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The Fast Solution of Sequences of Linear Systems via Subspace Recycling

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Overview

- **Introduction and Examples**
  - **Introduction: Sequential linear systems**
  - **Motivating example problems**
  - **Krylov subspace methods crash course (Why recycle?)**
  - **Meet the family of recycling methods (How to select a recycle space?)**
- **Convergence analysis: Deflated restarting**
  - **Effect of recycling *approximate* invariant subspaces?**
  - **Do we achieve deflation?**
  - **Symmetric case**
  - **Nonsymmetric case**
  - **Numerical examples**
  - **Results**
- **Software**
- **Light Reading**
- **Conclusions**

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Collaborators (Incomplete List)

- Eric de Sturler (Virginia Tech/Mathematics)
- Shun Wang (Illinois/Computer Science)
- Phani Nukala (ORNL)
- Philippe Geubelle (Illinois/Aerospace Engineering)
- Glaucio Paulino and Bob Dodds (Illinois/Civil & Env. Eng.)
- Misha Kilmer (Tufts University/Mathematics)
- Numerous Sandia collaborators…

Introduction and Examples

Solvers for SEQUENCES of Linear Systems

- Consider sequence of linear systems

$$A^{(i)}x^{(i)} = b^{(i)} \qquad i=1,2,3,\ldots$$

- Matrix is (non) symmetric, possibly ill-conditioned
- Applications:
  - Newton/Broyden method for nonlinear equations
  - Materials science and computational physics
  - Transient circuit simulation
  - Fatigue and fracture
  - Crack propagation
  - Optical tomography
  - Topology optimization
  - Large-scale fracture in disordered materials
  - Electronic structure calculations
  - Stochastic finite element methods NEW

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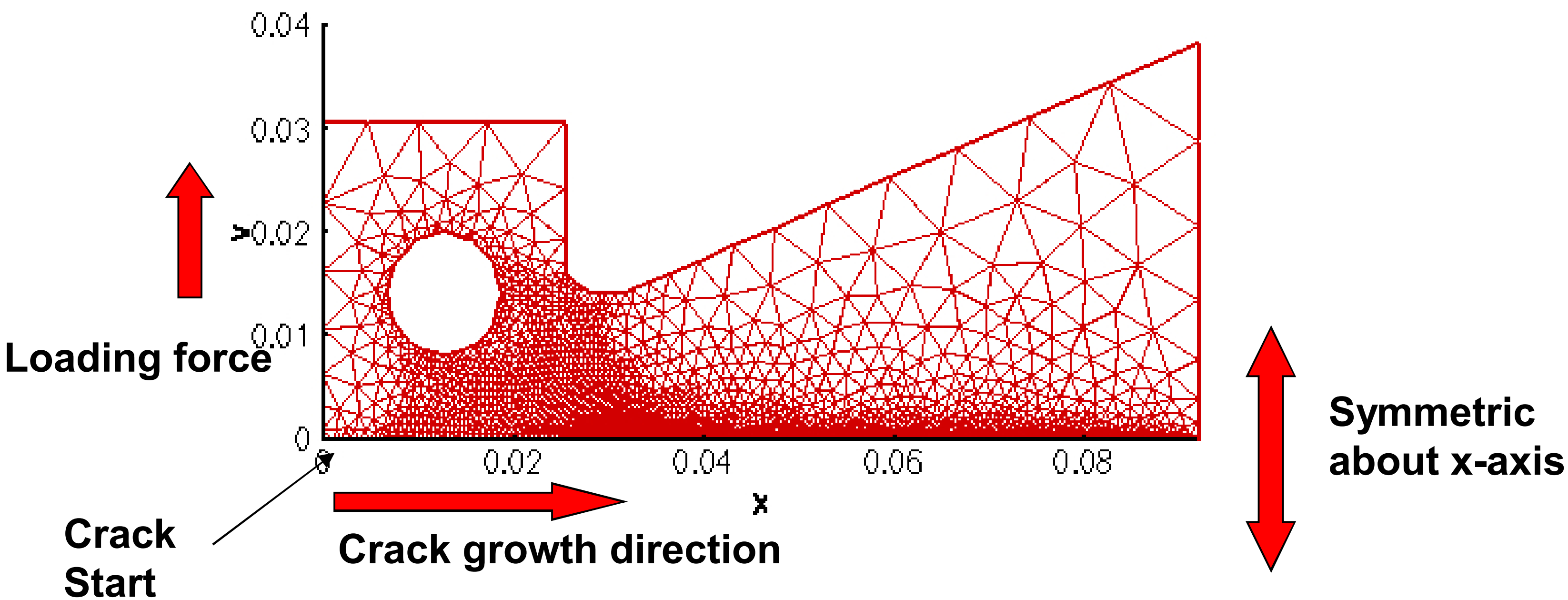
Example #1: Crack Propagation*

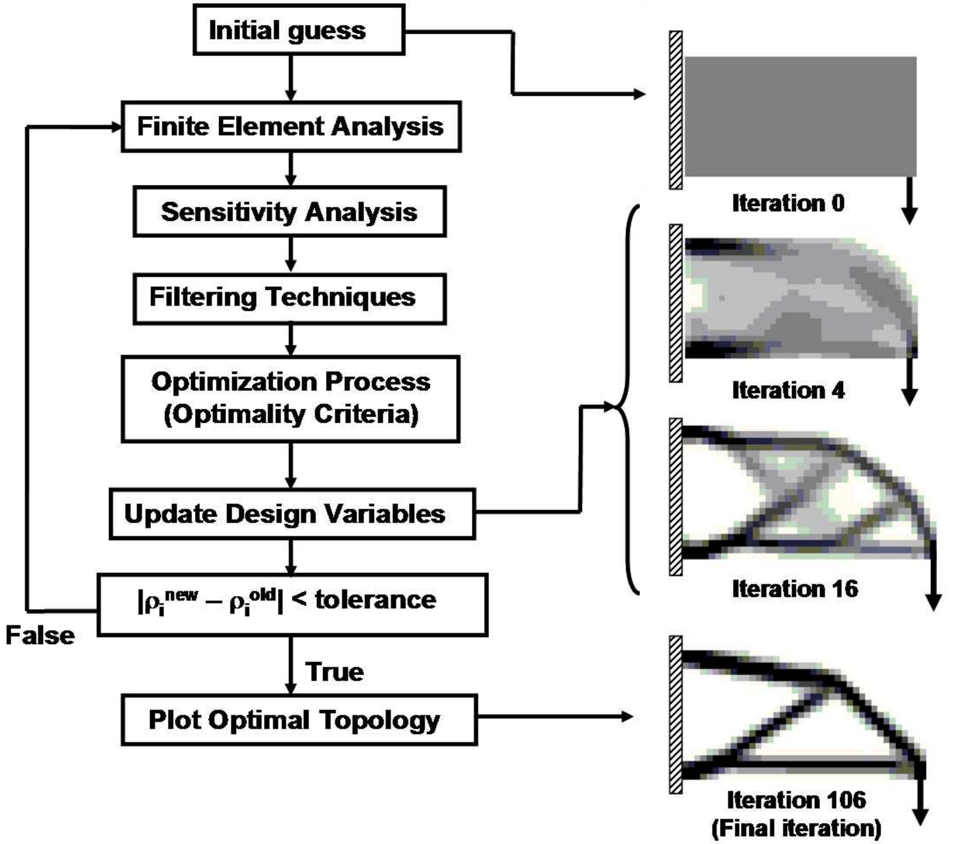
- Finite element crack propagation model
  - P. Geubelle (AE/UIUC), S. Maiti, (ME/Michigan Tech.)
- Thousands of loading steps (thousands of linear systems)



*MLP, E. de Sturler, G. Mackey, D.D. Johonson, and S. Maiti, *Recycling Krylov Subspaces for Sequences of Linear Systems*, SIAM Journal on Scientific Computing, Vol. 28, Issue 5, pp. 1651—1674, 2006.

Example #2: Topology Optimization*

- **Optimize material distribution, ρ, in design domain**
- **Minimize compliance $u^T K(\rho) u$, where $K(\rho)u=f$**



*S. Wang, E. de Sturler, and G. H. Paulino, *Large-scale topology optimization using preconditioned Krylov subspace methods with recycling*, International Journal for Numerical Methods in Engineering, Vol. 69, Issue 12, pp. 2441—2468, 2007.

Example #3: Stochastic PDEs*

- **Stochastic elliptic equation**

$$
\begin{aligned}
-\nabla \cdot \left(\mathbf{a}(\mathbf{x},\omega)\right)\nabla \mathbf{u}(\mathbf{x},\omega) &= \mathbf{f}(\mathbf{x}) \qquad && \mathbf{x} \in \mathbf{D}, \omega \in \Omega \\
\mathbf{u}(\mathbf{x},\omega) &= \mathbf{0} && \mathbf{x} \in \partial\mathbf{D}, \omega \in \Omega
\end{aligned}
$$

- **KL expansion + double orthogonal basis + discretization**
  - **Separate deterministic and stochastic components**
  - **Yield sequence of uncoupled equations**

$$
\mathbf{A}^{(i)}\mathbf{x}^{(i)} = \mathbf{b}^{(i)} \qquad \mathbf{i=1,2,3,}\ldots
$$

- **Preprocess for recycling Krylov solver**
  - **Use reordering scheme to minimize change in spectra of linear system**

*C. Jin, X-C. Cai, and C. Li, *Parallel Domain Decomposition Methods for Stochastic Elliptic Equations,* SIAM Journal on Scientific Computing, Vol. 29, Issue 5, pp. 2069—2114, 2007.

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Solvers for SEQUENCES of Linear Systems

- **Must solve thousands of linear systems!**
- **How to speed up solution of sequence of systems?**

- **Iterative (Krylov) methods build search space and select optimal solution from that space**
- **Building search space is dominant cost**

- **For sequences of systems, get fast convergence rate and good initial guess immediately by <u>recycling</u> selected search spaces from previous systems**

Krylov Subspace Methods Crash Course

- Consider: Ax=b (A is general nonsingular matrix)

- Given x_0, $r_0 = b - Ax_0$, compute optimal update

$$z \in K^m(A, r_0) = \text{span}\left\{ r_0, Ar_0, A^2 r_0, \ldots, A^{m-1} r_0 \right\}$$

by solving

$$\min_{z \in K^m(A, r_0)} \left\| r_0 - Az \right\|_2$$

Krylov Subspace Methods Crash Course

- Solve with least-squares
- Let $K_m = \left[r_0, Ar_0, A^2 r_0, \ldots, A^{m-1} r_0 \right]$. Then, $z = K_m y$ for some y.
- We must solve

$$AK_m y \approx r_0 \quad \Leftrightarrow \quad \left[Ar_0, A^2 r_0, \ldots, A^m r_0 \right] y \approx r_0$$

- Do so accurately and efficiently using Arnoldi

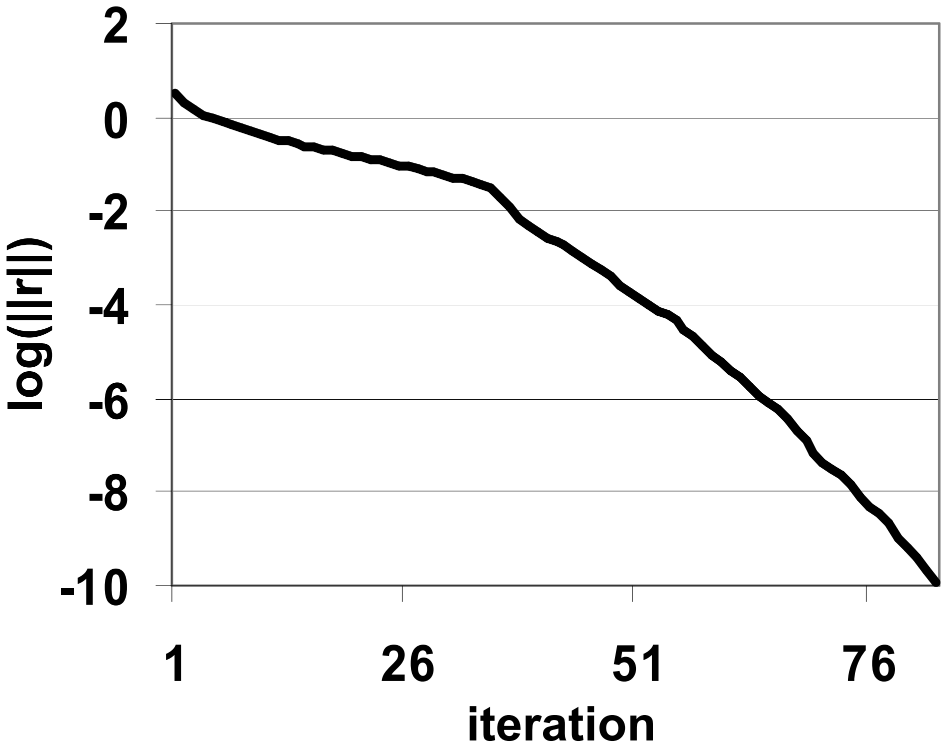
$$AV_m = V_{m+1} \bar{H}_m \qquad v_1 = r_0 / \|r_0\|$$

$$V_{m+1}^T V_{m+1} = I_{m+1} \qquad \text{range}(V_{m+1}) = \text{range}(K_{m+1})$$

$$\|r_0 - Az\| = \|r_0 - AV_m y\| = \|r_0 - V_{m+1} \bar{H}_m y\| = \left\| \|r_0\| e_1 - \bar{H}_m y \right\|$$

Why Recycle?

- Typically, a dominant subspace exists such that almost any Krylov space (from any starting vector) has large components in that space (why restarting is bad)



Why Recycle?

- **Typically, a dominant subspace exists such that almost any Krylov space (from any starting vector) has large components in that space (why restarting is bad)**
- **Optimality derives from orthogonal projection**
  - **new search directions should be far from this dominant subspace for fast convergence**
- **If such a dominant subspace persists (approximately) from one system to the next, it can be recycled**
  - **Typically true when changes to problem are small and/or highly localized**
- **Family of "recycling" solvers: GCRO-DR, RMINRES GCROT/Recycle (differ in how they define the dominant subspace)**

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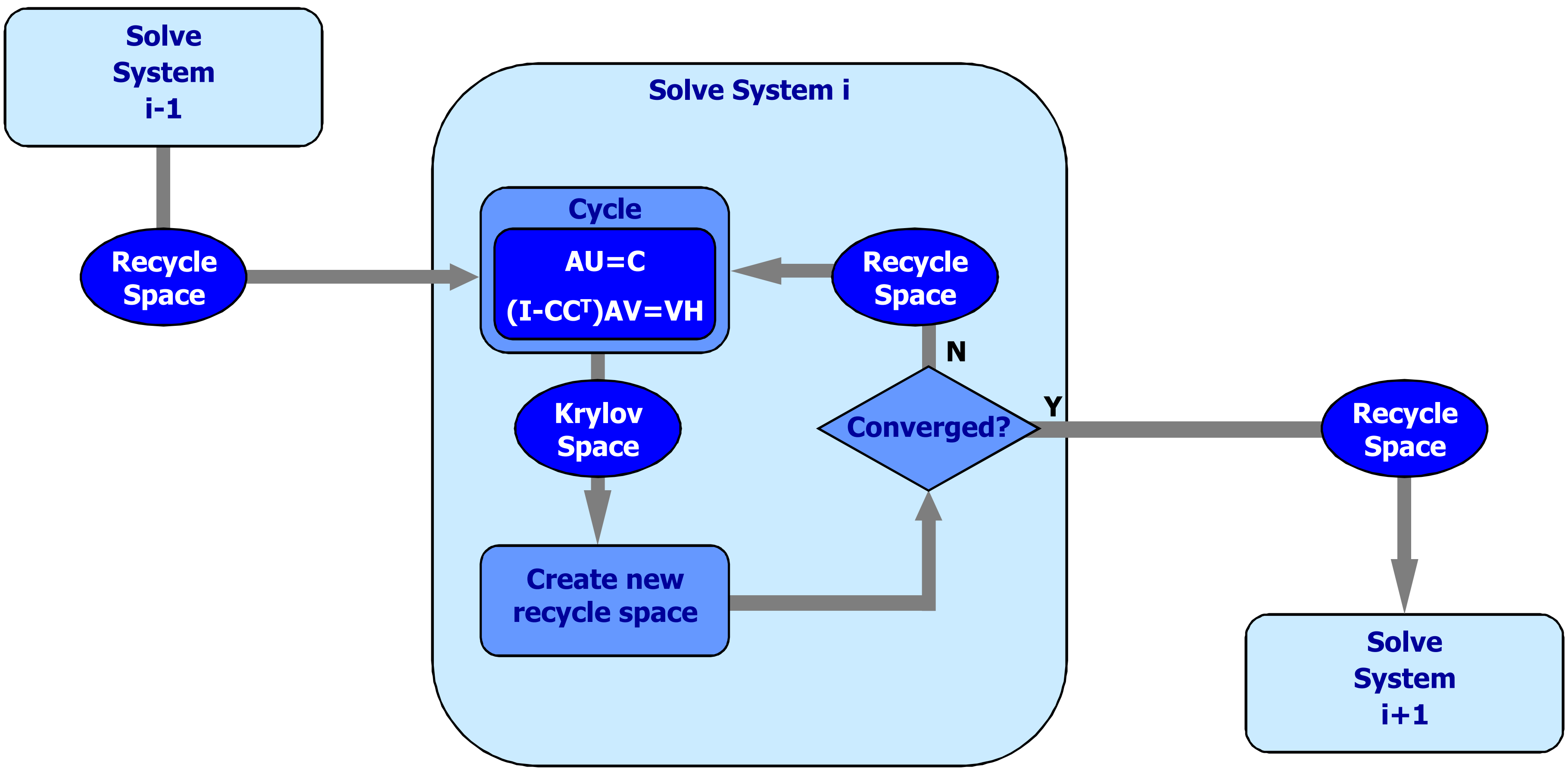
Structure of Recycling Solver



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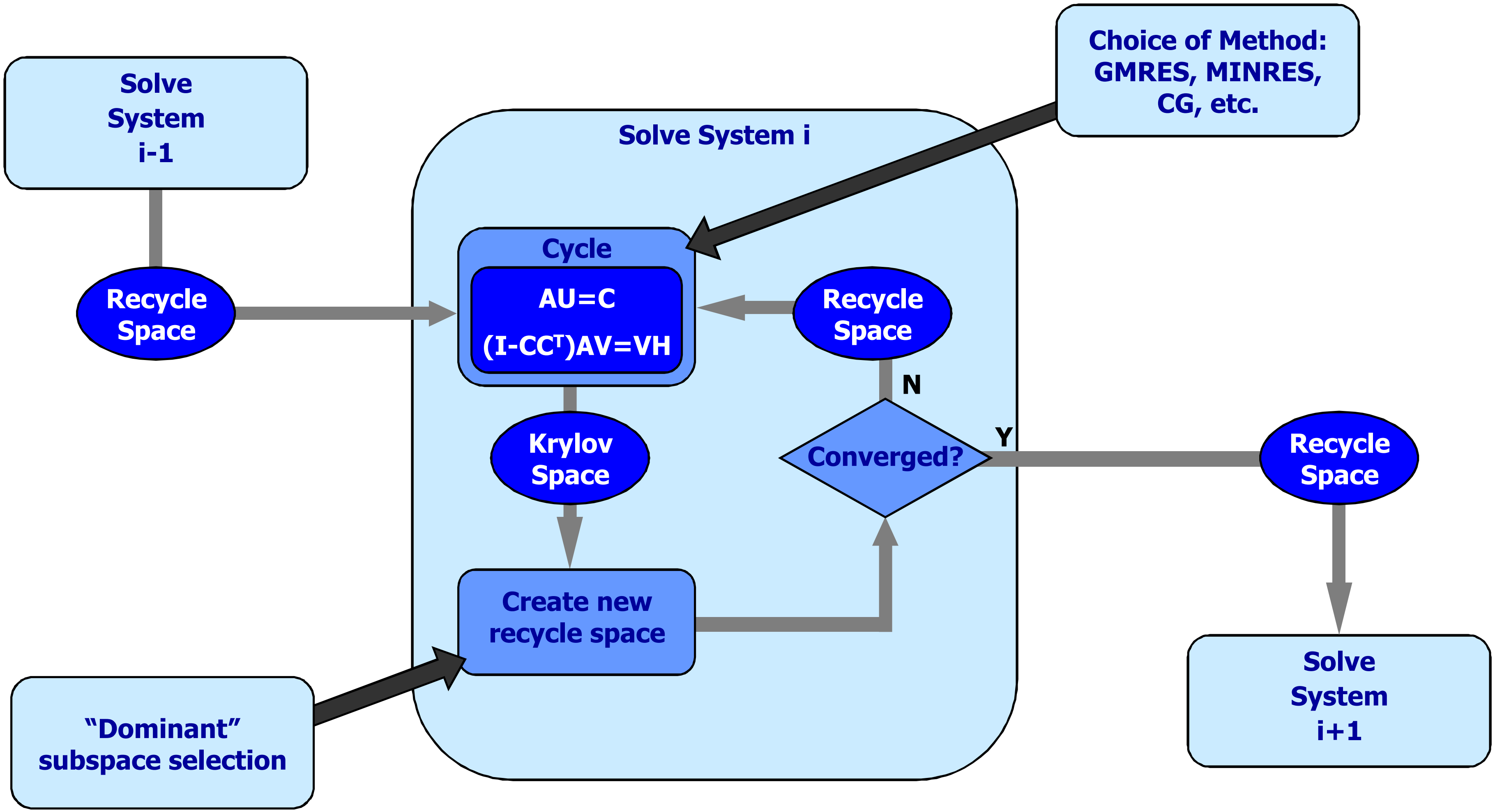
Structure of Recycling Solver



GCRO-DR / RMINRES

- In (nearly) symmetric problems, convergence delays caused by invariant subspace associated with small eigenvalues
  - corresponds to smooth modes that change little for small localized changes in the problem
- Remove them to improve convergence!
  - Recycle space = approximate eigenspace

$$\min_{z \in K^m(A, r_0)} \|r_0 - Az\|_2 = \min_{P_m(0)=1} \|p_m(A) r_0\|_2$$
$$\leq \kappa(V) \|r_0\|_2 \min_{P_m(0)=1} \max_{\lambda \in \Lambda(A)} |p_m(\lambda)|$$

- If $\kappa(V)$ is not large (normality assumption) we can improve bound by removing select eigenvalues
- RMINRES is specialization of GCRO-DR to symmetric (but not definite) case

GCROT/Recycle

- **Approximate b using 2 search spaces, range(C) & range(V) where $C^TC=I$, $V^TV=I$, but $C^TV \neq 0$**
- **Typically V generated after C**
- **Optimal approximation (one step)**

$$r_1 = (I - QQ^T)b \qquad \text{where} \qquad QR = qr([CV])$$

- **Suboptimal approximation (two steps)**

$$\tilde{r} = (I - CC^T)b$$

$$r_2 = (I - VV^T)\tilde{r}$$

- **Improve by taking into account "most relevant" parts of C**

$$\|r_1 - r_2\|_2^2 = \sum_i \nu_i^2 \cos(\angle_i(C,V))$$

- **Method measures "locally dominant" subspace**

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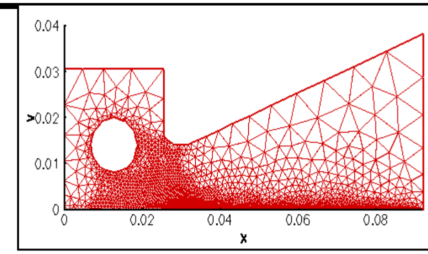
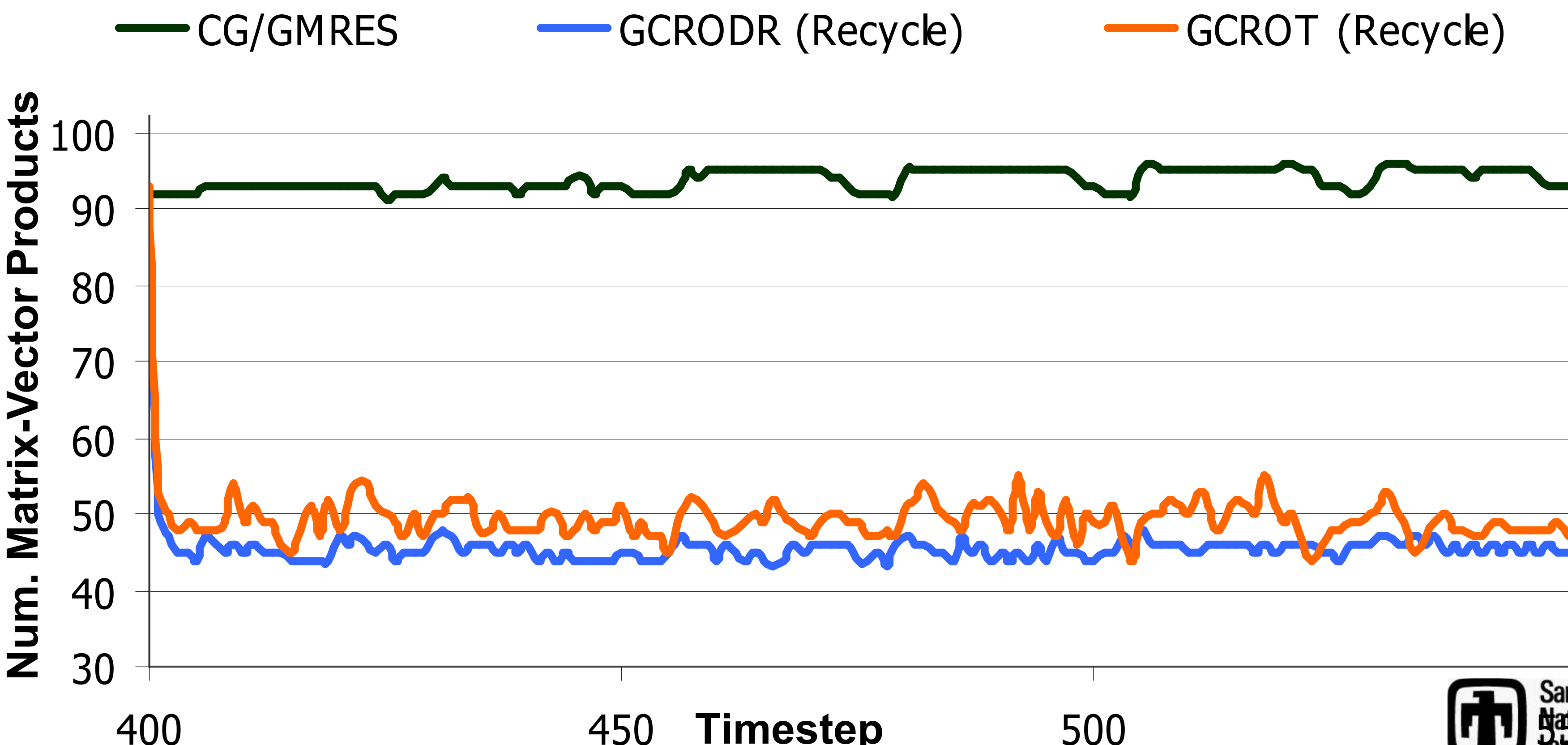
Example #1 Results: Crack Propagation

- IC(0) preconditioner
- GMRES – full recurrence
- All Others – Max subspace size 40





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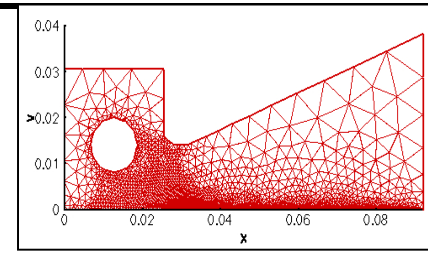
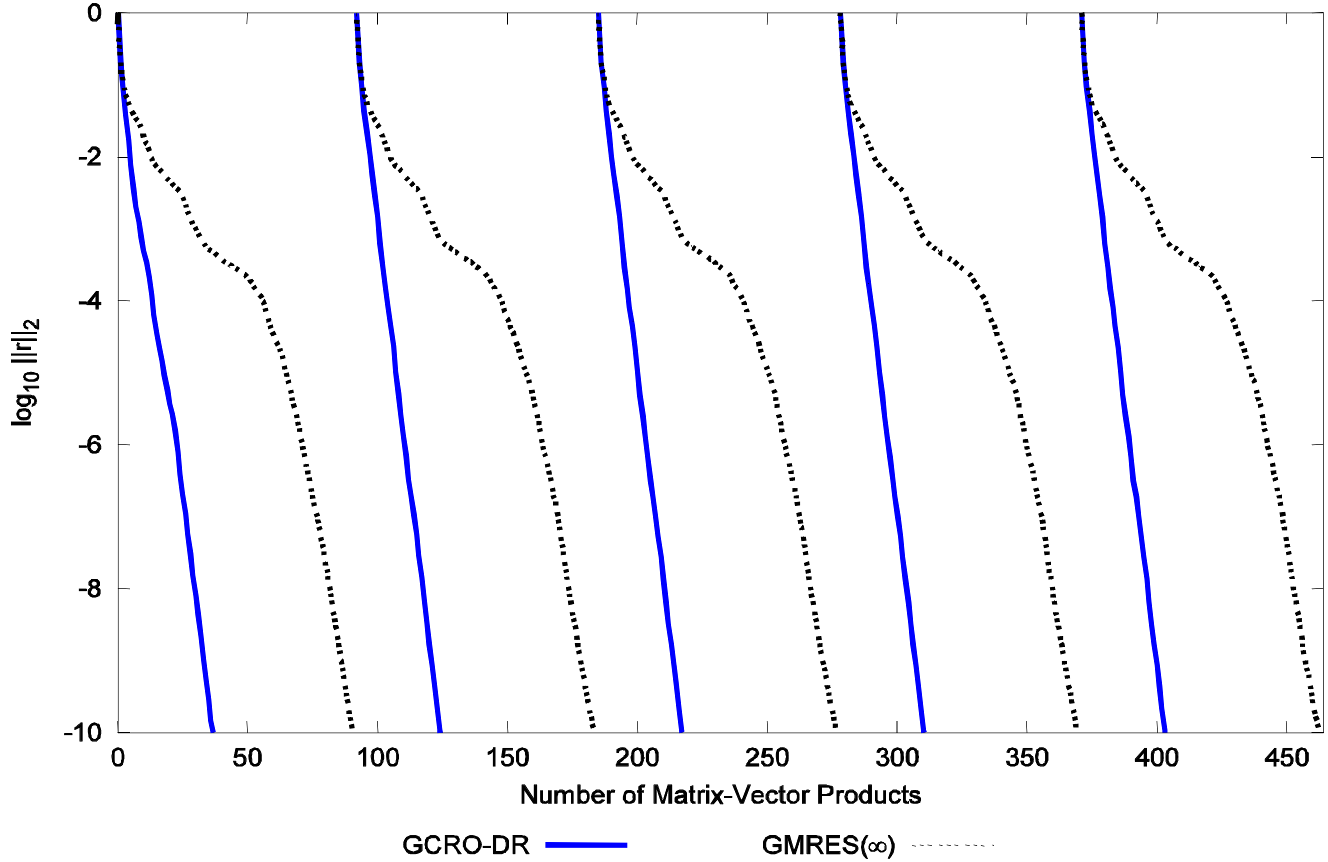
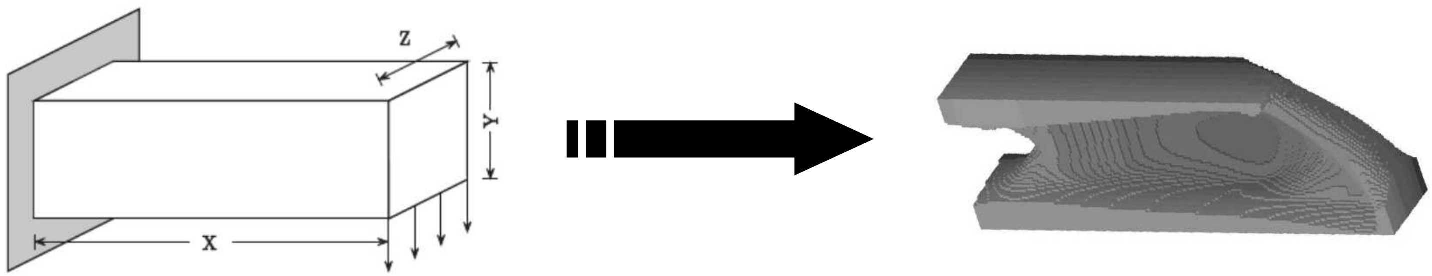




Example #2 Results: Topology Optimization*



Size	Num. DOFs	Direct Solve Time	Recycling Solve Time
Small	9,360	0.96	1.68
Medium	107,184	179.30	50.41
Large	1,010,160	26154.00	1196.30

Recycling Solve = RMINRES + IC(0) PC

Direct Solve = multifrontal, supernodal Cholesky factorization from TAUCS

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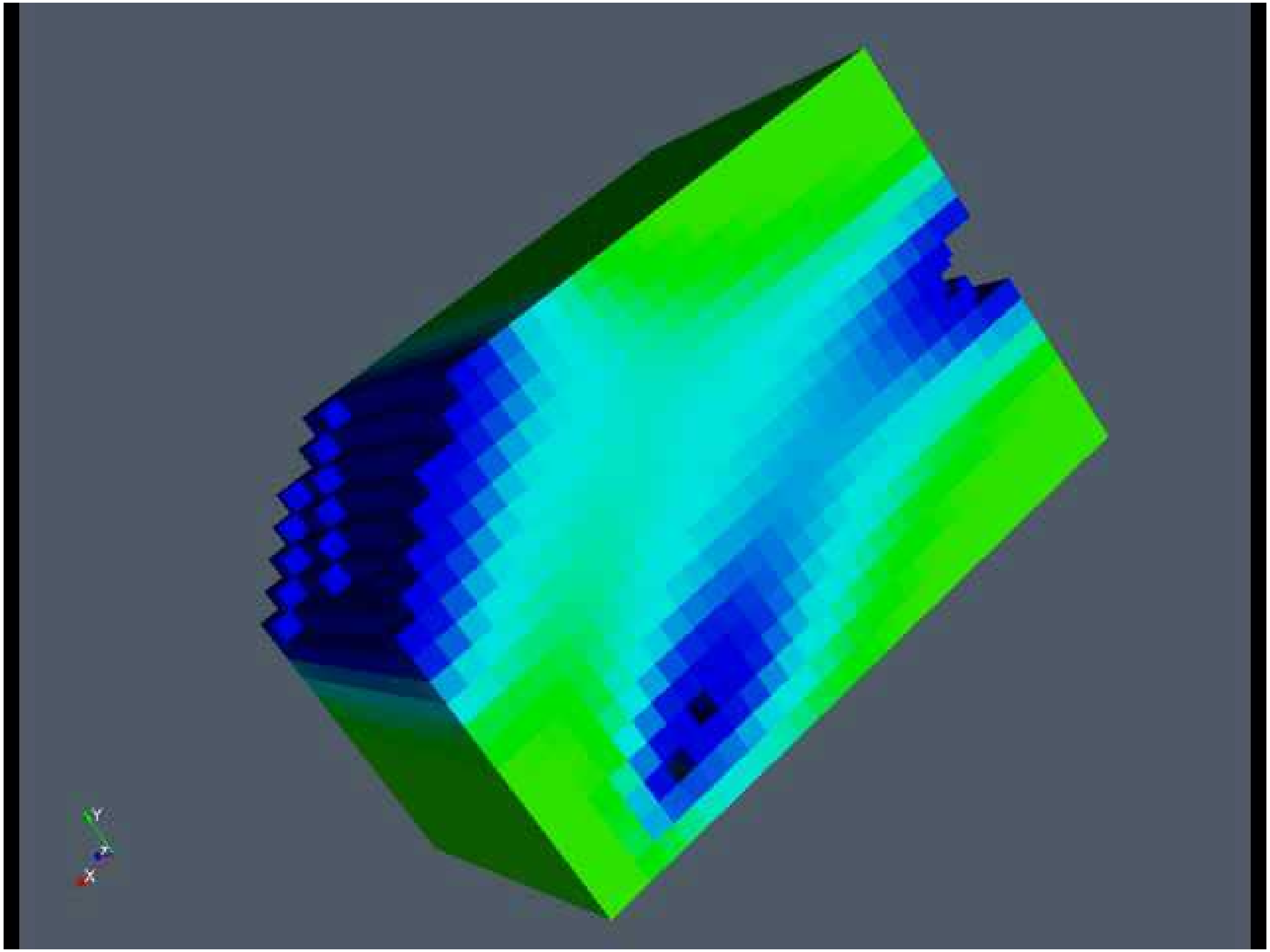
Example #2 Results: Topology Optimization



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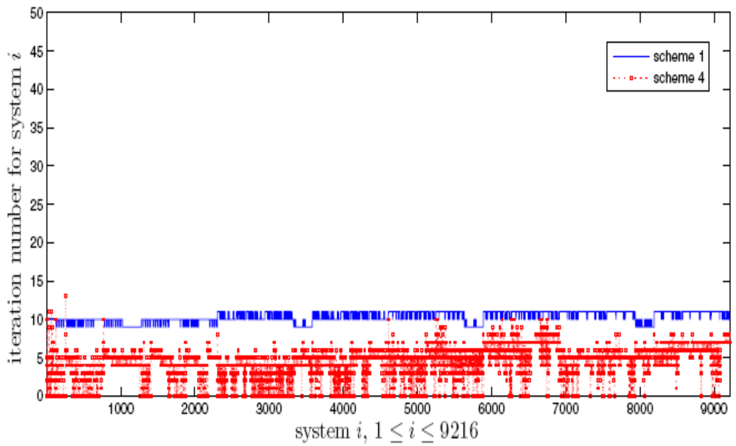
Example #3 Results: Stochastic PDEs*

- **Scheme #1: No Krylov recycling**
- **Scheme #4: Recycle Krylov spaces using reordering**
- **Many systems require zero iterations!**

One-Level ASM



Two-Level ASM

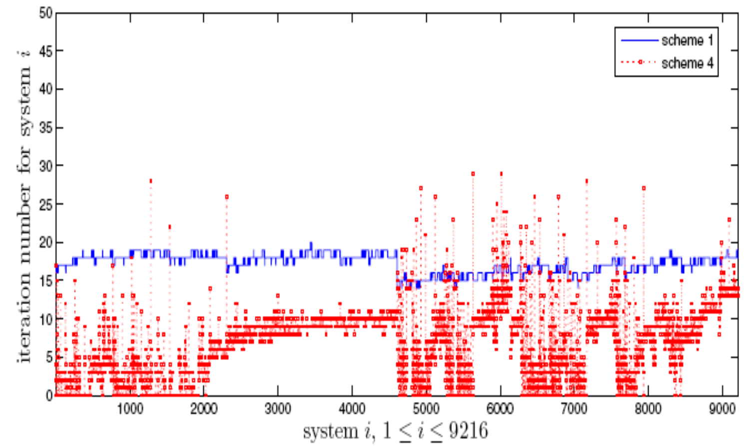


TABLE 4.1

Running time for different schemes and preconditioning (seconds).

Preconditioner	Scheme 1	Scheme 2	Scheme 3	Scheme 4
One-level ASM	12030	7693	4205	3882
Two-level ASM	20980	14130	10740	8476

*C. Jin, X-C. Cai, and C. Li, *Parallel Domain Decomposition Methods for Stochastic Elliptic Equations,* SIAM Journal on Scientific Computing, Vol. 29, Issue 5, pp. 2069—2114, 2007.

What makes a good recycling method?

- Methods need to satisfy three main requirements
  - Identify and converge to effective recycle space (invariant subspaces, dominant subspace) in modest number of iterations and do so over solution of multiple (changing) systems
  - Yield significant convergence improvement for recycle space of modest dimension
  - Converge quickly to perturbed recycle space for updated matrix, effective mechanism for cheaply updating recycle space to reflect changes

- Use knowledge of application to tune the recycling (dominant subspace, invariant subspace, solution space)

Convergence Analysis: Deflated Restarting

GCRO-DR

- Deflated Restarting within context of GCRO
- At end of cycle, GCRO-DR retains subspace spanned by k columns of U
- Let $\mathbf{AU} = \mathbf{C}$

  $\mathbf{C^H C} = \mathbf{I}$

- GCRO-DR generates Arnoldi relation

$$\left(\mathbf{I} - \mathbf{CC^H}\right)\mathbf{AV_m} = \mathbf{V_{m+1}}\underline{\mathbf{H}}$$

- RMINRES is specialization of algorithm for symmetric case
  - Will consider convergence of symmetric case separately

GCRO-DR

- We can rewrite GCRO-DR relation as

$$A\begin{bmatrix} U & V_m \end{bmatrix} = \begin{bmatrix} C & V_{m+1} \end{bmatrix} \begin{bmatrix} I & B \\ 0 & \underline{H} \end{bmatrix}$$

where

$$B = C^H A V_m$$

- Comments:
  - U arbitrary (harmonic Ritz vectors, Ritz vectors, etc.)
  - Focus on removing eigenvalues of smallest magnitude
  - V_{m+1} orthogonal to C
  - Designed for sequences of linear systems

Analysis: Symmetric Case

- For the symmetric case, convergence depends on spectrum

$$\left(\mathbf{I}-\mathbf{C}\mathbf{C}^H\right)\mathbf{A}\left(\mathbf{I}-\mathbf{C}\mathbf{C}^H\right)\mathbf{V}_m=\mathbf{V}_{m+1}\underline{\mathbf{T}}$$

  - Let C be k-dimensional matrix (recycle space)
  - Let $\Re(Q)$ be ℓ-dimensional invariant subspace of A, $\ell \leq k$

- Let Π_C be orthogonal projector onto $\Re(C)$
- Let P_Q be spectral projector onto $\Re(Q)$

- Let $\boldsymbol{\delta}(\mathbf{Q},\mathbf{C})=\left\|\left(\mathbf{I}-\boldsymbol{\Pi}_C\right)\boldsymbol{\Pi}_Q\right\|_2 \leq \mathbf{1}$
- δ is maximum component of unit vector in invariant subspace sticking out of recycle space
- We assume $\delta(Q,C) < 1$ (Desire $\delta(Q,C) << 1$)

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Analysis: Symmetric Case

- **For the symmetric case, convergence depends on spectrum**

$$\left(\mathbf{I}-\mathbf{C}\mathbf{C}^H\right)\mathbf{A}\left(\mathbf{I}-\mathbf{C}\mathbf{C}^H\right)\mathbf{V}_m = \mathbf{V}_{m+1}\underline{\mathbf{T}}$$

  - **Let C be k-dimensional matrix (recycle space)**
  - **Let $\Re(Q)$ be ℓ-dimensional invariant subspace of A, $\ell \le k$**

- **Let [Q Y_1 Y_2] be unitary, where**

$$\mathbf{A} = \left[\mathbf{Q} \quad \mathbf{Y}_1 \quad \mathbf{Y}_2\right]\begin{bmatrix} \Lambda_Q & & \\ & \Lambda_{Y,1} & \\ & & \Lambda_{Y,2} \end{bmatrix}\left[\mathbf{Q} \quad \mathbf{Y}_1 \quad \mathbf{Y}_2\right]^*$$

- **Assume $\Re(C) \subseteq \Re(Q,Y_1)$**

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Analysis: Symmetric Case

- After tedious analysis…

$$(I - \Pi_C)A(I - \Pi_C) = W\Gamma \begin{bmatrix} M & \\ & \Lambda_{Y,2} \end{bmatrix} \Gamma^* W^*$$

- Let

$$\alpha = \frac{1}{2}\left(\lambda_{max}(\lambda_{Y,1}) + \lambda_{min}(\lambda_{Y,1})\right)$$

$$\eta \equiv \lambda_{min}(\lambda_{Y,1})$$

- Then

$$\lambda_{min}(M) \geq \alpha - \eta - \delta^2(\alpha + \eta + \lambda_{max}(\Lambda_Q))$$

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Analysis: Symmetric Case

- For A HPD, residual norm bound $\sim \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{j}$
- For original matrix, $\kappa(A)=\frac{\lambda_n}{\lambda_1}$
- For projected operator, $\kappa((I-\Pi_C)A(I-\Pi_C)) \geq \frac{\lambda_n}{\lambda_{k+1}}$

- Numerical example
  - Let eigenvalues be {0.1, 0.2, 0.3, 0.4, 5, 6, … 100}

$$\kappa(A)=1000 \xrightarrow{\text{100 iter}} \|r\| \sim 0.8187$$

$$\kappa((I-\Pi_C)A(I-\Pi_C)) \approx 20 \xrightarrow{\text{100 iter}} \|r\| \sim 4.5023\times 10^{-5}$$

Analysis: Symmetric Case

- For A indefinite, residual norm bound ~ $\left(\dfrac{d/c - 1}{d/c + 1}\right)^{[j/2]}$

- If only a few negative eigenvalues, they may be eliminated by deflation

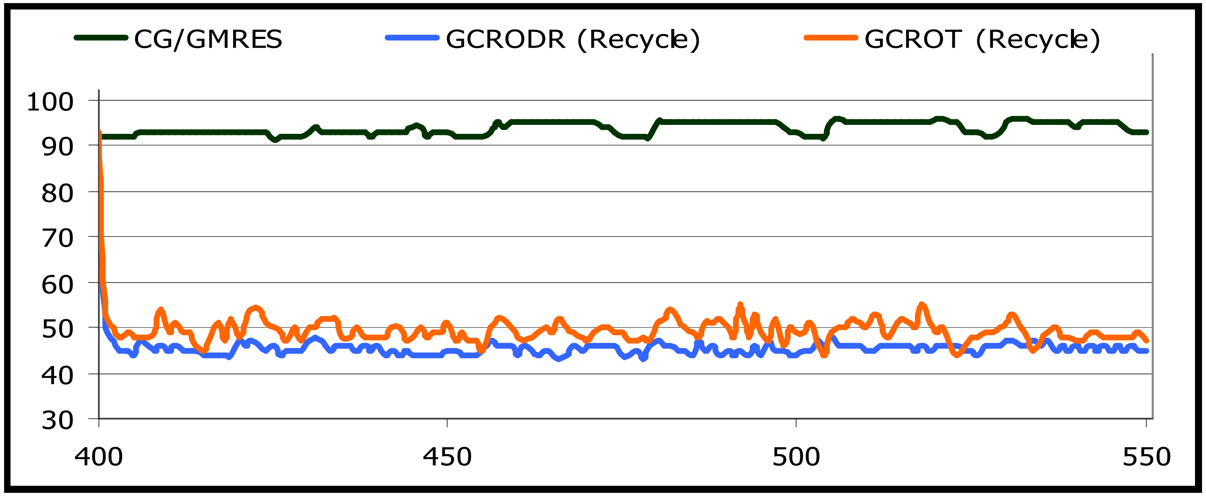
  residual norm bound ~ $\left(\dfrac{d/c - 1}{d/c + 1}\right)^{j}$

- Removes "squaring of condition number" effect

Example: Crack Propagation

- We assumed $\delta(Q, C) = \left\| (I - \Pi_C)\Pi_Q \right\|_2 < 1$

System	401	402	403	404	405
Before Cycle 1	0.9994	0.2380	0.0464	0.0607	0.0794
After Cycle 1	0.9180	0.1448	0.0463	0.0606	0.0787
After Cycle 2	0.2446	0.0302	0.0416	0.0568	0.0690
After Cycle 3	0.2331	0.0302	0.0415	0.0567	0.0684



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Example: Crack Propagation

- **Max/Min eigenvalues and condition number**

System	400	401	402	403	404
$\lambda_{max}(A)$	1.389687	1.389687	1.389687	1.389687	1.389687
$\lambda_{max}((I-\Pi_C)A(I-\Pi_C))$	1.389687	1.387698	1.389677	1.389687	1.389687
$\lambda_{min}(A)$	0.002732	0.002732	0.002732	0.002732	0.002732
$\lambda_{min}((I-\Pi_C)A(I-\Pi_C))$	0.002732	0.074453	0.148986	0.147848	0.149206
$\kappa(A)$	508.61	508.61	508.61	508.62	508.63
$\kappa((I-\Pi_C)A(I-\Pi_C))$	508.61	18.63	9.33	9.40	9.31

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Analysis: Nonsymmetric Case

- Let $\gamma(\mathbf{Q},\mathbf{C}) \equiv \left\|(\mathbf{I}-\mathbf{\Pi}_{\mathbf{C}})\mathbf{P}_{\mathbf{Q}}\right\|_2$

- Note $\gamma = \left\|(\mathbf{I}-\mathbf{\Pi}_{\mathbf{C}})\mathbf{\Pi}_{\mathbf{Q}}\mathbf{P}_{\mathbf{Q}}\right\|_2 \leq \left\|(\mathbf{I}-\mathbf{\Pi}_{\mathbf{C}})\mathbf{\Pi}_{\mathbf{Q}}\right\|_2 \left\|\mathbf{P}_{\mathbf{Q}}\right\|_2$

  $= \boldsymbol{\delta}(\mathbf{Q},\mathbf{C})\left\|\mathbf{P}_{\mathbf{Q}}\right\|_2$

- δ **is maximum component of unit vector in invariant subspace sticking out of recycle space**

- **We again assume δ(Q,C) < 1 (Desire δ(Q,C) << 1)**

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Analysis: Nonsymmetric Case

- **First bound:**

$$\min_{d_1 \in R(V_j, C)} \left\| r_0 - d_1 \right\|_2 \le \min_{d_2 \in R((I - P_Q) V_j)} \left\| \left(I - P_Q \right) r_1 - d_2 \right\|_2 + \left(\frac{\gamma}{1 - \delta} \right) \left\| P_Q \right\|_2 \left\| \left(I - \Pi_V \right) r_1 \right\|_2$$

where $r_1 = \left(I - \Pi_C \right) r_0$

V_j **is j-dimensional Krylov space (GCRO-DR)**

Analysis: Nonsymmetric Case

- **Second bound:**

$$\min_{d_1 \in R(V_j, C)} \|r_0 - d_1\|_2 \le \left\| \left(I - \Pi_{\tilde{V}}\right)\left(I - P_Q\right) r_1 - d_2 \right\|_2 + \left(\frac{\gamma}{1-\delta}\right) \|P_Q\|_2 + O(\delta^2)$$

- $\tilde{V}_j \equiv \left(I - P_Q\right) V_j$
- **Free to choose Q (select for best bound)**
- **Good bound if $\|P_Q\|_2$ not large**
- δ **need not be very small (unless $\|P_Q\|_2$ very large)**

Analysis: Nonsymmetric Case

- **Second bound:**

$$\min_{d_1 \in R(V_j, C)} \|r_0 - d_1\|_2 \leq \left\|\left(I - \Pi_{\tilde{V}}\right)\left(I - P_Q\right) r_1 - d_2\right\|_2$$
$$+ \left(\frac{\gamma}{1 - \delta}\right)\|P_Q\|_2 + O(\delta^2)$$

- **Must analyze Krylov process that generates space**

$$\tilde{V}_j \equiv \left(I - P_C\right) V_j$$

Analysis: Nonsymmetric Case

- **Second bound:**

$$\min_{d_1 \in R(V_j, C)} \|r_0 - d_1\|_2 \leq \left\| \left(I - \Pi_{\tilde{V}}\right)\left(I - P_Q\right) r_1 - d_2 \right\|_2 + \left(\frac{\gamma}{1-\delta}\right) \|P_Q\|_2 + O(\delta^2)$$

- **Following spirit of [Stewart, 2002], we observe**

$$\begin{bmatrix} (I - P_Q)(I - \Pi_C)A(I - \Pi_C)(I - P_Q) + \\ (I - P_Q)A_C P_Q V_j (\tilde{V}_j^H \tilde{V}_j)^{-1} \tilde{V}_j \end{bmatrix} \tilde{V}_j = \tilde{V}_{j+1} \underline{H}_j$$

- **Second operator is small perturbation of first**
  - **Consider spectrum of first**

Analysis: Nonsymmetric Case

- **Need additional assumptions…**
  - $\cos(\angle(\Re(Q),\Re(Y)))$ □ 1
- **After similar tedious analysis, expect similar result:**

$$(I - P_Q)(I - \Pi_C)A(I - \Pi_C)(I - P_Q) = Z\begin{bmatrix} M & \\ & L_Y \end{bmatrix}Z^*$$

where

$$\lambda_{min}(M) > \lambda_{min}(A)$$

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GCRO-DR: Numerical Examples

- **Main bound:**

BOUND

$$\min_{d_1 \in R(V_j, C)} \left\| r_0 - d_1 \right\|_2 \le \min_{d_2 \in R((I - P_Q) V_j)} \left\| (I - P_Q) r_1 - d_2 \right\|_2 + \left(\frac{\gamma}{1 - \delta} \right) \left\| P_Q \right\|_2 \left\| (I - \Pi_V) r_1 \right\|_2$$

where $r_1 = (I - \Pi_C) r_0$

V_j **is j-dimensional Krylov space (GCRO-DR)**

GCRO-DR: Numerical Examples

- **Main bound:**

DEFLATED

$$\min_{d_1 \in R(V_j, C)} \left\| r_0 - d_1 \right\|_2 \le \boxed{\min_{d_2 \in R((I - P_Q) V_j)} \left\| (I - P_Q) r_1 - d_2 \right\|_2}$$

$$+ \left(\frac{\gamma}{1 - \delta} \right) \left\| P_Q \right\|_2 \left\| (I - \Pi_V) r_1 \right\|_2$$

where $r_1 = (I - \Pi_C) r_0$

V_j **is j-dimensional Krylov space (GCRO-DR)**

GCRO-DR: Numerical Examples

- **Numerical Experiment***
  - **100 × 100 matrices**
  - $\mathbf{A}^{(i)} = \mathbf{S}^{(i)} \Lambda \left(\mathbf{S}^{(i)}\right)^{-1}$
  - $\kappa\left(\mathbf{S}^{(1)}\right) = 1, \quad \kappa\left(\mathbf{S}^{(2)}\right) = 10^{6}$

$$\Lambda = \mathrm{diag}\left(0.1, 0.2, 0.3, 0.4, 5, 6, 7, \ldots, 100\right)$$

- **Does GCRO-DR select and remove four small eigenvalues?**

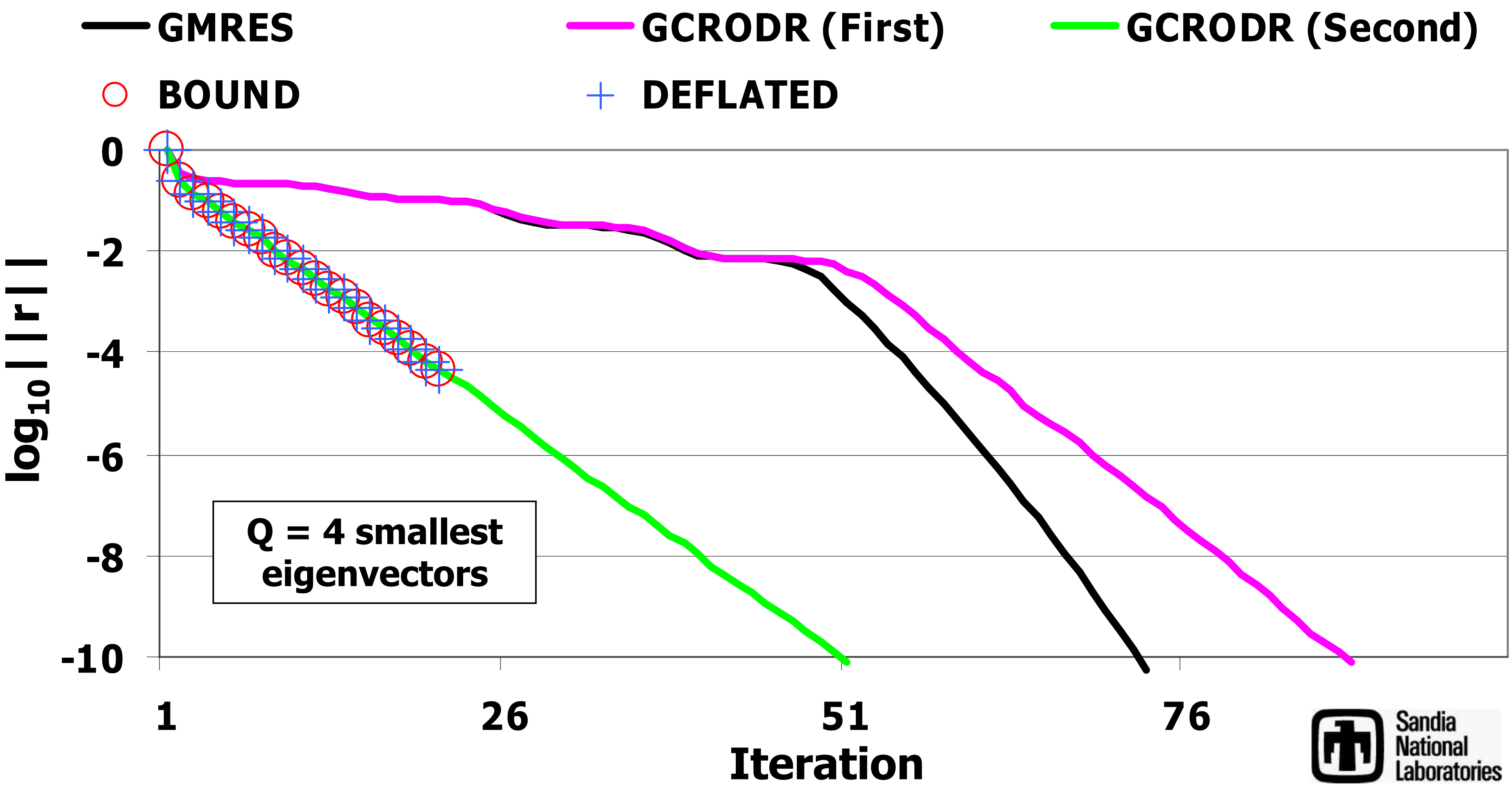
$$\begin{cases} \kappa\left(\mathbf{A}\right) = 1000 \\ \kappa\left(\hat{\mathbf{A}}\right) = 20 \end{cases}$$

- **Run GCRO-DR**
  - ***twice* on same problem**

* Simoncini & Szyld, 2005

Numerical Examples: $\kappa(S) = 1$

- GMRES – full recurrence
- GCRO-DR(24,4) – Max subspace size 24



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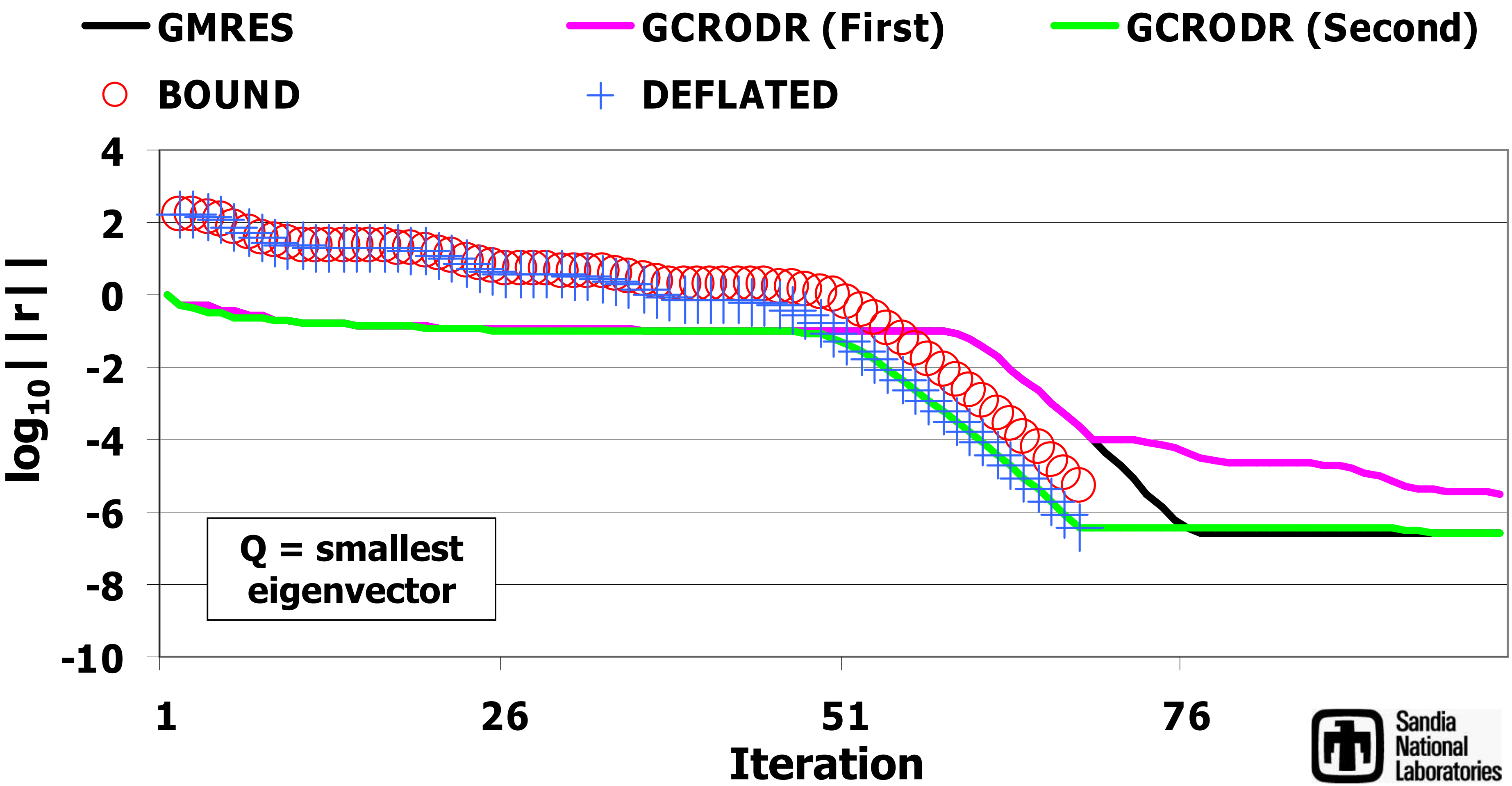
Numerical Examples: $\kappa(S) = 10^6$

- GMRES – full recurrence
- GCRO-DR(68,1) – Max subspace size 68



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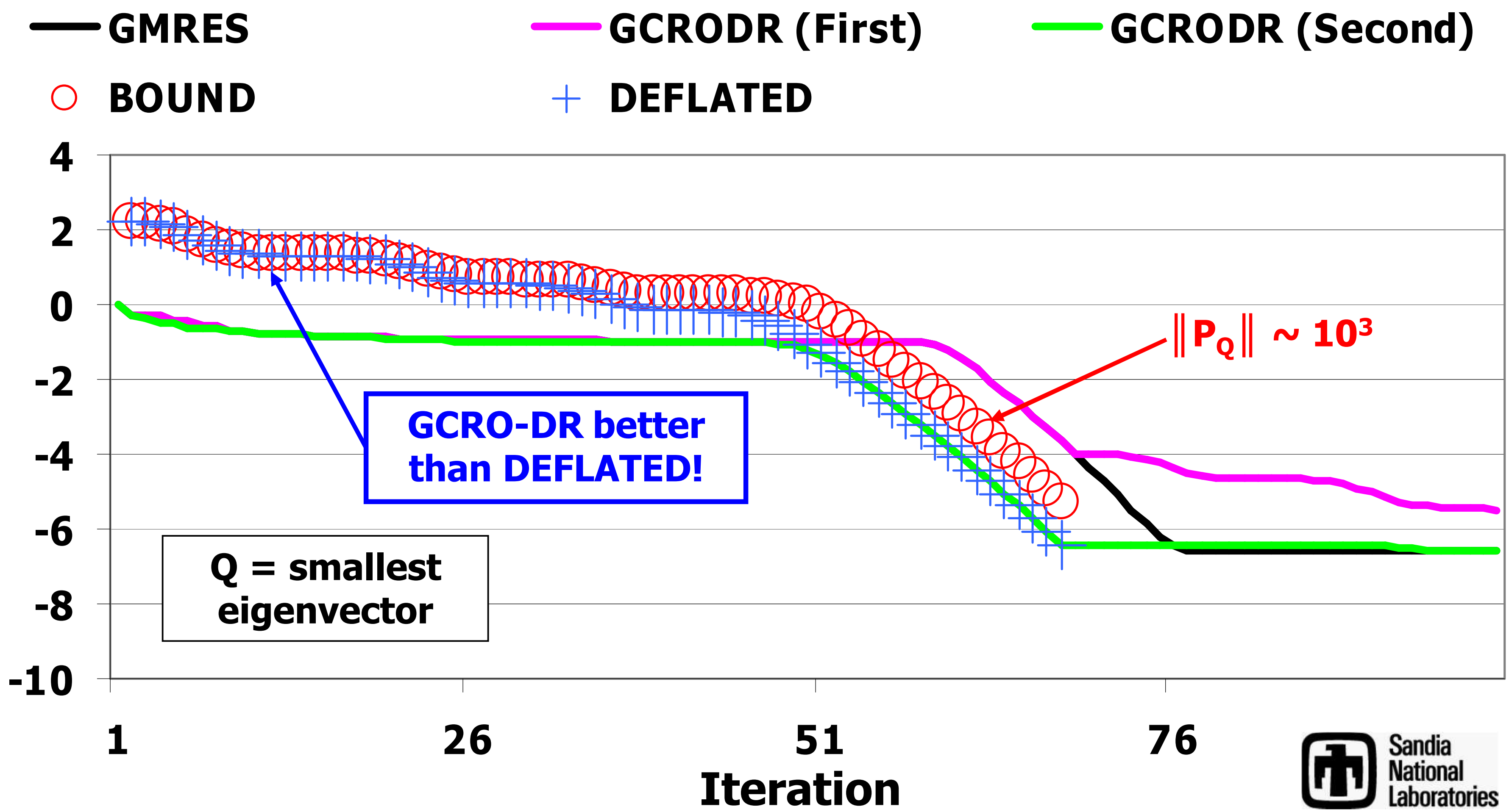
Numerical Examples: $\kappa(S) = 10^6$

- GMRES – full recurrence
- GCRO-DR(68,1) – Max subspace size 68



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Summary

- **Krylov recycling overview**
  - **GCRO-DR, RMINRES**
  - **Numerical example**

- **Convergence result (Symmetric case)**
  - **Improve conditioning if $\delta(Q,C)$ small**

- **Convergence result (Nonsymmetric case)**
  - **Less successful if $\|P_Q\|_2$ large**
  - **Less successful if highly nonnormal**

- **Numerical examples**

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Software

- **Matlab GCRO-DR**
  - Publicly available for download (www.sandia.gov/~mlparks)
  - Click on "software"

- **Fortran 90 GCRO-DR (serial)**
  - Limited release; Ask me

- **Matlab, PETSc RMINRES (ask EdS)**

- **Trilinos/Belos GCRO-DR (parallel)**
  - Available in Trilinos v8.0 public release
  - trilinos.sandia.gov

Recommended Reading

- **MLP, EdS, Greg Mackey, Duane D. Johnson, and Spandan Maiti, Recycling Krylov Subspaces for Sequences of Linear Systems, SIAM Journal on Scientific Computing, Vol. 28, No. 5, pp. 1651-1674, 2006.**
  - **GCRO-DR, GCROT/Recycle**
- **Shun Wang, EdS, and Glaucio H. Paulino, Large-Scale Topology Optimization using Preconditioned Krylov Subspace Methods with Recycling, International Journal for Numerical Methods in Engineering, Vol. 69, Issue 12, pp. 2441—2468, 2007.**
  - **RMINRES**

- **Available at**
  - **http://www.sandia.gov/~mlparks/**
  - **http://www.math.vt.edu/people/sturler/**