mathbf{P} \widetilde{\mathbf{A}}_\mu^* - 2\ \mathrm{Re}(\ \mu) \widetilde{\mathbf{B}}_\mu \widetilde{\mathbf{B}}_\mu^*.$$

where

$$\widetilde{\mathbf{A}}_\mu \equiv \left(\widetilde{\mathbf{E}} + \mu\,\widetilde{\mathbf{A}}\right)^I \left(\widetilde{\mathbf{E}} - \bar{\mu}\,\widetilde{\mathbf{A}}\right), \quad \text{and} \quad \widetilde{\mathbf{B}}_\mu \equiv \left(\widetilde{\mathbf{E}} + \mu\,\widetilde{\mathbf{A}}\right)^I \widetilde{\mathbf{B}}$$

Solution:

$$\mathbf{P} = -2\ \mathrm{Re}(\mu) \sum_{j=0}^{\infty} \widetilde{\mathbf{A}}_\mu^j \widetilde{\mathbf{B}}_\mu \widetilde{\mathbf{B}}_\mu^* \left(\widetilde{\mathbf{A}}_\mu^*\right)^j.$$

Convergent for stable pencil with $\mathrm{Real}(\mu) < 0$

Algorithm:Single Shift ADI

1. Solve $\begin{pmatrix} \mathbf{E}_{11} + \mu\,\mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{12}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{Z} \\ \mathbf{\Lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{B} \\ \mathbf{0} \end{pmatrix};$
2. $\mathbf{U} = \mathbf{Z}$;
3. **while** ('not converged')
   - 3.1 $\mathbf{Z} \leftarrow (\mathbf{E}_{11} - \bar{\mu}\,\mathbf{A}_{11})\,\mathbf{Z}$;
   - 3.2 Solve (in place) $\begin{pmatrix} \mathbf{E}_{11} + \mu\,\mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{12}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{Z} \\ \mathbf{\Lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{Z} \\ \mathbf{0} \end{pmatrix};$
   - 3.3 $\mathbf{U} \leftarrow [\mathbf{U}, \mathbf{Z}]$;

   end
4. $\mathbf{U} \leftarrow \sqrt{2|\ \mathrm{Re}(\mu)|}\,\mathbf{U}$.

Derivation Multi-Shift ADI

Easy to see $(\mathbf{P} - \mathbf{P}_k) = \widetilde{\mathbf{A}}_\mu^k \mathbf{P} \left(\widetilde{\mathbf{A}}_\mu^*\right)^k$.
Hence

$$\begin{aligned}\widetilde{\mathbf{A}}(\mathbf{P}-\mathbf{P}_k)\widetilde{\mathbf{E}}+\widetilde{\mathbf{E}}(\mathbf{P}-\mathbf{P}_k)\widetilde{\mathbf{A}}^* &= \widetilde{\mathbf{A}}\widetilde{\mathbf{A}}_\mu^k\mathbf{P}\left(\widetilde{\mathbf{A}}_\mu^k\right)^*\widetilde{\mathbf{E}}+\widetilde{\mathbf{E}}\widetilde{\mathbf{A}}_\mu^k\mathbf{P}\left(\widetilde{\mathbf{A}}_\mu^k\right)^*\widetilde{\mathbf{A}}^* \\ &= \widehat{\mathbf{A}}_\mu^k\left(\widetilde{\mathbf{A}}\mathbf{P}\widetilde{\mathbf{E}}+\widetilde{\mathbf{E}}\mathbf{P}\widetilde{\mathbf{A}}^*\right)\left(\widehat{\mathbf{A}}_\mu^k\right)^*.\end{aligned}$$

To get

$$\widetilde{\mathbf{A}}\left(\mathbf{P}-\mathbf{P}_k\right)\widetilde{\mathbf{E}}+\widetilde{\mathbf{E}}\left(\mathbf{P}-\mathbf{P}_k\right)\widetilde{\mathbf{A}}^* = -\widehat{\mathbf{A}}_\mu^k\left(\widetilde{\mathbf{B}}\widetilde{\mathbf{B}}^*\right)\left(\widehat{\mathbf{A}}_\mu^k\right)^*.$$

Where

$$\widehat{\mathbf{A}}_\mu \equiv \left(\widetilde{\mathbf{E}}-\bar{\mu}\,\widetilde{\mathbf{A}}\right)\left(\widetilde{\mathbf{E}}+\mu\,\widetilde{\mathbf{A}}\right)^I.$$

Algorithm:Multi-Shift ADI

1. $\mathbf{U} = [\ \ ]$;
2. **while** ('not converged')

   for i = 1:m,

   2.1 Solve $\begin{pmatrix} \mathbf{E}_{11}+\mu_i\mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{12}^T & \mathbf{0}\end{pmatrix}\begin{pmatrix}\mathbf{Z}\\ \mathbf{\Lambda}\end{pmatrix} = \begin{pmatrix}\mathbf{B}\\ \mathbf{0}\end{pmatrix}$;

   2.2 $\mathbf{U}_0 = \mathbf{Z}$;

   2.3 **for** j = 1:k-1,

   2.3.1 $\mathbf{Z} \leftarrow (\mathbf{E}_{11} - \bar{\mu}_i\mathbf{A}_{11})\mathbf{Z}$;

   2.3.2 Solve (in place) $\begin{pmatrix} \mathbf{E}_{11}+\mu_i\mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{12}^T & \mathbf{0}\end{pmatrix}\begin{pmatrix}\mathbf{Z}\\ \mathbf{\Lambda}\end{pmatrix} = \begin{pmatrix}\mathbf{Z}\\ \mathbf{0}\end{pmatrix}$;

   2.3.3 $\mathbf{U}_0 \leftarrow [\mathbf{U}_0, \mathbf{Z}]$;

   end

   2.4 $\mathbf{U} \leftarrow \left[\mathbf{U}, \sqrt{2|\operatorname{Re}(\mu_i)|}\,\mathbf{U}_0\right]$;

   % *Update and truncate* SVD($\mathbf{U}$);

   2.5 $\mathbf{B} \leftarrow (\mathbf{E}_{11} - \bar{\mu}_i\mathbf{A}_{11})\mathbf{Z}$.

   end

end

Model Problem: Oseen Equations

$$\begin{aligned}
\frac{\partial}{\partial t}v(x,t) + (a(x)\cdot\nabla)v(x,t) &- \nu\Delta v(x,t) + \nabla p(x,t) \\
&= \chi_{\Omega_g}(x) g_\Omega(x,t) \quad \text{in } \Omega\times(0,T), \\
\nabla\cdot v(x,t) &= 0 \quad \text{in } \Omega\times(0,T), \\
(-p(x,t)I + \nu\nabla v(x,t))n(x) &= 0 \quad \text{on } \Gamma_n\times(0,T), \\
v(x,t) &= 0 \quad \text{on } \Gamma_d\times(0,T), \\
v(x,t) &= g_\Gamma(x,t) \quad \text{on } \Gamma_g\times(0,T), \\
v(x,0) &= v_0(x) \quad \text{in } \Omega,
\end{aligned}$$

Channel Geometry and Grid

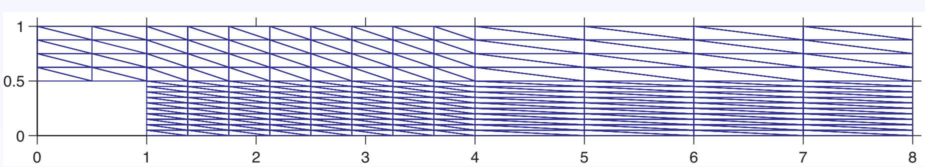


Figure: The channel geometry and coarse grid

EXAMPLE 1.

$$\mathbf{y}(t) = \int_{\Omega_{\text{obs}}} -\partial_{x_2} v_1(x,t) + \partial_{x_1} v_2(x,t)dx$$

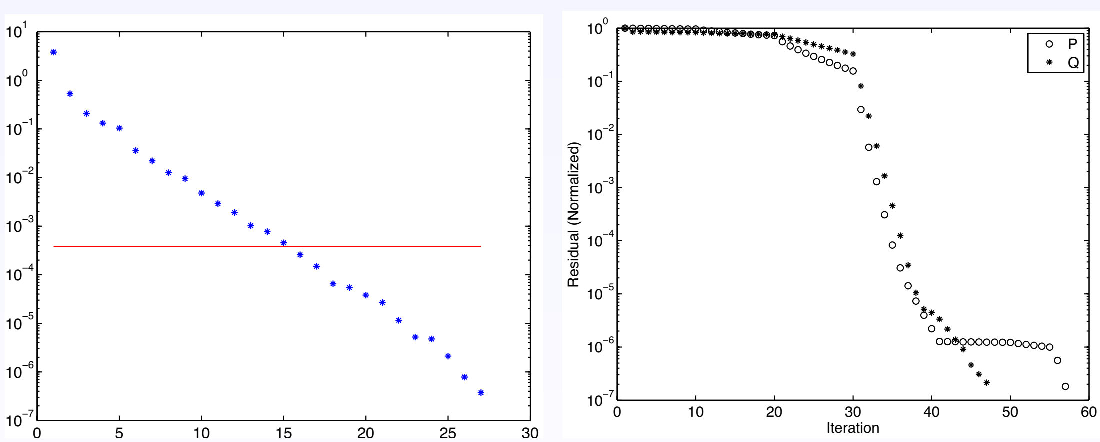
over the subdomain $\Omega_{\text{obs}} = (1,3)\times(0,1/2)$.

Model Reduction Results

n_v	n_p	k
1352	205	13
5520	761	14
12504	1669	15
22304	2929	15

Table: Number n_v of semidiscrete velocities $\mathbf{v}(t)$, number n_p of semidiscrete pressures $\mathbf{p}(t)$, and and size k of the reduced order velocities $\widehat{\mathbf{v}}(t)$ for various uniform refinements of the coarse grid.

Hankel S-vals and Convergence ADI



The largest Hankel singular values

Convergence of the multishift ADI Algorithm

Figure: The left plot shows the largest Hankel singular values and the threshold $\tau\sigma_1$. The right plot shows the normalized residuals $\|\widetilde{\mathbf{B}}_k\|_2$ generated by the multishift ADI Algorithm . for the approximate solution of the controllability Lyapunov equation ($\circ$) and of the observability Lyapunov equation ($*$).

Time (left) and Frequency (right) Responses

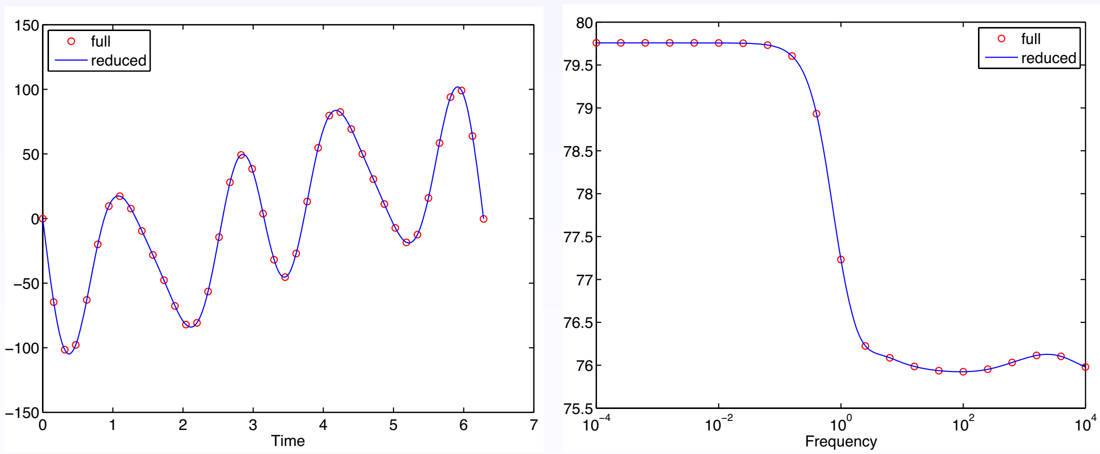


Figure: Time response (left) and frequency response (right) for the full order model (circles) and for the reduced order model (solid line).

Velocity Profile

full $>$ 20K DOF   reduced 15 DOF

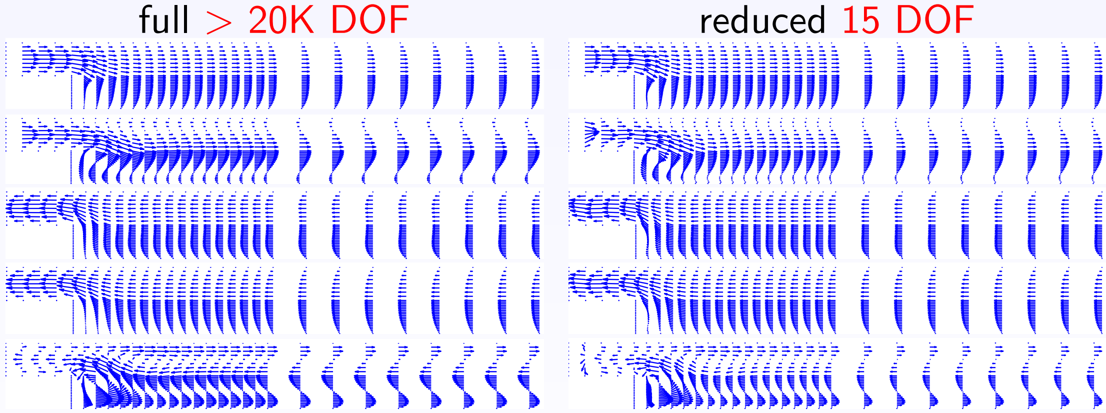


Figure: Velocities generated with the full order model (left column) and with the reduced order model (right column) at $t = 1.0996, 2.9845, 3.7699, 4.86965, 6.2832$ (top to bottom).

Approximate Power Method (Hodel)

$$\mathbf{A}\mathcal{P}\mathbf{U} + \mathcal{P}\mathbf{A}^T\mathbf{U} + \mathbf{B}\mathbf{B}^T\mathbf{U} = \mathbf{0}$$
$$\mathbf{A}\mathcal{P}\mathbf{U} + \mathcal{P}\mathbf{U}\mathbf{U}^T\mathbf{A}^T\mathbf{U} + \mathbf{B}\mathbf{B}^T\mathbf{U} + \mathcal{P}(\mathbf{I} - \mathbf{U}\mathbf{U}^T)\mathbf{A}^T\mathbf{U} = \mathbf{0}$$

Thus

$$\mathbf{A}\mathcal{P}\mathbf{U} + \mathcal{P}\mathbf{U}\mathbf{H}^T + \mathbf{B}\mathbf{B}^T\mathbf{U} \approx \mathbf{0} \quad \text{where} \quad \mathbf{H} = \mathbf{U}^T\mathbf{A}\mathbf{U}$$

Solving

$$\mathbf{A}\mathbf{Z} + \mathbf{Z}\mathbf{H}^T + \mathbf{B}\mathbf{B}^T\mathbf{U} = \mathbf{0}$$

gives approximation to

$$\mathbf{Z} \approx \mathcal{P}\mathbf{U}$$

Iterate $\Rightarrow$ *Approximate Power Method* $\mathbf{Z}_j \rightarrow \mathbf{U}\mathbf{S}$ with $\mathcal{P}\mathbf{U} = \mathbf{U}\mathbf{S}$
(also see Vasilyev and White 05)

A Parameter Free Synthesis ($\mathcal{P} \approx \mathbf{U}\mathbf{S}^2\mathbf{U}^T$)

Step 1: Solve the reduced order Lyapunov equation
Solve $\mathbf{H}\hat{\mathcal{P}} + \hat{\mathcal{P}}\mathbf{H}^T + \hat{\mathbf{B}}\hat{\mathbf{B}}^T = \mathbf{0}$.
with $\mathbf{H} = \mathbf{U}_k{}^T\mathbf{A}\mathbf{U}_k$, $\hat{\mathbf{B}} = \mathbf{U}_k{}^T\mathbf{B}$.

Step 2: (APM step) Solve a projected Sylvester equation

$$\mathbf{A}\mathbf{Z} + \mathbf{Z}\mathbf{H}^T + \mathbf{B}\hat{\mathbf{B}}^T = \mathbf{0},$$

Step 3: Modify **B**

Update $\mathbf{B} \leftarrow (\mathbf{I} - \mathbf{Z}\hat{\mathcal{P}}^{-1}\mathbf{U}^T)\mathbf{B}$.

Step 4: (ADI step) Update factorization and basis $\mathbf{U}_k$

Re-scale $\mathbf{Z} \leftarrow \mathbf{Z}\hat{\mathcal{P}}^{-1/2}$.
Update (and truncate) $[\mathbf{U}, \mathbf{S}] \leftarrow svd[\mathbf{U}\mathbf{S}, \mathbf{Z}]$.
$\mathbf{U}_k \leftarrow \mathbf{U}(:, 1:k)$, basis for dominant subspace.

Implementation Details

Note: $\mathbf{A}\mathcal{P}_j + \mathcal{P}_j\mathbf{A}^T + \mathbf{B}\mathbf{B}^T = \mathbf{B}_j\mathbf{B}_j^T$ gives Residual Norm for Free!

Stopping Rules:

1. $\frac{\|\mathcal{P}_{j+1}-\mathcal{P}_j\|_2}{\|\mathcal{P}_{j+1}\|_2} = \frac{\|\mathbf{Z}_j\hat{\mathcal{P}}_j^{-1/2}\|_2^2}{\|\mathbf{S}_{j+1}\|_2^2} \leq tol$
2. $\frac{\|\mathbf{B}_j\|_2}{\|\mathbf{B}\|_2} \leq \sqrt{tol}$

Montone Convergence!

$$\mathcal{P}_j \preceq \mathcal{P}_{j+1} \preceq \mathcal{P} \quad \text{for} \quad j = 1, 2, \ldots$$

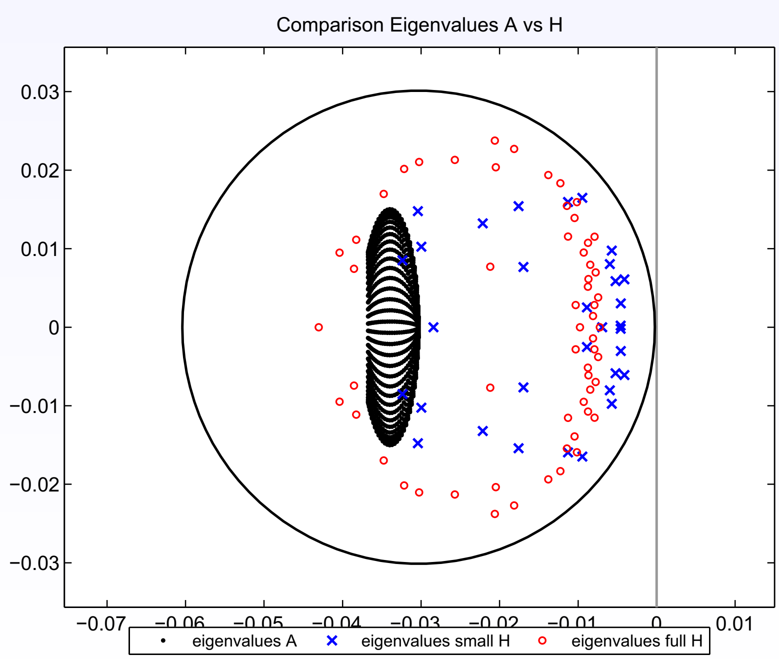
This implies

$$\lim_{j\to\infty} \mathcal{P}_j = \mathcal{P}_o \preceq \mathcal{P}, \quad \text{monotonically}$$

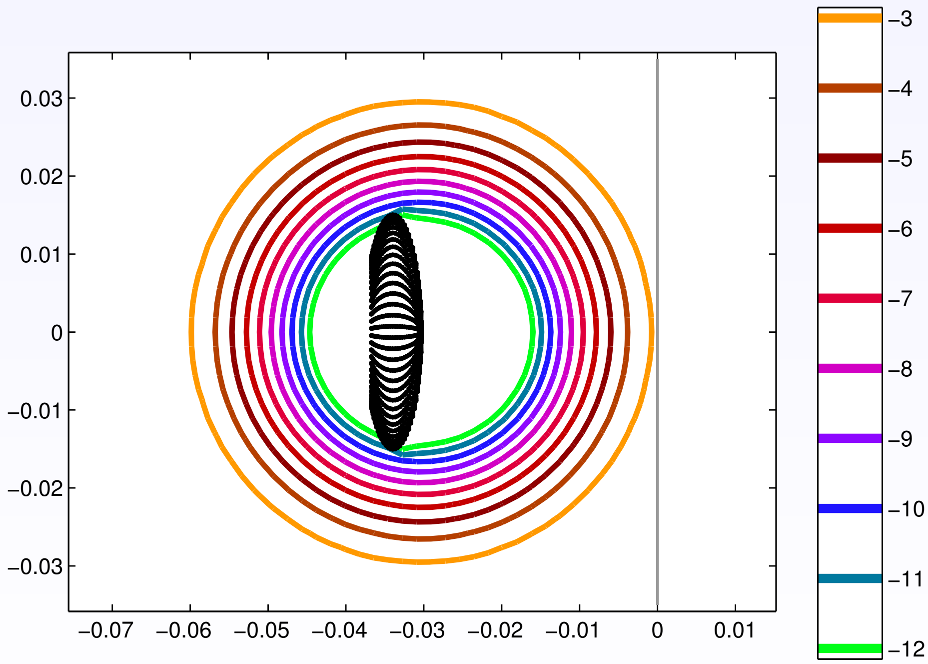
Automatic Shift Selection - Placement?

SUPG discretization advection-diffusion operator on square grid

k = 32, m = 59 , n = 32*32, Thanks Embree



ϵ-*Pseudospectra for* **A** *from SUPG, n=32*32*



Convergence History , Supg, $n = 800$, $N = 640{,}000$

CaamPC

Iter	$\frac{\lVert\mathcal{P}_+ - \mathcal{P}\rVert}{\lVert\mathcal{P}_+\rVert}$	$\lVert\mathbf{B}_j\rVert$	$\lVert\hat{\mathbf{B}}_j\rVert$
6	1.3e-01	2.5e+00	2.4e+00
7	7.5e-02	1.1e+00	1.2e+00
8	3.5e-02	6.74e-01	5.0e-01
9	2.0e-02	1.2e-02	6.7e-01
10	2.0e-04	7.1e-07	1.2e-02
11	1.0e-08	2.3e-11	6.4e-07

$\mathcal{P}_f$ is rank $k = 120$ Comptime($\mathcal{P}_f$) $= 157$ mins $= 2.6$ hrs

Preserving Passivity

Passive Systems:

$Re \int_{-\infty}^{t} \mathbf{u}(\tau)^T \mathbf{y}(\tau) \mathrm{d}\tau \geq 0$
for all $t \in \mathbb{R}$ and all $\mathbf{u} \in \mathcal{L}_2(\mathbb{R})$,

Positive Real: $\mathbf{G}(s) \equiv \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D}$.

(1) $\mathbf{G}(s)$ is analytic for $Re(s) > 0$,
(2) $\mathbf{G}(\bar{s}) = \overline{\mathbf{G}(s)}$ for all $s \in \mathbb{C}$,
(3) $\mathbf{G}(s) + (\mathbf{G}(s))^* \succeq \mathbf{0}$ for $Re(s) > 0$.

Spectral Zeros:

Property (3) $\Rightarrow$ $\mathbf{W}(s)$ (with stable inverse) s.t.
$\mathbf{G}(s) + \mathbf{G}^T(-s) = \mathbf{W}(s)\mathbf{W}^T(-s)$.
$\mathcal{S}_\mathbf{G} := \{s \in \mathbb{C} : \det[\mathbf{G}(s) + \mathbf{G}^T(-s)] = 0\}$

Spectral Zeros $\mathcal{S}_\mathbf{G}$

Finite generalized eigenvalues $\lambda \in \sigma(\mathcal{A}, \mathcal{E})$:

$$Rank(\mathcal{A} - \lambda\mathcal{E}) < 2n + p,$$

where

$$\mathcal{A} := \begin{bmatrix} \mathbf{A} & & \mathbf{B} \\ & -\mathbf{A}^T & -\mathbf{C}^T \\ \mathbf{C} & \mathbf{B}^T & \mathcal{D} \end{bmatrix} \text{ and } \mathcal{E} := \begin{bmatrix} \mathbf{I} & & \\ & \mathbf{I} & \\ & & \mathbf{0} \end{bmatrix}$$

Reflection Properties: $\lambda \in \mathcal{S}_\mathbf{G} \iff -\bar{\lambda} \in \mathcal{S}_\mathbf{G}$.

Equivalent Structured Formulations

Symmetric - SkewSymmetric $(\mathcal{A}, \mathcal{E})$ eigenproblem

$$\mathcal{A} = \begin{bmatrix} \mathbf{0} & \mathbf{A}^T & \mathbf{C}^T \\ \mathbf{A} & \mathbf{0} & \mathbf{B} \\ \mathbf{C} & \mathbf{B}^T & \mathcal{D} \end{bmatrix} \quad \text{and} \quad \mathcal{E} = \begin{bmatrix} \mathbf{0} & -\mathbf{I} & \mathbf{0} \\ \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}$$

Hamiltonian eigenproblem

$$\mathcal{H} = \begin{bmatrix} \mathbf{A} - \mathbf{B}\mathcal{D}^{-1}\mathbf{C} & -\mathbf{B}\mathcal{D}^{-1}\mathbf{B}^T \\ \mathbf{C}^T\mathcal{D}^{-1}\mathbf{C} & -(\mathbf{A} - \mathbf{B}\mathcal{D}^{-1}\mathbf{C})^T \end{bmatrix}$$

Interpolation via Invariant Subspace

Antoulas: *Interpolation at Spectral Zeros* $\Rightarrow$ *Passivity*
Invariant Subspace Formulation(S., 2005):

$$\begin{bmatrix} \mathbf{A} & & \mathbf{B} \\ & -\mathbf{A}^T & -\mathbf{C}^T \\ \mathbf{C} & \mathbf{B}^T & \mathcal{D} \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \\ \mathbf{Z} \end{bmatrix} = \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \\ \mathbf{0} \end{bmatrix} \mathbf{R}.$$

Construct $\mathbf{X} = \mathbf{V}\hat{\mathbf{X}}, \quad \mathbf{Y} = \mathbf{W}\hat{\mathbf{Y}}, \quad \hat{\mathbf{A}} := \mathbf{W}^T\mathbf{A}\mathbf{V}, \quad \mathbf{W}^T\mathbf{V} = \mathbf{I}$

$$\begin{bmatrix} \hat{\mathbf{A}} & & \hat{\mathbf{B}} \\ & -\hat{\mathbf{A}}^T & -\hat{\mathbf{C}}^T \\ \hat{\mathbf{C}} & \hat{\mathbf{B}}^T & \mathcal{D} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{X}} \\ \hat{\mathbf{Y}} \\ \mathbf{Z} \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{X}} \\ \hat{\mathbf{Y}} \\ \mathbf{0} \end{bmatrix} \mathbf{R}.$$

Summary

Gramian Based Model Reduction: Balanced Reduction

Solving Large Lyapunov Equations: Approximate Balancing
1M vars now possible
Parameter Free

Balanced Reduction of Oseen Eqns: Extension to
Descriptor System

Multi-Shift ADI Without Explicit Projectors:
Only need Saddle Point Solver Sparse Direct or Iterative

A-Priori Error Bounds and Preservation of Stability in ROM