High-Performance Variants of Krylov Subspace Methods: II/II

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Development and Education

MINISTRY OF EDUCATION,
YOUTH AND SPORTS

Review

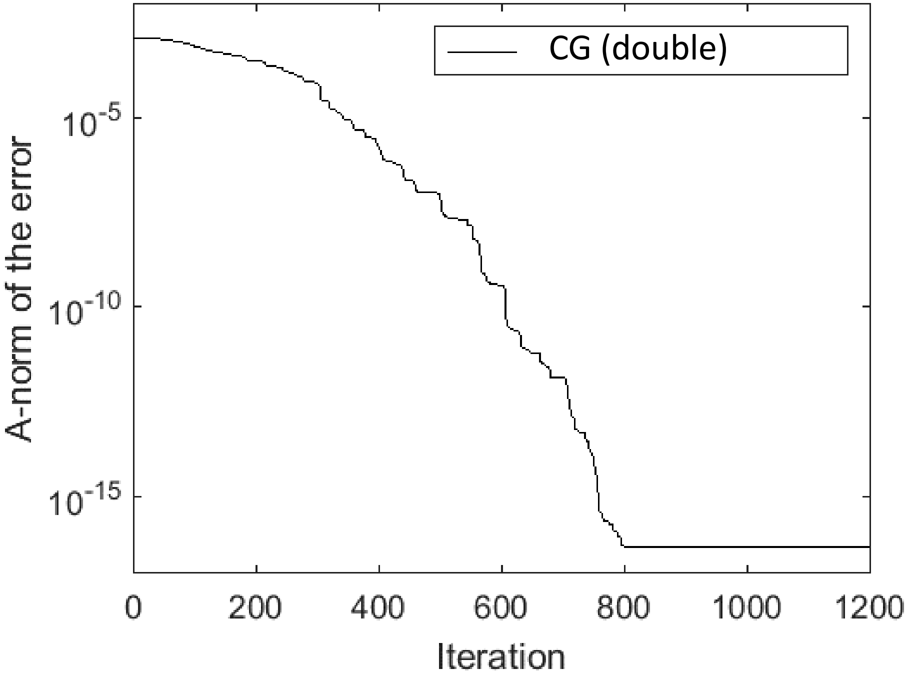
- Cost of data movement (relative to low computational cost) causes bottlenecks in classical formulations of Krylov subspace methods
- Motivates various approaches
    - Pipelined Krylov subspace methods
        - Add auxiliary recurrences to enable decoupling of inner products and SpMVs; can then be overlapped using non-blocking MPI
        - Effectively hides the cost of synchronization in each iteration
    - s-step Krylov subspace methods
        - Block iterations in groups of s; use block computation of O(s) basis vectors and block orthogonalization
        - Increases temporal locality, allowing asymptotic reduction in number of messages per iteration
    - Many practical implementation details: choosing parameters, preconditioning, etc.
- For certain (e.g., latency-bound) problems, these approaches can reduce the time-per-iteration cost

The effects of finite precision

Well-known that roundoff error has two effects:

1. Delay of convergence
   - No longer have exact Krylov subspace
   - Can lose numerical rank deficiency
   - Residuals no longer orthogonal - Minimization of $||x - x_i||_A$ no longer exact

2. Loss of attainable accuracy
   - Rounding errors cause true residual $b - Ax_i$ and updated residual r_i deviate!



A: bcsstk03 from SuiteSparse,
b: equal components in the eigenbasis of A,$||b|| = 1$
$N = 112, \kappa(A) \approx 7\text{e}6$

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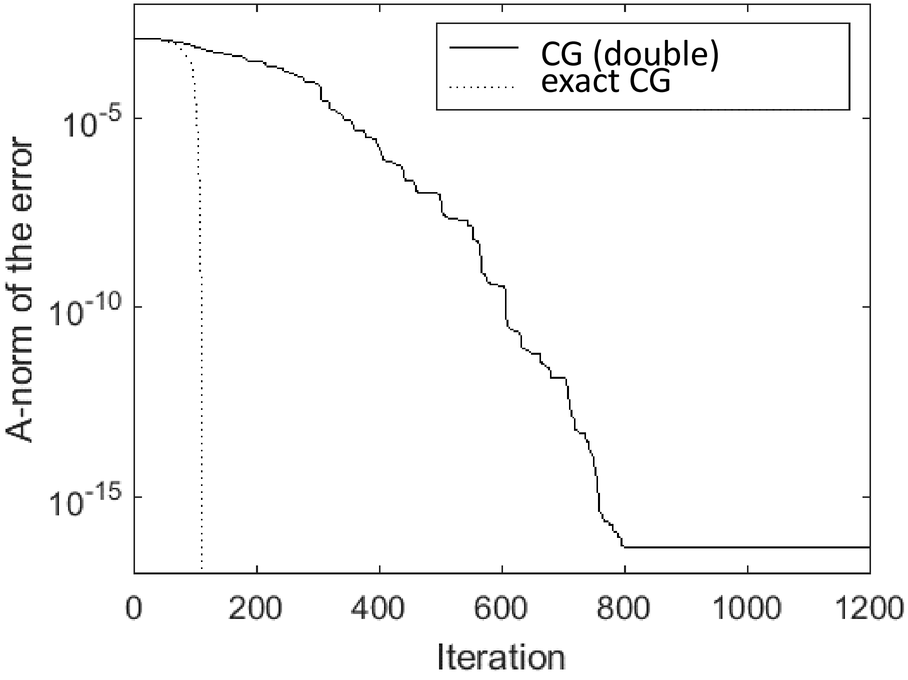

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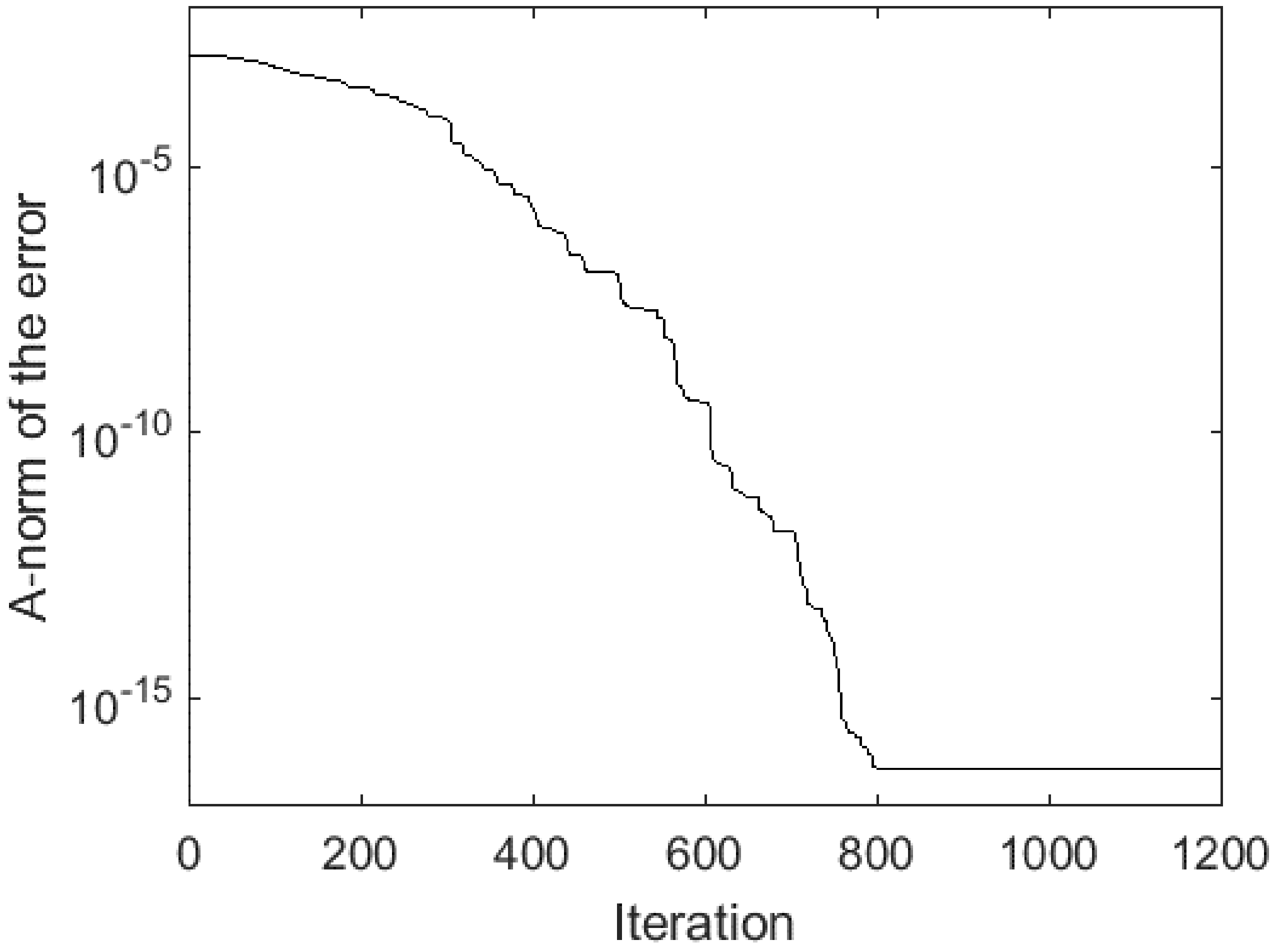
Much work on these results for CG; See Meurant and Strakoš (2006) for a thorough summary of early developments in finite precision analysis of Lanczos and CG

Conjugate Gradient method for solving Ax = b
double precision ($\varepsilon = 2^{-53}$)

$$\|x_i - x\|_A = \sqrt{(x_i - x)^T A (x_i - x)}$$

$$\boxed{\begin{aligned} x_i &= x_{i-1} + \alpha_i p_i \\ r_i &= r_{i-1} - \alpha_i A p_i \\ p_i &= r_i + \beta_i p_i \end{aligned}}$$



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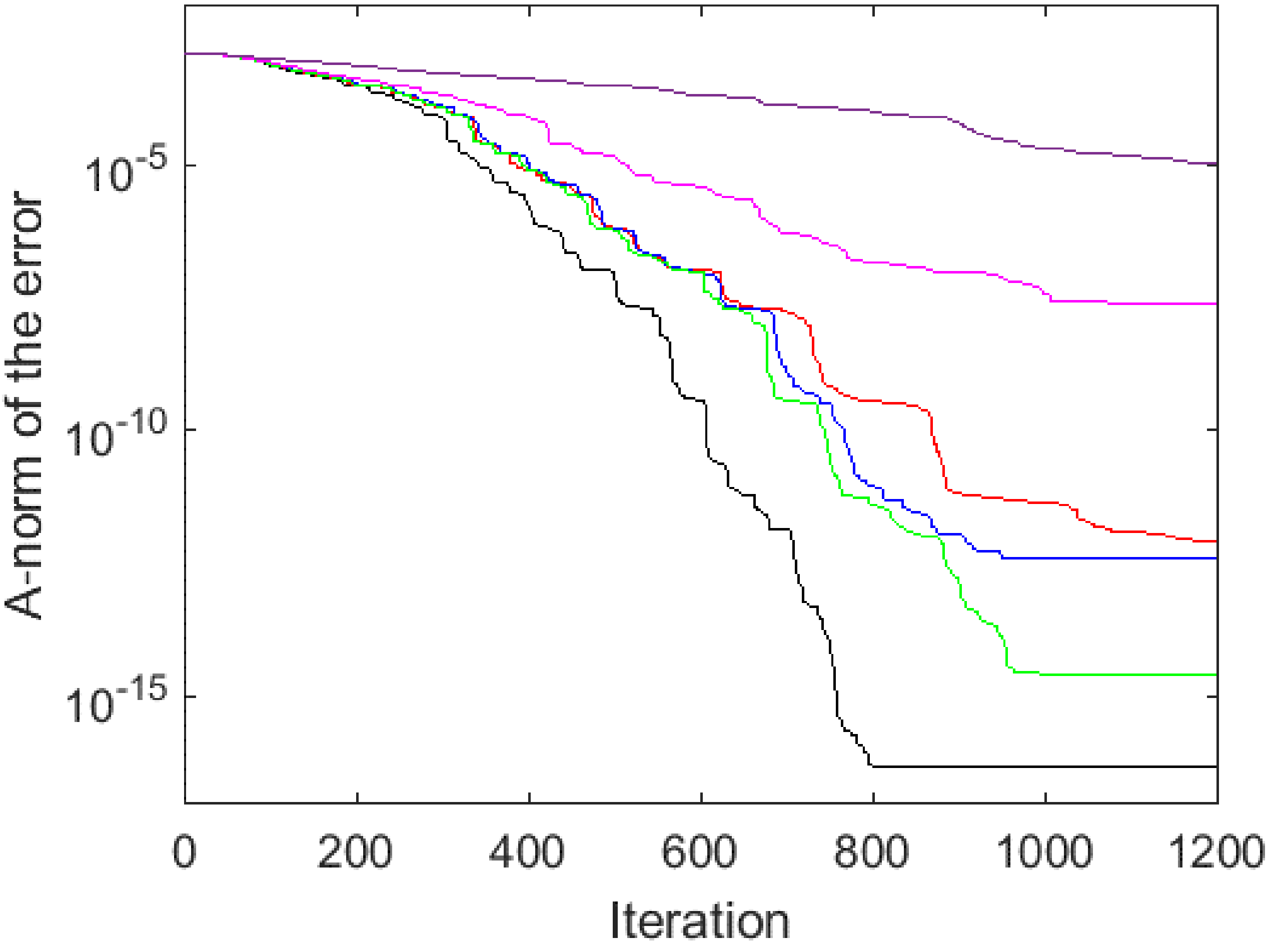

Improving Performance of Iterative Solvers

$$\text{runtime} = \begin{pmatrix}\text{time per}\\ \text{iteration}\end{pmatrix} \times \begin{pmatrix}\text{number of iterations}\\ \text{until convergence}\end{pmatrix}$$

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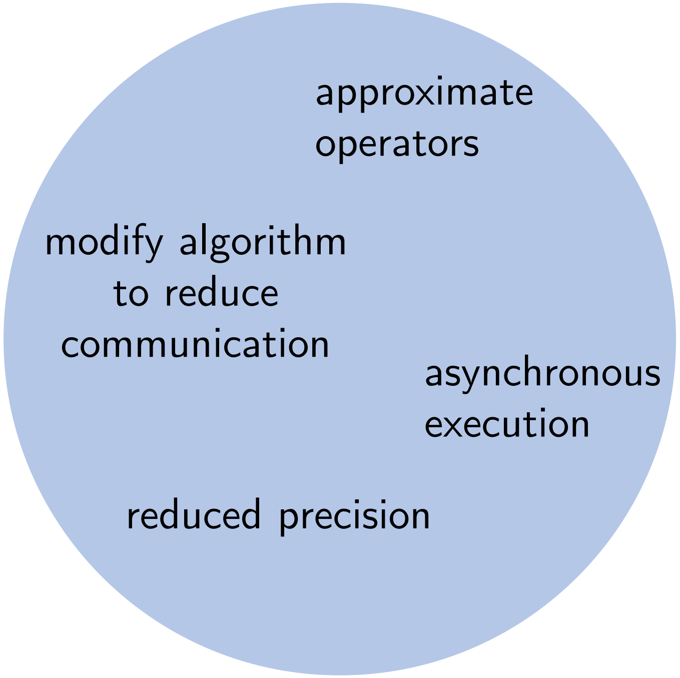

approximate operators

modify algorithm to reduce communication

asynchronous execution

reduced precision

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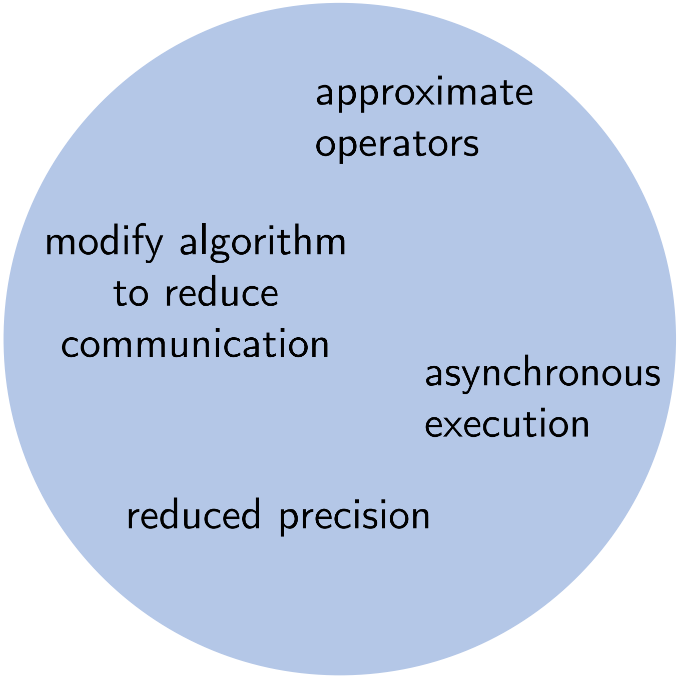

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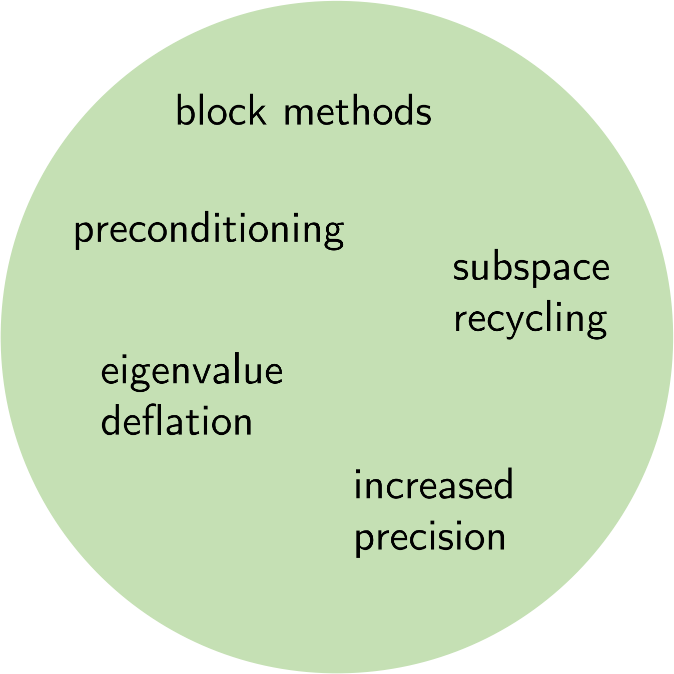

block methods

preconditioning

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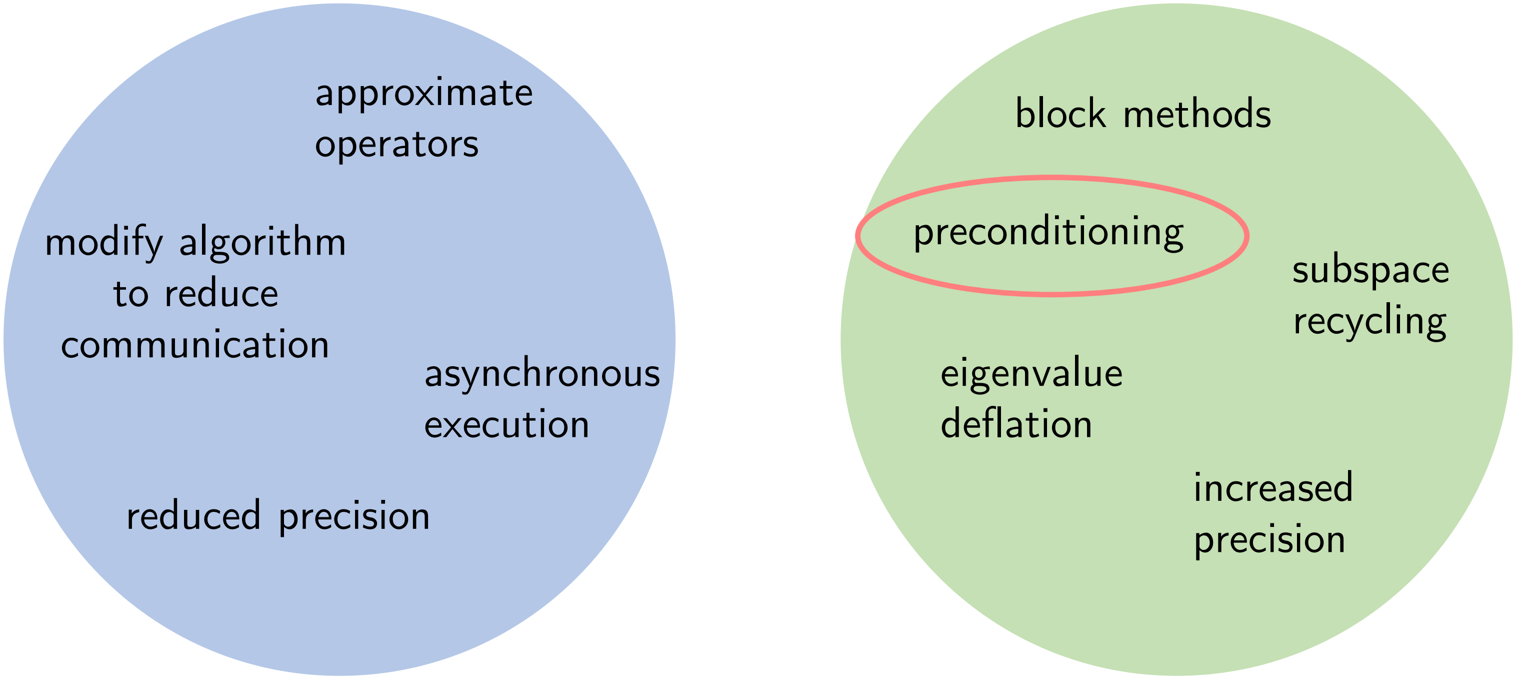

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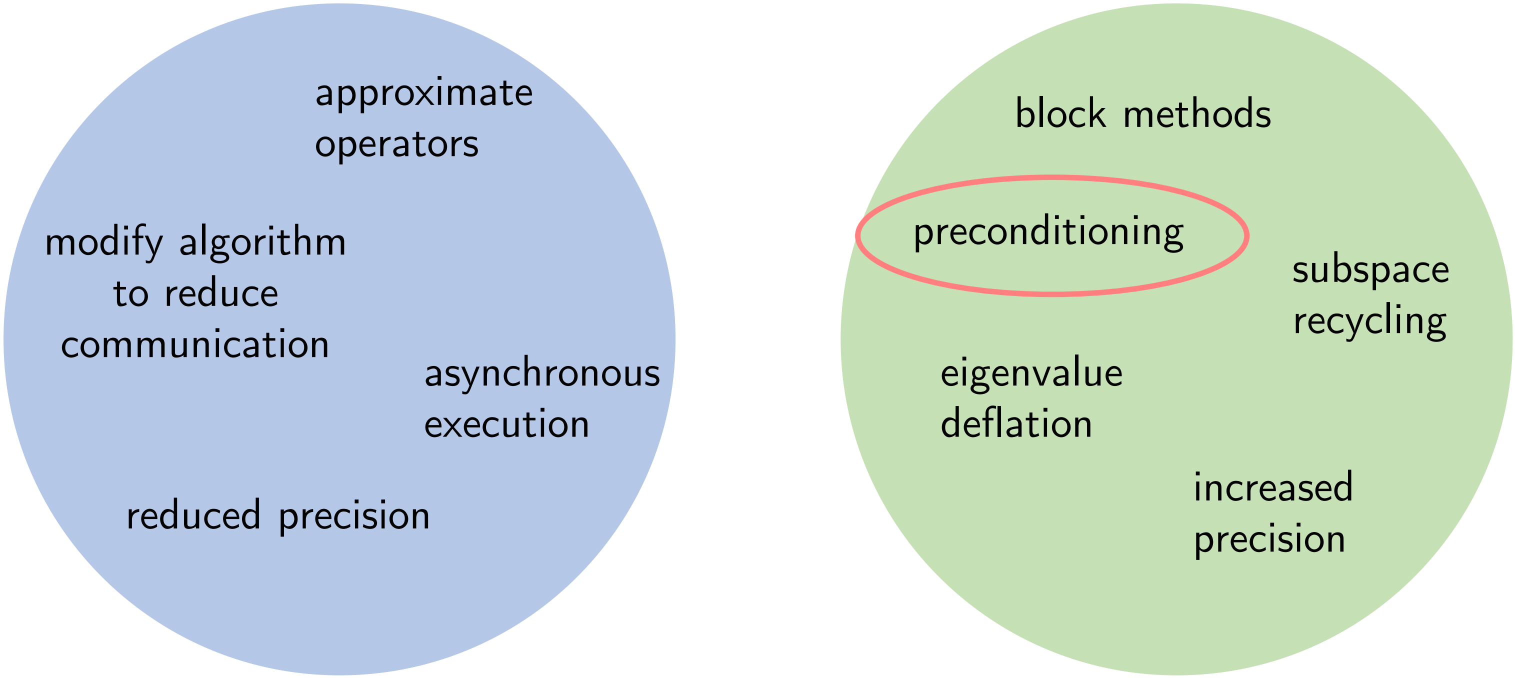

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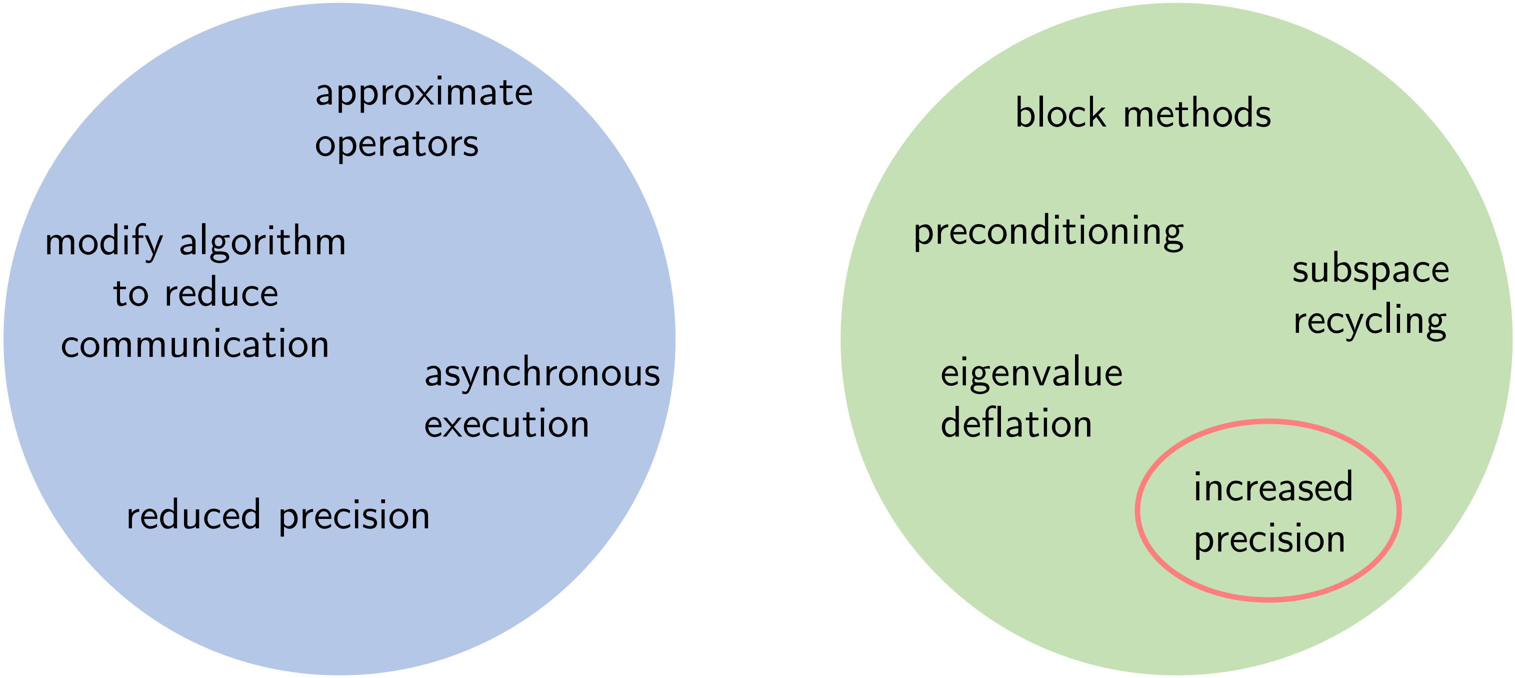

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- asynchronous execution
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Reduce number of iterations

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doubled precision → twice as many bits moved

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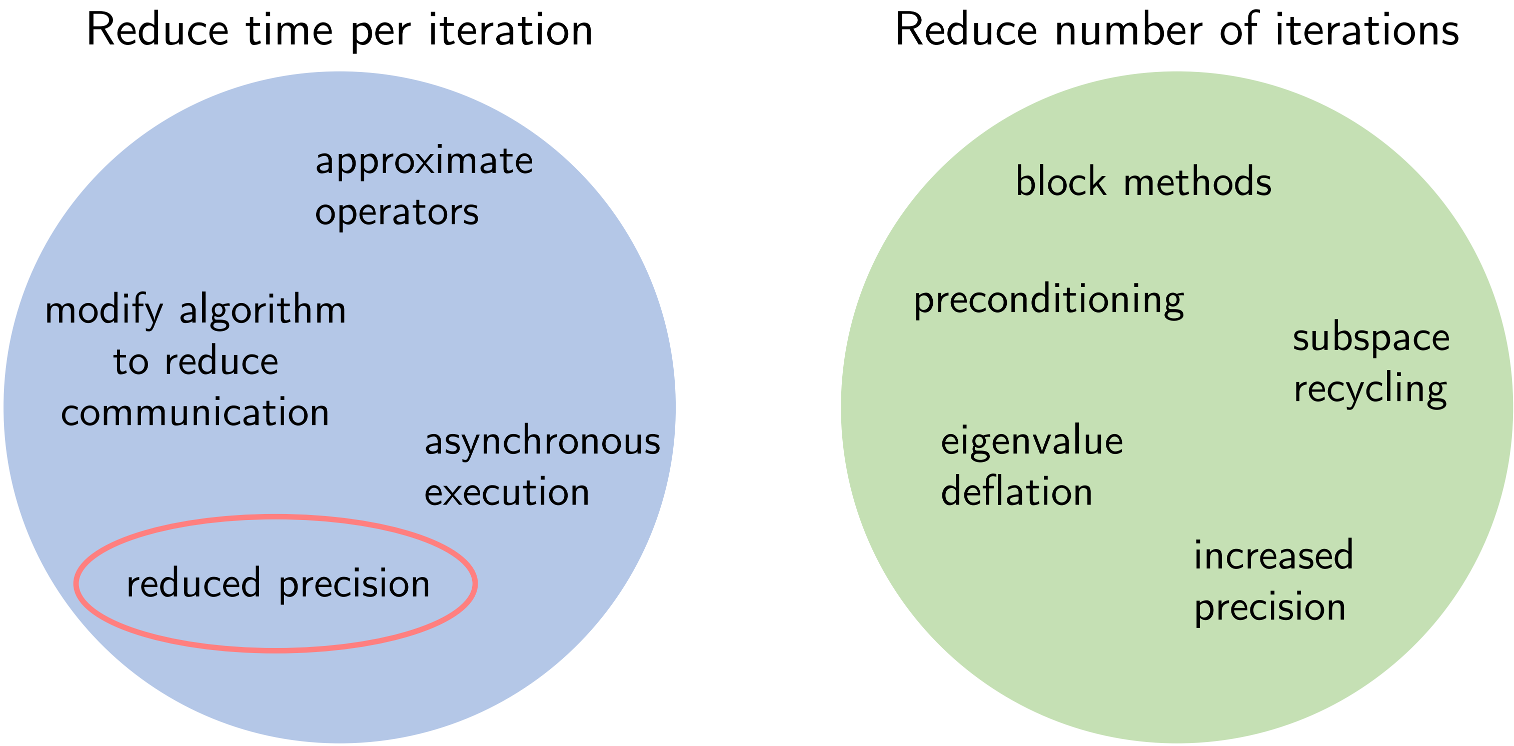

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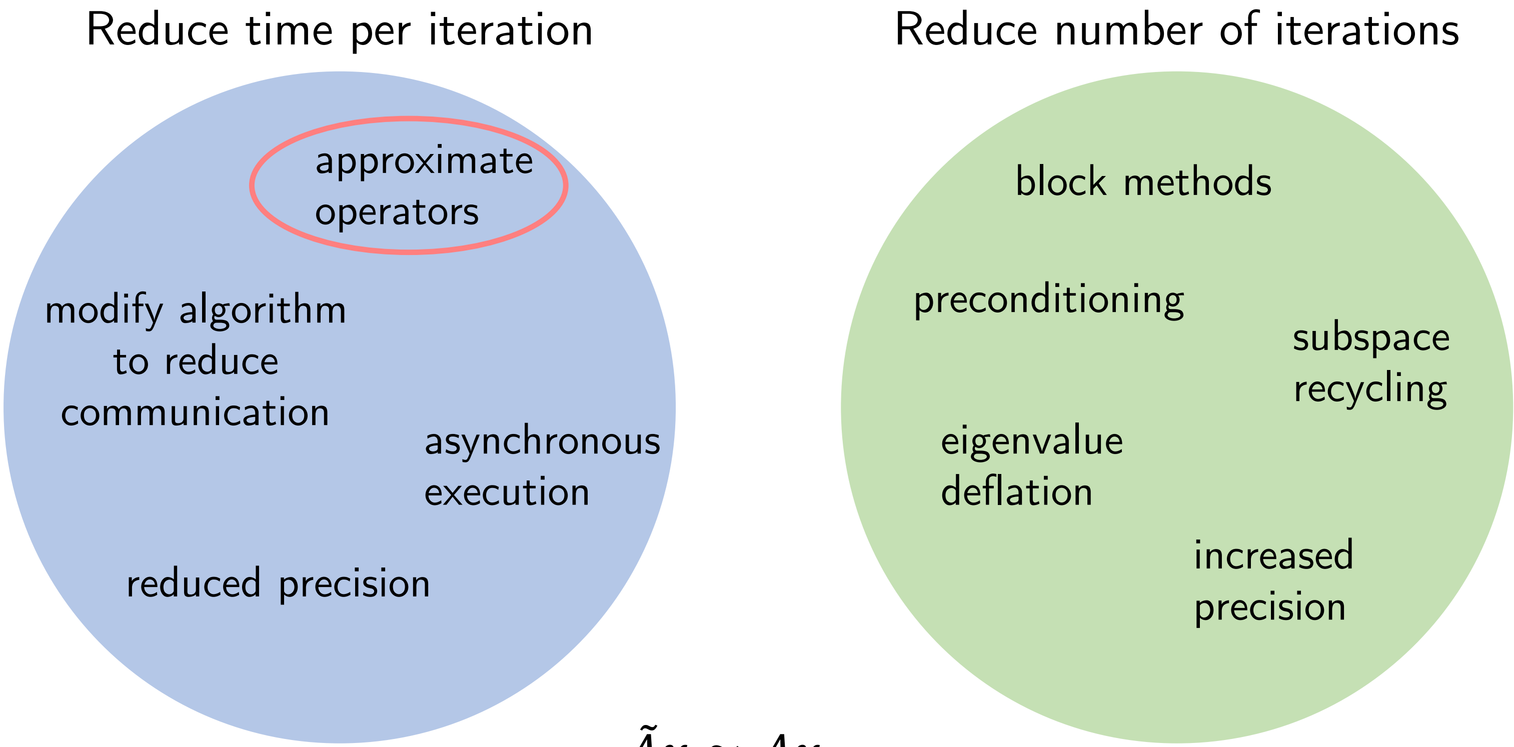

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$$\tilde{A}x \approx Ax$$

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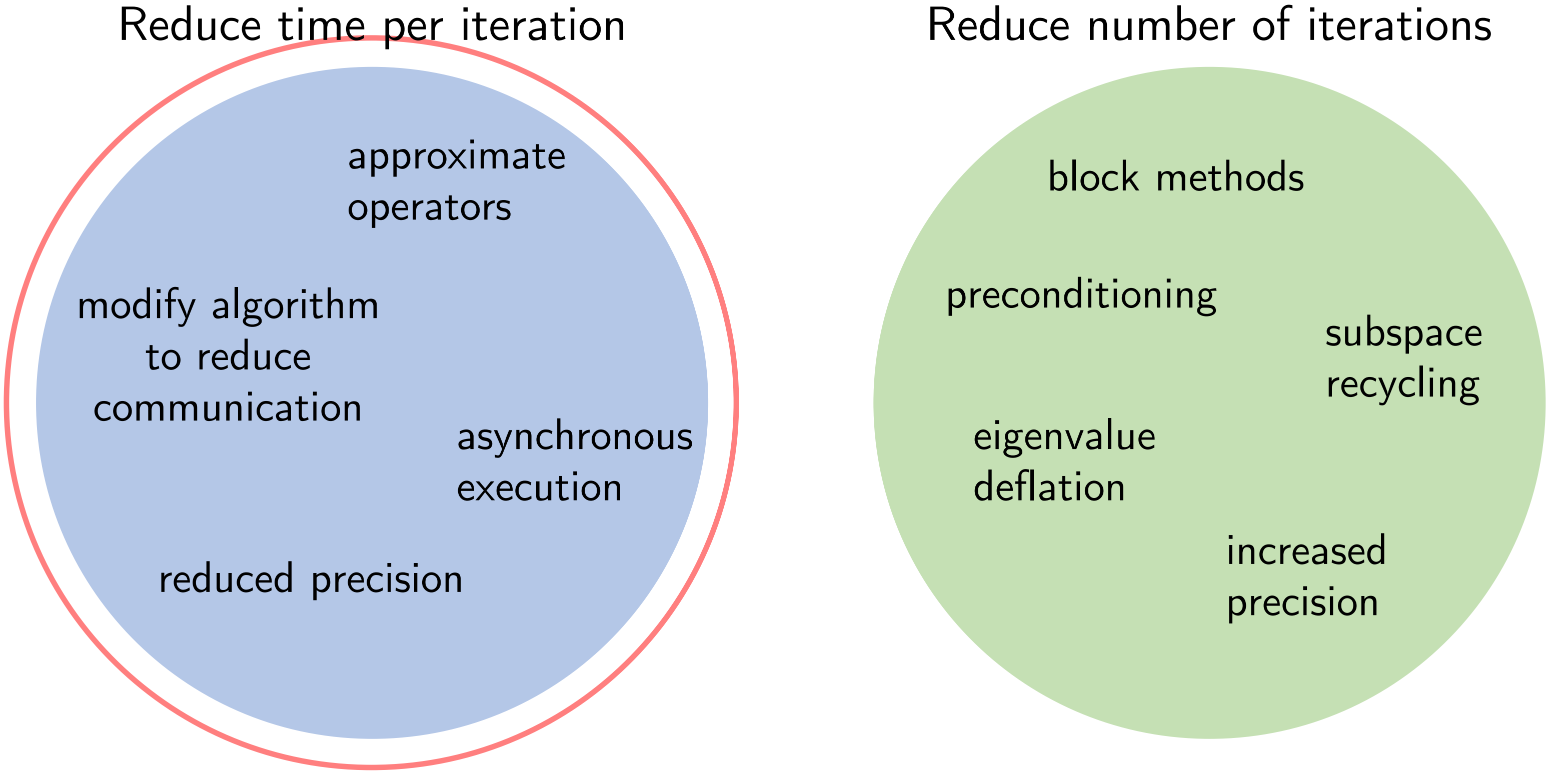

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convergence criteria never met: divergence, or convergence to inaccurate solution

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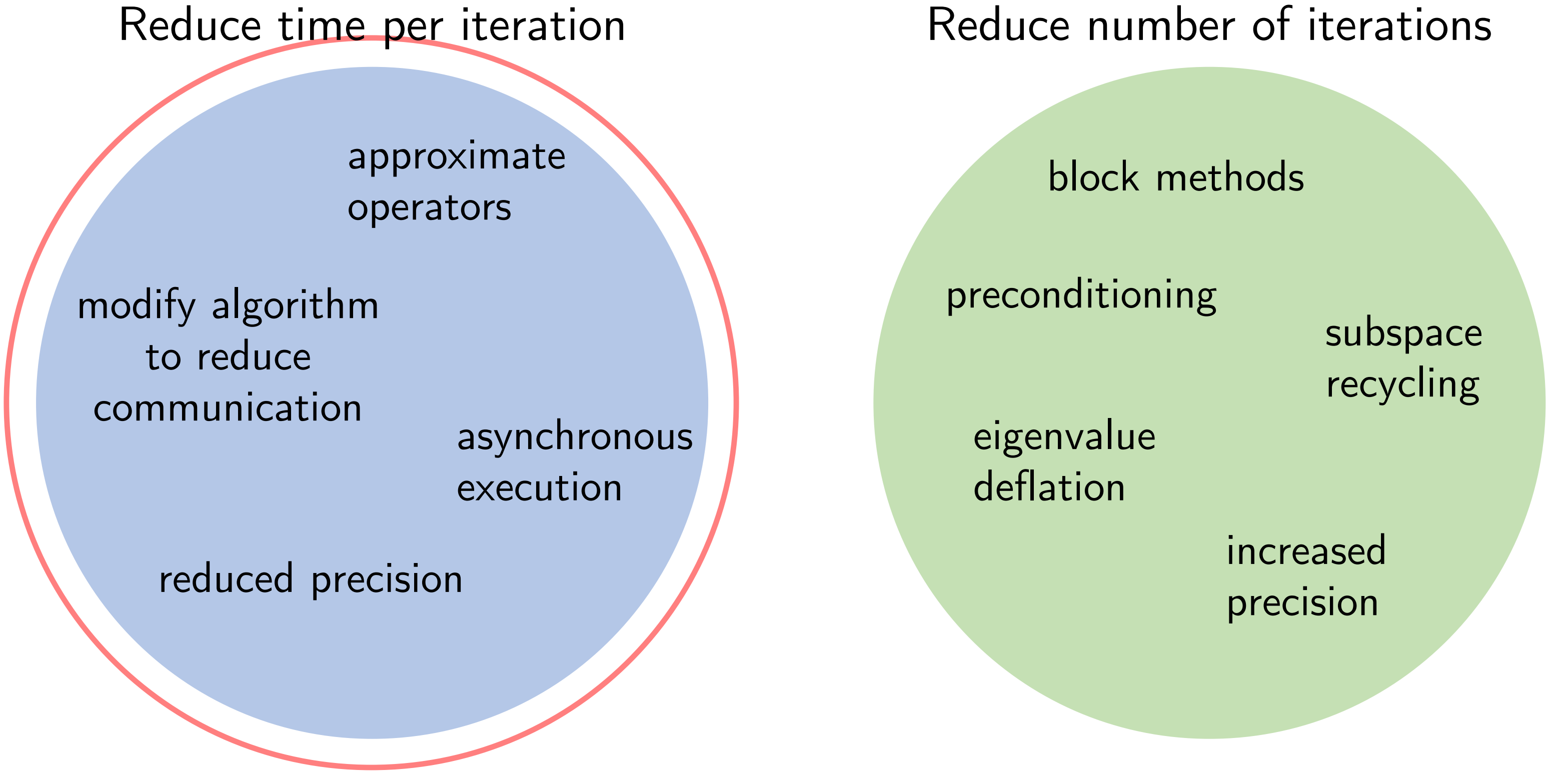

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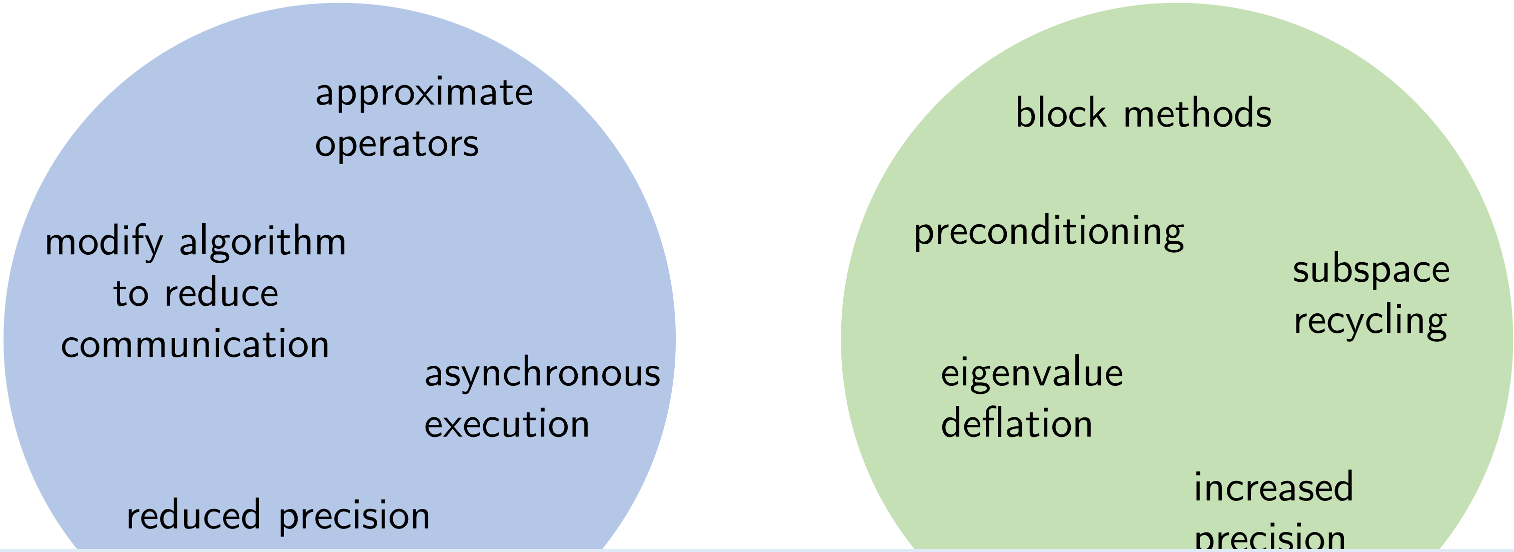

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To minimize runtime, must understand how modifications affect:

1) attainable accuracy 2) convergence rate 3) time per iteration

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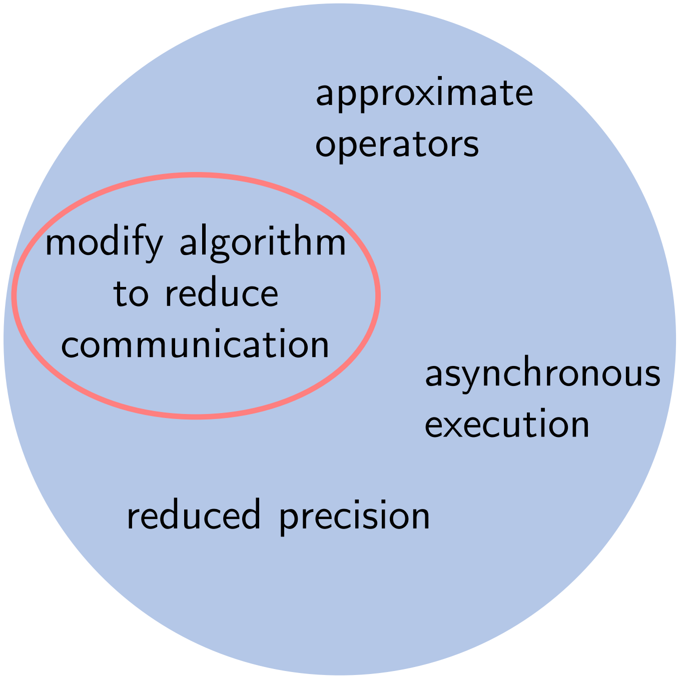

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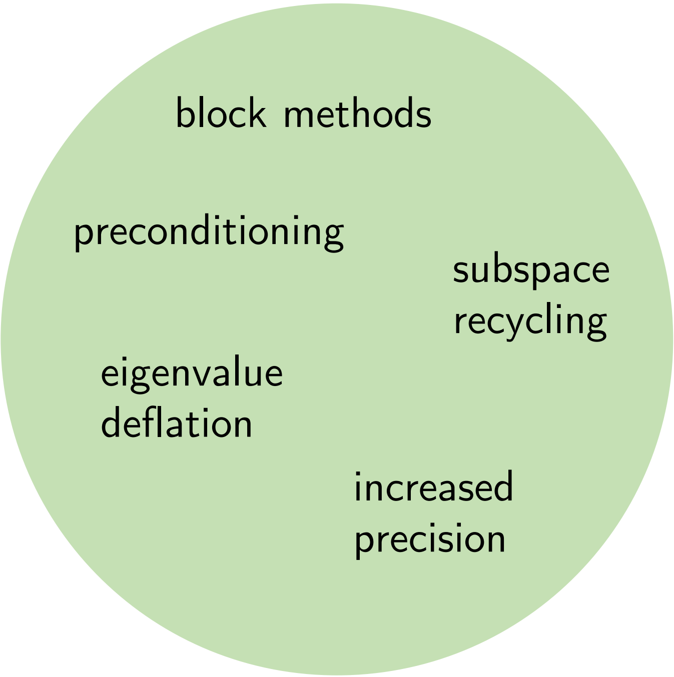

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Lecture Outline

- Effects of finite precision in Krylov subspace methods
  - Maximum attainable accuracy
  - Convergence delay
- Existing results for classical Krylov subspace methods
- Results for pipelined and s-step Krylov subspace methods
- Potential remedies for finite precision error in high-performance variants
- Choosing a method in practice
- The future of Krylov subspace methods

Maximum attainable accuracy

- Accuracy $\|x - \hat{x}_i\|$ generally not computable, *but* $x - \hat{x}_i = A^{-1}(b - A\hat{x}_i)$
- Size of the true residual, $\|b - A\hat{x}_i\|$, used as computable measure of accuracy

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- Writing $b - A\hat{x}_i = \hat{r}_i + b - A\hat{x}_i - \hat{r}_i$,

$$\|b - A\hat{x}_i\| \leq \|\hat{r}_i\| + \|b - A\hat{x}_i - \hat{r}_i\|$$

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- Many results on bounding 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).

Maximum attainable accuracy of HSCG

- In finite precision HSCG, iterates are updated by

$$\hat{x}_i = \hat{x}_{i-1} + \hat{\alpha}_{i-1}\hat{p}_{i-1} - \boldsymbol{\delta x_i}$$ and $$\hat{r}_i = \hat{r}_{i-1} - \hat{\alpha}_{i-1}A\hat{p}_{i-1} - \boldsymbol{\delta r_i}$$

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$\|f_i\| \leq O(\varepsilon)\sum_{m=0}^{i} N_A\|A\|\|\hat{x}_m\| + \|\hat{r}_m\|$ van der Vorst and Ye, 2000

$\|f_i\| \leq O(\varepsilon)\|A\|\left(\|x\| + \max_{m=0,\dots,i}\|\hat{x}_m\|\right)$ Greenbaum, 1997

$\|f_i\| \leq O(\varepsilon)N_A\||A|\|\|A^{-1}\|\sum_{m=0}^{i}\|\hat{r}_m\|$ Sleijpen and van der Vorst, 1995

Maximum Attainable Accuracy in HPC Variants

- Various synchronization-reducing modifications/variants discussed in Part I
  - Modified recurrence coefficient computation
  - 3-term CG (STCG)
  - Addition of auxiliary recurrences
  - Pipelined CG
  - s-step methods

Modified recurrence coefficient computation

- What is the effect of changing the way the recurrence coefficients (α and β) are computed in HSCG?

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- Notice that neither α nor β appear in the bounds on $\|f_i\|$

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$$f_i = f_{i-1} + A\delta x_i + \delta r_i$$

still holds

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still holds

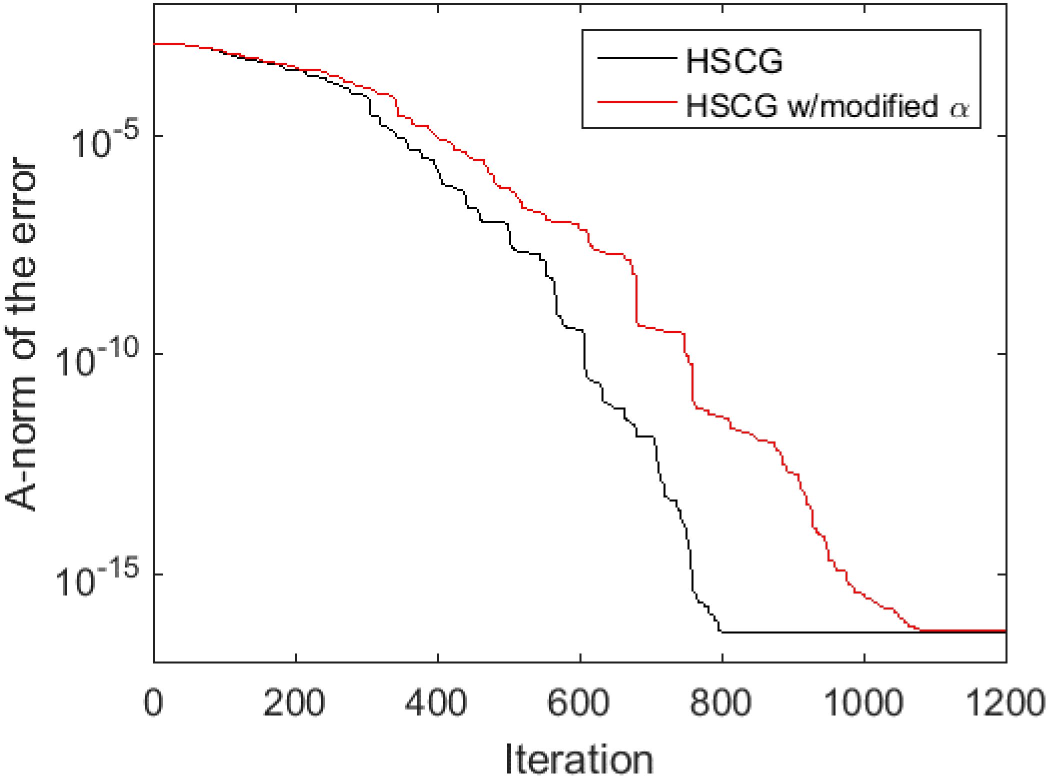
- Rounding errors made in computing $\hat{\alpha}_{i-1}$ do not contribute to the residual gap

- But may change computed $\hat{x}_i$, $\hat{r}_i$, which can affect convergence rate...

Modified recurrence coefficient computation

Example: HSCG with modified formula for α_{i-1}

$$\alpha_{i-1} = \left(\frac{r_{i-1}^T A r_{i-1}}{r_{i-1}^T r_{i-1}} - \frac{\beta_{i-1}}{\alpha_{i-2}} \right)^{-1}$$



Attainable accuracy of STCG

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- Residual gap bounded by sum of local errors PLUS local errors multiplied by factors which depend on

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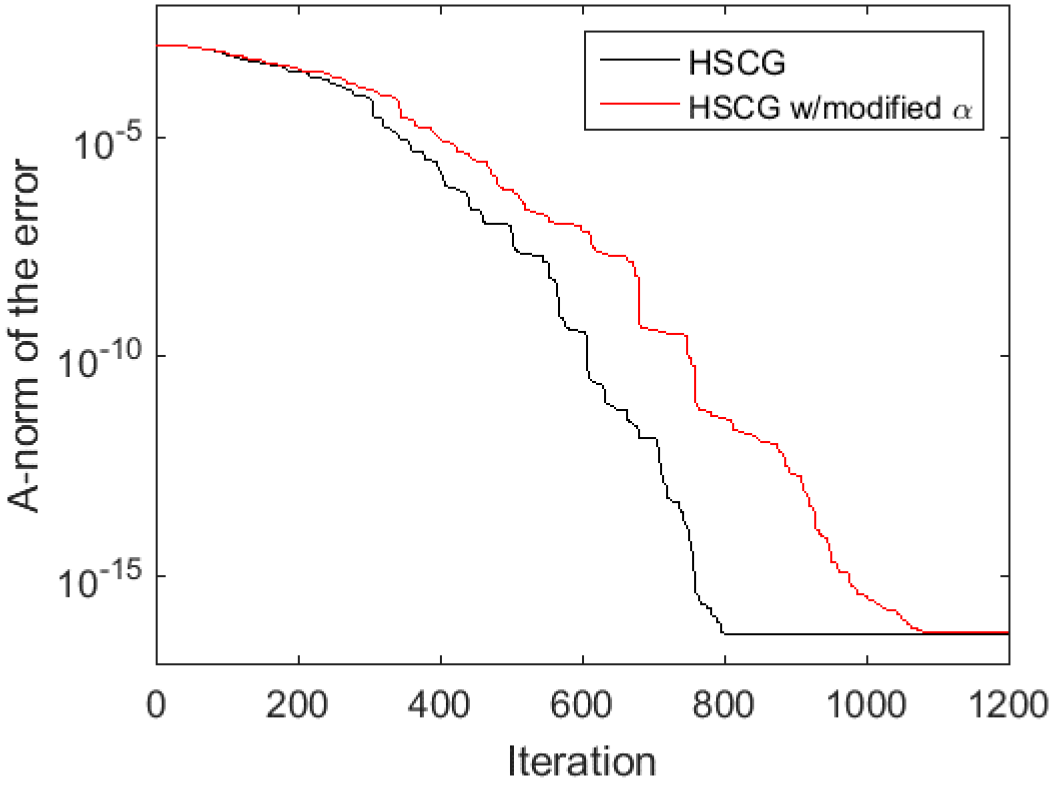
⇒ Large residual oscillations can cause these factors to be large!

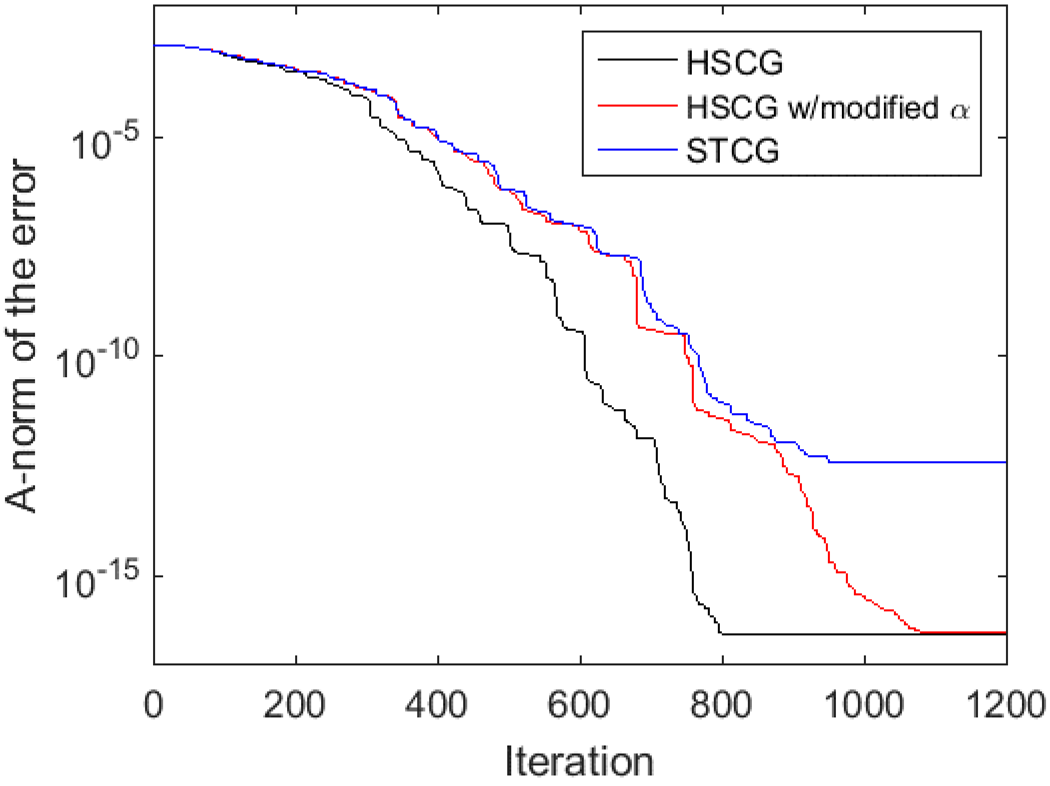
⇒ Local errors can be amplified!

STCG



A-norm of the error
10^{-5}
10^{-10}
10^{-15}
0
200
400
600
800
1000
1200
Iteration
HSCG
HSCG w/modified α

STCG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Attainable accuracy of pipelined CG

- What is the effect of adding auxiliary recurrences to the CG method?

Attainable accuracy of pipelined CG

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- To isolate the effects, we consider a simplified version of a pipelined method

```
$r_0 = b - Ax_0, p_0 = r_0, s_0 = Ap_0$
for $i = 1$:nmax
        $\alpha_{i-1} = \frac{(r_{i-1},r_{i-1})}{(p_{i-1},s_{i-1})}$
        $x_i = x_{i-1} + \alpha_{i-1} p_{i-1}$
        $r_i = r_{i-1} - \alpha_{i-1} s_{i-1}$
        $\beta_i = \frac{(r_i,r_i)}{(r_{i-1},r_{i-1})}$
        $p_i = r_i + \beta_i p_{i-1}$
        $s_i = Ar_i + \beta_i s_{i-1}$
end
```

Attainable accuracy of pipelined CG

- What is the effect of adding auxiliary recurrences to the CG method?
- To isolate the effects, we consider a simplified version of a pipelined method
  - Uses same update formulas for α and β as HSCG, but uses additional recurrence for Ap_i

```
$r_0 = b - Ax_0, p_0 = r_0, s_0 = Ap_0$
for $i$ = 1:nmax
    $\alpha_{i-1} = \frac{(r_{i-1}, r_{i-1})}{(p_{i-1}, s_{i-1})}$
    $x_i = x_{i-1} + \alpha_{i-1} p_{i-1}$
    $r_i = r_{i-1} - \alpha_{i-1} s_{i-1}$
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    $p_i = r_i + \beta_i p_{i-1}$
    $s_i = Ar_i + \beta_i s_{i-1}$
end
```

see [C., Rozložník, Strakoš, Tichý, Tůma, 2018]

Attainable accuracy of simple pipelined CG

$$\hat{x}_i = \hat{x}_{i-1} + \hat{\alpha}_{i-1}\hat{p}_{i-1} + \boldsymbol{\delta x_i} \qquad \hat{r}_i = \hat{r}_{i-1} - \hat{\alpha}_{i-1}\,\hat{s}_{i-1} + \boldsymbol{\delta r_i}$$

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$$f_i = \hat{r}_i - (b - A\hat{x}_i)$$

see [C., Rozložník, Strakoš, Tichý, Tůma, 2018]

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$$\begin{aligned} f_i &= \hat{r}_i - (b - A\hat{x}_i) \\ &= f_{i-1} - \hat{\alpha}_{i-1}(\hat{s}_{i-1} - A\hat{p}_{i-1}) + \delta r_i + A\delta x_i \end{aligned}$$

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where

$$G_i = \hat{S}_i - A\hat{P}_i, \quad d_i = [\hat{\alpha}_0, \dots, \hat{\alpha}_{i-1}]^T$$

see [C., Rozložník, Strakoš, Tichý, Tůma, 2018]

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Attainable accuracy of simple pipelined CG

$$\|G_i\| \leq \frac{O(\varepsilon)}{1 - O(\varepsilon)} \left(\kappa(\widehat{U}_i)\|A\| \left\|\widehat{P}_i\right\| + \|A\| \left\|\widehat{R}_i\right\| \left\|\widehat{U}_i^{-1}\right\| \right)$$

$$\widehat{U}_i = \begin{bmatrix} 1 & -\hat{\beta}_1 & 0 & 0 \\ 0 & 1 & \ddots & 0 \\ \vdots & \ddots & 1 & -\hat{\beta}_{i-1} \\ 0 & \dots & 0 & 1 \end{bmatrix} \qquad \widehat{U}_i^{-1} = \begin{bmatrix} 1 & \hat{\beta}_1 & \dots & \dots & \hat{\beta}_1\hat{\beta}_2 \cdots \hat{\beta}_{i-1} \\ 0 & 1 & \hat{\beta}_2 & \dots & \hat{\beta}_2 \cdots \hat{\beta}_{i-1} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & 1 & \hat{\beta}_{i-1} \\ 0 & \cdots & \cdots & 0 & 1 \end{bmatrix}$$

see [C., Rozložník, Strakoš, Tichý, Tůma, 2018]

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$$\beta_\ell \beta_{\ell+1} \cdots \beta_j = \frac{\left\|r_j\right\|^2}{\|r_{\ell-1}\|^2}, \qquad \ell < j$$

see [C., Rozložník, Strakoš, Tichý, Tůma, 2018]

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- Residual oscillations can cause these factors to be large!
- Errors in computed recurrence coefficients can be amplified!

see [C., Rozložník, Strakoš, Tichý, Tůma, 2018]

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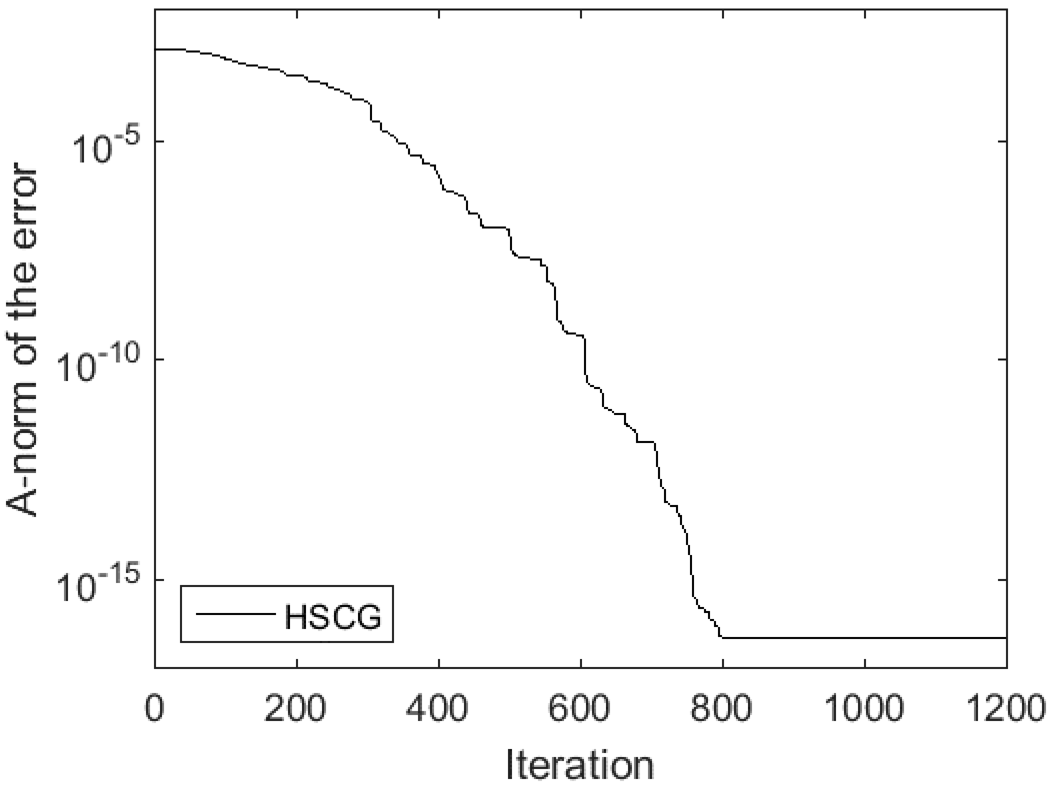
- Residual oscillations can cause these factors to be large!
- Errors in computed recurrence coefficients can be amplified!

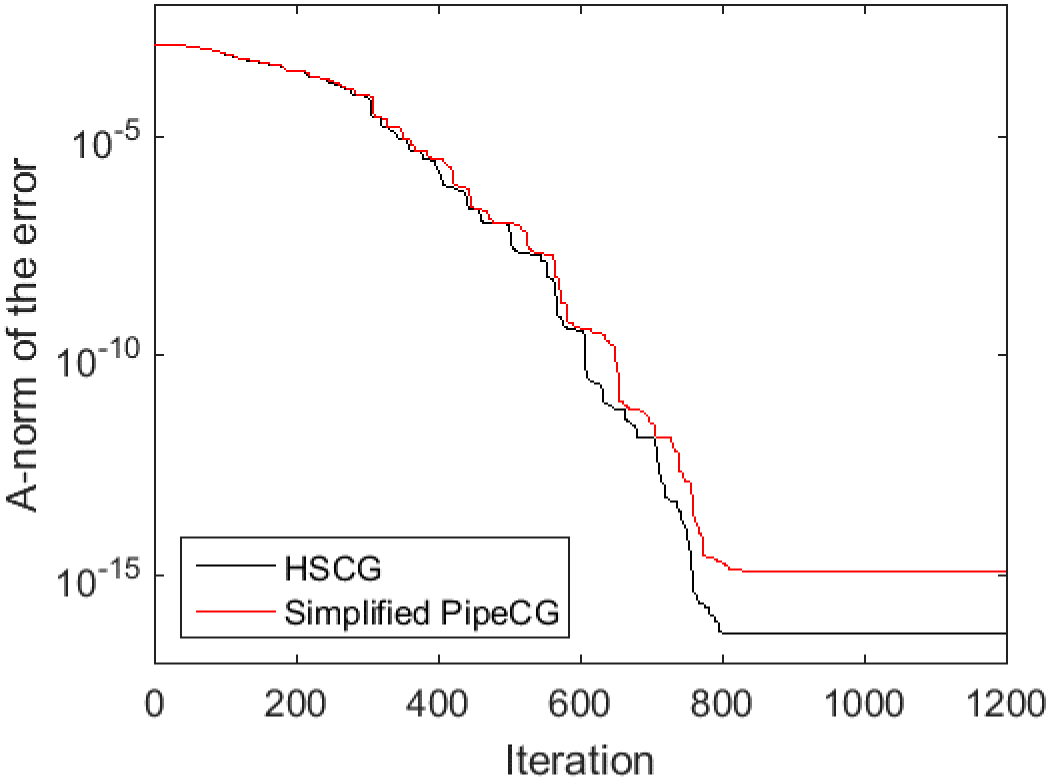
- Very similar to the results for attainable accuracy in the 3-term STCG
- Seemingly innocuous change can cause drastic loss of accuracy

see [C., Rozložník, Strakoš, Tichý, Tůma, 2018]

Simple pipelined CG

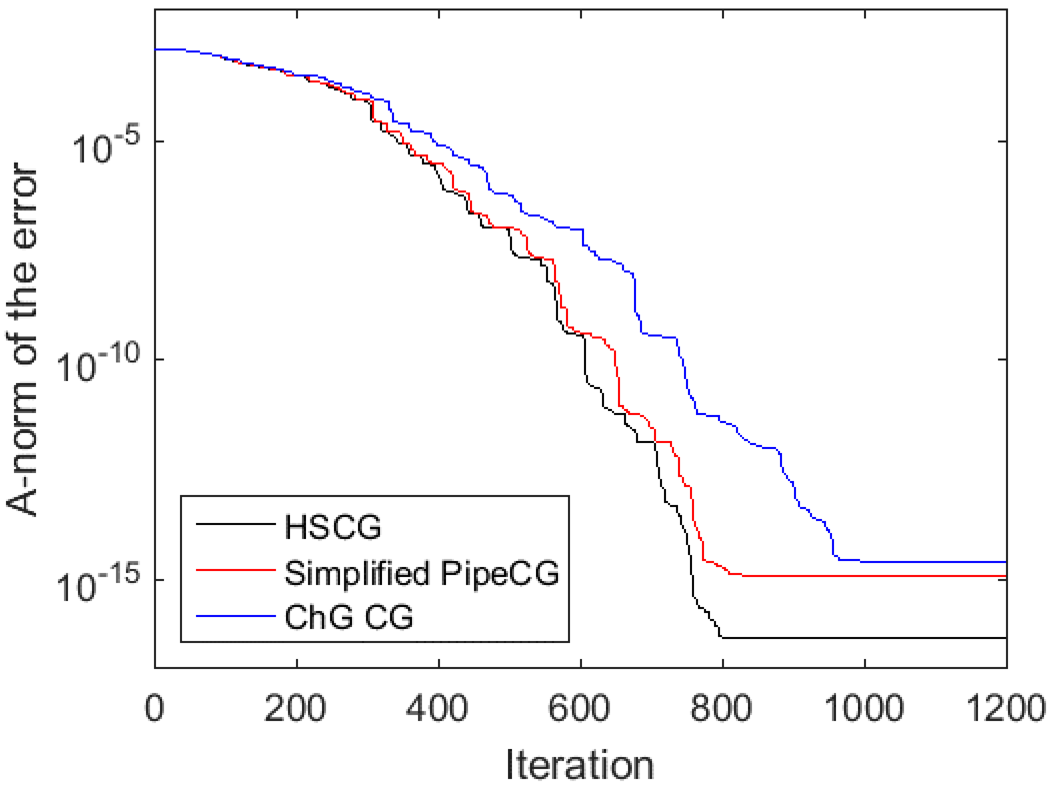


Simple pipelined CG



effect of using auxiliary vector $s_i \equiv Ap_i$

Simple pipelined CG



effect of changing formula for recurrence coefficient α and using auxiliary vector $s_i \equiv Ap_i$

Attainable Accuracy of Pipelined CG

(Cools, et al., 2018)

Pipelined CG uses 5 auxiliary recurrences:

$s_i \equiv Ap_i, \qquad q_i \equiv M^{-1}Ap_i, \qquad u_i \equiv M^{-1}r_i, \qquad w_i = AM^{-1}r_i, \qquad z_i \equiv AM^{-1}Ap_i$

Computed explicitly: $m_i \equiv M^{-1}w_i \; (\equiv M^{-1}AM^{-1}r_i), \;\; v_i = Am_i \; (\equiv AM^{-1}AM^{-1}r_i)$

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$$\begin{aligned}
\hat{p}_i &= \hat{u}_i + \hat{\beta}_i \hat{p}_{i-1} + \delta_i^p \\
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\hat{z}_i &= A\widehat{m}_i + \hat{\beta}_i \hat{z}_{i-1} + \delta_i^z \\
\hat{q}_i &= \widehat{m}_i + \hat{\beta}_i \hat{q}_{i-1} + \delta_i^q
\end{aligned}$$

$$\begin{aligned}
\hat{x}_{i+1} &= \hat{x}_i + \hat{\alpha}_i \hat{p}_i + \delta_i^x \\
\hat{r}_{i+1} &= \hat{r}_i - \hat{\alpha}_i \hat{s}_i + \delta_i^r \\
\widehat{w}_{i+1} &= \widehat{w}_i - \hat{\alpha}_i \hat{z}_i + \delta_i^w \\
\hat{u}_{i+1} &= u_i - \hat{\alpha}_i \hat{q}_i + \delta_i^u
\end{aligned}$$

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$$\begin{aligned} \hat{p}_i &= \hat{u}_i + \hat{\beta}_i \hat{p}_{i-1} + \delta_i^p \\ \hat{s}_i &= \widehat{w}_i + \hat{\beta}_i \hat{s}_{i-1} + \delta_i^s \\ \hat{z}_i &= A\widehat{m}_i + \hat{\beta}_i \hat{z}_{i-1} + \delta_i^z \\ \hat{q}_i &= \widehat{m}_i + \hat{\beta}_i \hat{q}_{i-1} + \delta_i^q \end{aligned} \qquad\qquad \begin{aligned} \hat{x}_{i+1} &= \hat{x}_i + \hat{\alpha}_i \hat{p}_i + \delta_i^x \\ \hat{r}_{i+1} &= \hat{r}_i - \hat{\alpha}_i \hat{s}_i + \delta_i^r \\ \widehat{w}_{i+1} &= \widehat{w}_i - \hat{\alpha}_i \hat{z}_i + \delta_i^w \\ \hat{u}_{i+1} &= u_i - \hat{\alpha}_i \hat{q}_i + \delta_i^u \end{aligned}$$

$$\begin{aligned} f_{i+1} &= (b - A\hat{x}_{i+1}) - \hat{r}_{i+1} \\ &= f_i - \hat{\alpha}_i (A\hat{p}_i - \hat{s}_i) - A\delta_i^x - \delta_i^r \end{aligned}$$

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$$\begin{aligned} f_{i+1} &= (b - A\hat{x}_{i+1}) - \hat{r}_{i+1} \\ &= f_i - \hat{\alpha}_i (\underbrace{A\hat{p}_i - \hat{s}_i}_{g_i \,=\, \hat{\beta}_i g_{i-1} + (A\hat{u}_{i+1} - \widehat{w}_{i+1}) + A\delta_i^p - \delta_i^s}) - A\delta_i^x - \delta_i^r \end{aligned}$$

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\hat{u}_{i+1} &= u_i - \hat{\alpha}_i \hat{q}_i + \delta_i^u
\end{aligned}$$

$$f_{i+1} = (b - A\hat{x}_{i+1}) - \hat{r}_{i+1}$$

$$= f_i - \hat{\alpha}_i \underbrace{(A\hat{p}_i - \hat{s}_i)} - A\delta_i^x - \delta_i^r$$

$$g_i = \hat{\beta}_i g_{i-1} + \underbrace{(A\hat{u}_{i+1} - \widehat{w}_{i+1})} + A\delta_i^p - \delta_i^s$$

$$h_{i+1} = h_i - \hat{\alpha}_i (A\hat{q}_i - \hat{z}_i) + A\delta_i^u - \delta_i^w$$

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$$f_{i+1} = (b - A\hat{x}_{i+1}) - \hat{r}_{i+1}$$

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$$j_i = \hat{\beta}_i j_{i-1} + A\delta_i^q - \delta_i^z$$

Attainable Accuracy of Pipelined CG

$$f_{i+1} = f_0 - \sum_{j=0}^{i} \hat{\alpha}_j g_j - \sum_{j=0}^{i} (A\delta_j^x + \delta_j^r)$$

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$$f_{i+1} = f_0 - \sum_{j=0}^{i} \hat{\alpha}_j g_j - \sum_{j=0}^{i} (A\delta_j^x + \delta_j^r)$$

$$g_j = \left(\prod_{k=1}^{j} \hat{\beta}_k\right) g_0 + \sum_{k=1}^{j} \left(\prod_{\ell=k+1}^{j} \hat{\beta}_\ell\right) \left(A\delta_k^p - \delta_k^s\right) + \sum_{k=1}^{j} \left(\prod_{\ell=k+1}^{j} \hat{\beta}_\ell\right) h_k$$

$$h_k = h_0 - \sum_{\ell=0}^{k-1} \hat{\alpha}_\ell j_\ell + \sum_{\ell=0}^{k-1} (A\delta_\ell^u + \delta_\ell^w)$$

$$j_\ell = \left(\prod_{m=1}^{\ell} \hat{\beta}_m\right) j_0 + \sum_{m=1}^{\ell} \left(\prod_{n=m+1}^{\ell} \hat{\beta}_n\right) \left(A\delta_m^q - \delta_m^z\right)$$

Attainable Accuracy of Pipelined CG

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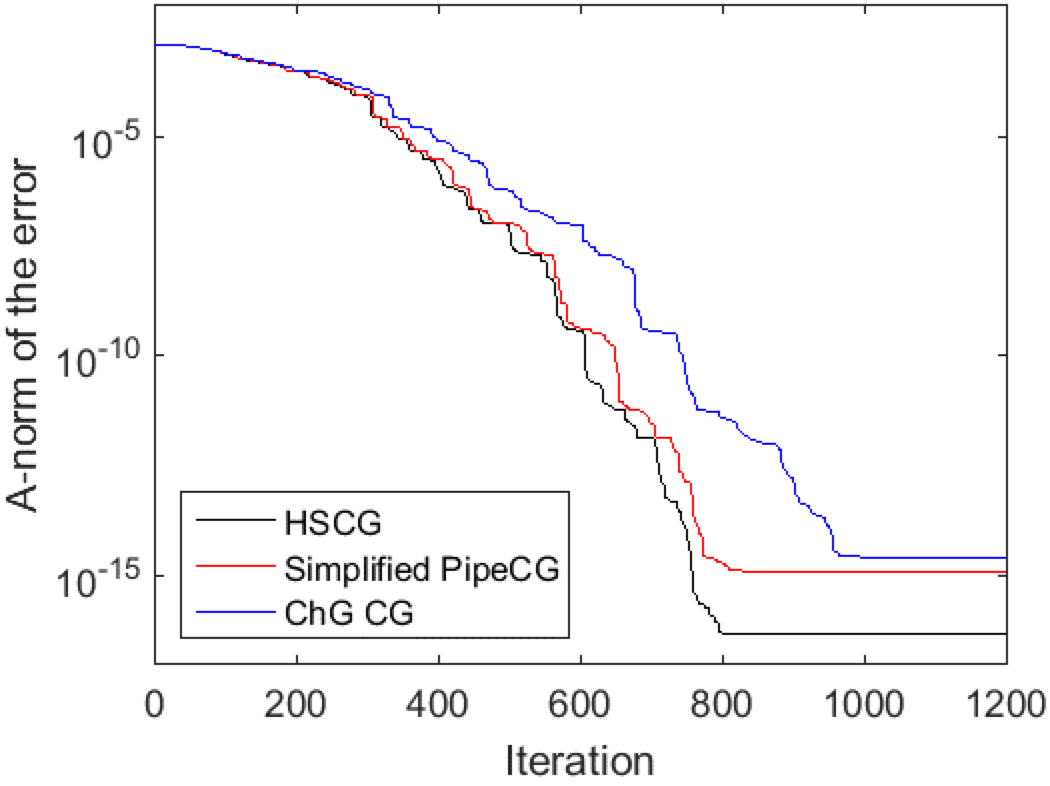
$$g_j = \left(\prod_{k=1}^{j} \hat{\beta}_k\right) g_0 + \sum_{k=1}^{j} \left(\prod_{\ell=k+1}^{j} \hat{\beta}_\ell\right) \left(A\delta_k^p - \delta_k^s\right) + \sum_{k=1}^{j} \left(\prod_{\ell=k+1}^{j} \hat{\beta}_\ell\right) h_k$$

$$h_k = h_0 - \sum_{\ell=0}^{k-1} \hat{\alpha}_\ell j_\ell + \sum_{\ell=0}^{k-1} (A\delta_\ell^u - \delta_\ell^w)$$

$$j_\ell = \left(\prod_{m=1}^{\ell} \hat{\beta}_m\right) j_0 + \sum_{m=1}^{\ell} \left(\prod_{n=m+1}^{\ell} \hat{\beta}_n\right) \left(A\delta_m^q - \delta_m^z\right)$$

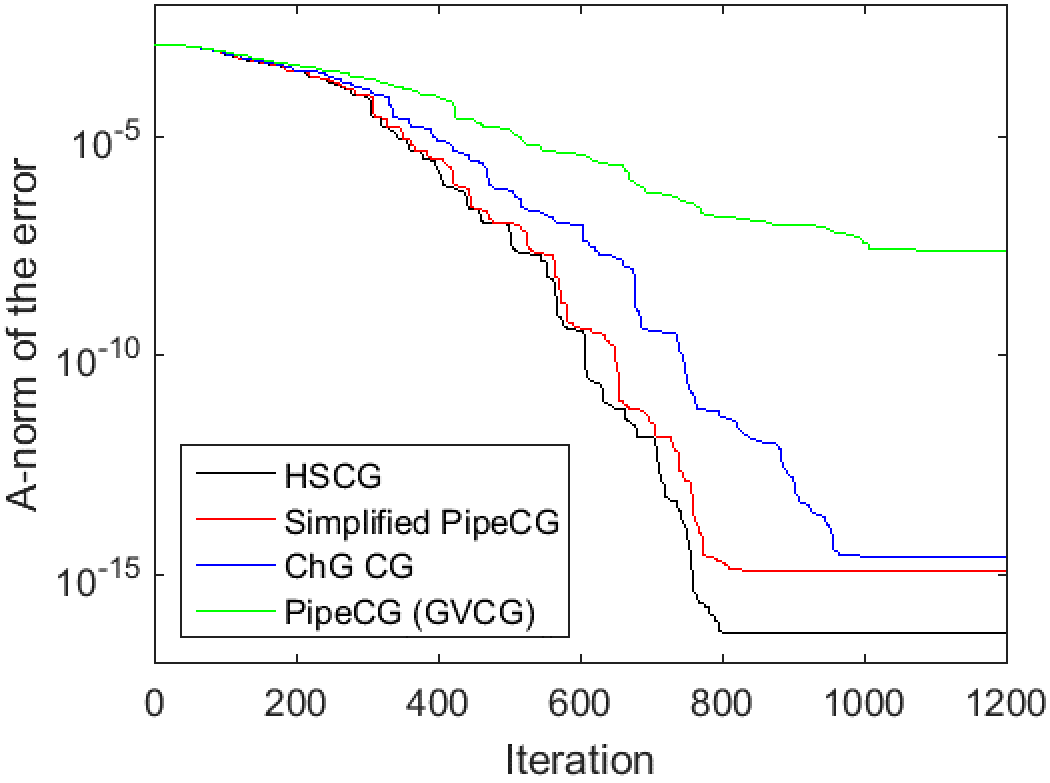
Local rounding errors
all potentially
amplified!

Pipelined CG



effect of changing formula for recurrence coefficient α and using auxiliary vector $s_i \equiv Ap_i$

Pipelined CG

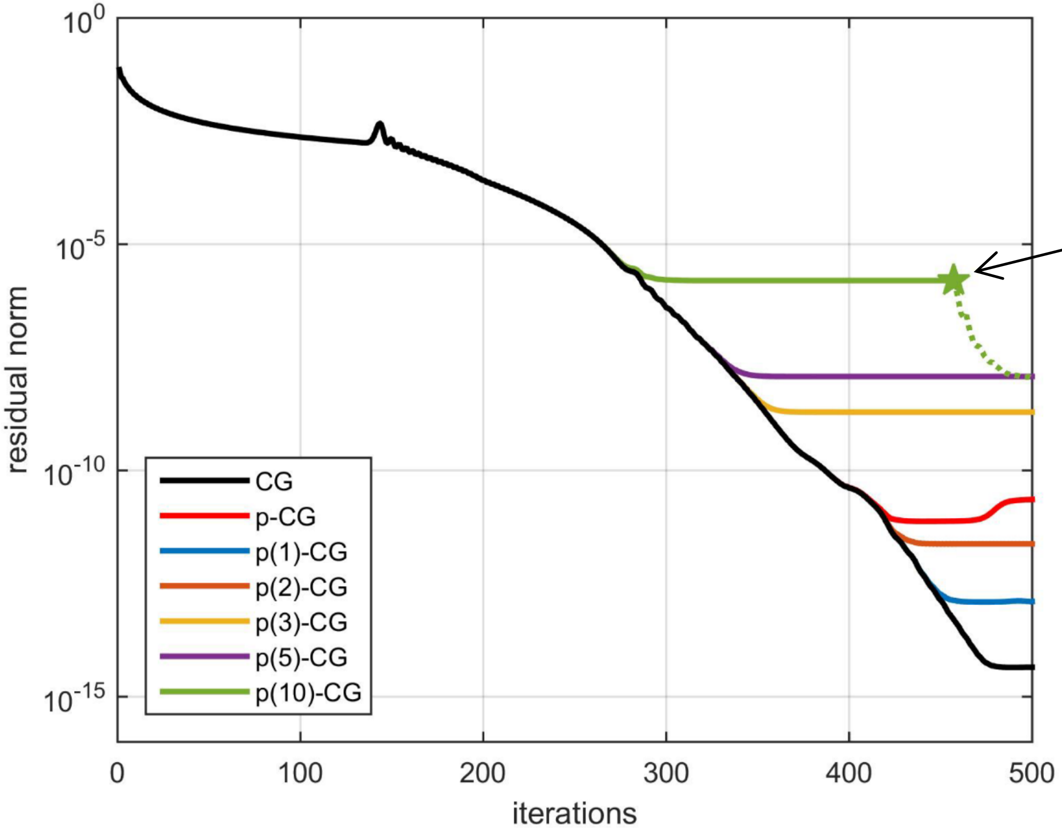


effect of changing formula for recurrence coefficient α and using auxiliary vectors $s_i \equiv Ap_i, w_i \equiv Ar_i, z_i \equiv A^2 r_i$

Effect of Deeper Pipelines

- Deeper pipeline -> effectively adding more auxiliary recurrences
- We expect residual gap to increase with increasing pipeline depth
- Some initial work (Cools, 2018) uses Chebyshev shifts to attempt to stabilize (deep) pipelined CG; but increasing gap is still apparent

2D Poisson problem, $N = 200$, b set such that $x_i = 1/\sqrt{N}$



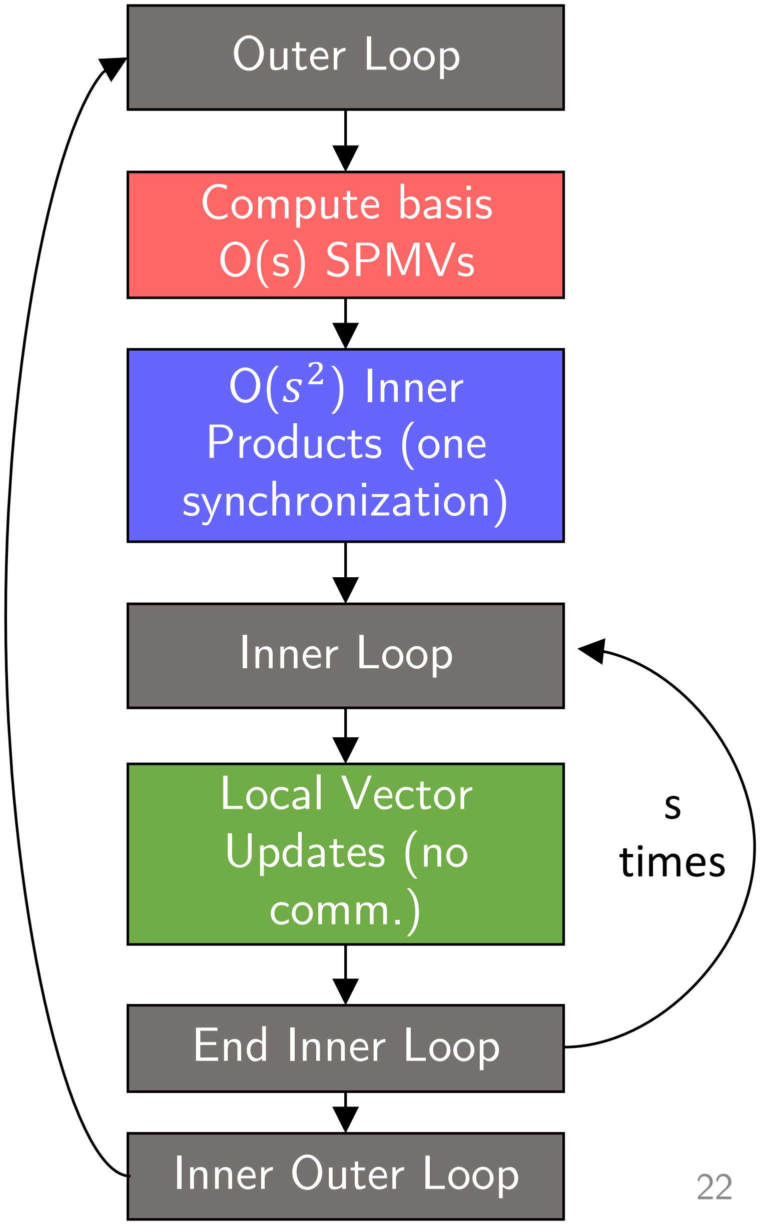
square root breakdown + explicit restart

(Cools, 2018)

s-step CG

```
$r_0 = b - Ax_0, p_0 = r_0$
for $k = 0$:nmax/$s$
    Compute $\mathcal{Y}_k$ and $\mathcal{B}_k$ such that $A\underline{\mathcal{Y}}_k = \mathcal{Y}_k\mathcal{B}_k$ and
        span($\mathcal{Y}_k$) $= \mathcal{K}_{s+1}(A, p_{sk}) + \mathcal{K}_s(A, r_{sk})$
    $\mathcal{G}_k = \mathcal{Y}_k^T\mathcal{Y}_k$
    $x_0' = 0, r_0' = e_{s+2}, p_0' = e_1$
    for $j = 1: s$
        $\alpha_{sk+j-1} = \frac{r_{j-1}'^T \mathcal{G}_k r_{j-1}'}{p_{j-1}'^T \mathcal{G}_k \mathcal{B}_k p_{j-1}'}$
        $x_j' = x_{j-1}' + \alpha_{sk+j-1} p_{j-1}'$
        $r_j' = r_{j-1}' - \alpha_{sk+j-1} \mathcal{B}_k p_{j-1}'$
        $\beta_{sk+j} = \frac{r_j'^T \mathcal{G}_k r_j'}{r_{j-1}'^T \mathcal{G}_k r_{j-1}'}$
        $p_j' = r_j' + \beta_{sk+j} p_{j-1}'$
    end

$[x_{s(k+1)} - x_{sk}, r_{s(k+1)}, p_{s(k+1)}] = \mathcal{Y}_k[x_s', r_s', p_s']$
end
```



Outer Loop

Compute basis O(s) SPMVs

O(s^2) Inner Products (one synchronization)

Inner Loop

Local Vector Updates (no comm.)

End Inner Loop

Inner Outer Loop

s times

Sources of local roundoff error in s-step CG

Computing the s-step Krylov subspace basis:

$$A\underline{\hat{\mathcal{Y}}}_k = \hat{\mathcal{Y}}_k\mathcal{B}_k + \Delta\mathcal{Y}_k$$

Updating coordinate vectors in the inner loop:

$$\hat{x}'_{k,j} = \hat{x}'_{k,j-1} + \hat{q}'_{k,j-1} + \xi_{k,j}$$

$$\hat{r}'_{k,j} = \hat{r}'_{k,j-1} - \mathcal{B}_k\,\hat{q}'_{k,j-1} + \eta_{k,j}$$

$$\text{with} \quad \hat{q}'_{k,j-1} = \mathrm{fl}(\hat{\alpha}_{sk+j-1}\hat{p}'_{k,j-1})$$

Recovering CG vectors for use in next outer loop:

$$\hat{x}_{sk+j} = \hat{\mathcal{Y}}_k\hat{x}'_{k,j} + \hat{x}_{sk} + \phi_{sk+j}$$

$$\hat{r}_{sk+j} = \hat{\mathcal{Y}}_k\hat{r}'_{k,j} + \psi_{sk+j}$$

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Error in computing s-step basis

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Error in basis change

Attainable accuracy of s-step CG

- We can write the gap between the true and updated residuals f in terms of these errors:

$$
\boxed{
\begin{aligned}
f_{sk+j} &= f_0 \\
&\quad - \sum_{\ell=0}^{k-1} \left[A\phi_{s\ell+s} + \psi_{s\ell+s} + \sum_{i=1}^{s} \left[A\hat{\mathcal{Y}}_{\ell}\xi_{\ell,i} + \hat{\mathcal{Y}}_{\ell}\eta_{\ell,i} - \Delta\mathcal{Y}_{\ell}\hat{q}'_{\ell,i-1} \right] \right] \\
&\quad - A\phi_{sk+j} - \psi_{sk+j} - \sum_{i=1}^{j} \left[A\hat{\mathcal{Y}}_{k}\xi_{k,i} + \hat{\mathcal{Y}}_{k}\eta_{k,i} - \Delta\mathcal{Y}_{\ell}\hat{q}'_{k,i-1} \right]
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}
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- Using standard rounding error results, this allows us to obtain an upper bound on $\|f_{sk+j}\|$.

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Attainable accuracy of s-step CG

$f_i \equiv b - A\hat{x}_i - \hat{r}_i$

For CG:

$$\|f_i\| \leq \|f_0\| + \varepsilon \sum_{m=1}^{i} (1+N)\|A\|\|\hat{x}_m\| + \|\hat{r}_m\|$$

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For s-step CG: $i \equiv sk + j$

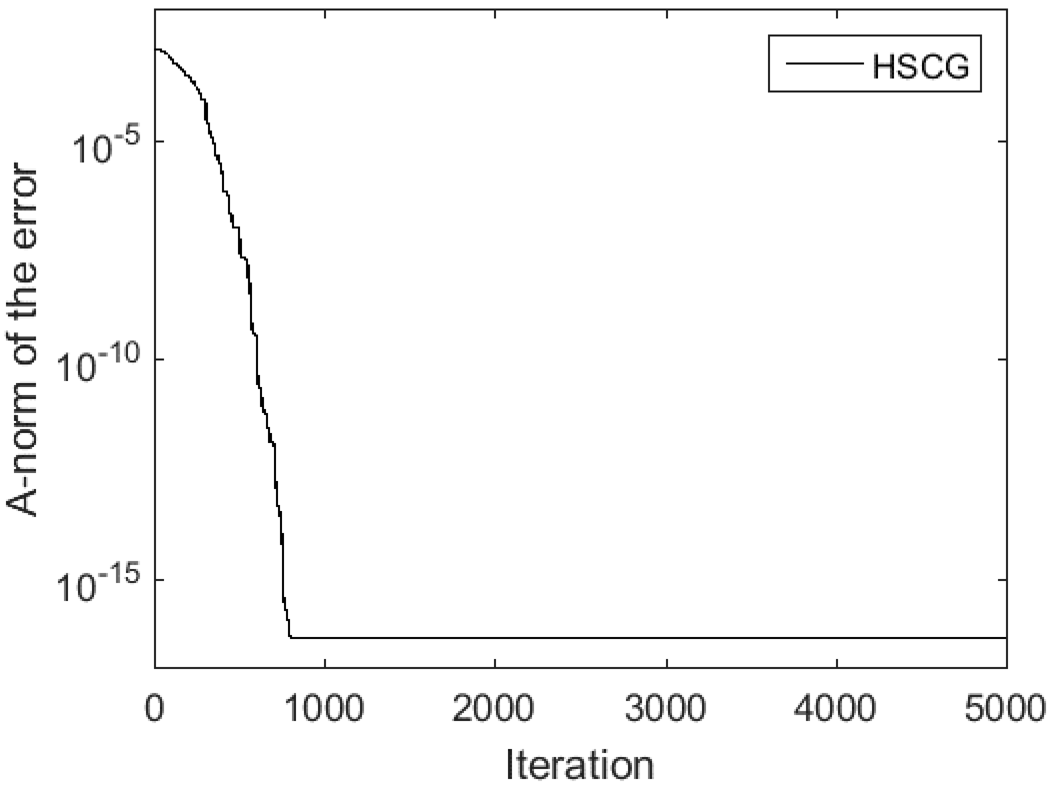
$$\|f_{sk+j}\| \leq \|f_0\| + \varepsilon \boldsymbol{c}\boldsymbol{\bar{\Gamma}_k} \sum_{m=1}^{sk+j} (1+N)\|A\|\|\hat{x}_m\| + \|\hat{r}_m\|$$

where c is a low-degree polynomial in s, and

$$\bar{\Gamma}_k = \max_{\ell \leq k} \Gamma_\ell \;, \qquad \text{where} \qquad \Gamma_\ell = \|\hat{\mathcal{Y}}_\ell^+\| \cdot \||\hat{\mathcal{Y}}_\ell|\|$$

(see C., 2015)

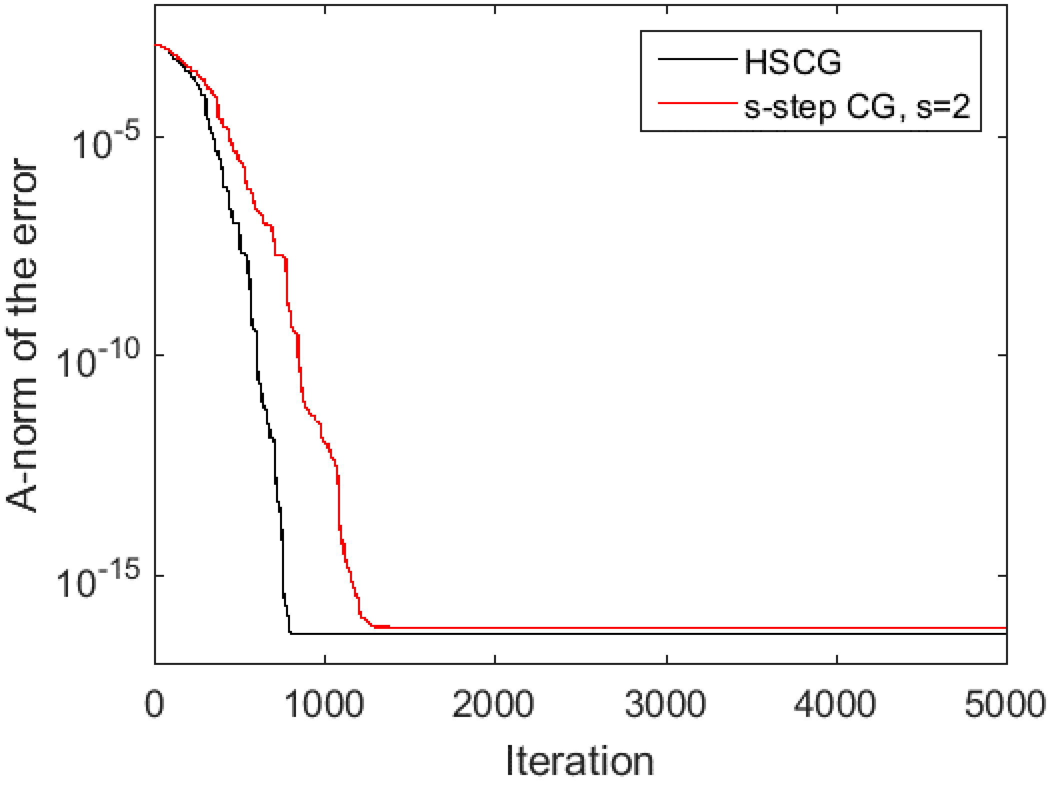
s-step CG



HSCG
A-norm of the error
10^{-5}
10^{-10}
10^{-15}
0
1000
2000
3000
4000
5000
Iteration

s-step CG

s-step CG with monomial basis ($\mathcal{Y} = [p_i, Ap_i, \ldots, A^s p_i, r_i, Ar_i, \ldots A^{s-1} r_i]$)



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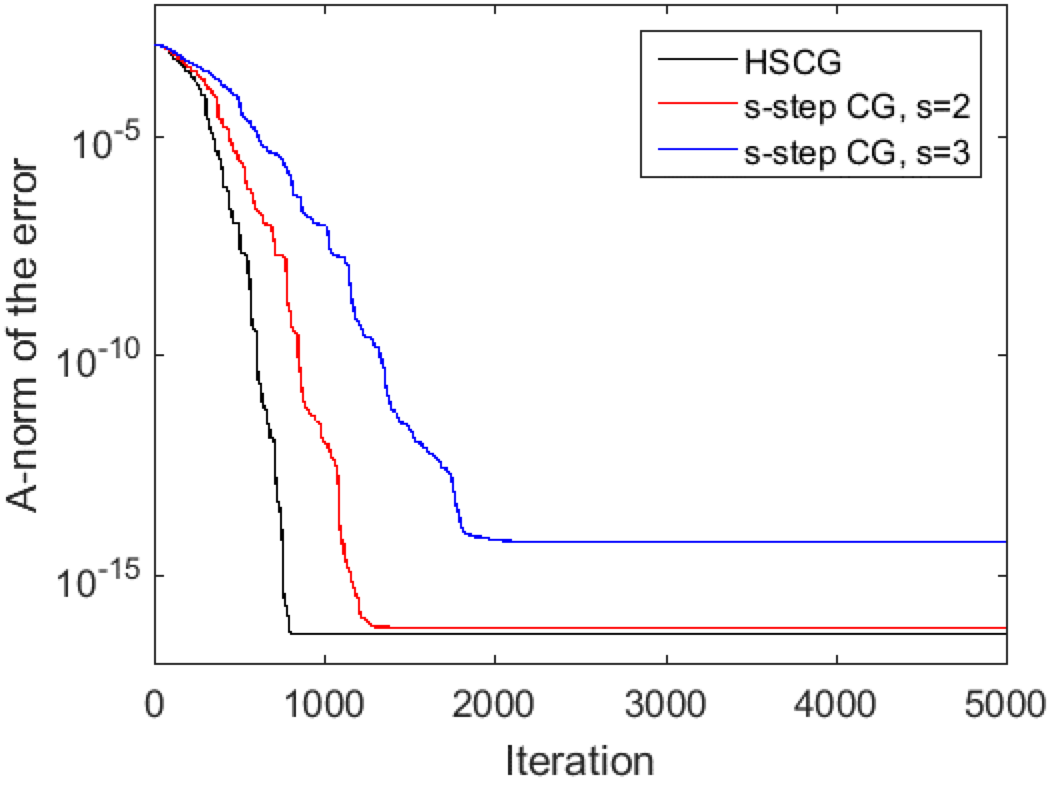

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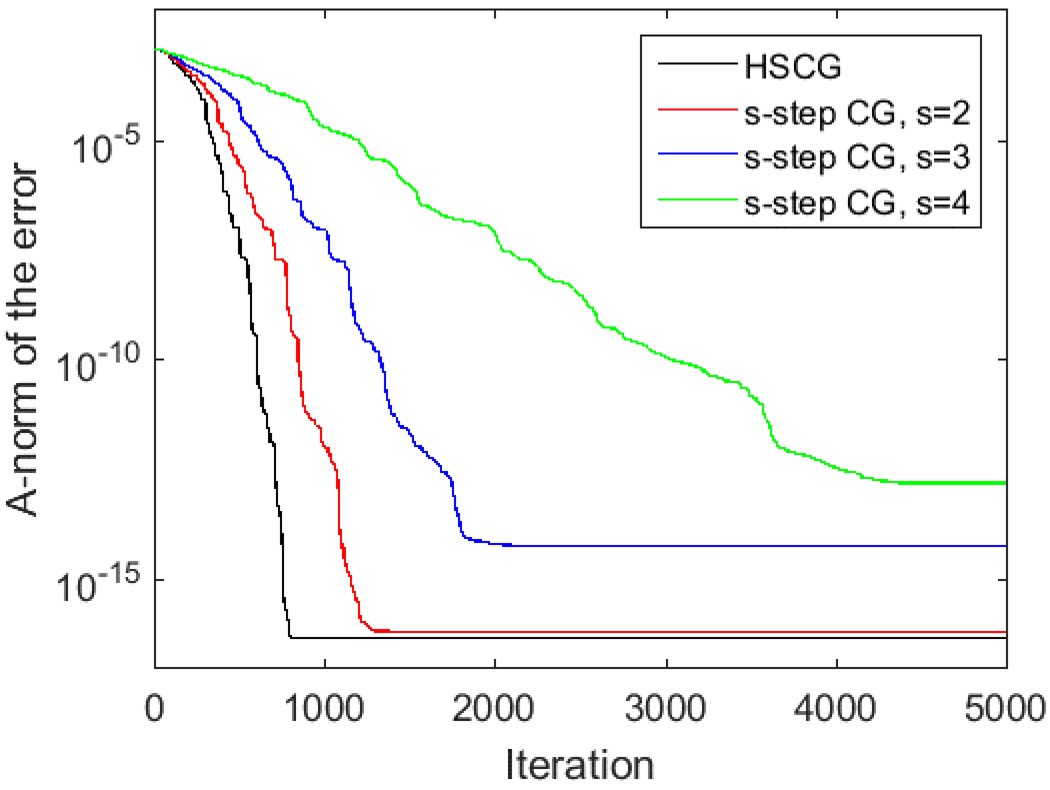
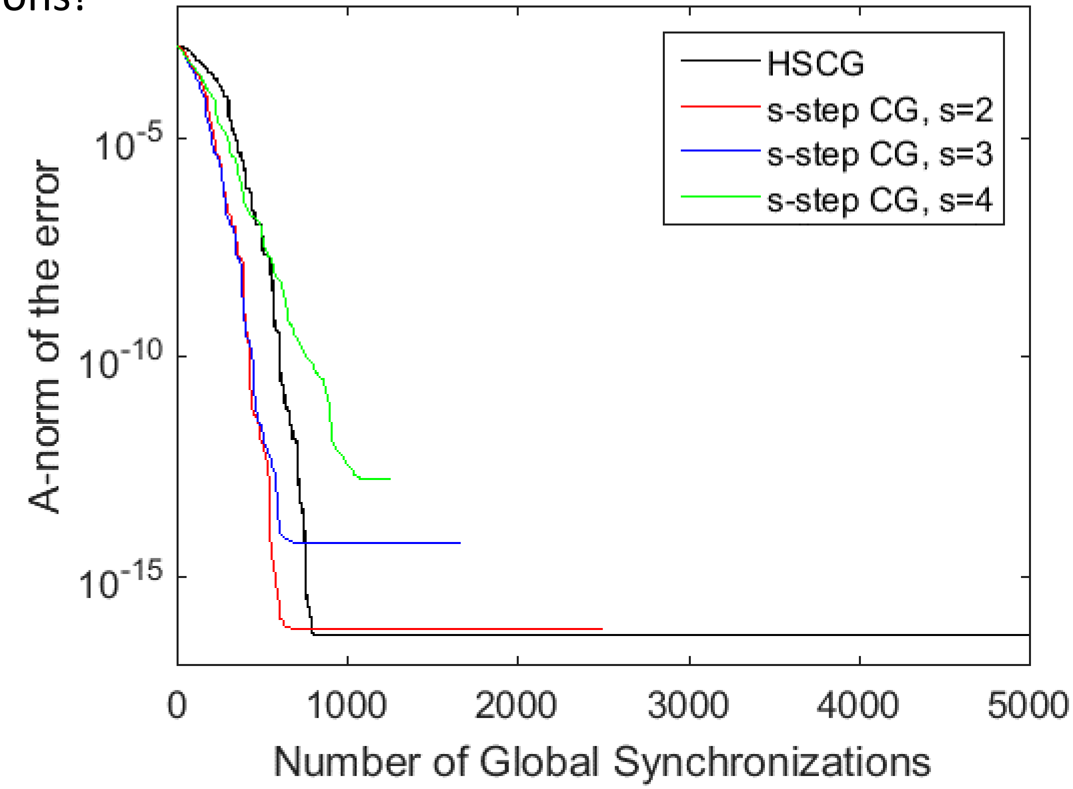


s-step CG

Even assuming perfect parallel scalability with s (which is usually not the case due to extra SpMVs and inner products), already at $s = 4$ we are worse than HSCG in terms of number of synchronizations!



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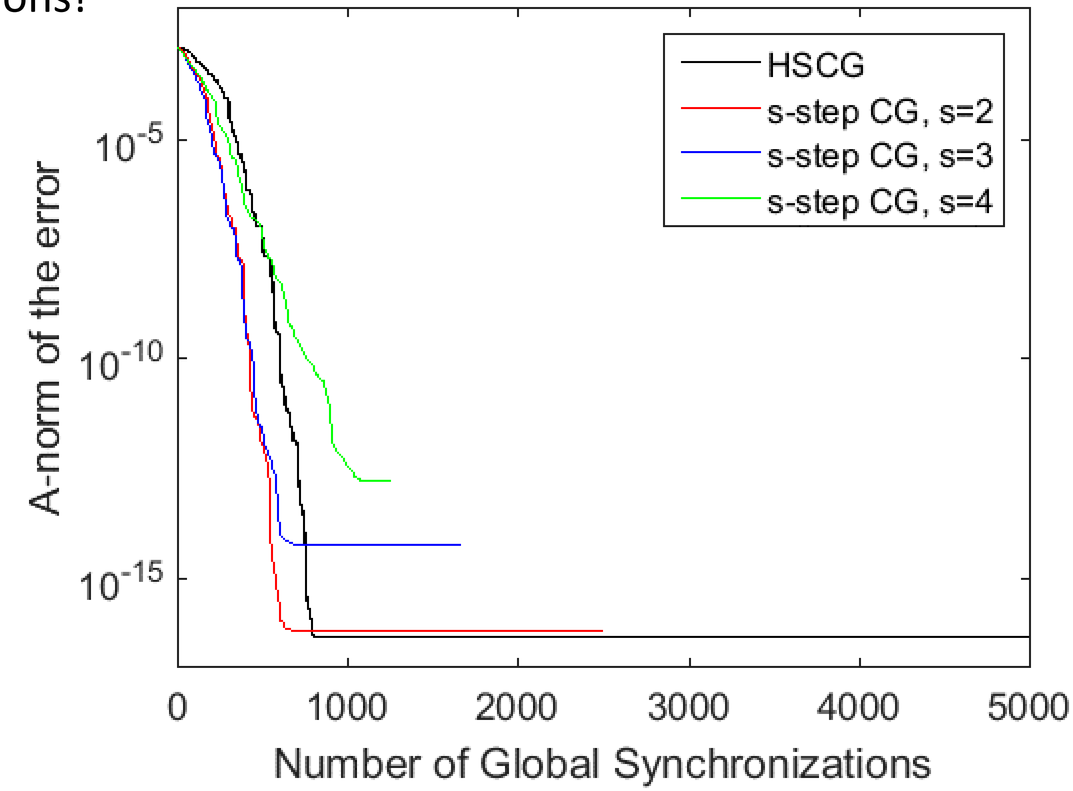

⇒ Can use other, more well-conditioned bases to improve convergence rate and accuracy (see, e.g. Philippe and Reichel, 2012).

Choosing a Polynomial Basis

- Recall: in each outer loop of s-step CG, we compute bases for some Krylov subspaces, e.g., $\mathcal{K}_{s+1}(A, p_i) = \text{span}\{p_i, Ap_i, \dots, A^s p_i\}$

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  - Recognized early on that this negatively affects convergence and accuracy (Leland, 1989), (Chronopoulous & Swanson, 1995)

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- **Improve basis condition number to improve numerical behavior**: Use different polynomials to compute a basis for the same subspace.

- Two choices based on spectral information that usually lead to well-conditioned bases:
  - **Newton polynomials**
  - **Chebyshev polynomials**

Better conditioned bases

- The Newton basis:

$$\{v, (A-\theta_1)v, (A-\theta_2)(A-\theta_1)v, \dots, (A-\theta_s)\cdots(A-\theta_1)v\}$$

  where $\{\theta_1, \dots, \theta_s\}$ are approximate eigenvalues of A, ordered according to Leja ordering

  – In practice: recover Ritz values from the first few iterations, iteratively refine eigenvalue estimates to improve basis

  – Used by many to improve s-step variants: e.g., Bai, Hu, and Reichel (1991), Erhel (1995), Hoemmen (2010)

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- Chebyshev basis: given ellipse enclosing spectrum of A with foci at $d \pm c$, we can generate the scaled and shifted Chebyshev polynomials as:

$$\tilde{\tau}_j(z) = \left(\tau_j\left(\frac{d-z}{c}\right)\right) \Big/ \left(\tau_j\left(\frac{d}{c}\right)\right)$$

  where $\{\tau_j\}_{j\geq 0}$ are the Chebyshev polynomials of the first kind

  – In practice: estimate d and c parameters from Ritz values recovered from the first few iterations

  – Used by many to improve s-step variants: e.g., de Sturler (1991), Joubert and Carey (1992), de Sturler and van der Vorst (1995)

"Backwards-like" analysis of Greenbaum

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    - Complete rounding error analysis
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- Can we make similar statements for HPC variants?

Roundoff Error in Lanczos vs. s-step Lanczos

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

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

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

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

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

$$\sigma \equiv \|A\|_2$$
$$\theta\sigma \equiv \||A|\|_2$$

Lanczos [Paige, 1976]

$$\varepsilon_0 = O(\varepsilon N)$$
$$\varepsilon_1 = O(\varepsilon n \theta)$$

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

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

$$\sigma \equiv \|A\|_2$$
$$\theta\sigma \equiv \||A|\|_2$$

Lanczos [Paige, 1976]

$$\varepsilon_0 = O(\varepsilon N)$$
$$\varepsilon_1 = O(\varepsilon n \theta)$$

s-step Lanczos [C., Demmel, 2015]:

$$\varepsilon_0 = O\left(\varepsilon N \boldsymbol{\Gamma}^2\right)$$
$$\varepsilon_1 = O(\varepsilon n \theta \boldsymbol{\Gamma})$$

$$\Gamma = c \cdot \max_{\ell \leq k} \|\hat{\mathcal{Y}}_\ell^+\| \, \||\hat{\mathcal{Y}}_\ell|\|$$

The amplification term

- Roundoff errors in s-step variant follow same pattern as classical variant, but amplified by factor of Γ or Γ^2
    - Theoretically confirms empirical observations on importance of basis conditioning (dating back to late ‘80s)

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- Using the definition

$$\Gamma \equiv \Gamma_k = \max_{\ell \leq k} \|\mathcal{Y}_\ell^+\| \cdot \||\mathcal{Y}_\ell|\|$$

  gives simple, but loose bounds

- What we really need: $\||\mathcal{Y}||y'|\| \leq \Gamma \|\mathcal{Y}y'\|$ to hold for the computed basis $\mathcal{Y}$ and coordinate vector y' in every bound.

The amplification term

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    - **Theoretically confirms empirical observations** on importance of basis conditioning (dating back to late ‘80s)

- Using the definition
$$\Gamma \equiv \Gamma_k = \max_{\ell \leq k} \|\mathcal{Y}_\ell^+\| \cdot \||\mathcal{Y}_\ell|\|$$
gives simple, but loose bounds

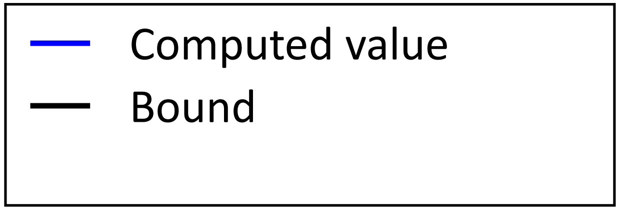
- What we really need: $\||\mathcal{Y}||y'|\| \leq \Gamma \|\mathcal{Y}y'\|$ to hold for the computed basis $\mathcal{Y}$ and coordinate vector y' in every bound.

- **Alternate definition of Γ gives tighter bounds**; requires light bookkeeping

- Example: for bounds on $\hat{\beta}_{i+1}\left|\hat{v}_i^T \hat{v}_{i+1}\right|$ and $\left|\hat{v}_{i+1}^T \hat{v}_{i+1} - 1\right|$, we can use the definition

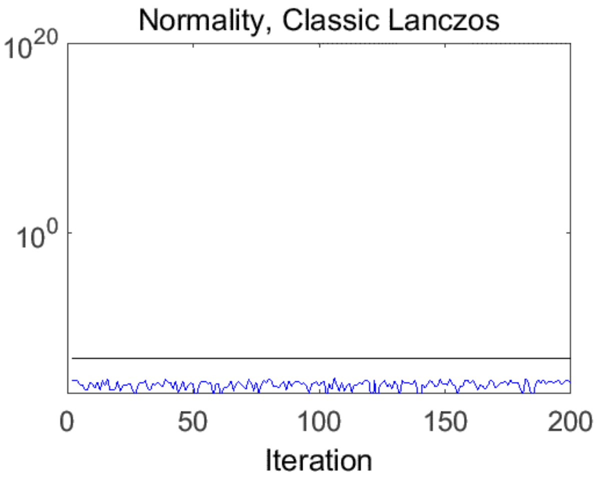
$$\Gamma_{k,j} \equiv \max_{x \in \{\hat{w}'_{k,j}, \hat{u}'_{k,j}, \hat{v}'_{k,j}, \hat{v}'_{k,j-1}\}} \frac{\||\hat{\mathcal{Y}}_k||x|\|}{\|\hat{\mathcal{Y}}_k x\|}$$

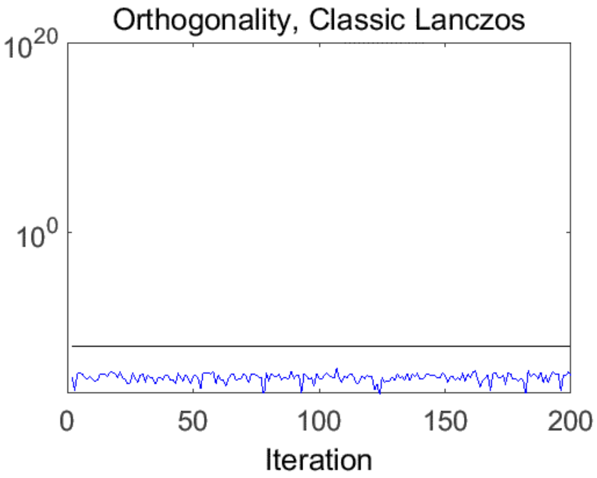
Problem: 2D Poisson,
$n = 256$,
random starting vector



$$\left|\hat{v}_{i+1}^T\hat{v}_{i+1} - 1\right| \le \varepsilon_0/2$$

$$\hat{\beta}_{i+1}\left|\hat{v}_i^T\hat{v}_{i+1}\right| \le 2\varepsilon_0\sigma$$





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🟦	Computed value
⬛	Bound
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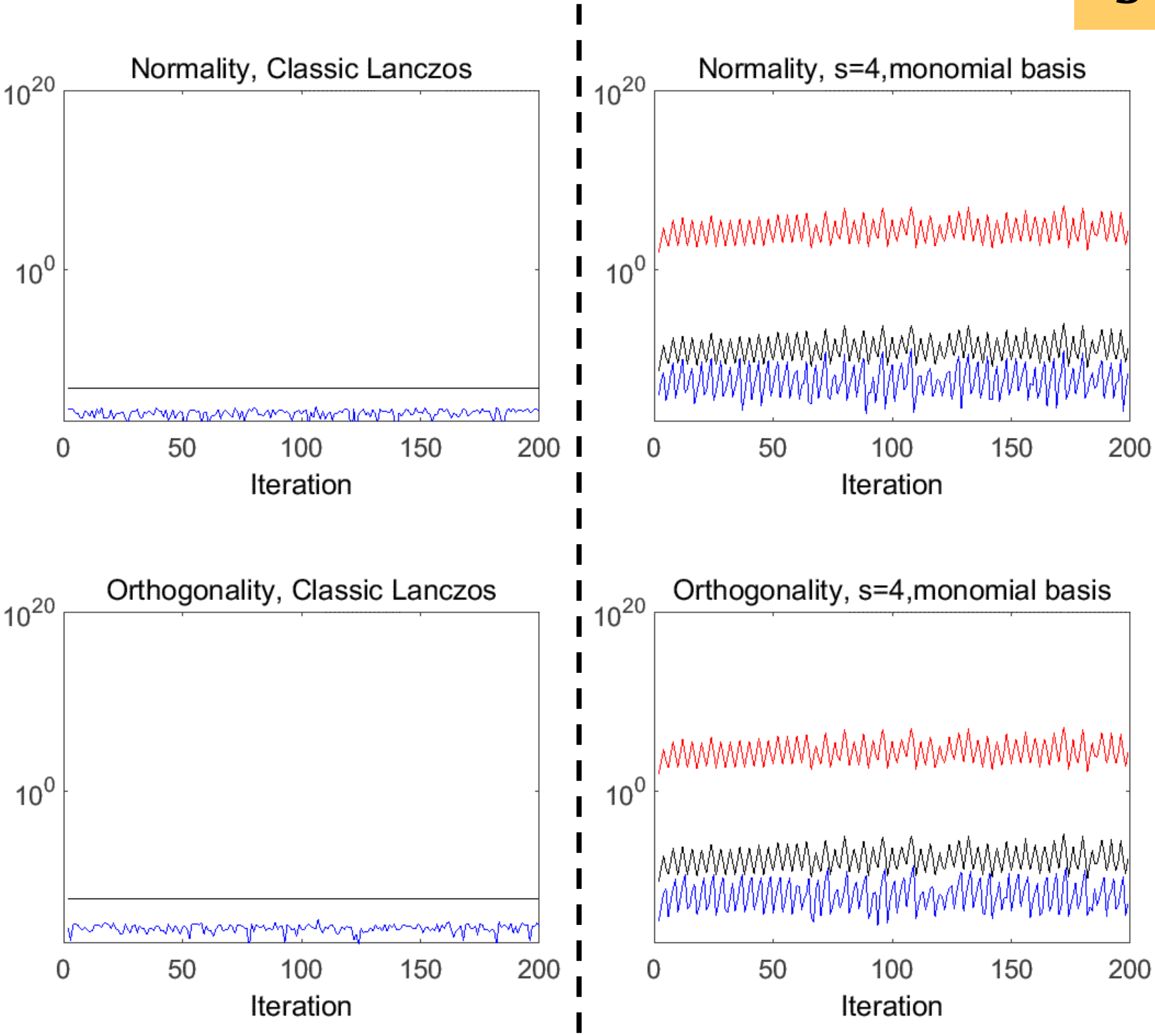
$\boldsymbol{s = 4}$



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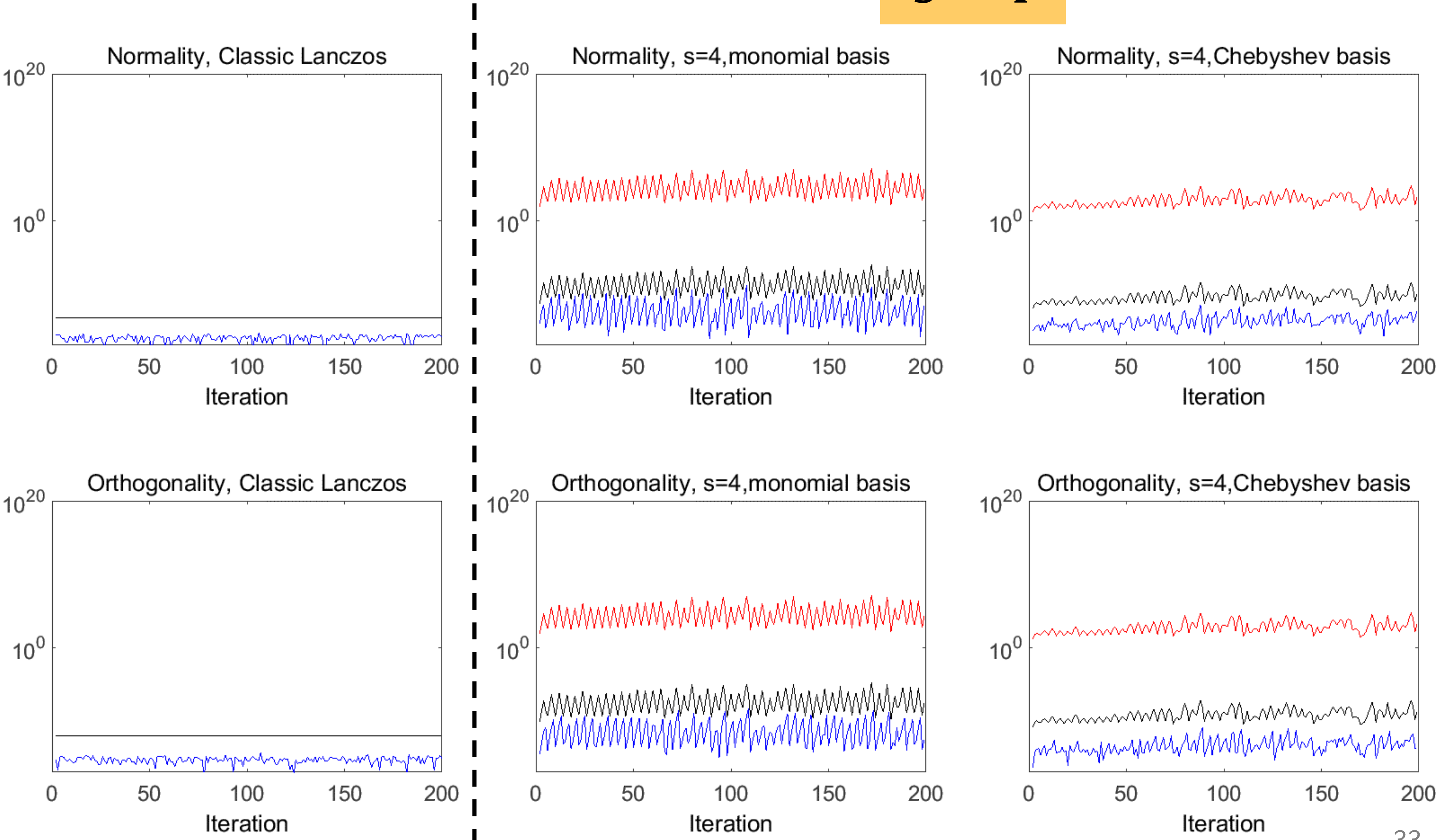

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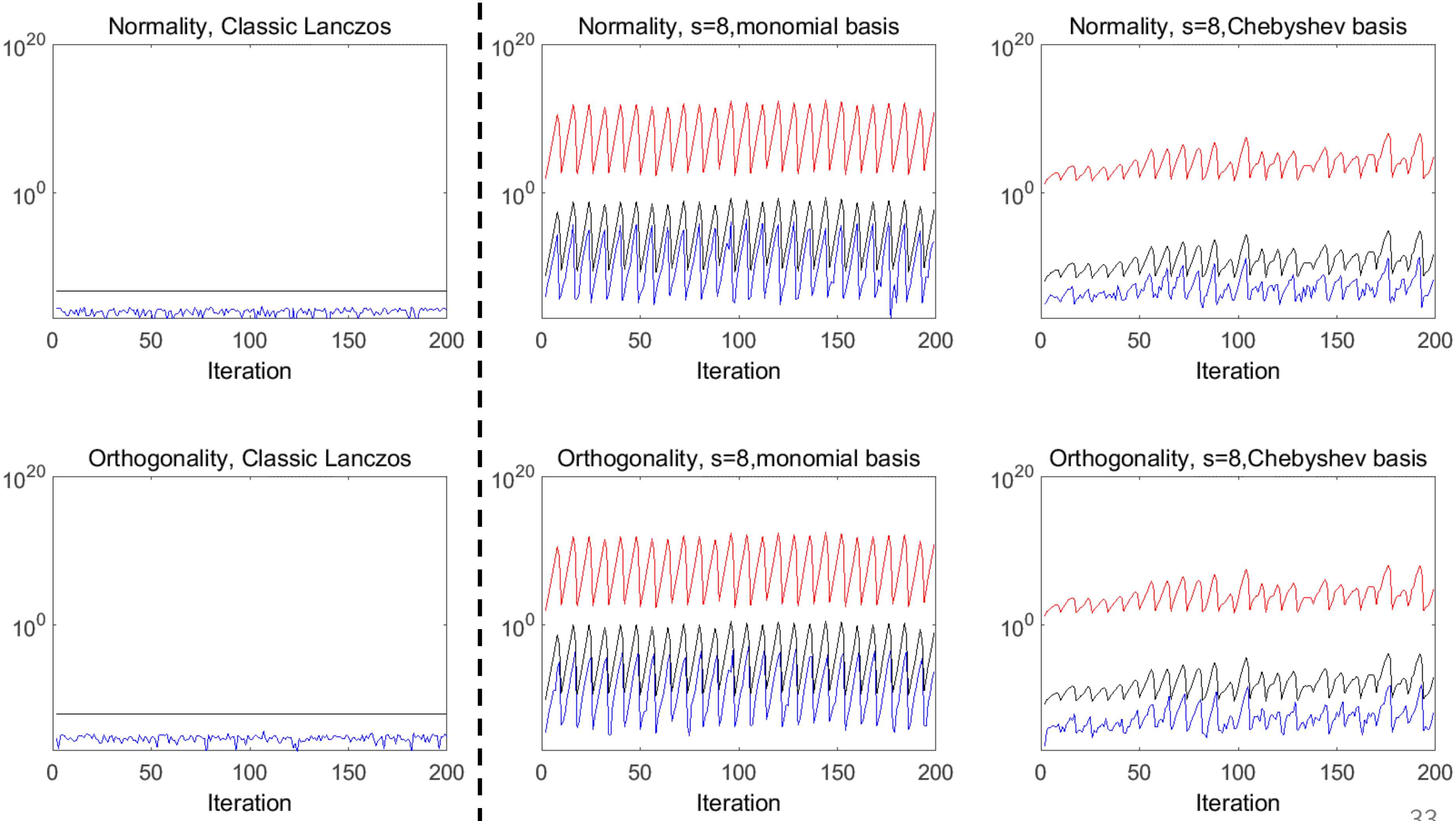

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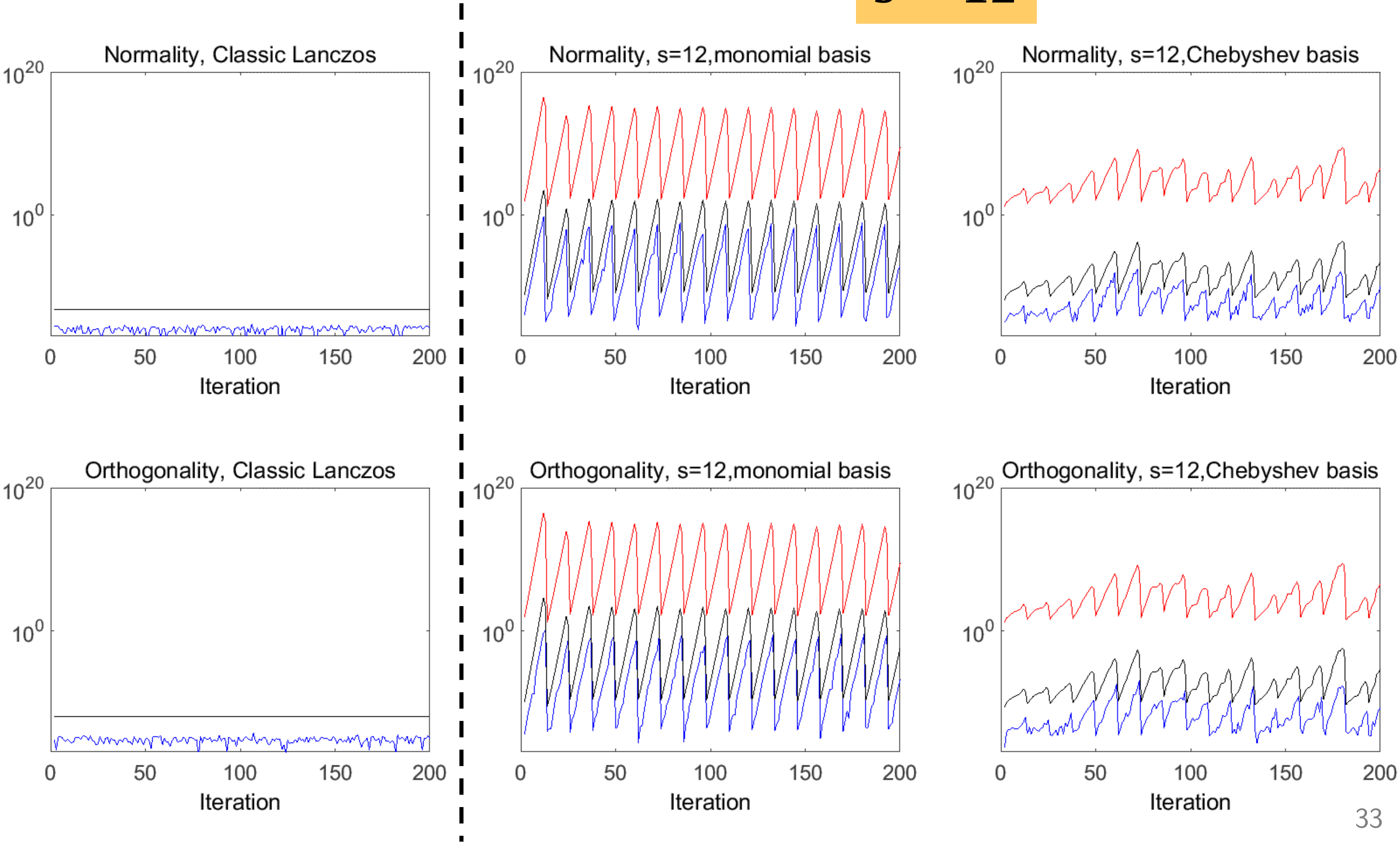

Convergence of Ritz Values in s-step Lanczos

- All results of Paige [1980], e.g., loss of orthogonality → eigenvalue convergence, hold for s-step Lanczos as long as

$$\left(\Gamma = c \cdot \max_{\ell \le k} \|\hat{\mathcal{Y}}_\ell^+\| \, \||\hat{\mathcal{Y}}_\ell|\|\right)$$

$$\Gamma \le \left(24\varepsilon(N + 11s + 15)\right)^{-1/2} \approx \frac{1}{\sqrt{N\varepsilon}}$$

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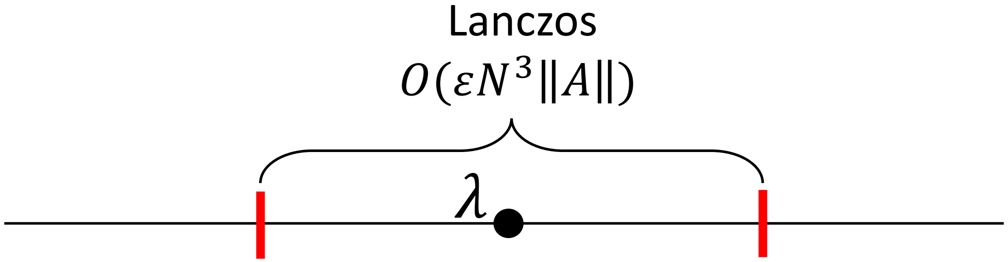
Lanczos

$O(\varepsilon N^3 \|A\|)$

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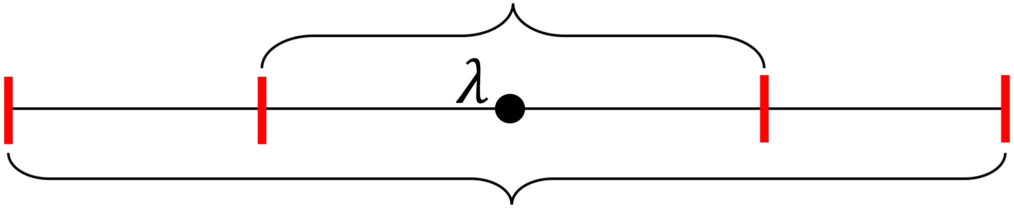

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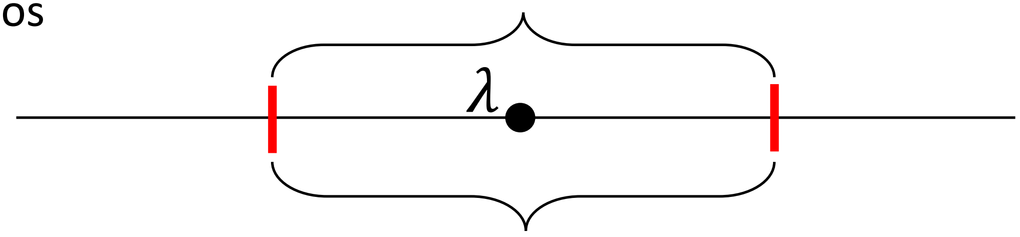
If $\boldsymbol{\Gamma \approx 1}$:

s-step Lanczos behaves the same numerically as classical Lanczos

Lanczos

$O(\varepsilon N^3\|A\|)$



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s-step Lanczos

Problem: Diagonal matrix with $n = 100$ with evenly spaced eigenvalues between $\lambda_{min} = 0.1$ and $\lambda_{max} = 100$; random starting vector

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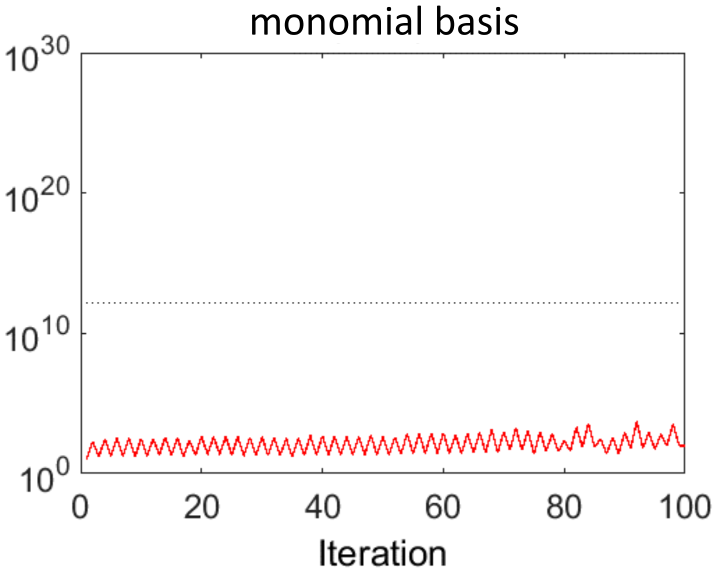
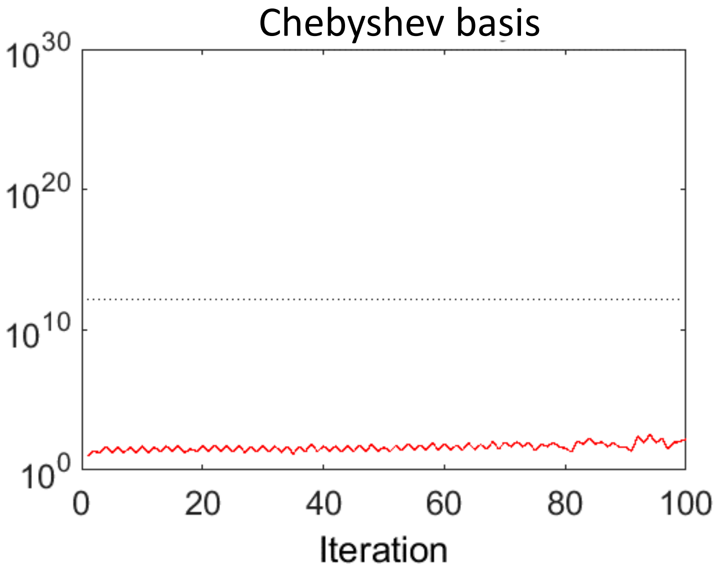
$$\boldsymbol{s = 2}$$

Top plots:

— Computed $\Gamma_{k,j}^2$

┈ $(24(\varepsilon(n + 11s + 15))^{-1}$





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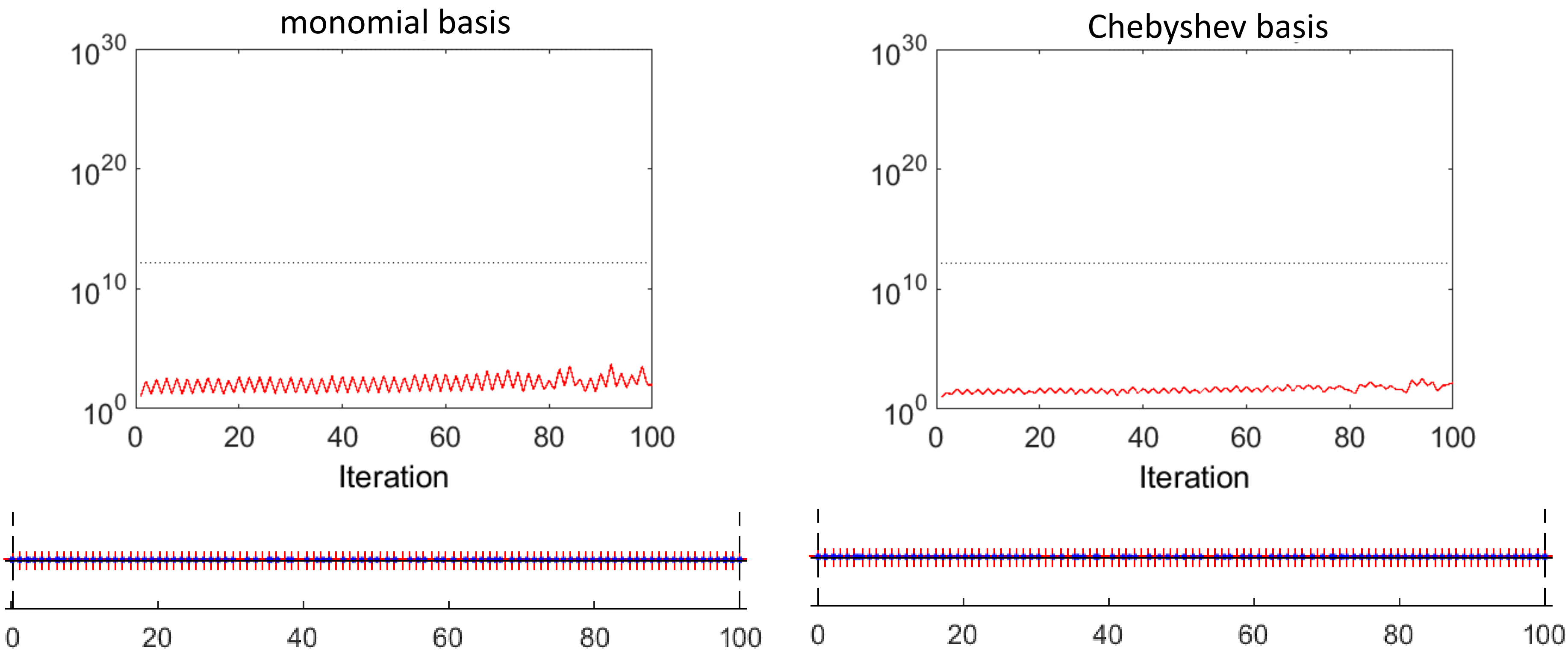

Bottom Plots:

+ True eigenvalues ● Computed Ritz values

¦ Bounds on range of computed Ritz values

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Top plots:

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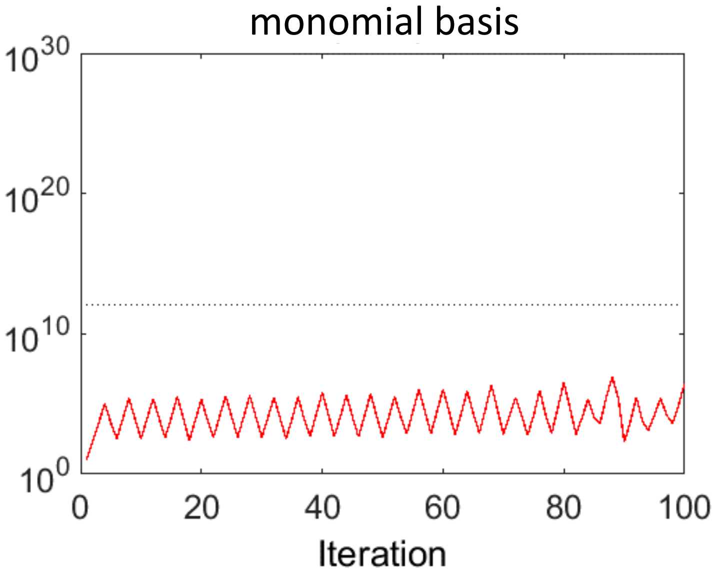

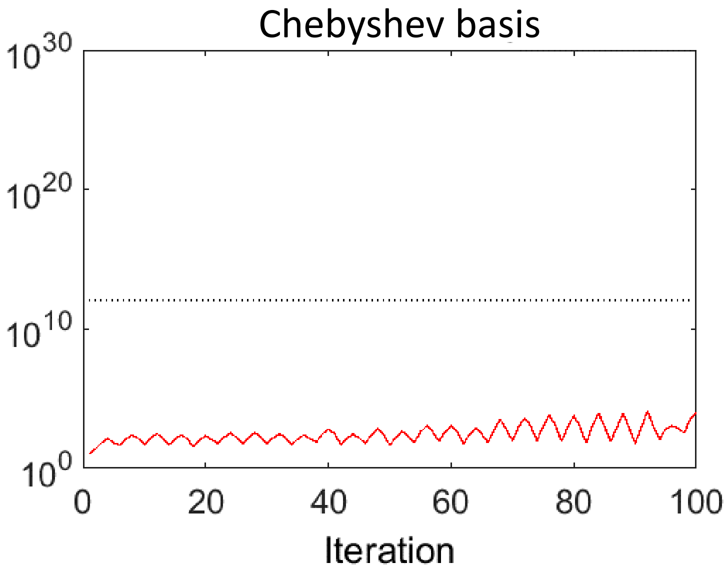

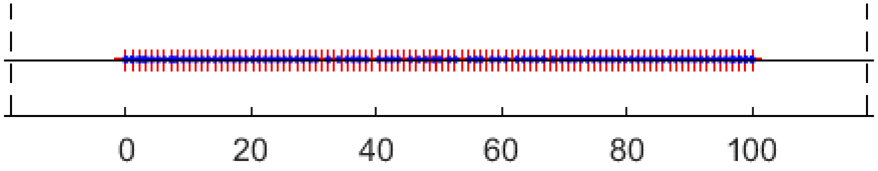

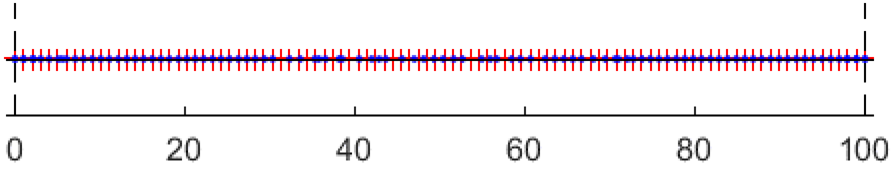

Bottom Plots:

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● Computed Ritz values

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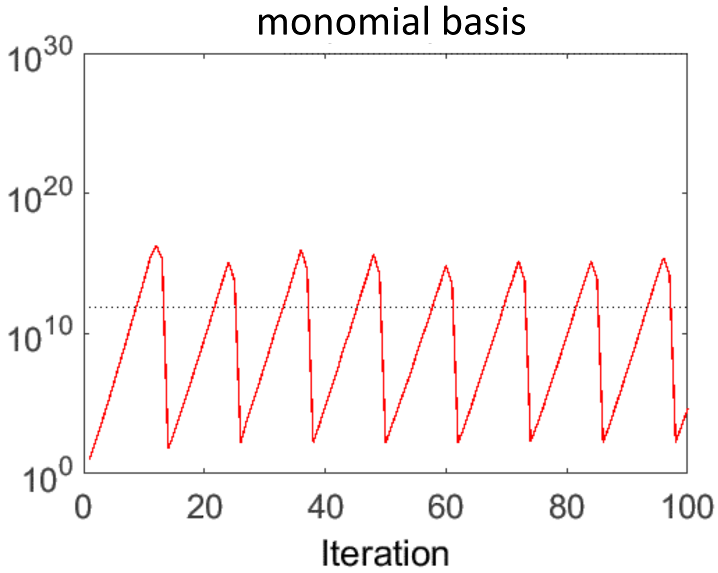
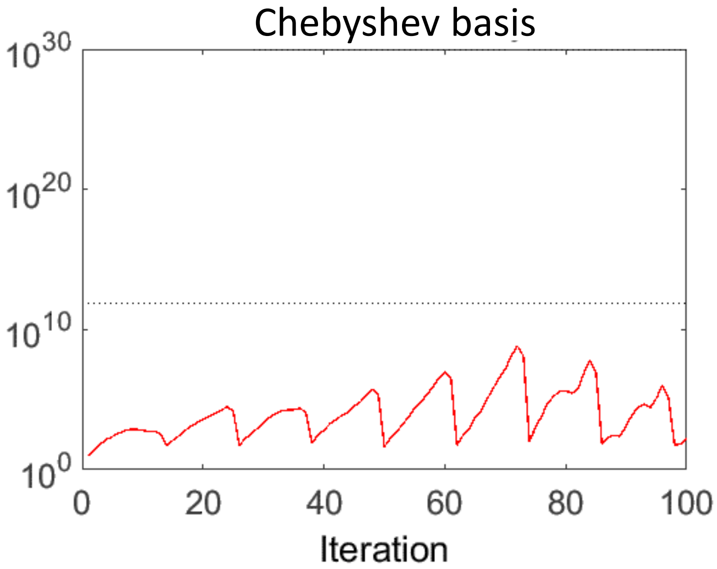
Problem: Diagonal matrix with $n = 100$ with evenly spaced eigenvalues between $\lambda_{min} = 0.1$ and $\lambda_{max} = 100$; random starting vector

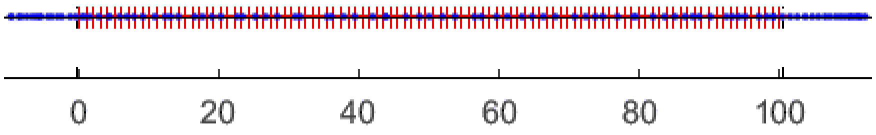
$\boldsymbol{s = 12}$

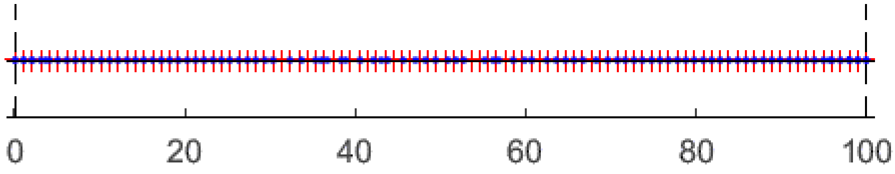
Top plots:

—	Computed $\Gamma_{k,j}^2$
┈	$(24(\varepsilon(n+11s+15))^{-1}$









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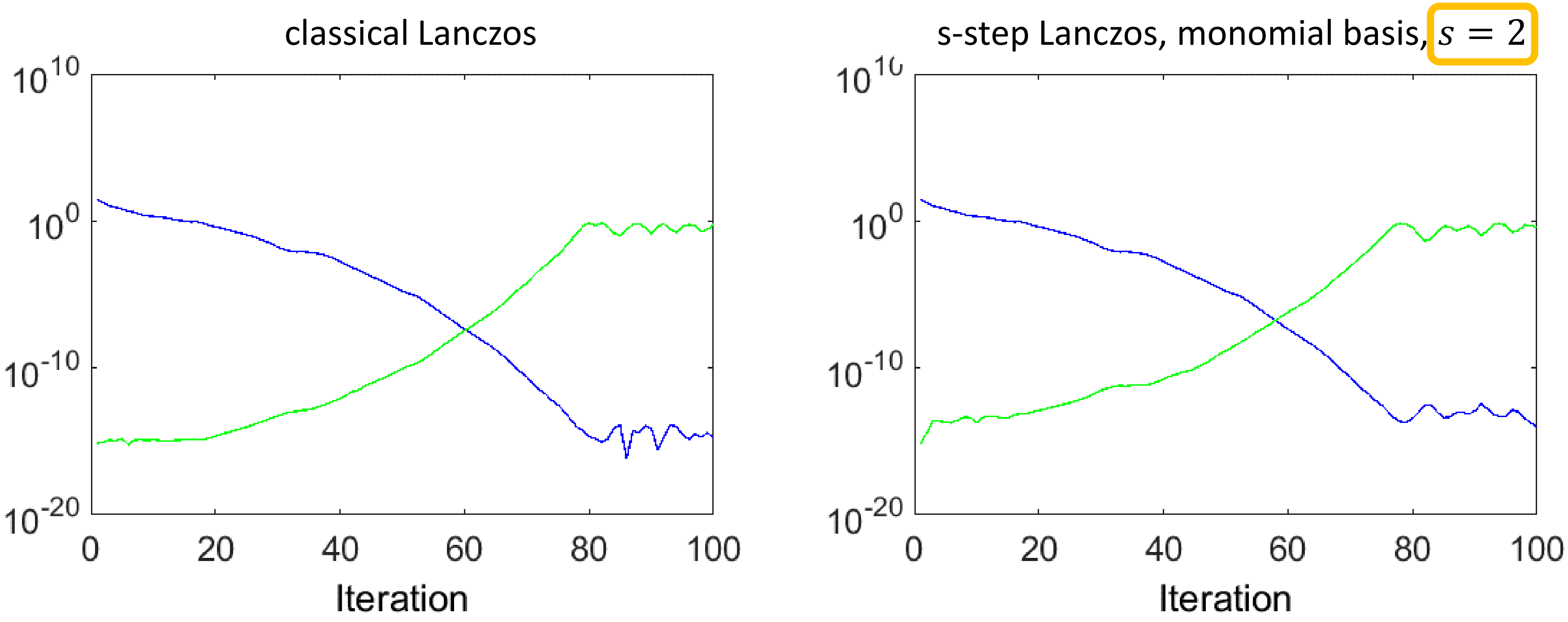
¦	Bounds on range of computed Ritz values		

Problem: Diagonal matrix with $n = 100$ with evenly spaced eigenvalues between $\lambda_{min} = 0.1$ and $\lambda_{max} = 100$; random starting vector

$\Gamma \leq 7 \times 10^2$



classical Lanczos

s-step Lanczos, monomial basis, $\boxed{s = 2}$

Measure of loss of orthogonality ⟵

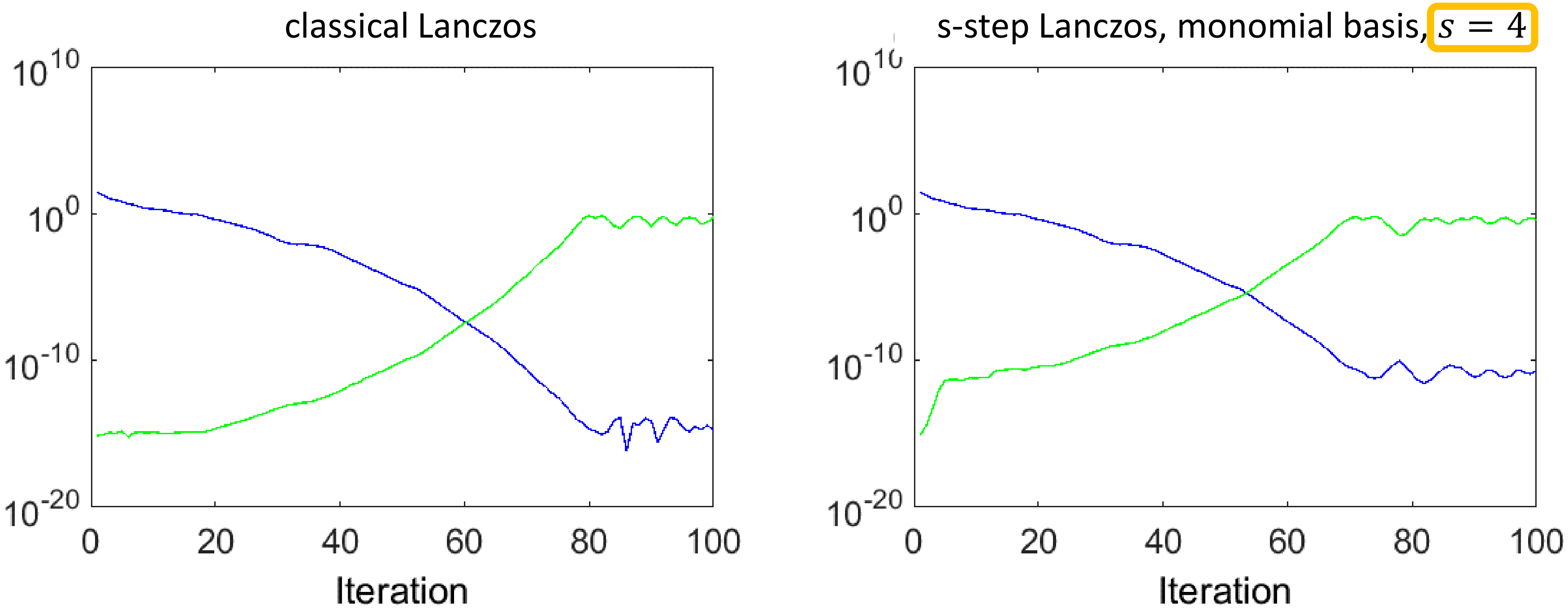
🟩 $\max_i |z_i^{(m)T} \hat{v}_{m+1}|$

🟦 $\min_i \hat{\beta}_{m+1} \eta_{m,i}^{(m)}$

Measure of Ritz value convergence ⟶

Problem: Diagonal matrix with $n = 100$ with evenly spaced eigenvalues between $\lambda_{min} = 0.1$ and $\lambda_{max} = 100$; random starting vector

$\Gamma \lesssim 3 \times 10^3$

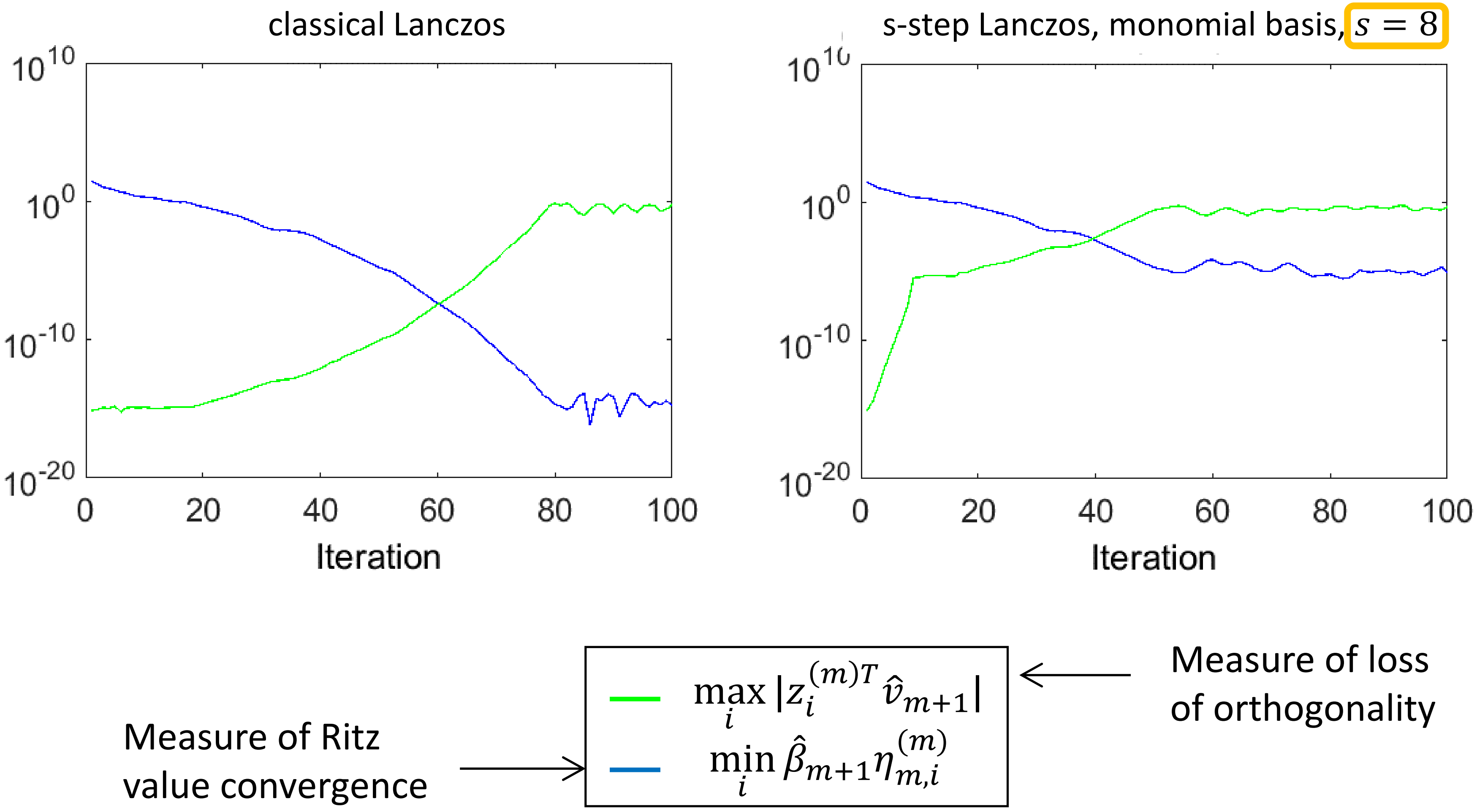


🟩 $\max_i |z_i^{(m)T} \hat{v}_{m+1}|$ ← Measure of loss of orthogonality

Measure of Ritz value convergence → 🟦 $\min_i \hat{\beta}_{m+1} \eta_{m,i}^{(m)}$

Problem: Diagonal matrix with $n = 100$ with evenly spaced eigenvalues between $\lambda_{min} = 0.1$ and $\lambda_{max} = 100$; random starting vector

$\Gamma \leq 2 \times 10^6$



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Measure of loss of orthogonality

Measure of Ritz value convergence

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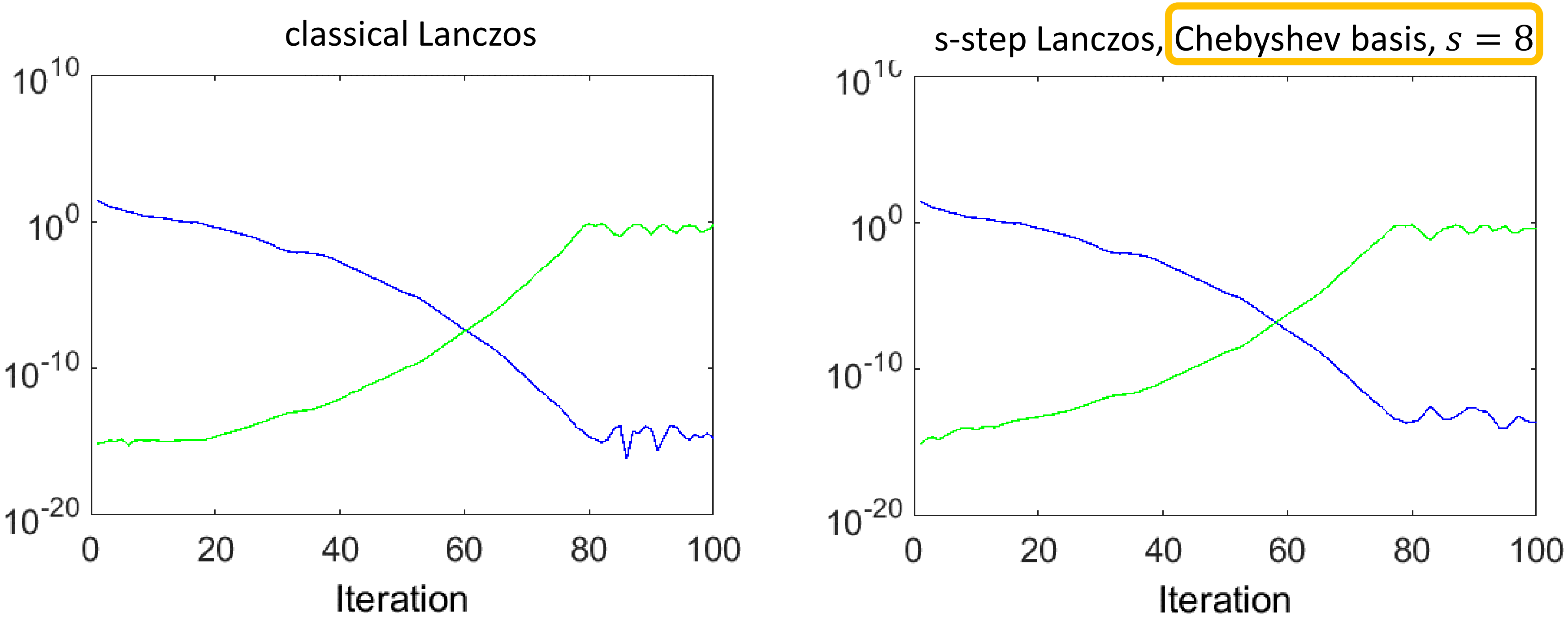

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Towards understanding convergence delay

- Coefficients α and β (related to entries of T_i) determine distribution functions $\omega^{(i)}(\lambda)$ which approximate distribution function $\omega(\lambda)$ determined by inputs A, b, x_0 in terms of the ith Gauss-Christoffel quadrature
- CG method = matrix formulation of Gauss-Christoffel quadrature (see, e.g., [Liesen & Strakoš, 2013])
- A-norm of CG error for $f(\lambda) = \lambda^{-1}$ given as scaled quadrature error

$$\int \lambda^{-1} d\omega(\lambda) = \sum_{\ell=1}^{i} \omega_\ell^{(i)} \left\{\theta_\ell^{(i)}\right\}^{-1} + \frac{\|x - x_i\|_A^2}{\|r_0\|^2}$$

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where F_i is small relative to error term?

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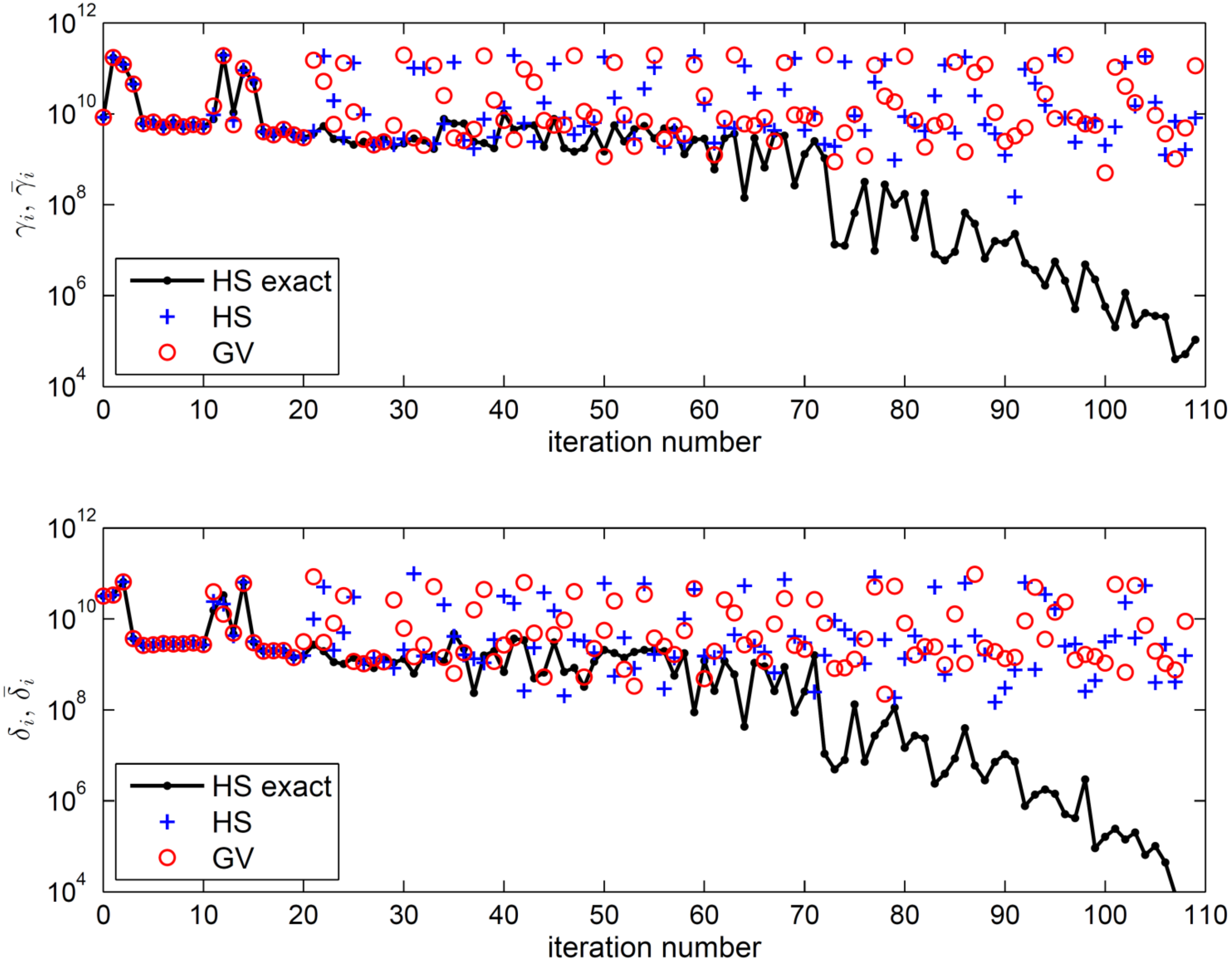
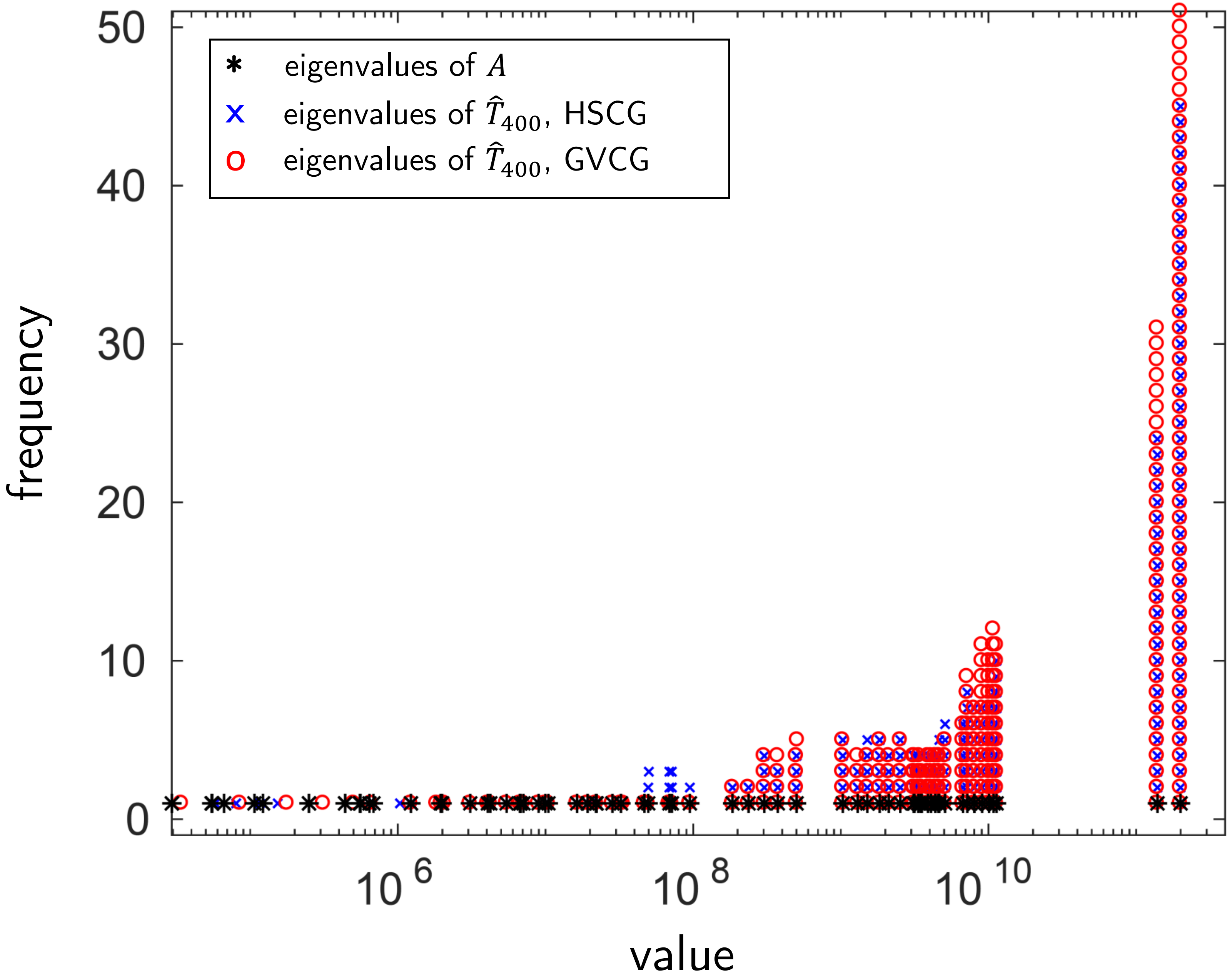
- For pipelined CG and s-step CG, THOROUGH ANALYSIS NEEDED!

Differences in entries γ_i, δ_i in Jacobi matrices T_i in HSCG vs. GVCG (matrix bcsstk03)



see [C., Rozložník, Strakoš, Tichý, Tůma, 2018]



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A different problem…

A: **nos4** from UFSMC,
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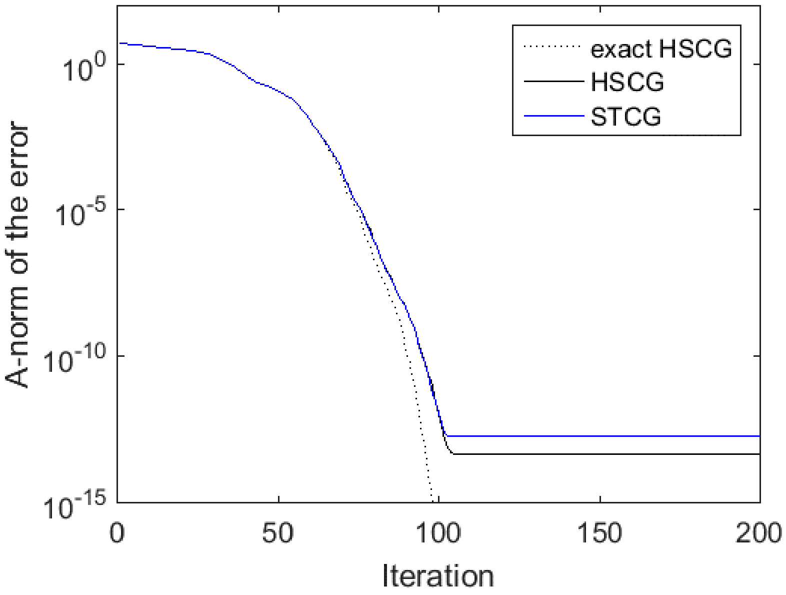

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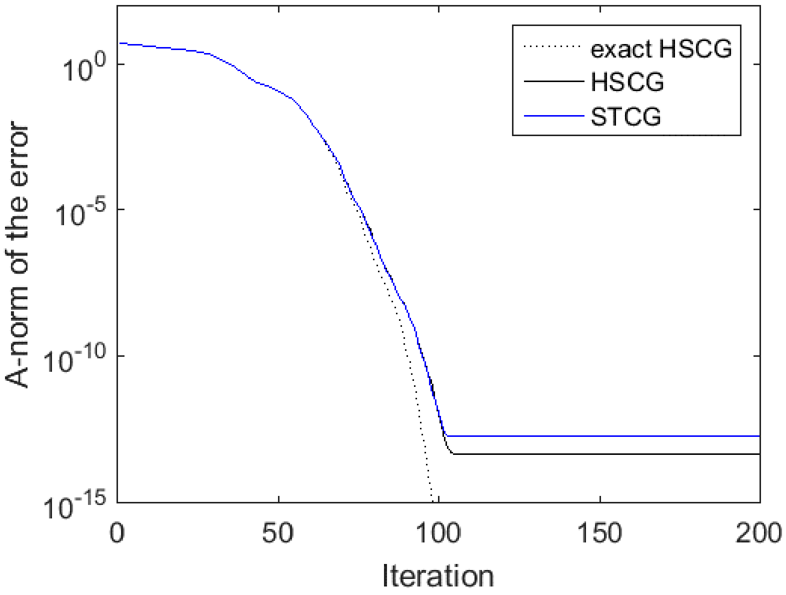

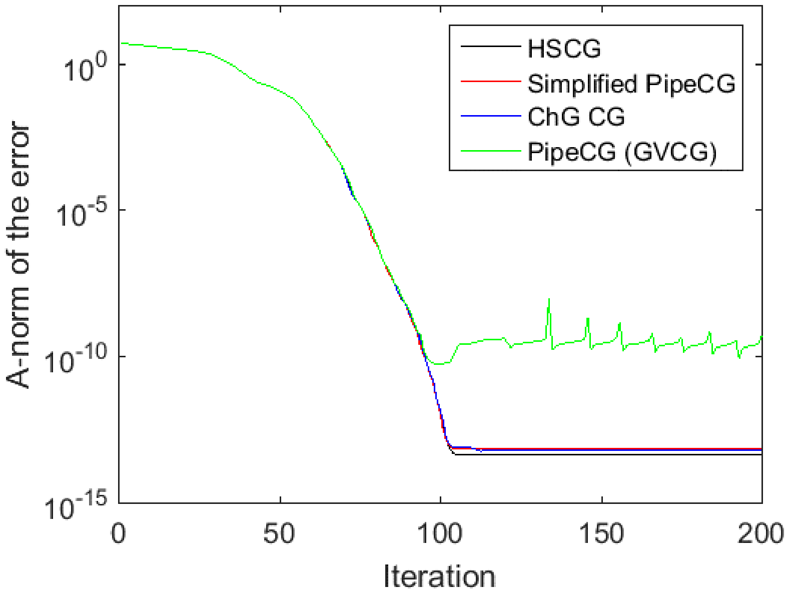

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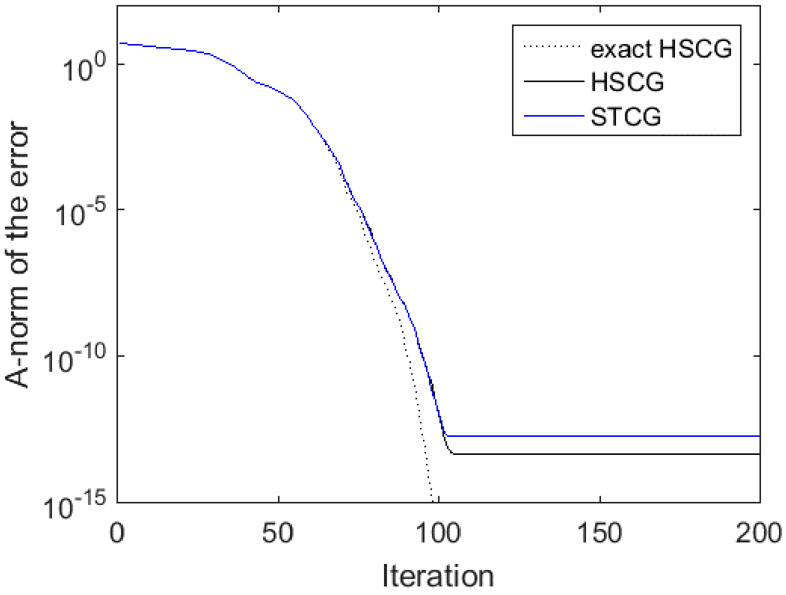

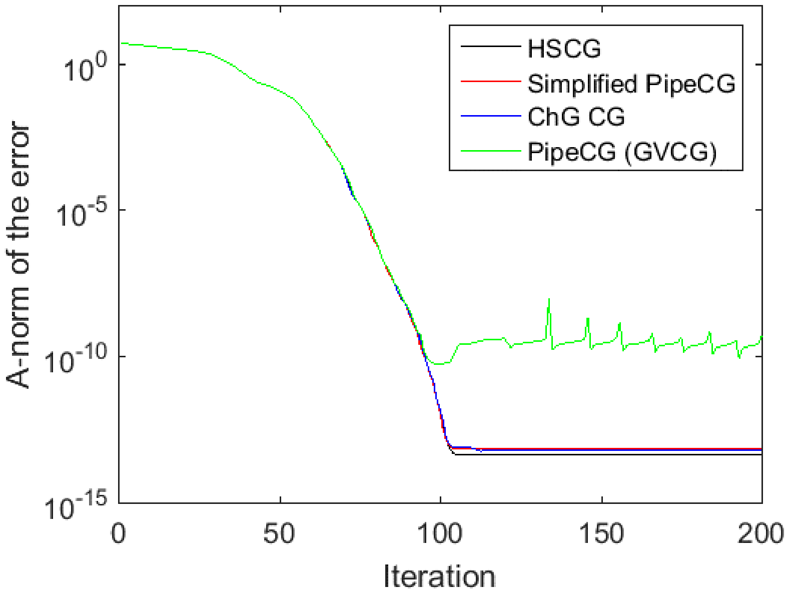

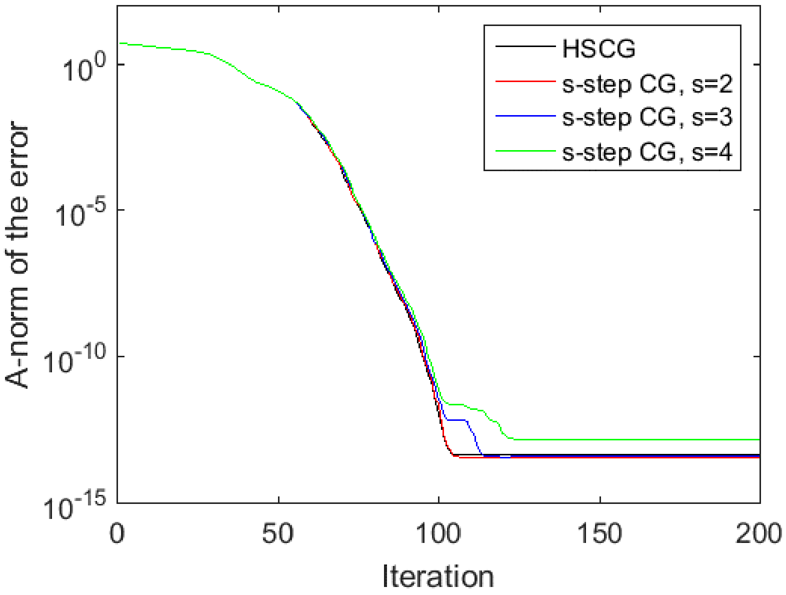

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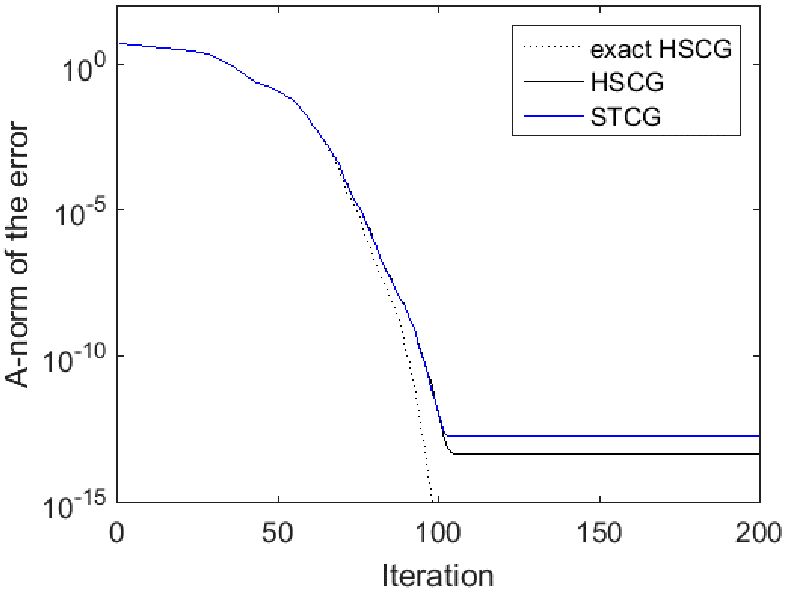
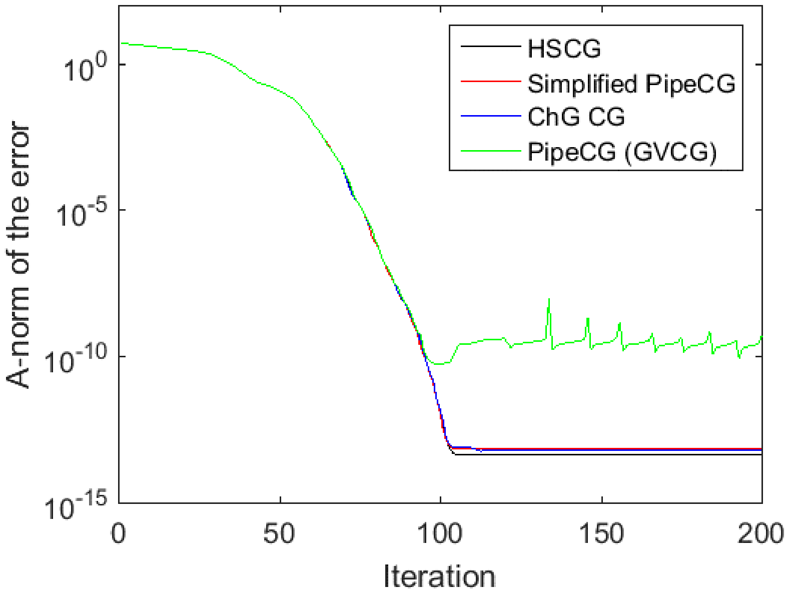
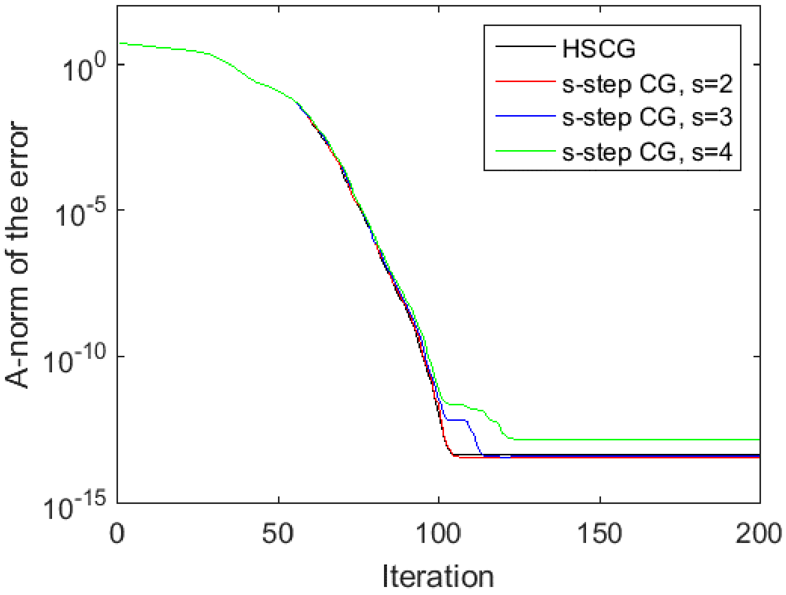


If application only requires
$\|x - x_i\|_A \leq 10^{-10}$,
any of these methods will work!

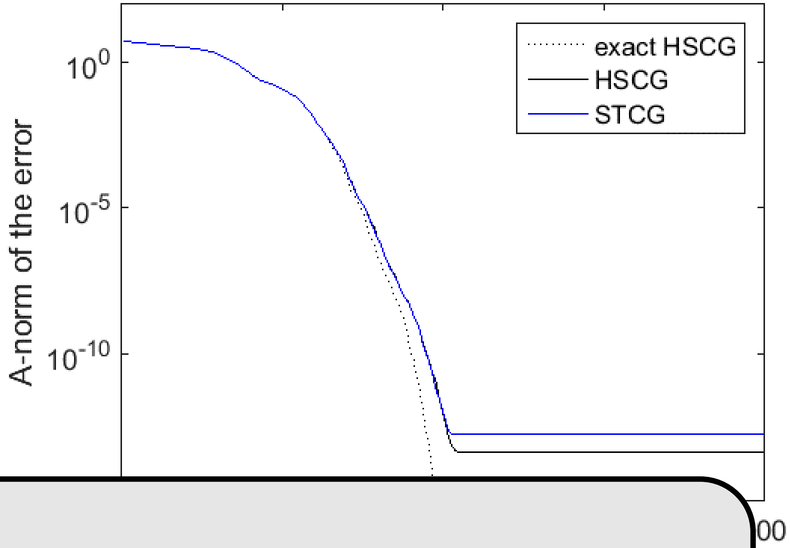




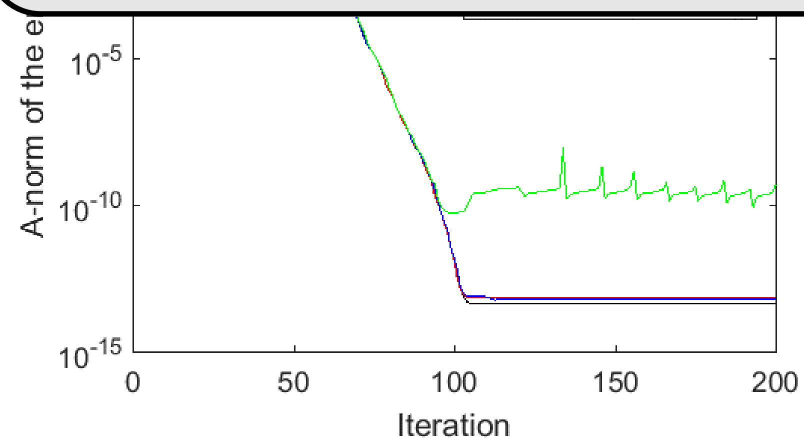
A different problem...

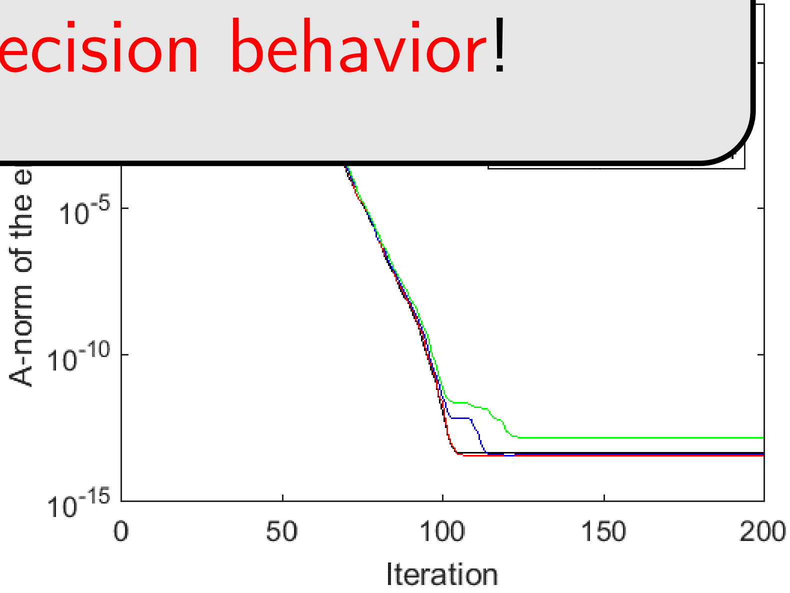
A: **nos4** from UFSMC,
b: equal components in the eigenbasis of A and $\|b\| = 1$
$N = 100, \kappa(A) \approx 2\text{e}3$

If application only requires
$\|x - x_i\|_A \leq 10^{-10}$,
any of these methods will work!



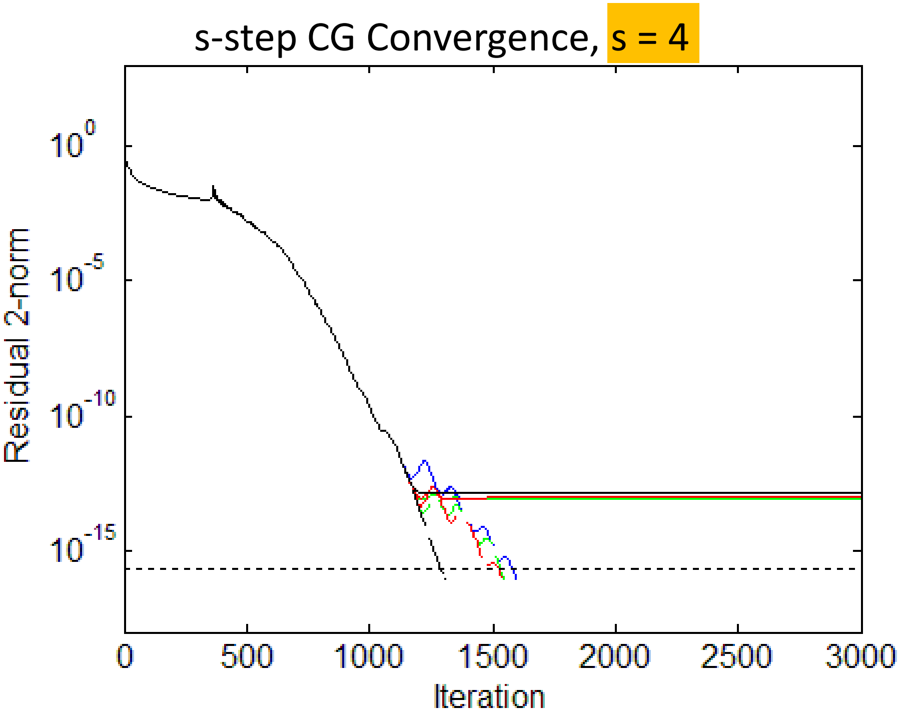
Need adaptive, problem-dependent approach based on understanding of finite precision behavior!



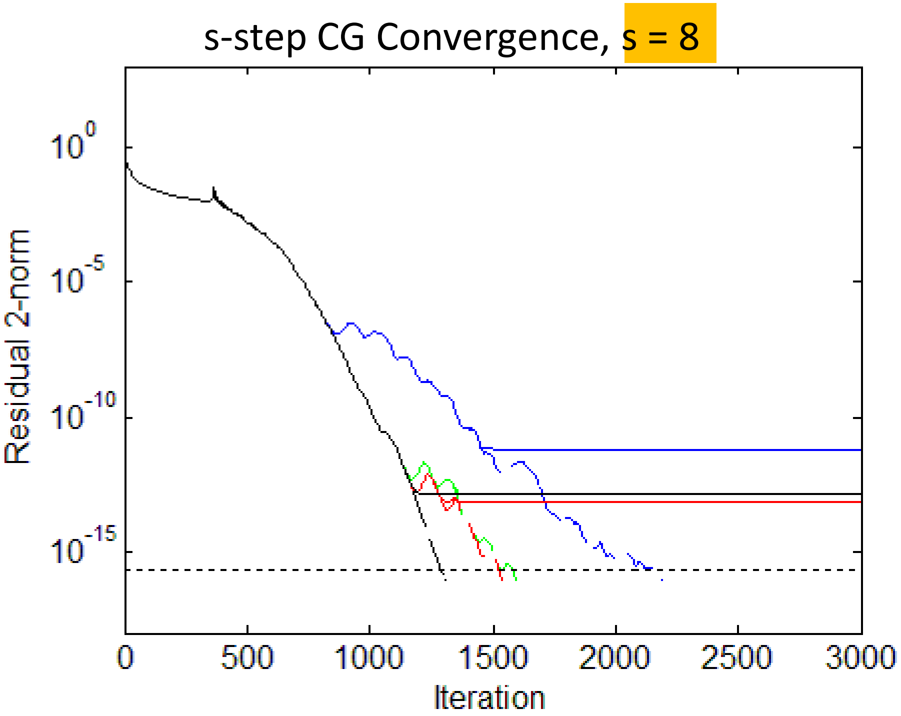


Summary

- Finite precision errors cause loss of attainable accuracy and convergence delay
- In classical CG, attainable accuracy limited only by sum of local rounding errors
- In pipelined CG, sum of many different local rounding errors can be (globally!) amplified
    - Amplification depends on CG recurrence coefficients α and β
        - Not much to do except try to decrease local errors (e.g., by stabilizing shifts)
- In s-step CG, local rounding errors in each outer loop are amplified by a factor related to the condition number of the generated s-step basis matrix
    - Amplification effects are still "local" within an outer loop (block of s iterations)
    - Suggests that basis condition number plays a huge role
- More difficult to precisely characterize convergence delay; further work needed



s-step CG Convergence, s = 4



s-step CG Convergence, s = 8

— CG true
- - CG updated
— s-step CG (monomial) true
- - s-step CG (monomial) updated
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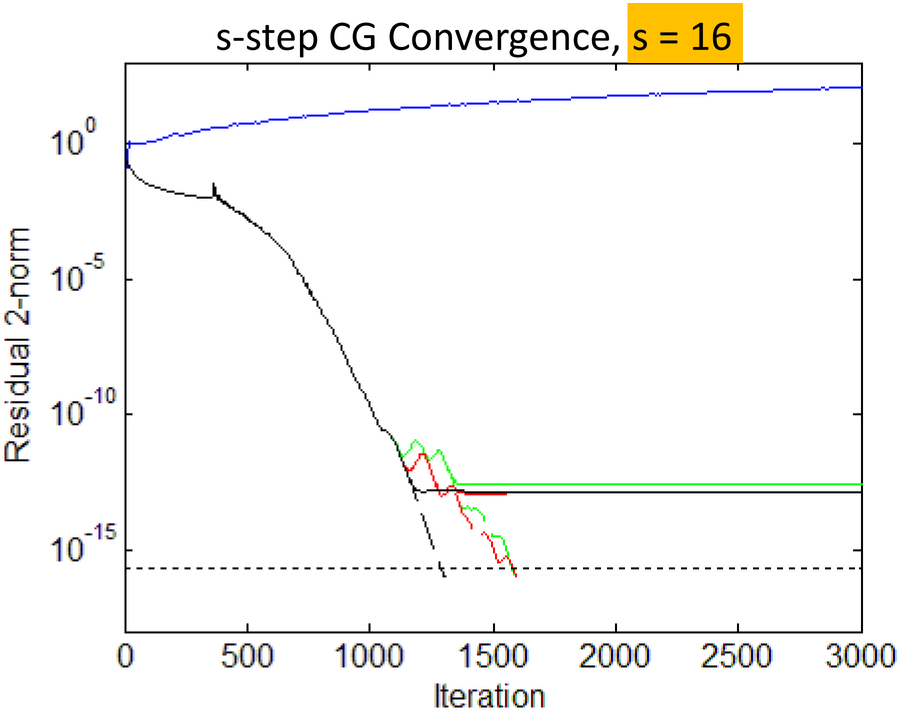
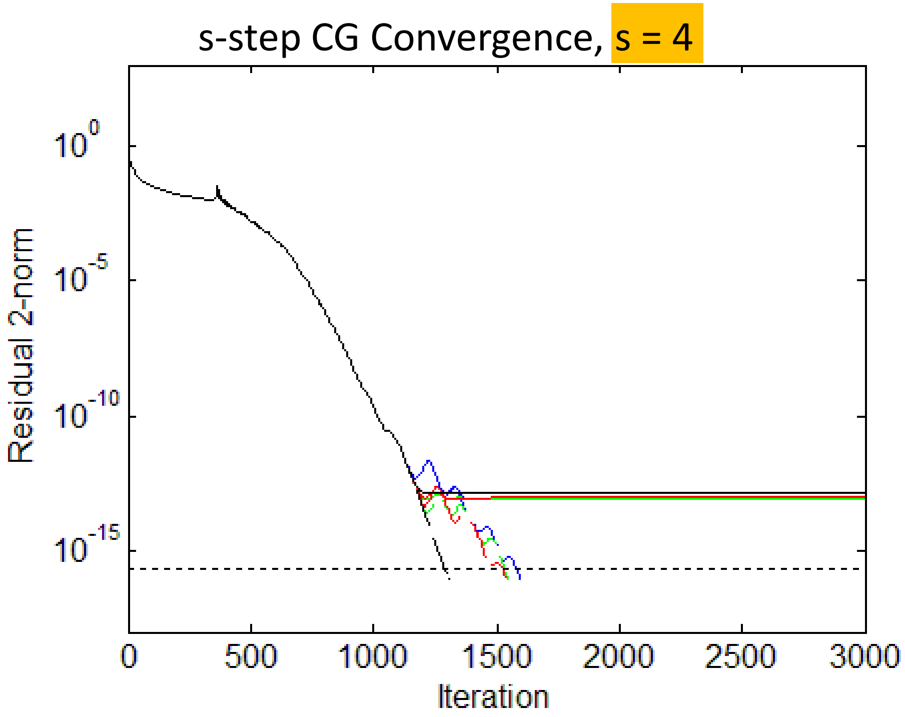


s-step CG Convergence, s = 16

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



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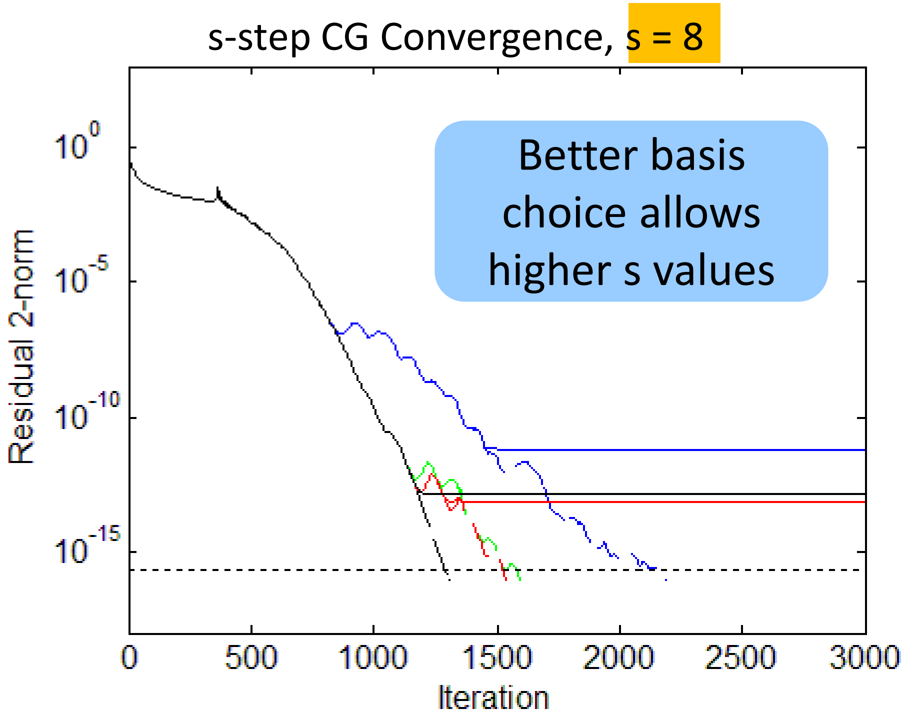
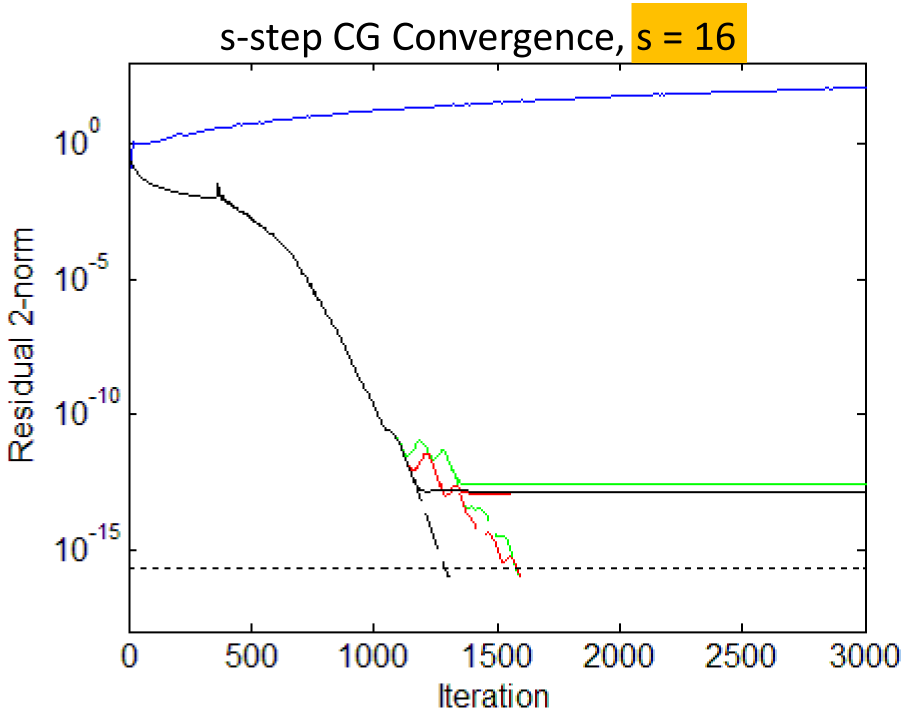


s-step CG Convergence, s = 8

Better basis choice allows higher s values



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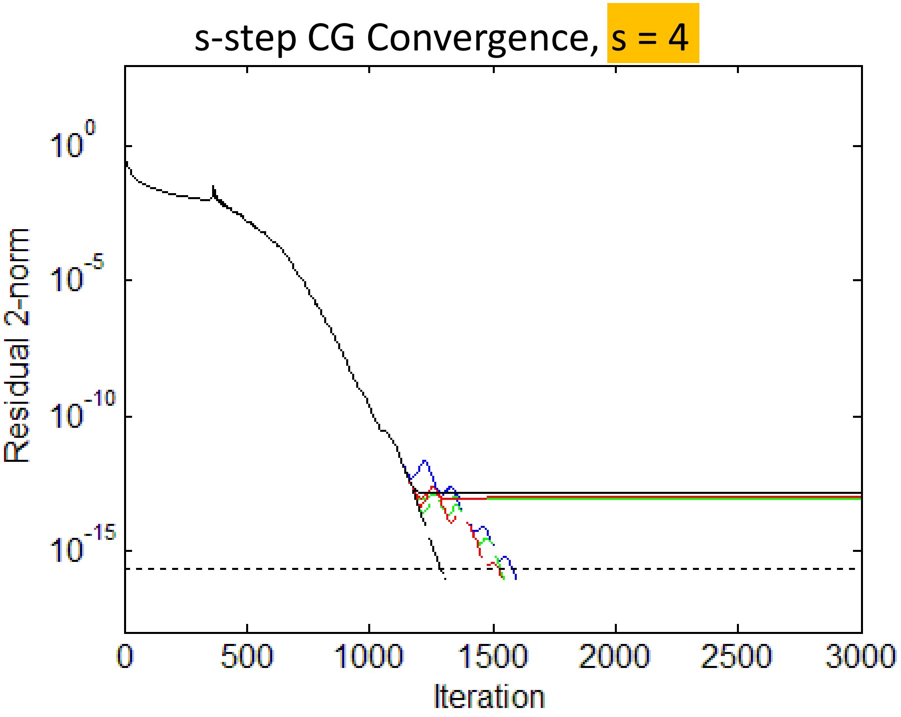

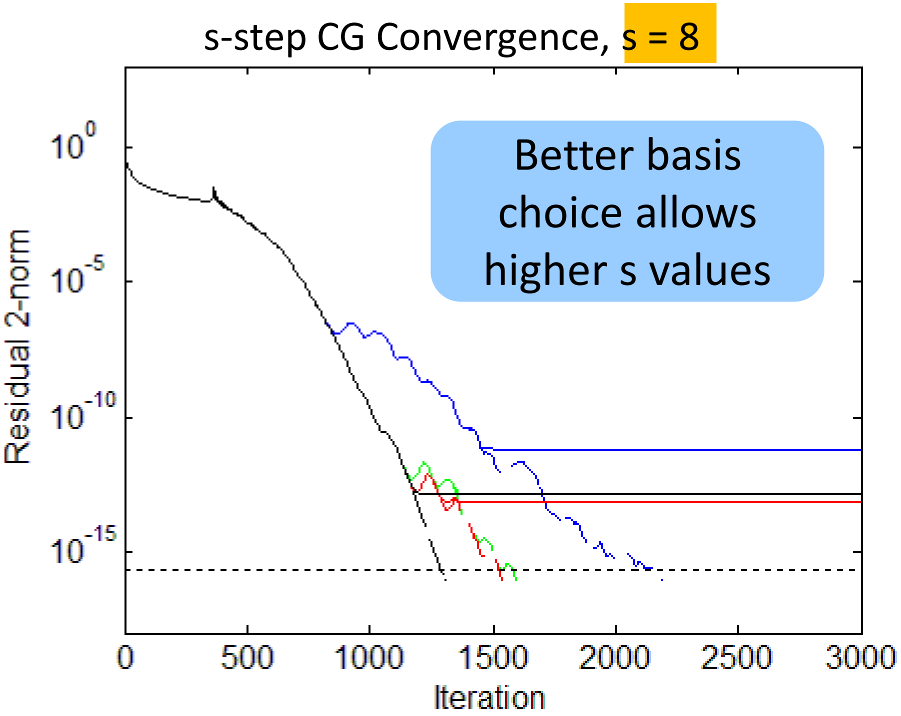

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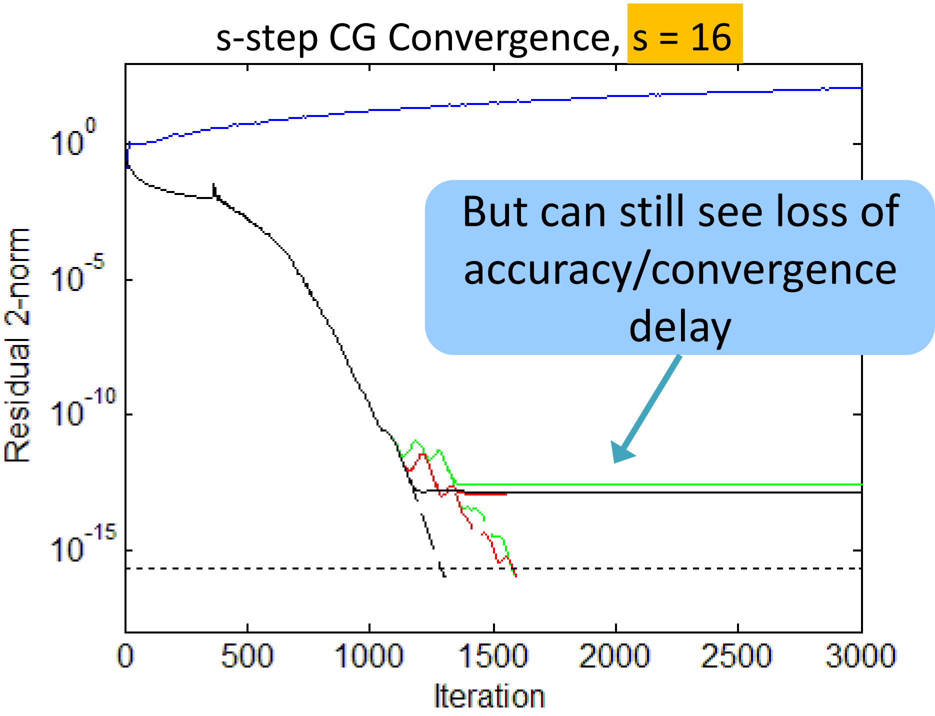

But can still see loss of accuracy/convergence delay

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Residual replacement strategy

- Improve accuracy by replacing **computed residual** $\hat{r}_i$ by the **true residual** $\boldsymbol{b} - \boldsymbol{A}\hat{x}_{\boldsymbol{i}}$ in certain iterations
  - Related work for classical CG: van der Vorst and Ye (1999)

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- Based on derived bound on deviation of residuals, can devise a residual replacement strategy for s-step CG

- Implementation has **negligible cost**

Residual replacement for s-step CG

- Use computable bound for$\|b - A\hat{x}_i - \hat{r}_i\|$ to update d_i, an estimate of error in computing r_i, in each iteration
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Pseudo-code for residual replacement with group update for s-step CG:

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if  $d_{i-1} \le \hat{\varepsilon}\|r_{i-1}\|$  and  $d_i > \hat{\varepsilon}\|r_i\|$  and  $d_i > 1.1 d_{init}$
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        $x_i = 0$
        $r_i = b - Az$
        $d_{init} = d_i = \varepsilon\big((1 + 2N')\|A\|\|z\| + \|r_i\|\big)$
        $p_i = \mathcal{Y}_k p'_{k,j}$
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set residual to true residual

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group update of approximate solution

set residual to true residual

A computable bound

- In each iteration, update error estimate d_i $(i \equiv sk + j)$ by:

$$
\begin{aligned}
d_i &\equiv d_{i-1} \\
&+\varepsilon\Big[(4+N')\big(\|A\|\,\big\||\hat{\mathcal{Y}}_k|\cdot|\hat{x}'_{k,j}|\big\| + \big\||\hat{\mathcal{Y}}_k|\cdot|\mathcal{B}_k|\cdot|\hat{x}'_{k,j}|\big\|\big) + \big\||\hat{\mathcal{Y}}_k|\cdot|\hat{r}'_{k,j}|\big\|\Big] \\
&+\varepsilon\begin{cases} \|A\|\|\hat{x}_{sk+s}\|+(2+2N')\|A\|\big\||\hat{\mathcal{Y}}_k|\cdot|\hat{x}'_{k,s}|\big\|+N'\big\||\hat{\mathcal{Y}}_k|\cdot|\hat{r}'_{k,s}|\big\|, & j = s \\ 0, & \text{o.w.} \end{cases}
\end{aligned}
$$

where $N' = \max(N, 2s + 1)$.

A computable bound

- In each iteration, update error estimate d_i $(i \equiv sk + j)$ by:

Estimated only once

$$
\begin{aligned}
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where $N' = \max(N, 2s + 1)$.

A computable bound

- In each iteration, update error estimate d_i $(i \equiv sk + j)$ by:

$O(s^3)$ flops per s iterations; ≤1 reduction per s iterations to compute $\left(|\hat{\mathcal{Y}}_k|^T|\hat{\mathcal{Y}}_k|\right)$

$$d_i \equiv d_{i-1}$$

$$+\varepsilon\left[(4+N')\left(\|A\| \left\| |\hat{\mathcal{Y}}_k| \cdot |\hat{x}'_{k,j}| \right\| + \left\| |\hat{\mathcal{Y}}_k| \cdot |\mathcal{B}_k| \cdot |\hat{x}'_{k,j}| \right\|\right) + \left\| |\hat{\mathcal{Y}}_k| \cdot |\hat{r}'_{k,j}| \right\|\right]$$

$$+\varepsilon\begin{cases} \|A\|\|\hat{x}_{sk+s}\| + (2+2N')\|A\|\left\| |\hat{\mathcal{Y}}_k| \cdot |\hat{x}'_{k,s}| \right\| + N'\left\| |\hat{\mathcal{Y}}_k| \cdot |\hat{r}'_{k,s}| \right\|, & j = s \\ 0, & \text{o.w.} \end{cases}$$

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A computable bound

- In each iteration, update error estimate d_i $(i \equiv sk + j)$ by:

$O(s^2)$ flops per s iterations; no communication

$$d_i \equiv d_{i-1}$$

$$+\varepsilon\Big[(4+N')\Big(\|A\| \, \big\||\hat{\mathcal{Y}}_k|\cdot|\hat{x}'_{k,j}|\big\| + \big\||\hat{\mathcal{Y}}_k|\cdot|\mathcal{B}_k|\cdot|\hat{x}'_{k,j}|\big\|\Big) + \big\||\hat{\mathcal{Y}}_k|\cdot|\hat{r}'_{k,j}|\big\|\Big]$$

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A computable bound

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Extra computation all lower order terms, communication only increased by *at most* factor of 2

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$$+\varepsilon\Big[(4+N')\Big(\|A\|\,\big\||\hat{\mathcal{Y}}_k|\cdot|\hat{x}'_{k,j}|\big\| + \big\||\hat{\mathcal{Y}}_k|\cdot|\mathcal{B}_k|\cdot|\hat{x}'_{k,j}|\big\|\Big) + \big\||\hat{\mathcal{Y}}_k|\cdot|\hat{r}'_{k,j}|\big\|\Big]$$

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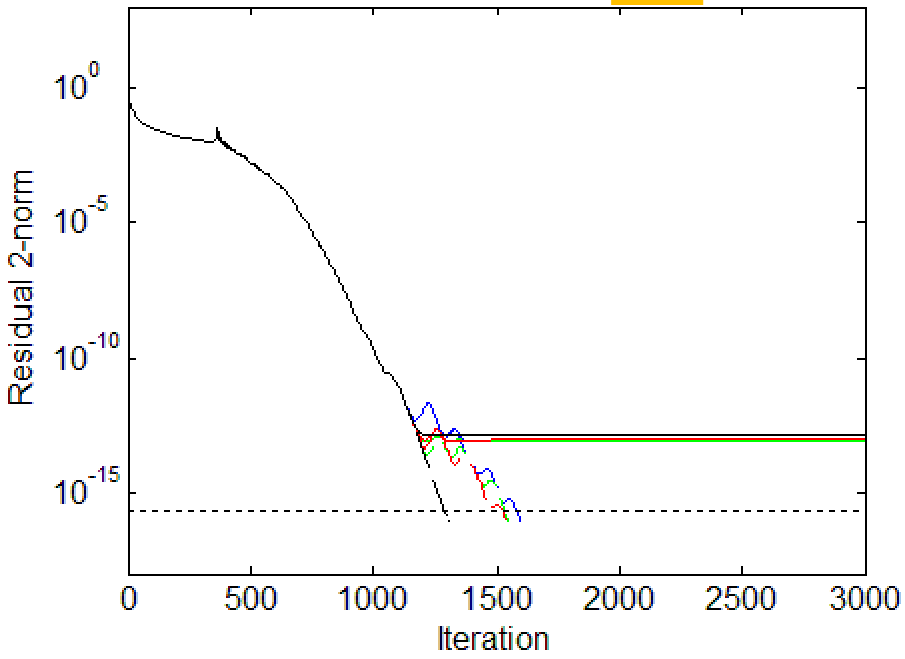
s-step CG Convergence, s = 4



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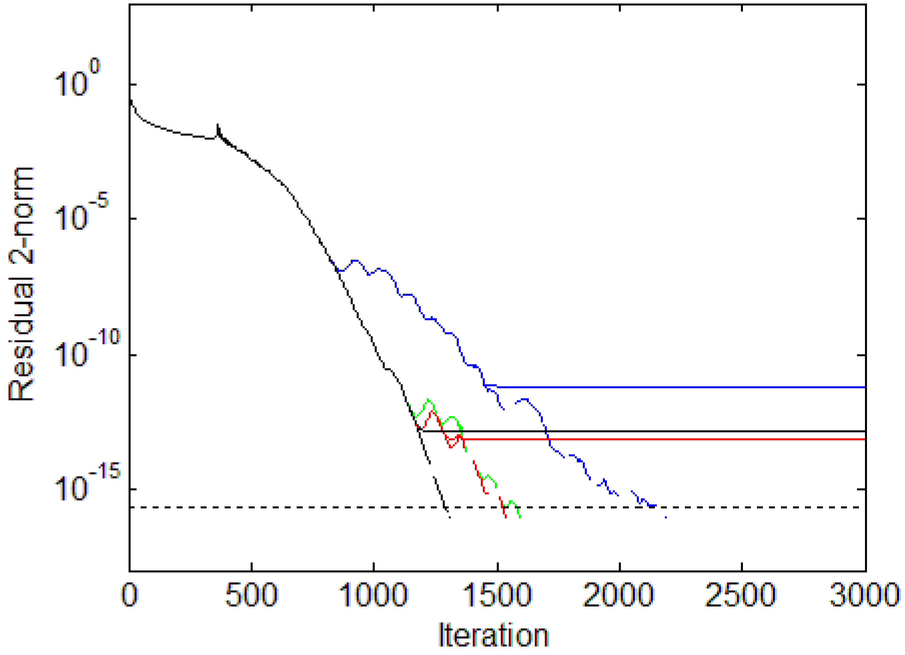

— CG true

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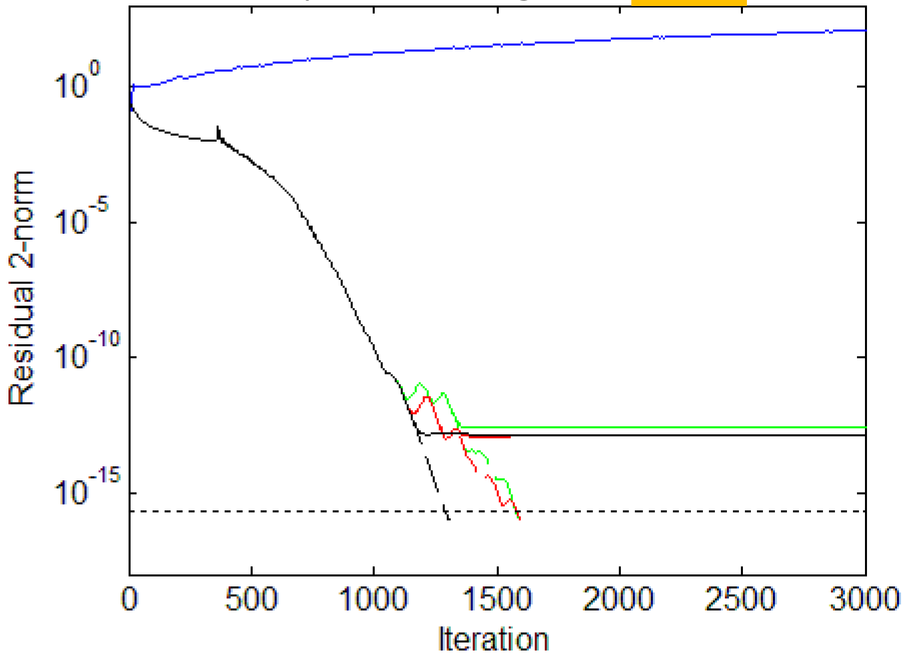

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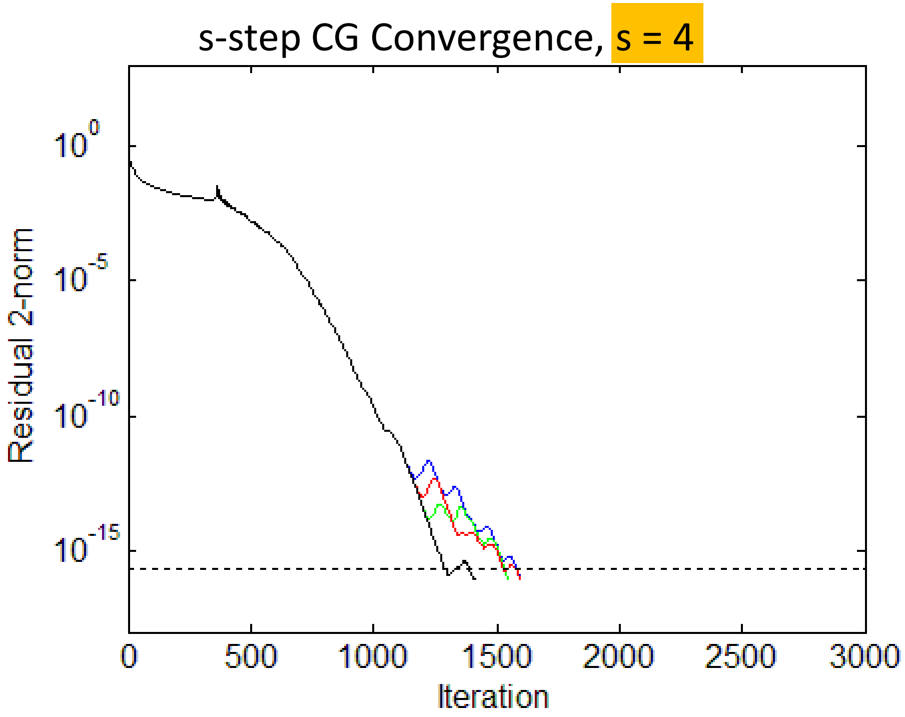

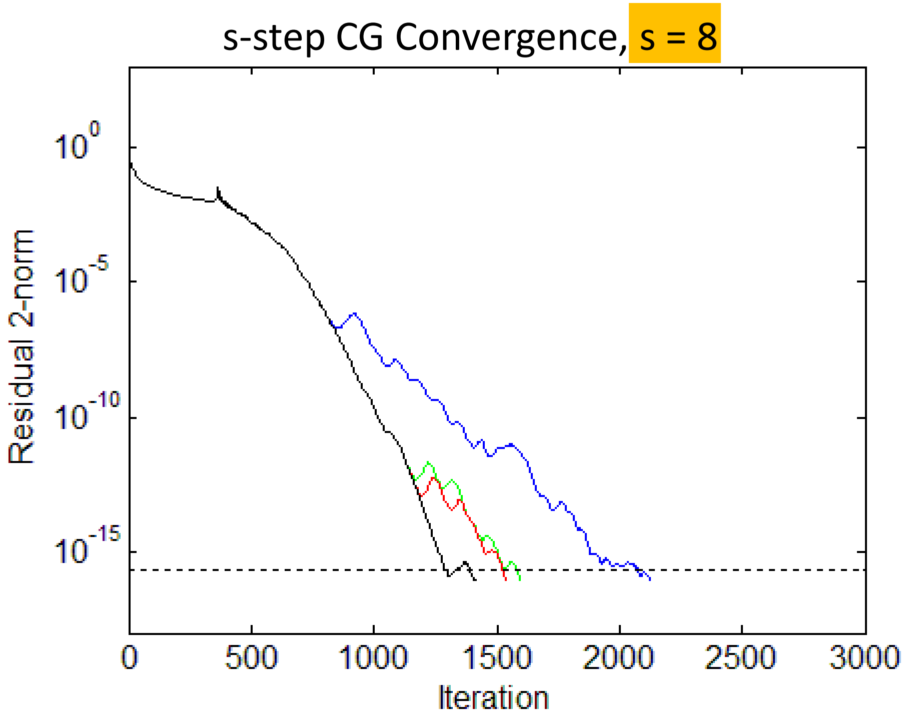

— CG+**RR** true

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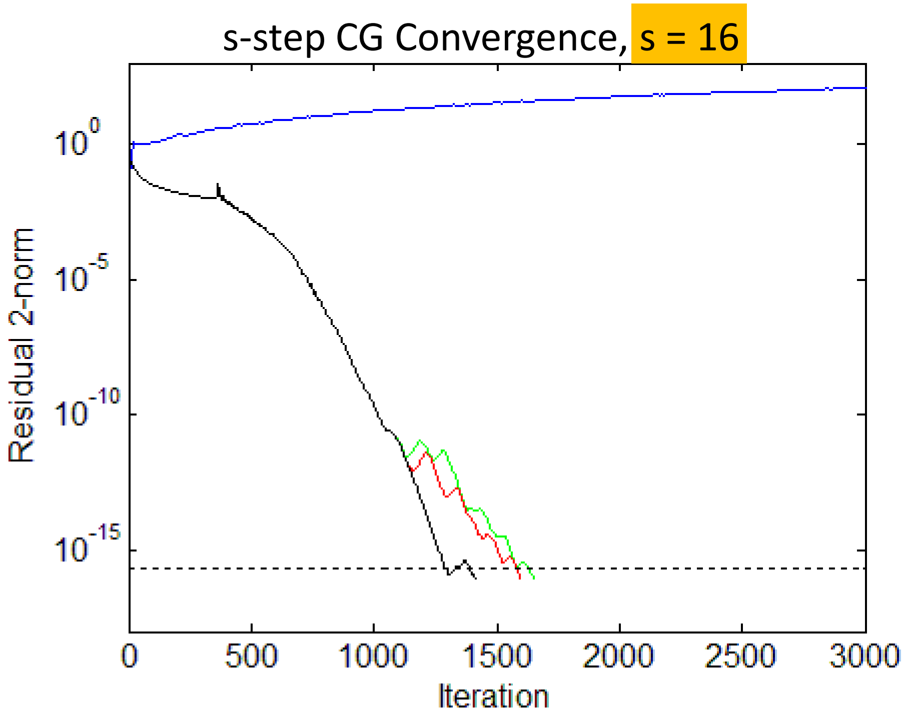

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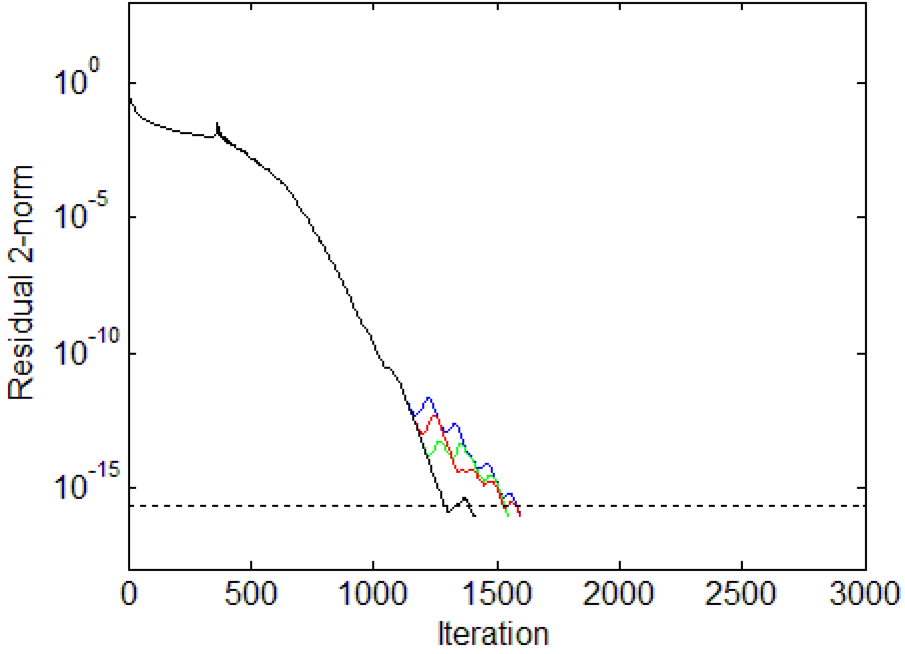

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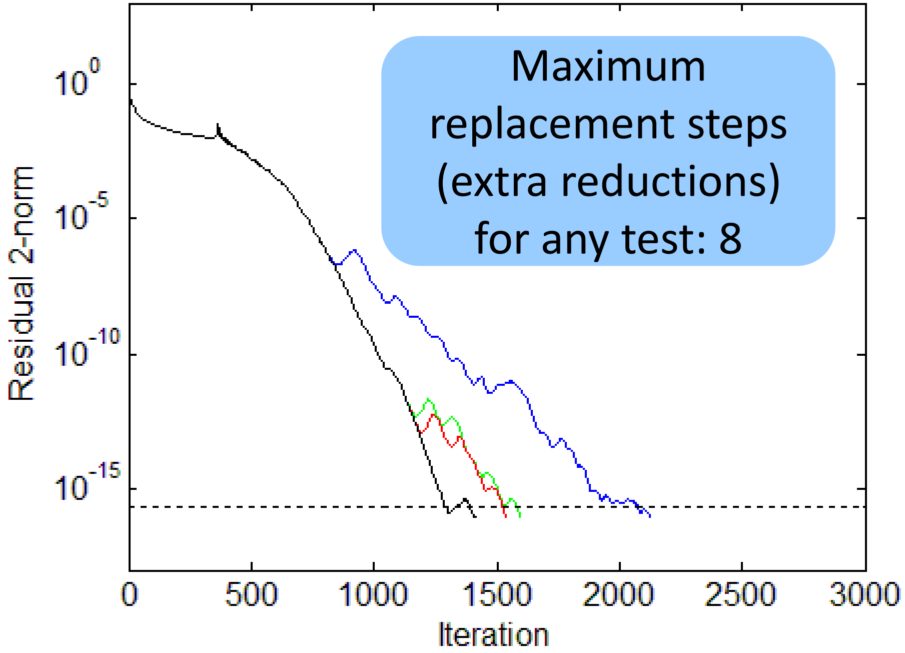

Maximum replacement steps (extra reductions) for any test: 8

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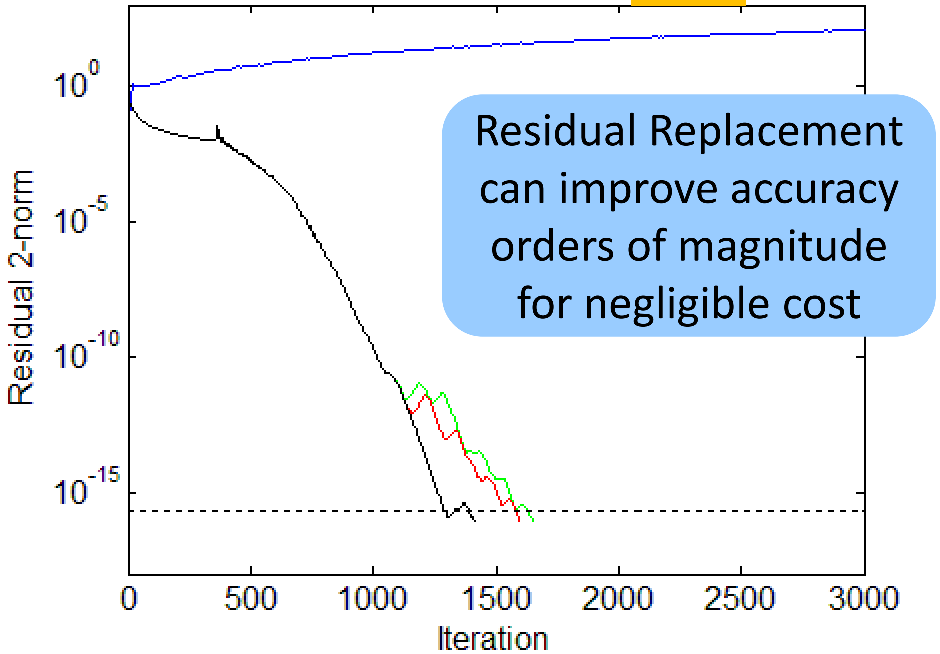
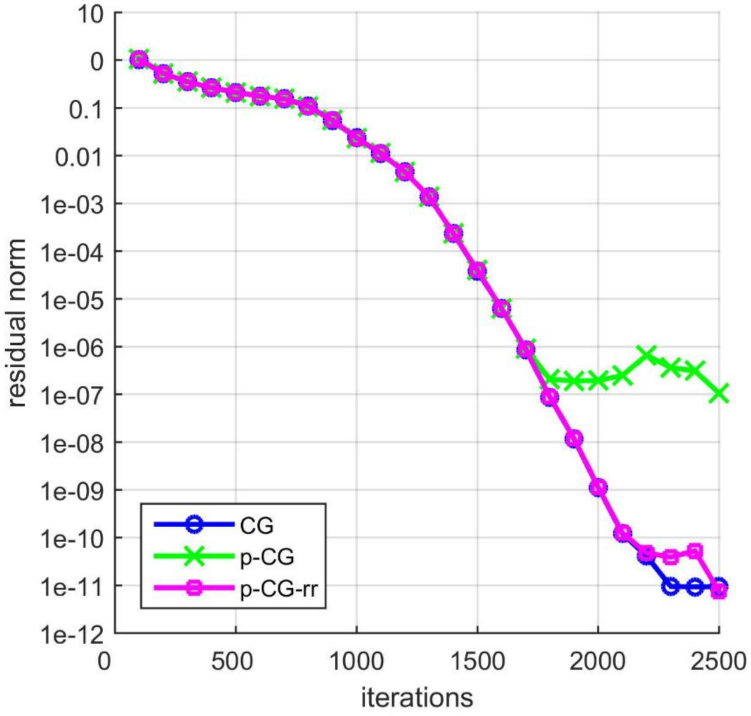


Residual Replacement can improve accuracy orders of magnitude for negligible cost

Pipelined CG with residual replacement

Similar approach possible for pipelined CG; see (Cools et al., 2018)



20 nodes (two 6-core Intel Xeon X5660 Nehalem 2:80-GHz processors per node),
2D Poisson problem with 1e6 unknowns;
in pipelined CG with residual replacement, 39 replacements were performed.

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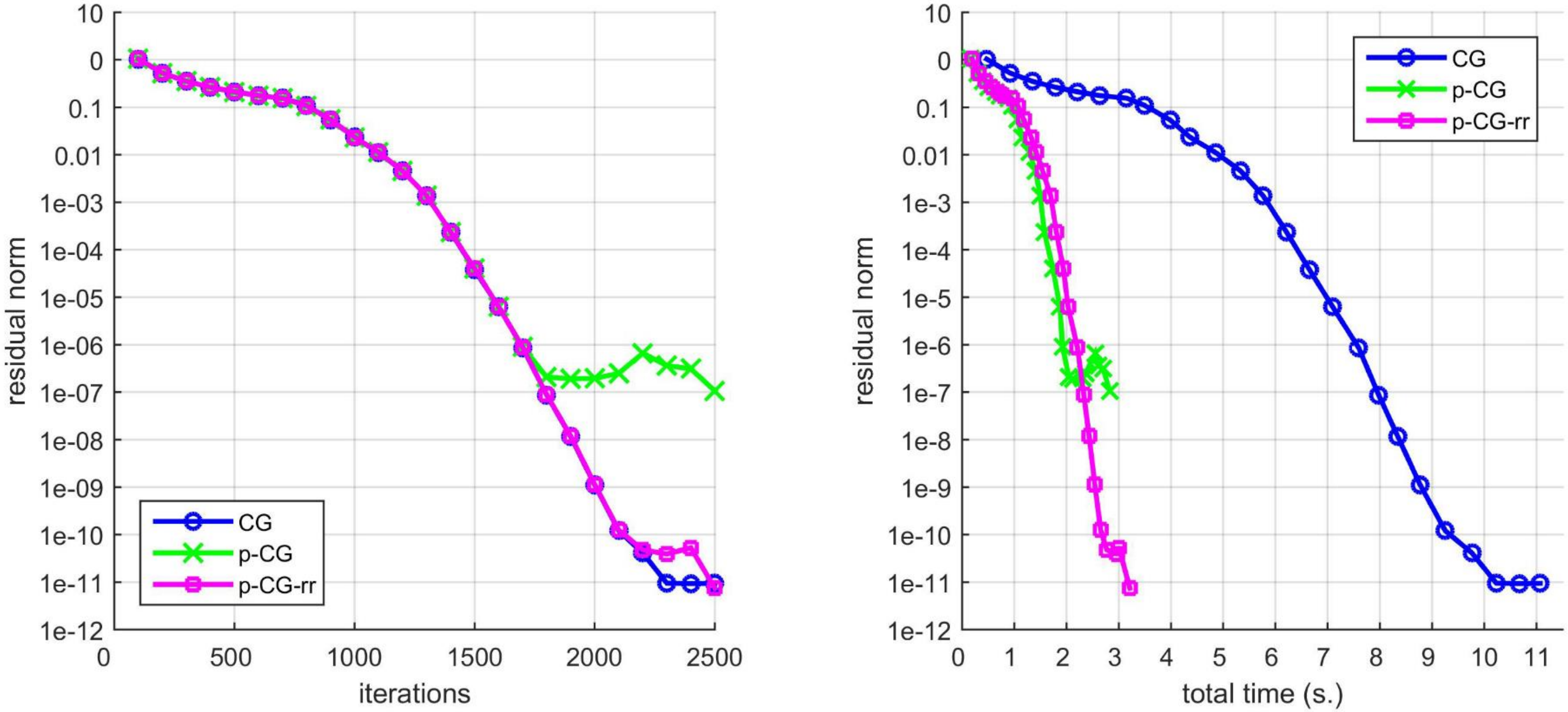

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- $\|\hat{r}_i\|$ large → Γ_k must be small; $\|\hat{r}_i\|$ small → Γ_k can grow

Adaptive s-step CG

- Consider the growth of the relative residual gap caused by errors in outer loop k, which begins with global iteration number m
- We can approximate an upper bound on this quantity by

$$\frac{\|f_{m+s} - f_m\|}{\|A\|\|x\|} \lesssim \varepsilon \left(1 + \kappa(A)\Gamma_k \frac{\max_{j\in\{0,\dots,s\}} \|\hat{r}_{m+j}\|}{\|A\|\|x\|} \right)$$

$f_i \equiv b - A\hat{x}_i - \hat{r}_i$

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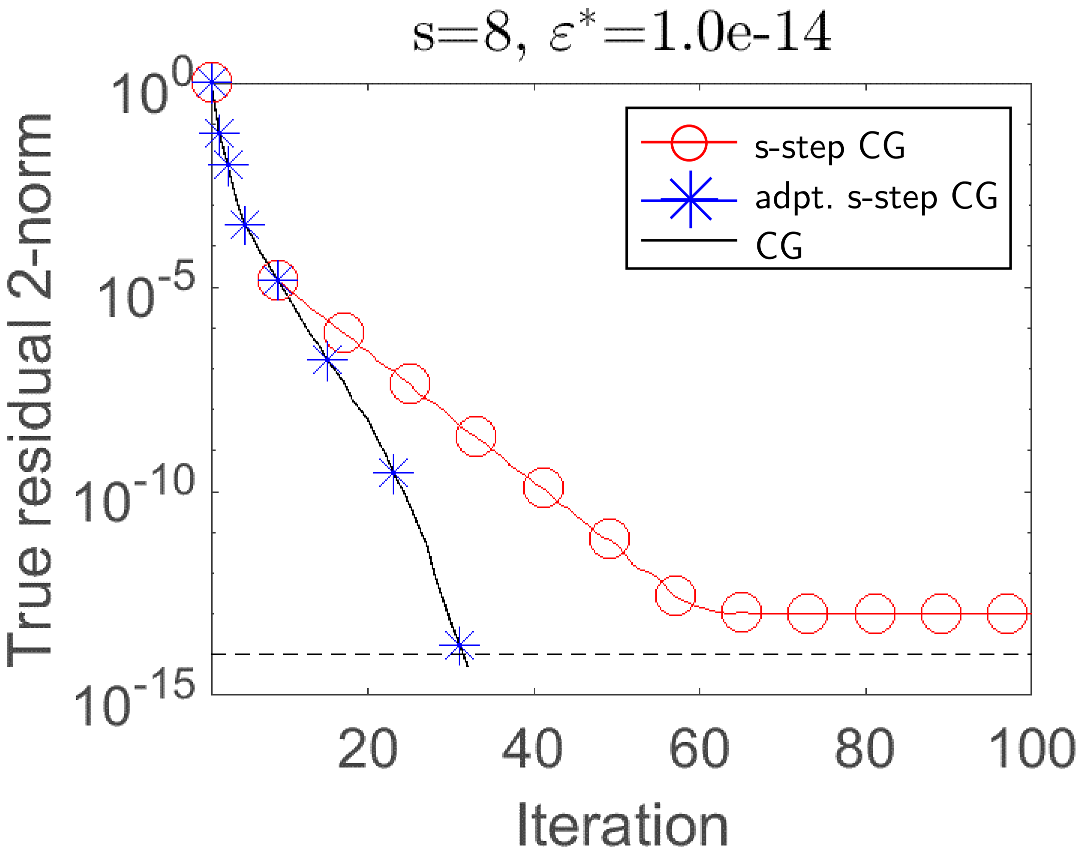
$\Rightarrow$ adaptive s-step approach [C., 2018]

  - s starts off small, increases at rate depending on $\|\hat{r}_i\|$ and ε^*

Adaptive s-step CG

mesh3e1 (SuiteSparse)
$n = 289$
$\kappa(A) \approx 10$
$b_i = 1/\sqrt{N}$



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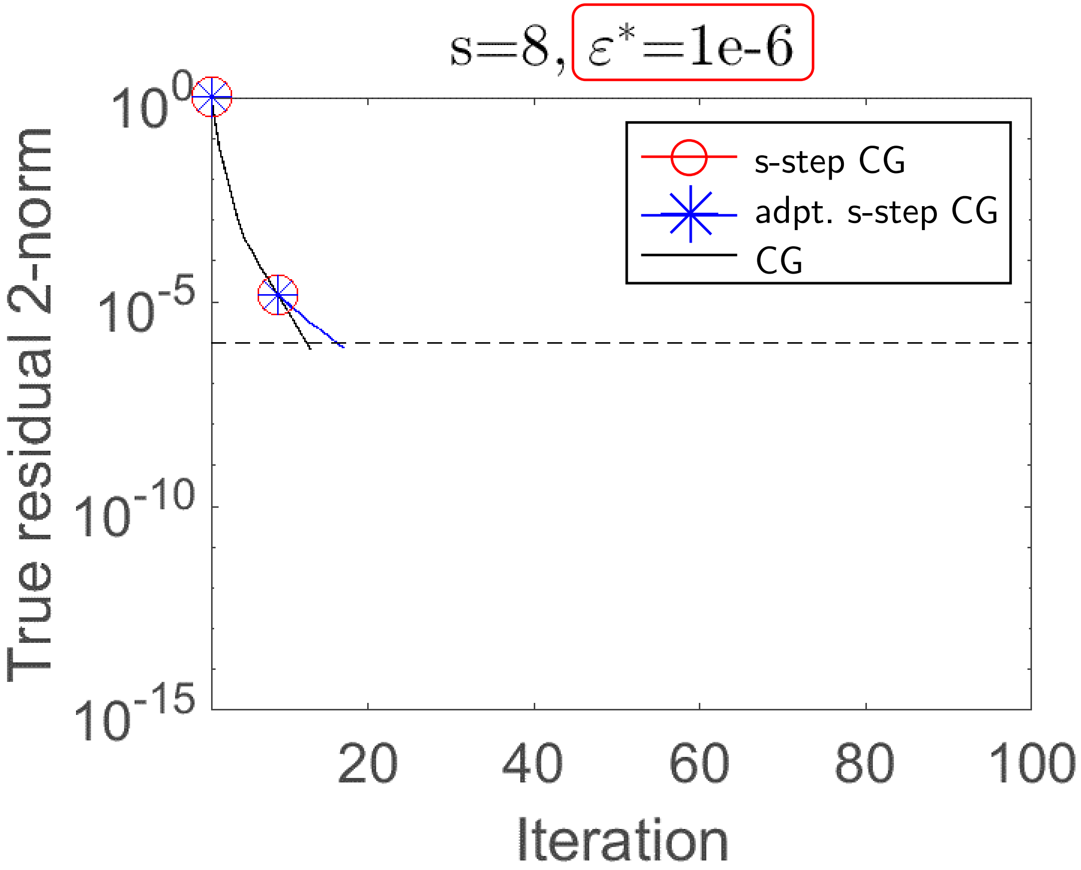

Extensions to adaptive s-step CG

- Method of Meurant and Tichý (2018) for cheap approximation of extremal Ritz values
  - Uses Cholesky factors of Lanczos tridiagonal T_i, $T_i = L_i L_i^T$
  - Use α and β computed during each iteration to incrementally update estimates of $\|L_i\|_2^2 = \lambda_{max}(T_i) \approx \lambda_{max}(A)$, $\left\|L_i^{-1}\right\|_2^{-2} = \lambda_{min}(T_i) \approx \lambda_{min}(A)$
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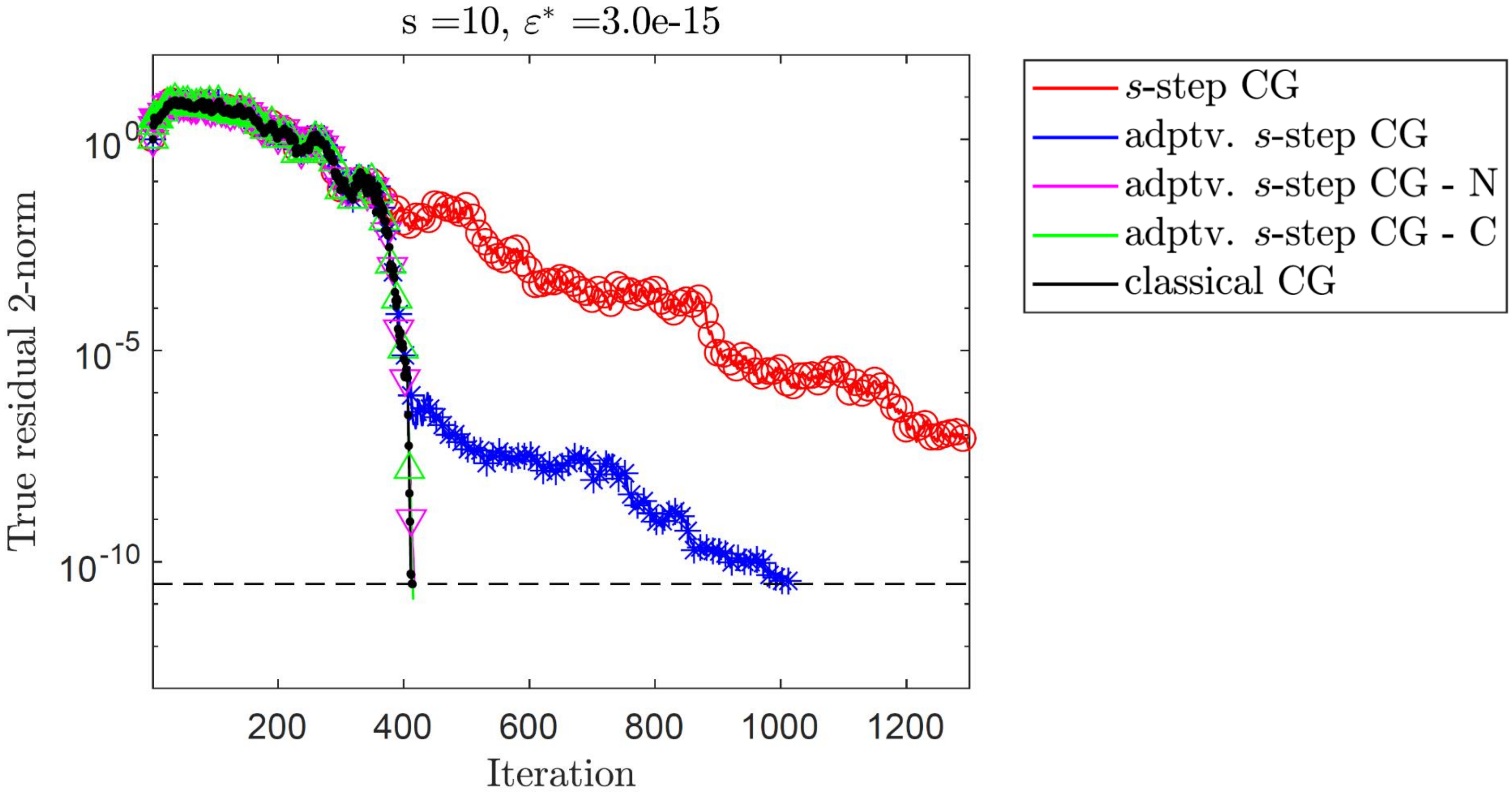
- Can be used in two ways in adaptive algorithm
  1. Incrementally refine estimate of $\kappa(A)$ (used in determining which s to use)
  2. Incrementally refine parameters used to construct Newton or Chebyshev polynomials

$A =$ 494bus from SuiteSparse

$b_i = 1/\sqrt{N}$



Number of global synchronizations

Fixed s-step	Old adaptive s-step	Improved adaptive s-step w/Newton	Improved adaptive s-step w/Chebyshev	classical CG
-	132	**59**	**53**	414

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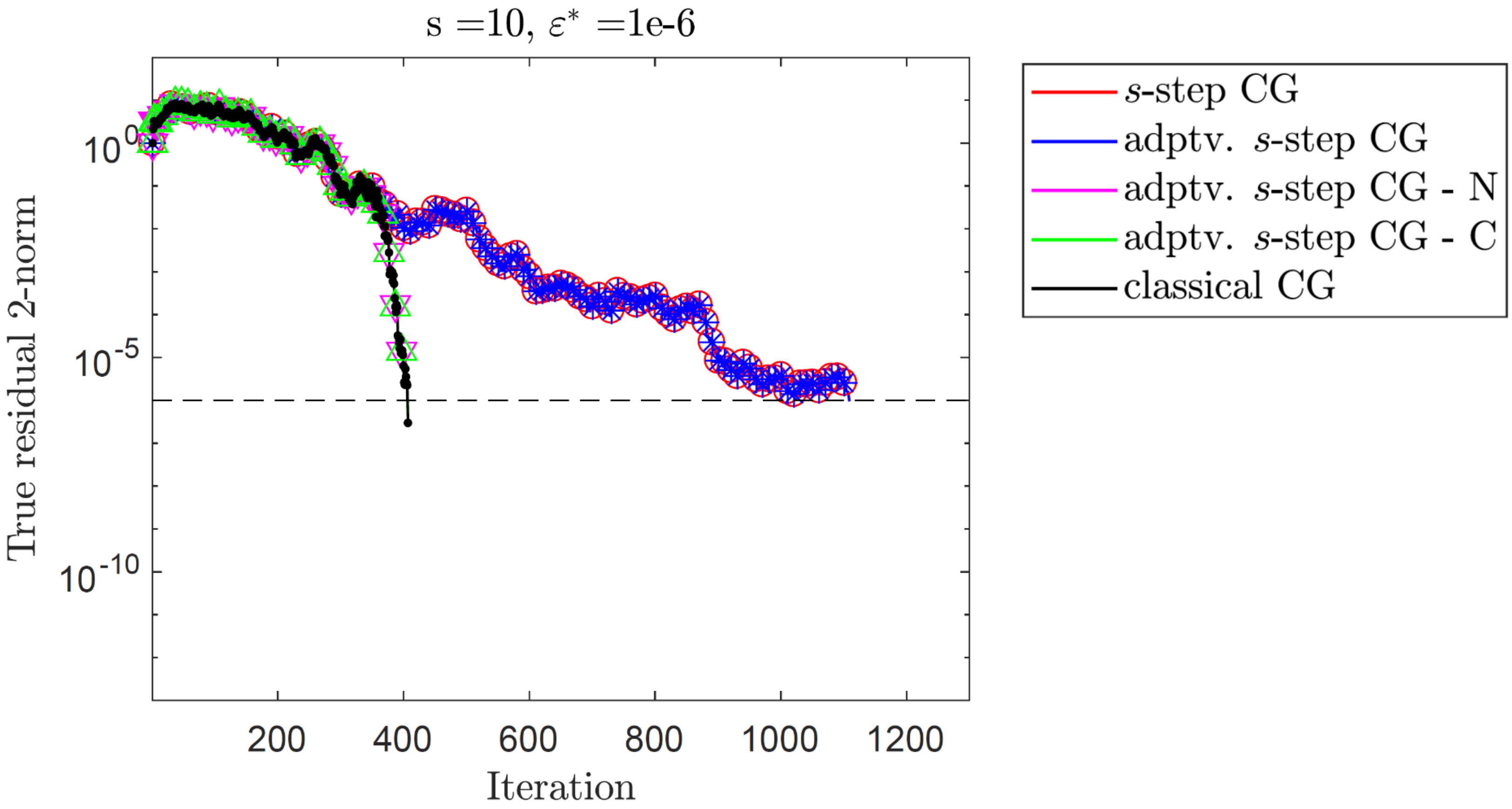

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- (deep) pipelined methods
  - cost of applying preconditioner + SpMV is less than or the same as a global synchronization
  - improvement only for large numbers of nodes

Looking Forward

- Better understanding of finite precision behavior

- Improved usability
  - More adaptivity, autotuning; less left to the user

- Hybrid methods?
  - stationary iterative method + Krylov subspace method

- Fault tolerance?
  - MTTF=0 on an exascale machine
  - A problem to be handled at the algorithm level, or...?

- Making use of specialized hardware
  - accelerators, GPUs, etc.
  - multiple precisions?
  - new performance model, new programming model, bigger tuning space

Thank you!

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