



# Analyzing and Improving Attainable Accuracy for the Communication Hiding Pipelined Conjugate Gradient Method

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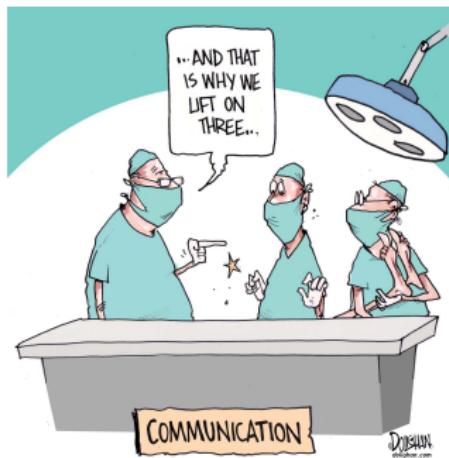
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# Motivation

## Communication is hard for humans

Introducing some buzzwords you will frequently hear during this talk ...



*"synchronization bottleneck"*

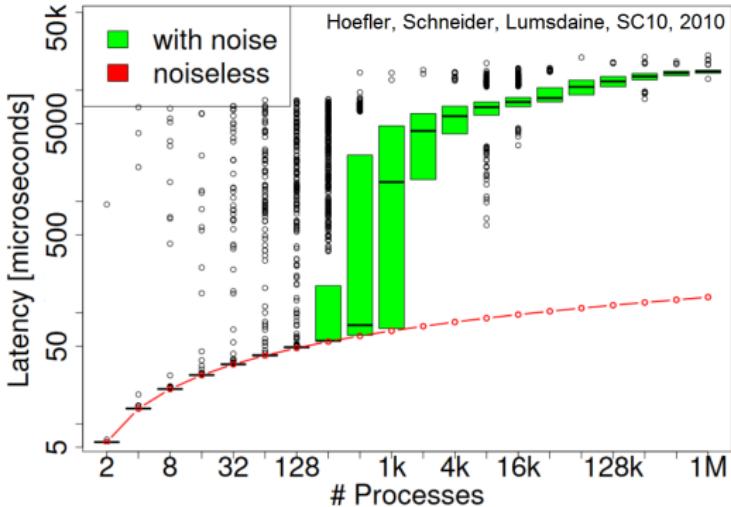
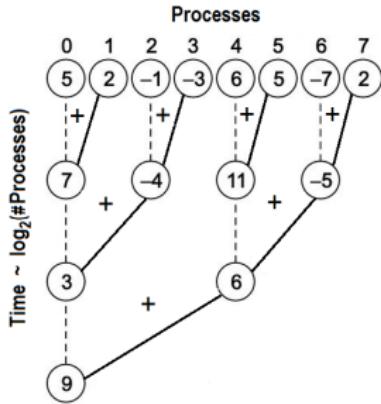
*"communication latency" / "error propagation"*



## Motivation

# Communication is hard for computers

Global reduction using tree-structured sum



Data movement (communication) is much more time consuming than flops (computations), so reducing time spent communicating data is essential for HPC

⇒ Communication avoiding / Communication hiding



## Krylov subspace methods Communication reducing methods

High communication cost has motivated several approaches to reducing the global synchronization bottleneck in Krylov subspace methods:

### Avoiding communication: *s*-step Krylov subspace methods \*

[A. Chronopoulos, E. de Sturler, J. Demmel, M. Hoemmen, E. Carson, L. Grigori, J. Erhel, ...]

- Compute iterations in blocks of  $s$ , allows use of matrix power kernels
- Reduces number of synchronizations per iteration by a factor of  $\mathcal{O}(s)$

### Hiding communication: Pipelined Krylov subspace methods \*

[P. Ghysels, W. Vanroose, S. C., P. Sanan, B. Gropp, I. Yamazaki, P. Luszczek, ...]

- Introduce auxiliary (basis) vectors to decouple SpMV and inner products
- Enables overlapping of communication and computations

\* All methods are equivalent to their corresponding Krylov subspace methods in exact arithmetic



Iteratively improve an approximate solution of the linear system  $Ax = b$ , with

$$x_i \in x_0 + \mathcal{K}_i(A, r_0) = x_0 + \text{span}\{r_0, Ar_0, A^2r_0, \dots, A^{i-1}r_0\}, \quad r_i = b - Ax_i.$$

- ▶ minimize certain error measure over Krylov subspace  $\mathcal{K}_i(A, r_0)$

- ▶ Krylov subspace methods:

**Conjugate Gradients (CG),**  
Lanczos, GMRES, MinRES,  
BiCG, BiCGStab, CGLS, ...

- ▶ Preconditioners:

AMG & GMG, Domain  
Decomposition Methods, FETI,  
BDDC, Incomplete factorization,  
Physics based preconditioners, ...



## Krylov subspace methods General concepts

Iteratively improve an approximate solution of the linear system  $Ax = b$ , with

$$x_i \in x_0 + \mathcal{K}_i(A, r_0) = x_0 + \text{span}\{r_0, Ar_0, A^2r_0, \dots, A^{i-1}r_0\}, \quad r_i = b - Ax_i.$$

- ▶ minimize certain error measure over Krylov subspace  $\mathcal{K}_i(A, r_0)$
- ▶ Krylov subspace methods:  
**Conjugate Gradients (CG),**  
Lanczos, GMRES, MinRES,  
BiCG, BiCGStab, CGLS, ...
- ▶ Preconditioners:  
AMG & GMG, Domain Decomposition Methods, FETI,  
BDDC, Incomplete factorization,  
Physics based preconditioners, ...
- ▶ usually in combination with sparse linear algebra/stencil application
- ▶ three algorithmic building blocks:
  - i. **dot-product**
    - $\mathcal{O}(N)$  flops
    - global synchronization (MPI\_Allreduce)
  - ii. **SpMV**
    - $\mathcal{O}(\text{nnz})$  flops
    - neighbor communication only
  - iii. **axpy**
    - $\mathcal{O}(N)$  flops
    - no communication



# Krylov subspace methods

## Classic Conjugate Gradients (CG)

Algorithm CG

```
1: procedure CG( $A, b, x_0$ )
2:    $r_0 := b - Ax_0; p_0 = r_0$ 
3:   for  $i = 0, \dots$  do
4:      $s_i := Ap_i$                                 dot-pr
5:      $\alpha_i := (r_i, r_i) / (s_i, p_i)$           SpMV
6:      $x_{i+1} := x_i + \alpha_i p_i$             axpy
7:      $r_{i+1} := r_i - \alpha_i s_i$ 
8:      $\beta_{i+1} := (r_{i+1}, r_{i+1}) / (r_i, r_i)$ 
9:      $p_{i+1} := r_{i+1} + \beta_{i+1} p_i$ 
10:    end for
11:  end procedure
```

✉ Hestenes & Stiefel (1952)

### i. dot-products

- ▶ 2 global reductions: latency dominated
- ▶ time scales as  $\log_2(\#partitions)$

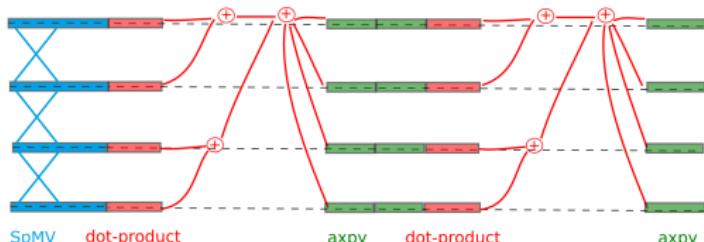
### ii. SpMV

- ▶ computationally expensive
- ▶ good scaling (minor communication)

### iii. axpy's

- ▶ vector operations (recurrences)
- ▶ perfect scaling (no communication)

Essentially sequential operations (line-per-line execution)





# Krylov subspace methods

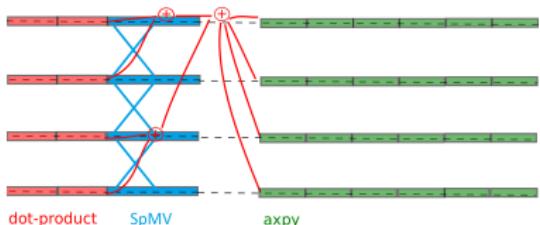
## Pipelined Conjugate Gradients

### Algorithm Pipelined CG

```
1: procedure PIPE-CG( $A, b, x_0$ )
2:    $r_0 := b - Ax_0; w_0 := Ar_0$ 
3:   for  $i = 0, \dots$  do
4:      $\gamma_i := (r_i, r_i)$ 
5:      $\delta := (w_i, r_i)$ 
6:      $q_i := Aw_i$ 
7:     if  $i > 0$  then
8:        $\beta_i := \gamma_i / \gamma_{i-1}; \alpha_i := (\delta / \gamma_i - \beta_i / \alpha_{i-1})^{-1}$ 
9:     else
10:       $\beta_i := 0; \alpha := \gamma_i / \delta$ 
11:    end if
12:     $z_i := q_i + \beta_i z_{i-1}$ 
13:     $s_i := w_i + \beta_i s_{i-1}$ 
14:     $p_i := r_i + \beta_i p_{i-1}$ 
15:     $x_{i+1} := x_i + \alpha_i p_i$ 
16:     $r_{i+1} := r_i - \alpha_i s_i$ 
17:     $w_{i+1} := w_i - \alpha_i z_i$ 
18:  end for
19: end procedure
```

dot-pr  
SpMV  
axpy

- i. **Communication avoiding:** dot-products grouped in one global reduction phase per iteration
- ii. **Communication hiding:** overlap global synchronization with SpMV (+ Prec) computation
- iii. **No free lunch:** Additional recurrence relations (axpy's) for the auxiliary vectors  $s_i = Ap_i$ ,  $w_i = Ar_i$ ,  $z_i = As_i$

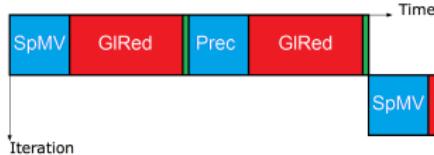


■ Ghysels & Vanroose (2014)

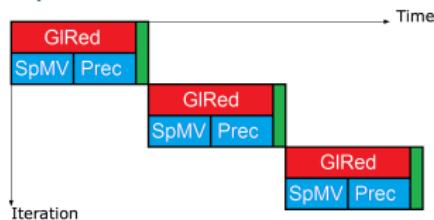


# Krylov subspace methods Deep $\ell$ -length pipelined CG

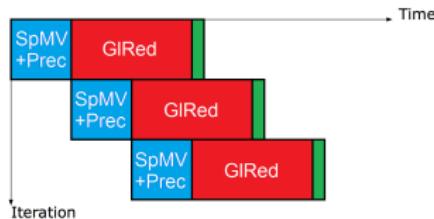
## Classic KSM:



## Pipelined KSM:



## Deep pipelined KSM:

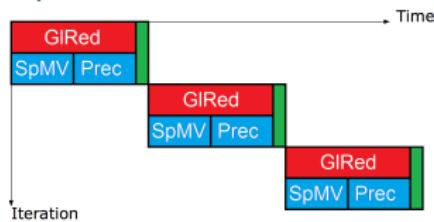




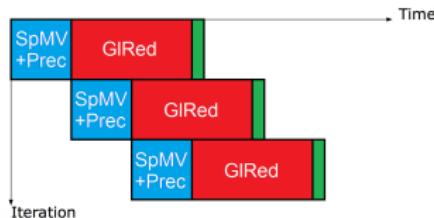
## Classic KSM:



## Pipelined KSM:



## Deep pipelined KSM:



## Krylov subspace methods Deep $\ell$ -length pipelined CG

### Pipelined “D-Lanczos”

✉ Saad (2003)

Consider the Lanczos relation

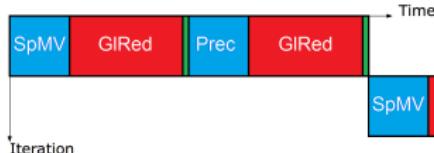
$$AV_i = V_{i+1} T_{i+1,i}$$

with  $A$  symmetric,  $V_{i+1} = [v_0, v_1, \dots, v_i]$  the Krylov subspace basis and  $T_{i+1,i}$  a symmetric tridiagonal matrix

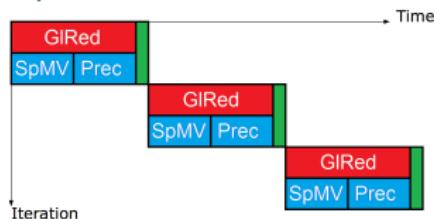
$$T_{i+1,i} = \begin{pmatrix} \gamma_0 & \delta_0 & & \\ \delta_0 & \gamma_1 & \ddots & \\ \ddots & \ddots & \ddots & \delta_{i-2} \\ & & \delta_{i-2} & \gamma_{i-1} \\ & & & \delta_{i-1} \end{pmatrix}.$$



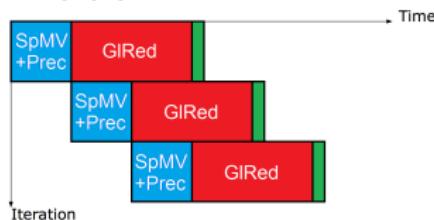
## Classic KSM:



## Pipelined KSM:



## Deep pipelined KSM:



## Krylov subspace methods Deep $\ell$ -length pipelined CG

### Pipelined “D-Lanczos”

Saad (2003)

Introduce the auxiliary Krylov subspace basis  $Z_{i+1} = [z_0, z_1, \dots, z_i]$  that **runs / SpMVs ahead** of the basis  $V_{i-l+1}$  as

$$z_i := \begin{cases} v_0 & j = 0, \\ P_i(A)v_0 & 0 < i \leq l, \\ P_i(A)v_{i-l} & i > l, \end{cases}$$

with polynomials  $P_l(t)$  of fixed order  $l$

$$P_l(t) := \prod_{j=0}^{l-1} (t - \sigma_j),$$

where  $l$  is the pipeline length.

Ghysels et al. (2013)



- ▶ Applying  $P_l(A)$  to  $AV_i = V_{i+1}T_{i+1,i}$  yields a Lanczos-type relation

$$AZ_i = Z_{i+1}B_{i+1,i}$$

with  $B_{i+1,i}$  shifted tridiagonal matrix.

- ▶ Auxiliary basis vectors are computed using a three-term recurrence relation

$$z_{i+1} = (\underbrace{Az_i - \gamma_{i-1}z_i - \delta_{i-1}z_{i-1}}_{\text{SpMV}}) / \delta_{i-1}$$



## Krylov subspace methods Deep $\ell$ -length pipelined CG

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- ▶ Basis transformation.  $Z_i$  and  $V_i$  both span  $i$ -th Krylov subspace, thus  $\exists$  an upper triangular basis transformation matrix  $G_i$  with

$$Z_i = V_i G_i.$$

- ▶ Band structure of  $G_i$ . Matrix  $G_i$  has only  $2l + 1$  nonzero diagonals

$$\begin{aligned} g_{j,i} &= (z_i, v_j) = (P_l(A)v_{i-l}, v_j) \\ &= (v_{i-l}, P_l(A)v_j) = g_{i-l,j+l}. \end{aligned}$$



## Krylov subspace methods Deep $\ell$ -length pipelined CG

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- ▶ Band structure of  $G_i$ . Matrix  $G_i$  has only  $2l + 1$  nonzero diagonals

$$\begin{aligned} g_{j,i} &= (z_i, v_j) = (P_l(A)v_{i-1}, v_j) \\ &= (v_{i-1}, P_l(A)v_j) = g_{i-1,j+l}. \end{aligned}$$

- ▶ Original basis vectors are computed using a multi-term recurrence relation

$$v_{i-l+1} = \left( z_{i-l+1} - \sum_{j=i-3l+1}^{i-l} g_{j,i-l+1} v_j \right) / g_{i-l+1,i-l+1}.$$



# Krylov subspace methods

## Deep $\ell$ -length pipelined CG

**Algorithm 1**  $\ell$ -length pipelined p( $\ell$ )-CG

**Input:**  $A, b, x_0, l, m, \tau$

```
1:  $r_0 := b - Ax_0; v_0 := r_0/\|r_0\|_2; z_0 := v_0; g_{0,0} := 1;$ 
2: for  $i = 0, \dots, m + l$  do
3:    $z_{i+1} := \begin{cases} (A - \sigma_i I)z_i, & i < l \\ Az_i, & i \geq l \end{cases}$ 
4:   if  $i \geq l$  then
5:      $g_{j,i-l+1} := (g_{j,i-l+1} - \sum_{k=i-3l+1}^{j-1} g_{k,j}g_{k,i-l+1})/g_{j,j}; \quad j = i-2l+2, \dots, i-l$ 
6:      $g_{i-l+1,i-l+1} := \sqrt{g_{i-l+1,i-l+1} - \sum_{k=i-3l+1}^{i-l} g_{k,i-l+1}^2};$ 
7:     # Check for breakdown and restart if required
8:     if  $i < 2l$  then
9:        $\gamma_{i-l} := (g_{i-l,i-l+1} + \sigma_{i-l}g_{i-l,i-l} - g_{i-l-1,i-l}\delta_{i-l-1})/g_{i-l,i-l};$ 
10:       $\delta_{i-l} := g_{i-l+1,i-l+1}/g_{i-l,i-l};$ 
11:    else
12:       $\gamma_{i-l} := (g_{i-l,i-l}\gamma_{i-2l} + g_{i-l,i-l+1}\delta_{i-2l} - g_{i-l-1,i-l}\delta_{i-l-1})/g_{i-l,i-l};$ 
13:       $\delta_{i-l} := (g_{i-l+1,i-l+1}\delta_{i-2l})/g_{i-l,i-l};$ 
14:    end if
15:     $v_{i-l+1} := (z_{i-l+1} - \sum_{j=i-3l+1}^{i-l} g_{j,i-l+1}v_j)/g_{i-l+1,i-l+1};$ 
16:     $z_{i+1} := (z_{i+1} - \gamma_{i-l}z_i - \delta_{i-l-1}z_{i-1})/\delta_{i-l};$ 
17:  end if
18:   $g_{j,i+1} := \begin{cases} (z_{i+1}, v_j); & j = \max(0, i-2l+1), \dots, i-l+1 \\ (z_{i+1}, z_j); & j = i-l+2, \dots, i+1 \end{cases}$ 
19:  if  $i = l$  then
20:     $\eta_0 := \gamma_0; \quad \zeta_0 := \|r_0\|_2; \quad p_0 := v_0/\eta_0;$ 
21:  else if  $i \geq l+1$  then
22:     $\lambda_{i-l} := \delta_{i-l-1}/\eta_{i-l-1};$ 
23:     $\eta_{i-l} := \gamma_{i-l} - \lambda_{i-l}\delta_{i-l-1};$ 
24:     $\zeta_{i-l} = -\lambda_{i-l}\zeta_{i-l-1};$ 
25:     $p_{i-l} = (v_{i-l} - \delta_{i-l-1}p_{i-l-1})/\eta_{i-l};$ 
26:     $x_{i-l} = x_{i-l-1} + \zeta_{i-l-1}p_{i-l-1};$ 
27:    if  $|\zeta_{i-l}|/\|r_0\| < \tau$  then RETURN; end if
28:  end if
29: end for
```



# Krylov subspace methods Deep $\ell$ -length pipelined CG

## Algorithm 1 $\ell$ -length pipelined p( $\ell$ )-CG

```

1:  $r_0 := b - Ax_0; v_0 := r_0/\|r_0\|_2; z_0 := v_0; g_{0,0} := 1;$ 
2: for  $i = 0, \dots, m + l$  do
3:    $z_{i+1} := \begin{cases} (A - \sigma_i I)z_i, & i < l \\ Az_i, & i \geq l \end{cases}$  ←
4:   if  $i \geq l$  then
5:      $g_{j,i-l+1} := (g_{j,i-l+1} - \sum_{k=i-3l+1}^{j-1} g_{k,j}g_{k,i-l+1})/g_{j,j}; \quad j = i-2l+2, \dots, i$ 
6:      $g_{i-l+1,i-l+1} := \sqrt{g_{i-l+1,i-l+1} - \sum_{k=i-3l+1}^{i-l} g_{k,i-l+1}^2};$ 
7:     # Check for breakdown and restart if required
8:     if  $i < 2l$  then
9:        $\gamma_{i-l} := (g_{i-l,i-l+1} + \sigma_{i-l}g_{i-l,i-l} - g_{i-l-1,i-l}\delta_{i-l-1})/g_{i-l,i-l};$ 
10:       $\delta_{i-l} := g_{i-l+1,i-l+1}/g_{i-l,i-l};$ 
11:    else
12:       $\gamma_{i-l} := (g_{i-l,i-l}\gamma_{i-2l} + g_{i-l,i-l+1}\delta_{i-2l} - g_{i-l-1,i-l}\delta_{i-l-1})/g_{i-l,i-l};$ 
13:       $\delta_{i-l} := (g_{i-l+1,i-l+1}\delta_{i-2l})/g_{i-l,i-l};$ 
14:    end if
15:     $v_{i-l+1} := (z_{i-l+1} - \sum_{j=i-3l+1}^{i-l} g_{j,i-l+1}v_j)/g_{i-l+1,i-l+1};$ 
16:     $z_{i+1} := (z_{i+1} - \gamma_{i-l}z_i - \delta_{i-l-1}z_{i-1})/\delta_{i-l};$ 
17:  end if
18:   $g_{j,i+1} := \begin{cases} (z_{i+1}, v_j); & j = \max(0, i-2l+1), \dots, i-l+1 \\ (z_{i+1}, z_j); & j = i-l+2, \dots, i+1 \end{cases}$  ←
19:  if  $i = l$  then
20:     $\eta_0 := \gamma_0; \quad \zeta_0 := \|r_0\|_2; \quad p_0 := v_0/\eta_0;$ 
21:    else if  $i \geq l + 1$  then
22:       $\lambda_{i-l} := \delta_{i-l-1}/\eta_{i-l-1};$ 
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27:      if  $|\zeta_{i-l}|/\|r_0\| < \tau$  then RETURN; end if
28:    end if
29:  end for

```

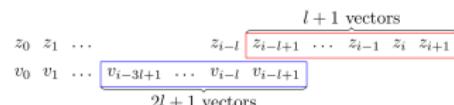
**Input:**  $A, b, x_0, l, m, \tau$

## SpMV (+ preconditioner)

- 1 SpMV on  $z_i$  per iteration

## Recurrence relations for $V_{i-l+1}$ and $Z_{i+1}$ basis vectors

- computation:  $2l + 2$  axpy's
- storage:  $3l + 2$  basis vectors



## Dot-products

- $2l + 1$  band structure of  $G_i$
- one global reduction phase is initiated per iteration



# Krylov subspace methods

## Deep $\ell$ -length pipelined CG

**Algorithm 1**  $l$ -length pipelined p( $l$ )-CG

```

1:  $r_0 := b - Ax_0; v_0 := r_0/\|r_0\|_2; z_0 := v_0; g_{0,0} := 1;$ 
2: for  $i = 0, \dots, m + l$  do
3:    $z_{i+1} := \begin{cases} (A - \sigma_i I)z_i, & i < l \\ Az_i, & i \geq l \end{cases}$ 
4:   if  $i \geq l$  then
5:      $g_{j,i-l+1} := (g_{j,i-l+1} - \sum_{k=i-3l+1}^{j-1} g_{k,j}g_{k,i-l+1})/g_{j,j}; \quad j = i - 2l + 2, \dots, i$ 
6:      $g_{i-l+1,i-l+1} := \sqrt{g_{i-l+1,i-l+1} - \sum_{k=i-3l+1}^{i-l} g_{k,i-l+1}^2};$ 
7:     # Check for breakdown and restart if required
8:     if  $i < 2l$  then
9:        $\gamma_{i-l} := (g_{i-l,i-l+1} + \sigma_{i-l}g_{i-l,i-l} - g_{i-l-1,i-l}\delta_{i-l-1})/g_{i-l,i-l};$ 
10:       $\delta_{i-l} := g_{i-l+1,i-l+1}/$ 
11:    else
12:       $\gamma_{i-l} := (g_{i-l,i-l}\gamma_{i-2} + \delta_{i-l})/g_{i-l+1,i-l+1}$ 
13:       $\delta_{i-l} := g_{i-l+1,i-l+1}/$ 
14:    end if
15:     $v_{i-l+1} := (z_{i-l+1} - \sum_j^i v_j);$ 
16:     $z_{i+1} := (z_{i+1} - \gamma_{i-l}z_i -$ 
17:    end if
18:     $g_{j,i+1} := \begin{cases} (z_{i+1}, v_j); & j = \\ (z_{i+1}, z_j); & \end{cases}$ 
19:    if  $i = l$  then
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25:         $p_{i-l} = (v_{i-l} - \delta_{i-l-1}p_{i-l-1})/\eta_{i-l};$ 
26:         $x_{i-l} = x_{i-l-1} + \zeta_{i-l-1}p_{i-l-1};$ 
27:        if  $|\zeta_{i-l}|/\|r_0\| < \tau$  then RETURN; end if
28:    end if
29:  end for

```

**Input:**  $A, b, x_0, l, m, \tau$ 
**SpMV (+ preconditioner)**

- 1 SpMV on  $z_i$  per iteration

Recurrence relations for  
 $V_{i-l+1}$  and  $Z_{i+1}$  basis vectors

- computation:  $2l + 2$  axpy's
- storage:  $3l + 2$  basis vectors

$z_0 \ z_1 \ \dots$	$\underbrace{z_{i-l} \ z_{i-l+1} \ \dots \ z_{i-1} \ z_i}_{l+1 \text{ vectors}}$
$v_0 \ v_1 \ \dots$	$\underbrace{v_{i-3l+1} \ \dots \ v_{i-l} \ v_{i-l+1}}_{2l+1 \text{ vectors}}$

Results of global sync.  
are needed  $l$  iterations  
later to update  $G_{:,i-l+1}$

Each global reduction is  
overlapped by  $\ell$  SpMVs

## Dot-products

- $2l + 1$  band structure of  $G_i$
- one global reduction phase  
is initiated per iteration

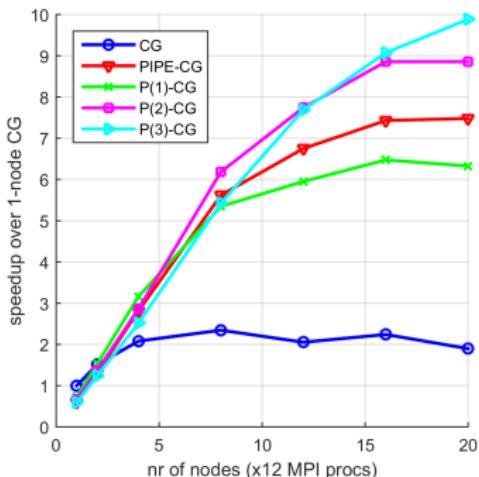


# Krylov subspace methods

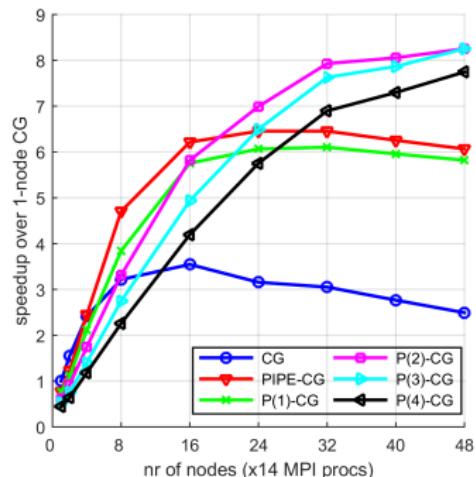
## Parallel performance of pipelined CG

Strong scaling experiments - PETSc 3.6.3/3.7.6 library - MPICH 3.1.3/3.3a2

Per node: Two 6-core Intel Xeon X5660 Nehalem  
2.80 GHz - 2D Poisson (5pt) - 1 million unknowns



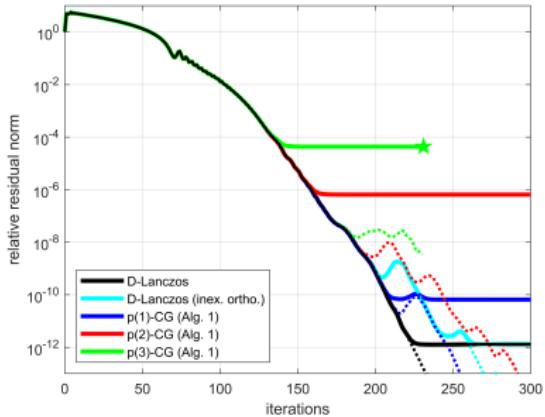
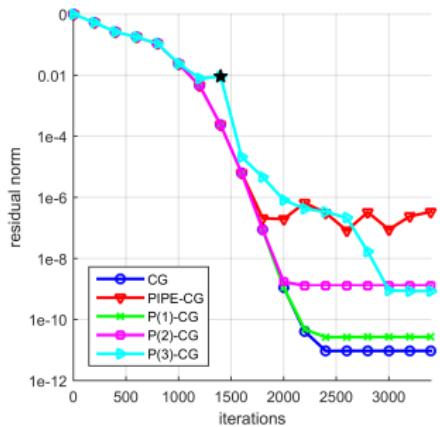
Per node: Two 14-core Intel E5-2680v4 Broadwell  
2.40 GHz - 2D Poisson (5pt) - 3 million unknowns





# Pipelined Conjugate Gradients

## Numerical stability in finite precision

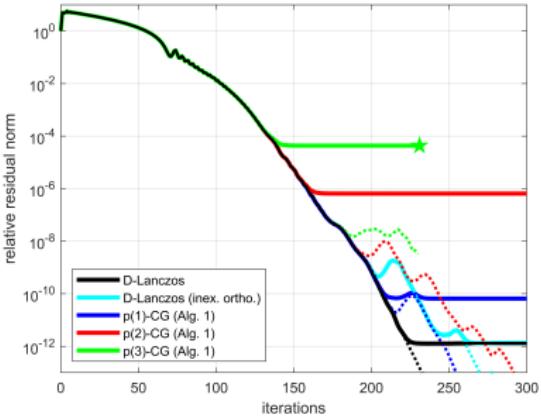
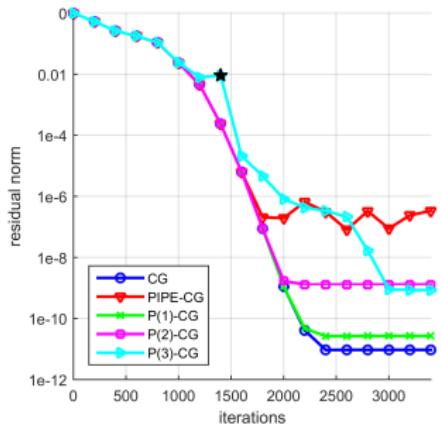


Pipelined CG produces identical iterates to classic CG in exact arithmetic; but ...



# Pipelined Conjugate Gradients

## Numerical stability in finite precision



Pipelined CG produces identical iterates to classic CG in exact arithmetic; but ...

Finite precision computations introduce roundoff errors that may lead to

1. *Delayed convergence* due to loss of basis orthogonality
2. *Loss of attainable accuracy* due to propagation of local rounding errors introduced by the recurrence relations



## Classic Conjugate Gradients Analyzing rounding error behavior in CG

Rounding errors due to **recurrence relations** for residual and solution update:

$$\bar{x}_{i+1} = \bar{x}_i + \bar{\alpha}_i \bar{p}_i + \xi_{i+1}^x, \quad \bar{r}_{i+1} = \bar{r}_i - \bar{\alpha}_i A \bar{p}_i + \xi_{i+1}^r,$$

with  $\xi_{i+1}^x \leq (\|\bar{x}_i\| + 2|\bar{\alpha}_i| \|\bar{p}_i\|) \epsilon$  and  $\xi_{i+1}^r \leq (\|\bar{r}_i\| + \mathcal{O}(\sqrt{n}) |\bar{\alpha}_i| \|A\| \|\bar{p}_i\|) \epsilon$ .



## Classic Conjugate Gradients Analyzing rounding error behavior in CG

Rounding errors due to **recurrence relations** for residual and solution update:

$$\bar{x}_{i+1} = \bar{x}_i + \bar{\alpha}_i \bar{p}_i + \xi_{i+1}^x, \quad \bar{r}_{i+1} = \bar{r}_i - \bar{\alpha}_i A \bar{p}_i + \xi_{i+1}^r,$$

Computed residual  $\bar{r}_i$  deviates from the true residual  $b - A\bar{x}_i$  in finite precision:

$$\begin{aligned} (b - A\bar{x}_{i+1}) - \bar{r}_{i+1} &= b - A(\bar{x}_i + \bar{\alpha}_i \bar{p}_i + \xi_{i+1}^x) - (\bar{r}_i - \bar{\alpha}_i A \bar{p}_i + \xi_{i+1}^r) \\ &= \sum_{k=0}^{i+1} (A\xi_k^x + \xi_k^r). \end{aligned}$$

■ Sleijpen et al. (1995)  
■ Greenbaum (1997)



# Classic Conjugate Gradients

## Analyzing rounding error behavior in CG

Rounding errors due to **recurrence relations** for residual and solution update:

$$\bar{x}_{i+1} = \bar{x}_i + \bar{\alpha}_i \bar{p}_i + \xi_{i+1}^x, \quad \bar{r}_{i+1} = \bar{r}_i - \bar{\alpha}_i A \bar{p}_i + \xi_{i+1}^r,$$

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■ Sleijpen et al. (1995)  
■ Greenbaum (1997)

Matrix notation:  $\bar{R}_{i+1} = [\bar{r}_0, \dots, \bar{r}_i]$ ,  $\bar{X}_{i+1} = [\bar{x}_0, \dots, \bar{x}_i]$ ,  $\Theta_i^x, \Theta_i^r$  rounding errors

$$(B - A\bar{X}_{i+1}) - \bar{R}_{i+1} = (A\Theta_{i+1}^x + \Theta_{i+1}^r) E_{i+1},$$

with  $E_{i+1}$  an upper triangular matrix with **all entries one**.



## Classic Conjugate Gradients Analyzing rounding error behavior in CG

Rounding errors due to **recurrence relations** for residual and solution update:

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with  $E_{i+1}$  an upper triangular matrix with **all entries one**.

*Accumulation of local rounding errors in classic CG, but no amplification.*



## Pipelined Conjugate Gradients Analyzing pipelined CG by Ghysels et al.

Additional recurrence relations in pipelined CG all introduce local rounding errors:

$$\begin{array}{ll} \bar{x}_{i+1} = \bar{x}_i + \bar{\alpha}_i \bar{p}_i + \xi_{i+1}^x, & \bar{s}_i = \bar{w}_i + \bar{\beta}_i \bar{s}_{i-1} + \xi_i^s, \\ \bar{r}_{i+1} = \bar{r}_i - \bar{\alpha}_i \bar{s}_i + \xi_{i+1}^r, & \bar{w}_{i+1} = \bar{w}_i - \bar{\alpha}_i \bar{z}_i + \xi_{i+1}^w, \\ \bar{p}_i = \bar{r}_i + \bar{\beta}_i \bar{p}_{i-1} + \xi_i^p, & \bar{z}_i = A\bar{w}_i + \bar{\beta}_i \bar{z}_{i-1} + \xi_i^z, \end{array}$$



# Pipelined Conjugate Gradients

## Analyzing pipelined CG by Ghysels et al.

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The gap on the residual is coupled to the gaps on the auxiliary variables:

$$\begin{aligned}(B - A\bar{X}_i) - \bar{R}_i &= (A\Theta_i^{\bar{x}} + \Theta_i^{\bar{r}}) E_i + (A\Theta_i^{\bar{p}} + \Theta_i^{\bar{s}}) \bar{\mathcal{B}}_i^{-1} \bar{\mathcal{A}}_i \\ &\quad + (A\Theta_i^{\bar{u}} + \Theta_i^{\bar{w}}) E_i \bar{\mathcal{B}}_i^{-1} \bar{\mathcal{A}}_i + (A\Theta_i^{\bar{q}} + \Theta_i^{\bar{z}}) \bar{\mathcal{B}}_i^{-1} \bar{\mathcal{A}}_i \bar{\mathcal{B}}_i^{-1} \bar{\mathcal{A}}_i\end{aligned}$$



# Pipelined Conjugate Gradients

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with  $\bar{\mathcal{A}}_i = \begin{pmatrix} 0 & \bar{\alpha}_0 & \bar{\alpha}_0 & \cdots & \bar{\alpha}_0 \\ 0 & \bar{\alpha}_1 & \cdots & & \bar{\alpha}_1 \\ \ddots & & \vdots & & \\ & 0 & \bar{\alpha}_{i-2} & & \\ & & 0 & & \end{pmatrix}, \bar{\mathcal{B}}_i^{-1} = \begin{pmatrix} 1 & \bar{\beta}_1 & \bar{\beta}_1 \bar{\beta}_2 & \cdots & \bar{\beta}_1 \bar{\beta}_2 \cdots \bar{\beta}_{i-1} \\ 1 & \bar{\beta}_2 & \ddots & & \bar{\beta}_2 \cdots \bar{\beta}_{i-1} \\ & \ddots & & & \vdots \\ & & 1 & & \bar{\beta}_{i-1} \\ & & & 1 & \end{pmatrix}$

Remark:  $\beta_i \beta_{i+1} \dots \beta_j = \|r_j\|^2 / \|r_{i-1}\|^2$ , so entries of  $\bar{\mathcal{B}}_i^{-1}$  may be arbitrarily large.



# Pipelined Conjugate Gradients Analyzing pipelined CG by Ghysels et al.

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The gap on the residual is coupled to the gaps on the auxiliary variables:

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with  $\bar{\mathcal{A}}_i = \begin{pmatrix} 0 & \bar{\alpha}_0 & \bar{\alpha}_0 & \cdots & \bar{\alpha}_0 \\ 0 & \bar{\alpha}_1 & \cdots & & \bar{\alpha}_1 \\ \ddots & & \vdots & & \\ & 0 & \bar{\alpha}_{i-2} & & \\ & & 0 & & \end{pmatrix}$ ,  $\bar{\mathcal{B}}_i^{-1} = \begin{pmatrix} 1 & \bar{\beta}_1 & \bar{\beta}_1 \bar{\beta}_2 & \cdots & \bar{\beta}_1 \bar{\beta}_2 \cdots \bar{\beta}_{i-1} \\ 1 & \bar{\beta}_2 & \ddots & & \bar{\beta}_2 \cdots \bar{\beta}_{i-1} \\ & \ddots & & & \vdots \\ & & 1 & & \bar{\beta}_{i-1} \\ & & & 1 & \end{pmatrix}$

*Amplification of local rounding errors possible, depending on values  $\bar{\alpha}_i$  and  $\bar{\beta}_i$ .*



## Pipelined Conjugate Gradients Analyzing deep $\ell$ -length pipelined CG

The recurrence relations for  $\bar{x}_i$  and  $\bar{p}_i$  in finite precision  $p(I)$ -CG are

$$\begin{aligned}\bar{x}_i &= \bar{x}_{i-1} + \bar{\zeta}_{i-1} \bar{p}_{i-1} + \xi_i^{\bar{x}} &\Leftrightarrow \quad \bar{x}_i &= \bar{x}_0 + \bar{P}_i \bar{q}_i + \Xi_i^{\bar{x}} \mathbf{1}, \\ \bar{p}_i &= (\bar{v}_i - \bar{\delta}_{i-1} \bar{p}_{i-1}) / \bar{\eta}_i + \xi_i^{\bar{p}} &\Leftrightarrow \quad \bar{V}_i &= \bar{P}_i \bar{U}_i + \Xi_i^{\bar{p}},\end{aligned}$$

with  $\bar{T}_i = \bar{L}_i \bar{U}_i$



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with  $\bar{T}_i = \bar{L}_i \bar{U}_i$ , implying the actual residual equals

$$\begin{aligned}b - A\bar{x}_i &= \bar{r}_0 - A\bar{V}_i \bar{U}_i^{-1} \bar{q}_i + \overbrace{A\Xi_i^{\bar{p}} \bar{U}_i^{-1} \bar{q}_i - A\Xi_i^{\bar{x}} \mathbf{1} + \xi_0^{\bar{r}}}^{\text{Local Rounding Errors (LRE)}} \\ &= \bar{r}_0 - \bar{V}_{i+1} \bar{T}_{i+1,i} \bar{U}_i^{-1} \bar{q}_i - (A\bar{V}_i - \bar{V}_{i+1} \bar{T}_{i+1,i}) \bar{U}_i^{-1} \bar{q}_i + \text{LRE} \\ &= \bar{r}_i - (A\bar{V}_i - \bar{V}_{i+1} \bar{T}_{i+1,i}) \bar{U}_i^{-1} \bar{q}_i + \text{LRE}\end{aligned}$$



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Computed residual  
tends to zero



# Pipelined Conjugate Gradients Analyzing deep $\ell$ -length pipelined CG

The recurrence relations for  $\bar{x}_i$  and  $\bar{p}_i$  in finite precision  $p(I)$ -CG are

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$\downarrow \qquad \downarrow$

Computed residual  
tends to zero

Inexact Lanczos relation ("gap on  $\bar{V}_{i+1}$ ")  
determines maximal attainable accuracy



## Pipelined Conjugate Gradients Analyzing deep $\ell$ -length pipelined CG

Basis vector recurrences in finite precision  $p(l)$ -CG

$$\bar{v}_{i+1} = \left( \bar{z}_{i+1} - \sum_{j=i-2l+1}^i \bar{g}_{j,i+1} \bar{v}_j \right) / \bar{g}_{i+1,i+1} + \xi_{i+1}^{\bar{v}}, \Leftrightarrow \bar{Z}_i = \bar{V}_i \bar{G}_i + \Xi_i^{\bar{v}} \quad (1)$$

$$\bar{z}_{i+1} = (A\bar{z}_i - \bar{\gamma}_{i-l}\bar{z}_i - \bar{\delta}_{i-l-1}\bar{z}_{i-1}) / \bar{\delta}_{i-l} + \xi_{i+1}^{\bar{z}}, \Leftrightarrow A\bar{Z}_i = \bar{Z}_{i+1} \bar{B}_{i+1,i} + \Xi_i^{\bar{z}} \quad (2)$$

$$\text{and the finite precision coefficient relation } \bar{G}_{i+1} \bar{B}_{i+1,i} = \bar{T}_{i+1,i} \bar{G}_i \quad (3)$$



# Pipelined Conjugate Gradients Analyzing deep $\ell$ -length pipelined CG

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$$\bar{z}_{i+1} = (A\bar{z}_i - \bar{\gamma}_{i-l}\bar{z}_i - \bar{\delta}_{i-l-1}\bar{z}_{i-1}) / \bar{\delta}_{i-l} + \xi_{i+1}^{\bar{z}}, \Leftrightarrow A\bar{Z}_i = \bar{Z}_{i+1} \bar{B}_{i+1,i} + \Xi_i^{\bar{z}} \quad (2)$$

and the finite precision coefficient relation  $\bar{G}_{i+1} \bar{B}_{i+1,i} = \bar{T}_{i+1,i} \bar{G}_i$  allow to compute the gap on the basis  $\bar{V}_{i+1}$  as

$$\begin{aligned} A\bar{V}_i - \bar{V}_{i+1} \bar{T}_{i+1,i} &\stackrel{(1)}{=} A\bar{Z}_i \bar{G}_i^{-1} - \bar{Z}_{i+1} \bar{G}_{i+1}^{-1} \bar{T}_{i+1,i} - A\Xi_i^{\bar{v}} \bar{G}_i^{-1} + \Xi_{i+1}^{\bar{v}} \bar{G}_{i+1}^{-1} \bar{T}_{i+1,i} \\ &\stackrel{(3)}{=} (A\bar{Z}_i - \bar{Z}_{i+1} \bar{B}_{i+1,i} - A\Xi_i^{\bar{v}} + \Xi_{i+1}^{\bar{v}} \bar{B}_{i+1,i}) \bar{G}_i^{-1} \\ &\stackrel{(2)}{=} (\Xi_i^{\bar{z}} - A\Xi_i^{\bar{v}} + \Xi_{i+1}^{\bar{v}} \bar{B}_{i+1,i}) \bar{G}_i^{-1}. \end{aligned}$$



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Basis vector recurrences in finite precision  $p(l)$ -CG

$$\bar{v}_{i+1} = \left( \bar{z}_{i+1} - \sum_{j=i-2l+1}^i \bar{g}_{j,i+1} \bar{v}_j \right) / \bar{g}_{i+1,i+1} + \xi_i^{\bar{v}}, \Leftrightarrow \bar{Z}_i = \bar{V}_i \bar{G}_i + \Xi_i^{\bar{v}} \quad (1)$$

$$\bar{z}_{i+1} = (A\bar{z}_i - \bar{\gamma}_{i-l}\bar{z}_i - \bar{\delta}_{i-l-1}\bar{z}_{i-1}) / \bar{\delta}_{i-l} + \xi_{i+1}^{\bar{z}}, \Leftrightarrow A\bar{Z}_i = \bar{Z}_{i+1} \bar{B}_{i+1,i} + \Xi_i^{\bar{z}} \quad (2)$$

and the finite precision coefficient relation  $\bar{G}_{i+1} \bar{B}_{i+1,i} = \bar{T}_{i+1,i} \bar{G}_i$  allow to compute the gap on the basis  $\bar{V}_{i+1}$  as

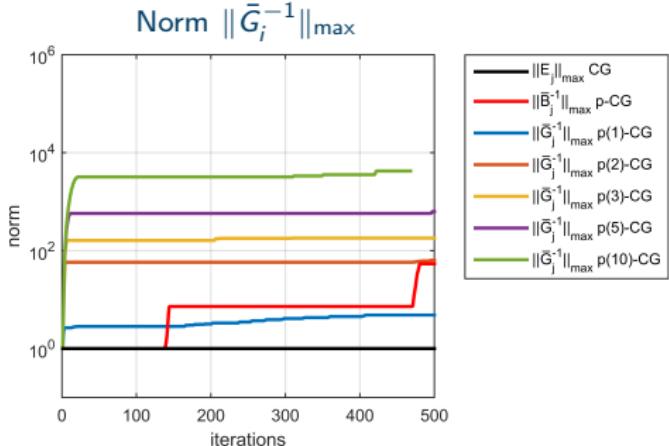
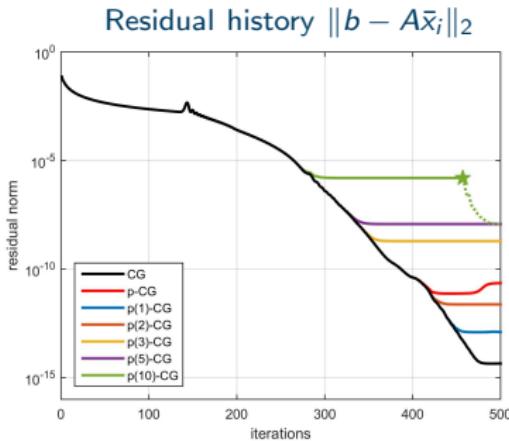
$$\begin{aligned} A\bar{V}_i - \bar{V}_{i+1} \bar{T}_{i+1,i} &\stackrel{(1)}{=} A\bar{Z}_i \bar{G}_i^{-1} - \bar{Z}_{i+1} \bar{G}_{i+1}^{-1} \bar{T}_{i+1,i} - A\Xi_i^{\bar{v}} \bar{G}_i^{-1} + \Xi_{i+1}^{\bar{v}} \bar{G}_{i+1}^{-1} \bar{T}_{i+1,i} \\ &\stackrel{(3)}{=} (A\bar{Z}_i - \bar{Z}_{i+1} \bar{B}_{i+1,i} - A\Xi_i^{\bar{v}} + \Xi_{i+1}^{\bar{v}} \bar{B}_{i+1,i}) \bar{G}_i^{-1} \\ &\stackrel{(2)}{=} (\Xi_i^{\bar{z}} - A\Xi_i^{\bar{v}} + \Xi_{i+1}^{\bar{v}} \bar{B}_{i+1,i}) \bar{G}_i^{-1}. \end{aligned}$$

*Amplification of local rounding errors possible, depending on  $\bar{G}_i^{-1}$ .*



# Pipelined Conjugate Gradients

## Analyzing deep $\ell$ -length pipelined CG



- The norm  $\|\bar{G}_i^{-1}\|_{\max}$  quantifies the impact of rounding error amplification on attainable accuracy in  $p(\ell)$ -CG.
- The Cholesky factorization  $Z_i^T Z_i = G_i^T G_i$  relates the conditioning of  $G_i$  and the auxiliary basis  $Z_i$ ; numerical stability depends on the polynomial  $P_\ell(A)$ .

Hoemmen (2010) Ghysels et al. (2013)



## Countermeasures against error propagation Residual replacement in p-CG by Ghysels et al.

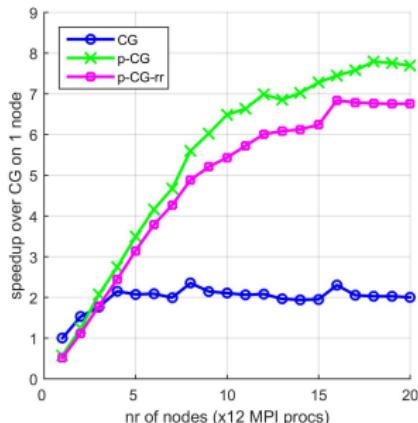
- ▶ Replace  $\bar{r}_i = \text{fl}(b - A\bar{x}_i)$ ,  $\bar{w}_i = \text{fl}(A\bar{r}_i)$ ,  $\bar{s}_i = \text{fl}(A\bar{p}_i)$ ,  $\bar{z}_i = \text{fl}(A\bar{s}_i)$  in selected iterations
  - ▣ Sleijpen et al. (1996)   ▣ van der Vorst & Ye (2000)   ▣ Strakos & Tichy (2002)
- ▶ Automated procedure based on estimate  $\|b - A\bar{x}_i - \bar{r}_i\|$  (computed inexpensively)
  - ▣ Carson & Demmel (2014)   ▣ C. et al. (2018)
    - Replace sufficiently often such that residual gap remains small
    - Don't replace if  $\|\bar{r}_i\|$  is small, which may cause delay of convergence



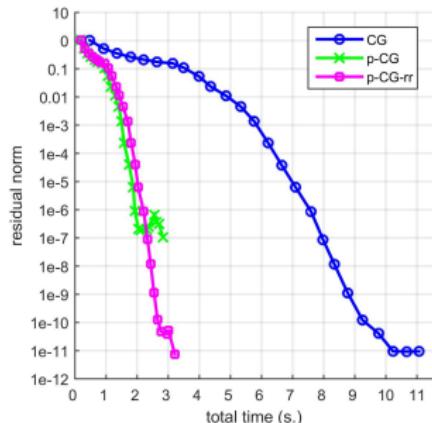
# Countermeasures against error propagation Residual replacement in p-CG by Ghysels et al.

- ▶ Replace  $\bar{r}_i = \text{fl}(b - A\bar{x}_i)$ ,  $\bar{w}_i = \text{fl}(A\bar{r}_i)$ ,  $\bar{s}_i = \text{fl}(A\bar{p}_i)$ ,  $\bar{z}_i = \text{fl}(A\bar{s}_i)$  in selected iterations
  - ▣ Sleijpen et al. (1996)   ▣ van der Vorst & Ye (2000)   ▣ Strakos & Tichy (2002)
- ▶ Automated procedure based on estimate  $\|b - A\bar{x}_i - \bar{r}_i\|$  (computed inexpensively)
  - ▣ Carson & Demmel (2014)   ▣ C. et al. (2018)
    - Replace sufficiently often such that residual gap remains small
    - Don't replace if  $\|\bar{r}_i\|$  is small, which may cause delay of convergence

Speedup over single-node CG (12-240 cores)



Accuracy vs. total time spent (240 cores)





# Countermeasures against error propagation Stable recurrences for deep $\ell$ -length pipelined CG

Introduce  $\ell$  auxiliary bases

$$Z_{i+1}^{(0)} = [v_0, \dots, v_i], \quad Z_{i+1}^{(1)} = [z_0^{(1)}, \dots, z_i^{(1)}], \quad \dots, \quad Z_{i+1}^{(\ell)} = [z_0, \dots, z_i],$$



# Countermeasures against error propagation

## Stable recurrences for deep $\ell$ -length pipelined CG

Introduce  $l$  auxiliary bases

$$Z_{i+1}^{(0)} = [v_0, \dots, v_i], \quad Z_{i+1}^{(1)} = [z_0^{(1)}, \dots, z_i^{(1)}], \quad \dots, \quad Z_{i+1}^{(l)} = [z_0, \dots, z_i],$$

and replace the multi-term recurrence relation for  $v_{i-l+1}$  ( $\sim 2l$  terms) by  $l+1$  coupled three-term recurrence relations

$$\left\{ \begin{array}{l} v_{i-l+1} = (z_{i-l+1}^{(1)} + (\sigma_0 - \gamma_{i-l})v_{i-l} - \delta_{i-l-1}v_{i-l-1})/\delta_{i-l}, \end{array} \right.$$



# Countermeasures against error propagation

## Stable recurrences for deep $\ell$ -length pipelined CG

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# Countermeasures against error propagation

## Stable recurrences for deep $\ell$ -length pipelined CG

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and replace the multi-term recurrence relation for  $v_{i-l+1}$  ( $\sim 2l$  terms) by  $l+1$  coupled three-term recurrence relations

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# Countermeasures against error propagation

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# Countermeasures against error propagation

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This modification causes (almost) no overhead

- the computational cost (#SpMVs and #axpy's) is identical to before,
- the storage cost increases by only  $l - 2$  vectors.



# Countermeasures against error propagation

## Stable recurrences for deep $\ell$ -length pipelined CG

### IN FINITE PRECISION ARITHMETIC

Introduce  $l$  auxiliary bases

$$\bar{Z}_{i+1}^{(0)} = [\bar{v}_0, \dots, \bar{v}_i], \quad \bar{Z}_{i+1}^{(1)} = [\bar{z}_0^{(1)}, \dots, \bar{z}_i^{(1)}], \quad \dots, \quad \bar{Z}_{i+1}^{(l)} = [\bar{z}_0, \dots, \bar{z}_i],$$

and replace the multi-term recurrence relation for  $\bar{v}_{i-l+1}$  ( $\sim 2l$  terms) by  $l+1$  coupled three-term recurrence relations **that all introduce local rounding errors**

$$\left\{ \begin{array}{lcl} \bar{v}_{i-l+1} &= (\bar{z}_{i-l+1}^{(1)} + (\sigma_0 - \bar{\gamma}_{i-l})\bar{v}_{i-l} - \bar{\delta}_{i-l-1}\bar{v}_{i-l-1})/\bar{\delta}_{i-l} + \xi_{i-l+1}^{(0)}, \\ \bar{z}_{i-l+2}^{(1)} &= (\bar{z}_{i-l+2}^{(2)} + (\sigma_1 - \bar{\gamma}_{i-l})\bar{z}_{i-l+1}^{(1)} - \bar{\delta}_{i-l-1}\bar{z}_{i-l}^{(1)})/\bar{\delta}_{i-l} + \xi_{i-l+2}^{(1)}, \\ \vdots && \vdots \\ \bar{z}_i^{(l-1)} &= (\bar{z}_i + (\sigma_{l-1} - \bar{\gamma}_{i-l})\bar{z}_{i-1}^{(l-1)} - \bar{\delta}_{i-l-1}\bar{z}_{i-2}^{(l-1)})/\bar{\delta}_{i-l} + \xi_i^{(l-1)}, \\ \bar{z}_{i+1} &= (A\bar{z}_i - \bar{\gamma}_{i-l}\bar{z}_i - \bar{\delta}_{i-l-1}\bar{z}_{i-1})/\bar{\delta}_{i-l} + \xi_{i+1}^{(l)}. \end{array} \right.$$



# Countermeasures against error propagation

## Stable recurrences for deep $\ell$ -length pipelined CG

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and replace the multi-term recurrence relation for  $\bar{v}_{i-l+1}$  ( $\sim 2l$  terms) by  $l+1$  coupled three-term recurrence relations **that are written in matrix notation as**

$$\left\{ \begin{array}{l} \bar{z}_{2:i-l+1}^{(1)} = \bar{z}_{i-l+1}^{(0)} \bar{T}_{i-l+1,i-l} - \sigma_0 \bar{z}_{i-l}^{(0)} - \Xi_{i-l+1}^{(0)} \bar{\Delta}_{i-l+1,i-l}, \\ \bar{z}_{2:i-l+2}^{(2)} = \bar{z}_{i-l+2}^{(1)} \bar{T}_{i-l+2,i-l+1} - \sigma_1 \bar{z}_{i-l+1}^{(1)} - \Xi_{i-l+2}^{(1)} \bar{\Delta}_{i-l+2,i-l+1}, \\ \vdots \qquad \qquad \qquad \vdots \\ \bar{z}_{2:i}^{(l)} = \bar{z}_i^{(l-1)} \bar{T}_{i,i-1} - \sigma_{l-1} \bar{z}_{i-1}^{(l-1)} - \Xi_i^{(l-1)} \bar{\Delta}_{i,i-1}, \\ A\bar{Z}_i^{(l)} = \bar{z}_{i+1}^{(l)} \bar{T}_{i+1,i} - \Xi_{i+1}^{(l)} \bar{\Delta}_{i+1,i}. \end{array} \right.$$



# Countermeasures against error propagation

## Stable recurrences for deep $\ell$ -length pipelined CG

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and replace the multi-term recurrence relation for  $\bar{v}_{i-l+1}$  ( $\sim 2l$  terms) by  $l+1$  coupled three-term recurrence relations that are written in matrix notation as

$$\rightarrow \left\{ \begin{array}{l} \bar{Z}_{2:i-l+1}^{(1)} = \bar{Z}_{i-l+1}^{(0)} \bar{T}_{i-l+1,i-l} - \sigma_0 \bar{Z}_{i-l}^{(0)} - \Xi_{i-l+1}^{(0)} \bar{\Delta}_{i-l+1,i-l}, \\ \bar{Z}_{2:i-l+2}^{(2)} = \bar{Z}_{i-l+2}^{(1)} \bar{T}_{i-l+2,i-l+1} - \sigma_1 \bar{Z}_{i-l+1}^{(1)} - \Xi_{i-l+2}^{(1)} \bar{\Delta}_{i-l+2,i-l+1}, \\ \vdots \qquad \qquad \qquad \vdots \\ \bar{Z}_{2:i}^{(l)} = \bar{Z}_i^{(l-1)} \bar{T}_{i,i-1} - \sigma_{l-1} \bar{Z}_{i-1}^{(l-1)} - \Xi_i^{(l-1)} \bar{\Delta}_{i,i-1}, \\ A\bar{Z}_i^{(l)} = \bar{Z}_{i+1}^{(l)} \bar{T}_{i+1,i} - \Xi_{i+1}^{(l)} \bar{\Delta}_{i+1,i}. \end{array} \right.$$

For  $\bar{Z}_{i+1}^{(l)}$  the gap is given by

$\bar{\Delta}_{i+1,i}$  diagonal matrix

$$A\bar{Z}_i^{(l)} - \bar{Z}_{i+1}^{(l)} \bar{T}_{i+1,i} = -\Xi_{i+1}^{(l)} \bar{\Delta}_{i+1,i}$$



# Countermeasures against error propagation

## Stable recurrences for deep $\ell$ -length pipelined CG

### IN FINITE PRECISION ARITHMETIC

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$$\bar{Z}_{i+1}^{(0)} = [\bar{v}_0, \dots, \bar{v}_i], \quad \bar{Z}_{i+1}^{(1)} = [\bar{z}_0^{(1)}, \dots, \bar{z}_i^{(1)}], \quad \dots, \quad \bar{Z}_{i+1}^{(\ell)} = [\bar{z}_0, \dots, \bar{z}_i],$$

and replace the multi-term recurrence relation for  $\bar{v}_{i-l+1}$  ( $\sim 2l$  terms) by  $\ell + 1$  coupled three-term recurrence relations that are written in matrix notation as

$$\rightarrow \left\{ \begin{array}{l} \bar{Z}_{2:i-l+1}^{(1)} = \bar{Z}_{i-l+1}^{(0)} \bar{T}_{i-l+1,i-l} - \sigma_0 \bar{Z}_{i-l}^{(0)} - \Xi_{i-l+1}^{(0)} \bar{\Delta}_{i-l+1,i-l}, \\ \bar{Z}_{2:i-l+2}^{(2)} = \bar{Z}_{i-l+2}^{(1)} \bar{T}_{i-l+2,i-l+1} - \sigma_1 \bar{Z}_{i-l+1}^{(1)} - \Xi_{i-l+2}^{(1)} \bar{\Delta}_{i-l+2,i-l+1}, \\ \vdots \qquad \qquad \qquad \vdots \\ \bar{Z}_{2:i}^{(\ell)} = \bar{Z}_i^{(\ell-1)} \bar{T}_{i,i-1} - \sigma_{\ell-1} \bar{Z}_{i-1}^{(\ell-1)} - \Xi_i^{(\ell-1)} \bar{\Delta}_{i,i-1}, \\ A\bar{Z}_i^{(\ell)} = \bar{Z}_{i+1}^{(\ell)} \bar{T}_{i+1,i} - \Xi_{i+1}^{(\ell)} \bar{\Delta}_{i+1,i}. \end{array} \right.$$

For  $\bar{Z}_{i+1}^{(\ell-1)}$  the gap is given by

$\bar{\Delta}_{i+1,i}$  diagonal matrix

$$A\bar{Z}_i^{(\ell-1)} - \bar{Z}_{i+1}^{(\ell-1)} \bar{T}_{i+1,i} = (A\bar{Z}_i^{(\ell)} - \bar{Z}_{i+1}^{(\ell)} \bar{T}_{i+1,i}) \bar{\Delta}_{i,i}^+ + \Xi_i^{(\ell)} - \Xi_{i+1}^{(\ell-1)} \bar{\Delta}_{i+1,i}$$



Countermeasures against error propagation  
Stable recurrences for deep  $\ell$ -length pipelined CG  
**IN FINITE PRECISION ARITHMETIC**

Introduce  $\ell$  auxiliary bases

$$\bar{Z}_{i+1}^{(0)} = [\bar{v}_0, \dots, \bar{v}_i], \quad \bar{Z}_{i+1}^{(1)} = [\bar{z}_0^{(1)}, \dots, \bar{z}_i^{(1)}], \quad \dots, \quad \bar{Z}_{i+1}^{(\ell)} = [\bar{z}_0, \dots, \bar{z}_i],$$

and replace the multi-term recurrence relation for  $\bar{v}_{i-l+1}$  ( $\sim 2l$  terms) by  $\ell + 1$  coupled three-term recurrence relations that are written in matrix notation as

$$\rightarrow \begin{cases} \bar{Z}_{2:i-l+1}^{(1)} = \bar{Z}_{i-l+1}^{(0)} \bar{T}_{i-l+1,i-l} - \sigma_0 \bar{Z}_{i-l}^{(0)} - \Xi_{i-l+1}^{(0)} \bar{\Delta}_{i-l+1,i-l}, \\ \bar{Z}_{2:i-l+2}^{(2)} = \bar{Z}_{i-l+2}^{(1)} \bar{T}_{i-l+2,i-l+1} - \sigma_1 \bar{Z}_{i-l+1}^{(1)} - \Xi_{i-l+2}^{(1)} \bar{\Delta}_{i-l+2,i-l+1}, \\ \vdots & \vdots \\ \bar{Z}_{2:i}^{(\ell)} & = \bar{Z}_i^{(\ell-1)} \bar{T}_{i,i-1} - \sigma_{\ell-1} \bar{Z}_{i-1}^{(\ell-1)} - \Xi_i^{(\ell-1)} \bar{\Delta}_{i,i-1}, \\ A\bar{Z}_i^{(\ell)} & = \bar{Z}_{i+1}^{(\ell)} \bar{T}_{i+1,i} - \Xi_{i+1}^{(\ell)} \bar{\Delta}_{i+1,i}. \end{cases}$$

For general  $\bar{Z}_{i+1}^{(k)}$  the gap is given by  $k \in \{0, 1, \dots, \ell - 1\}$

$$A\bar{Z}_i^{(k)} - \bar{Z}_{i+1}^{(k)} \bar{T}_{i+1,i} = (A\bar{Z}_i^{(k+1)} - \bar{Z}_{i+1}^{(k+1)} \bar{T}_{i+1,i}) \bar{\Delta}_{i,i}^+ + \Xi_i^{(k+1)} - \Xi_{i+1}^{(k)} \bar{\Delta}_{i+1,i}$$



# Countermeasures against error propagation

## Stable recurrences for deep $\ell$ -length pipelined CG

### IN FINITE PRECISION ARITHMETIC

Introduce  $\ell$  auxiliary bases

$$\bar{Z}_{i+1}^{(0)} = [\bar{v}_0, \dots, \bar{v}_i], \quad \bar{Z}_{i+1}^{(1)} = [\bar{z}_0^{(1)}, \dots, \bar{z}_i^{(1)}], \quad \dots, \quad \bar{Z}_{i+1}^{(\ell)} = [\bar{z}_0, \dots, \bar{z}_i],$$

and replace the multi-term recurrence relation for  $\bar{v}_{i-l+1}$  ( $\sim 2l$  terms) by  $\ell + 1$  coupled three-term recurrence relations that are written in matrix notation as

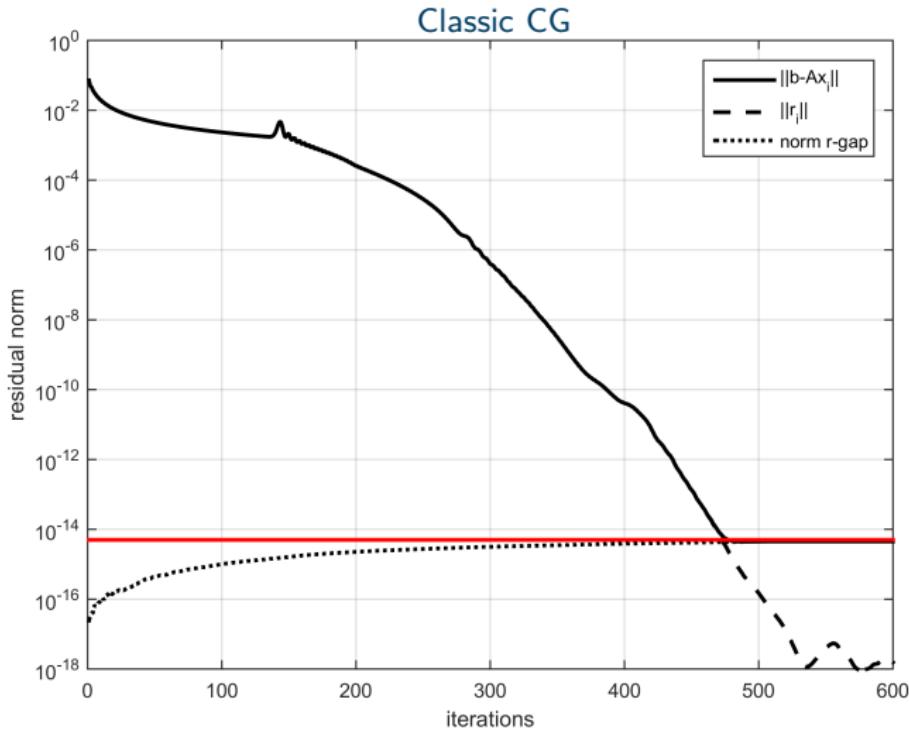
$$\rightarrow \left\{ \begin{array}{lcl} \bar{z}_{2:i-l+1}^{(1)} & = & \bar{z}_{i-l+1}^{(0)} \bar{T}_{i-l+1,i-l} - \sigma_0 \bar{z}_{i-l}^{(0)} - \Xi_{i-l+1}^{(0)} \bar{\Delta}_{i-l+1,i-l}, \\ \bar{z}_{2:i-l+2}^{(2)} & = & \bar{z}_{i-l+2}^{(1)} \bar{T}_{i-l+2,i-l+1} - \sigma_1 \bar{z}_{i-l+1}^{(1)} - \Xi_{i-l+2}^{(1)} \bar{\Delta}_{i-l+2,i-l+1}, \\ \vdots & & \vdots \\ \bar{z}_{2:i}^{(\ell)} & = & \bar{z}_i^{(\ell-1)} \bar{T}_{i,i-1} - \sigma_{\ell-1} \bar{z}_{i-1}^{(\ell-1)} - \Xi_i^{(\ell-1)} \bar{\Delta}_{i,i-1}, \\ A\bar{Z}_i^{(\ell)} & = & \bar{Z}_{i+1}^{(\ell)} \bar{T}_{i+1,i} - \Xi_{i+1}^{(\ell)} \bar{\Delta}_{i+1,i}. \end{array} \right.$$

Accumulation of local rounding errors, but no amplification, similar to classic CG.  
The method thus attains the same accuracy as classic CG!



# Countermeasures against error propagation

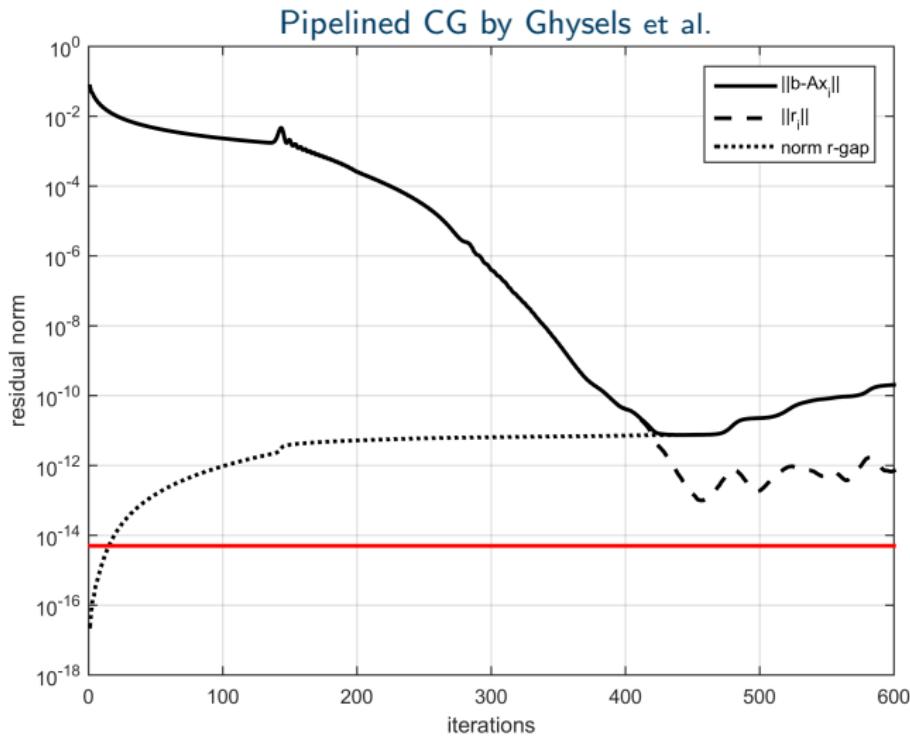
## Stable recurrences for deep $\ell$ -length pipelined CG





# Countermeasures against error propagation

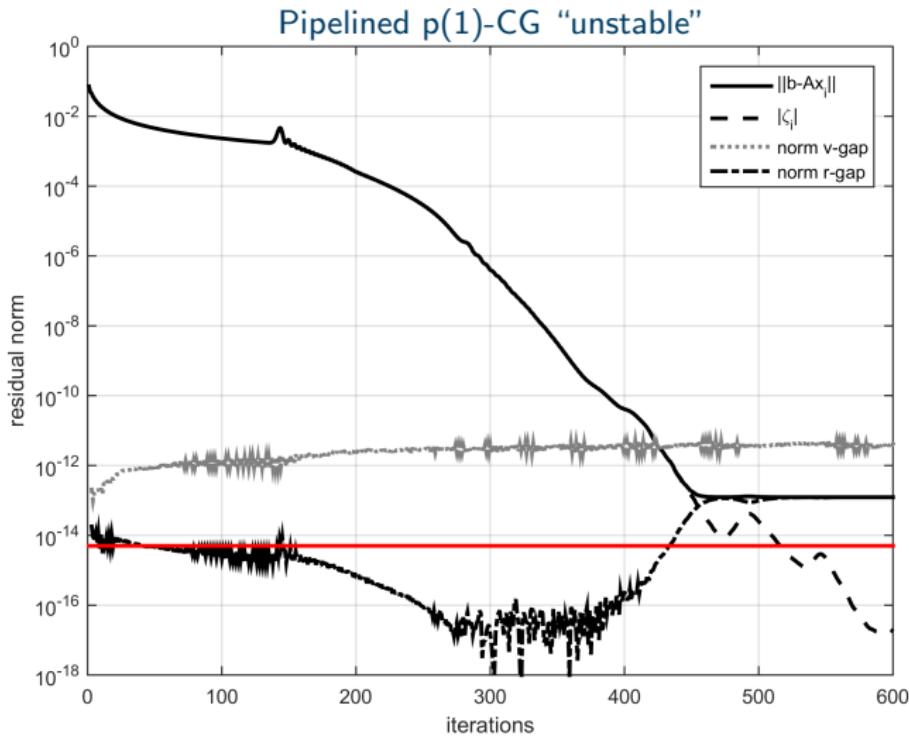
## Stable recurrences for deep $\ell$ -length pipelined CG





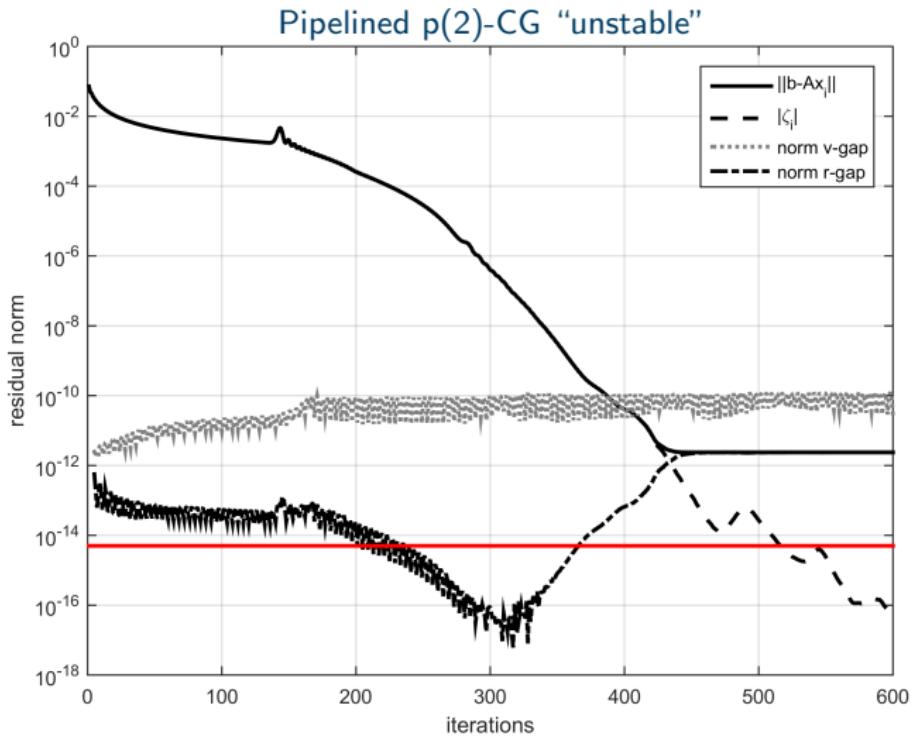
# Countermeasures against error propagation

## Stable recurrences for deep $\ell$ -length pipelined CG



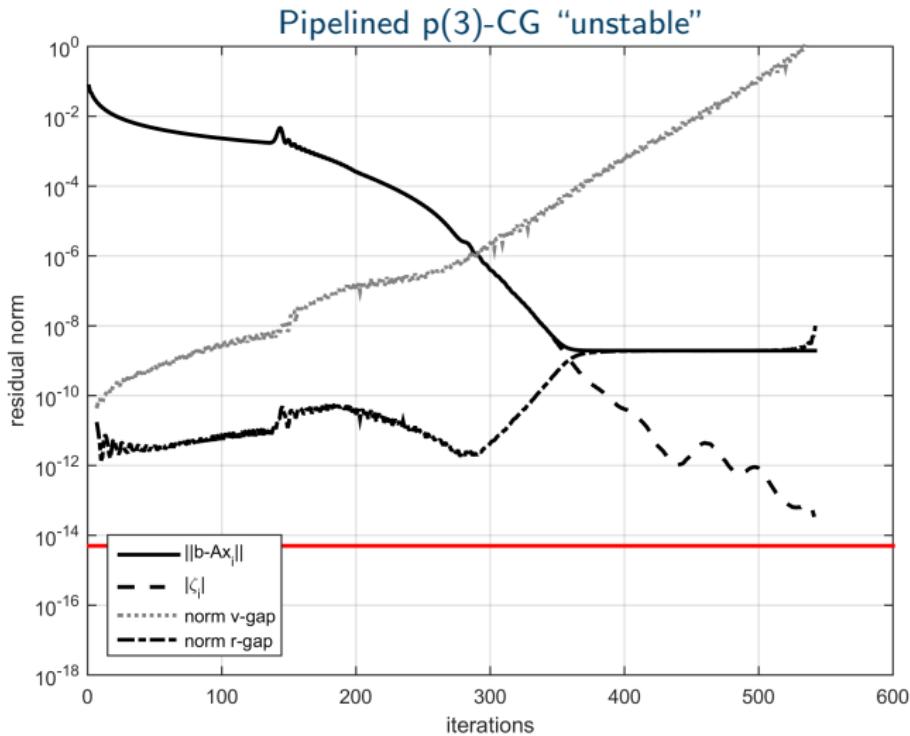


# Countermeasures against error propagation Stable recurrences for deep $\ell$ -length pipelined CG





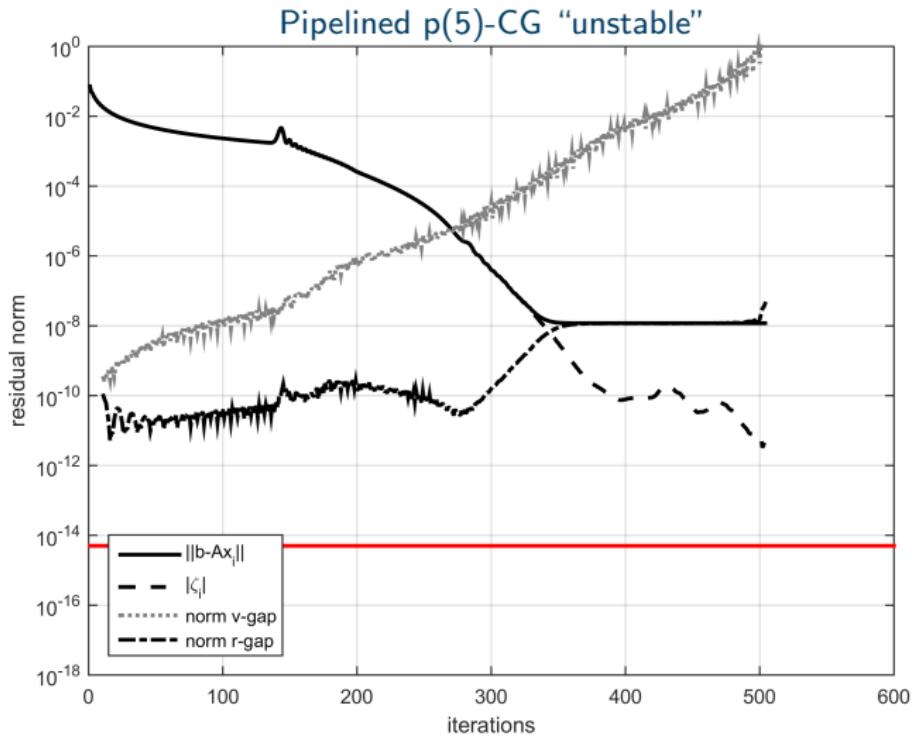
# Countermeasures against error propagation Stable recurrences for deep $\ell$ -length pipelined CG





# Countermeasures against error propagation

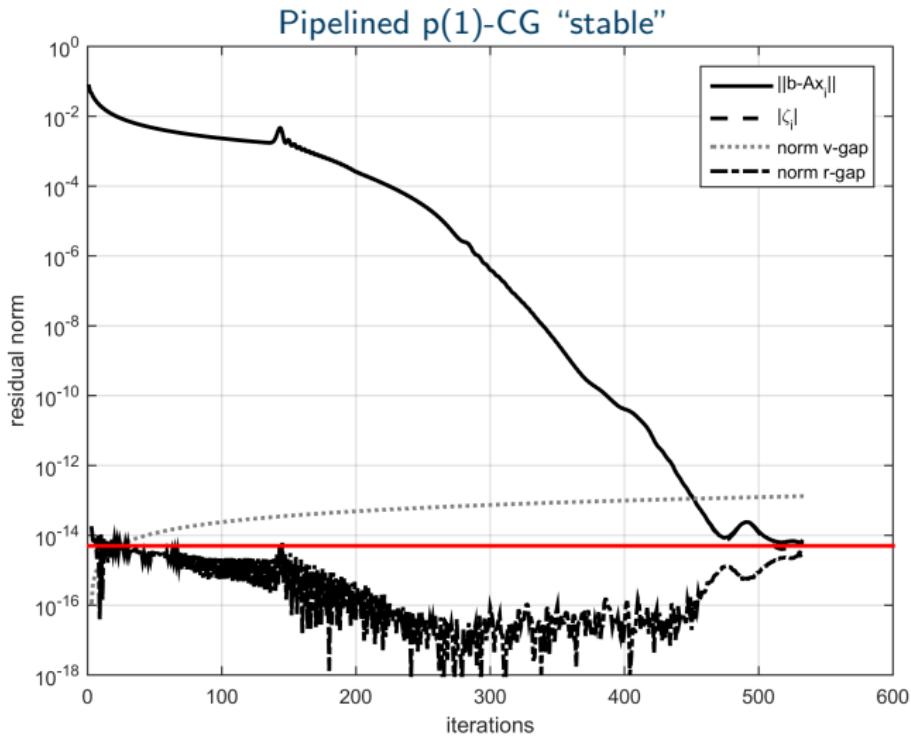
## Stable recurrences for deep $\ell$ -length pipelined CG





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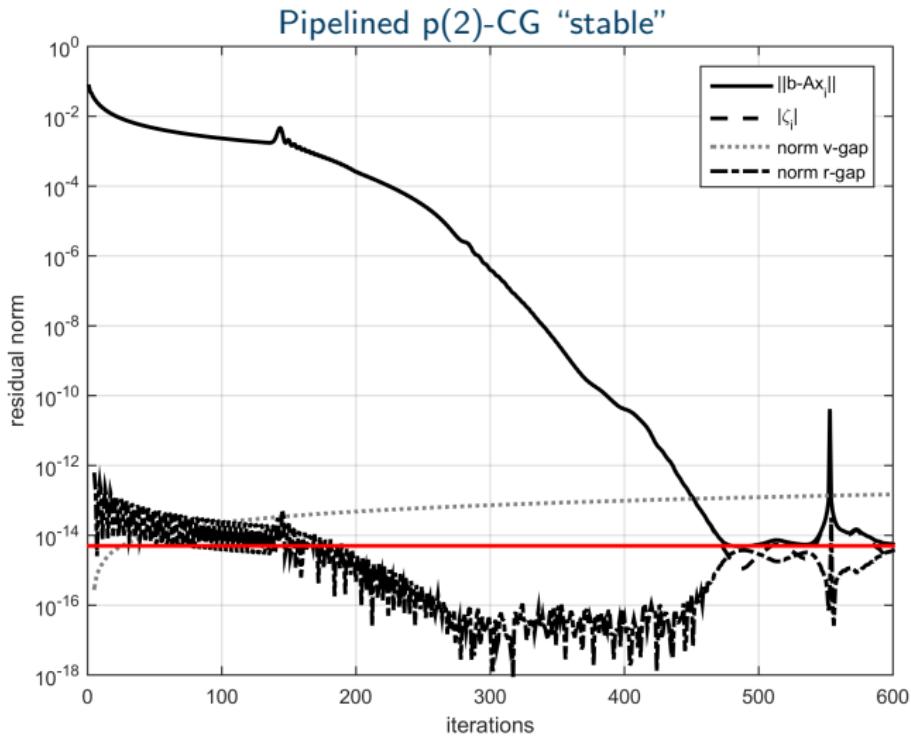
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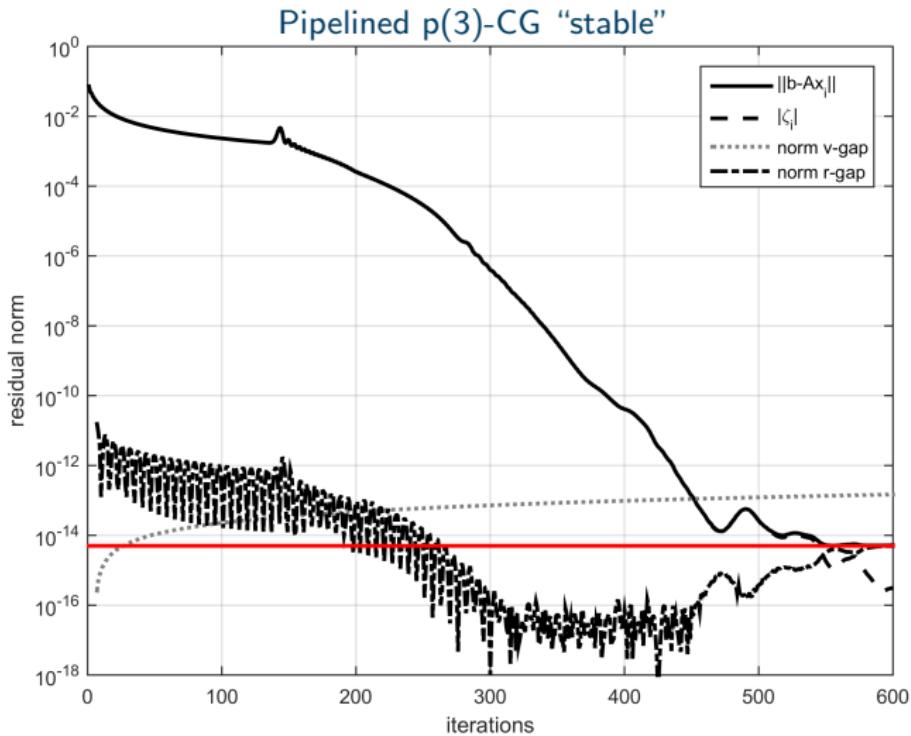
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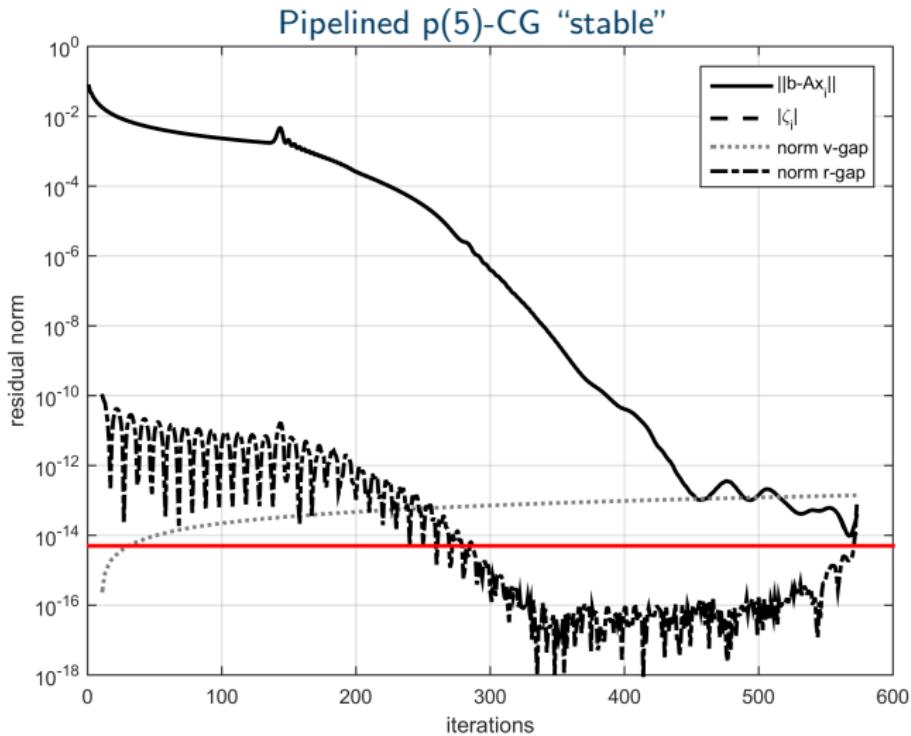
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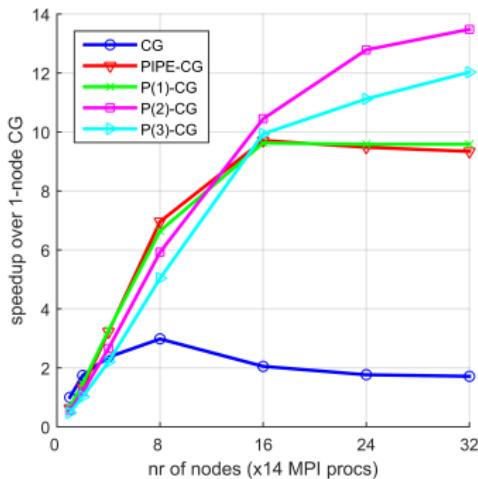




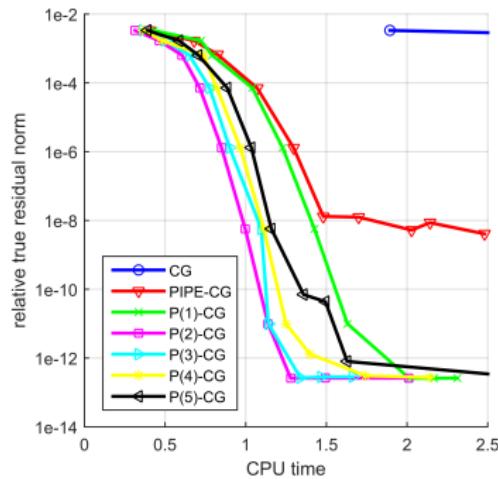
## Numerical experiments Deep $\ell$ -length pipelined CG

- Strong scaling on up to 32 14-core Intel E5-2680v4 Broadwell CPU nodes
- EDR Infiniband, Intel MPI 2018v3, PETSc v3.8.3, KSP ex2
- 2D 5-pt Poisson, 3 million unknowns, 1,500 iterations, no preconditioner

Speedup (over CG on 1 node)



Accuracy (vs. total CPU time)

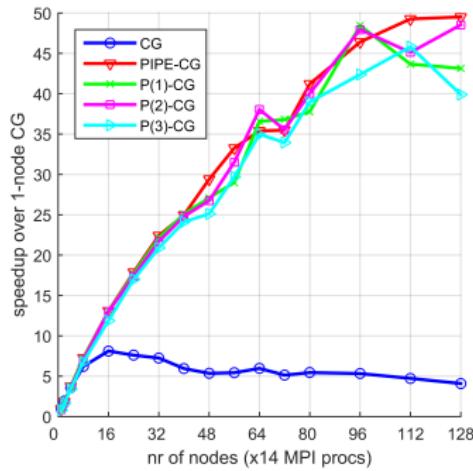




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- Strong scaling on up to 128 14-core Intel E5-2680v4 Broadwell CPU nodes
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- 3D Hydrostatic Ice Sheet Flow, 2.25 million FE, Newton-Krylov solver, 7 Newton steps, 4,500 total inner iter, block Jacobi preconditioner, inner tolerance: 1.0e-10, outer tolerance: 1.0e-8

Speedup (over CG on 1 node)

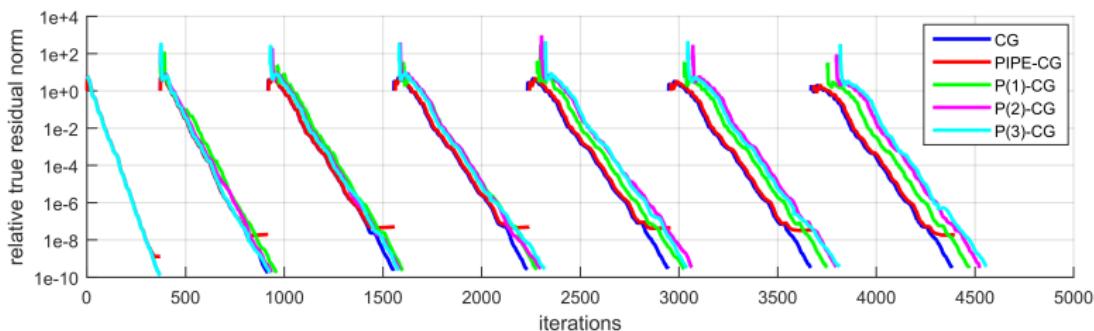




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Accuracy (vs. total number of inner iterations)





## Conclusions Takeaway messages

- Pipelined Krylov subspace methods are a promising approach
  - ▶ *Hide communication latency* behind computational kernels by adding auxiliary variables and recurrence relations
  - ▶ *p( $\ell$ )-CG*: *Deep pipelines* allow to hide global reduction phases behind multiple SpMV's/iterations
  - ▶ *Asynchronous implementation*: dot-products can take multiple iterations to complete; global reductions are implemented in an overlapping manner
  - ▶ *Improved scaling* over classic KSMs in strong scaling limit, where global reduction latencies rise and volume of computations per core diminishes



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- The finite precision behavior of communication avoiding- and hiding Krylov subspace algorithms should be carefully monitored
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- The finite precision behavior of communication avoiding- and hiding Krylov subspace algorithms should be carefully monitored
  - ▶ *Local rounding error analysis* allows to explain loss of attainable accuracy
- Insights to construct a more stable method are obtained from the analysis
  - ▶ *Fully restore attainable accuracy* in p( $\ell$ )-CG at *no increase in computational costs or storage costs* through residual replacement-type techniques
  - ▶ The issue of *loss of orthogonality* has not been addressed by the modifications to p( $\ell$ )-CG proposed in this talk



## Conclusions Contributions to PETSc

Open source HPC linear algebra toolkit: <https://www.mcs.anl.gov/petsc/>

The screenshot shows the GitHub repository page for PETSc. The left sidebar has icons for Issues, Pull requests, Pipelines, Branches, Pull requests, Pipelines, and +. The main area shows the repository overview with a blue header 'petsc'. Below it, there's a navigation bar with 'Overview' (selected), 'Source', 'Commits', 'Branches', 'Pull requests', and 'Pipelines'. The 'Overview' section includes a download button, an SSH link, and a git URL. It also displays information about the repository: last updated an hour ago, website <http://mcs.anl.gov/petsc>, language C, and access level Read. On the right, there are statistics: 107 Watchers, 135 Forks, and 9+ Branches. A large yellow starburst graphic with a red outline and border contains the text: "We are soliciting for feedback from your applications".

- ▶ KSPPGMRES: pipelined GMRES (thanks to J. Brown)
- ▶ KSPPIPECG: pipelined Conjugate Gradients
- ▶ KPPPIPECR: pipelined Conjugate Residuals
- ▶ KSPPIPECGRR: pipelined CG with automated residual replacement
- ▶ KSPPIPELCG: pipelined CG with deep pipelines
- ▶ KSPGROPPCG: asynchronous CG variant by W. Gropp and collaborators
- ▶ KSPPIPEBCGS: pipelined BiCGStab



## Related publications

# Thank you!



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☞ <https://www.uantwerpen.be/en/staff/wim-vanroose>

-  P. Ghysels, T. J. Ashby, K. Meerbergen, and W. Vanroose, *Hiding Global Communication Latency in the GMRES Algorithm on Massively Parallel Machines* SIAM J. Sci. Comput., 35(1), pp. C48–C71, 2013.
-  P. Ghysels and W. Vanroose, *Hiding global synchronization latency in the preconditioned Conjugate Gradient algorithm*, Parallel Computing, 40(7), pp. 224–238, 2014.
-  S. Cools, E.F. Yetkin, E. Agullo, L. Giraud, W. Vanroose, *Analyzing the effect of local rounding error propagation on the maximal attainable accuracy of the pipelined Conjugate Gradient method*. SIAM J. on Matrix Anal. Appl., 39(1), pp. 426–450, 2018.
-  J. Cornelis, S. Cools, W. Vanroose, *The communication-hiding Conjugate Gradient method with deep pipelines*. Submitted to SIAM J. Sci. Comput., 2018, Preprint: ArXiv 1801.04728.
-  S. Cools, J. Cornelis, W. Vanroose, *Numerically Stable Recurrence Relations for the Communication Hiding Pipelined Conjugate Gradient Method*. Submitted to IEEE Transactions on Parallel and Distributed Systems., 2019, Preprint: ArXiv 1902.03100.