High performance Krylov subspace method variants

and their behavior in finite precision

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Preprint NCMM/2016/08:
http://www.karlin.mff.cuni.cz/~strakos/download/2016_CarRozStrTicTum_16.pdf

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

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

$$x_i = x_{i-1} + \alpha_i p_i$$
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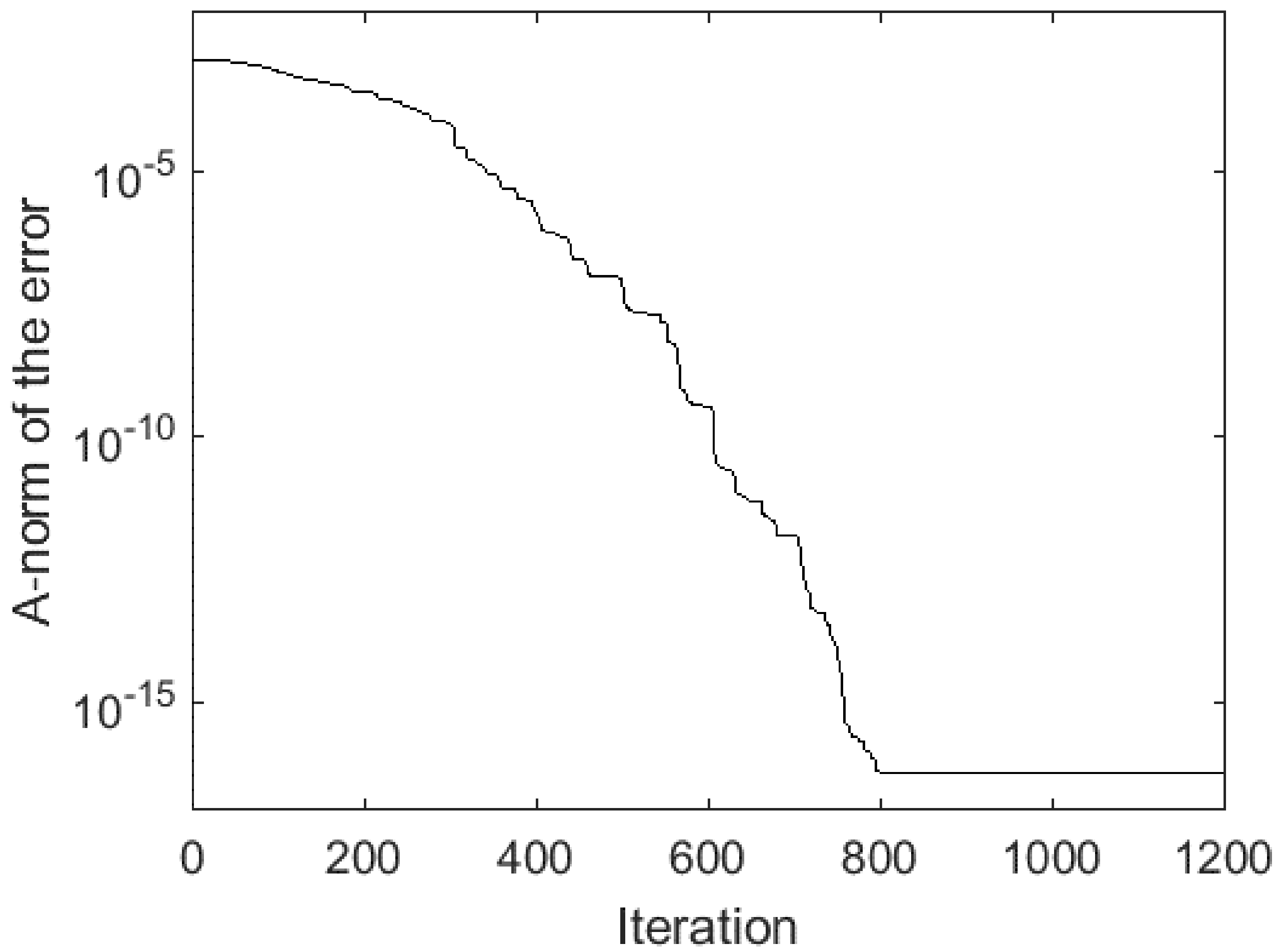

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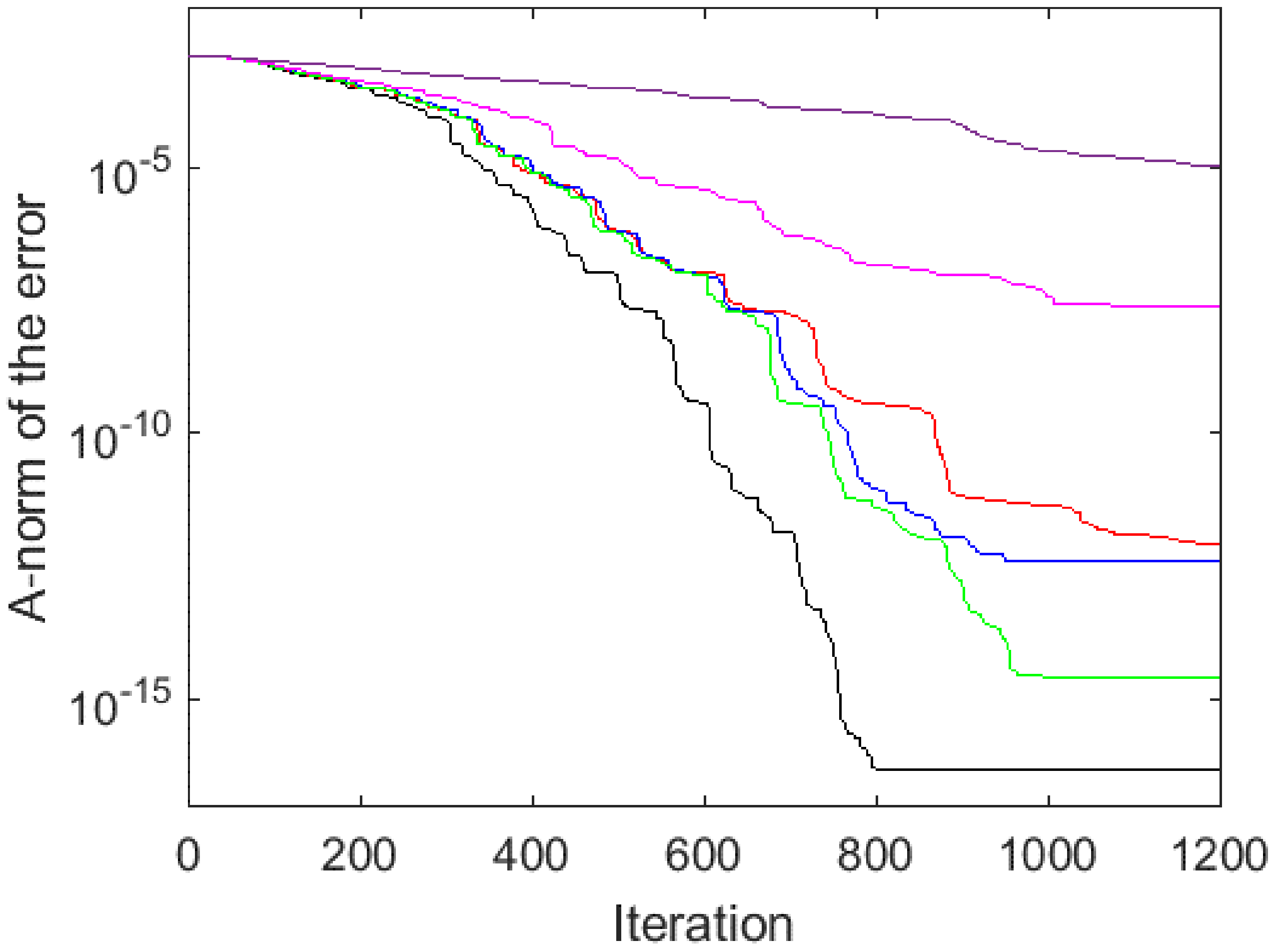


Krylov subspace methods

- **Linear systems** $Ax = b$, eigenvalue problems, singular value problems, least squares, etc.
- Best for: A large & very sparse, stored implicitly, or only approximation needed

- **Krylov Subspace Method** is a projection process onto the Krylov subspace

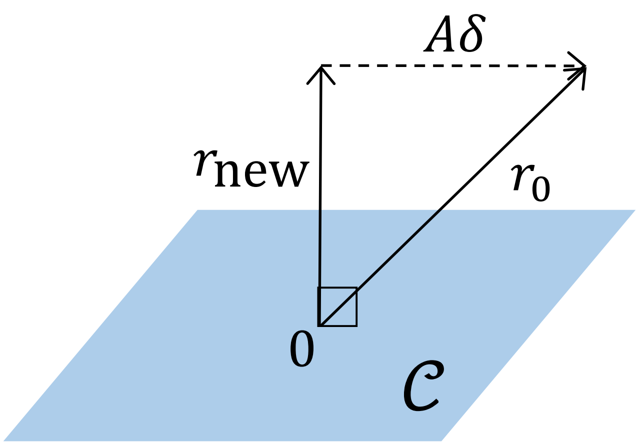
$$\mathcal{K}_i(A, r_0) = \text{span}\{r_0, Ar_0, A^2 r_0, \ldots, A^{i-1} r_0\}$$

where A is an $N \times N$ matrix and $r_0 = b - Ax_0$ is a length-N vector

- In each iteration,
  - Add a dimension to the Krylov subspace
    - Forms nested sequence of Krylov subspaces

$$\mathcal{K}_1(A, r_0) \subset \mathcal{K}_2(A, r_0) \subset \cdots \subset \mathcal{K}_i(A, r_0)$$

  - Orthogonalize (with respect to some $\mathcal{C}_i$)
  - Select approximate solution $x_i \in x_0 + \mathcal{K}_i(A, r_0)$ using $r_i = b - Ax_i \perp \mathcal{C}_i$



- Ex: Lanczos/**Conjugate Gradient (CG)**, Arnoldi/Generalized Minimum Residual (GMRES), Biconjugate Gradient (BICG), BICGSTAB, GKL, LSQR, etc.

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Connection with Lanczos

- With $v_1 = r_0 / \|r_0\|$, i iterations of Lanczos produces $N \times i$ matrix $V_i = [v_1, \dots, v_i]$, and $i \times i$ tridiagonal matrix T_i such that
$$AV_i = V_i T_i + \delta_{i+1} v_{i+1} e_i^T, \qquad T_i = V_i^* A V_i$$
- CG approximation x_i is obtained by solving the reduced model
$$T_i y_i = \|r_0\| e_1, \qquad x_i = x_0 + V_i y_i$$

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⇒ CG (and other Krylov subspace methods) are highly nonlinear

- Good for convergence, bad for ease of finite precision analysis

Implementation of CG

- Standard implementation due to Hestenes and Stiefel (1952) (HSCG)
- Uses three 2-term recurrences for updating x_i, r_i, p_i

$$r_0 = b - Ax_0, \quad p_0 = r_0$$

for i = 1:nmax

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If
$$p_i \perp_A p_j \text{ for } i \neq j,$$

1-dimensional minimizations in each iteration give i-dimensional minimization over the whole subspace

$$x_0 + \mathcal{K}_i(A, r_0) = x_0 + \operatorname{span}\{p_0, \dots p_{i-1}\}$$

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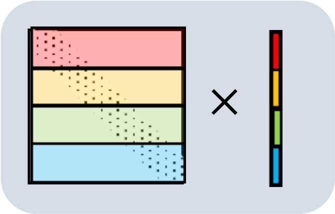
$\longrightarrow$ Sparse matrix-vector multiplication (SpMV)

- Must communicate vector entries w/ neighboring processors (P2P communication)



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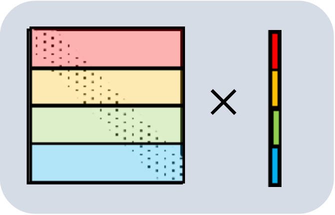

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$\rightarrow$ Inner products

- global synchronization (MPI_Allreduce)
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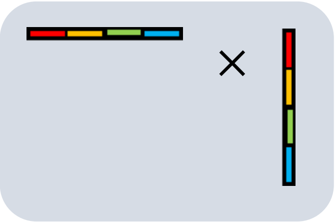

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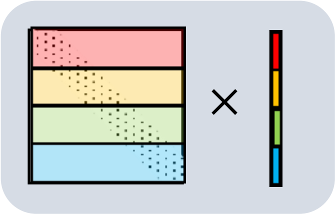

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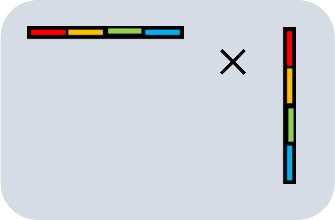

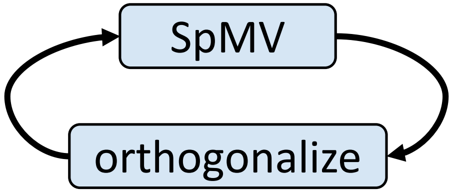

Dependencies between communication-bound kernels in each iteration limit performance!

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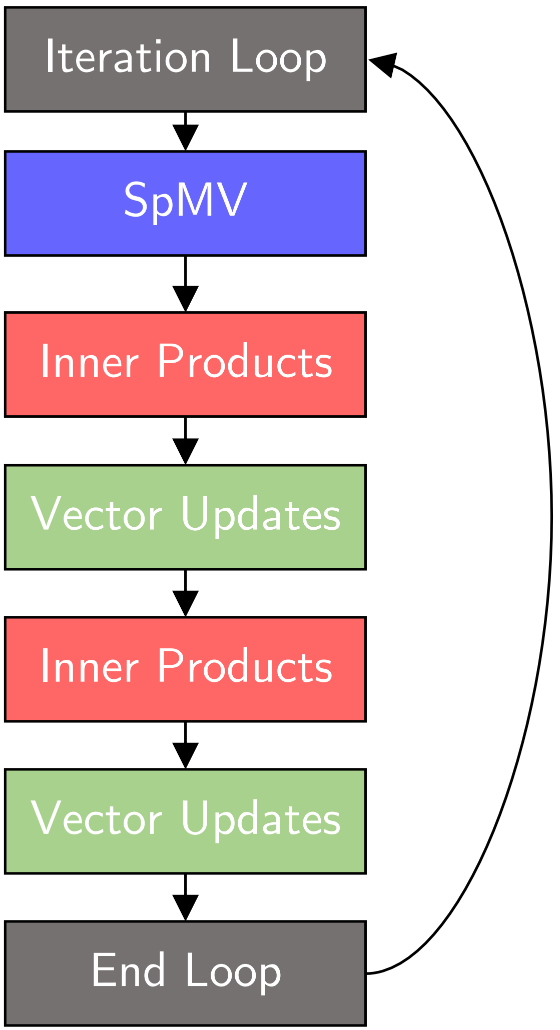

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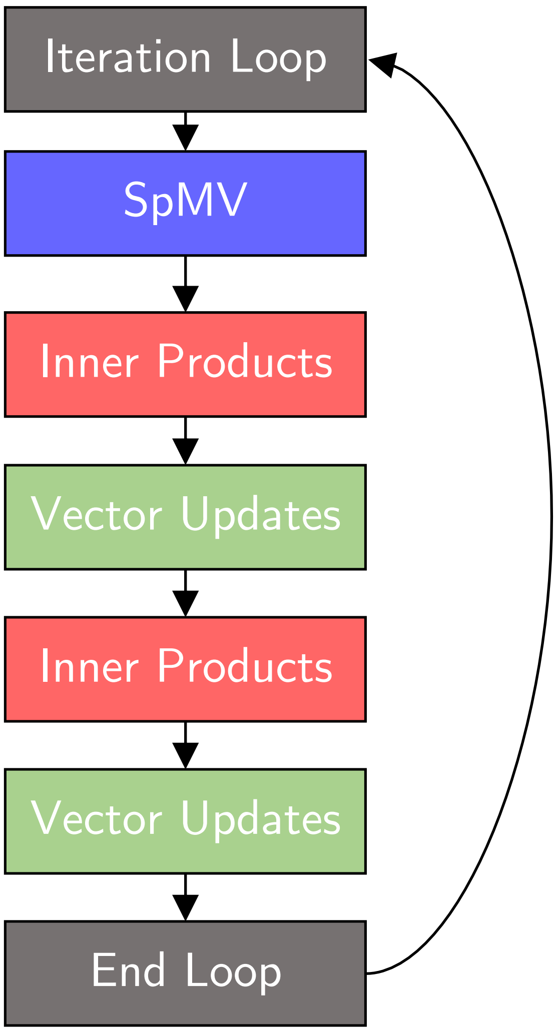

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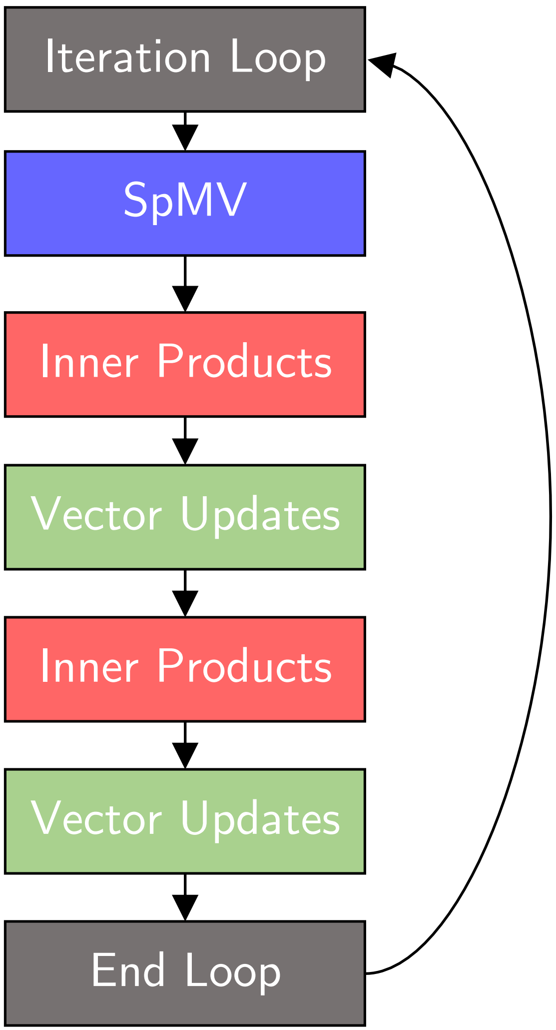

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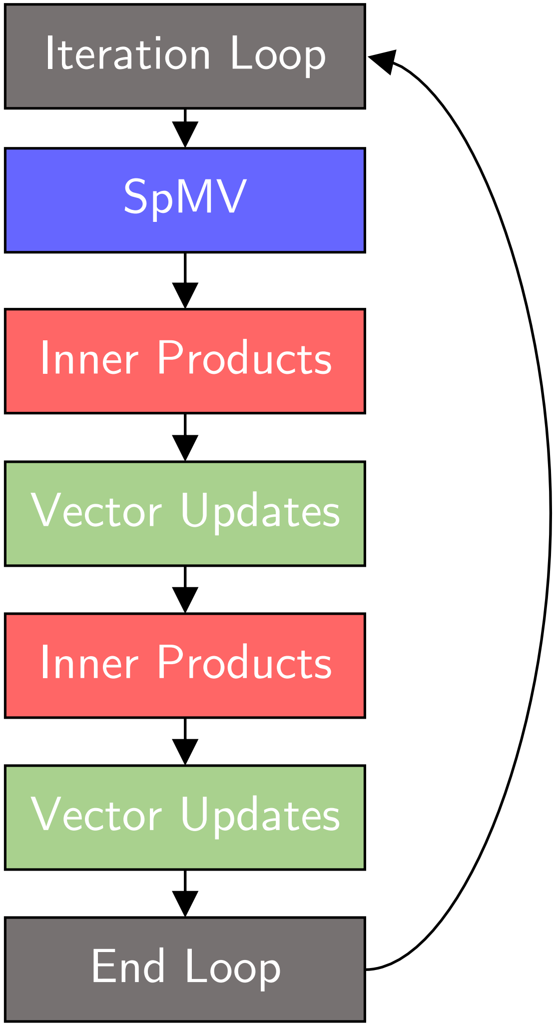

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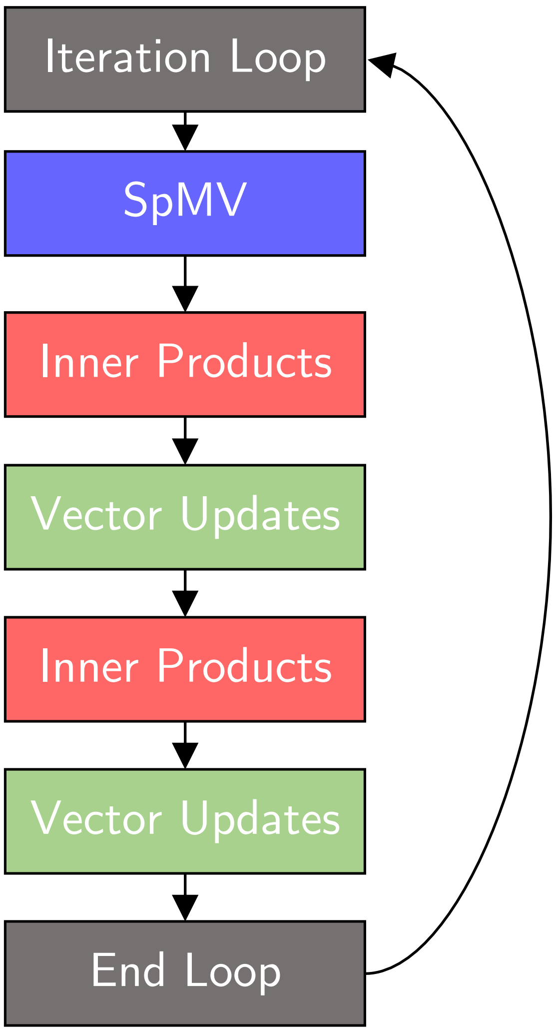

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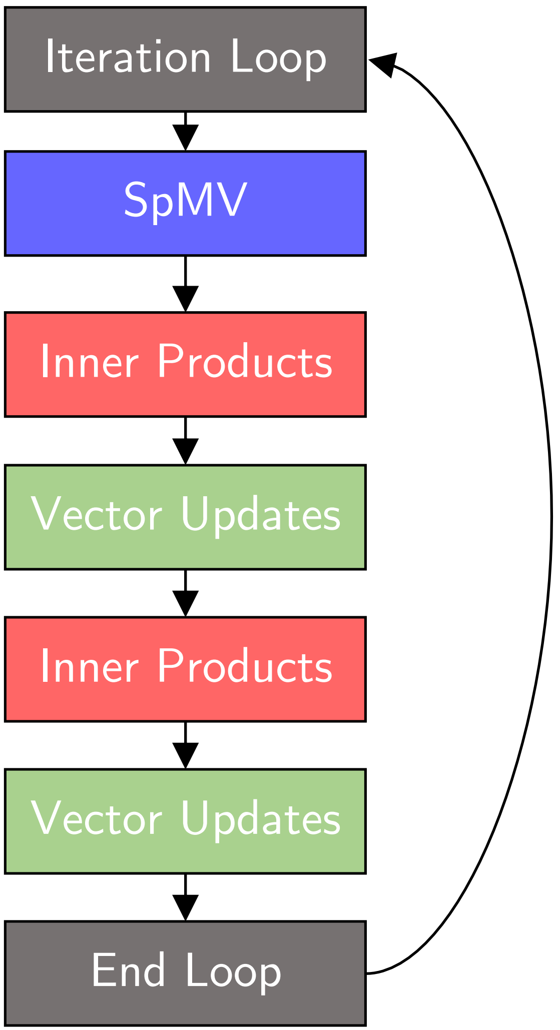

Future exascale systems

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Node Memory Bandwidth	25 GB/s
Total Node Interconnect Bandwidth	3.5 GB/s
Memory Latency	100 ns
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- Gaps between communication/computation cost only growing larger in future systems
- **Reducing time spent moving data/waiting for data will be essential for applications at exascale!**

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- s-step Krylov subspace methods
  - Compute iterations in blocks of s using a different Krylov subspace basis
  - Enables one synchronization per s iterations

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 no longer exact!

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

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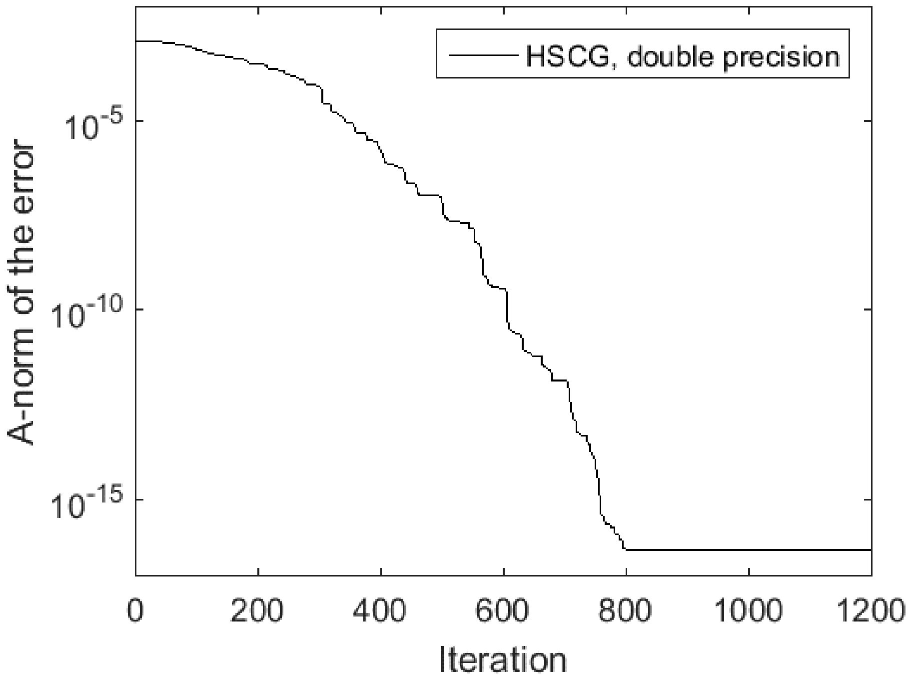

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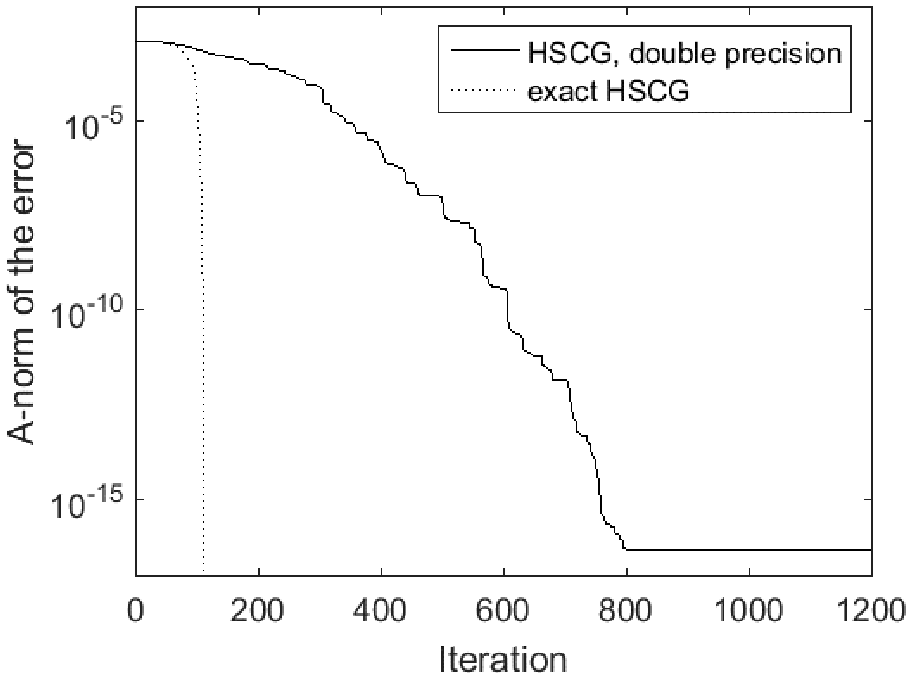

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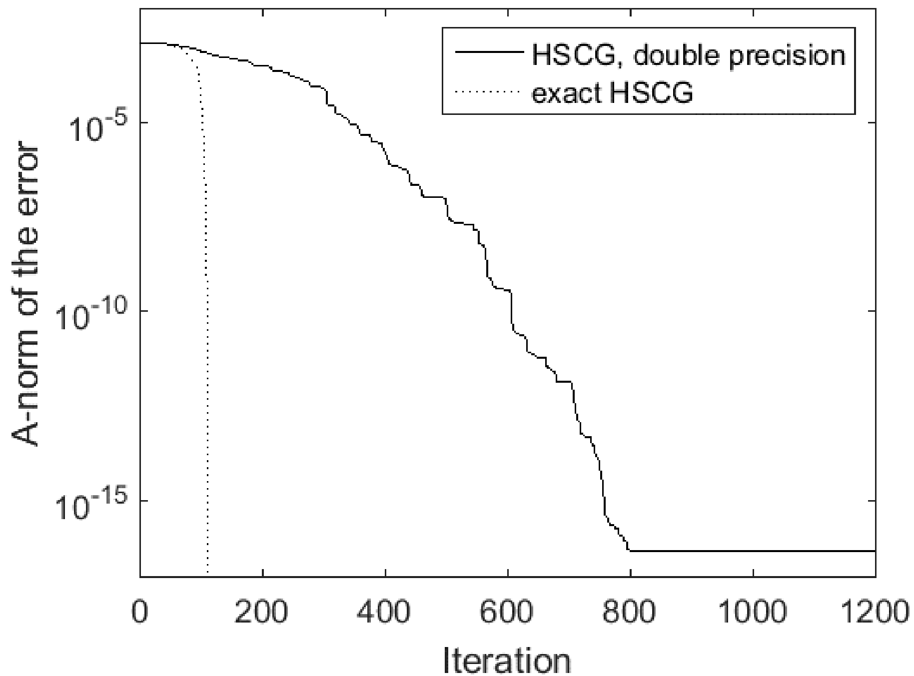

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Much work on these results for CG; See Meurant and Strakoš (2006) for a thorough summary of early developments in finite precision analysis of Lanczos and CG

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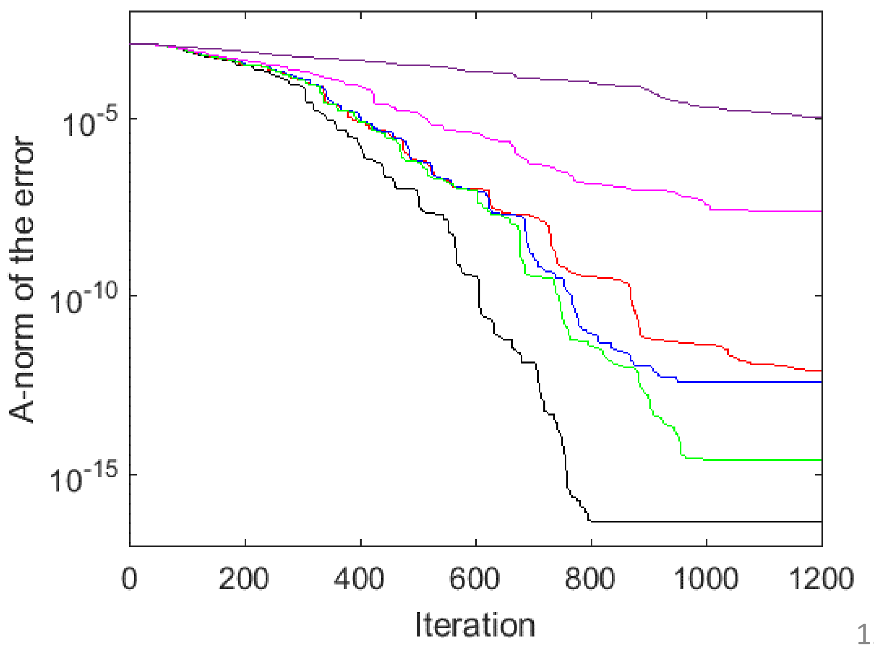
- Changes to how the recurrences are computed can exacerbate finite precision effects of convergence delay and loss of accuracy



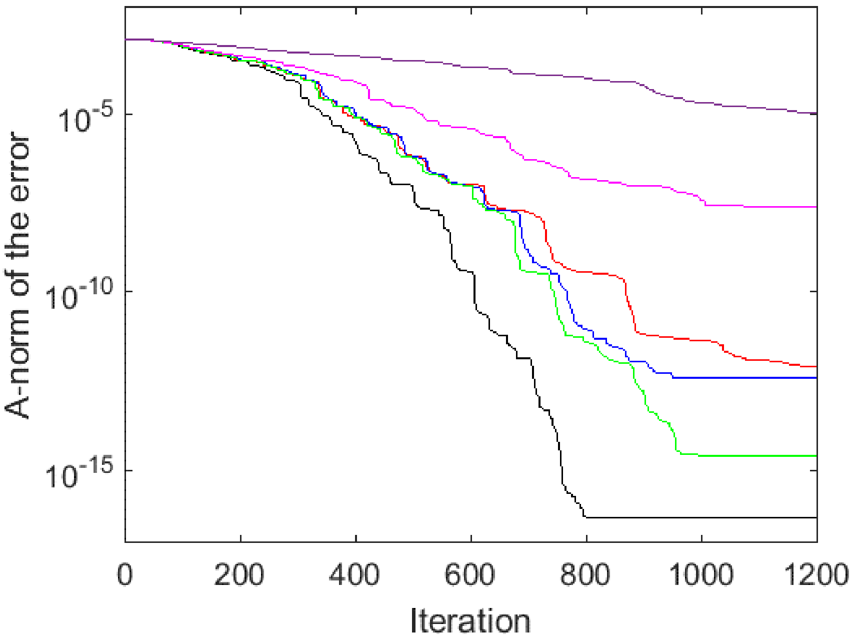
Optimizing high performance iterative solvers

- Synchronization-reducing variants are designed to reduce the time/iteration
- But this is not the whole story!
- What we really want to minimize is the **runtime, subject to some constraint on accuracy,**

runtime = (time/iteration) x (# iterations)

- Changes to how the recurrences are computed can exacerbate finite precision effects of convergence delay and loss of accuracy

- Crucial that we understand and take into account how algorithm modifications will affect the convergence rate and attainable accuracy!



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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).

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

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

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

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

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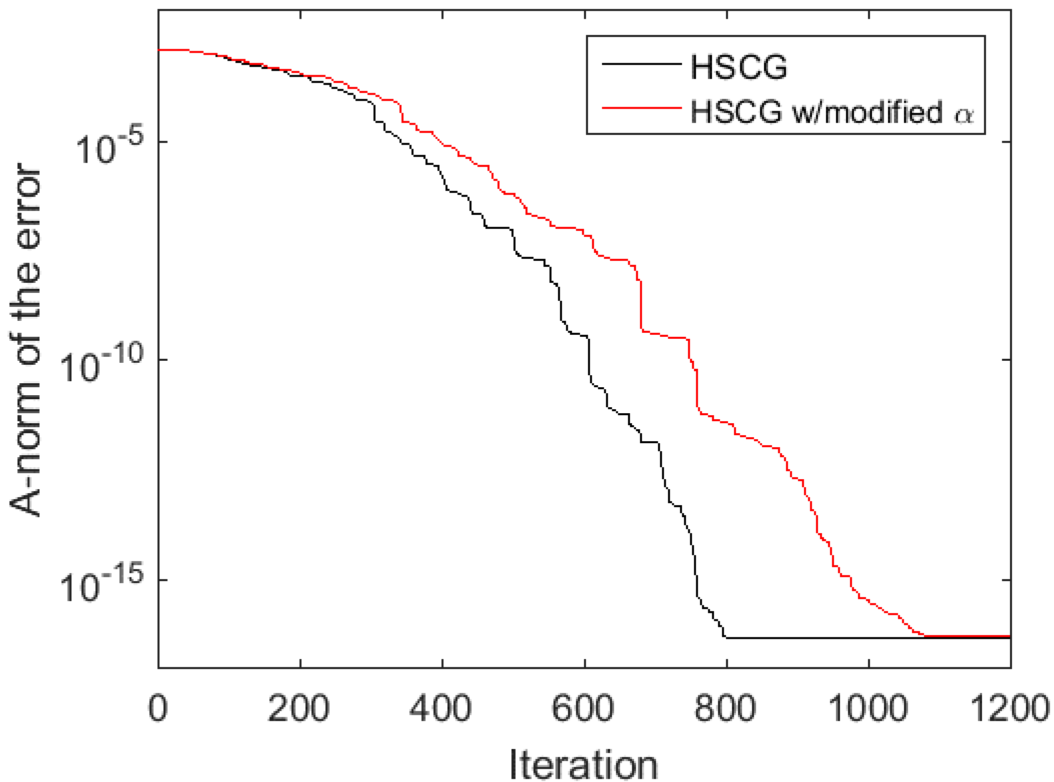

CG with two three-term recurrences (STCG)

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$$AP_i = R_{i+1}\underline{L}_i, \qquad R_i = P_i U_i$$

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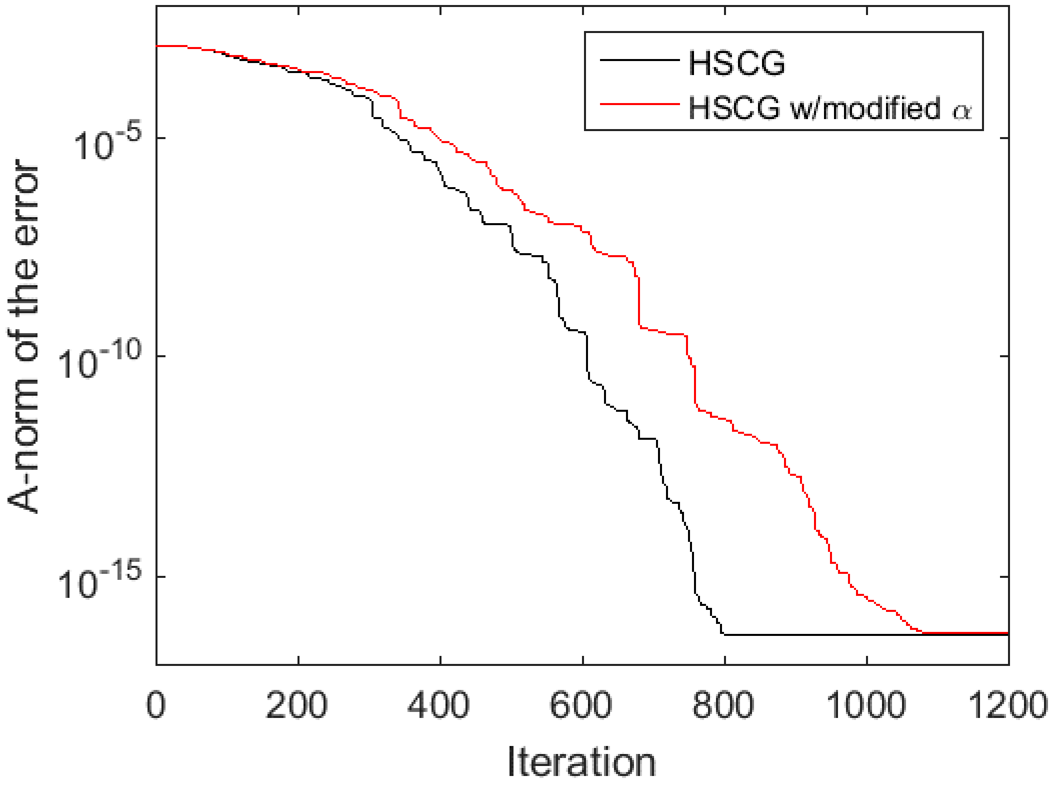
$\Rightarrow$ Large residual oscillations can cause these factors to be large!

$\Rightarrow$ Local errors can be amplified!

STCG



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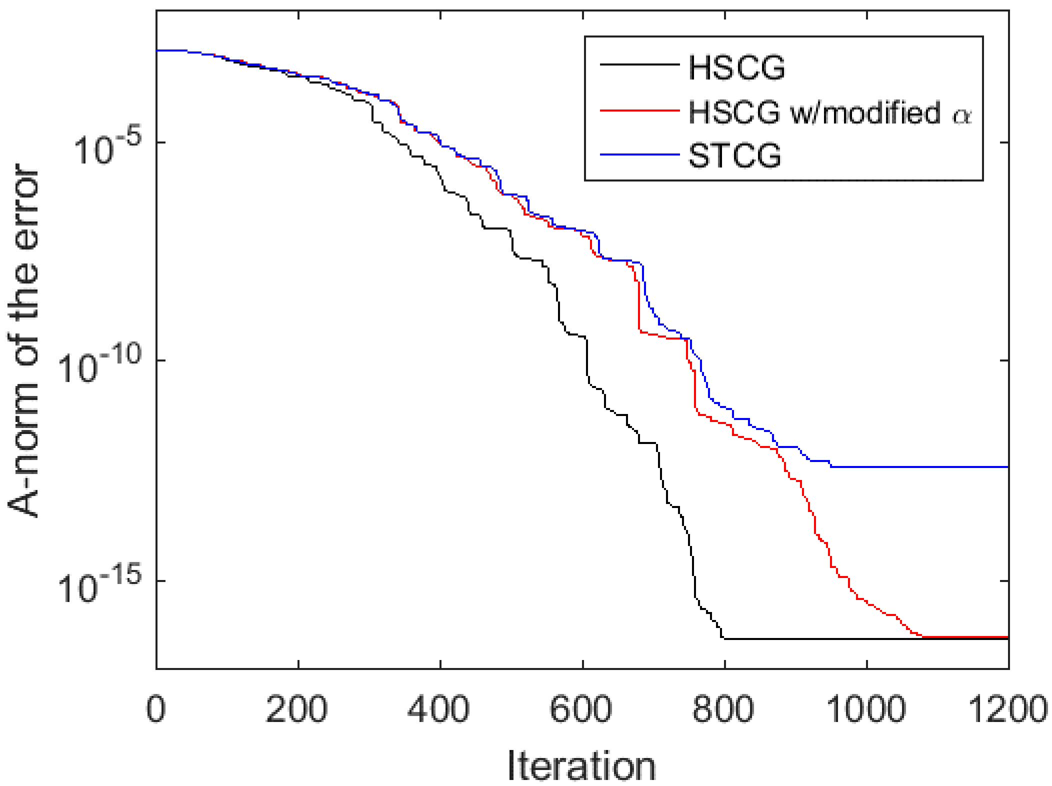
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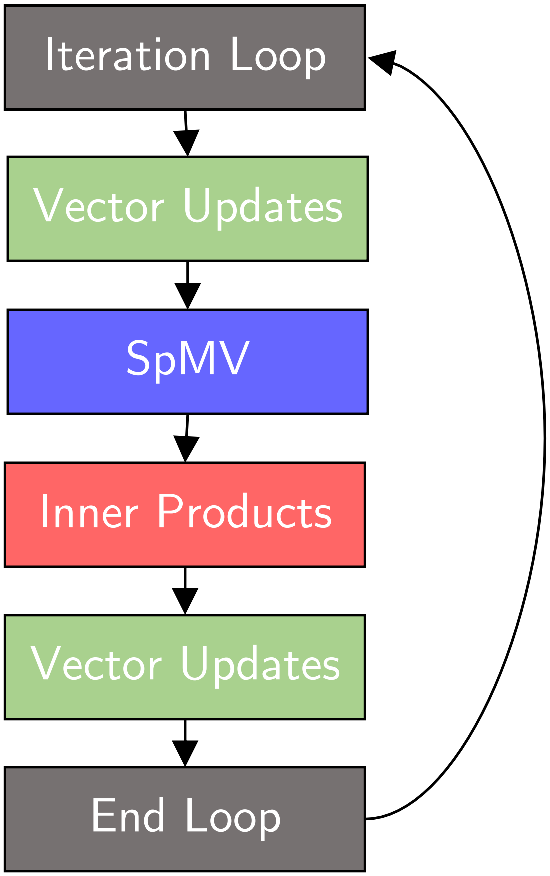

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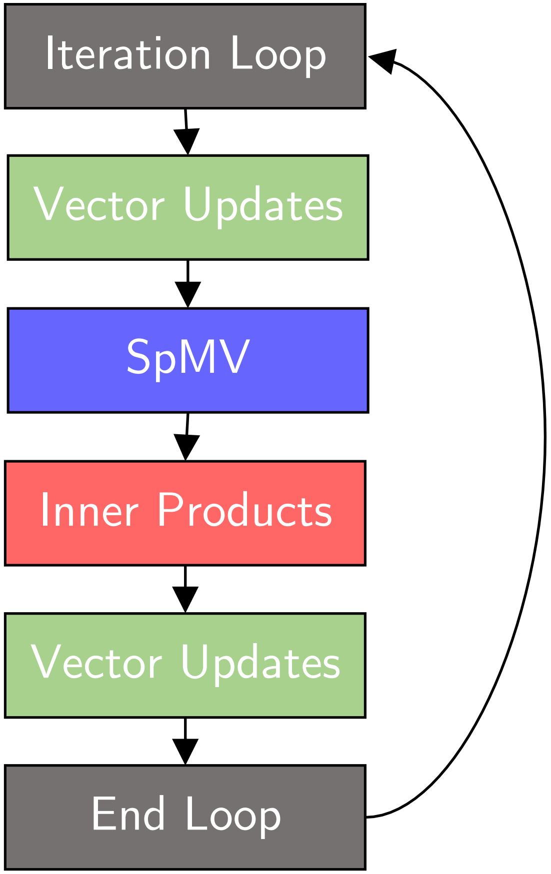

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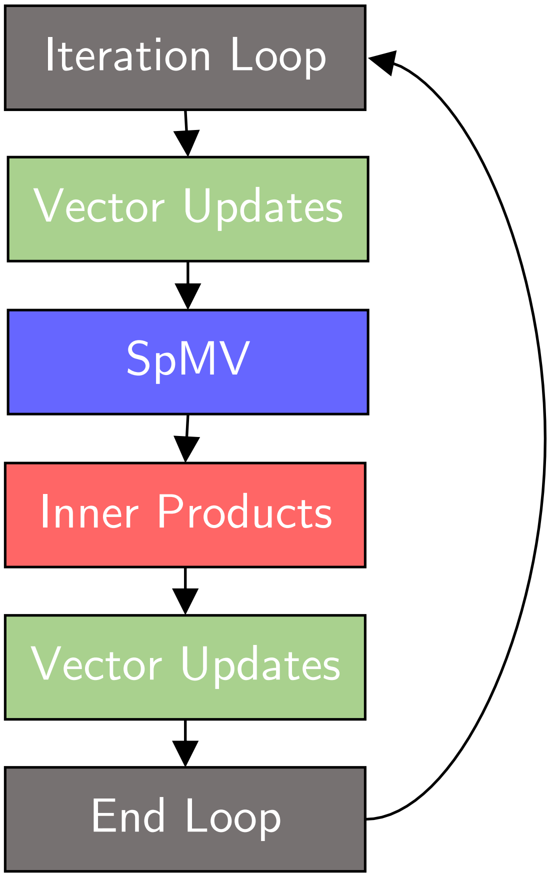

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- Looks like HSCG, but very similar to 3-term recurrence CG (STCG)
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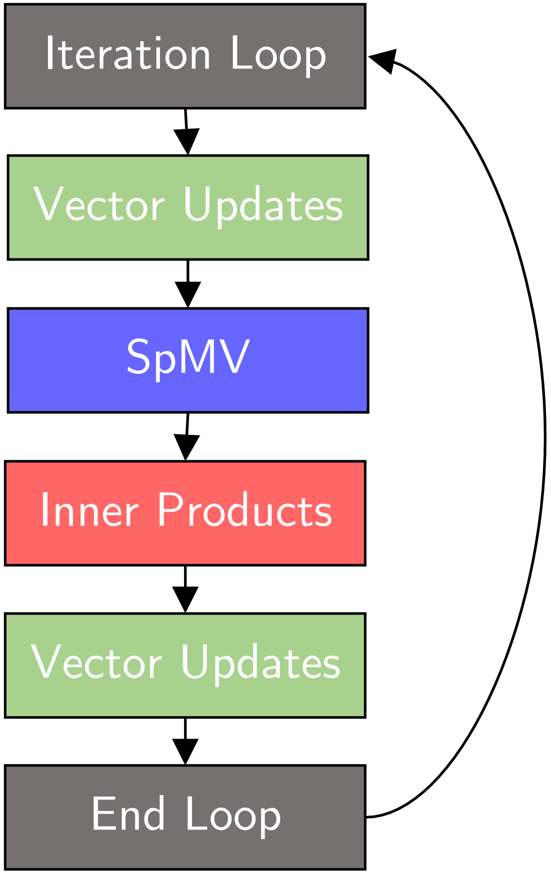

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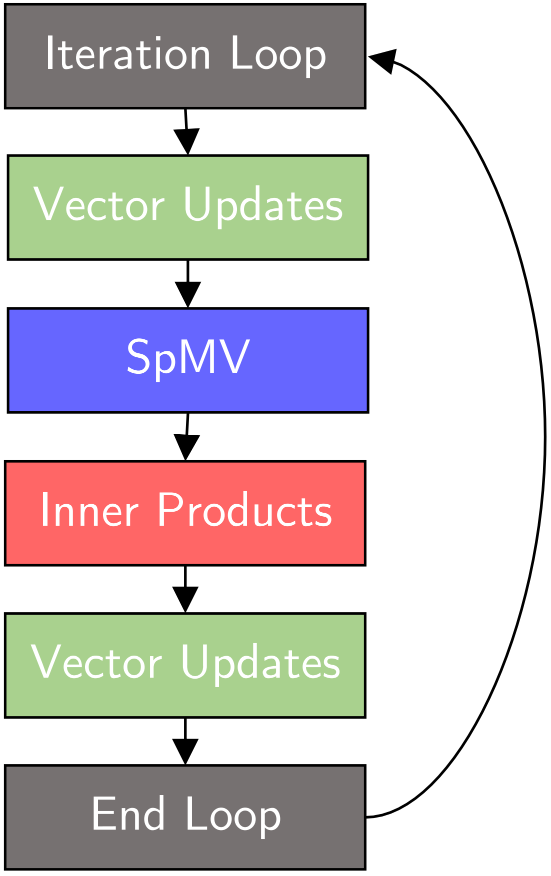

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  - Allows the use of nonblocking (asynchronous) MPI communication to *overlap* SpMV and inner products

  - Hides the latency of global communications

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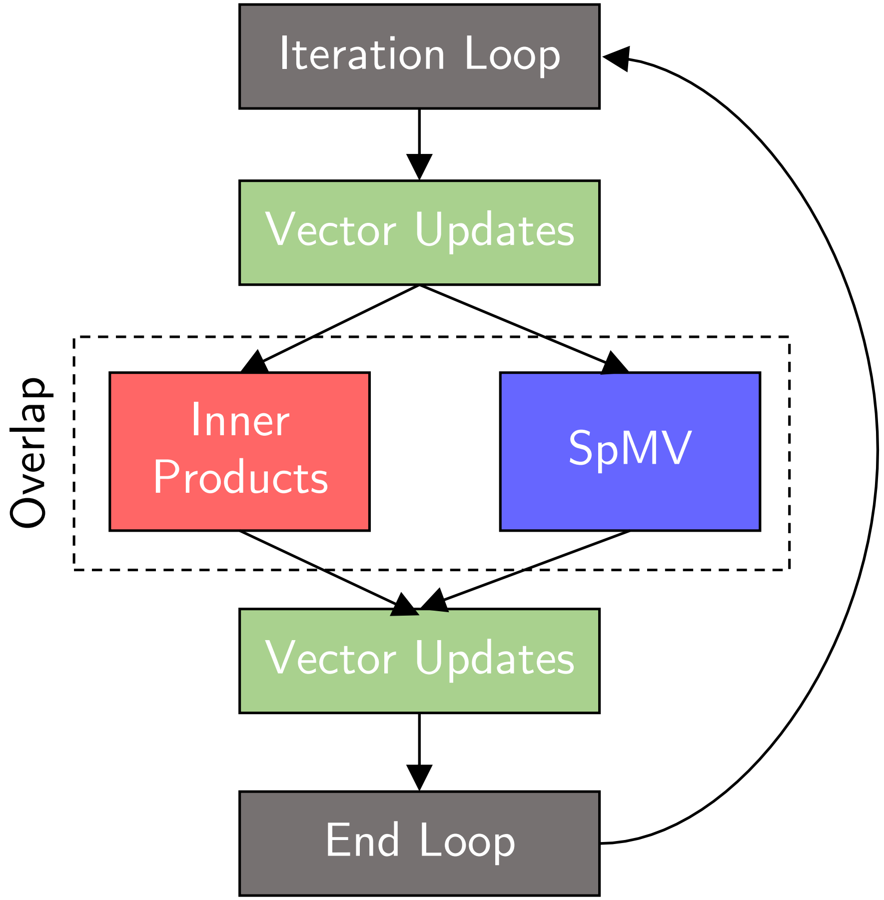

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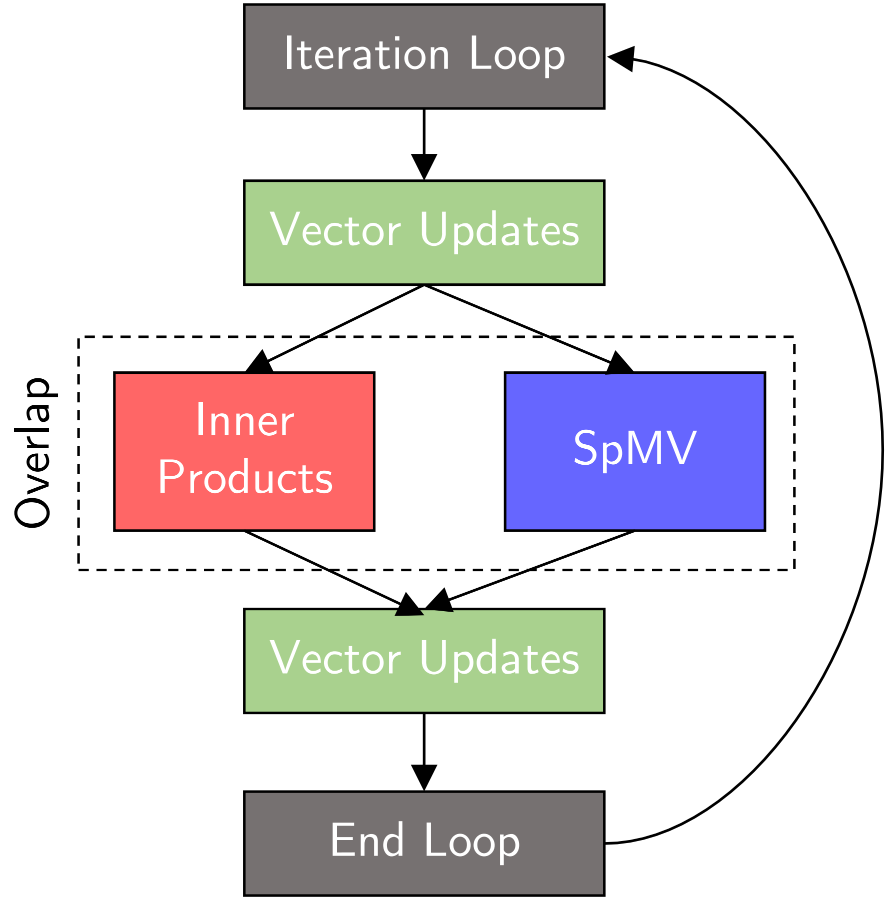

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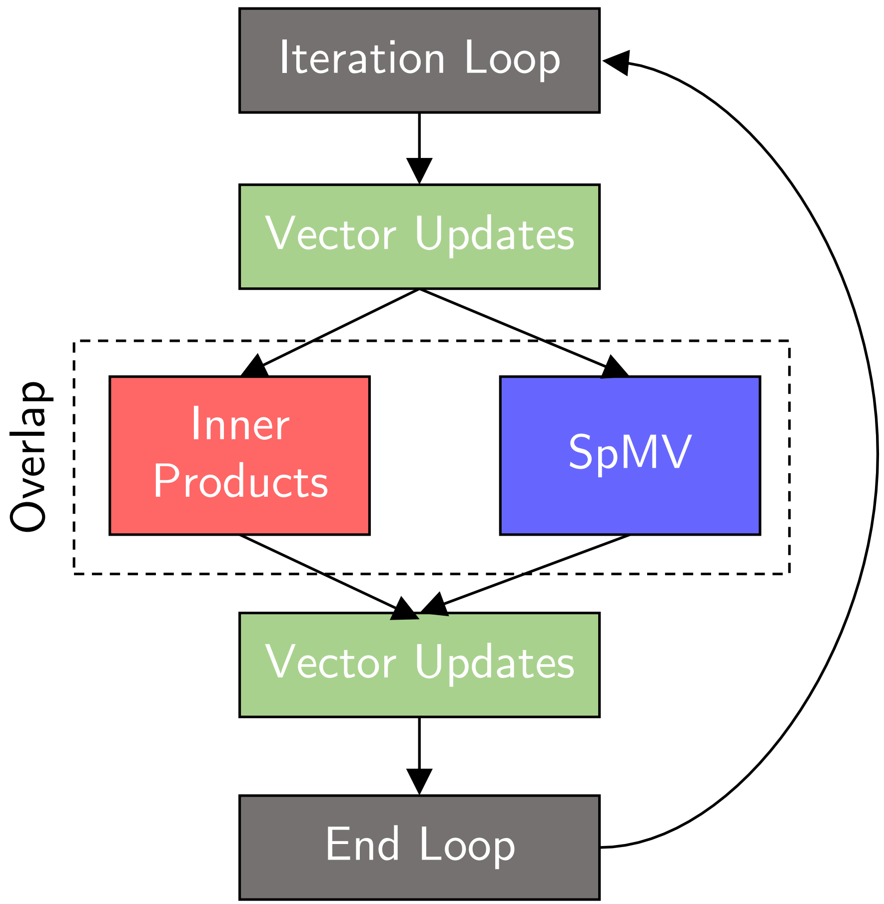

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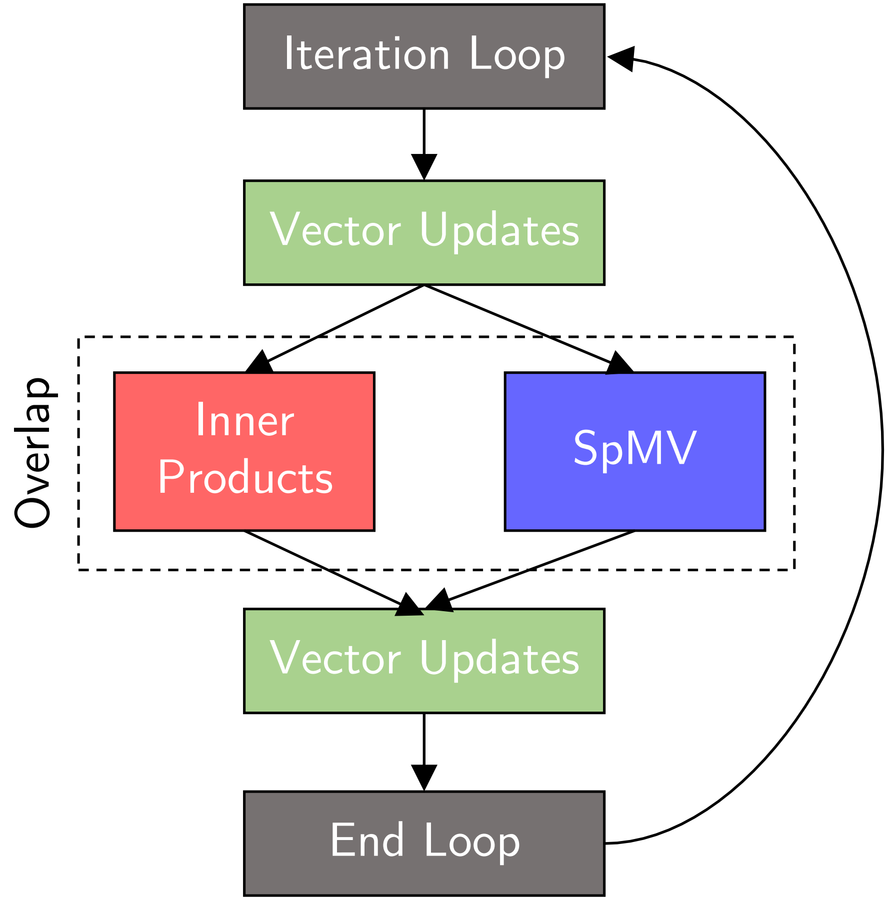

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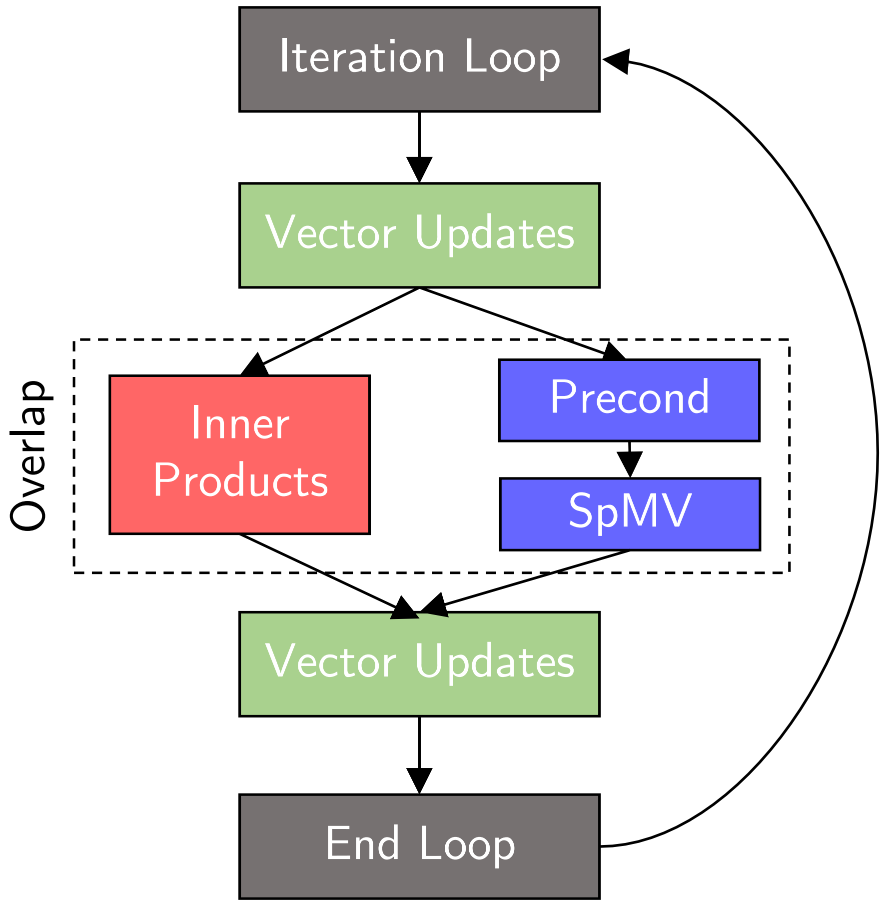

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  - Uses same update formulas for α and β as HSCG, but uses additional recurrence for Ap_i

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

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

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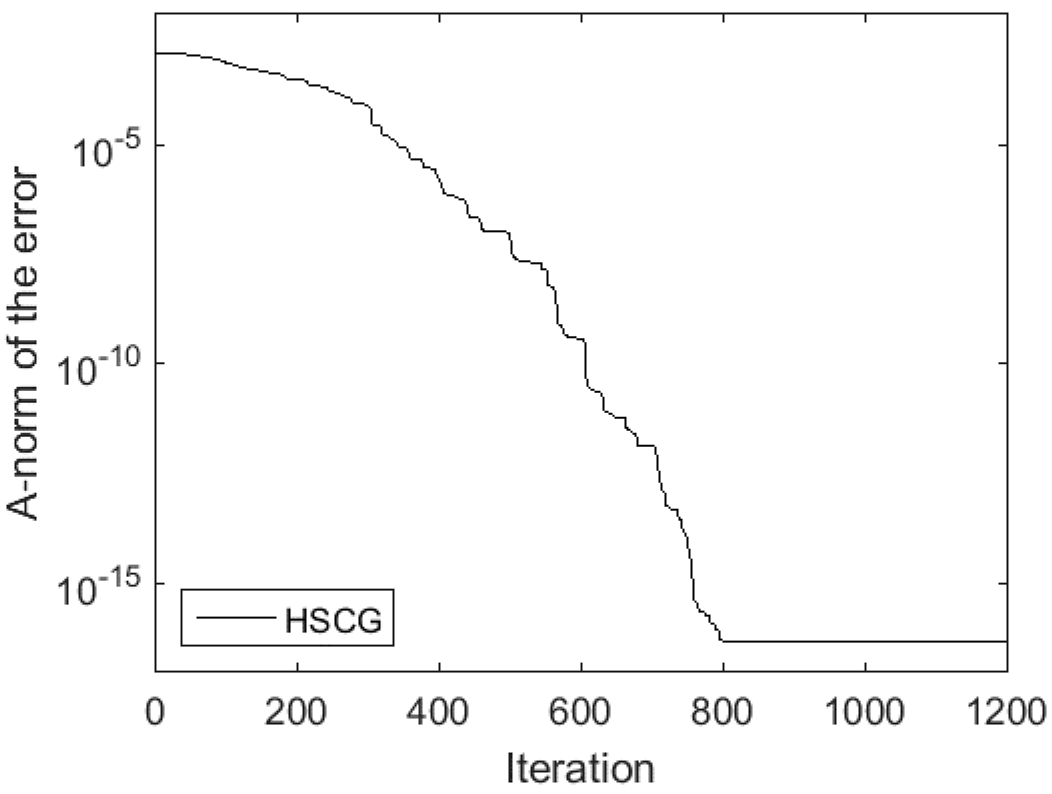
- Very similar to the results for attainable accuracy in the 3-term STCG
- Seemingly innocuous change can cause drastic loss of accuracy

Simple pipelined CG



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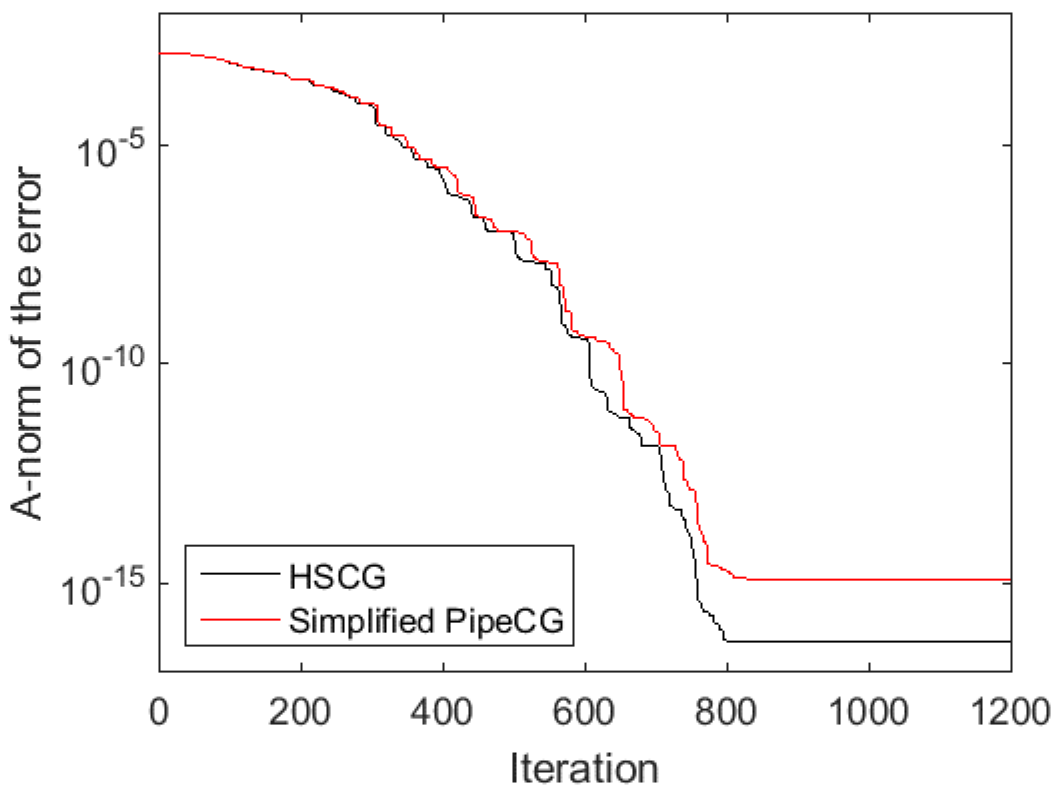

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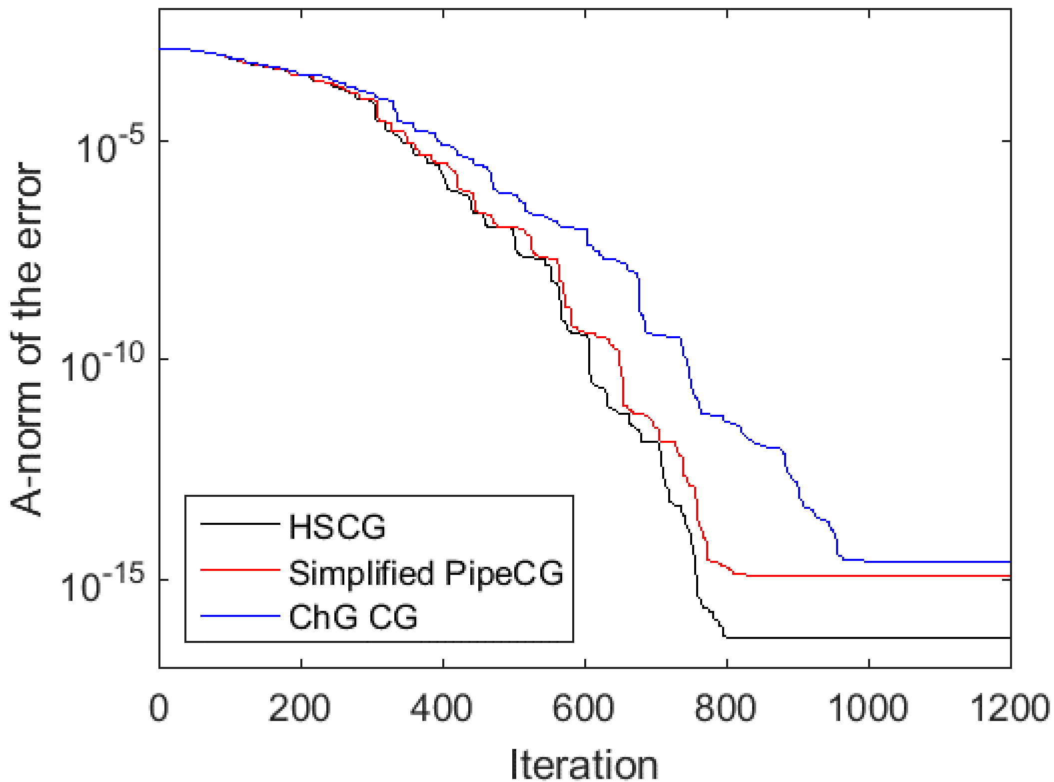

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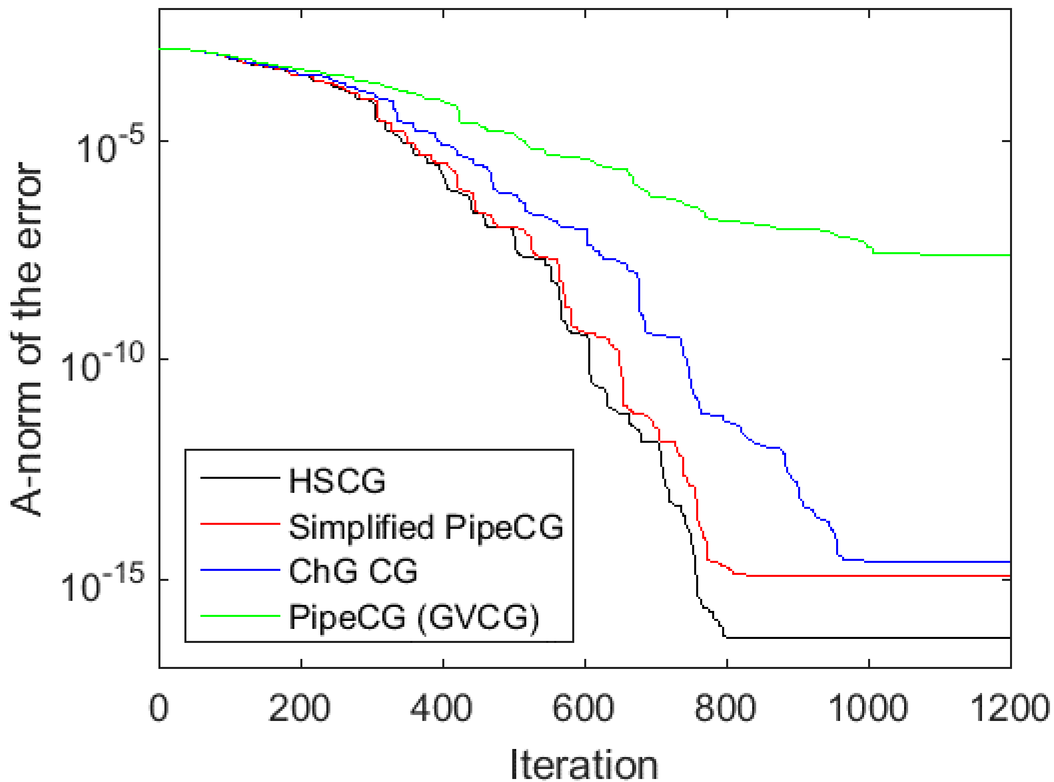

effect of changing formula for recurrence coefficient α and using auxiliary vectors $s_i \equiv Ap_i, w_i \equiv Ar_i, z_i \equiv A^2 r_i$

s-step CG

- Idea: Compute blocks of s iterations at once
  - Compute updates in a different basis
  - Communicate every s iterations instead of every iteration
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- An idea rediscovered many times…

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- Resurgence of interest in recent years due to growing problem sizes; growing relative cost of communication

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Key observation: After iteration i, for $j \in \{0, .., s\}$,

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Expand solution space s dimensions at once

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Compute s iterations of vector updates

Perform s iterations of vector updates by updating coordinates in basis $\mathcal{Y}$:

$$x_{i+j} - x_i = \mathcal{Y}x_j', \qquad r_{i+j} = \mathcal{Y}r_j', \qquad p_{i+j} = \mathcal{Y}p_j'$$

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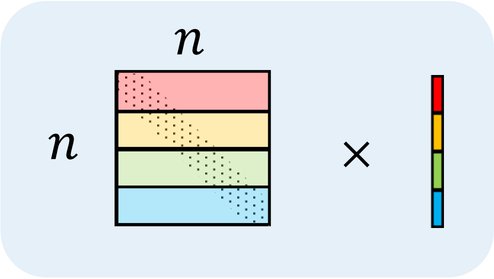

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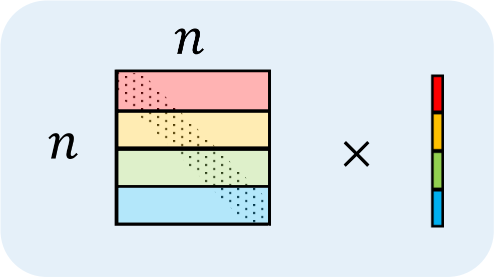

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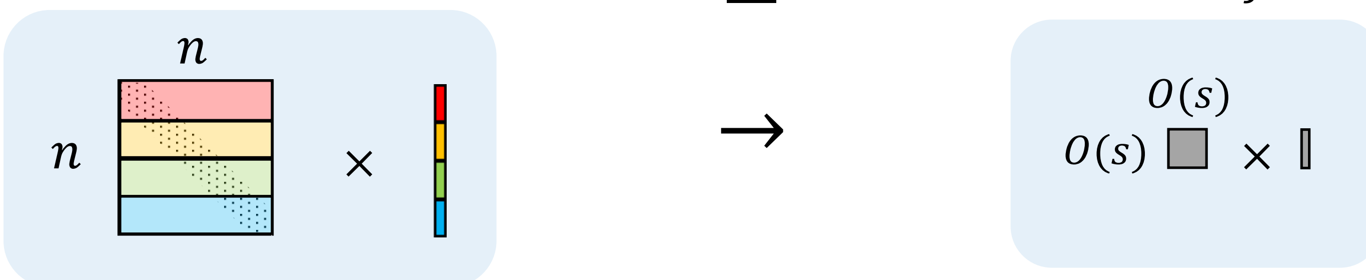

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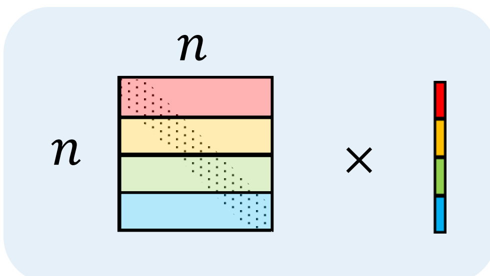

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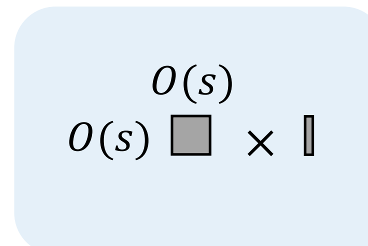

$$(r_{i+j}, r_{i+j})$$

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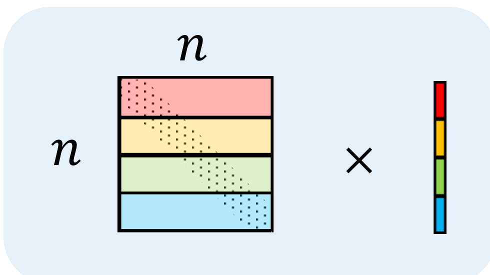

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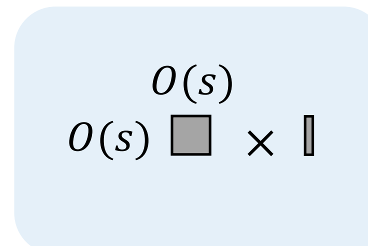

$$(r_{i+j}, r_{i+j}) \quad = \quad r_j'^T \mathcal{Y}^T \mathcal{Y} r_j'$$

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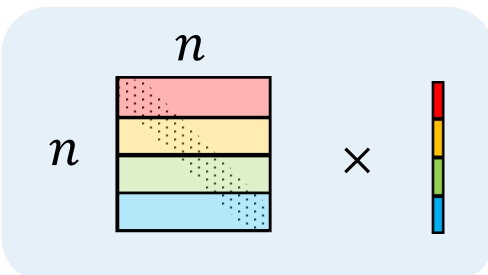

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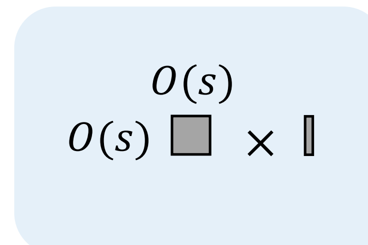

$$(r_{i+j}, r_{i+j}) \quad = \quad r_j'^T \mathcal{Y}^T \mathcal{Y} r_j' \quad = \quad r_j'^T \mathcal{G} r_j'$$

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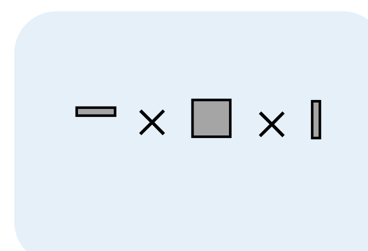

s-step CG

$r_0 = b - Ax_0, p_0 = r_0$

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

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$\mathcal{G}_k = \mathcal{Y}_k^T \mathcal{Y}_k$

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

for $j = 1: s$

$$\alpha_{sk+j-1} = \frac{r'^T_{j-1} \mathcal{G}_k r'_{j-1}}{p'^T_{j-1} \mathcal{G}_k \mathcal{B}_k p'_{j-1}}$$

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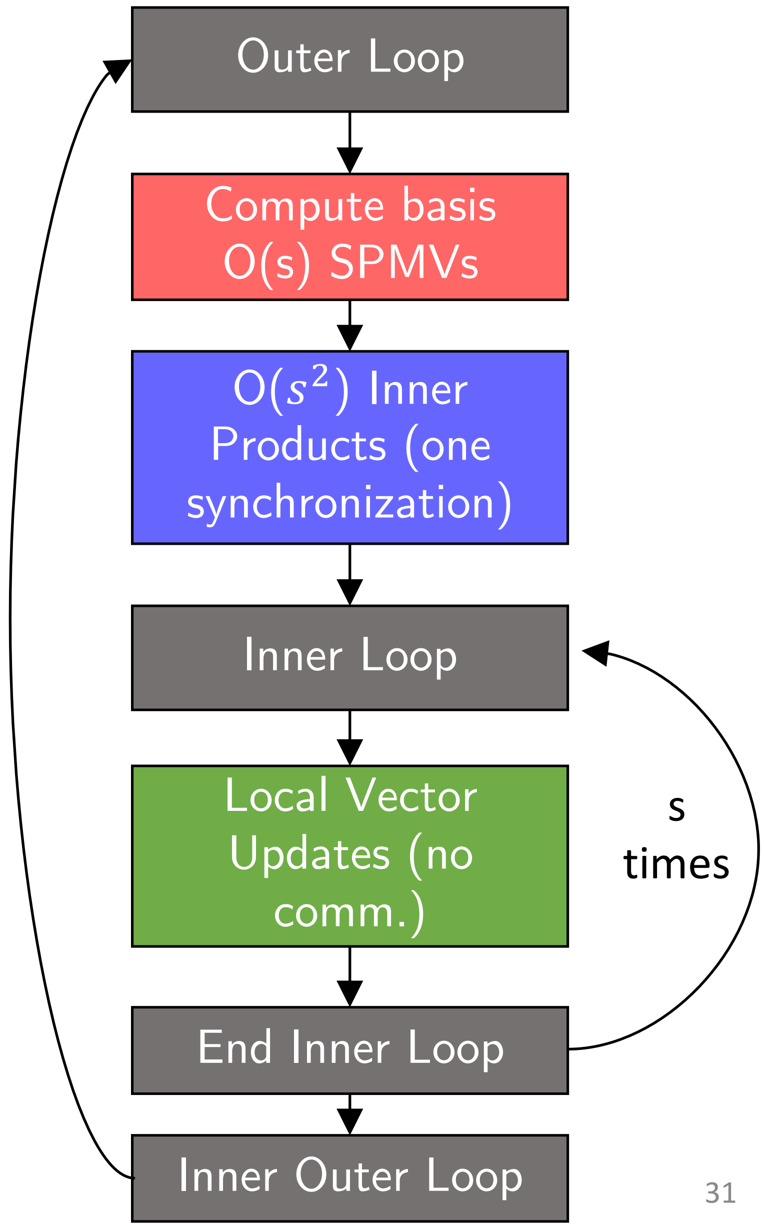

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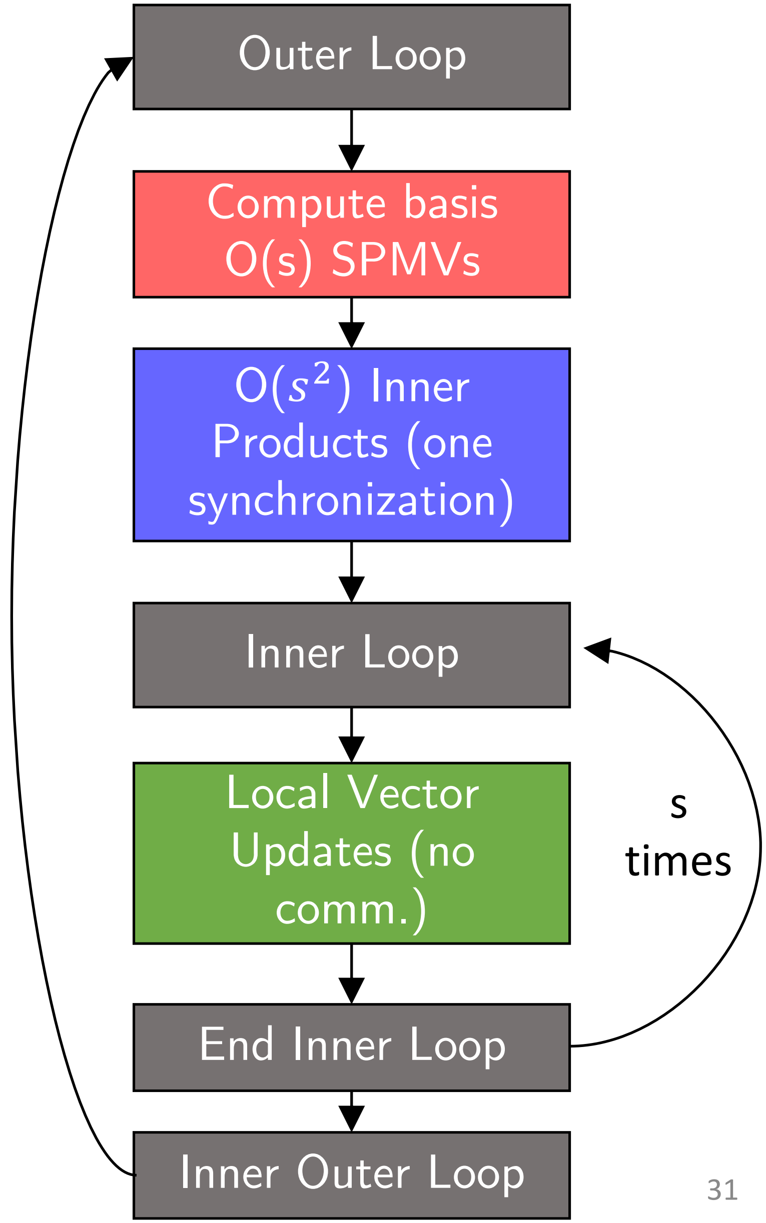

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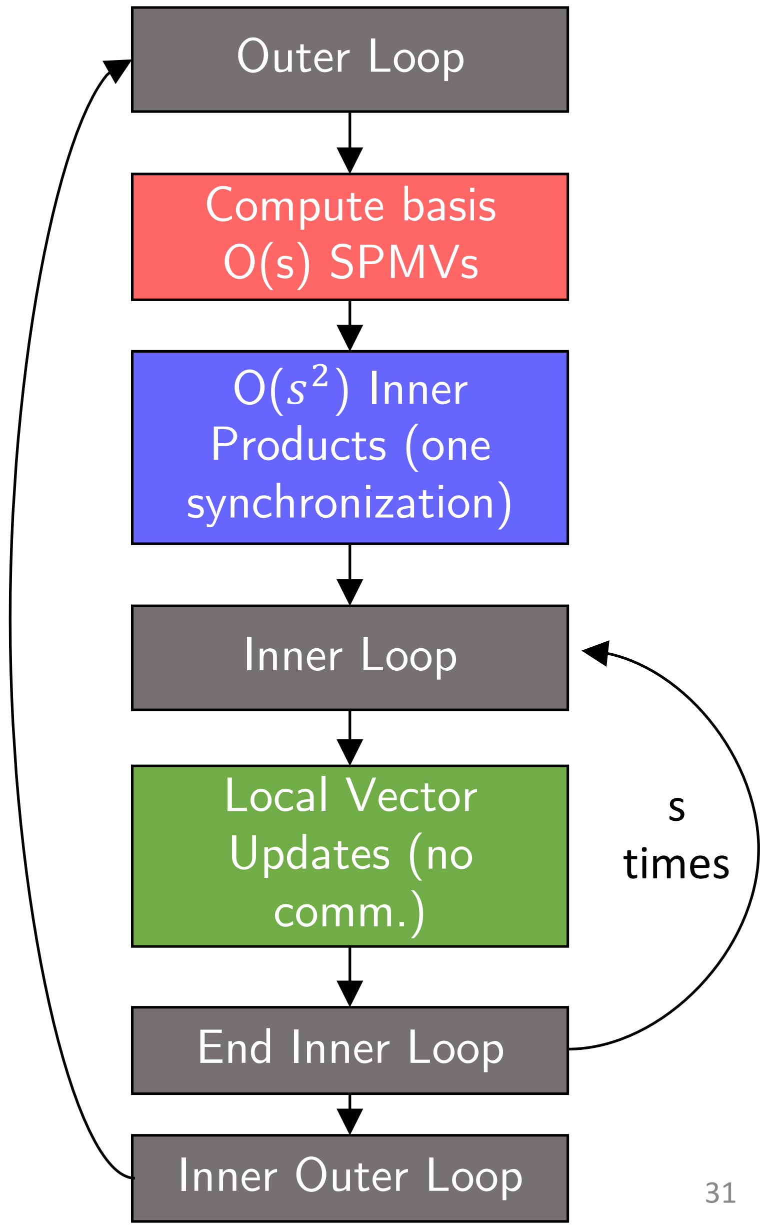

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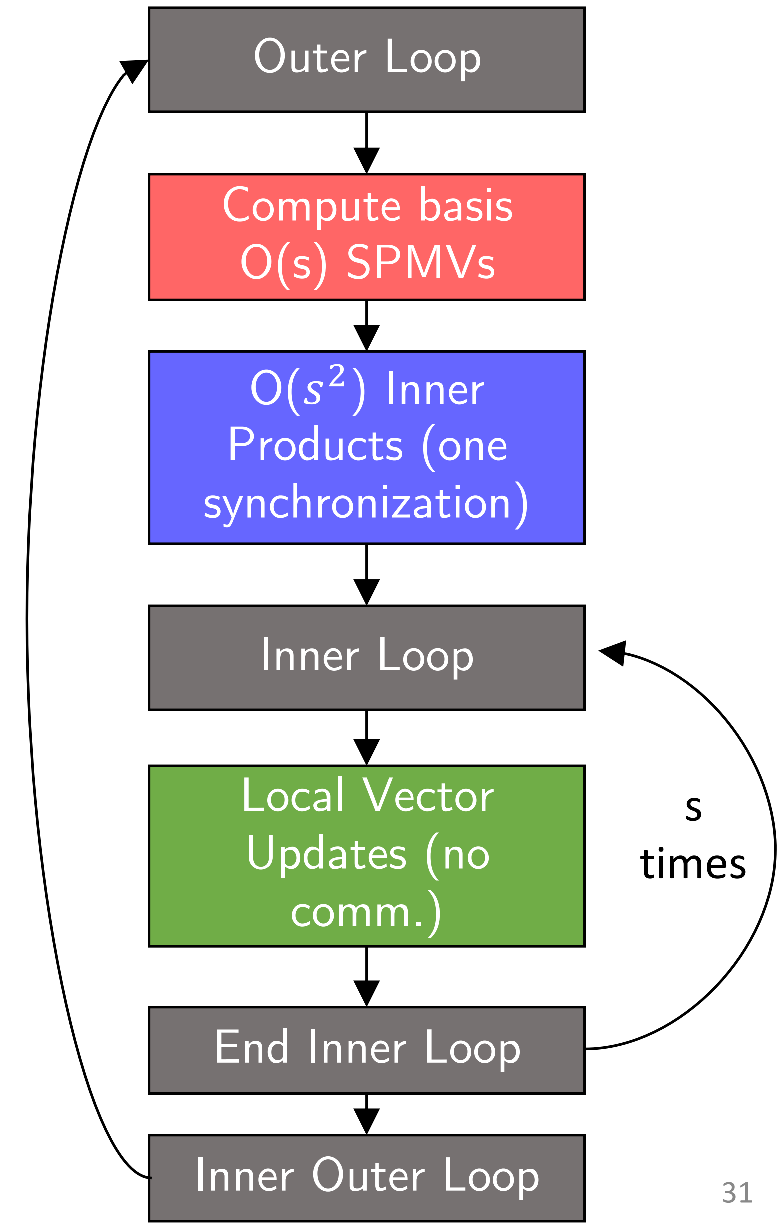

Sources of local roundoff error in s-step CG

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:

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

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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:

$$f_{sk+j} = f_0$$
$$-\sum_{\ell=0}^{k-1}\left[A\phi_{s\ell+s} + \psi_{s\ell+s} + \sum_{i=1}^{s}\left[A\hat{\mathcal{Y}}_\ell \xi_{\ell,i} + \hat{\mathcal{Y}}_\ell \eta_{\ell,i} - \Delta\mathcal{Y}_\ell \hat{q}'_{\ell,i-1}\right]\right]$$
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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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$$
\begin{aligned}
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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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$f_i \equiv b - A\hat{x}_i - \hat{r}_i$

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: $i \equiv sk + j$

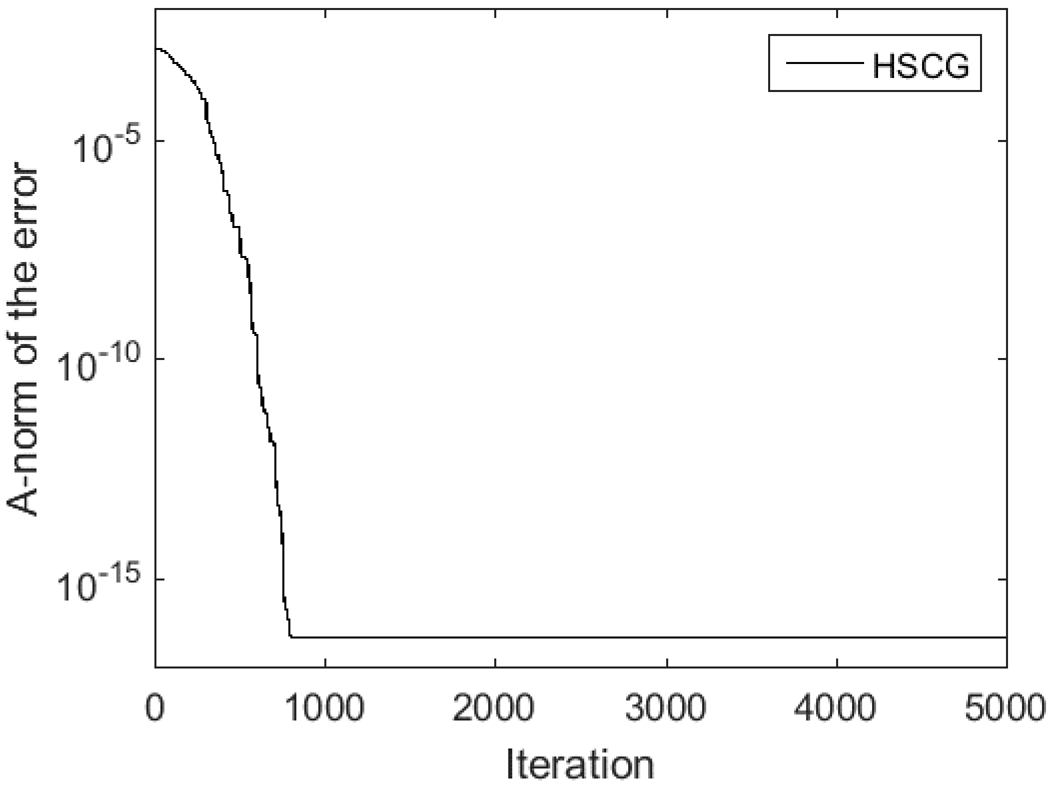
$$\|f_{sk+j}\| \leq \|f_0\| + \varepsilon \boldsymbol{c}\boldsymbol{\bar{\Gamma}_k} \sum_{m=1}^{sk+j} (1+N)\|A\|\|\hat{x}_m\| + \|\hat{r}_m\|$$

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)

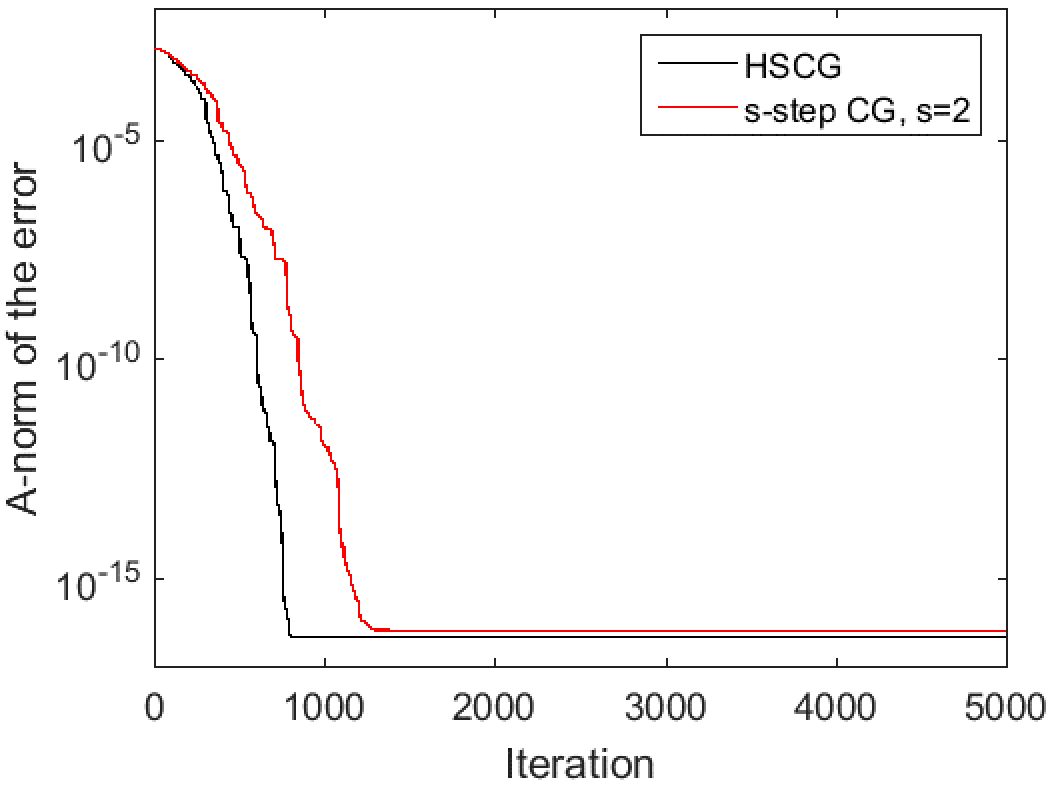
s-step CG



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

s-step CG

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



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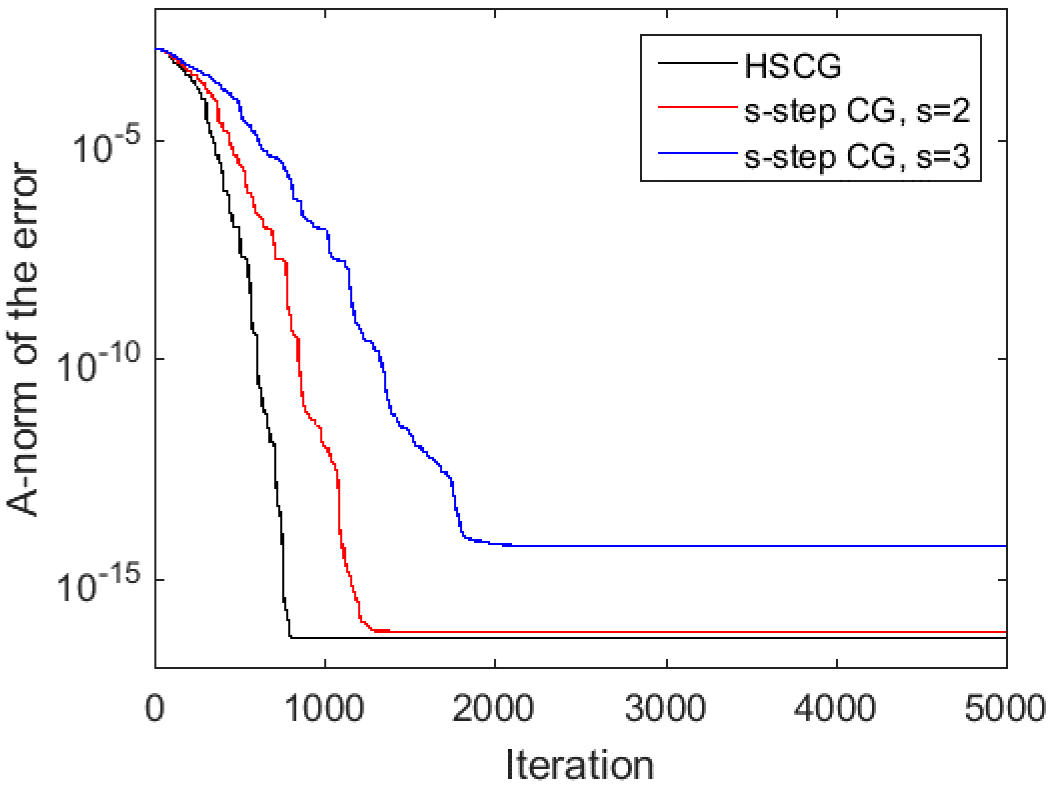

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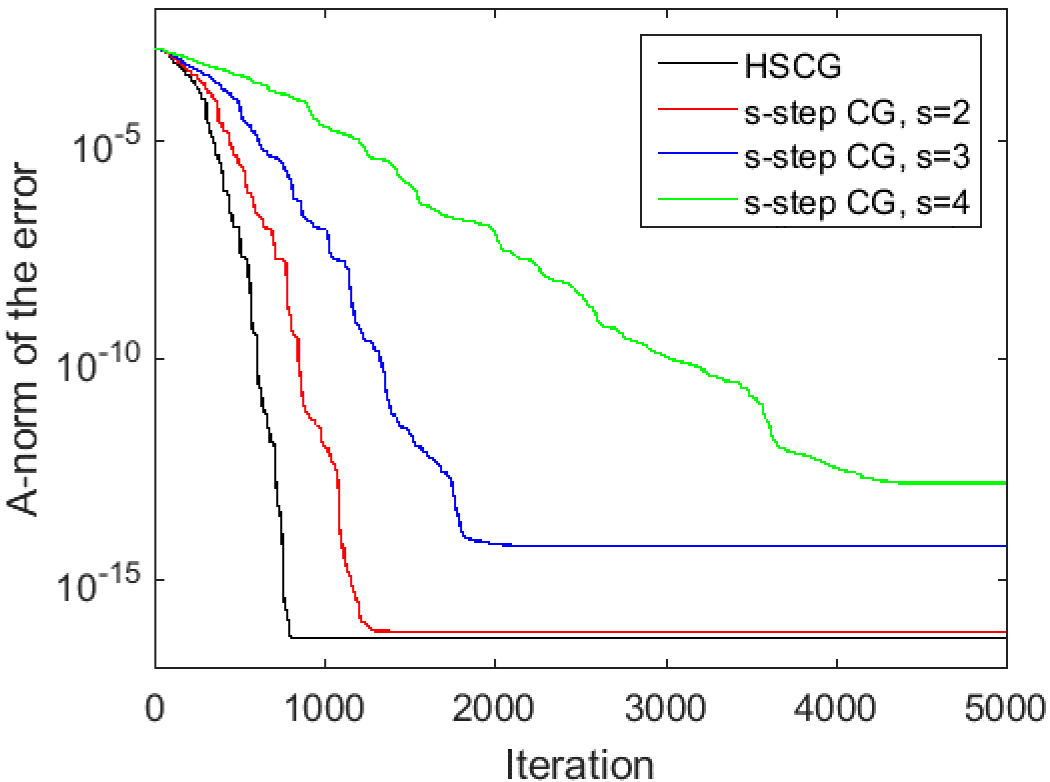
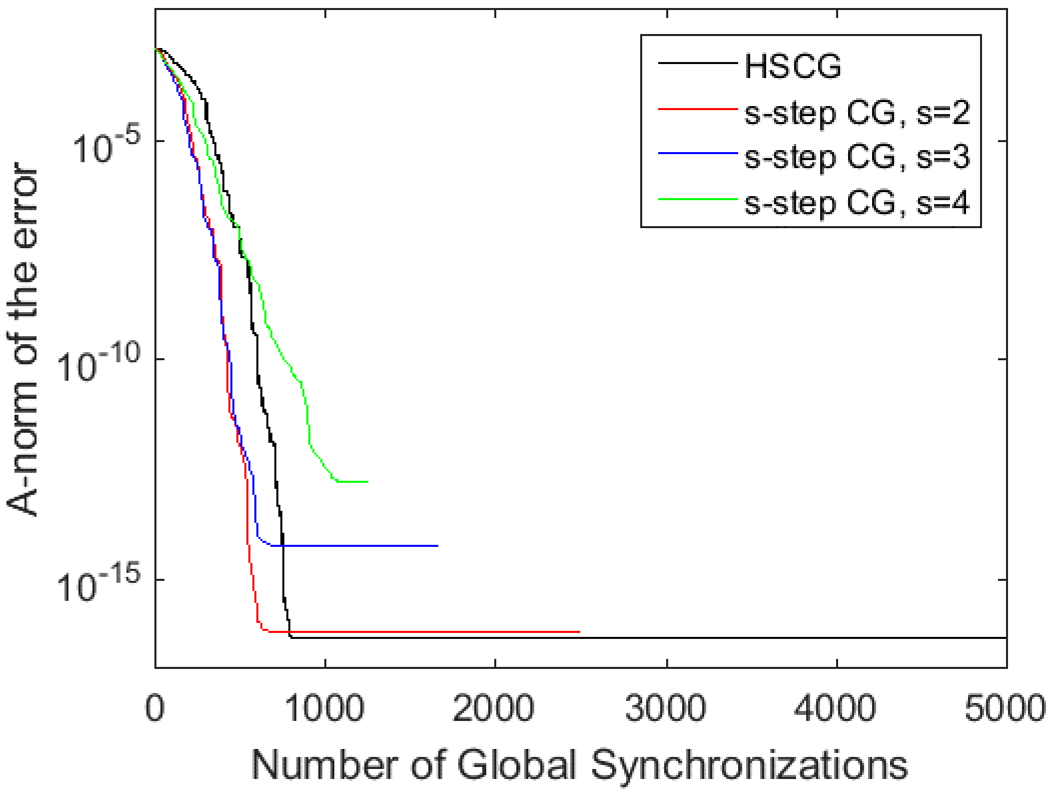


Can also use other, more well-conditioned bases to improve convergence rate and accuracy (see, e.g. Philippe and Reichel, 2012).

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!

A different problem...

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

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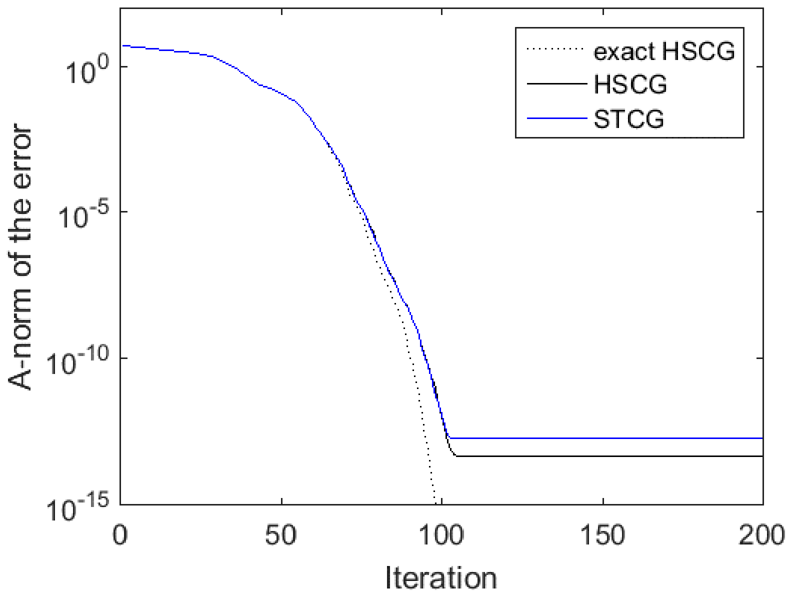

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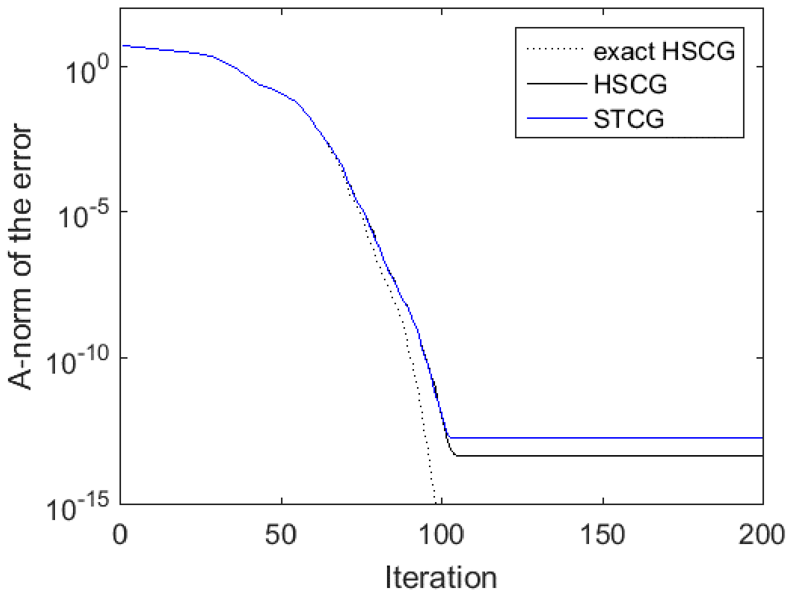

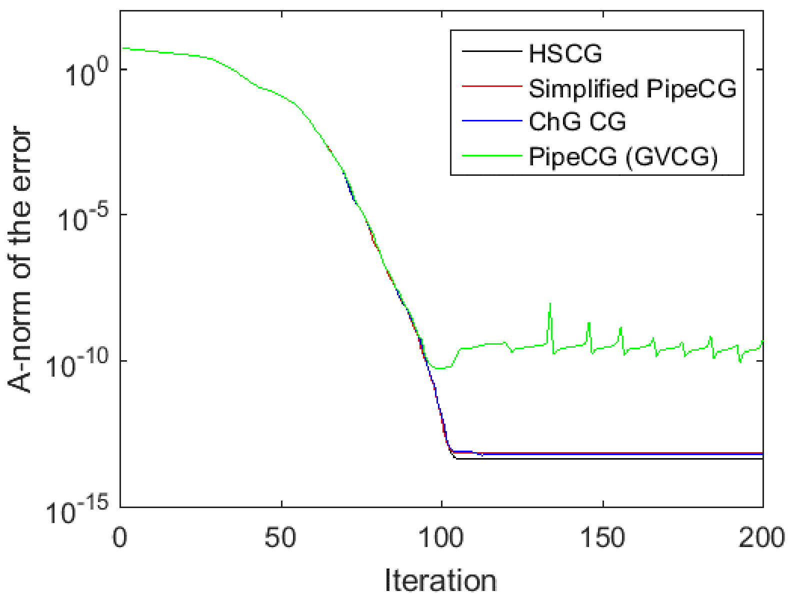

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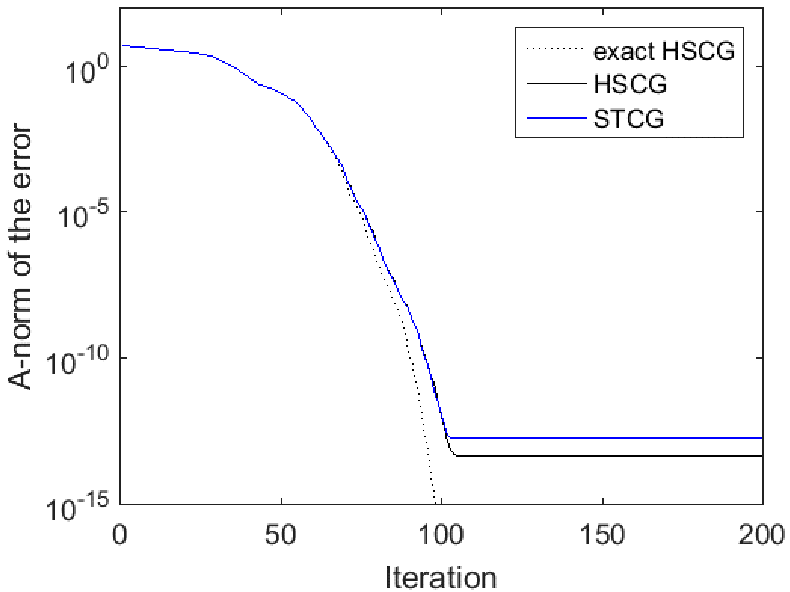

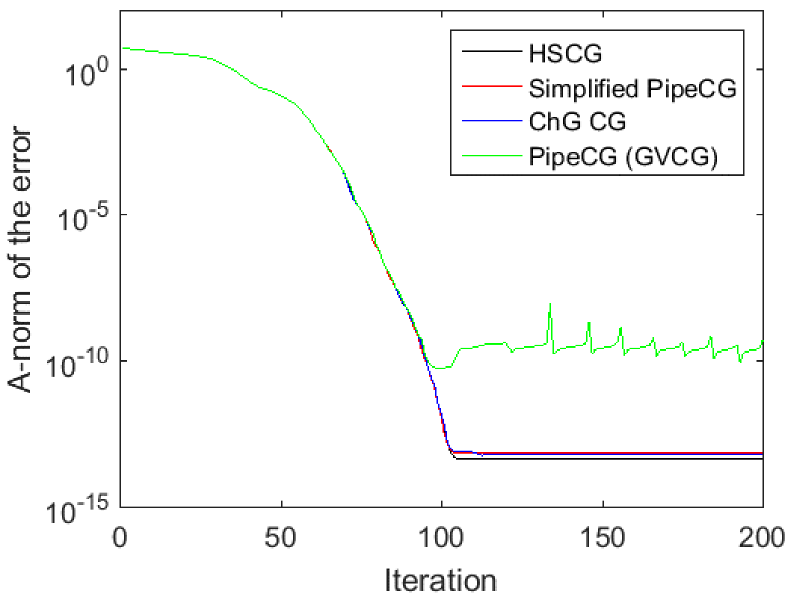

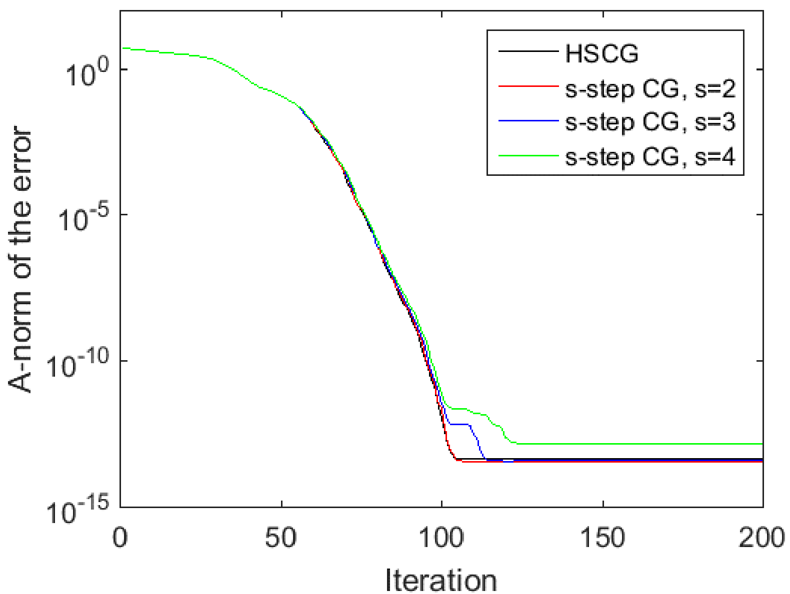

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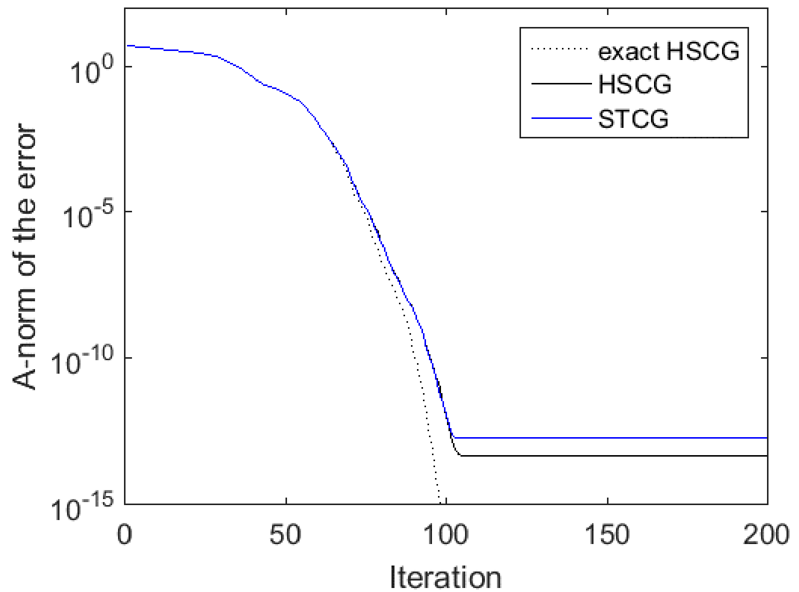
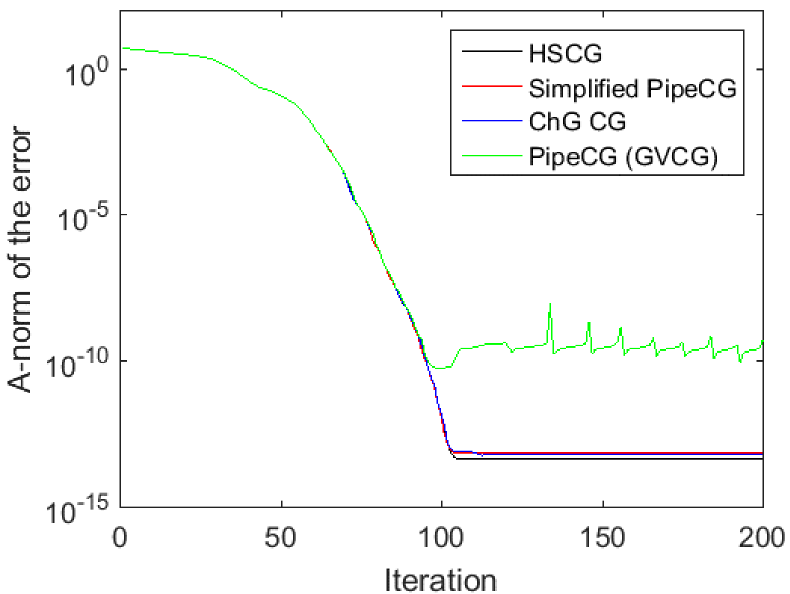
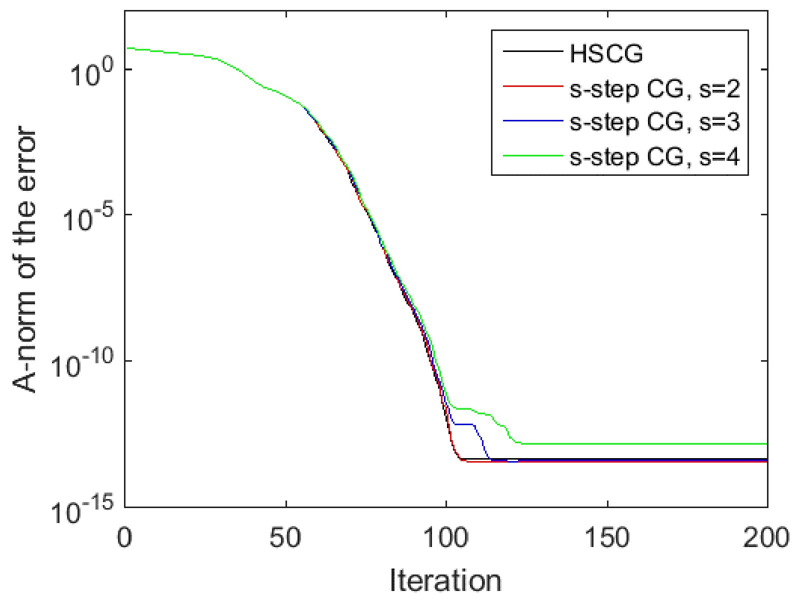
If application only requires $\|x - x_i\|_A \leq 10^{-10}$, any of these methods will work!





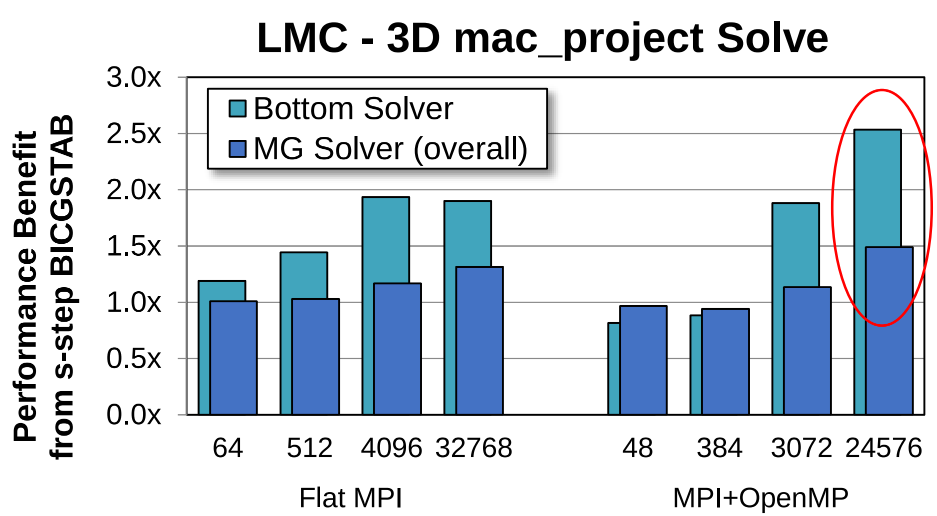


Speedups for real applications

- s-step BICGSTAB bottom-solver implemented in BoxLib (AMR framework from LBL)

Low Mach Number Combustion Code (LMC): gas-phase combustion simulation

- Compared GMG with BICGSTAB vs. GMG with s-step BICGSTAB (s=4) on a Cray XE6 for two different applications
- Up to 2.5x speedup in bottom solve; up to 1.5x in overall MG solve



(see Williams et al., IPDPS 2014)

Conclusions and takeaways

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  - Much focus on modifying methods to speed up iterations
  - But the speed of an iteration only part of the runtime:

runtime = (time/iteration) x (#iterations)

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- Key challenge: identify problems (or classes of problems) for which synchronization-reducing Krylov subspace methods can reduce runtime while meeting application-specific accuracy constraints

⇒ Requires understanding the effects of finite precision computations on convergence rate and accuracy

Thank You!

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