

# Communication-Avoiding Krylov Subspace Methods in Theory and Practice

---

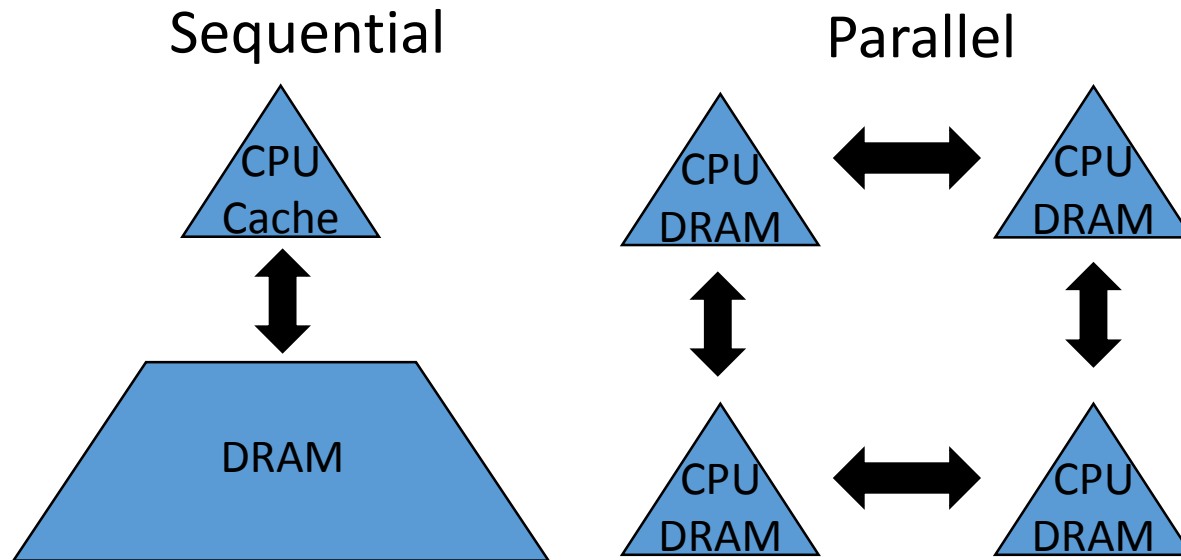
**Erin Carson, NYU**

DMML Workshop

October 23, 2015

# Why Avoid “Communication”?

- Algorithms have two costs: **computation** and **communication**
  - Communication : moving data** between levels of memory hierarchy (sequential), between processors (parallel)



- On today’s computers, communication is expensive, computation is cheap, in terms of both time and energy!

# Future Exascale Systems

---

	Petascale Systems (2009)	Predicted Exascale Systems*	Factor Improvement
System Peak	$2 \cdot 10^{15}$ flops	$10^{18}$ flops	~1000
Node Memory Bandwidth	25 GB/s	0.4-4 TB/s	~10-100
Total Node Interconnect Bandwidth	3.5 GB/s	100-400 GB/s	~100
Memory Latency	100 ns	50 ns	~1
Interconnect Latency	1 $\mu$ s	0.5 $\mu$ s	~1

\*Sources: from P. Beckman (ANL), J. Shalf (LBL), and D. Unat (LBL)

# Future Exascale Systems

	Petascale Systems (2009)	Predicted Exascale Systems*	Factor Improvement
System Peak	$2 \cdot 10^{15}$ flops	$10^{18}$ flops	~1000
Node Memory Bandwidth	25 GB/s	0.4-4 TB/s	~10-100
Total Node Interconnect Bandwidth	3.5 GB/s	100-400 GB/s	~100
Memory Latency	100 ns	50 ns	~1
Interconnect Latency	1 $\mu$ s	0.5 $\mu$ s	~1

\*Sources: from P. Beckman (ANL), J. Shalf (LBL), and D. Unat (LBL)

- Gaps between communication/computation cost only growing larger in future systems

# Future Exascale Systems

	Petascale Systems (2009)	Predicted Exascale Systems*	Factor Improvement
System Peak	$2 \cdot 10^{15}$ flops	$10^{18}$ flops	~1000
Node Memory Bandwidth	25 GB/s	0.4-4 TB/s	~10-100
Total Node Interconnect Bandwidth	3.5 GB/s	100-400 GB/s	~100
Memory Latency	100 ns	50 ns	~1
Interconnect Latency	1 $\mu$ s	0.5 $\mu$ s	~1

\*Sources: from P. Beckman (ANL), J. Shalf (LBL), and D. Unat (LBL)

- Gaps between communication/computation cost only growing larger in future systems
- **Avoiding communication will be essential for applications at exascale!**

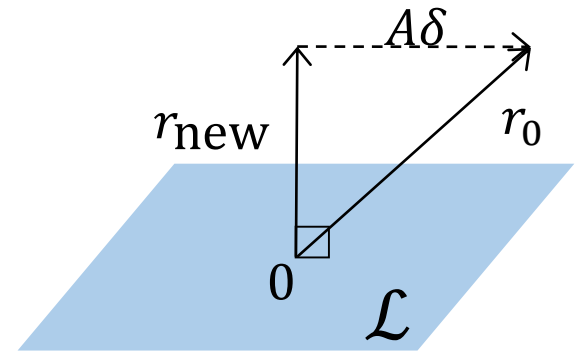
# Krylov Subspace Methods

---

- General class of iterative solvers: used for linear systems, eigenvalue problems, singular value problems, least squares, etc.
- Examples: Lanczos/Conjugate Gradient (CG), Arnoldi/Generalized Minimum Residual (GMRES), Biconjugate Gradient (BICG), BICGSTAB, GKL, LSQR, etc.
- Projection process onto the expanding **Krylov subspace**

$$\mathcal{K}_m(A, r_0) = \text{span}\{r_0, Ar_0, A^2r_0, \dots, A^{m-1}r_0\}$$

- In each iteration,
  - Add a dimension to the Krylov subspace  $\mathcal{K}_m$
  - Orthogonalize (with respect to some  $\mathcal{L}_m$ )



# Krylov Solvers: Limited by Communication

In terms of communication:

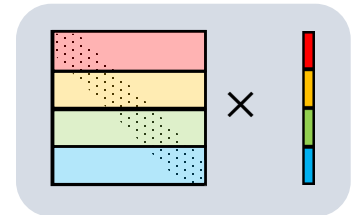
# Krylov Solvers: Limited by Communication

In terms of communication:

“Add a dimension to  $\mathcal{K}_m$ ”

→ Sparse Matrix-Vector Multiplication (SpMV)

- Parallel: comm. vector entries w/ neighbors
- Sequential: read  $A$ /vectors from slow memory





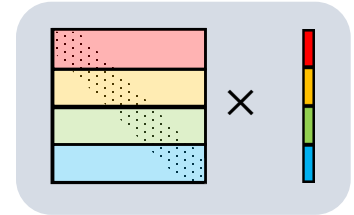
# Krylov Solvers: Limited by Communication

In terms of communication:

“Add a dimension to  $\mathcal{K}_m$ ”

→ Sparse Matrix-Vector Multiplication (SpMV)

- Parallel: comm. vector entries w/ neighbors
- Sequential: read  $A$ /vectors from slow memory



“Orthogonalize (with respect to some  $\mathcal{L}_m$ )”

→ Inner products

Parallel: global reduction (All-Reduce)

Sequential: multiple reads/writes to slow memory



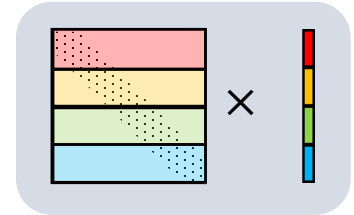
# Krylov Solvers: Limited by Communication

In terms of communication:

“Add a dimension to  $\mathcal{K}_m$ ”

→ Sparse Matrix-Vector Multiplication (SpMV)

- Parallel: comm. vector entries w/ neighbors
- Sequential: read  $A$ /vectors from slow memory

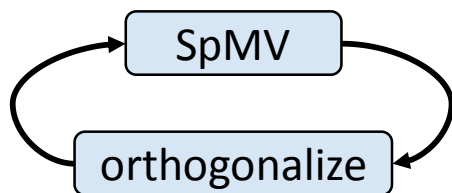


“Orthogonalize (with respect to some  $\mathcal{L}_m$ )”

→ Inner products

Parallel: global reduction (All-Reduce)

Sequential: multiple reads/writes to slow memory



**Dependencies between communication-bound kernels in each iteration limit performance!**

# Example: Classical Conjugate Gradient (CG)

---

Given: initial approximation  $x_0$  for solving  $Ax = b$

Let  $p_0 = r_0 = b - Ax_0$

**for**  $m = 0, 1, 2, \dots$ , until convergence **do**

$$\alpha_m = \frac{r_m^T r_m}{p_m^T A p_m}$$

$$x_{m+1} = x_m + \alpha_m p_m$$

$$r_{m+1} = r_m - \alpha_m A p_m$$

$$\beta_{m+1} = \frac{r_{m+1}^T r_{m+1}}{r_m^T r_m}$$

$$p_{m+1} = r_{m+1} + \beta_{m+1} p_m$$

**end for**

# Example: Classical Conjugate Gradient (CG)

---

Given: initial approximation  $x_0$  for solving  $Ax = b$

Let  $p_0 = r_0 = b - Ax_0$

**for**  $m = 0, 1, 2, \dots$ , until convergence **do**

$$\alpha_m = \frac{r_m^T r_m}{p_m^T A p_m}$$

SpMV

$$x_{m+1} = x_m + \alpha_m p_m$$

$$r_{m+1} = r_m - \alpha_m A p_m$$

$$\beta_{m+1} = \frac{r_{m+1}^T r_{m+1}}{r_m^T r_m}$$

$$p_{m+1} = r_{m+1} + \beta_{m+1} p_m$$

**end for**

# Example: Classical Conjugate Gradient (CG)

Given: initial approximation  $x_0$  for solving  $Ax = b$

Let  $p_0 = r_0 = b - Ax_0$

**for**  $m = 0, 1, 2, \dots$ , until convergence **do**

$$\alpha_m = \frac{r_m^T r_m}{p_m^T A p_m}$$
$$x_{m+1} = x_m + \alpha_m p_m$$
$$r_{m+1} = r_m - \alpha_m A p_m$$
$$\beta_{m+1} = \frac{r_{m+1}^T r_{m+1}}{r_m^T r_m}$$

SpMV

Inner products

$$p_{m+1} = r_{m+1} + \beta_{m+1} p_m$$

**end for**

# Communication-Avoiding KSMs

---

- Idea: Compute blocks of  $s$  iterations at once
  - Communicate every  $s$  iterations instead of every iteration
  - **Reduces communication cost by  $O(s)$ !**
    - (latency in parallel, latency and bandwidth in sequential)

# Communication-Avoiding KSMs

---

- Idea: Compute blocks of  $s$  iterations at once
  - Communicate every  $s$  iterations instead of every iteration
  - **Reduces communication cost by  $O(s)$ !**
    - (latency in parallel, latency and bandwidth in sequential)
- An idea rediscovered many times...
- First related work:  $s$ -dimensional steepest descent - Khabaza ('63), Forsythe ('68), Marchuk and Kuznecov ('68):
- Flurry of work on  $s$ -step Krylov methods in '80s/early '90s: see, e.g., Van Rosendale, 1983; Chronopoulos and Gear, 1989
  - Goals: increasing parallelism, avoiding I/O, increasing “convergence rate”

# Communication-Avoiding KSMs

---

- Idea: Compute blocks of  $s$  iterations at once
  - Communicate every  $s$  iterations instead of every iteration
  - **Reduces communication cost by  $O(s)$ !**
    - (latency in parallel, latency and bandwidth in sequential)
- An idea rediscovered many times...
- First related work:  $s$ -dimensional steepest descent - Khabaza ('63), Forsythe ('68), Marchuk and Kuznecov ('68):
- Flurry of work on  $s$ -step Krylov methods in '80s/early '90s: see, e.g., Van Rosendale, 1983; Chronopoulos and Gear, 1989
  - Goals: increasing parallelism, avoiding I/O, increasing “convergence rate”
- Resurgence of interest in recent years due to growing problem sizes; growing relative cost of communication



# Communication-Avoiding KSMs: CA-CG

---

- Main idea: Unroll iteration loop by a factor of  $s$ ; split iteration loop into an outer loop and an inner loop
- Key observation: starting at some iteration  $m$ ,

$$x_{m+j} - x_m, r_{m+j}, p_{m+j} \in \mathcal{K}_{s+1}(A, p_m) + \mathcal{K}_s(A, r_m) \quad \text{for } j \in \{0, \dots, s\}$$

# Communication-Avoiding KSMs: CA-CG

- Main idea: Unroll iteration loop by a factor of  $s$ ; split iteration loop into an outer loop and an inner loop
- Key observation: starting at some iteration  $m$ ,

$$x_{m+j} - x_m, r_{m+j}, p_{m+j} \in \mathcal{K}_{s+1}(A, p_m) + \mathcal{K}_s(A, r_m) \quad \text{for } j \in \{0, \dots, s\}$$

## Outer loop $k$ : Communication step

### Expand solution space $s$ dimensions at once

- Compute “basis matrix”  $Y_k$  with columns spanning

$$\mathcal{K}_{s+1}(A, p_m) + \mathcal{K}_s(A, r_m)$$

- Requires **reading  $A$ /communicating vectors only once**
  - Using “matrix powers kernel”

### Orthogonalize all at once

- Compute/store block of inner products between basis vectors in Gram matrix:

$$G_k = Y_k^T Y_k$$

- Communication cost of **one global reduction**

# Communication-Avoiding KSMs: CA-CG

---

**Inner loop:  
Computation  
steps, no  
communication!**

Perform  $s$  iterations of updates

- Using  $Y_k$  and  $G_k$ , this requires **no communication!**
- Represent  $n$ -vectors by their  $O(s)$  coordinates in  $Y_k$ :

$$x_{sk+j} - x_{sk} = Y_k x'_j, \quad r_{sk+j} = Y_k r'_j, \quad p_{sk+j} = Y_k p'_j$$

# Communication-Avoiding KSMs: CA-CG

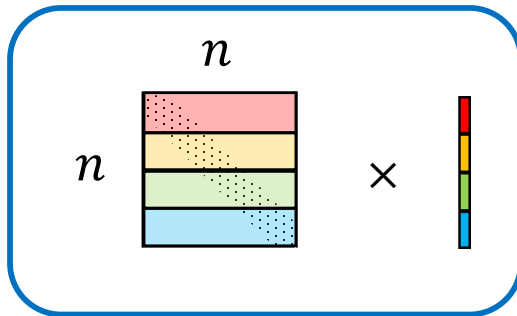
**Inner loop:  
Computation  
steps, no  
communication!**

Perform  $s$  iterations of updates

- Using  $Y_k$  and  $G_k$ , this requires **no communication!**
- Represent  $n$ -vectors by their  $O(s)$  coordinates in  $Y_k$ :

$$x_{sk+j} - x_{sk} = Y_k x'_j, \quad r_{sk+j} = Y_k r'_j, \quad p_{sk+j} = Y_k p'_j$$

$Ap_{sk+j}$



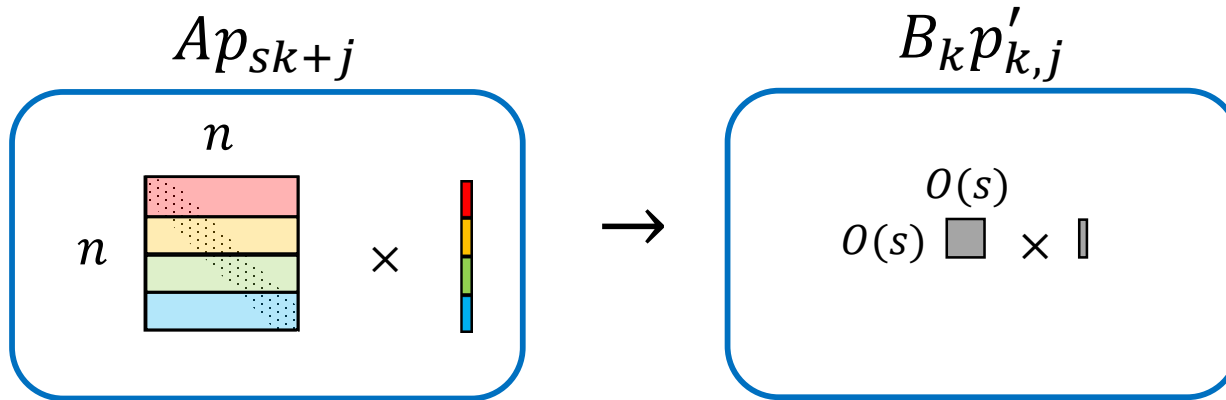
# Communication-Avoiding KSMs: CA-CG

**Inner loop:  
Computation  
steps, no  
communication!**

Perform  $s$  iterations of updates

- Using  $Y_k$  and  $G_k$ , this requires **no communication!**
- Represent  $n$ -vectors by their  $O(s)$  coordinates in  $Y_k$ :

$$x_{sk+j} - x_{sk} = Y_k x'_j, \quad r_{sk+j} = Y_k r'_j, \quad p_{sk+j} = Y_k p'_j$$



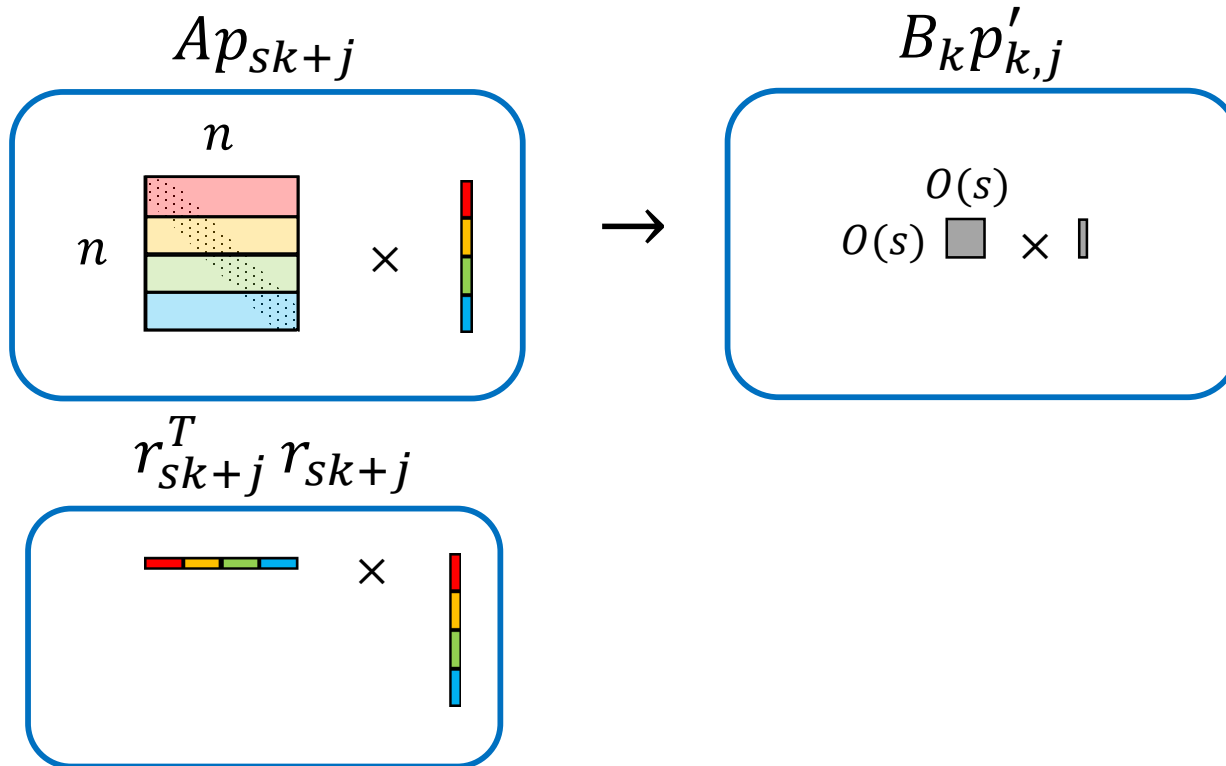
# Communication-Avoiding KSMs: CA-CG

**Inner loop:  
Computation  
steps, no  
communication!**

Perform  $s$  iterations of updates

- Using  $Y_k$  and  $G_k$ , this requires **no communication!**
- Represent  $n$ -vectors by their  $O(s)$  coordinates in  $Y_k$ :

$$x_{sk+j} - x_{sk} = Y_k x'_j, \quad r_{sk+j} = Y_k r'_j, \quad p_{sk+j} = Y_k p'_j$$



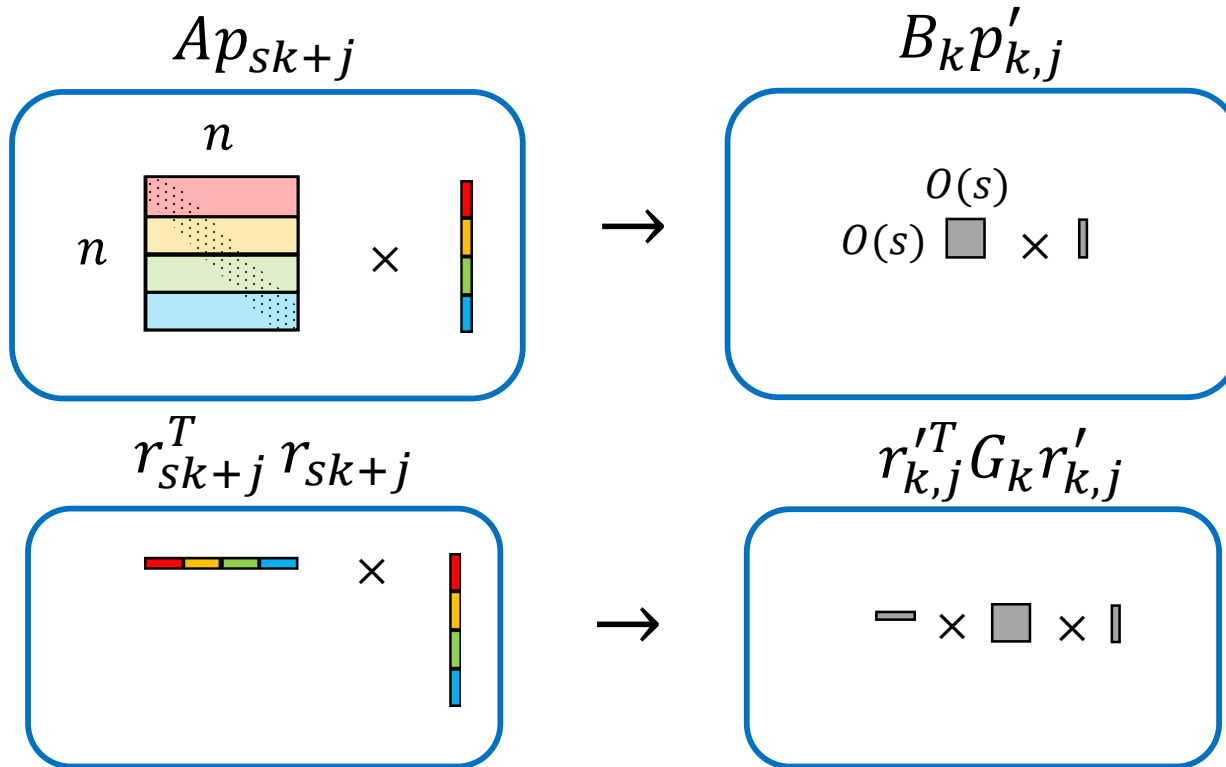
# Communication-Avoiding KSMs: CA-CG

**Inner loop:  
Computation  
steps, no  
communication!**

Perform  $s$  iterations of updates

- Using  $Y_k$  and  $G_k$ , this requires **no communication!**
- Represent  $n$ -vectors by their  $O(s)$  coordinates in  $Y_k$ :

$$x_{sk+j} - x_{sk} = Y_k x'_j, \quad r_{sk+j} = Y_k r'_j, \quad p_{sk+j} = Y_k p'_j$$



# Example: CA-Conjugate Gradient

---

Given: initial approximation  $x_0$  for solving  $Ax = b$

Let  $p_0 = r_0 = b - Ax_0$

**for**  $k = 0, 1, \dots$ , until convergence **do**

    Compute  $Y_k$ ,    compute  $G_k = Y_k^T Y_k$

    Let  $x'_0 = 0_{2s+1}$ ,  $r'_0 = e_{s+2}$ ,  $p'_0 = e_1$

**for**  $j = 0, \dots, s - 1$  **do**

$$\alpha_{sk+j} = \frac{(r'_j)^T G_k r'_j}{(p'_j)^T G_k B_k p'_j}$$

$$x'_{j+1} = x'_j + \alpha_{sk+j} p'_j$$

$$r'_{j+1} = r'_j - \alpha_{sk+j} B_k p'_j$$

$$\beta_{sk+j+1} = \frac{(r'_{j+1})^T G_k r'_{j+1}}{(r'_j)^T G_k r'_j}$$

$$p'_{j+1} = r'_{j+1} + \beta_{sk+j+1} p'_j$$

**end for**

    Compute  $x_{sk+s} = Y_k x'_s + x_{sk}$ ,  $r_{sk+s} = Y_k r'_s$ ,  $p_{sk+s} = Y_k p'_s$

**end for**



# Example: CA-Conjugate Gradient

Given: initial approximation  $x_0$  for solving  $Ax = b$

Let  $p_0 = r_0 = b - Ax_0$

for  $k = 0, 1, \dots$ , until convergence do

Compute  $Y_k$ , compute  $G_k = Y_k^T Y_k$

Let  $x'_0 = 0_{2s+1}$ ,  $r'_0 = e_{s+2}$ ,  $p'_0 = e_1$

for  $j = 0, \dots, s - 1$  do

$$\alpha_{sk+j} = \frac{(r'_j)^T G_k r'_j}{(p'_j)^T G_k B_k p'_j}$$

$$x'_{j+1} = x'_j + \alpha_{sk+j} p'_j$$

$$r'_{j+1} = r'_j - \alpha_{sk+j} B_k p'_j$$

$$\beta_{sk+j+1} = \frac{(r'_{j+1})^T G_k r'_{j+1}}{(r'_j)^T G_k r'_j}$$

$$p'_{j+1} = r'_{j+1} + \beta_{sk+j+1} p'_j$$

end for

Compute  $x_{sk+s} = Y_k x'_s + x_{sk}$ ,  $r_{sk+s} = Y_k r'_s$ ,  $p_{sk+s} = Y_k p'_s$

end for

via CA Matrix Powers Kernel

Global reduction to compute  $G_k$

# Example: CA-Conjugate Gradient

Given: initial approximation  $x_0$  for solving  $Ax = b$

Let  $p_0 = r_0 = b - Ax_0$

for  $k = 0, 1, \dots$ , until convergence do

Compute  $Y_k$ , compute  $G_k = Y_k^T Y_k$

Let  $x'_0 = 0_{2s+1}$ ,  $r'_0 = e_{s+2}$ ,  $p'_0 = e_1$

for  $j = 0, \dots, s - 1$  do

$$\alpha_{sk+j} = \frac{(r'_j)^T G_k r'_j}{(p'_j)^T G_k B_k p'_j}$$
$$x'_{j+1} = x'_j + \alpha_{sk+j} p'_j$$
$$r'_{j+1} = r'_j - \alpha_{sk+j} B_k p'_j$$
$$\beta_{sk+j+1} = \frac{(r'_{j+1})^T G_k r'_{j+1}}{(r'_j)^T G_k r'_j}$$
$$p'_{j+1} = r'_{j+1} + \beta_{sk+j+1} p'_j$$

end for

Compute  $x_{sk+s} = Y_k x'_s + x_{sk}$ ,  $r_{sk+s} = Y_k r'_s$ ,  $p_{sk+s} = Y_k p'_s$

end for

via CA Matrix Powers Kernel

Global reduction to compute  $G_k$

Local computations within inner loop require no communication!

# Complexity Comparison

---

Example of parallel (per processor) complexity for  $s$  iterations of CG vs. CA-CG for a 2D 9-point stencil:

(Assuming each of  $p$  processors owns  $n/p$  rows of the matrix and  $s \leq \sqrt{n/p}$ )

	Flops		Words Moved		Messages	
	SpMV	Orth.	SpMV	Orth.	SpMV	Orth.
Classical CG	$\frac{sn}{p}$	$\frac{sn}{p}$	$s\sqrt{n/p}$	$s \log_2 p$	$s$	$s \log_2 p$
CA-CG	$\frac{sn}{p}$	$\frac{s^2 n}{p}$	$s\sqrt{n/p}$	$s^2 \log_2 p$	1	$\log_2 p$

All values in the table meant in the Big-O sense (i.e., lower order terms and constants not included)

# Complexity Comparison

Example of parallel (per processor) complexity for  $s$  iterations of CG vs. CA-CG for a 2D 9-point stencil:

(Assuming each of  $p$  processors owns  $n/p$  rows of the matrix and  $s \leq \sqrt{n/p}$ )

	Flops		Words Moved		Messages	
	SpMV	Orth.	SpMV	Orth.	SpMV	Orth.
Classical CG	$\frac{sn}{p}$	$\frac{sn}{p}$	$s\sqrt{n/p}$	$s \log_2 p$	$s$	$s \log_2 p$
CA-CG	$\frac{sn}{p}$	$\frac{s^2 n}{p}$	$s\sqrt{n/p}$	$s^2 \log_2 p$	1	$\log_2 p$

All values in the table meant in the Big-O sense (i.e., lower order terms and constants not included)

# Complexity Comparison

Example of parallel (per processor) complexity for  $s$  iterations of CG vs. CA-CG for a 2D 9-point stencil:

(Assuming each of  $p$  processors owns  $n/p$  rows of the matrix and  $s \leq \sqrt{n/p}$ )

	Flops		Words Moved		Messages	
	SpMV	Orth.	SpMV	Orth.	SpMV	Orth.
Classical CG	$\frac{sn}{p}$	$\frac{sn}{p}$	$s\sqrt{n/p}$	$s \log_2 p$	$s$	$s \log_2 p$
CA-CG	$\frac{sn}{p}$	$\frac{s^2 n}{p}$	$s\sqrt{n/p}$	$s^2 \log_2 p$	1	$\log_2 p$

All values in the table meant in the Big-O sense (i.e., lower order terms and constants not included)

# From Theory to Practice

---

- Parameter  $s$  is limited by machine parameters and matrix sparsity structure
- We can auto-tune to find the best  $s$  based on these properties
  - That is, find  $s$  that gives the fastest **speed per iteration**

# From Theory to Practice

---

- Parameter  $s$  is limited by machine parameters and matrix sparsity structure
- We can auto-tune to find the best  $s$  based on these properties
  - That is, find  $s$  that gives the fastest **speed per iteration**
- In practice, we don't just care about speed per iteration, but also the number of iterations

$$\text{Runtime} = (\text{time/iteration}) \times (\# \text{ iterations})$$

# From Theory to Practice

---

- Parameter  $s$  is limited by machine parameters and matrix sparsity structure
- We can auto-tune to find the best  $s$  based on these properties
  - That is, find  $s$  that gives the fastest **speed per iteration**
- In practice, we don't just care about speed per iteration, but also the number of iterations

$$\text{Runtime} = (\text{time/iteration}) \times (\# \text{ iterations})$$

- We also need to consider how convergence rate and accuracy are affected by choice of  $s$ !



# From Theory to Practice

---

- CA-KSMs are mathematically equivalent to classical KSMs

# From Theory to Practice

---

- CA-KSMs are mathematically equivalent to classical KSMs
- But can behave much differently in finite precision!

# From Theory to Practice

---

- CA-KSMs are mathematically equivalent to classical KSMs
- But can behave much differently in finite precision!
- Roundoff error bounds generally grow with increasing  $s$

# From Theory to Practice

---

- CA-KSMs are mathematically equivalent to classical KSMs
- But can behave much differently in finite precision!
- Roundoff error bounds generally grow with increasing  $s$
- Two effects of roundoff error:

# From Theory to Practice

---

- CA-KSMs are mathematically equivalent to classical KSMs
- But can behave much differently in finite precision!
- Roundoff error bounds generally grow with increasing  $s$
- Two effects of roundoff error:
  1. **Decrease in accuracy** → Tradeoff: increasing blocking factor  $s$  past a certain point: **true residual  $\mathbf{b} - \mathbf{A}\mathbf{x}$**  stagnates

# From Theory to Practice

---

- CA-KSMs are mathematically equivalent to classical KSMs
- But can behave much differently in finite precision!
- Roundoff error bounds generally grow with increasing  $s$
- Two effects of roundoff error:
  1. **Decrease in accuracy** → Tradeoff: increasing blocking factor  $s$  past a certain point: **true residual  $\mathbf{b} - \mathbf{A}\mathbf{x}$**  stagnates
  2. **Delay of convergence** → Tradeoff: increasing blocking factor  $s$  past a certain point: no speedup expected

# From Theory to Practice

---

- CA-KSMs are mathematically equivalent to classical KSMs
- But can behave much differently in finite precision!
- Roundoff error bounds generally grow with increasing  $s$
- Two effects of roundoff error:
  1. **Decrease in accuracy** → Tradeoff: increasing blocking factor  $s$  past a certain point: **true residual  $\mathbf{b} - \mathbf{A}\mathbf{x}$**  stagnates
  2. **Delay of convergence** → Tradeoff: increasing blocking factor  $s$  past a certain point: no speedup expected

$$\text{Runtime} = (\text{time/iteration}) \times (\# \text{ iterations})$$

# From Theory to Practice

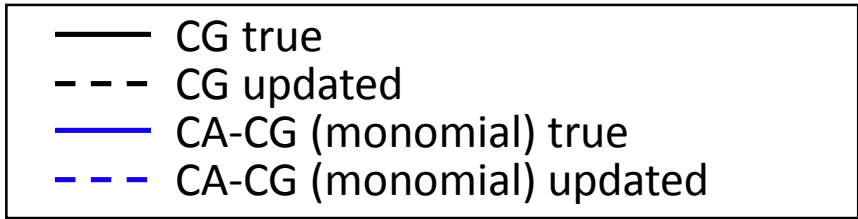
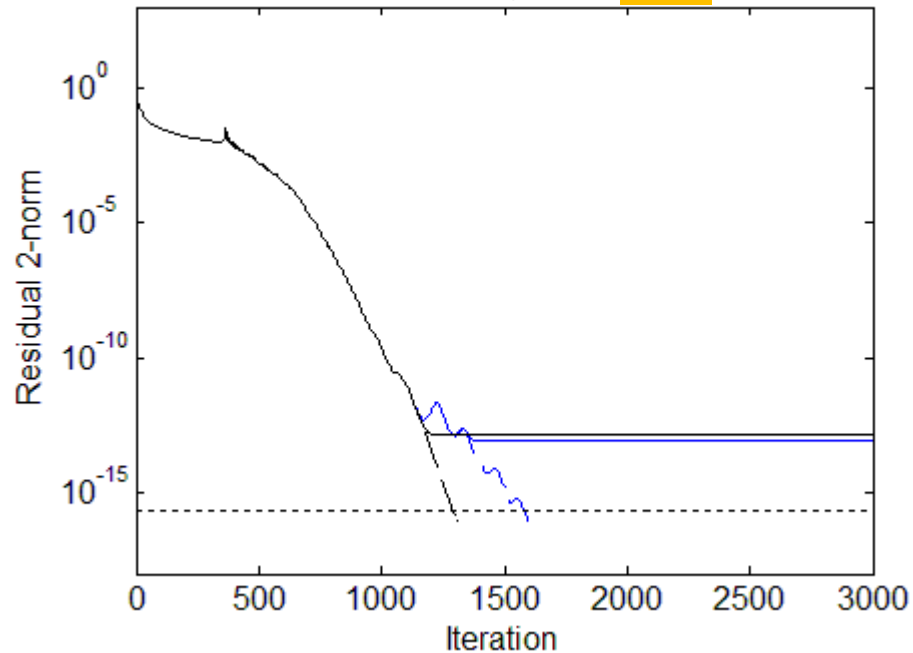
---

- CA-KSMs are mathematically equivalent to classical KSMs
- But can behave much differently in finite precision!
- Roundoff error bounds generally grow with increasing  $s$
- Two effects of roundoff error:
  1. **Decrease in accuracy** → Tradeoff: increasing blocking factor  $s$  past a certain point: **true residual  $\mathbf{b} - \mathbf{A}\mathbf{x}$**  stagnates
  2. **Delay of convergence** → Tradeoff: increasing blocking factor  $s$  past a certain point: no speedup expected

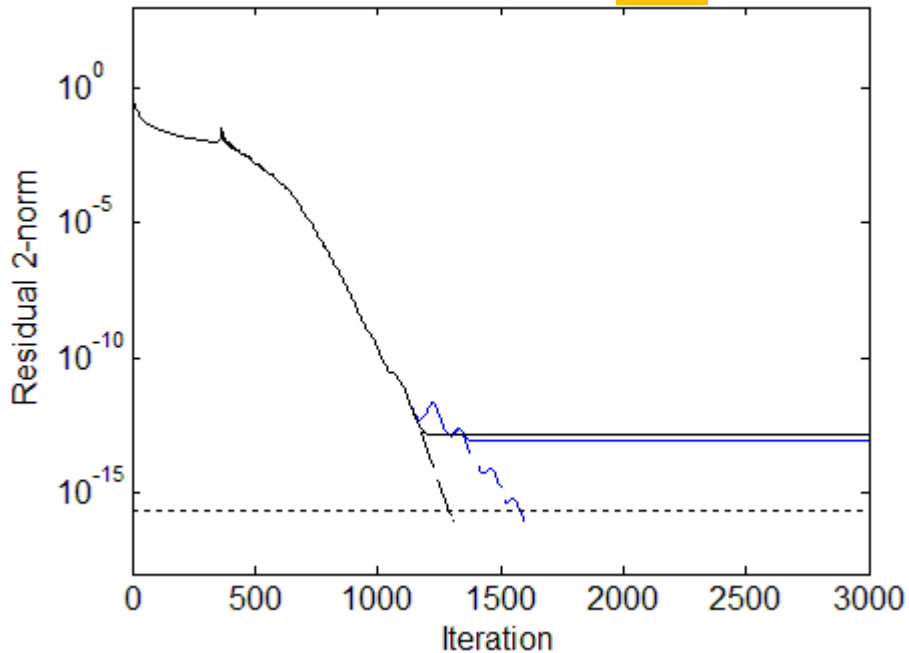
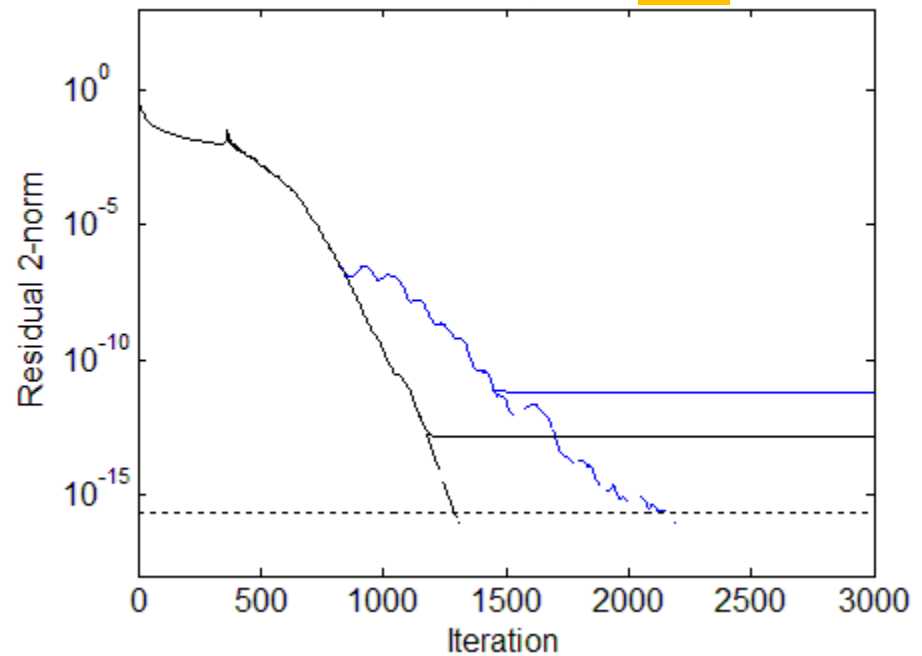

$$\text{Runtime} = (\text{time/iteration}) \times (\# \text{ iterations})$$



CA-CG Convergence,  $s = 4$



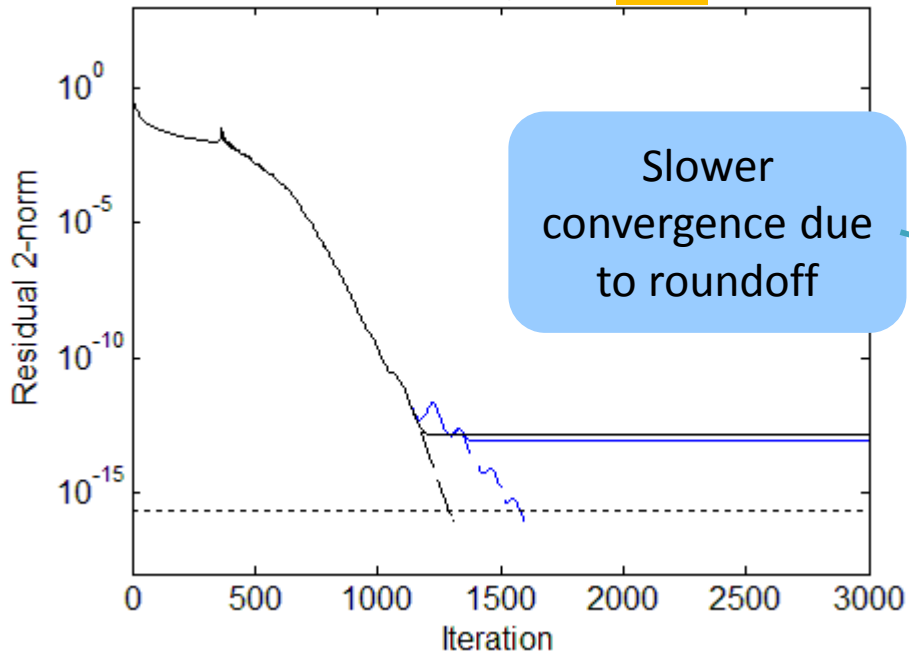
Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

CA-CG Convergence,  $s = 4$ CA-CG Convergence,  $s = 8$ 

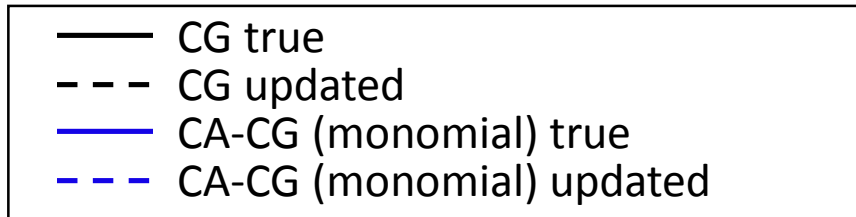
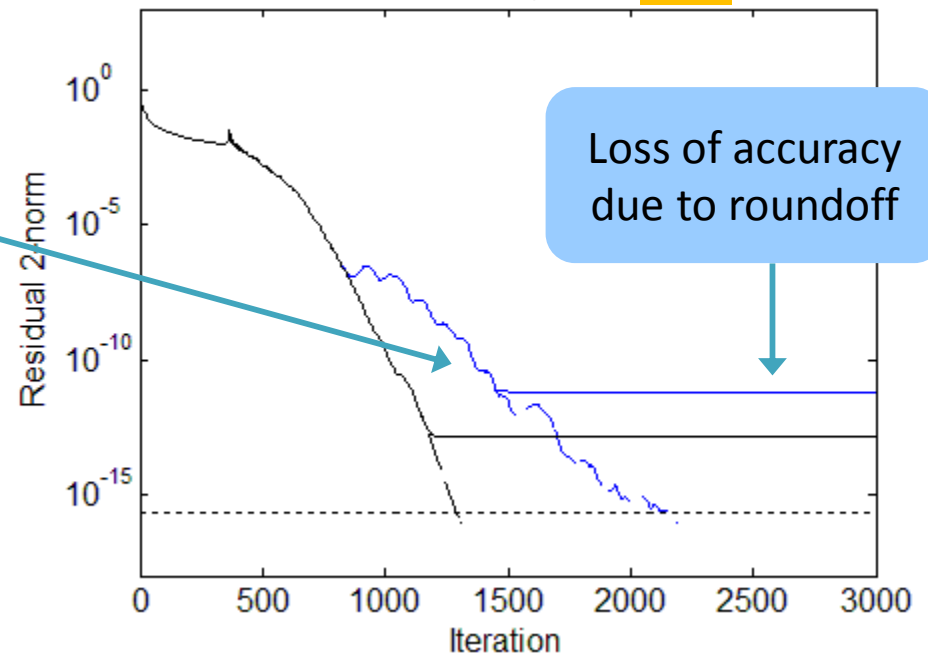
- CG true
- - - CG updated
- CA-CG (monomial) true
- - - CA-CG (monomial) updated

Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

CA-CG Convergence,  $s = 4$

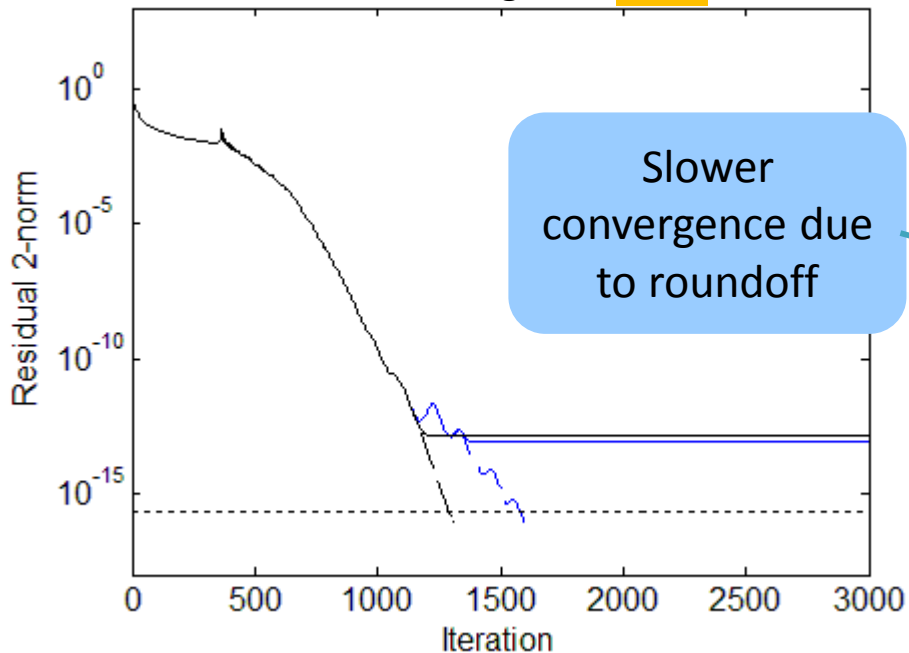


CA-CG Convergence,  $s = 8$

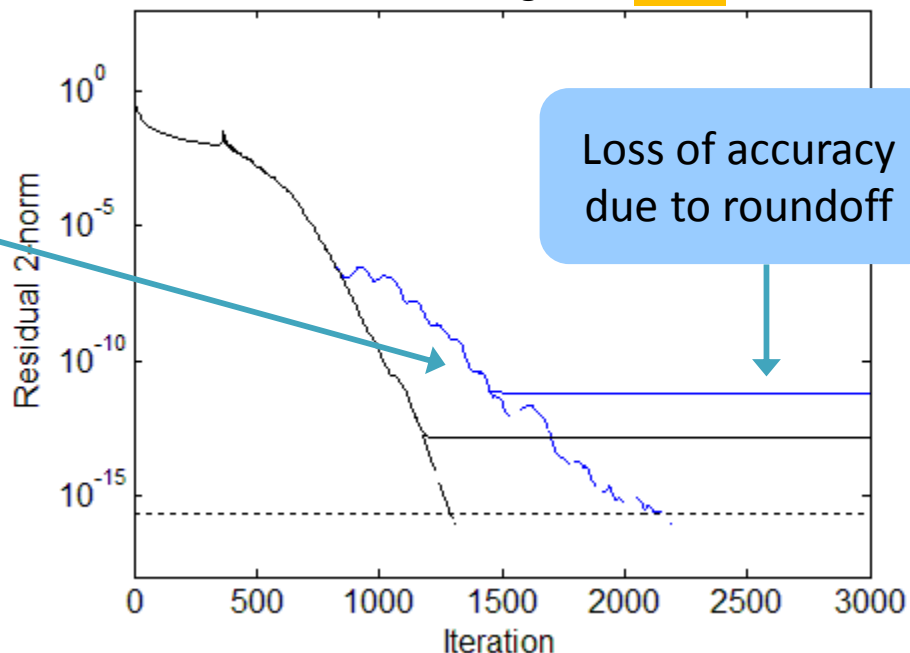


Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

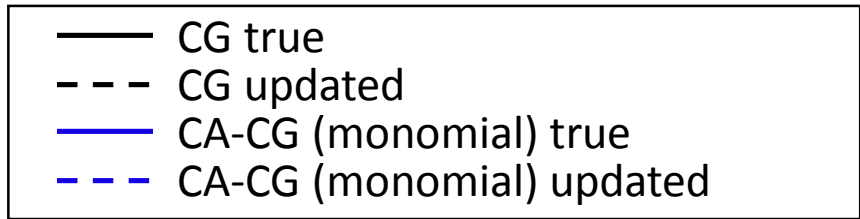
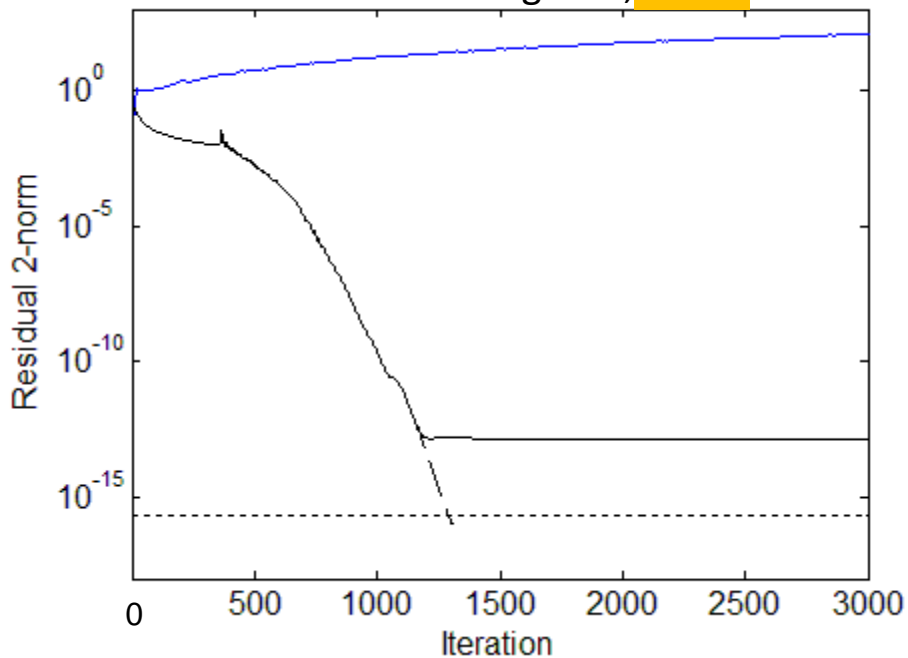
CA-CG Convergence,  $s = 4$



CA-CG Convergence,  $s = 8$

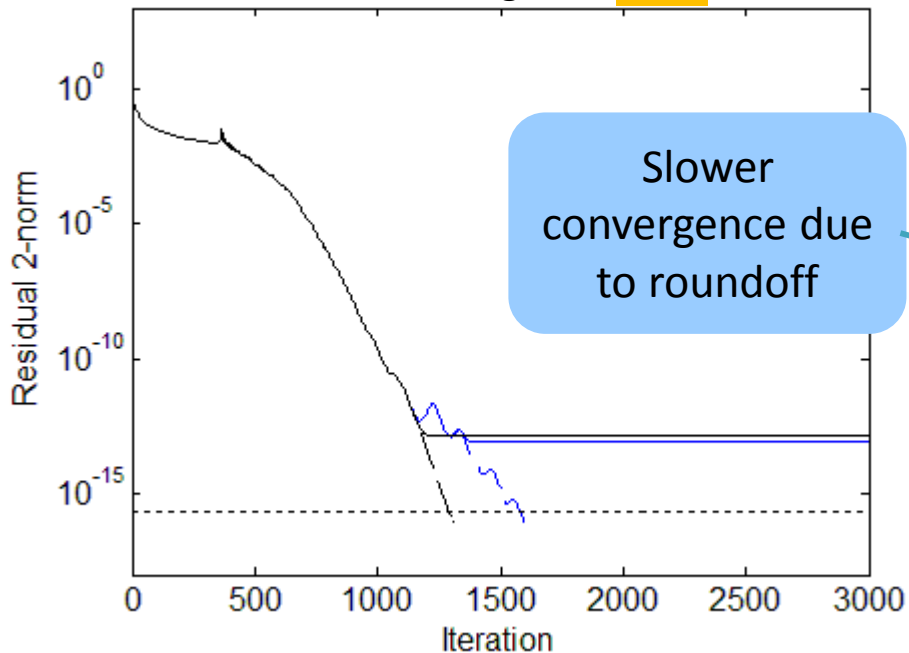


CA-CG Convergence,  $s = 16$

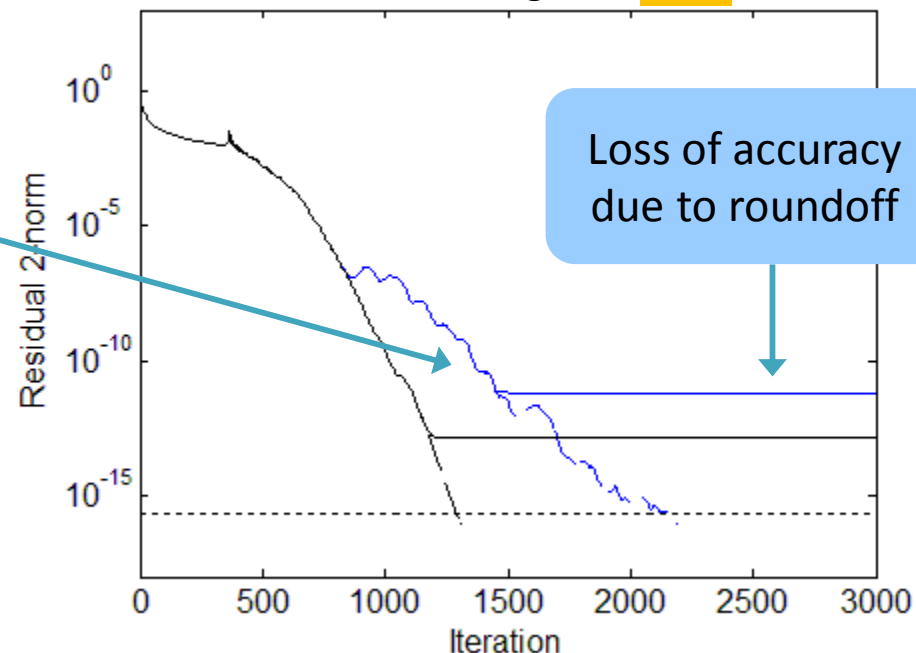


Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

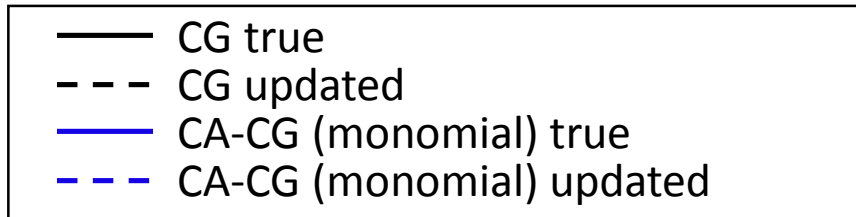
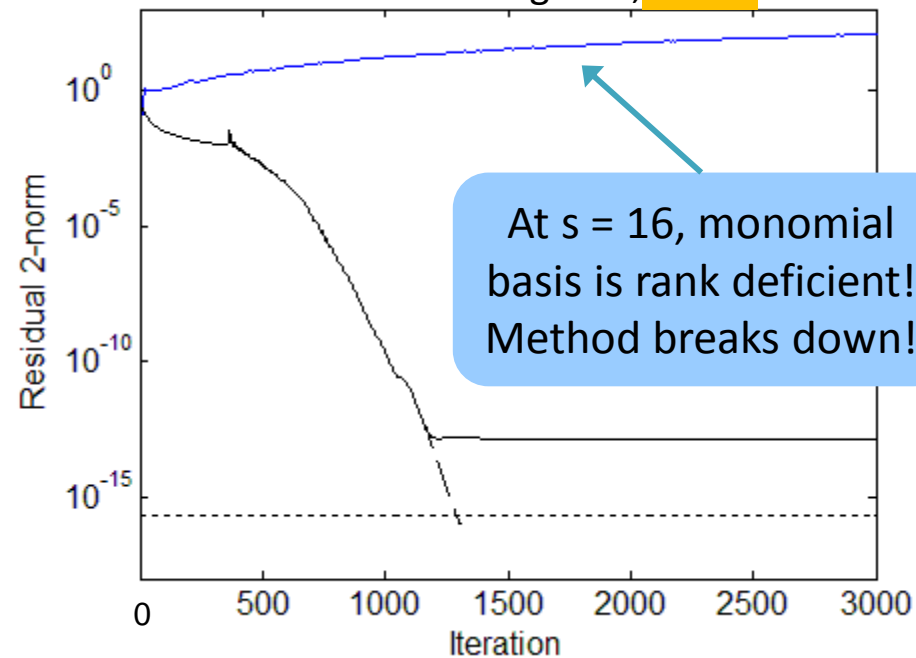
CA-CG Convergence,  $s = 4$



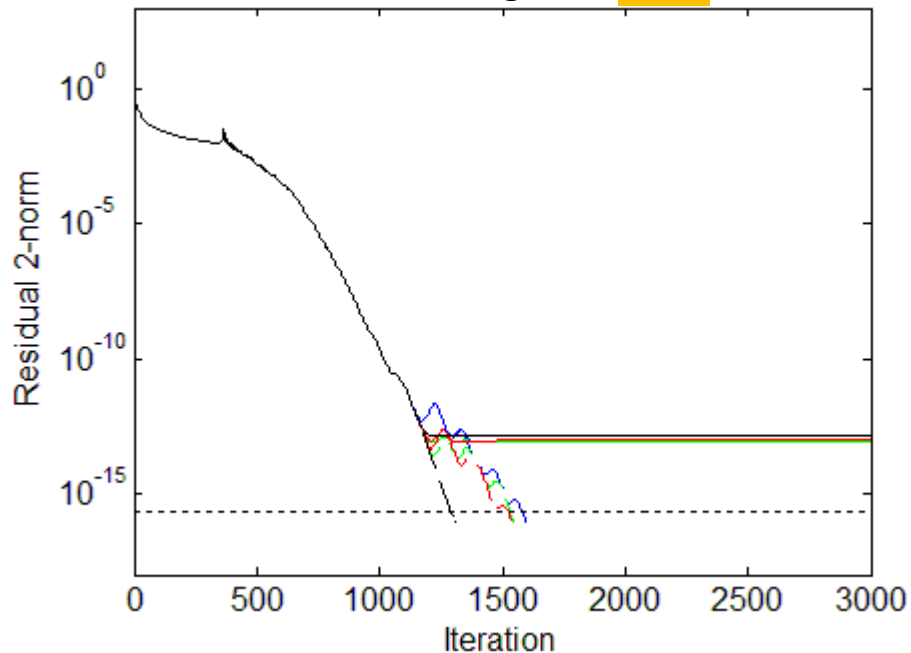
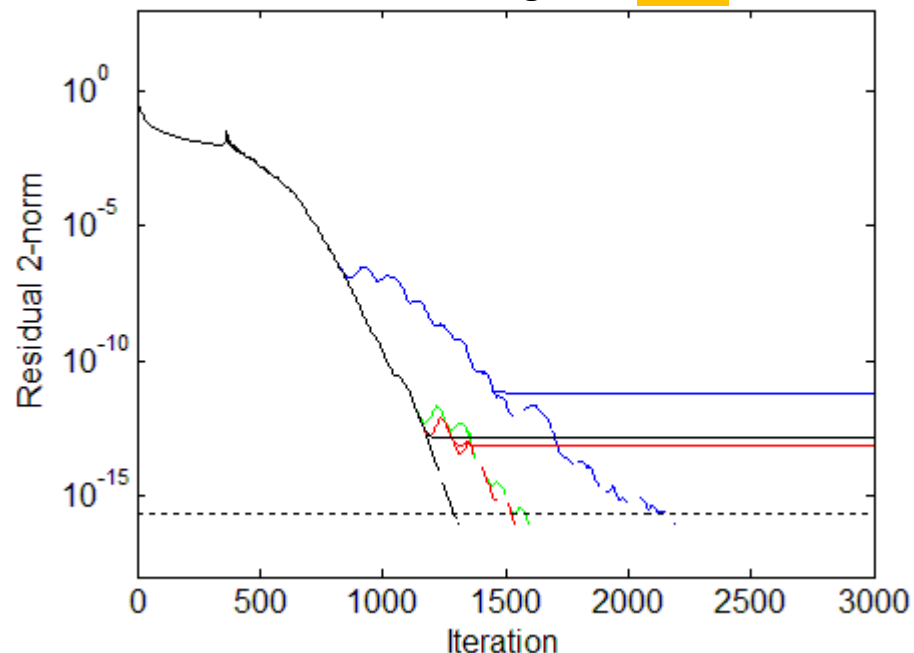
CA-CG Convergence,  $s = 8$



CA-CG Convergence,  $s = 16$

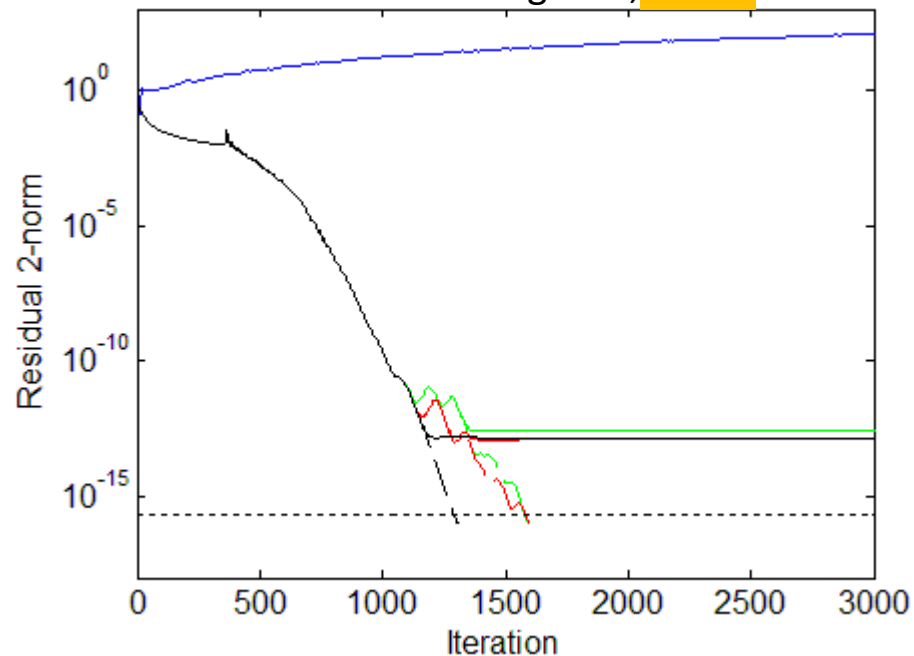


Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

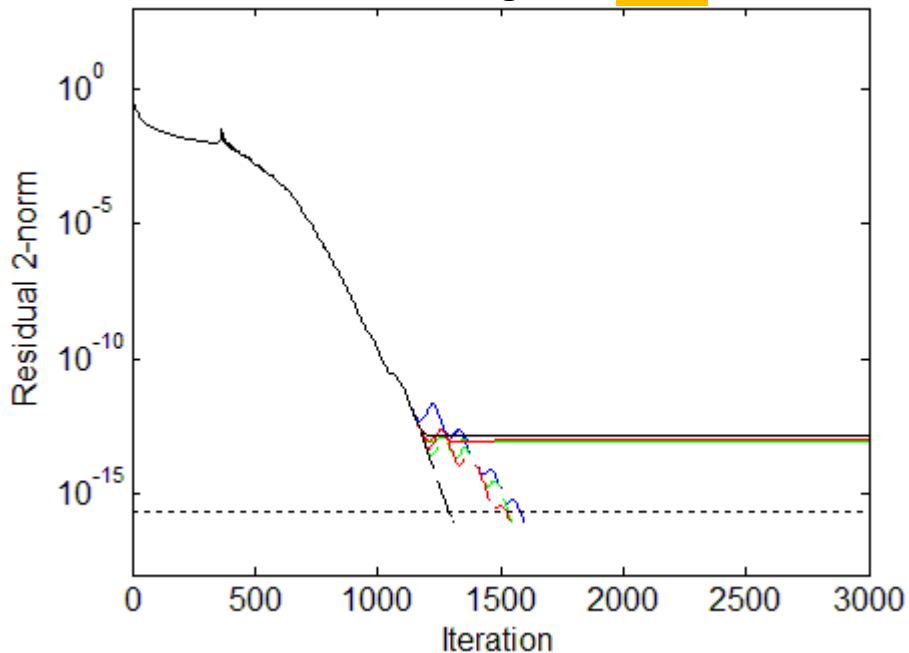
CA-CG Convergence,  $s = 4$ CA-CG Convergence,  $s = 8$ 

- CG true
- - - CG updated
- CA-CG (monomial) true
- - - CA-CG (monomial) updated
- CA-CG (Newton) true
- - - CA-CG (Newton) updated
- CA-CG (Chebyshev) true
- - - CA-CG (Chebyshev) updated

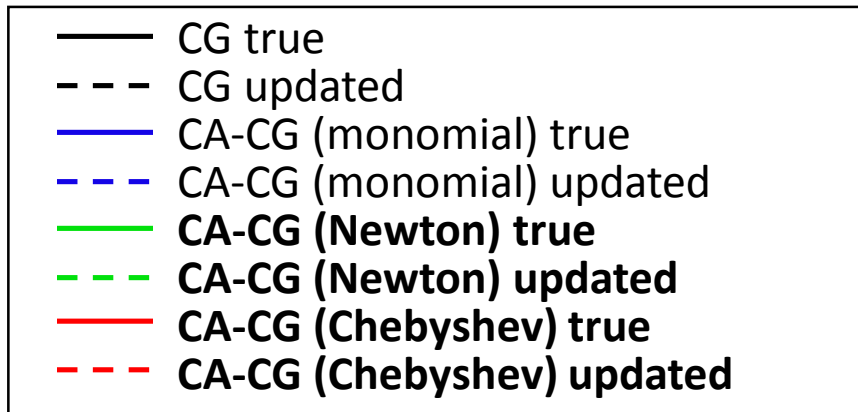
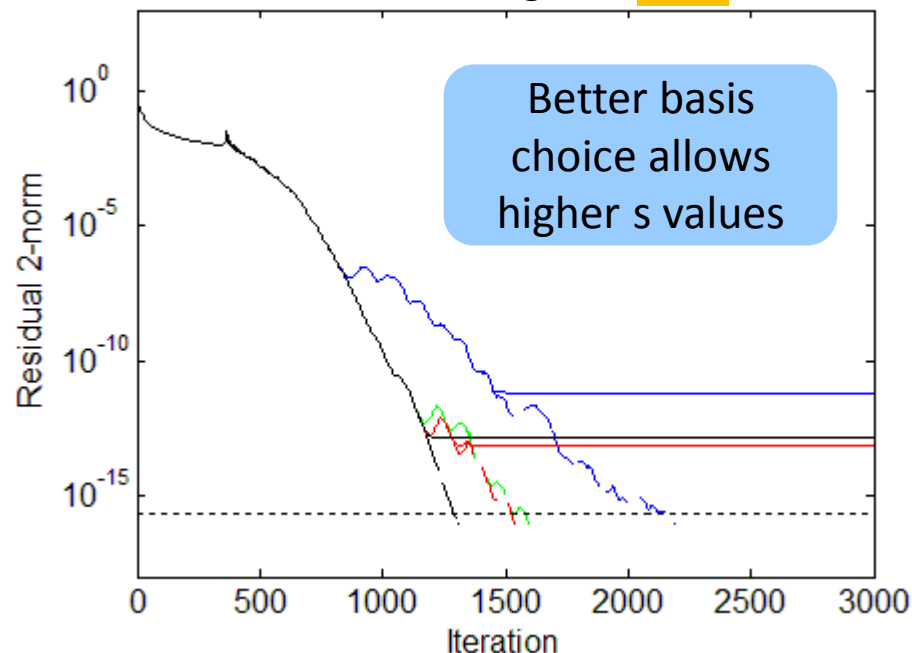
Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

CA-CG Convergence,  $s = 16$ 

CA-CG Convergence,  $s = 4$

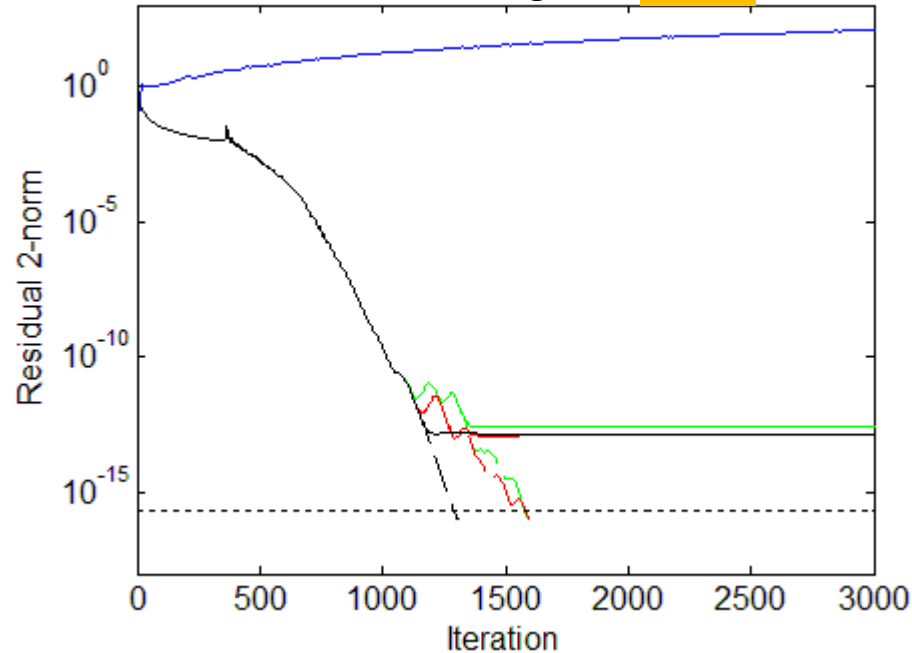


CA-CG Convergence,  $s = 8$

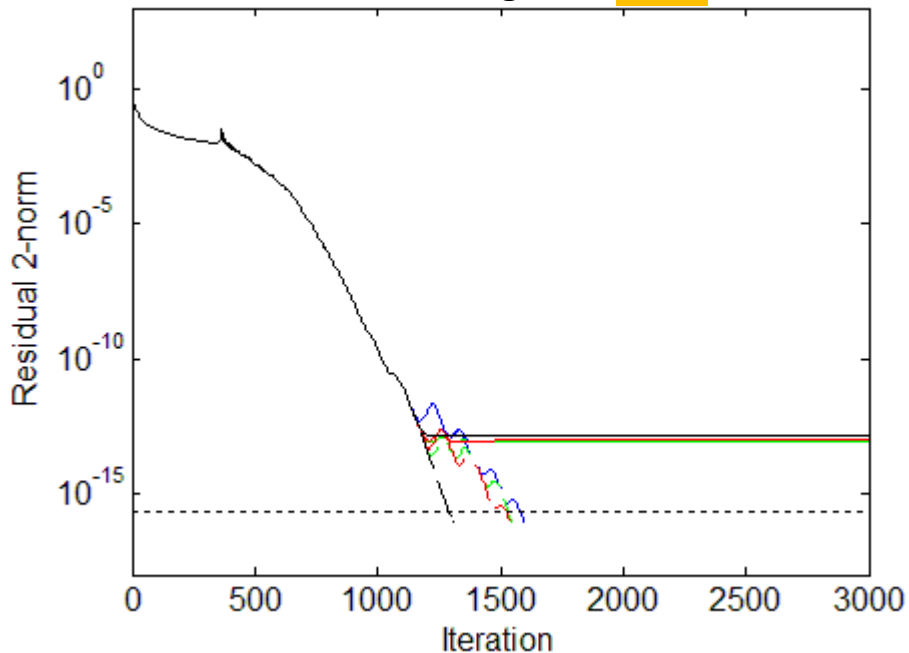


Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

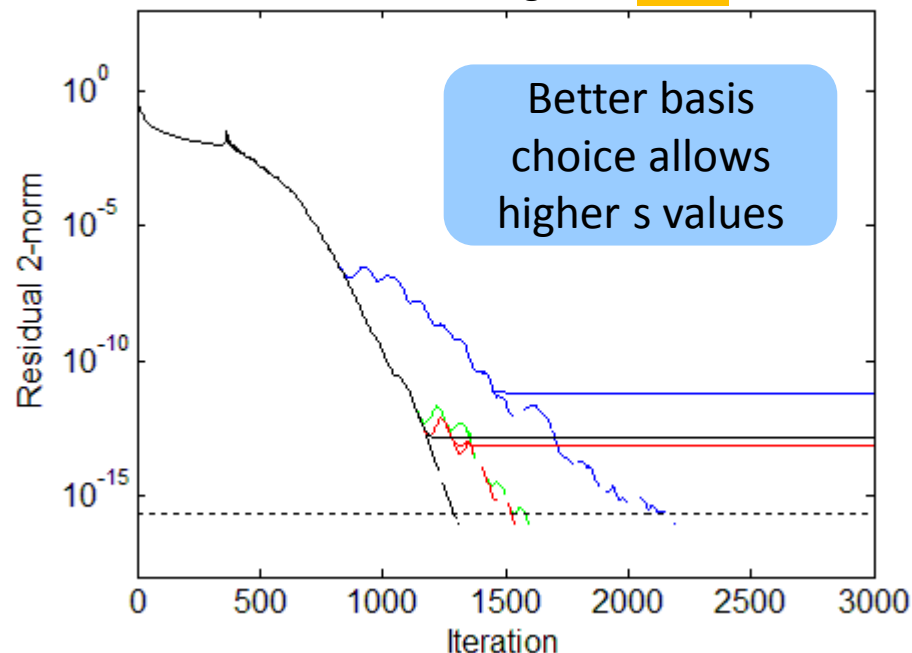
CA-CG Convergence,  $s = 16$



CA-CG Convergence,  $s = 4$



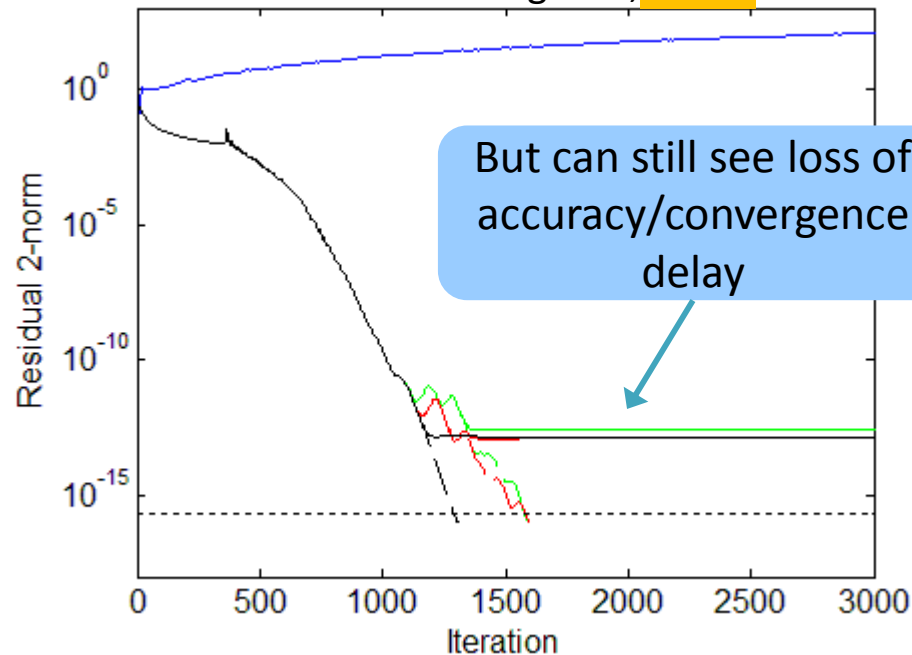
CA-CG Convergence,  $s = 8$



- CG true
- - - CG updated
- CA-CG (monomial) true
- - - CA-CG (monomial) updated
- CA-CG (Newton) true
- - - CA-CG (Newton) updated
- CA-CG (Chebyshev) true
- - - CA-CG (Chebyshev) updated

Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

CA-CG Convergence,  $s = 16$





# Maximum attainable accuracy of CG

---

- In classical CG, iterates are updated by

$$x_{m+1} = x_m + \alpha_m p_m \quad \text{and} \quad r_{m+1} = r_m - \alpha_m A p_m$$

- Formulas for  $x_{m+1}$  and  $r_{m+1}$  do not depend on each other - rounding errors cause the true residual,  $b - Ax_{m+1}$ , and the updated residual,  $r_{m+1}$ , to deviate

# Maximum attainable accuracy of CG

---

- In classical CG, iterates are updated by

$$x_{m+1} = x_m + \alpha_m p_m \quad \text{and} \quad r_{m+1} = r_m - \alpha_m A p_m$$

- Formulas for  $x_{m+1}$  and  $r_{m+1}$  do not depend on each other - rounding errors cause the true residual,  $b - Ax_{m+1}$ , and the updated residual,  $r_{m+1}$ , to deviate
- The size of the true residual is bounded by

$$\|b - Ax_{m+1}\| \leq \|r_{m+1}\| + \|b - Ax_{m+1} - r_{m+1}\|$$

- When  $\|r_{m+1}\| \gg \|b - Ax_{m+1} - r_{m+1}\|$ ,  $\|r_{m+1}\|$  and  $\|b - Ax_{m+1}\|$  have similar magnitude
- When  $\|r_{m+1}\| \rightarrow 0$ ,  $\|b - Ax_{m+1}\|$  depends on  $\|b - Ax_{m+1} - r_{m+1}\|$

# Maximum attainable accuracy of CG

---

- In classical CG, iterates are updated by

$$x_{m+1} = x_m + \alpha_m p_m \quad \text{and} \quad r_{m+1} = r_m - \alpha_m A p_m$$

- Formulas for  $x_{m+1}$  and  $r_{m+1}$  do not depend on each other - rounding errors cause the true residual,  $b - Ax_{m+1}$ , and the updated residual,  $r_{m+1}$ , to deviate
- The size of the true residual is bounded by

$$\|b - Ax_{m+1}\| \leq \|r_{m+1}\| + \|b - Ax_{m+1} - r_{m+1}\|$$

- When  $\|r_{m+1}\| \gg \|b - Ax_{m+1} - r_{m+1}\|$ ,  $\|r_{m+1}\|$  and  $\|b - Ax_{m+1}\|$  have similar magnitude
- When  $\|r_{m+1}\| \rightarrow 0$ ,  $\|b - Ax_{m+1}\|$  depends on  $\|b - Ax_{m+1} - r_{m+1}\|$
- Many results on attainable accuracy, e.g.: Greenbaum (1989, 1994, 1997), Sleijpen, van der Vorst and Fokkema (1994), Sleijpen, van der Vorst and Modersitzki (2001), Björck, Elfving and Strakoš (1998) and Gutknecht and Strakoš (2000).
- We have applied a similar analysis to upper bound the maximum attainable accuracy in finite precision CA-KSMs

# Residual Replacement Strategy for CG

---

- van der Vorst and Ye (1999): Improve accuracy by replacing **updated residual**  $r_{m+1}$  by the **true residual**  $b - Ax_{m+1}$  in certain iterations, combined with group update.

# Residual Replacement Strategy for CG

---

- van der Vorst and Ye (1999): Improve accuracy by replacing **updated residual**  $r_{m+1}$  by the **true residual**  $b - Ax_{m+1}$  in certain iterations, combined with group update.
- Choose when to replace  $r_{m+1}$  with  $b - Ax_{m+1}$  to meet two constraints:

# Residual Replacement Strategy for CG

---

- van der Vorst and Ye (1999): Improve accuracy by replacing **updated residual**  $r_{m+1}$  by the **true residual**  $b - Ax_{m+1}$  in certain iterations, combined with group update.
- Choose when to replace  $r_{m+1}$  with  $b - Ax_{m+1}$  to meet two constraints:
  1. **Replace often enough** so that at termination,  $\|b - Ax_{m+1} - r_{m+1}\|$  is small relative to  $\varepsilon N \|A\| \|x_{m+1}\|$

# Residual Replacement Strategy for CG

---

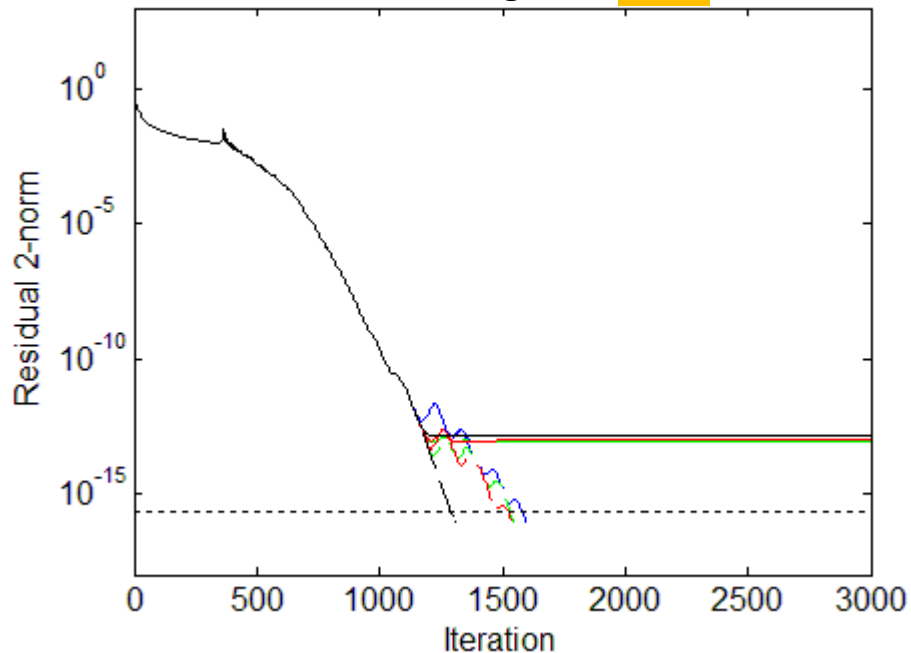
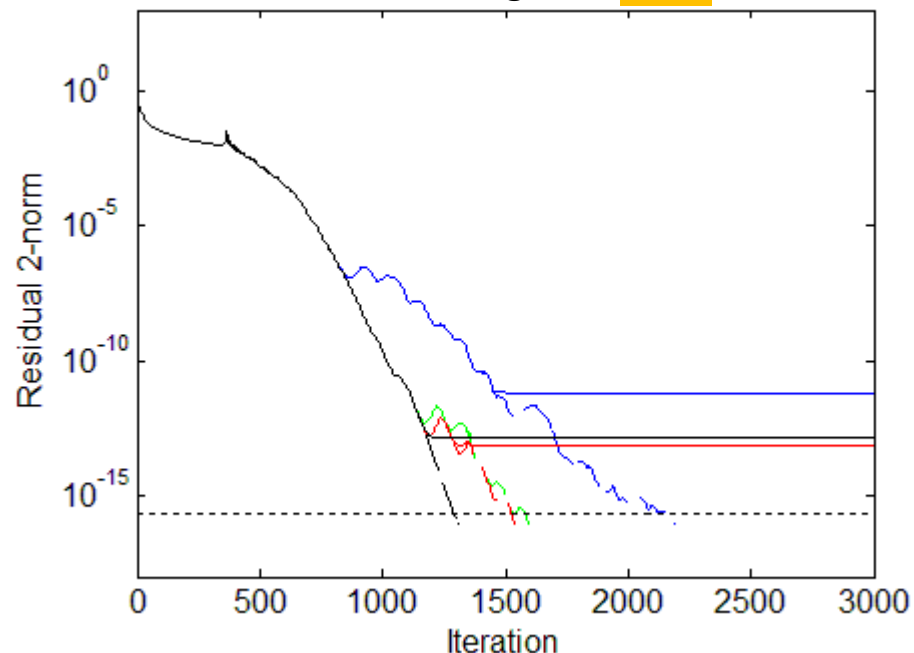
- van der Vorst and Ye (1999): Improve accuracy by replacing **updated residual**  $r_{m+1}$  by the **true residual**  $b - Ax_{m+1}$  in certain iterations, combined with group update.
- Choose when to replace  $r_{m+1}$  with  $b - Ax_{m+1}$  to meet two constraints:
  1. **Replace often enough** so that at termination,  $\|b - Ax_{m+1} - r_{m+1}\|$  is small relative to  $\varepsilon N \|A\| \|x_{m+1}\|$
  2. **Don't replace so often** that original convergence mechanism of updated residuals is destroyed (avoid large perturbations to finite precision CG recurrence)

# Residual Replacement Strategy for CG

---

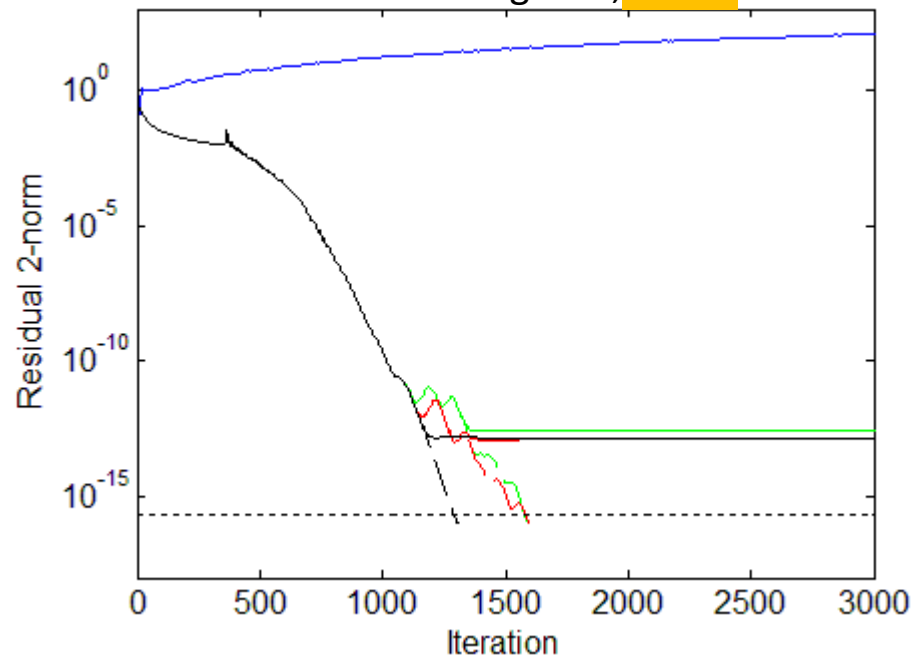
- van der Vorst and Ye (1999): Improve accuracy by replacing **updated residual**  $r_{m+1}$  by the **true residual**  $b - Ax_{m+1}$  in certain iterations, combined with group update.
- Choose when to replace  $r_{m+1}$  with  $b - Ax_{m+1}$  to meet two constraints:
  1. **Replace often enough** so that at termination,  $\|b - Ax_{m+1} - r_{m+1}\|$  is small relative to  $\varepsilon N \|A\| \|x_{m+1}\|$
  2. **Don't replace so often** that original convergence mechanism of updated residuals is destroyed (avoid large perturbations to finite precision CG recurrence)
- We can implement an analogous strategy for CA-CG and CA-BICG based on derived bound on deviation of residuals
  - Estimating quantities in bound has **negligible cost**  $\rightarrow$  residual replacement strategy does not asymptotically increase communication or computation!

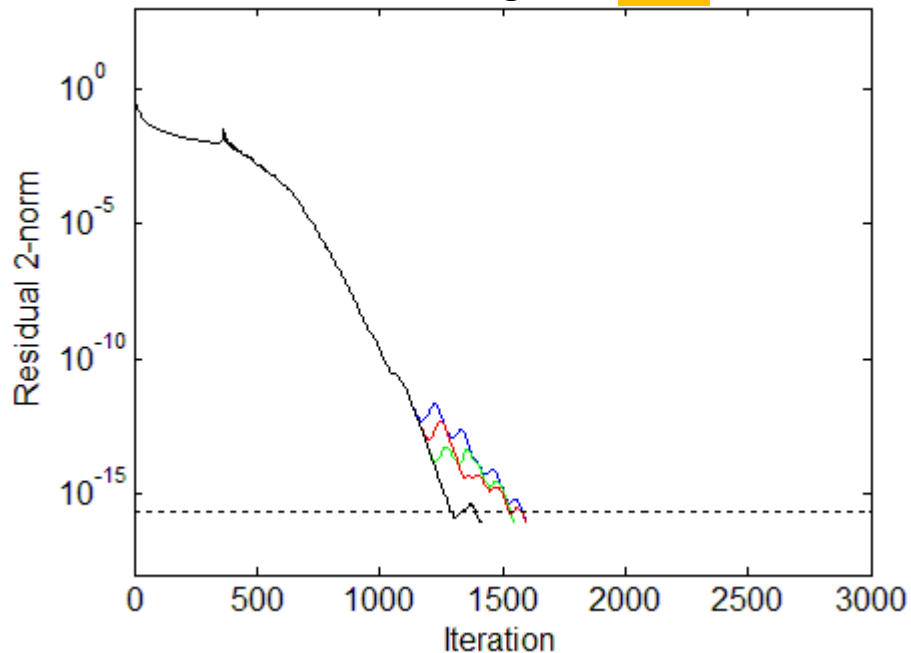
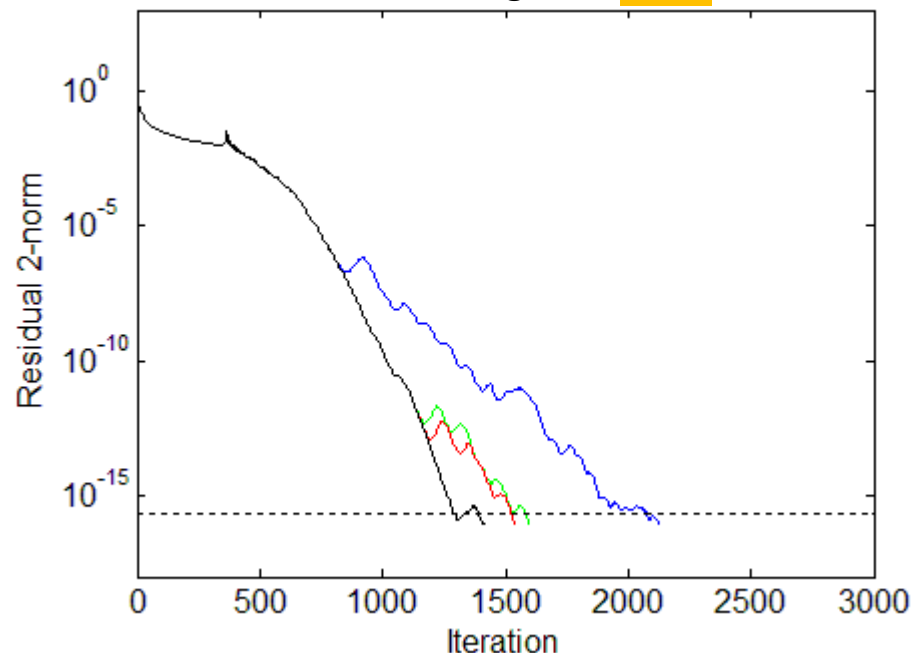
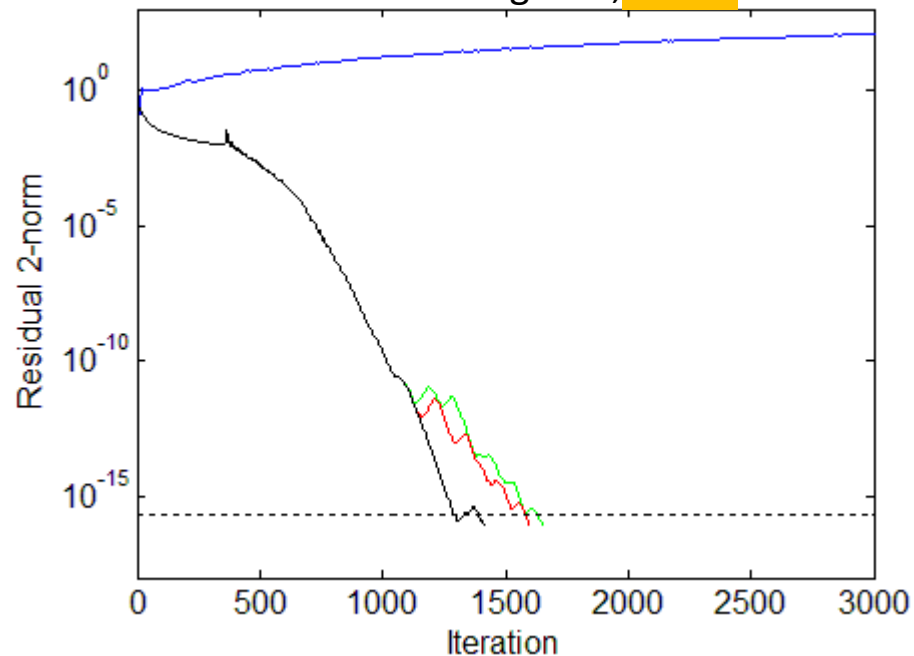


CA-CG Convergence,  $s = 4$ CA-CG Convergence,  $s = 8$ 

- CG true
- - - CG updated
- CA-CG (monomial) true
- - - CA-CG (monomial) updated
- CA-CG (Newton) true
- - - CA-CG (Newton) updated
- CA-CG (Chebyshev) true
- - - CA-CG (Chebyshev) updated

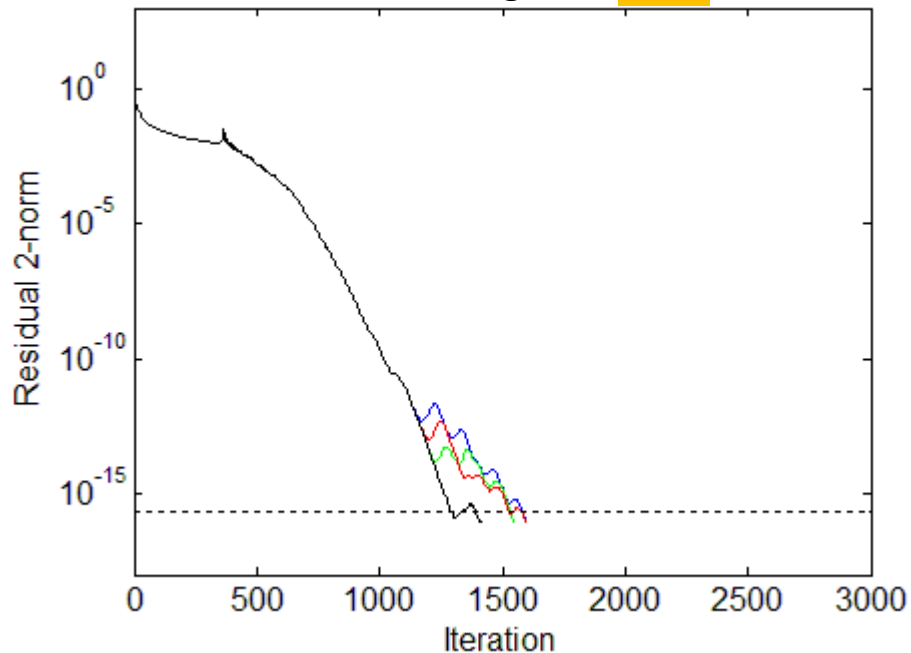
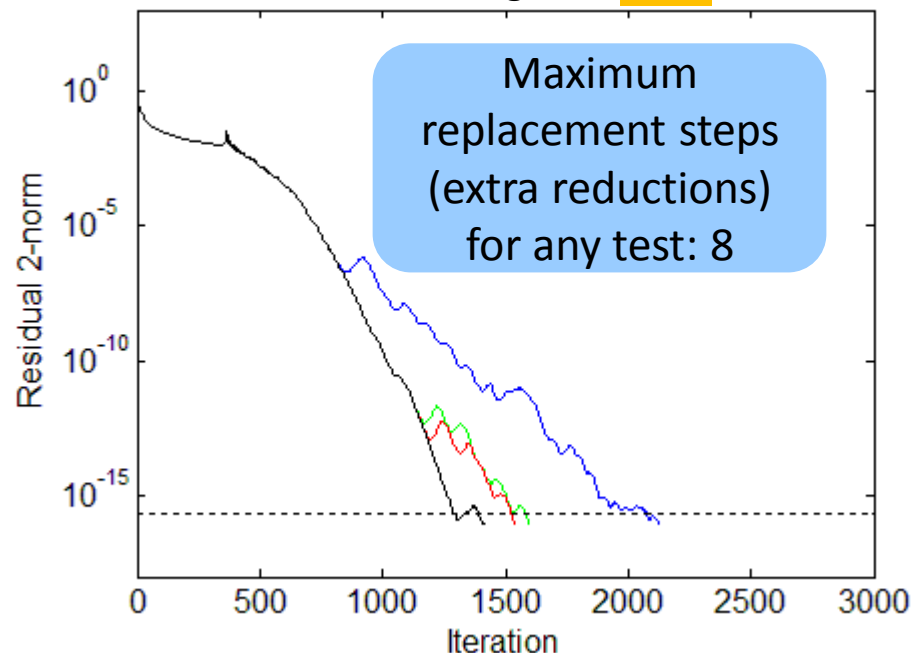
Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

CA-CG Convergence,  $s = 16$ 

CA-CG Convergence,  $s = 4$ CA-CG Convergence,  $s = 8$ CA-CG Convergence,  $s = 16$ 

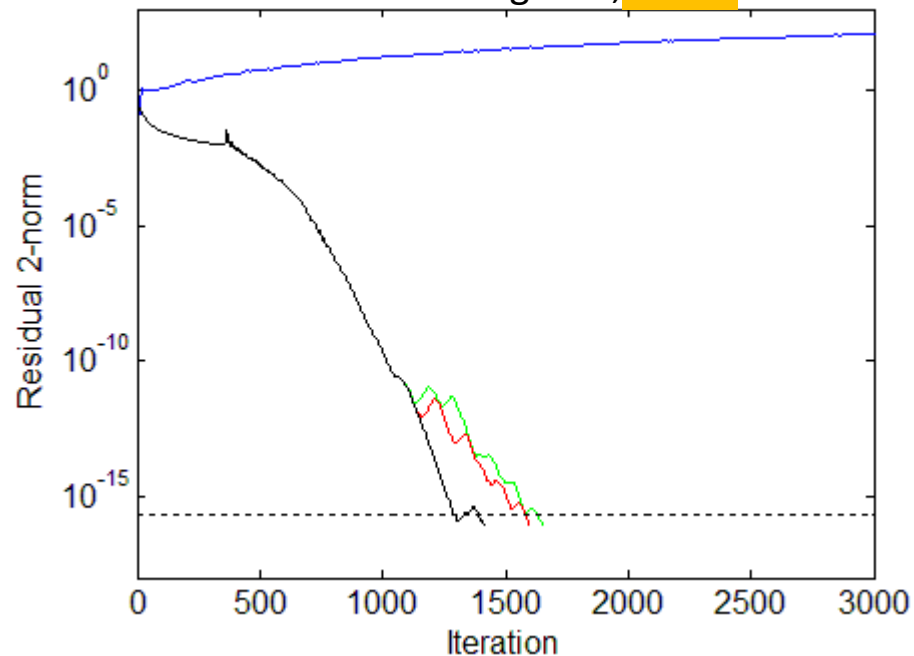
- CG-RR true
- - - CG-RR updated
- CA-CG-RR (monomial) true
- - - CA-CG-RR (monomial) updated
- CA-CG-RR (Newton) true
- - - CA-CG-RR (Newton) updated
- CA-CG-RR (Chebyshev) true
- - - CA-CG-RR (Chebyshev) updated

Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

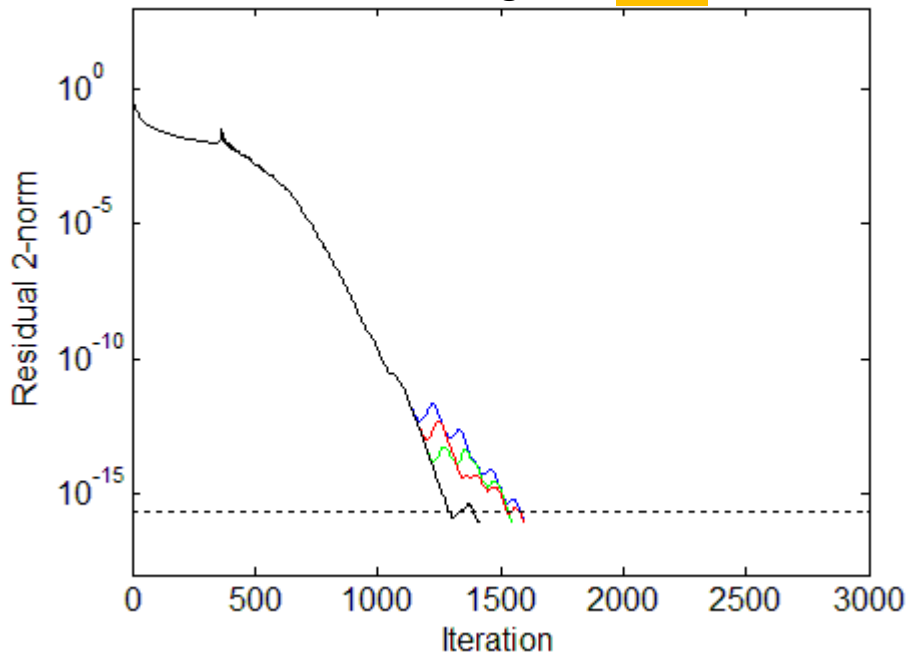
CA-CG Convergence,  $s = 4$ CA-CG Convergence,  $s = 8$ 

- CG-RR true
- - - CG-RR updated
- CA-CG-RR (monomial) true
- - - CA-CG-RR (monomial) updated
- CA-CG-RR (Newton) true
- - - CA-CG-RR (Newton) updated
- CA-CG-RR (Chebyshev) true
- - - CA-CG-RR (Chebyshev) updated

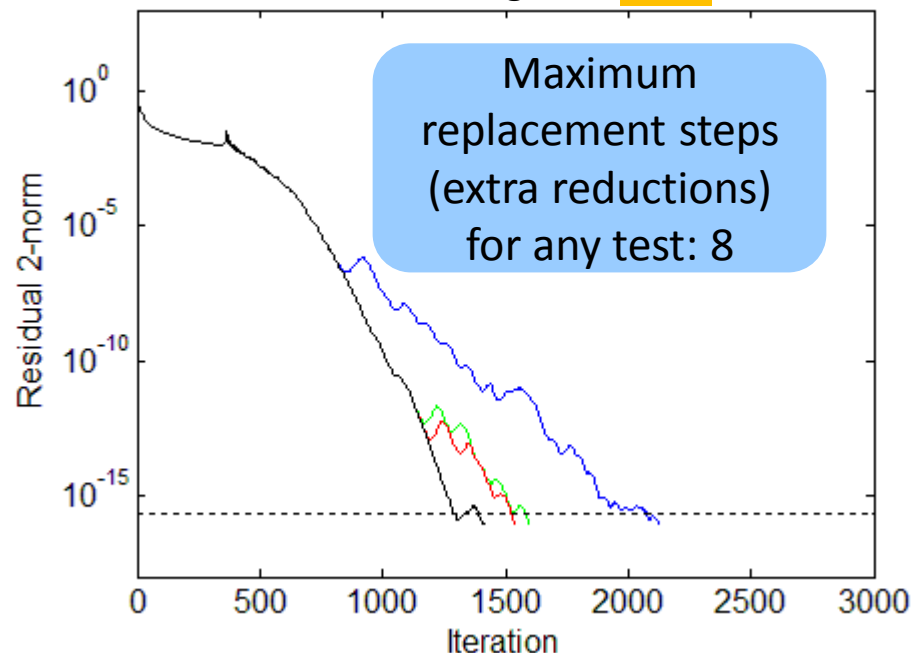
Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

CA-CG Convergence,  $s = 16$ 

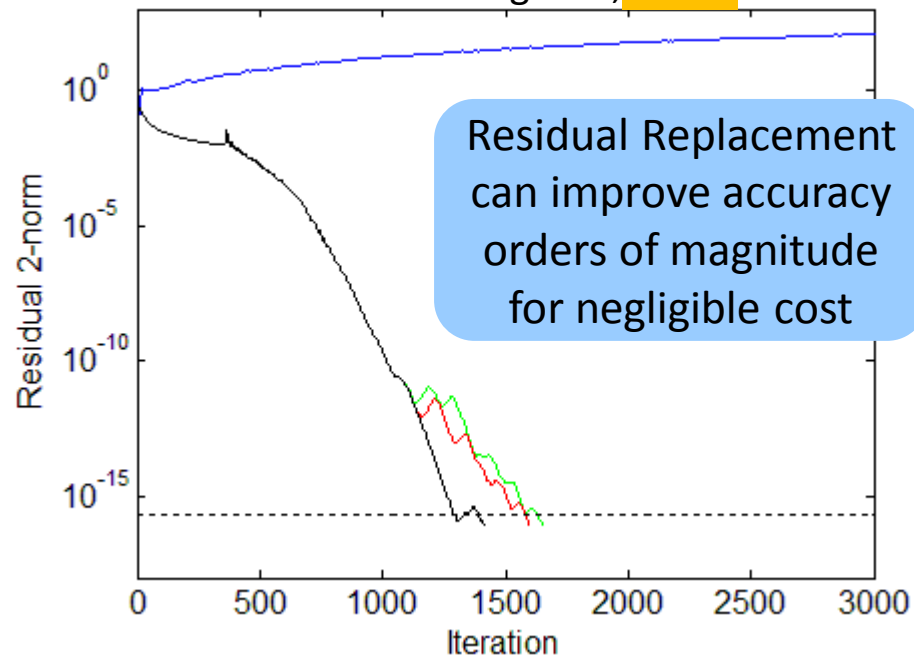
CA-CG Convergence,  $s = 4$



CA-CG Convergence,  $s = 8$



CA-CG Convergence,  $s = 16$



- CG-RR true
- - - CG-RR updated
- CA-CG-RR (monomial) true
- - - CA-CG-RR (monomial) updated
- CA-CG-RR (Newton) true
- - - CA-CG-RR (Newton) updated
- CA-CG-RR (Chebyshev) true
- - - CA-CG-RR (Chebyshev) updated

Model Problem: 2D Poisson (5-pt stencil),  
 $n = 512^2$ ,  $\text{nnz} \approx 10^6$ ,  $\kappa(A) \approx 10^4$   
 $b = A(1\sqrt{n} \cdot \text{ones}(n, 1))$

# Paige's Results for Classical Lanczos

---

- Using bounds on local rounding errors in Lanczos, Paige showed that
  1. The computed Ritz values always lie between the extreme eigenvalues of  $A$  to within a small multiple of machine precision.
  2. At least one small interval containing an eigenvalue of  $A$  is found by the  $n$ th iteration.
  3. The algorithm behaves numerically like Lanczos with full reorthogonalization until a very close eigenvalue approximation is found.
  4. The loss of orthogonality among basis vectors follows a rigorous pattern and implies that some Ritz values have converged.

# Paige's Results for Classical Lanczos

---

- Using bounds on local rounding errors in Lanczos, Paige showed that
  1. The computed Ritz values always lie between the extreme eigenvalues of  $A$  to within a small multiple of machine precision.
  2. At least one small interval containing an eigenvalue of  $A$  is found by the  $n$ th iteration.
  3. The algorithm behaves numerically like Lanczos with full reorthogonalization until a very close eigenvalue approximation is found.
  4. The loss of orthogonality among basis vectors follows a rigorous pattern and implies that some Ritz values have converged.

Do the same statements hold for CA-Lanczos?

# Paige's Lanczos Convergence Analysis

---

Finite precision Lanczos process: ( $A$  is  $n \times n$  with at most  $N$  nonzeros per row)

$$A\hat{V}_m = \hat{V}_m\hat{T}_m + \hat{\beta}_{m+1}\hat{v}_{m+1}e_m^T + \delta\hat{V}_m$$

$$\hat{V}_m = [\hat{v}_1, \dots, \hat{v}_m], \quad \delta\hat{V}_m = [\delta\hat{v}_1, \dots, \delta\hat{v}_m], \quad \hat{T}_m = \begin{bmatrix} \hat{\alpha}_1 & \hat{\beta}_2 & & \\ \hat{\beta}_2 & \ddots & \ddots & \\ & \ddots & \ddots & \hat{\beta}_m \\ & & \hat{\beta}_m & \hat{\alpha}_m \end{bmatrix}$$

# Paige's Lanczos Convergence Analysis

Finite precision Lanczos process: ( $A$  is  $n \times n$  with at most  $N$  nonzeros per row)

$$A\hat{V}_m = \hat{V}_m\hat{T}_m + \hat{\beta}_{m+1}\hat{v}_{m+1}e_m^T + \delta\hat{V}_m$$

$$\hat{V}_m = [\hat{v}_1, \dots, \hat{v}_m], \quad \delta\hat{V}_m = [\delta\hat{v}_1, \dots, \delta\hat{v}_m], \quad \hat{T}_m = \begin{bmatrix} \hat{\alpha}_1 & \hat{\beta}_2 & & & \\ \hat{\beta}_2 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & \hat{\beta}_m & \\ & & & & \hat{\alpha}_m \end{bmatrix}$$

Classic Lanczos rounding  
error result of Paige (1976):

for  $i \in \{1, \dots, m\}$ ,

$$\begin{aligned} \|\delta\hat{v}_i\|_2 &\leq \varepsilon_1\sigma \\ \hat{\beta}_{i+1}|\hat{v}_i^T\hat{v}_{i+1}| &\leq 2\varepsilon_0\sigma \\ |\hat{v}_{i+1}^T\hat{v}_{i+1} - 1| &\leq \varepsilon_0/2 \\ |\hat{\beta}_{i+1}^2 + \hat{\alpha}_i^2 + \hat{\beta}_i^2 - \|A\hat{v}_i\|_2^2| &\leq 4i(3\varepsilon_0 + \varepsilon_1)\sigma^2 \end{aligned}$$

where  $\sigma \equiv \|A\|_2$ ,  $\theta\sigma \equiv \| \|A\| \|_2$ ,  $\varepsilon_0 \equiv 2\varepsilon(n+4)$ , and  $\varepsilon_1 \equiv 2\varepsilon(N\theta+7)$



# Paige's Lanczos Convergence Analysis

Finite precision Lanczos process: ( $A$  is  $n \times n$  with at most  $N$  nonzeros per row)

$$A\hat{V}_m = \hat{V}_m\hat{T}_m + \hat{\beta}_{m+1}\hat{v}_{m+1}e_m^T + \delta\hat{V}_m$$

$$\hat{V}_m = [\hat{v}_1, \dots, \hat{v}_m], \quad \delta\hat{V}_m = [\delta\hat{v}_1, \dots, \delta\hat{v}_m], \quad \hat{T}_m = \begin{bmatrix} \hat{\alpha}_1 & \hat{\beta}_2 & & & \\ \hat{\beta}_2 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & \hat{\beta}_m & \hat{\alpha}_m \\ & & & & \hat{\alpha}_m \end{bmatrix}$$

Classic Lanczos rounding error result of Paige (1976):

for  $i \in \{1, \dots, m\}$ ,

$$\begin{aligned} \|\delta\hat{v}_i\|_2 &\leq \varepsilon_1\sigma \\ \hat{\beta}_{i+1}|\hat{v}_i^T\hat{v}_{i+1}| &\leq 2\varepsilon_0\sigma \\ |\hat{v}_{i+1}^T\hat{v}_{i+1} - 1| &\leq \varepsilon_0/2 \\ |\hat{\beta}_{i+1}^2 + \hat{\alpha}_i^2 + \hat{\beta}_i^2 - \|A\hat{v}_i\|_2^2| &\leq 4i(3\varepsilon_0 + \varepsilon_1)\sigma^2 \end{aligned}$$

where  $\sigma \equiv \|A\|_2$ ,  $\theta\sigma \equiv \| \|A\| \|_2$ ,  $\varepsilon_0 \equiv 2\varepsilon(n+4)$ , and  $\varepsilon_1 \equiv 2\varepsilon(N\theta+7)$

$$\begin{array}{c} \uparrow \\ \varepsilon_0 = O(\varepsilon n) \end{array}$$

$$\begin{array}{c} \uparrow \\ \varepsilon_1 = O(\varepsilon N\theta) \end{array}$$

# Paige's Lanczos Convergence Analysis

Finite precision Lanczos process: ( $A$  is  $n \times n$  with at most  $N$  nonzeros per row)

$$A\hat{V}_m = \hat{V}_m\hat{T}_m + \hat{\beta}_{m+1}\hat{v}_{m+1}e_m^T + \delta\hat{V}_m$$

$$\hat{V}_m = [\hat{v}_1, \dots, \hat{v}_m], \quad \delta\hat{V}_m = [\delta\hat{v}_1, \dots, \delta\hat{v}_m], \quad \hat{T}_m = \begin{bmatrix} \hat{\alpha}_1 & \hat{\beta}_2 & & & \\ \hat{\beta}_2 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & \hat{\beta}_m & \\ & & & & \hat{\alpha}_m \end{bmatrix}$$

Classic Lanczos rounding error result of Paige (1976):

for  $i \in \{1, \dots, m\}$ ,

$$\begin{aligned} \|\delta\hat{v}_i\|_2 &\leq \varepsilon_1\sigma \\ \hat{\beta}_{i+1}|\hat{v}_i^T\hat{v}_{i+1}| &\leq 2\varepsilon_0\sigma \\ |\hat{v}_{i+1}^T\hat{v}_{i+1} - 1| &\leq \varepsilon_0/2 \\ |\hat{\beta}_{i+1}^2 + \hat{\alpha}_i^2 + \hat{\beta}_i^2 - \|A\hat{v}_i\|_2^2| &\leq 4i(3\varepsilon_0 + \varepsilon_1)\sigma^2 \end{aligned}$$

where  $\sigma \equiv \|A\|_2$ ,  $\theta\sigma \equiv \| \|A\| \|_2$ ,  $\varepsilon_0 \equiv 2\varepsilon(n + 4)$ , and  $\varepsilon_1 \equiv 2\varepsilon(N\theta + 7)$

↑  
 $\varepsilon_0 = O(\varepsilon n)$

↑  
 $\varepsilon_1 = O(\varepsilon N\theta)$

→ These results form the basis for Paige's influential results in (Paige, 1980).

# CA-Lanczos Convergence Analysis

For CA-Lanczos,  
we have:

for  $i \in \{1, \dots, m=sk+j\}$ ,

$$\begin{aligned} \|\delta \hat{v}_i\|_2 &\leq \varepsilon_1 \sigma \\ \hat{\beta}_{i+1} |\hat{v}_i^T \hat{v}_{i+1}| &\leq 2\varepsilon_0 \sigma \\ |\hat{v}_{i+1}^T \hat{v}_{i+1} - 1| &\leq \varepsilon_0/2 \\ |\hat{\beta}_{i+1}^2 + \hat{\alpha}_i^2 + \hat{\beta}_i^2 - \|A\hat{v}_i\|_2^2| &\leq 4i(3\varepsilon_0 + \varepsilon_1)\sigma^2 \end{aligned}$$

$$\varepsilon_0 \equiv 2\varepsilon(n+11s+15)\Gamma^2 = O(\varepsilon n\Gamma^2),$$

$$\varepsilon_1 \equiv 2\varepsilon((N+2s+5)\theta + (4s+9)\tau + 10s+16)\Gamma = O(\varepsilon N\theta\Gamma),$$

where  $\sigma \equiv \|A\|_2$ ,  $\theta\sigma \equiv \| \|A\| \| \|_2$ ,  $\tau\sigma \equiv \max_{\ell \leq k} \| \|B_\ell\| \|_2$ , and

$$\Gamma \leq \max_{\ell \leq k} \|Y_\ell^+\|_2 \cdot \| \|Y_\ell\| \|_2 \leq (2s+1) \cdot \max_{\ell \leq k} \kappa(Y_\ell).$$

# CA-Lanczos Convergence Analysis

For CA-Lanczos,  
we have:

for  $i \in \{1, \dots, m=sk+j\}$ ,

$$\begin{aligned} \|\delta \hat{v}_i\|_2 &\leq \varepsilon_1 \sigma \\ \hat{\beta}_{i+1} |\hat{v}_i^T \hat{v}_{i+1}| &\leq 2\varepsilon_0 \sigma \\ |\hat{v}_{i+1}^T \hat{v}_{i+1} - 1| &\leq \varepsilon_0/2 \\ |\hat{\beta}_{i+1}^2 + \hat{\alpha}_i^2 + \hat{\beta}_i^2 - \|A\hat{v}_i\|_2^2| &\leq 4i(3\varepsilon_0 + \varepsilon_1)\sigma^2 \end{aligned}$$

$$\varepsilon_0 \equiv 2\varepsilon(n+11s+15)\Gamma^2 = O(\varepsilon n \Gamma^2), \leftarrow \text{(vs. } O(\varepsilon n) \text{ for Lanczos)}$$

$$\varepsilon_1 \equiv 2\varepsilon((N+2s+5)\theta + (4s+9)\tau + 10s+16)\Gamma = O(\varepsilon N \theta \Gamma), \leftarrow \text{(vs. } O(\varepsilon N \theta) \text{ for Lanczos)}$$

where  $\sigma \equiv \|A\|_2$ ,  $\theta\sigma \equiv \| \|A\| \| \|_2$ ,  $\tau\sigma \equiv \max_{\ell \leq k} \| \|B_\ell\| \|_2$ , and

$$\Gamma \leq \max_{\ell \leq k} \|Y_\ell^+\|_2 \cdot \| \|Y_\ell\| \|_2 \leq (2s+1) \cdot \max_{\ell \leq k} \kappa(Y_\ell).$$

# The Amplification Term $\Gamma$

---

- Roundoff errors in CA variant follow same pattern as classical variant, but amplified by factor of  $\Gamma$  or  $\Gamma^2$ 
  - **Theoretically confirms empirical observations** on importance of basis conditioning (dating back to late '80s)

- A loose bound for the amplification term:

$$\Gamma \leq \max_{\ell \leq k} \|\mathbf{y}_\ell^+\|_2 \cdot \|\mathbf{y}_\ell\|_2 \leq (2s+1) \cdot \max_{\ell \leq k} \kappa(\mathbf{y}_\ell)$$

- What we really need:  $\|\mathbf{y}\|\|\mathbf{y}'\|_2 \leq \Gamma\|\mathbf{y}\mathbf{y}'\|_2$  to hold for the computed basis  $\mathbf{y}$  and coordinate vector  $\mathbf{y}'$  in every bound.
- **Tighter bound on  $\Gamma$  possible**; requires some light bookkeeping
- Example: for bounds on  $\hat{\beta}_{i+1} |\hat{\mathbf{v}}_i^T \hat{\mathbf{v}}_{i+1}|$  and  $|\hat{\mathbf{v}}_{i+1}^T \hat{\mathbf{v}}_{i+1} - 1|$ , we can use the definition

$$\Gamma_{k,j} \equiv \max_{x \in \{\hat{\mathbf{w}}'_{k,j}, \hat{\mathbf{u}}'_{k,j}, \hat{\mathbf{v}}'_{k,j}, \hat{\mathbf{v}}'_{k,j-1}\}} \frac{\|\hat{\mathbf{y}}_k\|_2 \|x\|_2}{\|\hat{\mathbf{y}}_k x\|_2}$$

# Results for CA-Lanczos

---

- Back to our question: Do Paige's results, e.g.,  
    loss of orthogonality  $\rightarrow$  eigenvalue convergence  
hold for CA-Lanczos?

# Results for CA-Lanczos

---

- Back to our question: Do Paige's results, e.g.,  
loss of orthogonality  $\rightarrow$  eigenvalue convergence  
hold for CA-Lanczos?
- The answer is **YES!** ...but

# Results for CA-Lanczos

---

- Back to our question: Do Paige's results, e.g.,  
loss of orthogonality  $\rightarrow$  eigenvalue convergence  
hold for CA-Lanczos?
- The answer is **YES!** ...but
- Only if:
  - $\varepsilon_0 \equiv 2\varepsilon(n+11s+15) \Gamma^2 \leq \frac{1}{12}$
  - i.e.,  $\Gamma \leq (24\varepsilon(n+11s+15))^{-1/2} = O(n\varepsilon)^{-1/2}$
- Otherwise, e.g., can lose orthogonality due to computation with  
(numerically) rank-deficient basis



# Results for CA-Lanczos

---

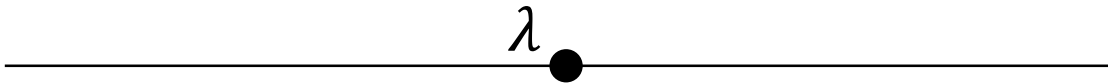
- Back to our question: Do Paige's results, e.g.,  
loss of orthogonality  $\rightarrow$  eigenvalue convergence  
hold for CA-Lanczos?
- The answer is **YES!** ...but
- Only if:
  - $\varepsilon_0 \equiv 2\varepsilon(n+11s+15) \Gamma^2 \leq \frac{1}{12}$
  - i.e.,  $\Gamma \leq (24\varepsilon(n + 11s + 15))^{-1/2} = O(n\varepsilon)^{-1/2}$
  - Otherwise, e.g., can lose orthogonality due to computation with  
(numerically) rank-deficient basis
- **Take-away: we can use this bound on  $\Gamma$  to design a better algorithm!**
  - Mixed precision, selective reorthogonalization, dynamic basis size, etc.

Extending the results of Greenbaum (1989):

Eigenvalue approximations generated at each step by a perturbed Lanczos recurrence for  $A$  are equal to those generated by exact Lanczos applied to a matrices whose eigenvalues lie within intervals about the eigenvalues of  $A$ .

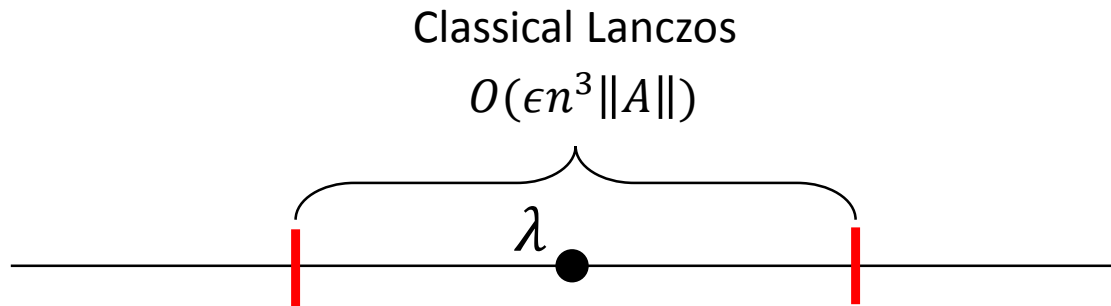
Extending the results of Greenbaum (1989):

Eigenvalue approximations generated at each step by a perturbed Lanczos recurrence for  $A$  are equal to those generated by exact Lanczos applied to a matrices whose eigenvalues lie within intervals about the eigenvalues of  $A$ .



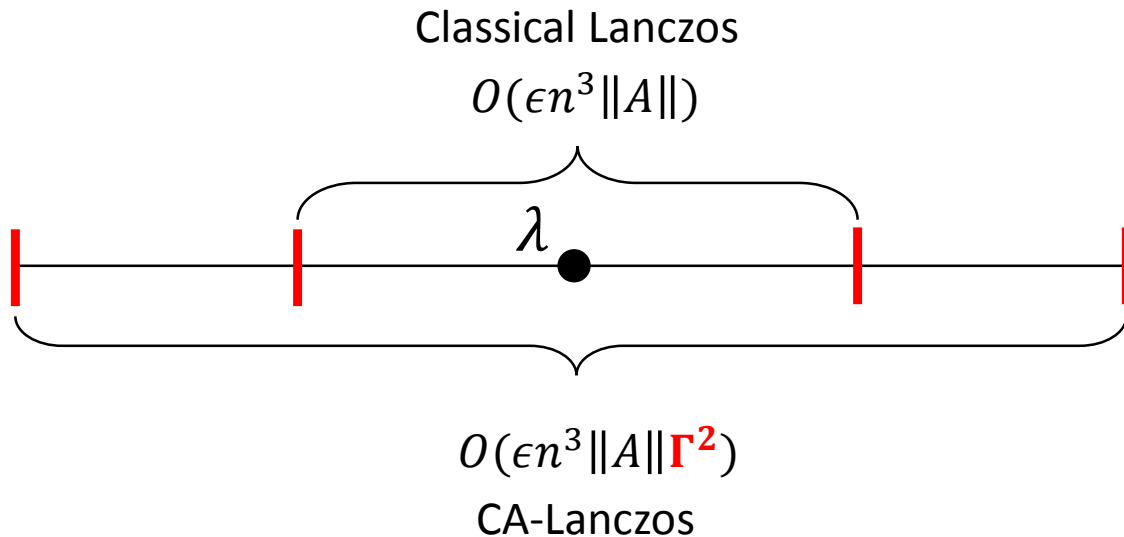
Extending the results of Greenbaum (1989):

Eigenvalue approximations generated at each step by a perturbed Lanczos recurrence for  $A$  are equal to those generated by exact Lanczos applied to a matrices whose eigenvalues lie within intervals about the eigenvalues of  $A$ .



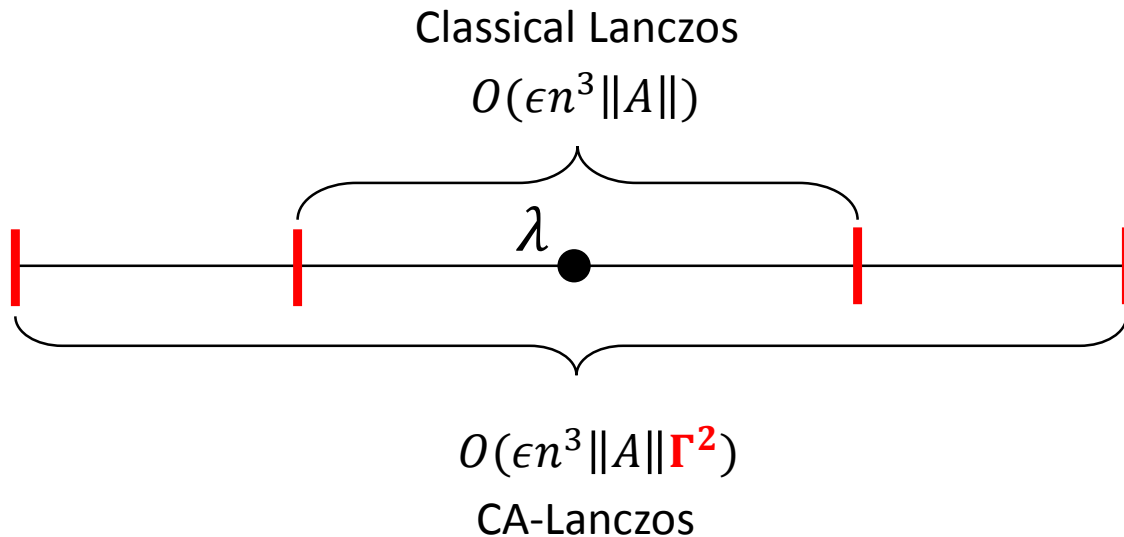
Extending the results of Greenbaum (1989):

Eigenvalue approximations generated at each step by a perturbed Lanczos recurrence for  $A$  are equal to those generated by exact Lanczos applied to a matrices whose eigenvalues lie within intervals about the eigenvalues of  $A$ .



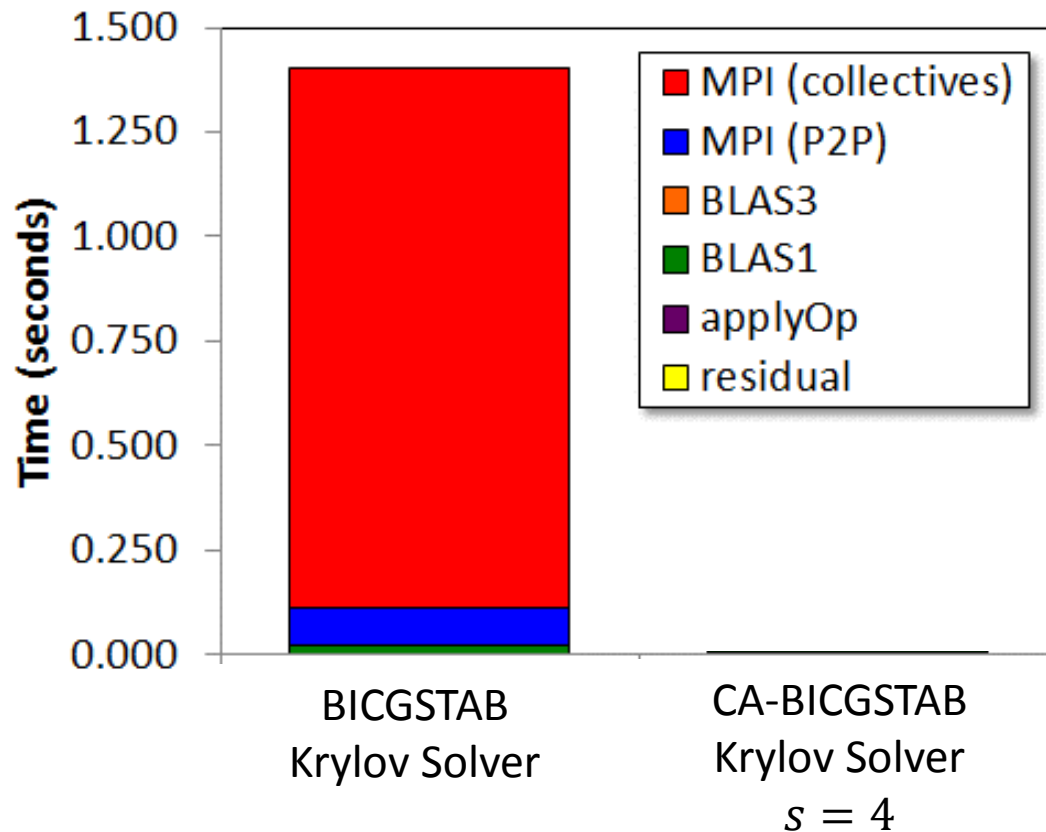
Extending the results of Greenbaum (1989):

Eigenvalue approximations generated at each step by a perturbed Lanczos recurrence for  $A$  are equal to those generated by exact Lanczos applied to a matrices whose eigenvalues lie within intervals about the eigenvalues of  $A$ .



Ongoing work...

- Timing for coarse grid solves in geometric multigrid method
- 3D Helmholtz equation with  $n = 1.6 \cdot 10^6$
- 24K cores on NERSC's Hopper (Cray XE6)



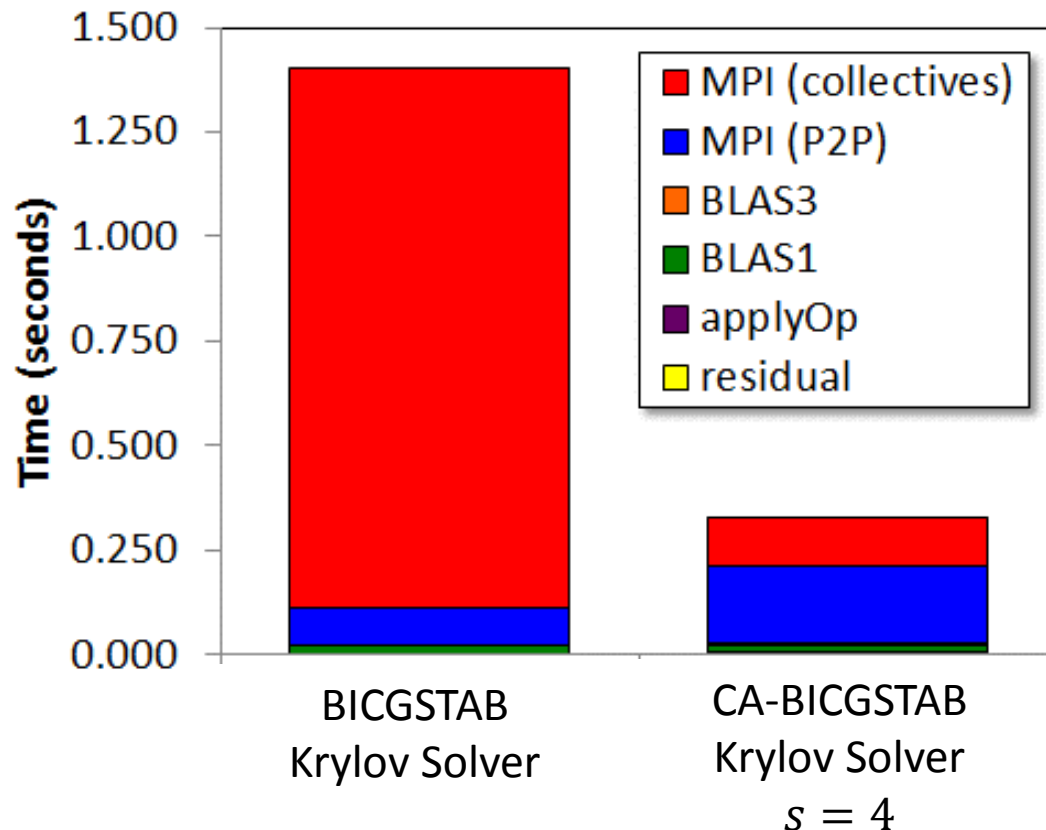
Problem specifics:

$$Lu = (a\alpha - b\nabla \cdot \beta\nabla)u = f$$

$$\alpha = \beta = 1.0, a = b = 0.9$$

- Periodic boundary conds.
- RHS: 3D triangle wave w/period spanning entire domain

- Timing for coarse grid solves in geometric multigrid method
- 3D Helmholtz equation with  $n = 1.6 \cdot 10^6$
- 24K cores on NERSC's Hopper (Cray XE6)



Problem specifics:

$$Lu = (a\alpha - b\nabla \cdot \beta\nabla)u = f$$

$$\alpha = \beta = 1.0, a = b = 0.9$$

- Periodic boundary conds.
- RHS: 3D triangle wave w/period spanning entire domain

**4.2x speedup in Krylov solve!**



# Future Directions

---

Broad research agenda: Design methods for large-scale problems that optimize performance subject to application-specific numerical constraints

- **New Algorithms/Applications**

- Application of communication-avoiding ideas and solvers to new computational science domains
- Design of new high-performance preconditioners

- **Finite-Precision Analysis**

- Bounds on stability and convergence for other Krylov methods (particularly in the nonsymmetric case)
- Extension of “Backwards-like” error analyses

- **Improving Usability**

- Automating parameter selection via “numerical auto-tuning”
- Integration into high-performance libraries

Thank you!

Happy Birthday, Jim!

contact: [erinc@cims.nyu.edu](mailto:erinc@cims.nyu.edu)  
<http://www.cims.nyu.edu/~erinc/>