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## Probing for Schur Complements and Preconditioning Generalized Saddle-Point Problems

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# Collaborators

- Jörg Liesen, TU Berlin
- Chris Siefert, Mike Parks, UIUC
- Armand Beaudoin, UIUC: metal deformation
- Lihua Zhu, UIUC: metal deformation
- Alla Sheffer, UBC: surface parameterization

# Overview

- Crash course on Krylov subspace methods
- Saddle-point problems
- Preconditioners
  - Numerical Example: Surface Parameterization
- Preconditioning Matrices with Nonzero (2,2) Block
- Approximating the Schur complement
- Probing
- Numerical results
  - Oseen Problem (lid driven cavity)
  - Metal Deformation
- Conclusions

# Krylov Methods Crash Course

Consider  $Ax = b$ . Given  $x_0$  and  $r_0 = b - Ax_0$ , compute optimal update from  $K^m(A, r_0) \equiv \text{span} \{r_0, Ar_0, \dots, A^{m-1}r_0\}$ :

$$\min_{z \in K^m(A, r_0)} \|b - A(x_0 + z)\|_2 \quad \Leftrightarrow \quad \min_{z \in K^m(A, r_0)} \|r_0 - Az\|_2$$

Let  $K_m = [r_0 \quad Ar_0 \quad A^2r_0 \quad \dots \quad A^{m-1}r_0]$ , then  $z = K_m \zeta$ ,

and we must solve the following least squares problem

$$AK_m \zeta \approx r_0 \quad \Leftrightarrow \quad [Ar_0 \quad A^2r_0 \quad \dots \quad A^m r_0] \zeta \approx r_0$$

Do this accurately and efficiently every iteration for increasing  $m$ .

Arnoldi recurrence:

$AV_m = V_{m+1} \underline{H}_m$ , where  $v_1 = r_0 / \|r_0\|_2$ ,  $V_{m+1}^H V_{m+1} = I_{m+1}$ , and

$\text{range}(V_{m+1}) = \text{range}(K_{m+1})$

$$\|r_0 - AV_m y_m\|_2 = \|V_{m+1} e_1 \|r_0\|_2 - V_{m+1} \underline{H}_m y_m\|_2 = \|e_1 \|r_0\|_2 - \underline{H}_m y_m\|_2$$

# Krylov Methods Crash Course

Consider  $Ax = b$ , and relate convergence to polynomials.

$$x_m = x_0 + z_m \text{ where } z_m \in \text{span}\{r_0, Ar_0, A^2r_0, \dots, A^{m-1}r_0\}$$
$$r_m = r_0 - Az_m \in \text{span}\{r_0, Ar_0, \dots, A^m r_0\}$$

Assume  $A = U\Lambda U^{-1}$  (diagonalizable), then residual at step  $m$

$$\min_{z \in K^m(A, r_0)} \|r_0 - Az\| = \min_{p_m(0)=1} \|p_m(A)r_0\| \leq \|r_0\| \|U\| \|U^{-1}\| \min_{p_m(0)=1} \max_{\lambda \in \Lambda(A)} |p_m(\lambda)|$$

For normal matrix this bound is sharp. For highly nonnormal matrix this bound may not be useful.

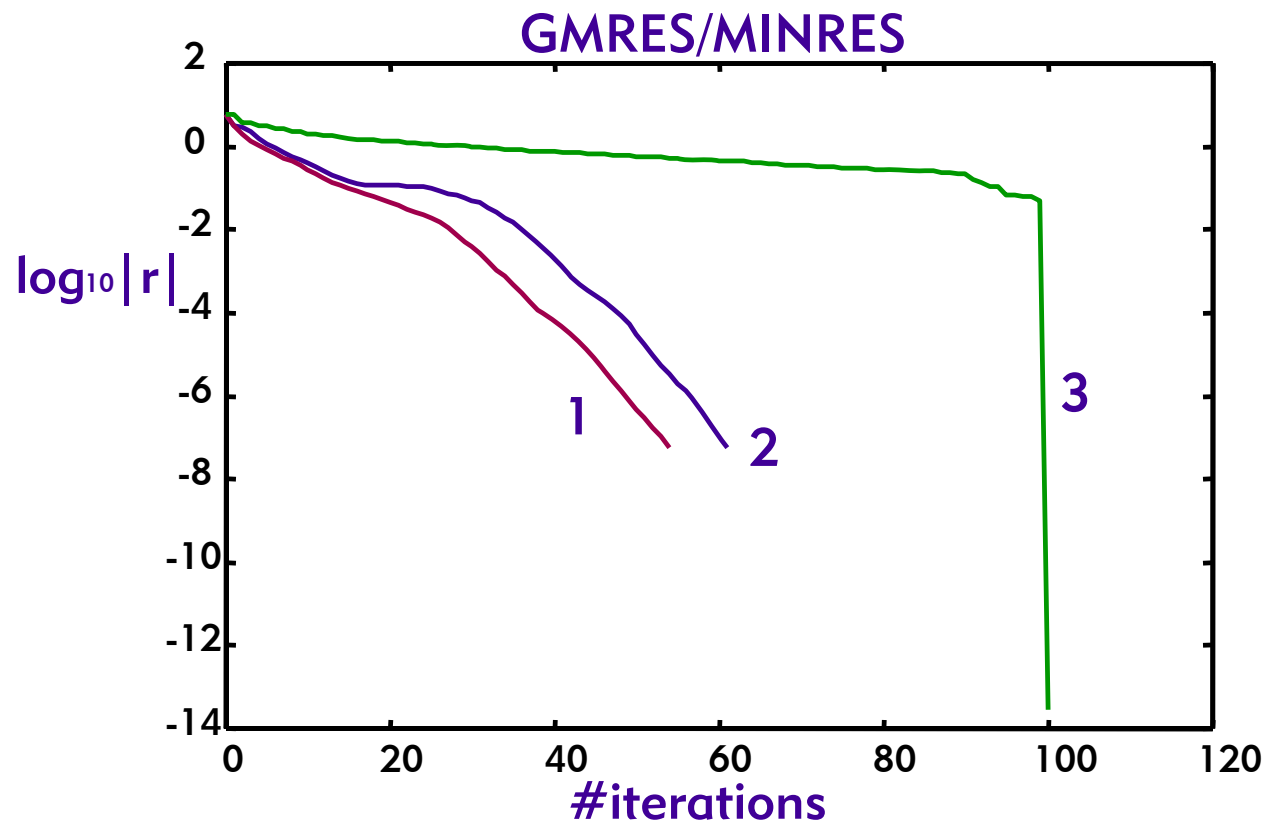
$\kappa(U)$  small: convergence determined by minimal polynomial

Clustered eigenvalues yield fast convergence: preconditioning

Eigenvalues surrounding origin yields very poor convergence.

# Krylov Methods Crash Course

1.  $A = \text{diag}(1, 2, 3, \dots, 100)$
2.  $A = \text{diag}(-1, -100, 1, 2, \dots, 49, 52, \dots, 100)$
3.  $A = \text{diag}(-99, -97, \dots, -1, 1, 3, \dots, 97, 99)$



# Generalized Saddle-point Problems

We consider systems of the type

$$\begin{pmatrix} A & B^T \\ C & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} A & B^T \\ C & D \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

Systems of this type arise in a variety of problems:

- Constrained optimization problems
  - FETI (type) methods (Mike Parks)
  - Surface parameterization
- Systems of PDEs with continuity constraints
  - Navier-Stokes
  - Potential flow in porous media
  - Polycrystal plasticity – metal deformation
  - Electrostatics / electromagnetics

# Preconditioners

- Various preconditioners have been proposed
  - Block diagonal preconditioner
  - Constraint preconditioner
  - Block upper triangular
- ‘Ideal version’ leads to small number of nonzero eigenvalues, and hence fast convergence for Krylov methods
- In general we use an approximation to these ideal versions (otherwise too expensive)
- Typically involve Schur complement type matrix



# Preconditioners

Significant body of work by Elman, Golub, Wathen, Benzi, Silvester, Gould, Nocedal, Hribar, Simoncini, Perugia, BP, ...

Use splitting  $A = F - E$  (dS&L):

$$\begin{pmatrix} F^{-1} & & \\ & (CF^{-1}B^T)^{-1} & \\ & & \end{pmatrix} \begin{pmatrix} F - E & B^T \\ C & 0 \end{pmatrix} = \begin{pmatrix} I - S & N \\ M & 0 \end{pmatrix}$$

$$M = (CF^{-1}B^T)^{-1}C, N = F^{-1}B^T, MN = I, (NM)^2 = NM$$

$$\text{Oblique projection: } NM = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} 0 & \\ & I \end{pmatrix} \begin{pmatrix} U_1 & U_2 \end{pmatrix}^{-1}$$

Principal angles ( $\omega_i = \cos \varphi_i$ ) between  $\text{null}(NM)$  and  $\text{range}(NM)$  play important role in eigenvalue bounds.

# Preconditioners

Preconditioned system: 
$$\begin{pmatrix} I - S & N \\ M & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \hat{f} \\ \hat{g} \end{pmatrix}$$

Eigenvalues: 
$$|\lambda_S - \lambda| \leq 1.5 \left( \frac{1 + \omega_{\max}}{1 - \omega_{\max}} \right)^{1/2} \|S\|, \lambda \in \{1, (1 \pm \sqrt{5})/2\}$$

Further splitting gives fixed point iteration that depends only on  $x$ : 
$$x_{k+1} = (I - NM)Sx_k + \tilde{f}$$

Solves *related system* 
$$(I - (I - NM)S)x = \tilde{f}$$

Eigenvalues 
$$|1 - \lambda_R| \leq (1 - \omega_{\max}^2)^{-1/2} \|S\|$$

# Preconditioners

This approach is applicable to general problems; for details and analysis see dS&L 2002.

- Eigenvalue bounds for general problems
- Regarding related system
  - Smaller system to solve
  - Good bounds on eigenvalues, single cluster
  - Shows bounds always better than for block diag. prec.
  - Satisfies constraints
  - Extends constraint preconditioners to general matrices and is more efficient (CPU and memory).

Problem is that (this type of) iteration involves  $(CF^{-1}B^T)^{-1}$ , which may be expensive to compute and iterate with.

In that case, we must look for alternatives.

# Invariance Property (also nonzero (2,2))

$$\hat{A} = \begin{pmatrix} A & B^T R_2 \\ R_1 C & 0 \end{pmatrix}, \quad \text{Preconditioner: } \begin{pmatrix} F^{-1} & 0 \\ 0 & (R_1 C F^{-1} B^T R_2)^{-1} \end{pmatrix}$$

$$\begin{pmatrix} I - S & \tilde{N} \\ \tilde{M} & 0 \end{pmatrix}, \quad \text{where } \tilde{N} = F^{-1} B^T R_2 \text{ and } \tilde{M} = R_2^{-1} (C F^{-1} B^T)^{-1} C$$

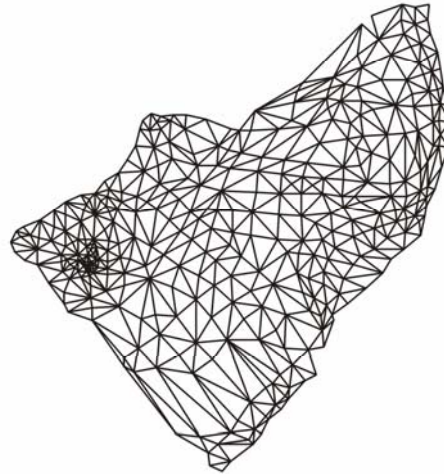
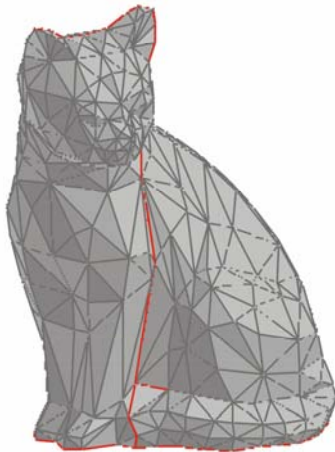
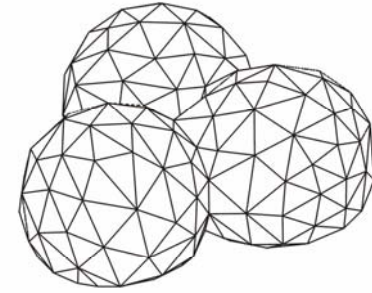
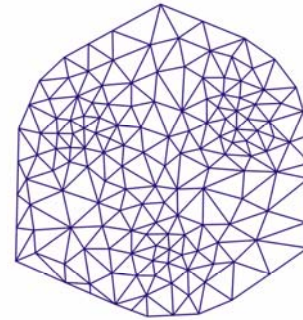
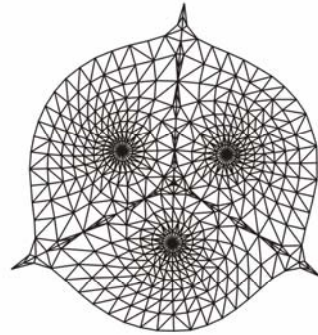
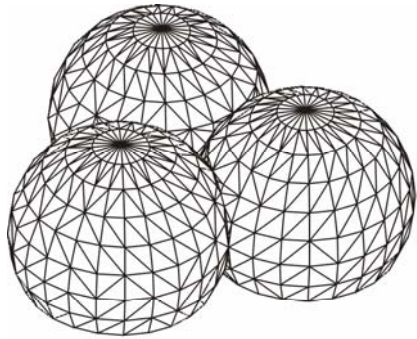
$$\tilde{M}\tilde{N} = R_2^{-1} M N R_2 = I, \quad \tilde{N}\tilde{M} = N M \text{ (oblique) projection.}$$

This matrix has exactly the same eigenvalues (and bounds) as the original matrix with block diagonal preconditioner.

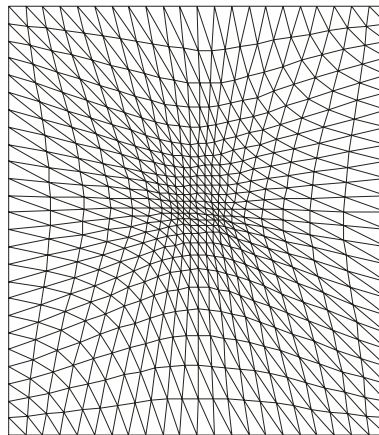
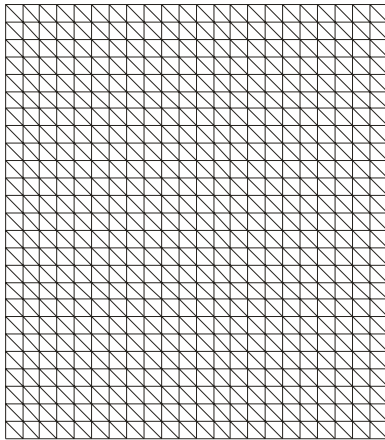
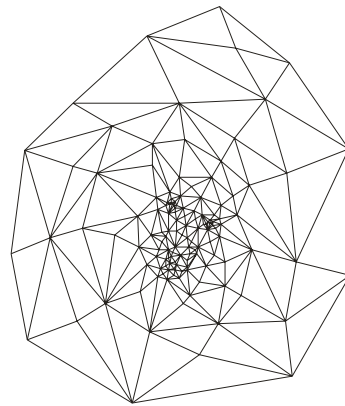
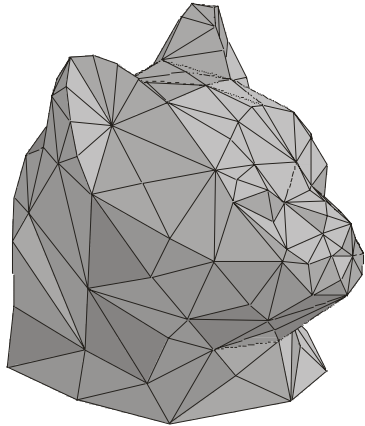
Also leads to the same fixed point iteration/related system

$$\left( I - (I - \tilde{N}\tilde{M})S \right) x = \left( I - (I - N M)S \right) x = \tilde{f}$$

# Surface Parameterization



# Example: Texture Mapping



# Angle-based Flattening

Solve mesh flattening as constrained optimization problem.

Minimize relative deformation of angles,  $\sum_{i,j} (\alpha_{i,j} - \phi_{i,j})^2 / \phi_{i,j}^2$ ,

Subject to constraints on valid 2D mesh

1. Angles between 0 and  $\pi$  (orientation), hardly ever a problem (dealt with algorithmically)
2. Angles in triangle sum to  $\pi$ ,
3. Angles around interior node sum to  $2\pi$ ,
4. Triangles at an interior node need to agree on edge lengths: **nonlinear constraint**.

$$\min \sum_{i,j} (\alpha_{i,j} - \phi_{i,j})^2 / \phi_{i,j}^2 \text{ subject to } \left[ g_2(\alpha) \ g_3(\alpha) \ g_4(\alpha) \right]^T = 0$$

Critical point of Lagrangian  $L(\alpha, \lambda) = F(\alpha) + \lambda^T g(\alpha)$

# Nonlinear System

Critical point of  $L(a, \lambda) = F(a) + \lambda^T g(a)$ :  $\nabla_{a,\lambda} L(a, \lambda) = \mathbf{0}$

Newton iteration:  $\nabla_{a,\lambda}^2 L(a, \lambda) \begin{bmatrix} \Delta a \\ \Delta \lambda \end{bmatrix} = -\nabla_{a,\lambda} L(a, \lambda)$

Jacobian:  $\begin{bmatrix} \nabla_a^2 [F(a) + \lambda^T g(a)] & [\nabla_a g(a)]^T \\ \nabla_a g(a) & \mathbf{0} \end{bmatrix} =$   
 $\begin{bmatrix} A + G_k & B^T & C_k^T \\ B & \mathbf{0} & \mathbf{0} \\ C_k & \mathbf{0} & \mathbf{0} \end{bmatrix}$  (symmetric and indefinite)

$A = \text{diag}(2w_i^j)$  and  $G_k$  depends only on  $\mathbf{g}^{(4)}(a)$

$B$  depends only on  $\mathbf{g}^{(2)}(a)$  and hence is constant (zero, one)

$C_k$  depends on  $\mathbf{g}^{(3)}$  and  $\mathbf{g}^{(4)}$  and is partially constant ( $\mathbf{g}^{(3)}$ )



# Preconditioning

Consider the following choice of blocks

$$\begin{bmatrix} F - E_k & C_k^T \\ C_k & 0 \end{bmatrix} \text{ with } F = \begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \text{ and } E_k = \begin{bmatrix} G_k & 0 \\ 0 & 0 \end{bmatrix}.$$

Explicit inverse of  $F$  known (very good splitting).

$$\begin{bmatrix} I - S_k & N_k \\ M_k & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix} \quad \text{and} \quad (I - (I - N_k M_k) S_k) x = \tilde{f}$$

$$|\lambda_S - \lambda| \leq 1.5 \left( \frac{1 + \omega_{\max}}{1 - \omega_{\max}} \right)^{1/2} \|S\| \quad \text{and} \quad |1 - \lambda_R| \leq (1 - \omega_{\max}^2)^{-1/2} \|S\|$$

# Scaling Constraints

Scale constraints  $g_3(\alpha)$  and  $g_4(\alpha)$  by  $\varepsilon$  and precondition:

Block diagonal preconditioner: 
$$\begin{bmatrix} I - \varepsilon S_k & \varepsilon N_k \\ \varepsilon^{-1} M_k & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \tilde{f} \\ \varepsilon^{-1} g \end{bmatrix}$$

Related system (after splitting):  $(I - \varepsilon(I - N_k M_k) S_k) x = \tilde{f}$

Eigenvalue bounds for the scaled system:

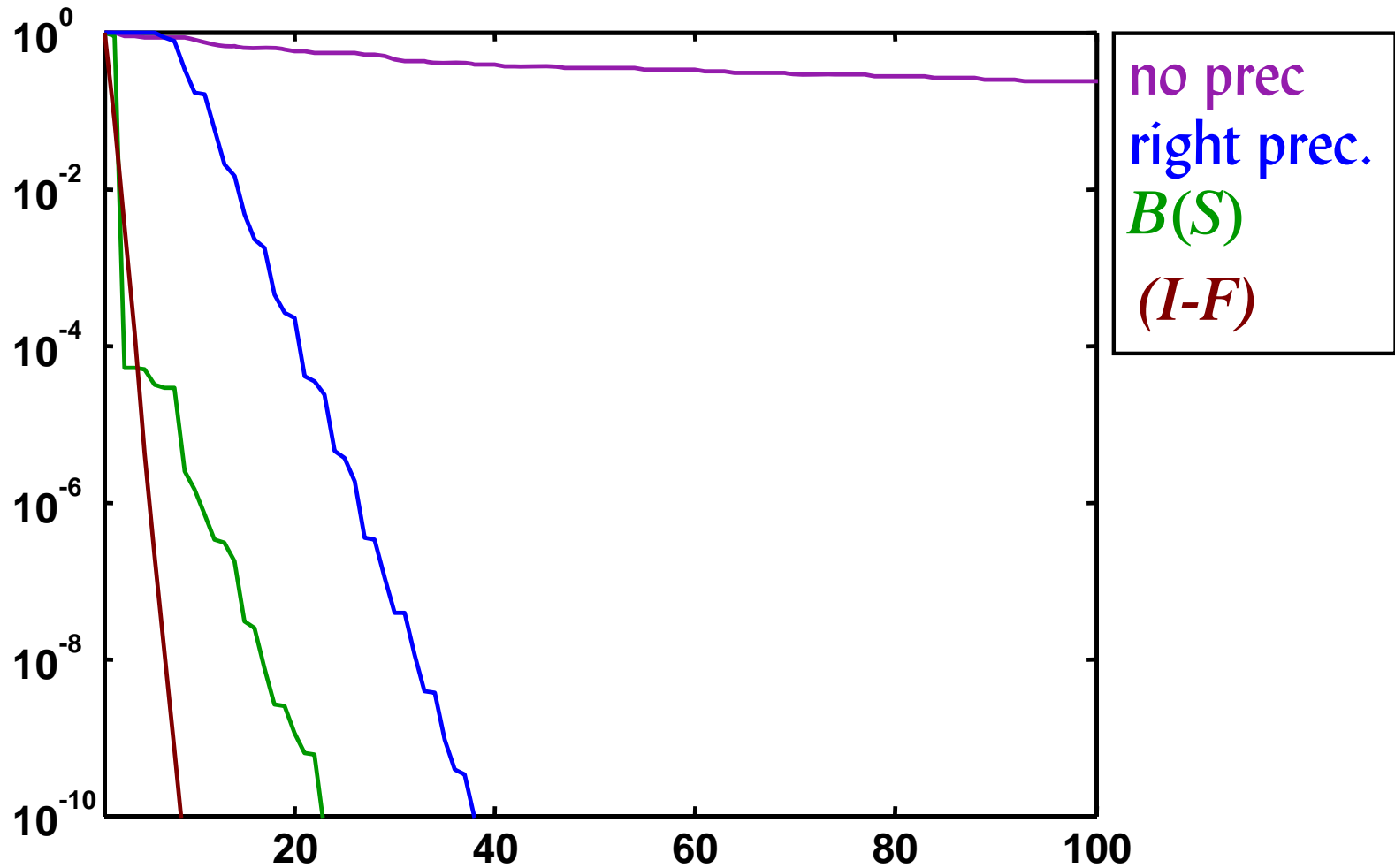
Block diagonal preconditioner: 
$$|\lambda_S - \lambda| \leq 1.5\varepsilon \left( \frac{1 + \omega_{\max}}{1 - \omega_{\max}} \right)^{1/2} \|S\|$$

Related 
$$|1 - \lambda_R| \leq \varepsilon (1 - \omega_{\max}^2)^{-1/2} \|S\|$$

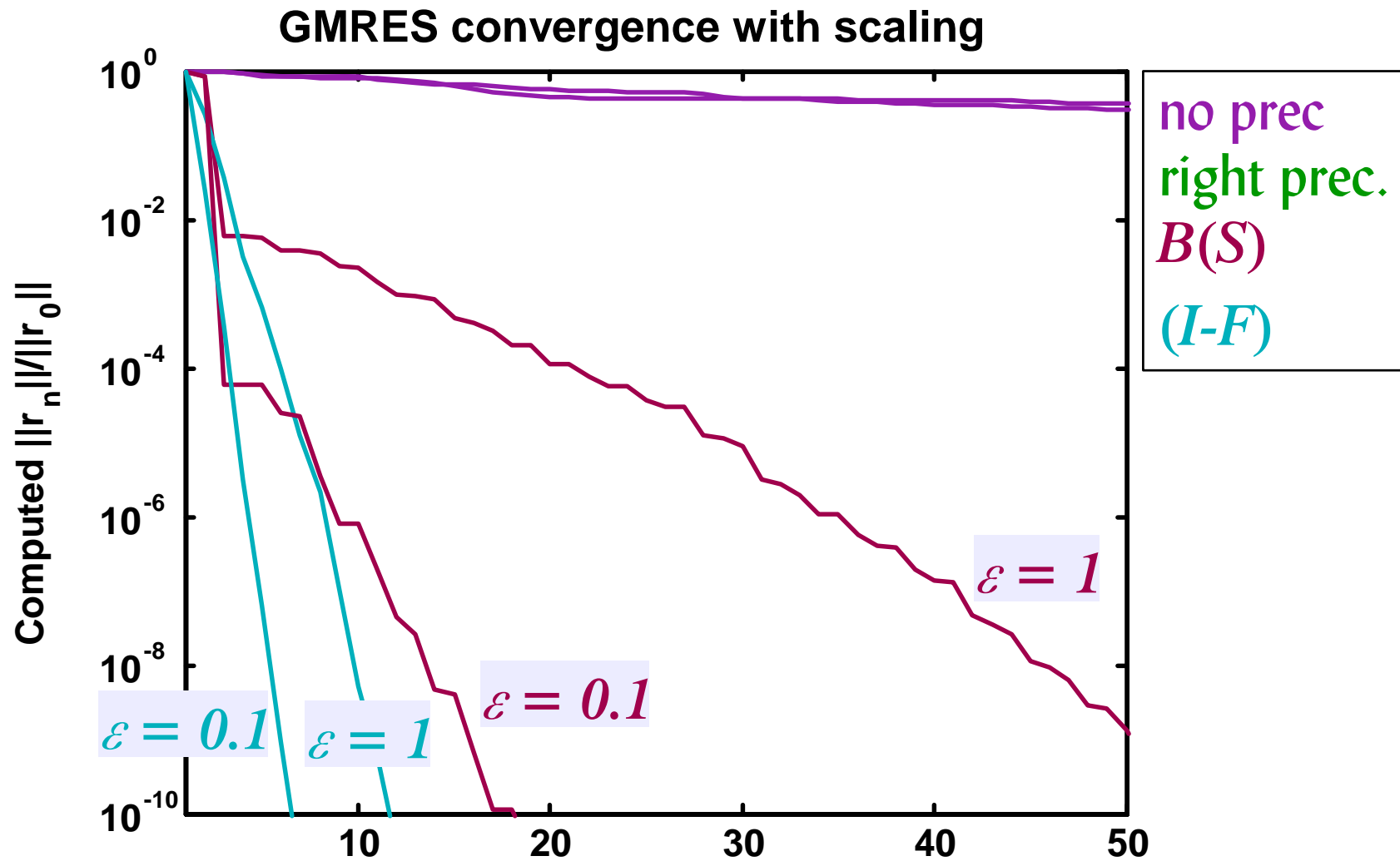
Very fast convergence even for modest  $\varepsilon$ , (but Newton ...)

# Convergence “Three Balls”

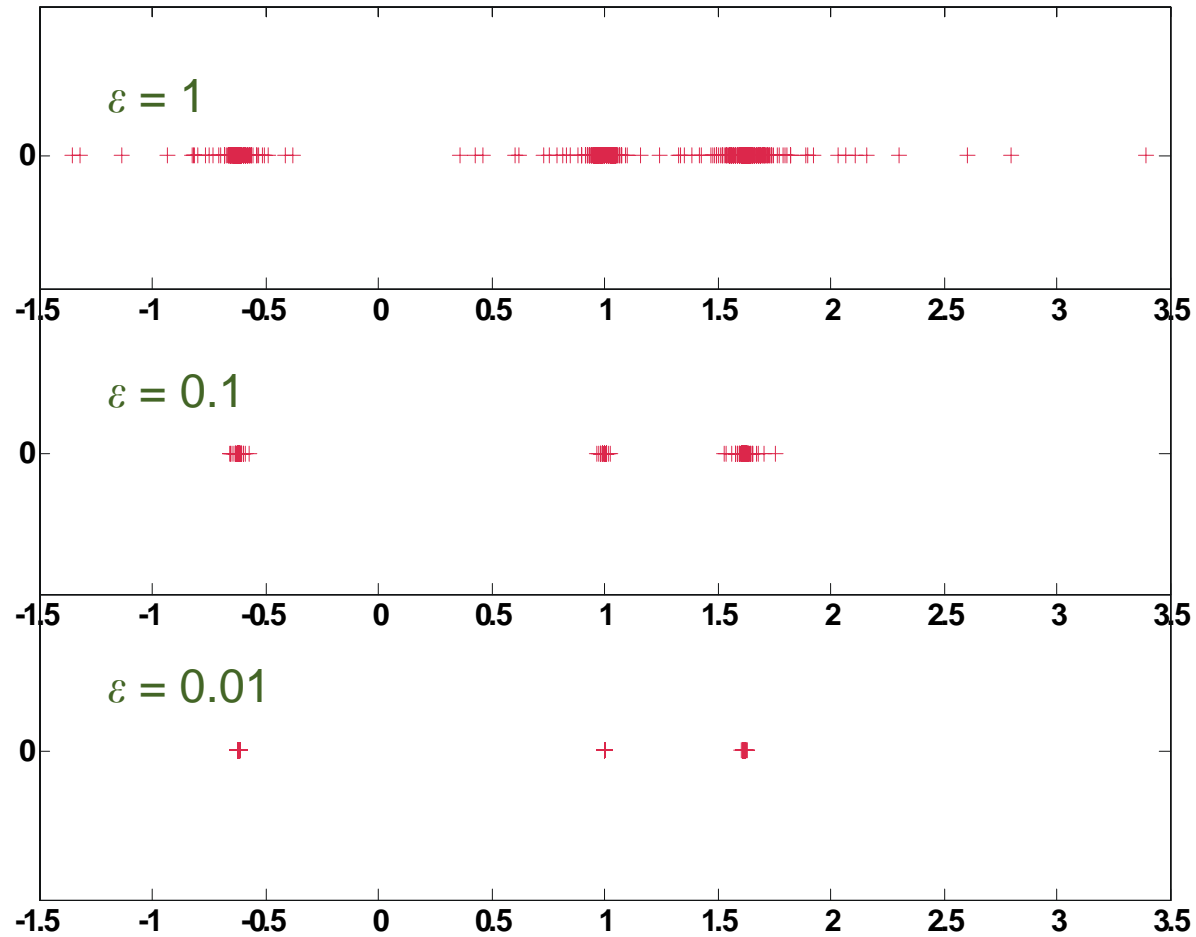
GMRES convergence (no scaling)



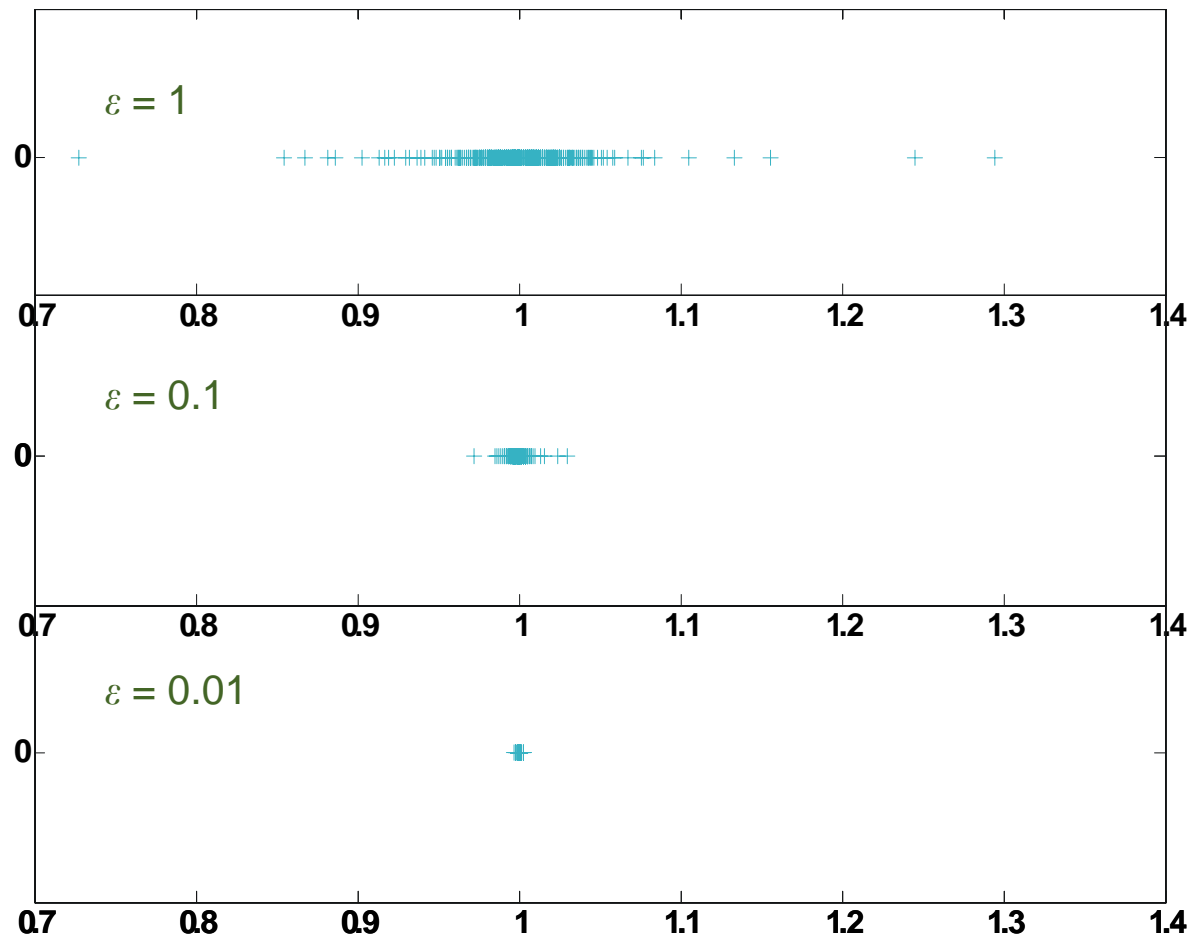
# Convergence “Three Balls”



# Eigenvalues of B(S)



# Eigenvalues of Related System



# Preconditioners – nonzero (2,2)

First, we consider saddle-point problems with nonzero (2,2) block, such as stabilized finite element discretizations.

Block-diagonal preconditioner from splitting (1,1) block

$$\begin{pmatrix} F - E & B^T \\ C & D \end{pmatrix} \rightarrow \begin{pmatrix} F^{-1} & 0 \\ 0 & -(D - CF^{-1}B^T)^{-1} \end{pmatrix}$$

Preconditioned system: 
$$\begin{pmatrix} I - S & N \\ M & Q \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \hat{f} \\ \hat{g} \end{pmatrix},$$

where  $MN = I + Q$  and  $(NM)^2 = NM + NQM$

Further splitting leads to fixed point iteration and a smaller

**related system:**  $(I - (I - NM)S)x = \tilde{f}$

# Preconditioners – nonzero (2,2)

Eigenvalues of  $B(S) = \begin{pmatrix} I - S & N \\ M & Q \end{pmatrix}$ ?

$$B(0) = \begin{pmatrix} I & N \\ M & Q \end{pmatrix}: \quad \lambda \in \left\{ 1, \frac{1}{2}(1 + \delta_j) \pm \sqrt{1 + \frac{1}{4}(1 + \delta_j)^2} \right\}$$

where  $\delta_j$  is an eigenvalue of  $Q$  and typically small.

Let  $\text{null}(NM) \rightarrow U_1$  and other eigenvectors  $NM \rightarrow \tilde{U}_2 = U_2\Theta$   
Eigenvalues of  $B(S)$  from perturbation of  $B(0)$ :

$$|\lambda_S - \lambda| \leq 2\gamma\kappa_\Theta \left( \frac{1 + \omega_{\max}}{1 - \omega_{\max}} \right)^{1/2} \|S\| \quad (\text{typically } \gamma\kappa_\Theta \text{ modest})$$

$$(I - (I - NM)S): \quad |1 - \lambda_R| \leq (1 + \omega_1\bar{\delta} + \omega_1\tilde{\delta}\kappa_\Theta)(1 - \omega_{\max}^2)^{-1/2} \|S\|$$



# Approximating the Schur complement

Replace Schur complement type matrix by approximation:

$\begin{pmatrix} F^{-1} & 0 \\ 0 & S_F^{-1} \end{pmatrix}$  by  $\begin{pmatrix} F^{-1} & 0 \\ 0 & S_{\tilde{F}}^{-1} \end{pmatrix}$ , where  $S_F^{-1}$  is approximated directly

Preconditioned system  $\begin{pmatrix} I - S & N \\ M_2 & 0 \end{pmatrix}$  or  $\begin{pmatrix} I - S & N \\ M_2 & Q_2 \end{pmatrix}$

where  $N = F^{-1}B^T$ ,  $M_2 = S_{\tilde{F}}^{-1}C$ ,  $M_2N = S_{\tilde{F}}^{-1}S_F \equiv I + \mathcal{E}$ , and  $(NM_2)^2 = N(I + \mathcal{E})M_2 = NM_2 + N\mathcal{E}M_2$

Bounds:  $\begin{pmatrix} I - S & N \\ M_2 & Q_2 \end{pmatrix} = \begin{pmatrix} I & N \\ M & Q \end{pmatrix} - \begin{pmatrix} S & 0 \\ \mathcal{E}M & \mathcal{E}Q \end{pmatrix}$

# Approximating the Schur complement

$$B(S, \mathcal{E}) = \begin{pmatrix} I - S & N \\ M_2 & Q_2 \end{pmatrix} = \begin{pmatrix} I & N \\ M & Q \end{pmatrix} - \begin{pmatrix} S & 0 \\ -\mathcal{E}M & -\mathcal{E}Q \end{pmatrix}$$

Eigenvalues of  $B(S, \mathcal{E})$  from perturbation of  $B(0, 0)$ :

$$|\lambda_{S, \mathcal{E}} - \lambda| \leq \gamma \kappa_{\Theta} \left( \frac{1 + \omega_{\max}}{1 - \omega_{\max}} \right)^{1/2} \|S\| + \hat{\gamma} \kappa_V \|\mathcal{E}\|$$

(typically  $\gamma \kappa_{\Theta}$  and  $\hat{\gamma} \kappa_V$  modest)

When  $D = 0$  (and hence  $Q, Q_2 = 0$ )

$$|\lambda_{S, \mathcal{E}} - \lambda| \leq 2 \left( \frac{1 + \omega_{\max}}{1 - \omega_{\max}} \right)^{1/2} \|S\| + \frac{2}{\sqrt{5}} \|\mathcal{E}\|$$

# Approximating the Schur complement

Splitting as before leads to exactly the same related system.

$$\text{New splitting: } \begin{pmatrix} I - S & N \\ M_2 & Q_2 \end{pmatrix} = \begin{pmatrix} I & N \\ M_2 & M_2 N - I \end{pmatrix} - \begin{pmatrix} S & 0 \\ 0 & \mathcal{E} \end{pmatrix}$$

$$\text{Linear system: } \begin{pmatrix} I - (I - NM_2)S & -N\mathcal{E} \\ -M_2S & I + \mathcal{E} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \tilde{f} \\ \tilde{g} \end{pmatrix}$$

Eigenvalues cluster around 1.

$$|1 - \lambda_R| \leq \sqrt{1 + \|N\|^2} \sqrt{1 + \|M_2\|^2} \max(\|S\|, \|\mathcal{E}\|)$$

We lose advantages of smaller system and satisfying the constraints.

# Probing for the Schur Complement

Approximate  $-(D - CF^{-1}B^T)^{-1}$  without having  $(D - CF^{-1}B^T)$

Probing (Chan&Mathew'92): reconstruct matrix with small bandwidth from products with selected vectors and invert. Based on rapid decay from diagonal in matrix (1D interface).

We use decay of  $F^{-1}$  on mesh with structure of  $C, B^T, D$  to select pattern of large coefficients in matrix to probe for  
Construct set of vectors to minimize lumping other coeff.s

Cheap to use multiple orderings and combine inverses of matrices with small bandwidth (convergence not great)

Better to approximate matrix structure for multidimensional problem directly and use incomplete decomposition

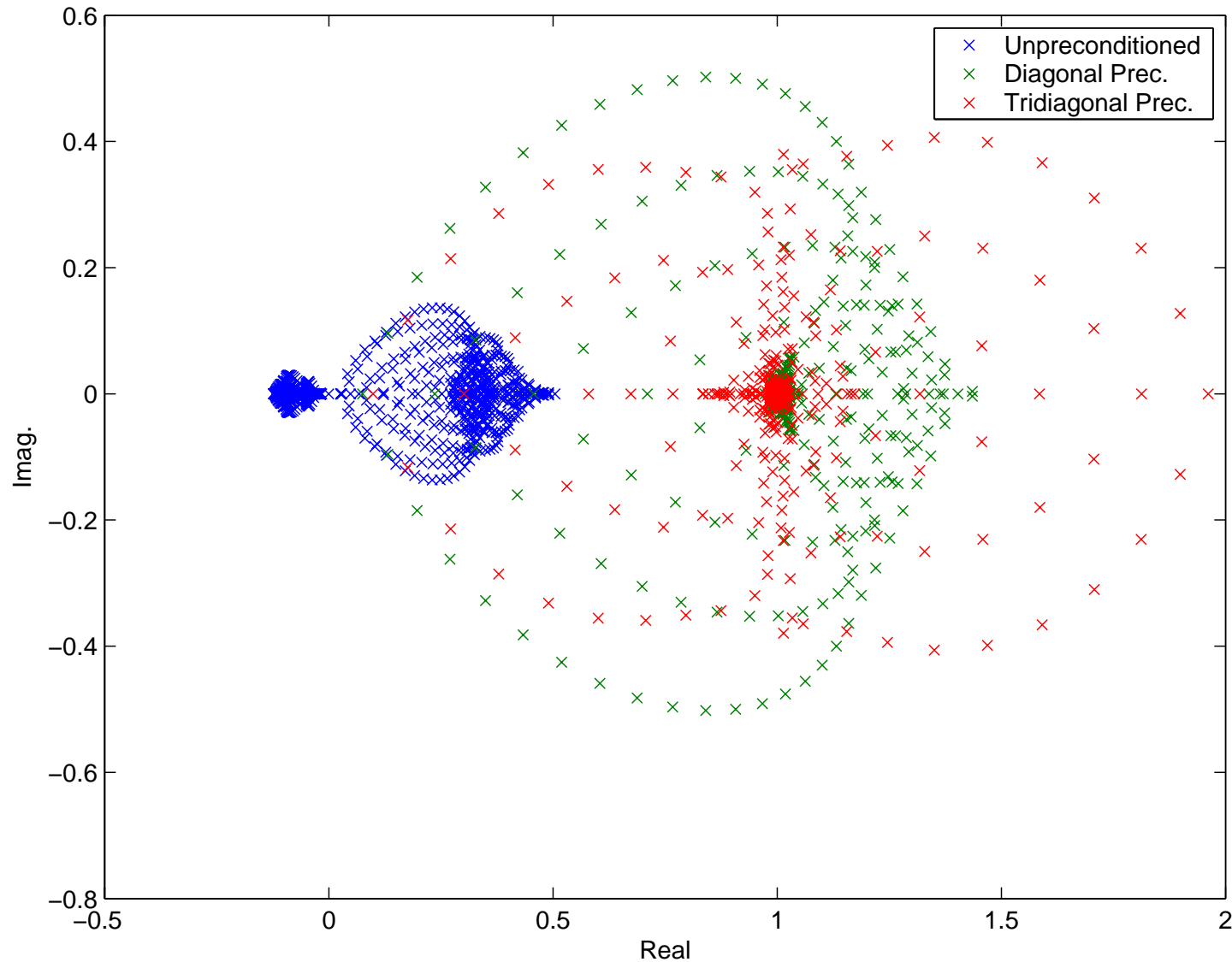
# Oseen problem, driven cavity

- Software by Elman, Silvester, Wathen, Ramage
- System (A nonsymmetric):

$$\begin{bmatrix} A & B^T \\ B & -\beta C \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

- viscosity  $\nu=1/10$  and stabilization  $\beta=1/4$

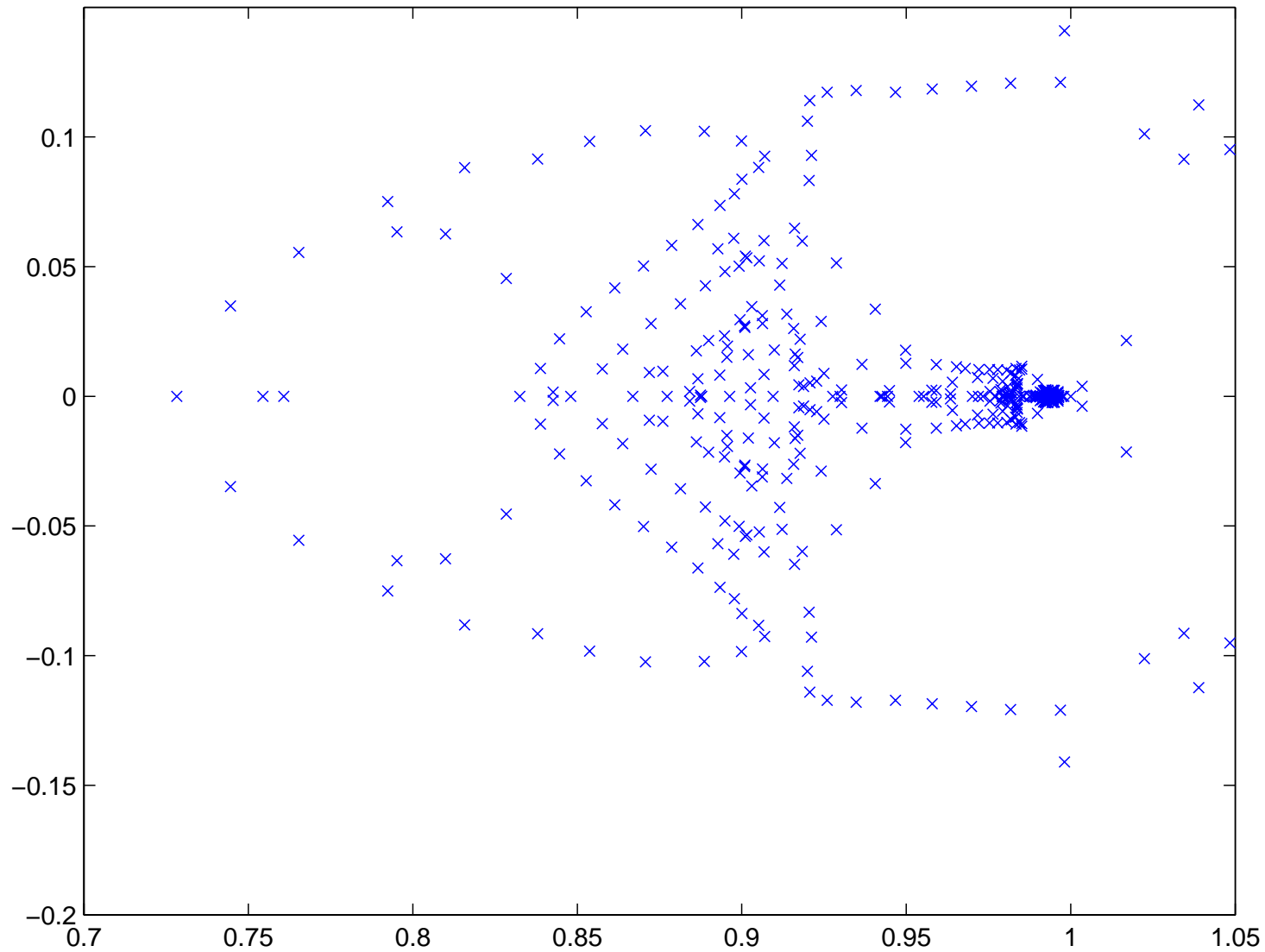
# Basic Splittings of (1,1) Block



# Oseen problem

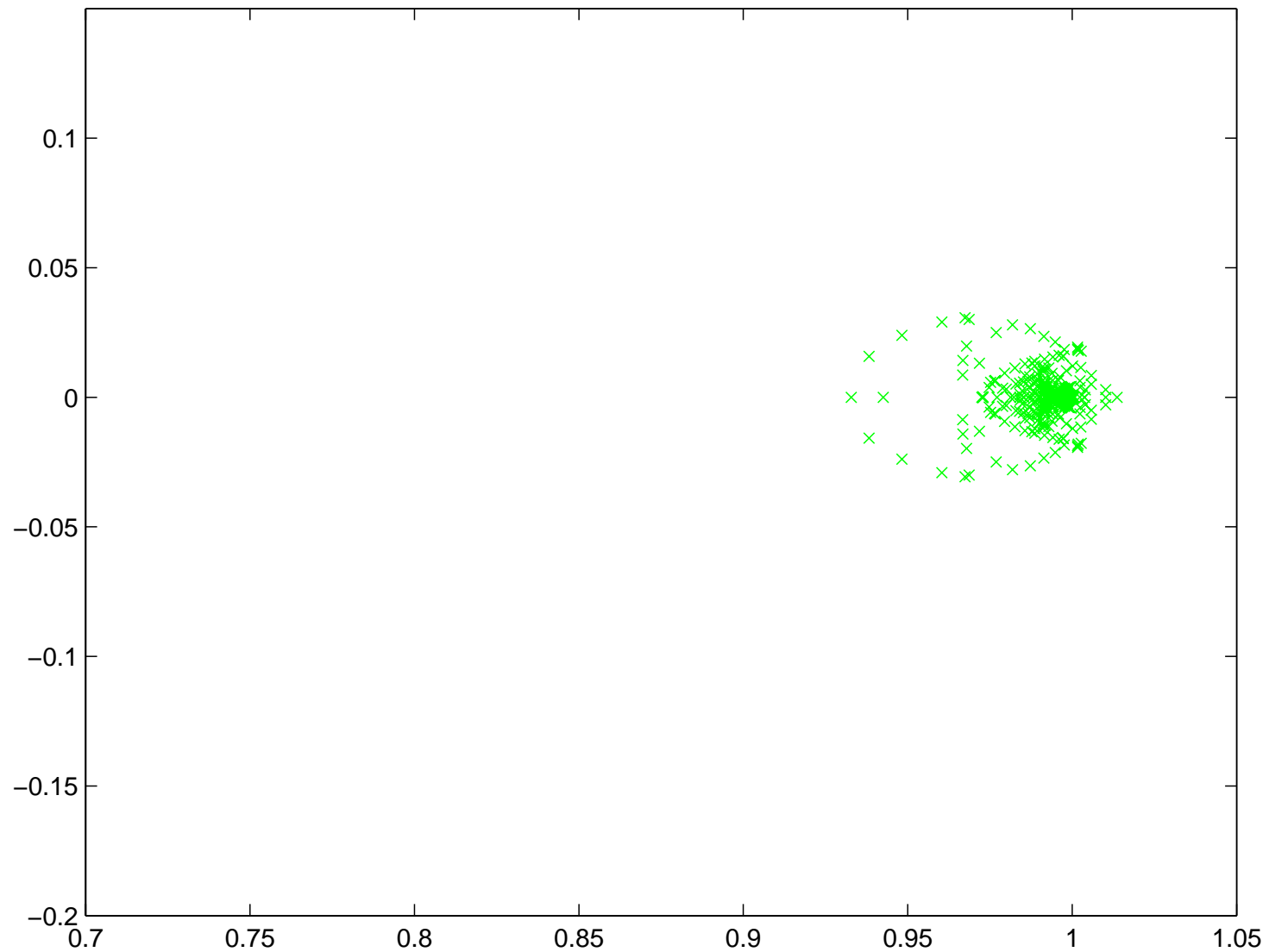
- Not constrained to ‘structured’ splittings  $A=F-E$
- Multigrid cycle is a (complicated) splitting
- Use number of V-cycles for  $F^{-1}$ .
- Useful because we can study convergence and eigenvalue (bounds) for sequence of problems with decreasing  $\|S\|$ .
- Likewise, we can analyze the effect of approximations to the Schur complement (not as easy)

# 1 V-cycle, Related System: Eigenvalues

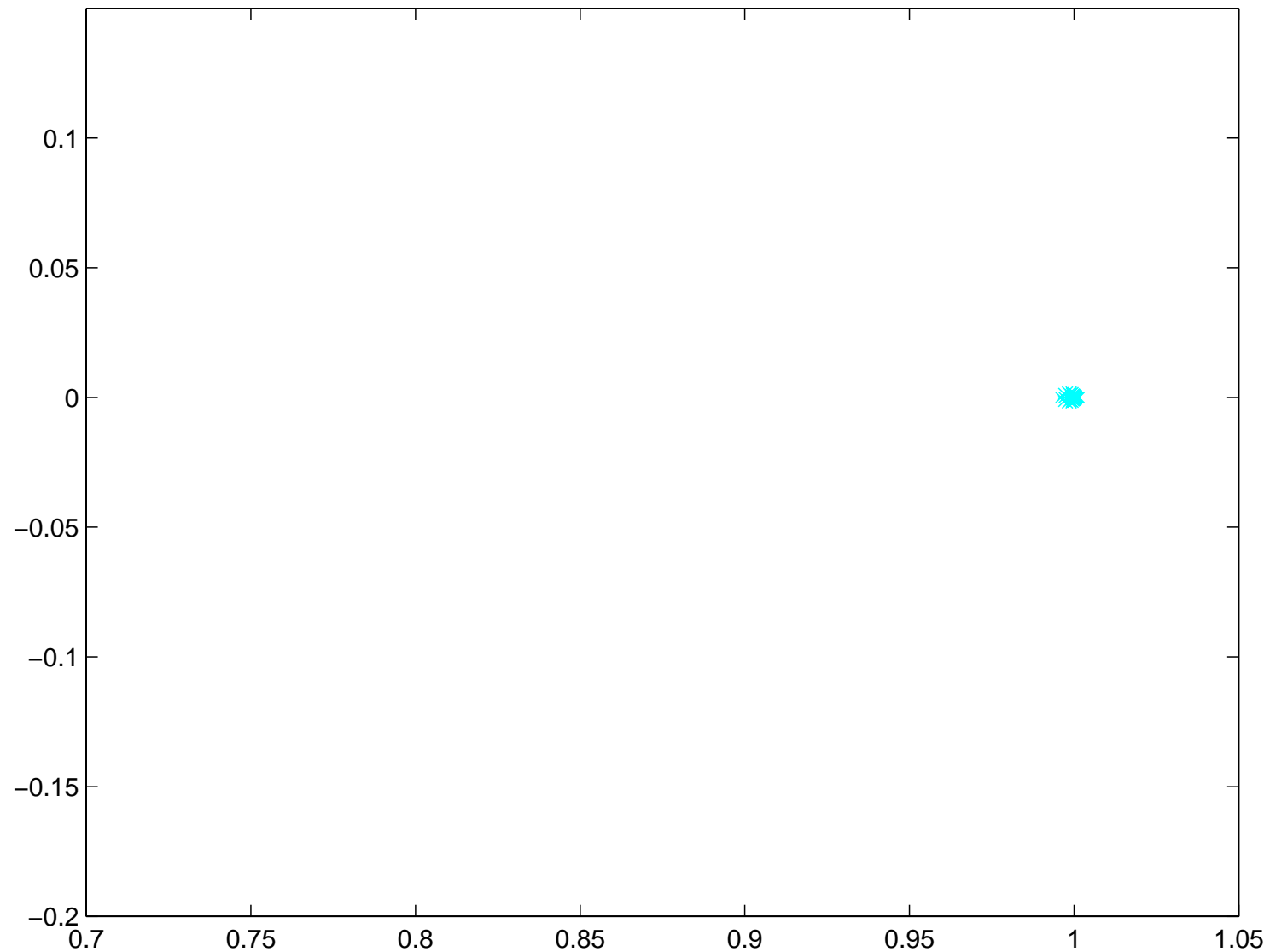




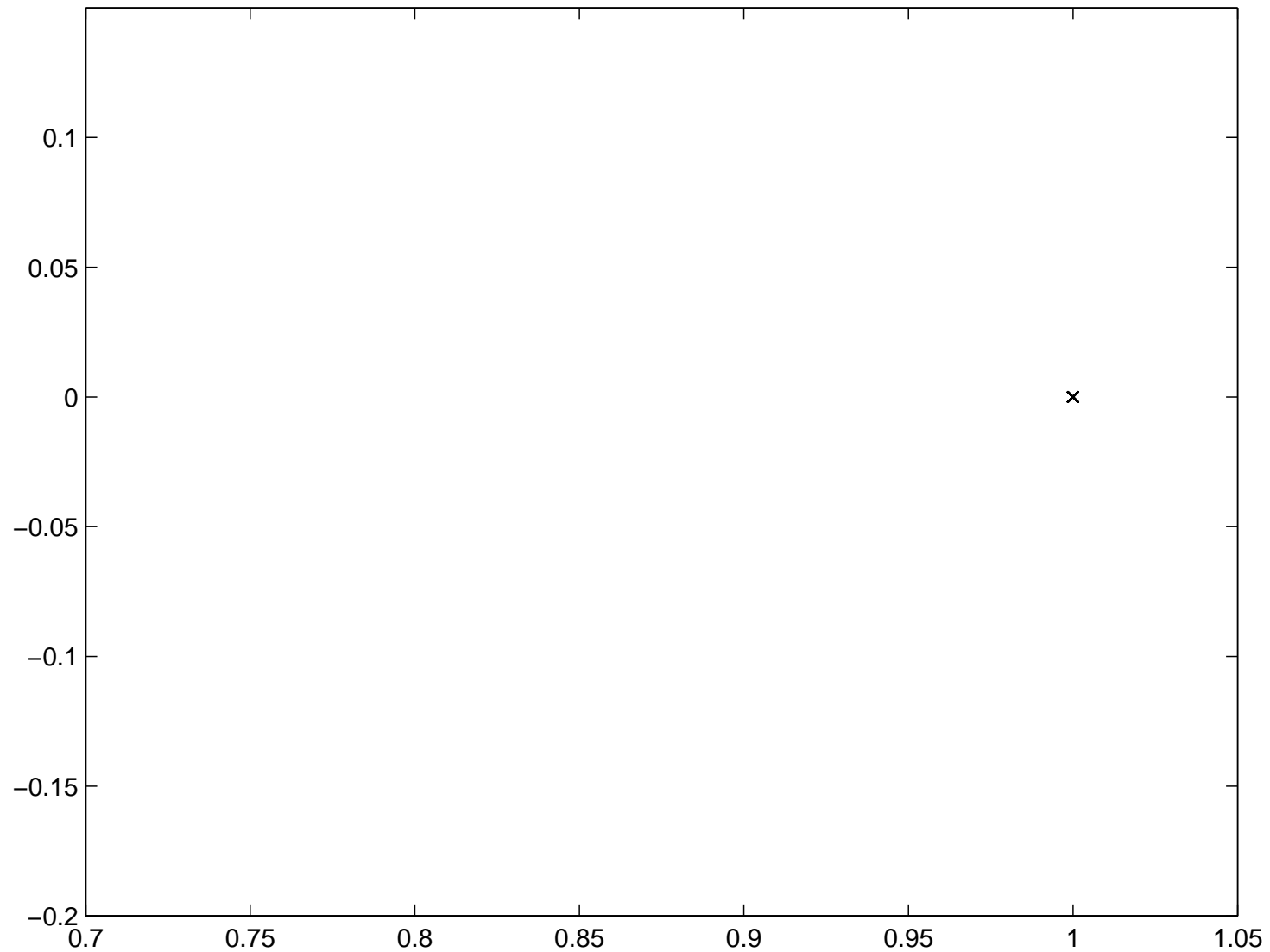
# 2 V-cycles, Related System: Eigenvalues



# 4 V-cycles, Related System: Eigenvalues

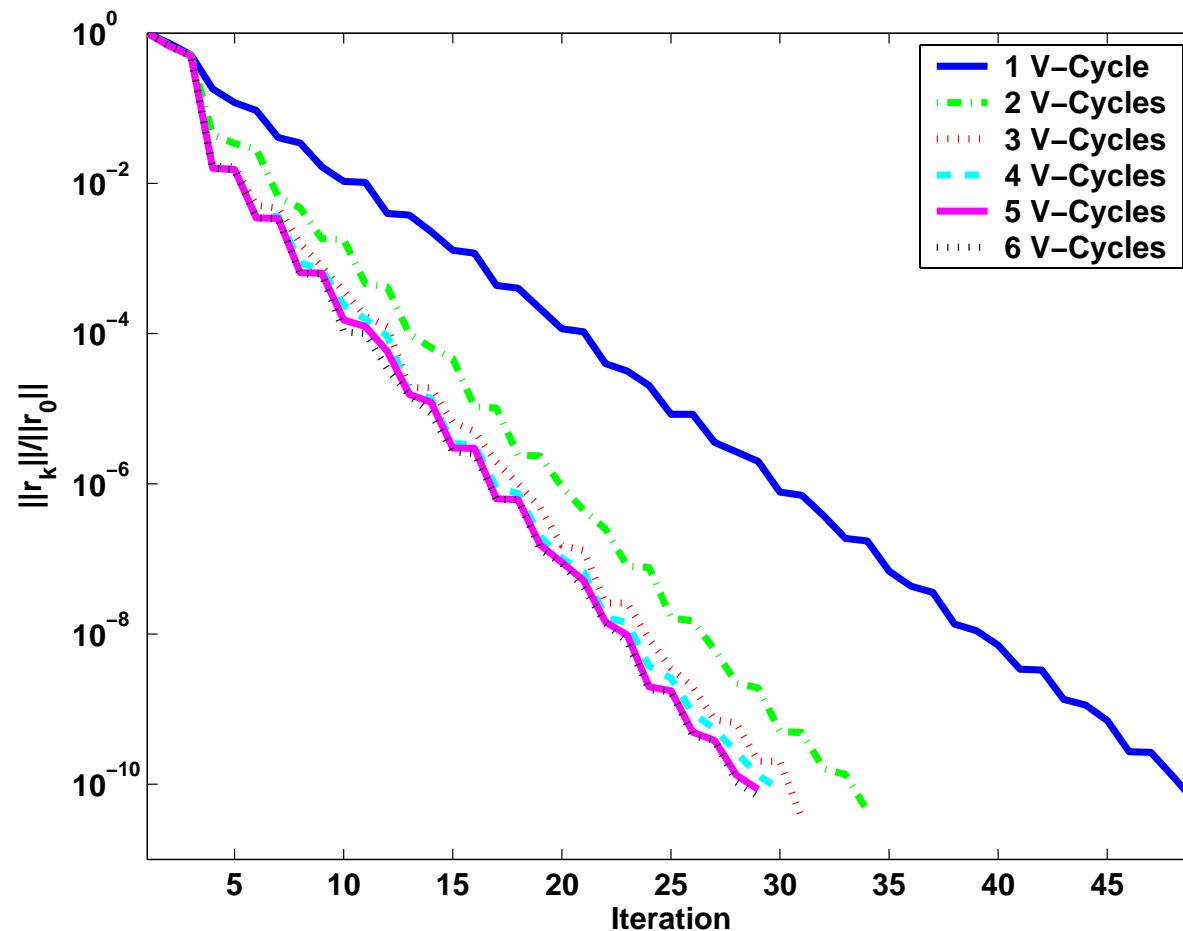


# 6 V-cycles, Related System: Eigenvalues



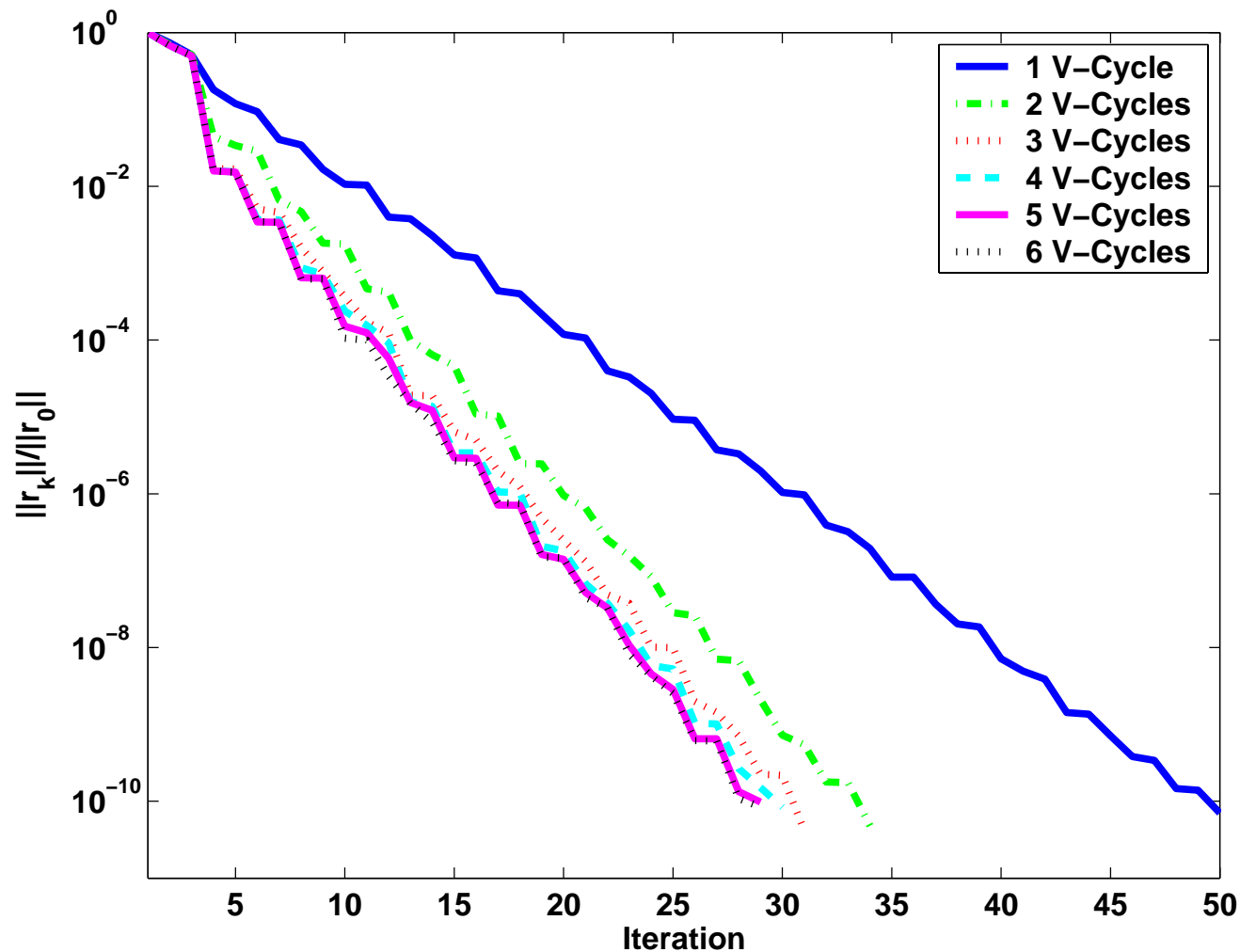
# Exact Schur Complement

Convergence for block-diagonal preconditioner for various numbers of V-cycles for the splitting



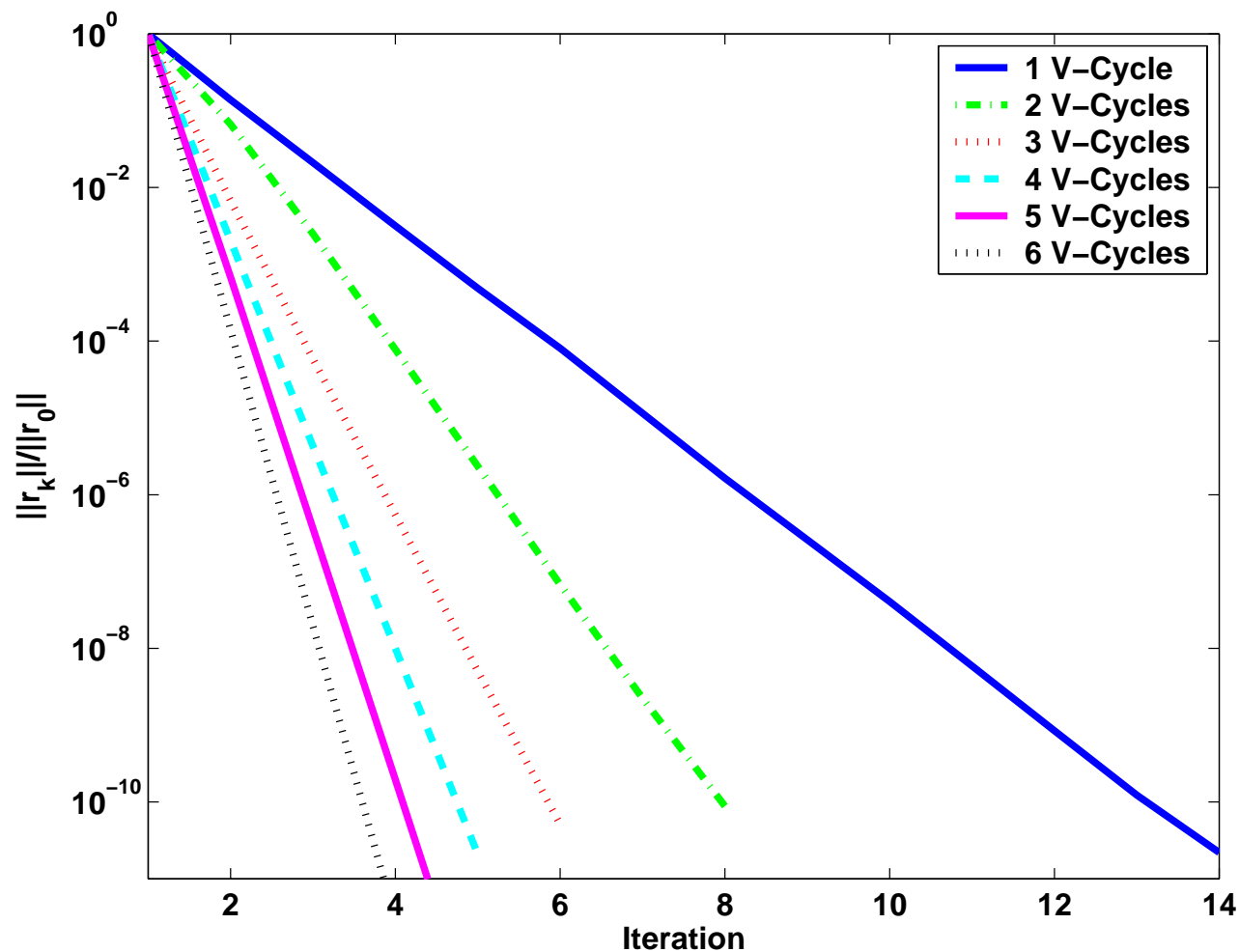
# Inexact Schur Complement - ILU(1.e-4)

Convergence for block-diagonal preconditioner for various numbers of V-cycles for the splitting



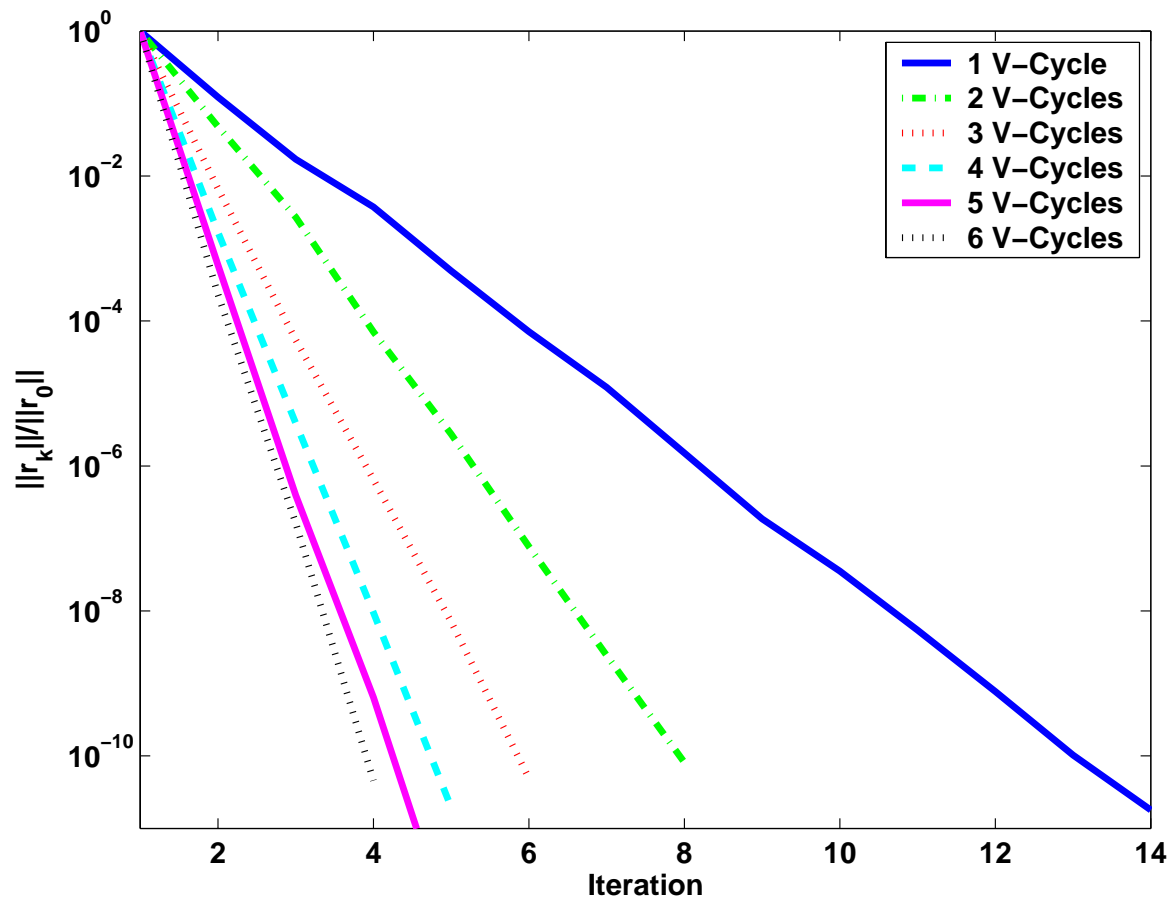
# Exact Schur Complement

Convergence for related system using various numbers of V-cycles for the splitting



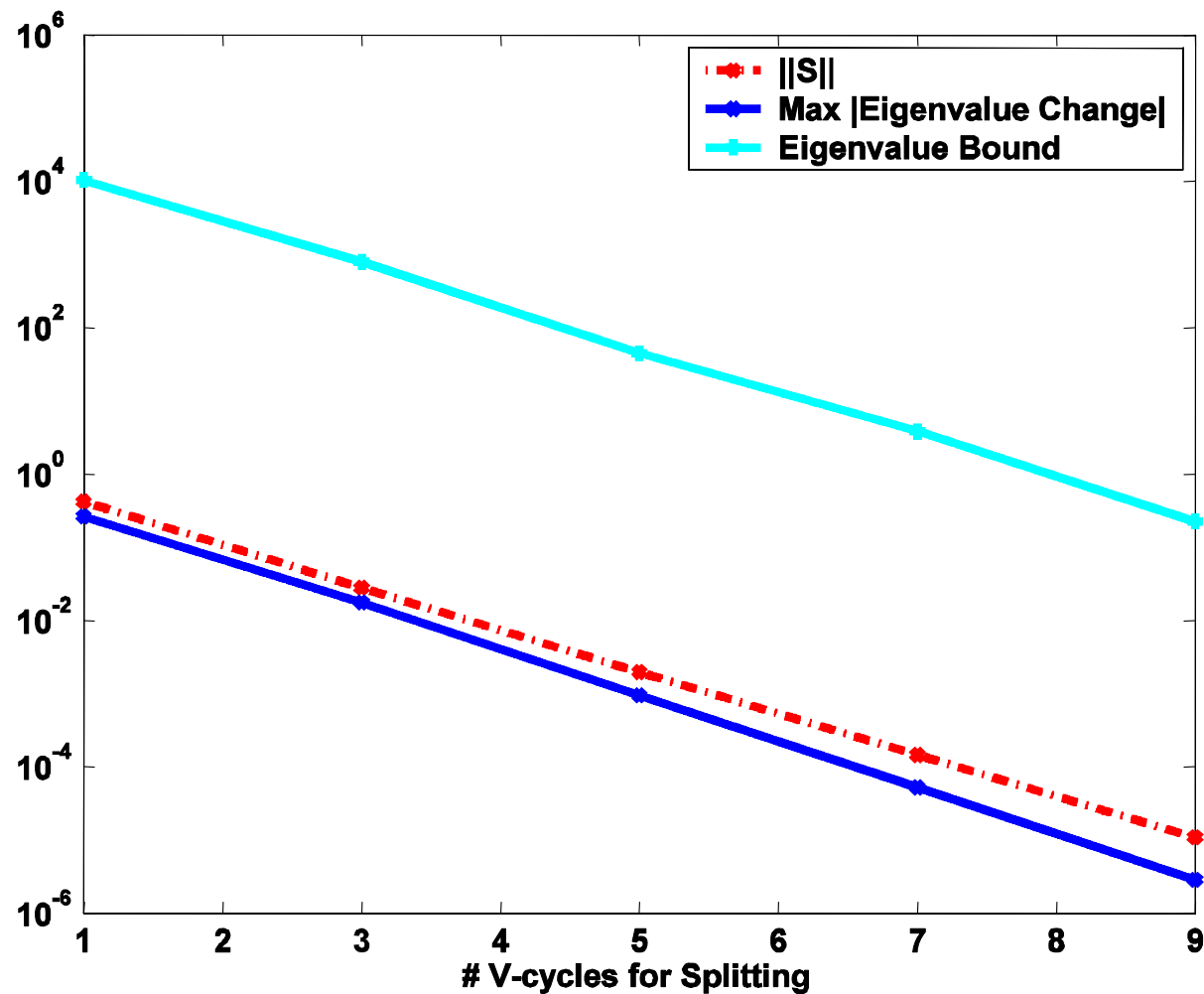
# Inexact Schur Complement - ILU(1.e-4)

Convergence for related system using various numbers of V-cycles for the splitting



# Exact Schur Complement

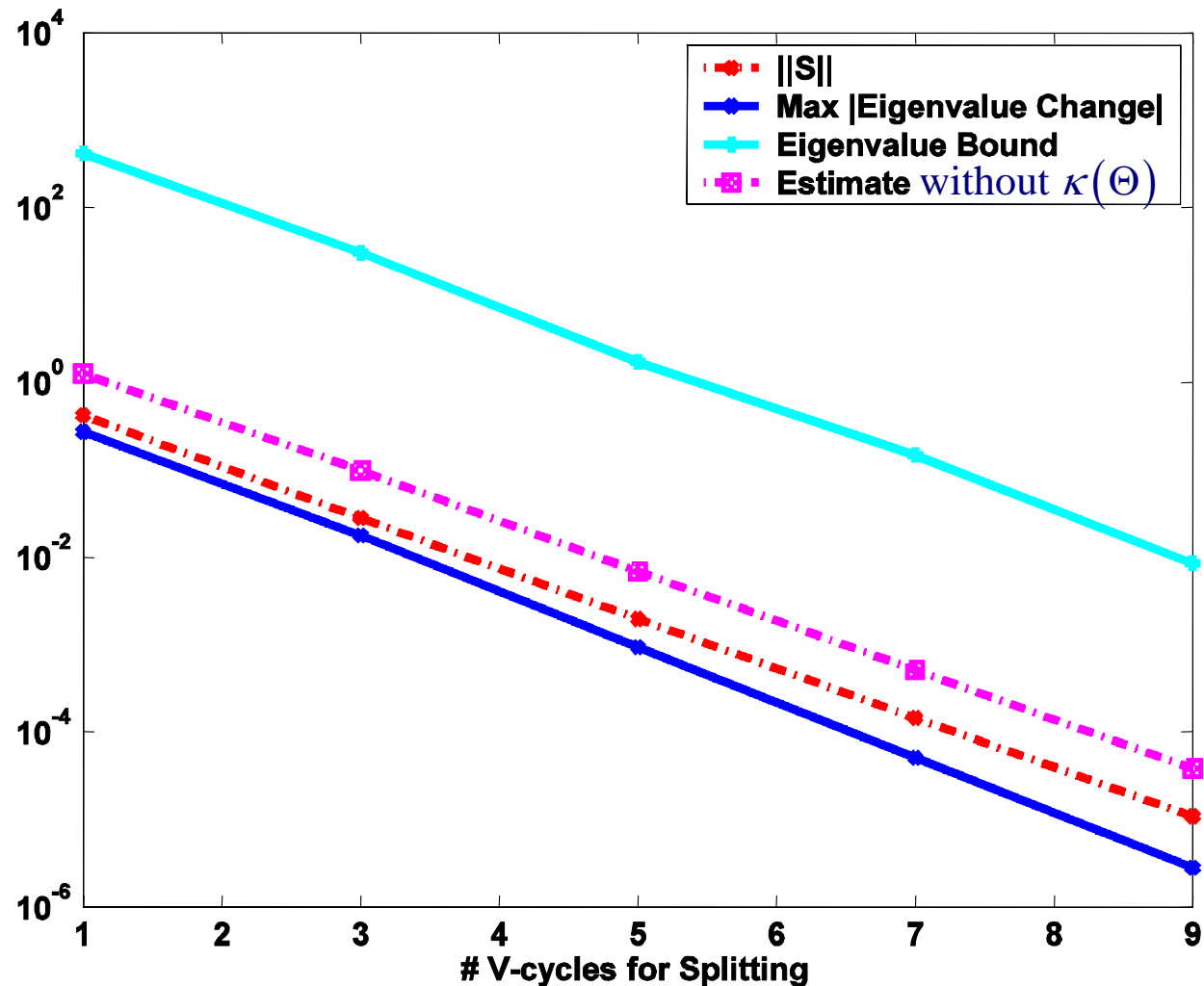
Eigenvalue perturbations and bounds for block-diagonal preconditioner using various numbers of V-Cycles for splitting





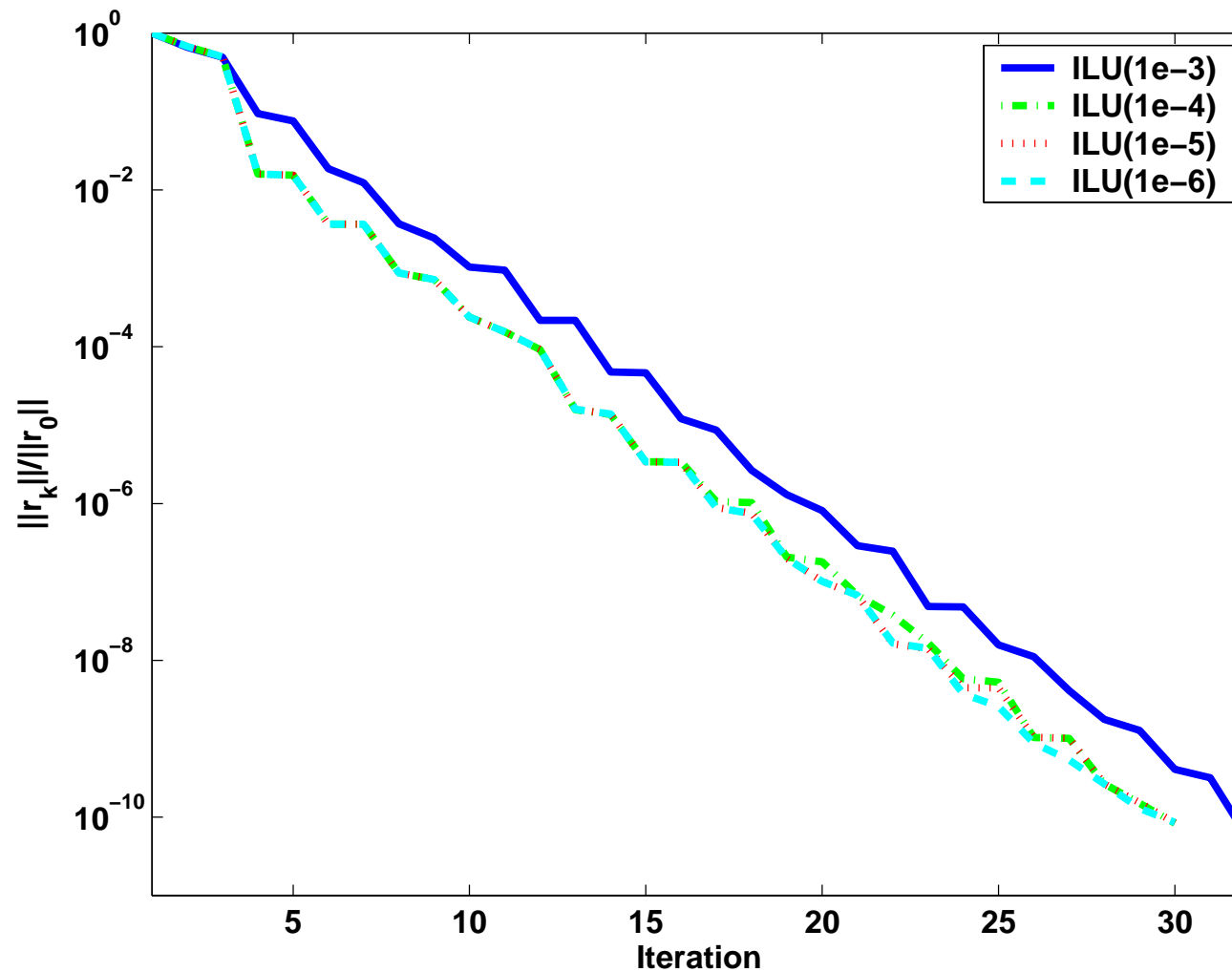
# Exact Schur Complement

Eigenvalue perturbations and bounds for related system using various numbers of V-Cycles for splitting



# Inexact Schur Complement – ILU

Convergence for block-diagonal preconditioner using various accuracies for Schur Complement ILU



# Inexact Schur Complement - ILU

Convergence for related system using various accuracies for Schur Complement ILU

