Efficient Iterative Algorithms for Linear Stability Analysis

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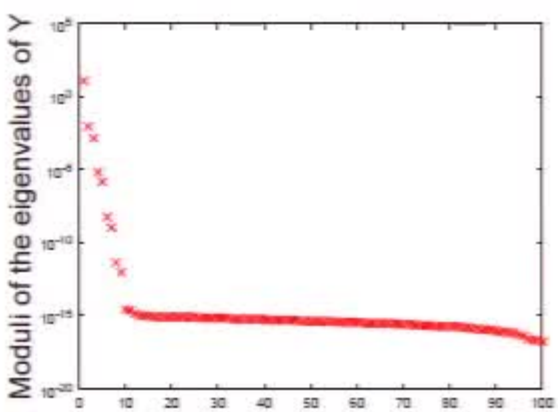
The problem

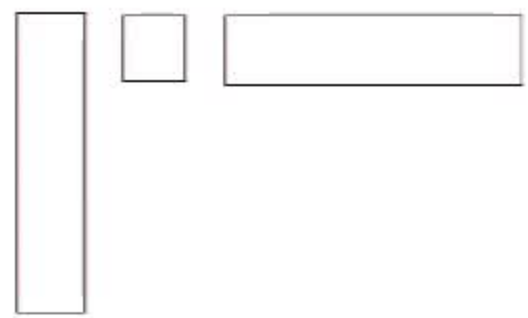
Solve the *Lyapunov equation*

$$SY + YS^T = \text{RHS}$$

efficiently, where

- $S = A^{-1}M$, where $A, M \in \mathbb{R}^{n \times n}$ large and sparse
  A: Jacobian matrix, M: mass matrix
- The RHS matrix is real, symmetric and has rank 1 or 2
- $Y \in \mathbb{R}^{n \times n}$: symmetric, typically has low-rank representation

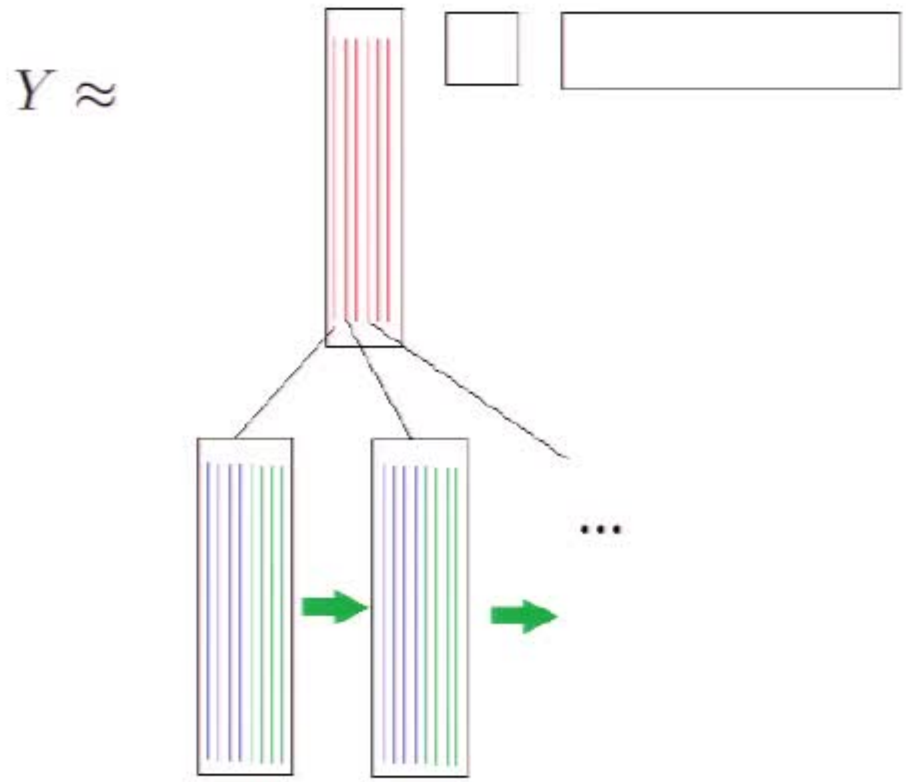


$Y \approx$ 

Krylov subspace methods!

[Penzl; Antoulas, Sorensen, & Zhou; Grasedyck; Kressner & Tobler; ...]

Hierarchy of the solution methods



We want

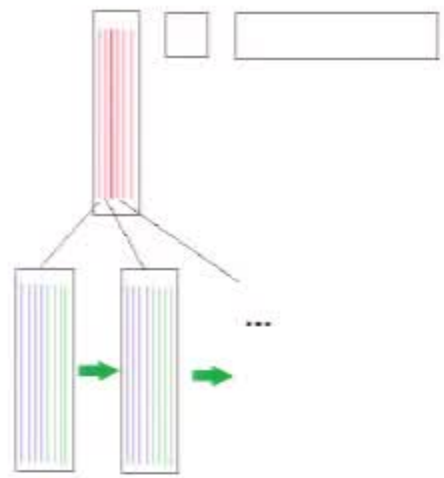
the size of the subspace to be as small as possible

the computation of each basis vector as cheap as possible

to re-use information obtained in previous iterations

Outline

- Motivation: linear stability analysis of large-scale dynamical systems
  - eigenvalue problem in the form of a Lyapunov equation
  - *Lyapunov inverse iteration*
- Strategies for solving $SY + YS^T = \text{RHS}$:
  - Krylov-type Lyapunov solvers and our modification
  - preconditioned GMRES
  - recycling Krylov subspaces



- Concluding remarks

Linear stability analysis

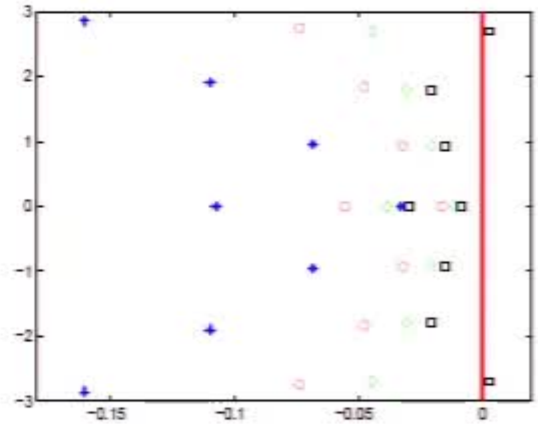
- The *stability* (sensitivity to small perturbations) of the dynamical system

$$M\dot{\mathbf{u}} = A(\alpha)\mathbf{u}$$

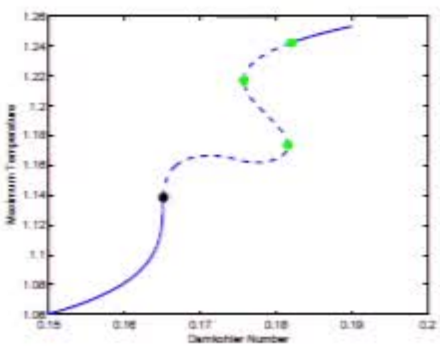
depends on the rightmost eigenvalue μ_{rm} of $A(\alpha)\mathbf{x} = \mu M\mathbf{x}$:

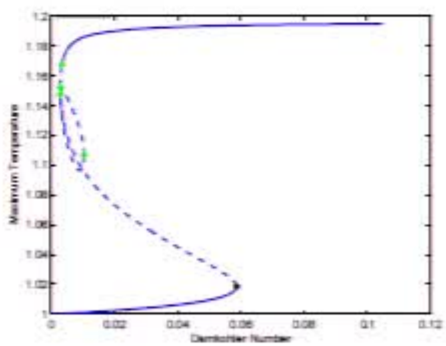
  - $\text{Re}(\mu_{\text{rm}}) < 0$: steady state is stable
  - $\text{Re}(\mu_{\text{rm}}) \geq 0$: unstable

$\alpha_1(*) < \alpha_2(\circ) < \alpha_3(\Diamond) < \alpha_4(\Box) \rightarrow$

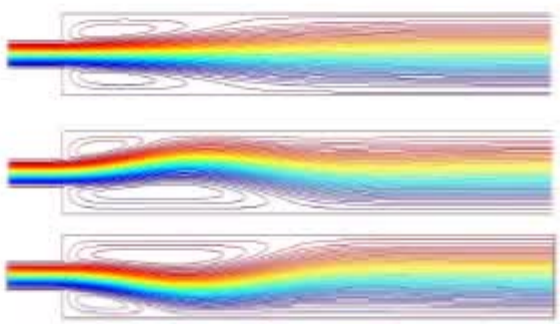


- Bifurcation phenomenon occurs as well





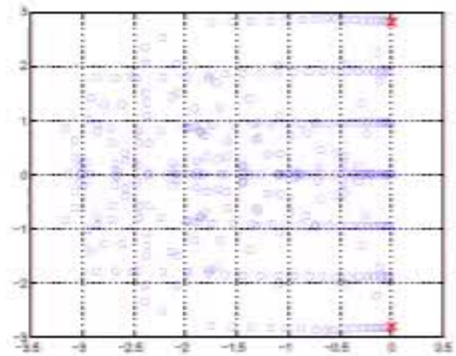
[Heinemann & Poore]



[Cliffe, Garratt & Spence]

The eigenvalue problem

- Finding the rightmost eigenvalue of $A\mathbf{x} = \mu M\mathbf{x}$ is difficult
  - direct methods (QR, QZ): not feasible for large-scale problems
  - iterative methods (subspace, Arnoldi, Jacobi-Davidson): not reliable without a rough estimate of μ_{rm}



- New strategy: solve a related, "easier" problem

Theorem 1 (joint with Elman; also in [Meerbergen & Vandebril])

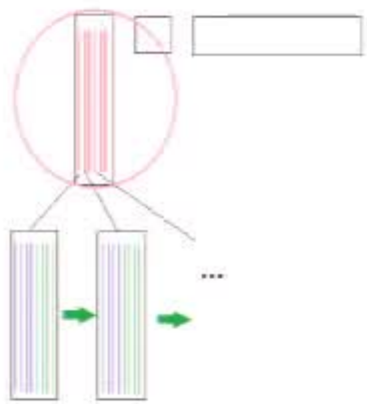
Assume $A\mathbf{x} = \mu M\mathbf{x}$ has a complete set of eigenvectors and all its eigenvalues lie to the left of the imaginary axis. Then the eigenvalue λ_{sm} of

$$SZ + ZS^T = \lambda\left(-2SZS^T\right),$$

with smallest modulus is $-\text{Re}(\mu_{\text{rm}})$, where $S = A^{-1}M$.

- the smallest eigenvlaue is easier to find
- Lyapunov inverse iteration [Meerbergen & Spence]

Iterative Lyapunov solvers

$Y \approx$ 

Iterative method for $SY + YS^T = BCB^T$

1. construct a small subspace span$\{V_m\}$
2. solve the small Lyapunov equation

$$\left(V_m^T S V_m\right) X + X \left(V_m^T S V_m\right)^T = \left(V_m^T B\right) C \left(V_m^T B\right)^T$$

[Bartels & Stewart; Hammarling]

3. $Y \approx V_m X V_m^T$

Choice of the subspace:

- standard Krylov subspace [Saad; Jaimoukha & Kasenally; ...]

$$\mathcal{K}_m(S, B) = \text{span}\left\{B, SB, S^2B, \ldots, S^{m-1}B\right\}$$

  At each step:
  - $S = A^{-1}M \Rightarrow$ a solve of type $A\mathbf{x} = \mathbf{b}$
  - $V_m^T S V_m$: upper-Hessenberg, available at no additional cost
- rational Krylov subspace

Rational Krylov subspace method

[Ruhe; Druskin & Simoncini]

$$\mathcal{K}_m(S, B, \mathbf{s}) = \text{span}\left\{B, (S - s_1 I)^{-1} B, (S - s_2 I)^{-1}(S - s_1 I)^{-1} B, \ldots, \prod_{j=1}^{m-1} (S - s_{m-j} I)^{-1} B\right\}$$

At each step:

- $S = A^{-1}M \Rightarrow$ a solve of type $(M - sA)\mathbf{x} = \mathbf{b}$
- $V_m^T S V_m$ requires $S\mathbf{v}_{m+1} \Rightarrow$ an extra solve of type $A\mathbf{x} = \mathbf{b}$

$$V_m^T S V_m = (I_m + H_m D_m - V_m^T S\mathbf{v}_{m+1} H_{m+1,m}\mathbf{e}_m^T)H_m^{-1}$$

- $A\mathbf{x} = \mathbf{b}$ is much more difficult to solve!
- shifts are real, adaptively chosen based on rough spectral information of S obtained from $V_m^T S V_m$ [Druskin, Lieberman & Zaslavksy; Druskin & Simoncini]

Iterative linear solves

Due to the fact that $S = A^{-1}M$

- standard Krylov subspace requires solves of type $A\mathbf{x} = \mathbf{b}$

$$\mathcal{K}_m(S, B) = \text{span}\left\{B, SB, S^2B, \ldots, S^{m-1}B\right\}$$

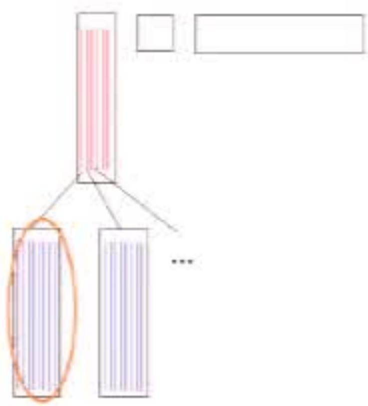
- rational Krylov subspace requires solves of types $A\mathbf{x} = \mathbf{b}$ and $(M - sA)\mathbf{x} = \mathbf{b}$

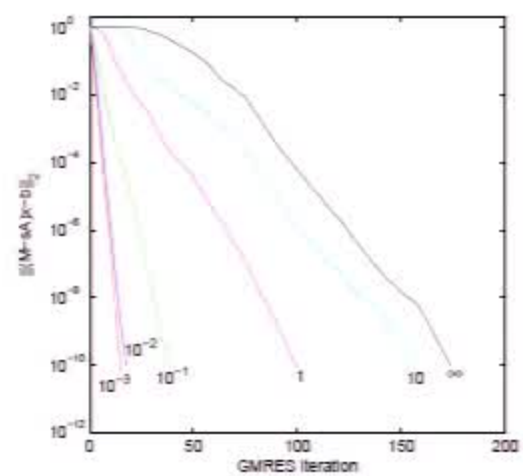
$$\mathcal{K}_m(S, B, \mathbf{s}) = \text{span}\left\{B, (S - s_1 I)^{-1}B, (S - s_2 I)^{-1}(S - s_1 I)^{-1}B, \ldots, \prod_{j=1}^{m-1}(S - s_{m-j}I)^{-1}B\right\}$$

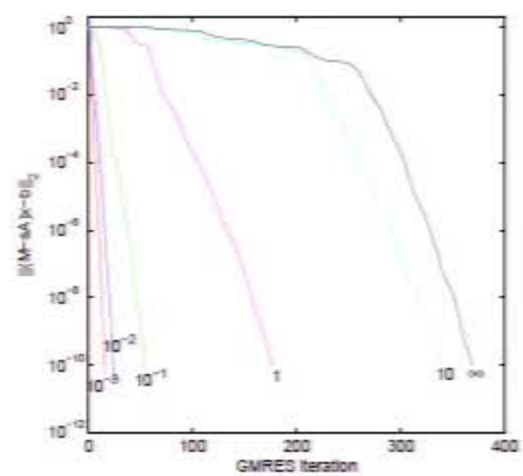
- preconditioned GMRES for the linear systems

$n \approx 10,000$, incompressible flows

$Y \approx$



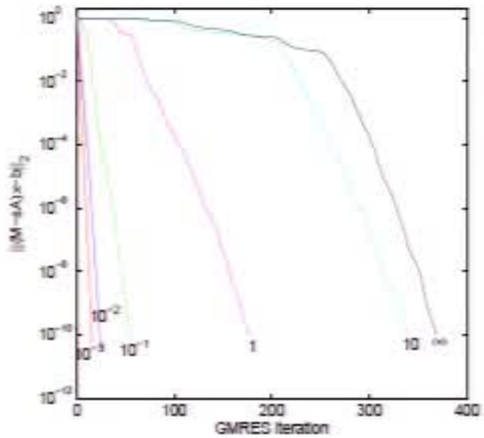


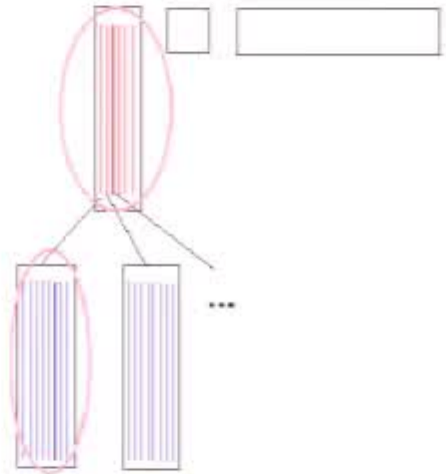


$$\mathcal{K}_d(AP^{-1}, \mathbf{b}) = \text{span}\left\{\mathbf{b}, AP^{-1}\mathbf{b}, (AP^{-1})^2\mathbf{b}, \ldots, (AP^{-1})^{m-1}\mathbf{b}\right\}$$

Iteration counts

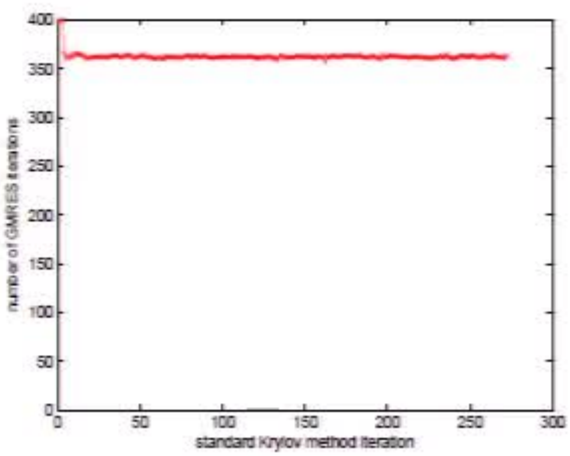
Solve $SY^T + YS^T = BCB^T$ iteratively. $Y \in \mathbb{R}^{n\times n}$ has low-rank representation.

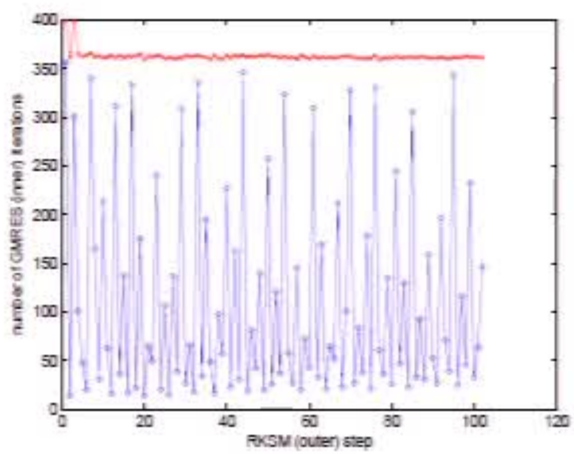


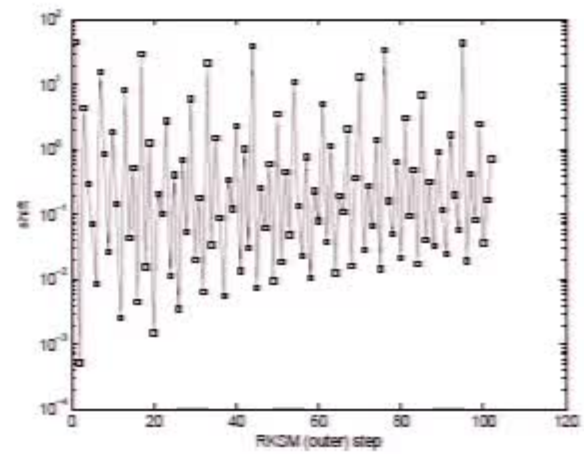


standard Krylov

rational Krylov



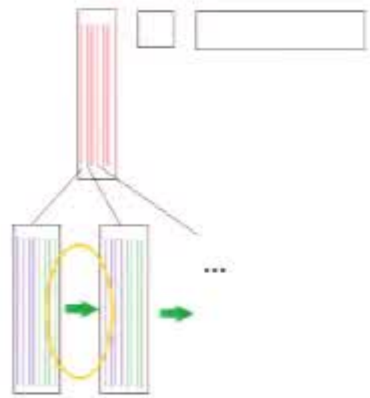




Krylov subspace recycling

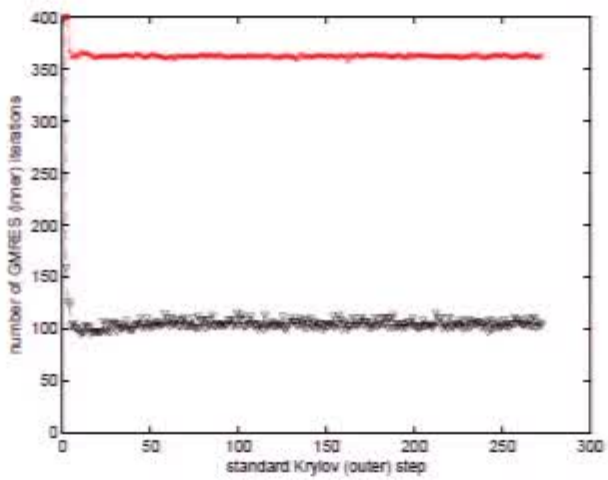
[Parks, De Sturler, Machey, Johnson, & Maiti]

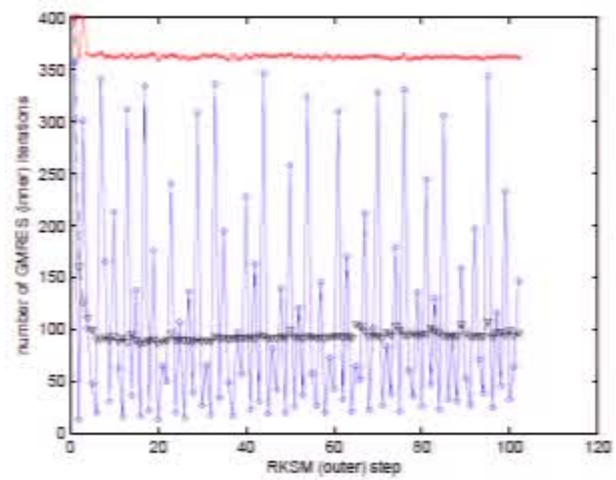
$Y \approx$



- In both Lyapunov solvers, we need to solve a sequence of linear systems $A\mathbf{x} = \mathbf{b}_i$.
- We construct a sequence of Krylov subspaces $\{\mathcal{K}_d(AP^{-1}, \mathbf{b}_i)\}$ for them
- $\mathcal{K}_d(AP^{-1}, \mathbf{b}_i)$ may contain spectral info of AP^{-1} that facilitates the solve of $A\mathbf{x} = \mathbf{b}_{i+1}$.

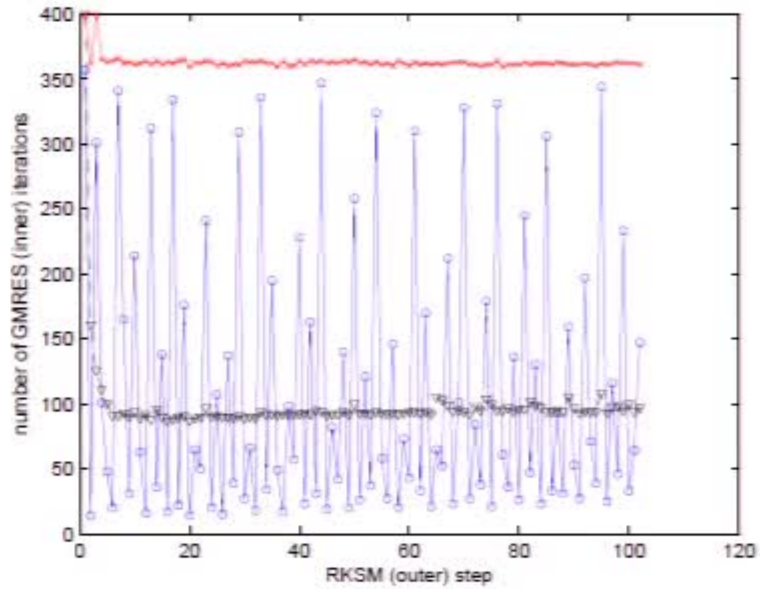
keep the half of $\mathcal{K}_d(AP^{-1}, \mathbf{b}_i)$ corresponding to the smaller eigenvalues of AP^{-1}





$\mathcal{K}_d((M - s_i A)P_{s_i}^{-1}, \mathbf{b}_i)$ are NOT recycled due to the oscillation in the shifts!

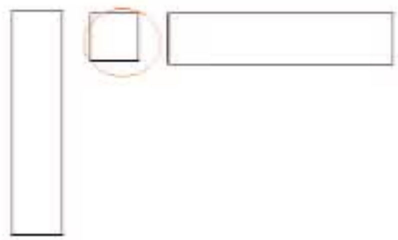
Let's cut more corners!



Can we get rid of the red (or black) curve completely?

Modified RKSM

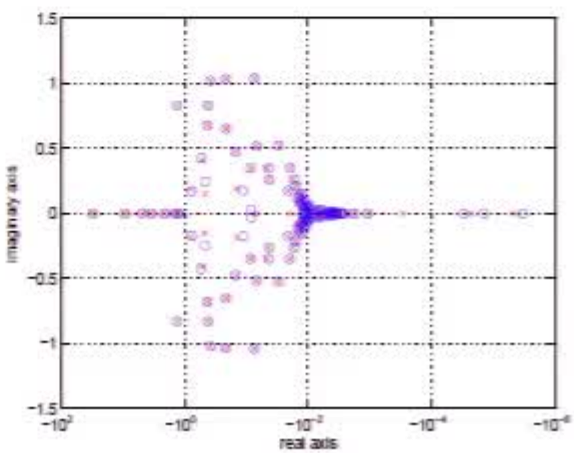
The matrix-vector product $S\mathbf{v}_{m+1}$ (solve $A\mathbf{x} = \mathbf{b}_i$) is needed to compute the small matrix $V_m^T S V_m$.

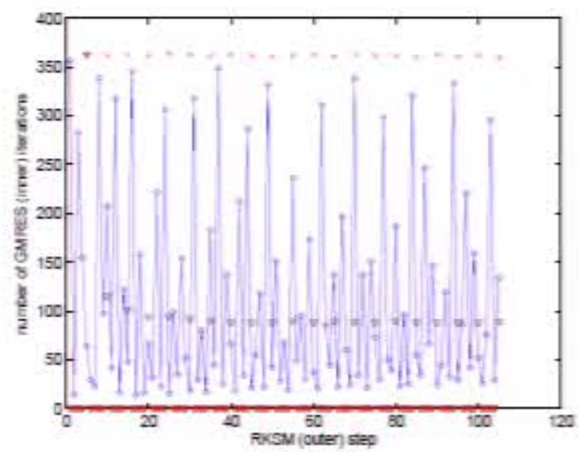
$Y \approx$ 

- need this matrix to construct Y (no need to form it at every step)
- produces spectral info about S used to generate shifts (explore alternatives)

Theorem 2 (joint with Elman)

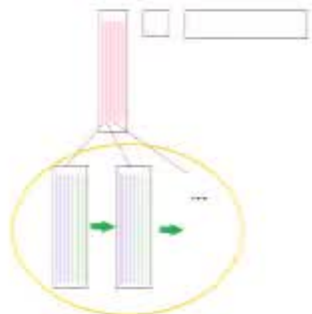
Suppose V_m holds an orthonormal basis of the rational Krylov subspace of $S = A^{-1}M$. Then $(V_m^T A V_m)^{-1}(V_m^T M V_m)$ and $V_m^T S V_m$ only differ by a rank-1 matrix.

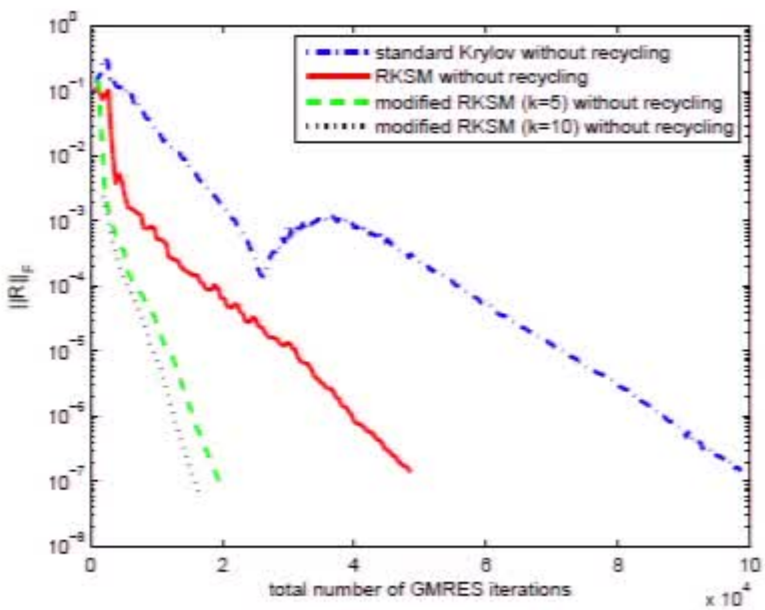


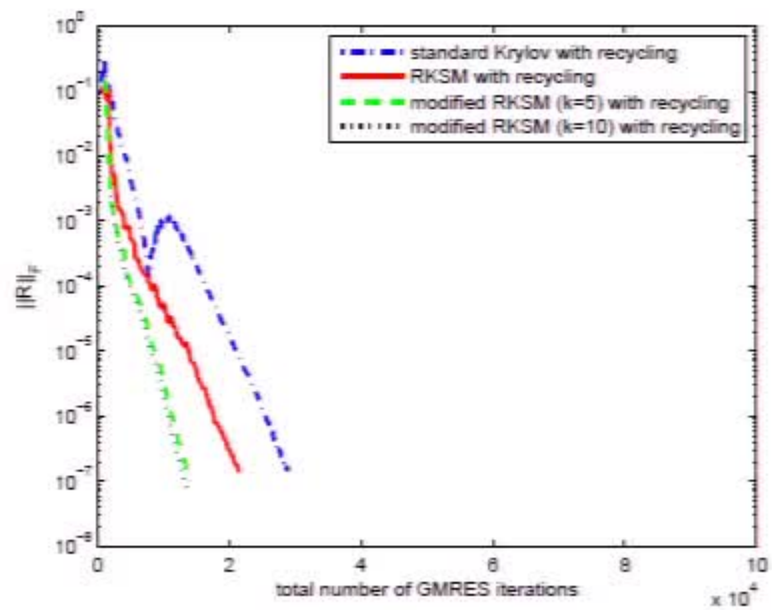


Total costs

- ✓ picked a good Lyapunov solver and improved it
- ✓ picked a good preconditioner for the linear systems (problem-specific)
- ✓ re-used intermediate computational results

$Y \approx$ 





A few details

- Preconditioner used: the Least-Squares Commutator preconditioner [Elman, Silvester, & Wathen; Elman & Tuminaro].
  - an important feature: does not require extra work to build as the shift s varies
  - techniques for preconditioning a family of shifted linear systems with different right-hand sides? [Bakhos, Ladenheim, Kitanidis, Saibaba, & Szyld; ...]
  - solves with P are approximated by one V-cycle of algebraic multigrid
- The choice of shifts $\{s_j\}_{j=1}^m$ [Druskin, Lieberman, & Zaslavksy; Druskin & Simoncini]
  - first introduced to approximate $\mathbf{u}(t) = \exp(St)\mathbf{u}(0)$
  - based on a representation of the error between the true $\mathbf{u}$ and its estimate obtained by RKSM
  - boils down to the following optimization problem

$$s_{m+1} = \arg\left(\max_{s\in\mathcal{I}} \frac{1}{|r_m(s)|}\right), \text{ where } r_m(s) = \frac{\prod_{j=1}^m (s-\theta_j)}{\prod_{j=1}^m (s-s_j)}$$

    $\{\theta_j\}_{j=1}^m$: Ritz values (eigenvalues of $V_m^T S V_m$)
  - connection with the Lyapunov equation: the analytic solution to $SY^T + YS^T = BCB^T$ is

$$Y = \int_0^\infty \exp(tS) BCB^T \exp\left(tS^T\right)\, dt$$

Conclusion

Papers (joint with Elman):

-On the robust computation of the rightmost eigenvalues:
Lyapunov inverse iteration for computing a few rightmost eigenvalues of large generalized eigenvalues problems, in SIMAX 2013
-On the efficient implementation of this eigenvalue solver: (this talk)
Efficient iterative algorithms for linear stability analysis of incompressible flows, in IMANUM 2015

- Discussed how to solve $AYM + MYA^T =$ RHS efficiently

  Lyapunov solver + preconditioner + recycling

- Proposed a modified RKSM that achieves significant computational savings
- Other applications besides linear stability analysis?
- Robust eigenvalue solver for finding the rightmost eigenvalues of large, *unstable*, *complex* matrices? (joint with Xue)