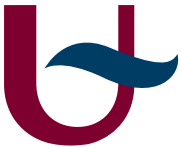


Parallel Performance and Numerical Stability of Communication Hiding Pipelined Krylov Subspace Methods

10th International Workshop on Parallel Matrix Algorithms and Applications (PMAA'18)

ETH Zürich, June 27-29, 2018

University of Antwerp* [Belgium], LBNL‡ [USA], INRIA Bordeaux† [France]

S. Cools*, J. Cornelis*, W. Vanroose*, T. Mijieux*, P. Ghysels‡, E. F. Yetkin†, E. Agullo†, L. Giraud†

* E-mail: siegfried.cools@uantwerp.be

Universiteit Antwerpen

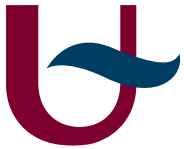
Exascale systems projection

	Today's Systems	Predicted Exascale Systems*	Factor Improvement
System Peak	10^{16} flops/s	10^{18} flops/s	100
Node Memory Bandwidth	10^{2} GB/s	10^{3} GB/s	10
Interconnect Bandwidth	10^{1} GB/s	10^{2} GB/s	10
Memory Latency	10^{-7} s	$5 \cdot 10^{-8}$ s	2
Interconnect Latency	10^{-6} s	$5 \cdot 10^{-7}$ s	2

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

- Data movement (communication) is much more expensive than flops (computation) in terms of both time and energy
- Reducing time spent moving data/waiting for data will be essential for exascale applications

$\Rightarrow$ Communication avoiding / Communication hiding



Communication hiding vs. communication avoiding

Communication cost has motivated several approaches to reducing global synchronization cost in Krylov subspace methods:

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

[A. Chronopoulous, J. Demmel, M. Hoemmen, E. Carson, L. Grigori, J. Erhel, ...]

- Compute iterations in blocks of s (change of Krylov subspace basis)
- 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, ...]

- Introduce auxiliary vectors to decouple SpMV and inner products
- Enables overlapping of communication and computation

* Both equivalent to corresponding Krylov subspace methods in exact arithmetic

Communication hiding vs. communication avoiding

Communication co g global synchronization co

Avoiding comm hods *

[A. Chronopoulous, J.]

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Hiding commur thods *

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June 27, 2018

10:15 AM – 12:15 PM

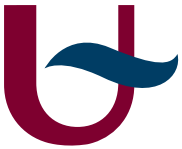
1.2.B: **Scalable communication-reducing Krylov subspace methods**

Organizers: **S. Cools**

Location: **CAB G61**

- 10:15 AM *Jeffrey Cornelis:* **Hiding global communication in the Conjugate Gradient method using deep pipelines**
- 10:45 AM *Hussam Al Daas:* **Recycling Krylov method for the solution of sequence of linear systems**
- 11:15 AM *Sicong Zhuang:* **Iteration-Fusing Conjugate Gradient**
- 11:45 AM *Emmanuel Agullo:* **Partial convergence in block Krylov solvers**

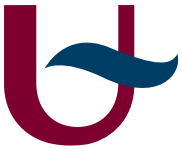
Thumbs up to all MS speakers!



General concepts

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

$$x_i \in x_0 + \mathcal{K}_i(A, r_0) = x_0 + \text{span}\{r_0, Ar_0, A^2 r_0, \ldots, A^{i-1} r_0\}$$



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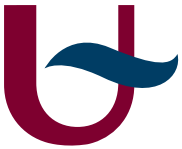
- minimize certain error measure over Krylov subspace $\mathcal{K}_i(A, r_0)$
- Krylov subspace methods:

  Conjugate Gradients (CG), Lanczos, GMRES, MinRES, BiCG, CGS, BiCGStab, CGLS, ...
- Preconditioners:

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



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- 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
     - $\mathcal{O}$(nnz) flops
     - neighbor communication only
  iii. axpy
     - $\mathcal{O}$(N) flops
     - no communication

Classical CG

Algorithm CG

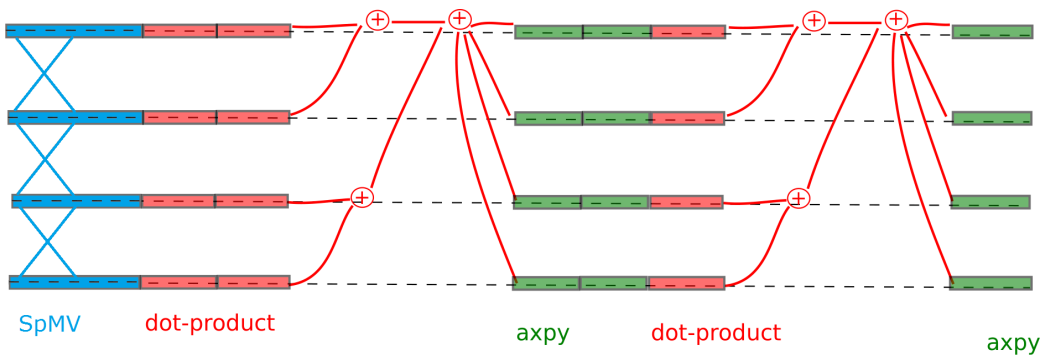
1: **procedure** CG(A, b, x_0)
2: $r_0 := b - Ax_0$; $p_0 = r_0$
3: **for** $i = 0, \ldots$ **do**
4: $s_i := Ap_i$ — **SpMV**
5: $\alpha_i := (r_i, r_i) / (s_i, p_i)$ — **dot-pr**
6: $x_{i+1} := x_i + \alpha_i p_i$ — **axpy**
7: $r_{i+1} := r_i - \alpha_i s_i$ — **axpy**
8: $\beta_{i+1} := (r_{i+1},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

Hestenes & Stiefel (1952)

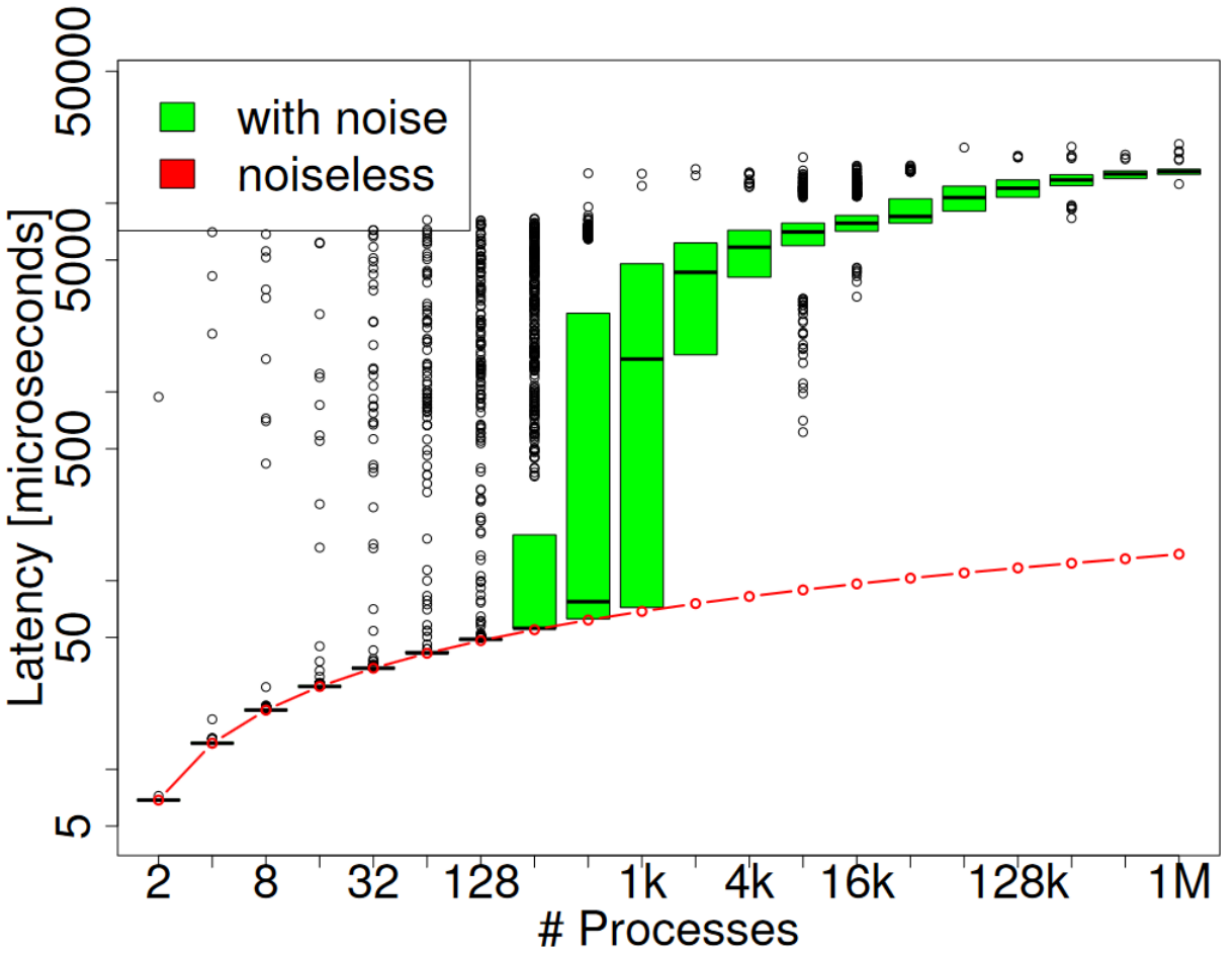
i. dot-products
- 2 global reductions: latency dominated
- scales as $log_2(\#partitions)$

ii. SpMV
- computationally expensive
- good scaling (minor comm.)

iii. axpy's
- vector operations (recurrence relations)
- perfect scaling (no comm.)



Global reduction latency



T. Hoeffler, T. Schneider and A. Lumsdaine, SC10, 2010

Pipelined CG

Algorithm Pipelined CG

1: **procedure** PIPE-CG(A, b, x_0)
2: $r_0 := b - Ax_0$; $w_0 := Ar_0$
3: **for** $i = 0, \ldots$ **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: $p_i := r_i + \beta_i p_{i-1}$
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16: $r_{i+1} := r_i - \alpha_i s_i$
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dot-pr
SpMV
axpy

Ghysels & Vanroose (2014)

Pipelined CG = re-engineered version of CG for improved parallel performance

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Pipelined CG = re-engineered version of CG for improved parallel performance

- Introduce new auxiliary variables ...

  $s_i = Ap_i$, $w_i = Ar_i$, $z_i = As_i = A^2 p_i$

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13: $s_i := w_i + \beta_i s_{i-1}$ — axpy
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Ghysels & Vanroose (2014)

Pipelined CG = re-engineered version of CG for improved parallel performance

- Introduce new auxiliary variables ...

  $s_i = Ap_i$, $w_i = Ar_i$, $z_i = As_i = A^2 p_i$

- that are computed recursively, e.g.:

$$p_i = r_i + \beta_i p_{i-1}$$

$$\Rightarrow s_i = Ap_i = w_i + \beta_i s_{i-1}$$

with $w_i := Ar_i$

Pipelined CG

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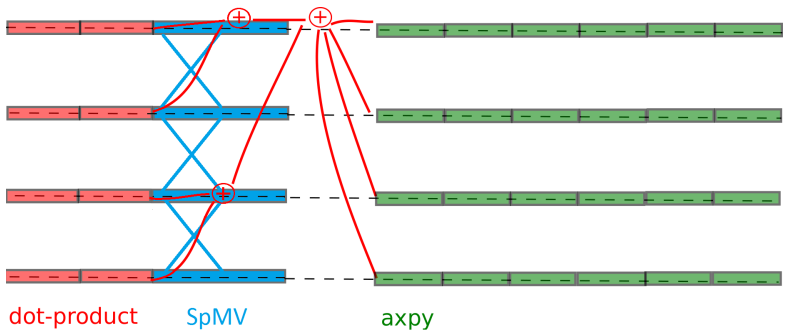
dot-pr
SpMV
axpy

Ghysels & Vanroose (2014)

i. Communication avoiding:
dot-products grouped in one global reduction phase per iteration

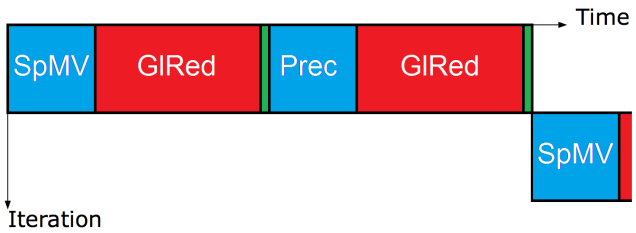
ii. Communication hiding:
overlap global synchronization with SpMV (+ Prec) computation

iii. No free lunch: Additional recurrence relations, i.e. axpy's, for auxiliary var's $s_i = Ap_i$, $w_i = Ar_i$, $z_i = As_i$

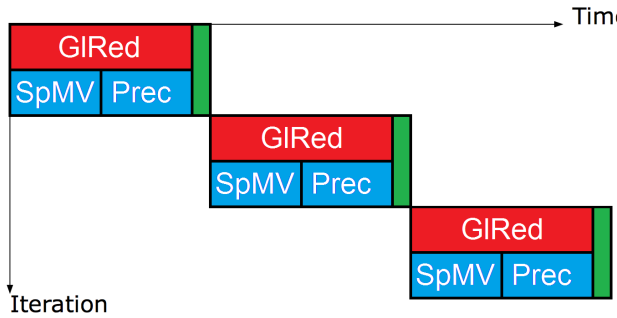


Generalization: deep pipelines

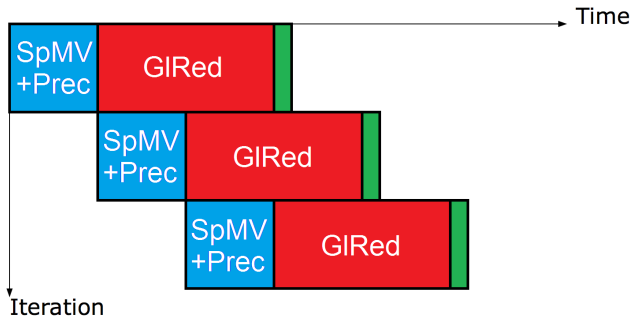
Classic KSM:



Pipelined KSM:



Deep pipelined KSM:



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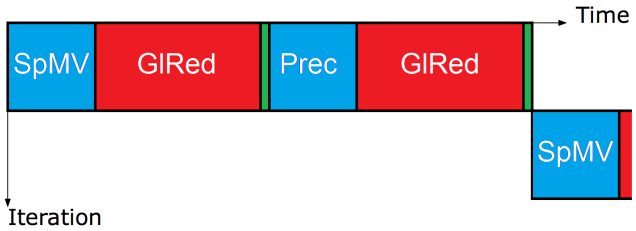

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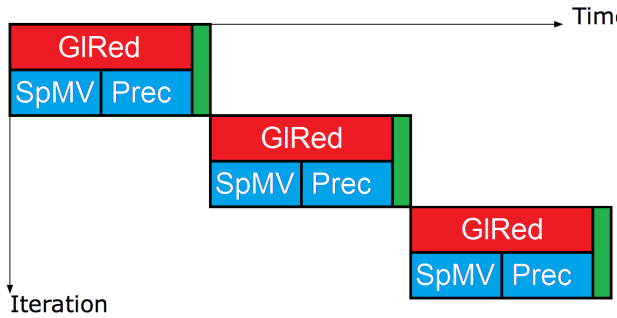

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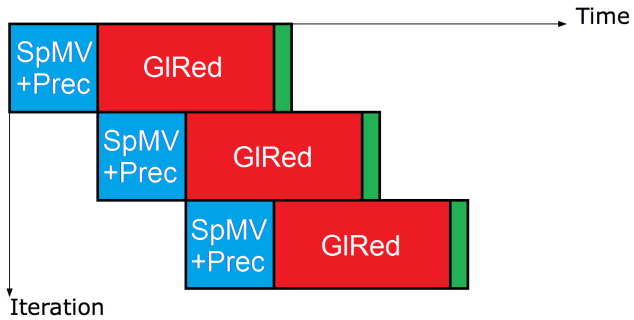


Consider the Arnoldi relation

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

with V_i the Krylov subspace basis and $H_{i+1,i}$ upper Hessenberg. Introduce the auxiliary vectors $Z_{i+1} = [z_0, z_1, \ldots, z_i]$ as

$$z_j := \begin{cases} v_0 & j = 0, \\ P_j(A) v_0 & 0 < j \leq l, \\ P_l(A) v_{j-l} & j > l, \end{cases}$$

with polynomials $P_l(t)$ of fixed order l, where l is the pipeline length

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

Pipelined KSM with deep pipeline

Writing the Arnoldi relation $AV_i = V_{i+1}H_{i+1,i}$ for basis vector v_{j-l} and applying $P_l(A)$ to both sides, we obtain recurrence relations for z_j:

$$v_{j-l} = \frac{Av_{j-l-1} - \sum_{k=0}^{j-l-1} h_{k,j-l-1}v_k}{h_{j-l,j-l-1}} \quad \Rightarrow \quad z_j = \frac{Az_{j-1} - \sum_{k=0}^{j-l-1} h_{k,j-l-1}z_{k+l}}{h_{j-l,j-l-1}}.$$

This implies an Arnoldi-like relation for the auxiliary variables

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

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

Basis transformation: *Z_i and V_i both span the i-th Krylov subspace, thus there an upper triangular transformation matrix G_i such that*

$$Z_i = V_i G_i.$$

Pipelined KSM with deep pipeline

- Recursive calculation of entries of G_i $(\forall j = 0, 1, \ldots, k \leq i)$:

$$g_{j,k} = (z_k, v_j) = \left(z_k, \frac{z_j - \sum_{m=0}^{j-1} g_{m,j} v_m}{g_{j,j}} \right) = \frac{(z_k, z_j) - \sum_{m=0}^{j-1} g_{m,j} g_{m,k}}{g_{j,j}}$$

- Recursive calculation of the Hessenberg matrix $H_{i+1,i}$:

$$\begin{aligned}
H_{k+1,k} &= V_{k+1}^T A V_k \\
&= V_{k+1}^T A Z_k G_k^{-1} \qquad \text{using} \quad Z_k = V_k G_k \\
&= V_{k+1}^T Z_{k+1} B_{k+1,k} G_k^{-1} \qquad \text{using} \quad A Z_k = Z_{k+1} B_{k+1,k} \\
&= G_{k+1} B_{k+1,k} G_k^{-1} \qquad \text{using} \quad G_{k+1} = V_{k+1}^T Z_{k+1} \\
&= \begin{pmatrix} H_{k,k-1} & \left(G_k b_{:,k} + g_{:,k+1} b_{k+1,k} - H_{k,k-1} g_{:,k}\right) g_{k,k}^{-1} \\ 0 & g_{k+1,k+1} b_{k+1,k} g_{k,k}^{-1} \end{pmatrix} \\
&\qquad \text{using} \quad H_{k,k-1} G_{k-1} = G_k B_{k,k-1}
\end{aligned}$$

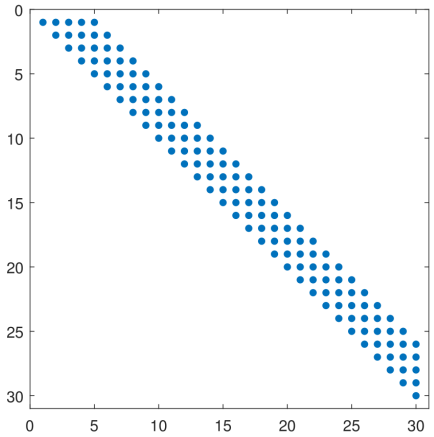
- Combining all relations leads to the deep pipelined p(l)-GMRES algorithm.

Ghysels & Vanroose (2013)

Pipelined CG with deep pipeline

In case of an SPD matrix A the following features simplify the algorithm:

- $H_{i+1,i}$ is tridiagonal
- G_i has a $(2l+1)$-nonzero diagonal band structure.
  E.g. $l = 2$:



Cornelis et al. (2018)

- The solution x_i can be constructed using a recursively computed search direction p_i, instead of using the entire Krylov basis V_i:

$$p_j = (v_j - \delta_{j-1} p_{j-1})/\eta_j, \qquad x_j = x_{j-1} + \xi_{j-1} p_{j-1}.$$

Liesen & Strakos, *Krylov Subspace Methods* (2012)

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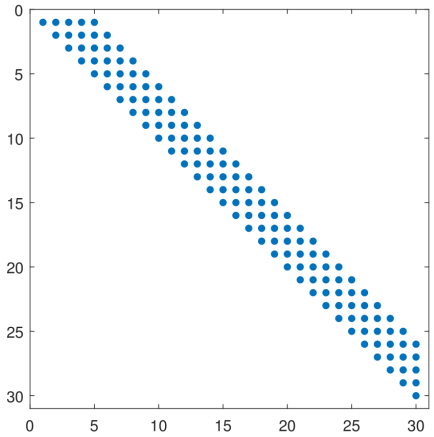

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June 27, 2018

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Liesen & Strakos, *Krylov Subspace Methods* (2012)

Pipelined CG with deep pipeline

Algorithm Deep pipelined Conjugate Gradients (p(ℓ)-CG)

$r_0 := b - Ax_0$;
$v_0 := r_0/\|r_0\|_2$;
$z_0 := v_0$; $g_{0,0} := 1$;
for $i = 0, \ldots, m + l$ **do**
  $z_{i+1} := \begin{cases} (A - \sigma_i I)z_i, & i < l \\ Az_i, & i \geq l \end{cases}$
  $a := i - l$
  if $a \geq 0$ **then**
    $g_{j,a+1} := (g_{j,a+1} - \sum_{k=a+1-2l}^{j-1} g_{k,j} g_{k,a+1})/g_{j,j}$; $\quad j = a - l + 2, \ldots, a$
    $g_{a+1,a+1} := \sqrt{g_{a+1,a+1} - \sum_{k=a+1-2l}^{a} g_{k,a+1}^2}$;
    # Check for breakdown and restart if required
    if $a < l$ **then**
      $\gamma_a := (g_{a,a+1} + \sigma_a g_{a,a} - \delta_{a-1} g_{a-1,a})/g_{a,a}$;
      $\delta_a := g_{a+1,a+1}/g_{a,a}$;
    else
      $\gamma_a := (g_{a,a}\gamma_{a-l} + g_{a,a+1}\delta_{a-l} - \delta_{a-1} g_{a-1,a})/g_{a,a}$;
      $\delta_a := (g_{a+1,a+1}\delta_{a-l})/g_{a,a}$;
    end if
    $v_{a+1} := (z_{a+1} - \sum_{j=a-2l+1}^{a} g_{j,a+1} v_j)/g_{a+1,a+1}$;
    $z_{i+1} := (z_{i+1} - \gamma_a z_i - \delta_{a-1} z_{i-1})/\delta_a$;
  end if
  if $a < 0$ **then**
    $g_{j,i+1} := (z_{i+1}, z_j)$; $\quad j = 0, \ldots, i + 1$
  else
    $g_{j,i+1} := \begin{cases} (z_{i+1}, v_j); & j = \max(0, i - 2l + 1), \ldots, a + 1 \\ (z_{i+1}, z_j); & j = a + 2, \ldots, i + 1 \end{cases}$
  end if

Cornelis et al. (2018)

Pipelined CG with deep pipeline

Algorithm Deep pipelined Conjugate Gradients (p(ℓ)-CG)

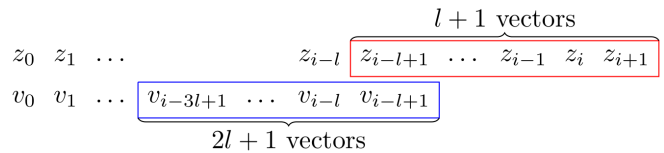
1: $r_0 := b - Ax_0$;
2: $v_0 := r_0/\|r_0\|_2$;
3: $z_0 := v_0$; $g_{0,0} := 1$;
4: **for** $i = 0, \ldots, m + l$ **do**
5: $\quad z_{i+1} := \begin{cases} (A - \sigma_i I)z_i, & i < l \\ Az_i, & i \geq l \end{cases}$
6: $\quad a := i - l$
7: $\quad$ **if** $a \geq 0$ **then**
8: $\quad\quad g_{j,a+1} := (g_{j,a+1} - \sum_{k=a+1-2l}^{j-1} g_{k,j}g_{k,a+1})/g_{j,j}$; $\quad j = a - l + 2, \ldots$
9: $\quad\quad g_{a+1,a+1} := \sqrt{g_{a+1,a+1} - \sum_{k=a+1-2l}^{a} g_{k,a+1}^2}$;
10: $\quad\quad$ # Check for breakdown and restart if required
11: $\quad\quad$ **if** $a < l$ **then**
12: $\quad\quad\quad \gamma_a := (g_{a,a+1} + \sigma_a g_{a,a} - \delta_{a-1}g_{a-1,a})/g_{a,a}$;
13: $\quad\quad\quad \delta_a := g_{a+1,a+1}/g_{a,a}$;
14: $\quad\quad$ **else**
15: $\quad\quad\quad \gamma_a := (g_{a,a}\gamma_{a-l} + g_{a,a+1}\delta_{a-l} - \delta_{a-1}g_{a-1,a})/g_{a,a}$;
16: $\quad\quad\quad \delta_a := (g_{a+1,a+1}\delta_{a-l})/g_{a,a}$;
17: $\quad\quad$ **end if**
18: $\quad\quad v_{a+1} := (z_{a+1} - \sum_{j=a-2l+1}^{a} g_{j,a+1}v_j)/g_{a+1,a+1}$;
19: $\quad\quad z_{i+1} := (z_{i+1} - \gamma_a z_i - \delta_{a-1}z_{i-1})/\delta_a$;
20: $\quad$ **end if**
21: $\quad$ **if** $a < 0$ **then**
22: $\quad\quad g_{j,i+1} := (z_{i+1}, z_j)$; $\quad j = 0, \ldots, i + 1$
23: $\quad$ **else**
24: $\quad\quad g_{j,i+1} := \begin{cases} (z_{i+1}, v_j); & j = \max(0, i - 2l + 1), \ldots, a + 1 \\ (z_{i+1}, z_j); & j = a + 2, \ldots, i + 1 \end{cases}$
25: $\quad$ **end if**

SpMV (+ preconditioner)

- one SpMV on z_i / iteration

Recurrence relations for V_{i-l} and Z_i basis vectors

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



Dot-products

- $2l + 1$ band structure of G_i
- one global synchronization phase / iteration

Cornelis et al. (2018)

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14: $\quad\quad$ **else**
15: $\quad\quad\quad \gamma_a := (g_{a,a}\gamma_{a-l}$
16: $\quad\quad\quad \delta_a := (g_{a+1,a+1}$
17: $\quad\quad$ **end if**
18: $\quad\quad v_{a+1} := (z_{a+1} - \sum$
19: $\quad\quad z_{i+1} := (z_{i+1} - \gamma_a z$
20: $\quad$ **end if**
21: $\quad$ **if** $a < 0$ **then**
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25: $\quad$ **end if**

Results of dot-products are needed l iterations later to update $G_{:,i-l+1}$

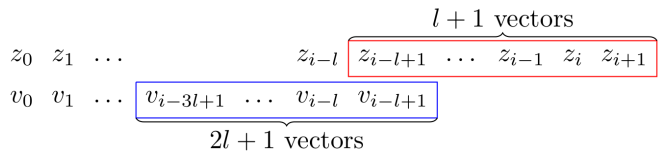
Each global reduction is overlapped by ℓ SpMVs

SpMV (+ preconditioner)

- one SpMV on z_i / iteration

Recurrence relations for V_{i-l} and Z_i basis vectors

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



Dot-products

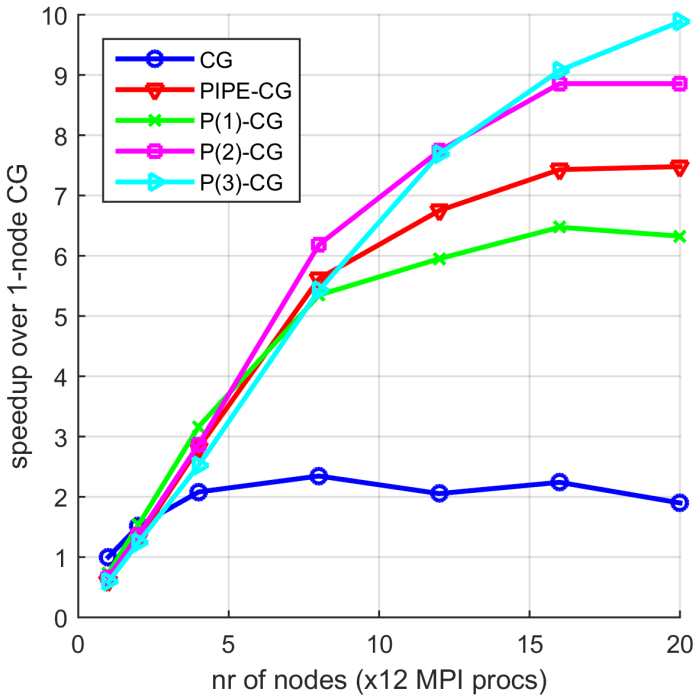
- $2l+1$ band structure of G_i
- one global synchronization phase / iteration

Cornelis et al. (2018)

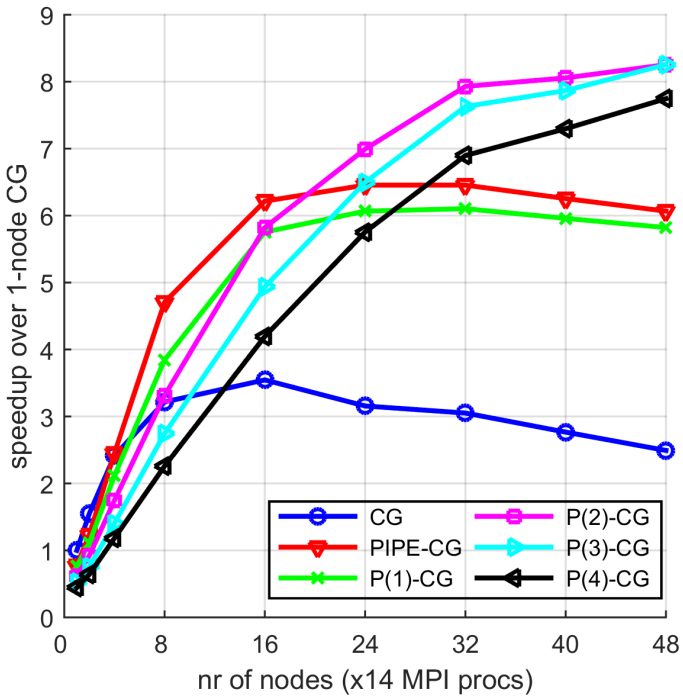
Parallel performance of pipelined CG

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

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



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



Overview of pipelined Krylov methods

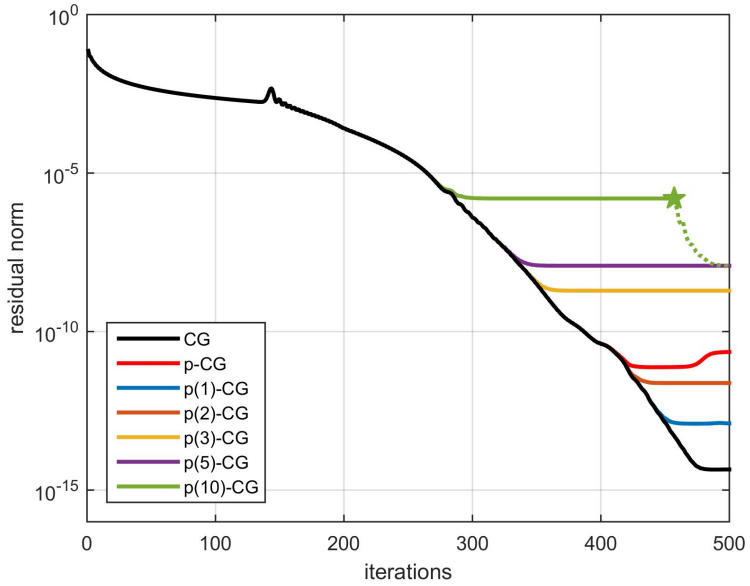
- Pipelined GMRES — Ghysels et al. (2013)
  - depth-one pipeline: p-GMRES
  - deep pipelines: p(ℓ)-GMRES: compute ℓ new Krylov subspace basis vectors (SpMV's) during global communication and orthogonalize after ℓ iterations.

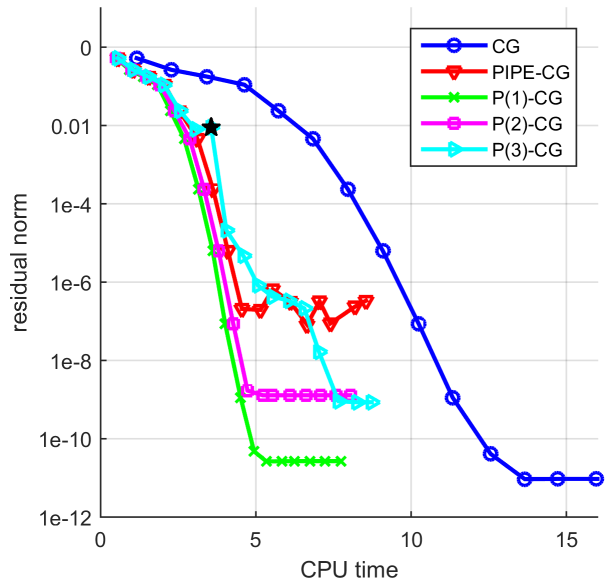
$$V_{i-\ell+1} = [v_0, v_1, \ldots, v_{i-\ell}]$$

$$Z_{i+1} = [z_0, z_1, \ldots, z_{i-\ell}, \underbrace{z_{i-\ell+1}, \ldots, z_i}_{\ell}]$$

- Pipelined CG
  - depth-one pipeline: p-CG — Ghysels et al. (2014)
  - deep pipelines: p(ℓ)-CG — Cornelis et al. (2018)
- Pipelined BiCGStab — C. & Vanroose (2017)
- Pipelined Block-CG/LOBPCG — (work in progress)
- Pipelined BiCG/CGLS/LSQR — (work in progress)
- Preconditioned pipelined variants
- Augmented/deflated/hybrid *s*-step pipelined methods — Yamazaki et al. (2017)

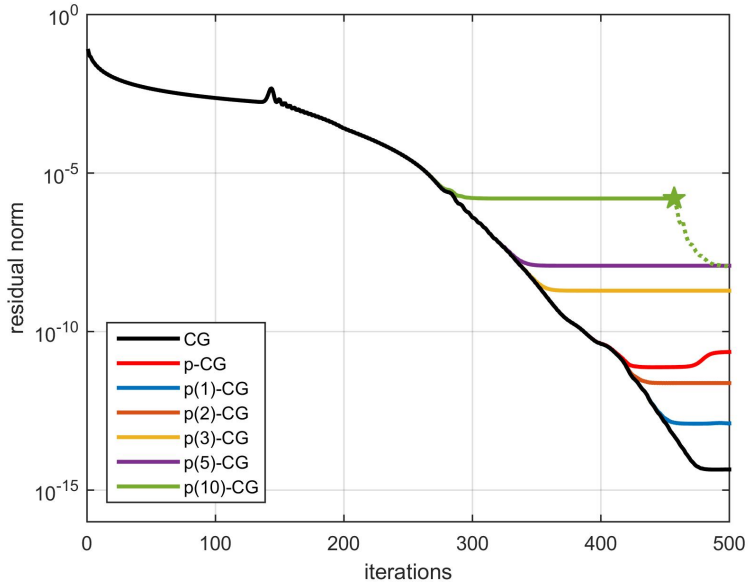
Numerical stability in finite precision

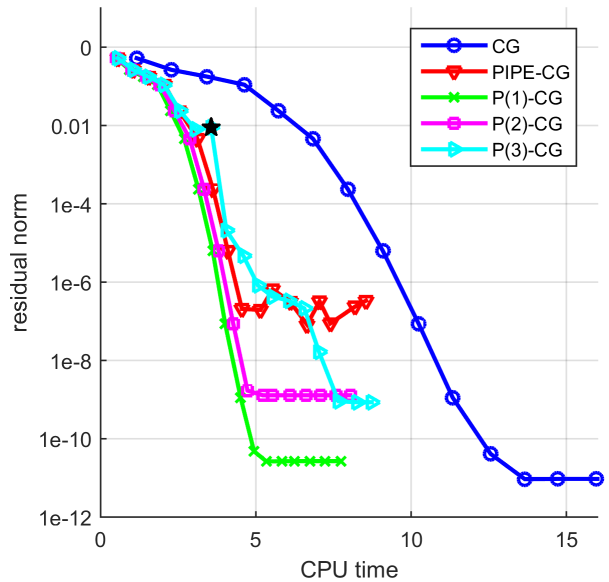




Pipelined KSM produce identical iterates to classic KSM in exact arithmetic. But finite precision computations introduce roundoff errors, which may lead to:

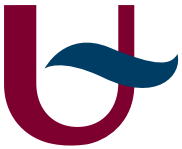
Numerical stability in finite precision





Pipelined KSM produce identical iterates to classic KSM in exact arithmetic. But finite precision computations introduce roundoff errors, which may lead to:

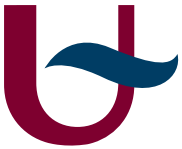
1. **Delay of convergence:** caused by loss of basis orthogonality
2. **Loss of attainable accuracy:** caused by propagation of local rounding errors in recurrences, and strongly dependent on:
   ▷ pipeline length l ▷ system size N ▷ polynomial $P_l(A)$ (basis Z_i)



Rounding error behavior in CG

Rounding errors due to recurrence relations for residual and auxiliary variables:

$$\bar{x}_{i+1} = \bar{x}_i + \bar{\alpha}_i \bar{p}_i + \xi^x_{i+1}, \qquad \bar{r}_{i+1} = \bar{r}_i - \bar{\alpha}_i A\bar{p}_i + \xi^r_{i+1}.$$



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Residual deviates from the true residual $b - A\bar{x}_{i+1}$ in finite precision:

$$\begin{aligned} f_{i+1} &= (b - A\bar{x}_{i+1}) - \bar{r}_{i+1} \\ &= b - A(\bar{x}_i + \bar{\alpha}_i \bar{p}_i + \xi^x_{i+1}) - (\bar{r}_i - \bar{\alpha}_i A\bar{p}_i + \xi^r_{i+1}) \\ &= f_0 - \sum_{k=0}^{i} (A\xi^x_{k+1} + \xi^r_{k+1}) \,. \end{aligned}$$

Sleijpen & van der Vorst (1995)

Greenbaum (1997)

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Greenbaum (1997)

Matrix notation: $\mathcal{F}_{i+1} = [f_0, \ldots, f_i]$, $\Theta^x_i = [0, \xi^x_1, \ldots, \xi^x_{i-1}]$, $\Theta^r_i = [f_0, \xi^r_1, \ldots, \xi^r_{i-1}]$

$$\mathcal{F}_{i+1} = -(A\Theta^x_{i+1} + \Theta^r_{i+1})\, U_{i+1},$$

with U_{i+1} an upper triangular matrix with all entries one.

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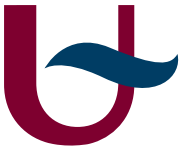
with U_{i+1} an upper triangular matrix with all entries one.

Only accumulation of local rounding errors in classical CG, no amplification.

Gutknecht & Strakos (2000)
van der Vorst & Ye (2000)



Rounding error behavior in pipelined CG

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

$$\bar{x}_{i+1} = \bar{x}_i + \bar{\alpha}_i \bar{p}_i + \xi^x_{i+1}, \qquad \bar{s}_i = \bar{w}_i + \bar{\beta}_i \bar{s}_{i-1} + \xi^s_i,$$

$$\bar{r}_{i+1} = \bar{r}_i - \bar{\alpha}_i \bar{s}_i + \xi^r_{i+1}, \qquad \bar{w}_{i+1} = \bar{w}_i - \bar{\alpha}_i \bar{z}_i + \xi^w_{i+1},$$

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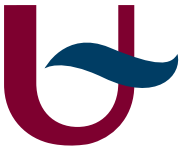

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$$\begin{pmatrix} 0 & \bar{\alpha}_0 & \bar{\alpha}_0 & \cdots & \bar{\alpha}_0 \\ & 0 & \bar{\alpha}_1 & \cdots & \bar{\alpha}_1 \\ & & \ddots & & \vdots \\ & & & 0 & \bar{\alpha}_{j-1} \\ & & & & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & \bar{\beta}_1 & \bar{\beta}_1\bar{\beta}_2 & \cdots & \bar{\beta}_1\bar{\beta}_2\ldots\bar{\beta}_j \\ & 1 & \bar{\beta}_2 & & \bar{\beta}_2\ldots\bar{\beta}_j \\ & & \ddots & & \vdots \\ & & & 1 & \bar{\beta}_j \\ & & & & 1 \end{pmatrix}$$

Note:

$\beta_i\, \beta_{i+1} \cdots \beta_j = \dfrac{\|r_j\|^2}{\|r_{i-1}\|^2} \Rightarrow$ arbitrarily large in CG!

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$$\begin{pmatrix} 0 & \bar{\alpha}_0 & \bar{\alpha}_0 & \cdots & \bar{\alpha}_0 \\ & 0 & \bar{\alpha}_1 & \cdots & \bar{\alpha}_1 \\ & & \ddots & & \vdots \\ & & & 0 & \bar{\alpha}_{j-1} \\ & & & & 0 \end{pmatrix}$$

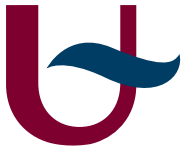
$$\begin{pmatrix} 1 & \bar{\beta}_1 & \bar{\beta}_1\bar{\beta}_2 & \cdots & \bar{\beta}_1\bar{\beta}_2\ldots\bar{\beta}_j \\ & 1 & \bar{\beta}_2 & & \bar{\beta}_2\ldots\bar{\beta}_j \\ & & \ddots & & \vdots \\ & & & 1 & \bar{\beta}_j \\ & & & & 1 \end{pmatrix}$$

Note:

$\beta_i\, \beta_{i+1} \cdots \beta_j = \dfrac{\|r_j\|^2}{\|r_{i-1}\|^2} \Rightarrow$ arbitrarily large in CG!

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

Carson et al. (2017) C. & Vanroose (2017)



Rounding error behavior in p(/)-CG

Numerical stability analysis of p(/)-CG in a nutshell

Rounding error behavior in p(*l*)-CG

Numerical stability analysis of p(*l*)-CG in a nutshell

True basis vector $\bar{\mathbf{v}}_{j+1}$ satisfies:

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Using 

, 

and 

the gap $\mathcal{F}_{j+1} = \bar{\boldsymbol{V}}_{j+1} - \bar{V}_{j+1}$ can be calculated as

$$\mathcal{F}_{j+1} = (\Theta_j^{\bar{z}}\bar{G}_j^{-1} - A\Theta_j^{\bar{v}}\bar{G}_j^{-1} + \Theta_{j+1}^{\bar{v}}\bar{B}_{j+1,j}\bar{G}_j^{-1})\bar{\Delta}_{j+1,j}^{-1}$$

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2 Computed basis vector $\bar{v}_{j+1}$ satisfies:

$$\bar{Z}_j = \bar{V}_j\bar{G}_j + \Theta_j^v$$

3 Computed basis vector $\bar{z}_{j+1}$ satisfies:

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Using 1, 2 and 3 the gap $\mathcal{F}_{j+1} = \bar{\boldsymbol{V}}_{j+1} - \bar{V}_{j+1}$ can be calculated as

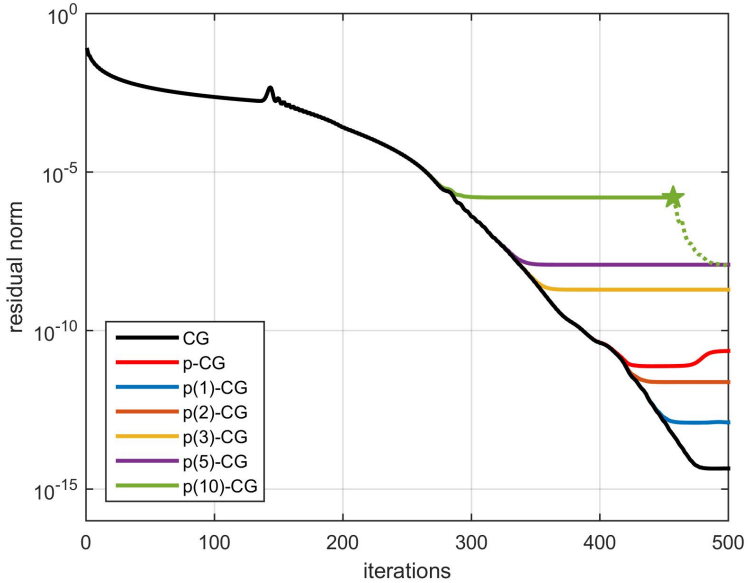
$$\mathcal{F}_{j+1} = (\Theta_j^v\bar{G}_j^{-1} - A\Theta_j^v\bar{G}_j^{-1} + \Theta_{j+1}^{\bar{v}}\bar{B}_{j+1,j}\bar{G}_j^{-1})\bar{\Delta}_{j+1,j}^{-1}$$

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

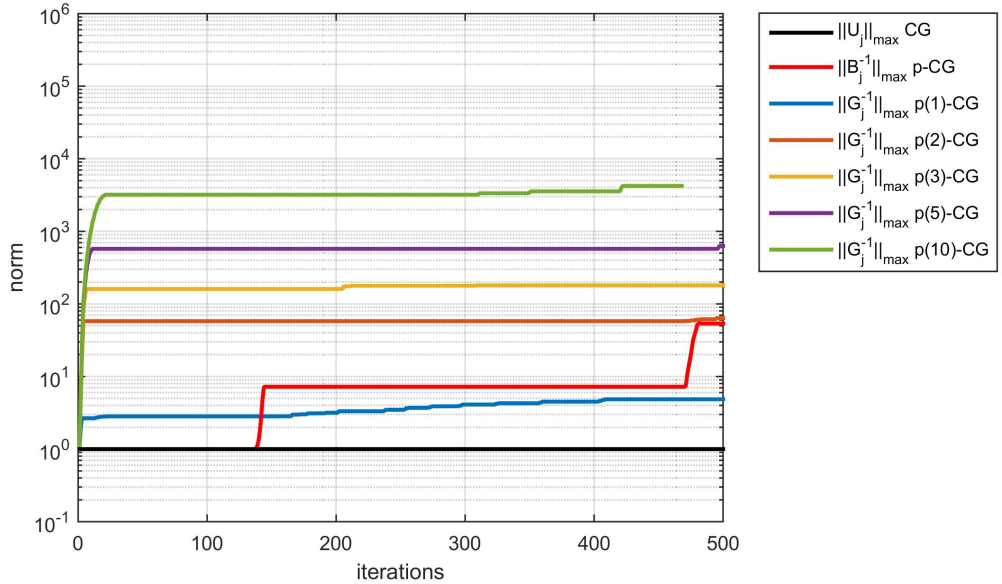
Carson & Demmel (2014) C. (2018)

Rounding error behavior in p(l)-CG

residual history $\|b - A\bar{x}_i\|_2$



$\|G_i^{-1}\|_{\max}$ for different l



- Maximum norm $\|G_i^{-1}\|_{\max}$ provides a measure for the impact of local rounding error propagation on maximal attainable accuracy in p(l)-CG

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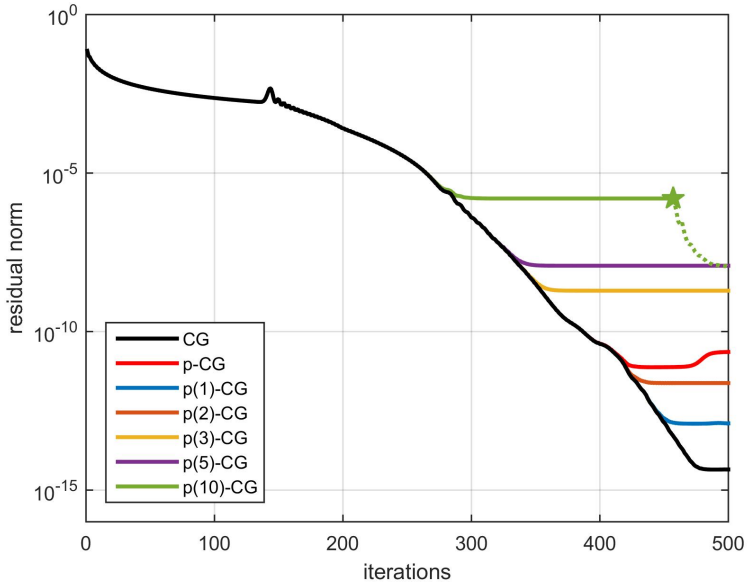

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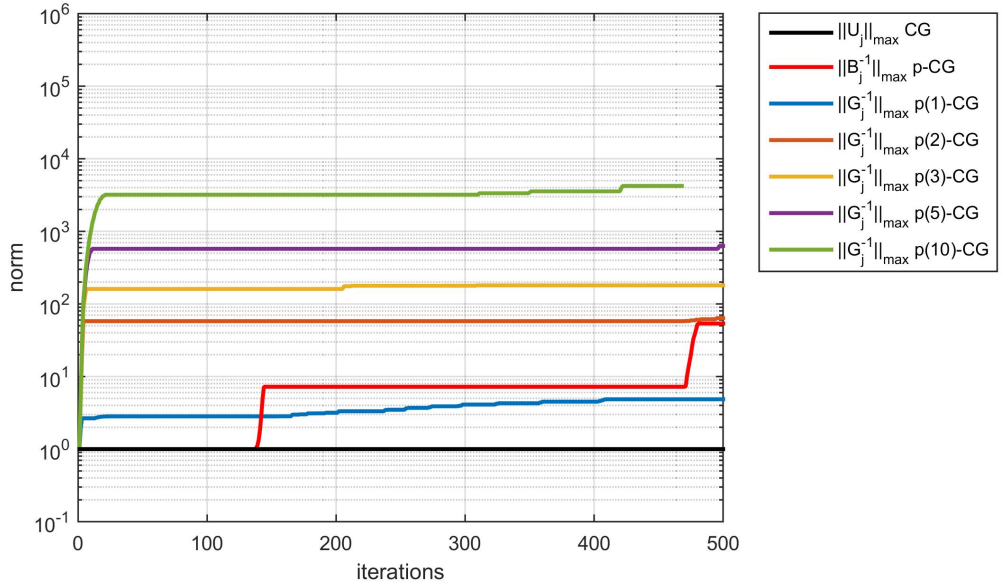
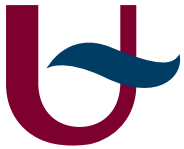


- Maximum norm $\|G_i^{-1}\|_{\max}$ provides a measure for the impact of local rounding error propagation on maximal attainable accuracy in p(l)-CG
- Rounding error analysis explains loss of attainable accuracy w.r.t.
  ▷ pipeline length l ▷ system size N ▷ polynomial $P_l(A)$ (basis Z_i)



Residual replacement in pipelined CG

- Core idea: improve accuracy by replacing $\bar{r}_i$, $\bar{s}_i$, $\bar{w}_i$ and $\bar{z}_i$ by their true values in selected iterations (causing minor computational overhead):

$$\bar{r}_i = \mathrm{fl}(b - A\bar{x}_i), \quad \bar{w}_i = \mathrm{fl}(A\bar{r}_i), \quad \bar{s}_i = \mathrm{fl}(A\bar{p}_i), \quad \bar{z}_i = \mathrm{fl}(A\bar{s}_i).$$

van der Vorst & Ye (2000)

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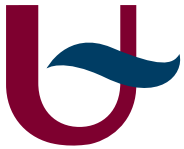
van der Vorst & Ye (2000)

- Replacement criterion: choose when to replace based on (an estimate of) the gap $\|f_i\| = \|(b - A\bar{x}_i) - \bar{r}_i\|$:

$$\|f_{i-1}\| \leq \tau \|\bar{r}_{i-1}\| \quad \text{and} \quad \|f_i\| > \tau \|\bar{r}_i\| \qquad \text{with } \tau = \sqrt{\epsilon}.$$

  - Replace sufficiently often such that $\|f_i\|$ remains small
  - Don't replace when $\|\bar{r}_i\|$ is too small, which may cause delay of convergence

Sleijpen & van der Vorst (1996) Strakos & Tichy (2002)



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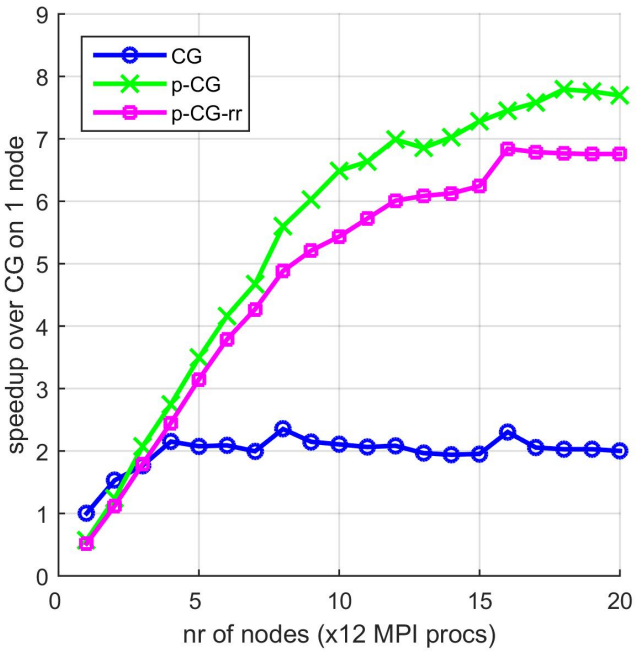
- Automated residual replacements: estimate of $\|f_i\|$ is computed at runtime (inexpensive). In many cases accuracy is significantly improved.

C. & Vanroose (2017)

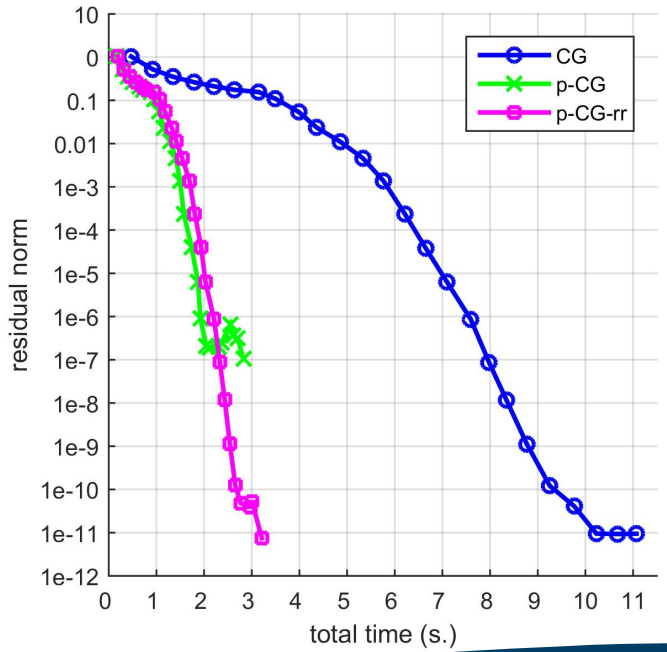
Residual replacement in pipelined CG

- PETSc implementation using MPICH-3.1.3 communication
- Benchmark problem: 2D Laplacian model, 1,000,000 unknowns
- System specs: 20 nodes, two 6-core Intel Xeon X5660 Nehalem 2.8GHz CPUs/node

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



Accuracy i.f.o. total time spent (240 cores)

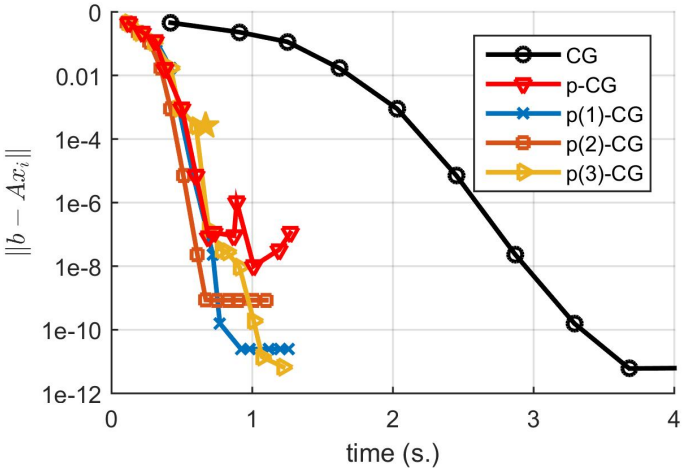


Numerically stable variant of p(l)-CG

Use idea similar to residual replacement to improve stability: replace recurrence for v_{j+1} by the Arnoldi relation:

Original p(l)-CG:

$$v_{j+1} = \left(z_{j+1} - \sum_{k=j-2l+1}^{j} g_{k,j+1} v_k \right) / g_{j+1,j+1}$$



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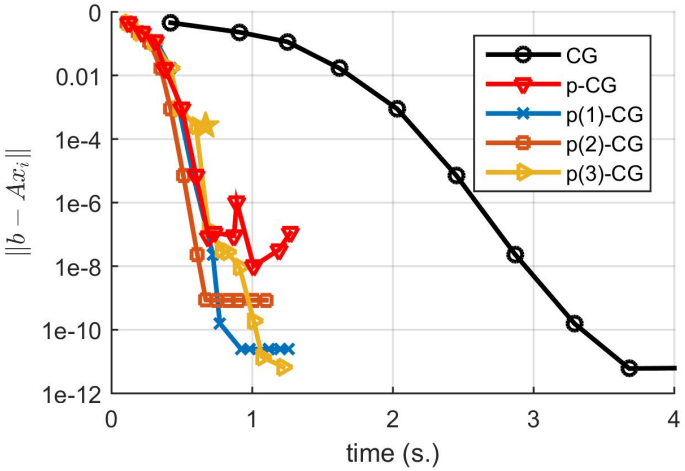
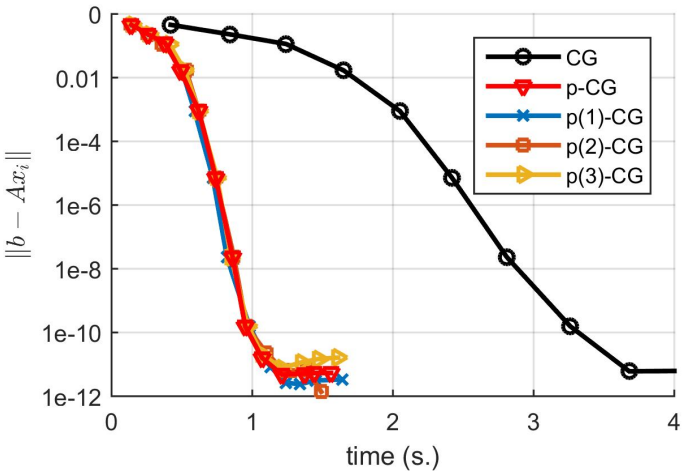
Stabilized p(l)-CG:

$$v_{j+1} = (A v_j - \gamma_j v_j - \delta_{j-1} v_{j-1}) / \delta_j$$





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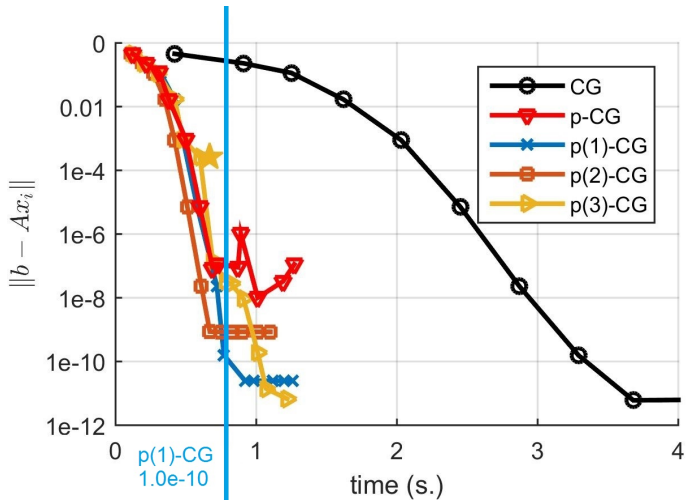
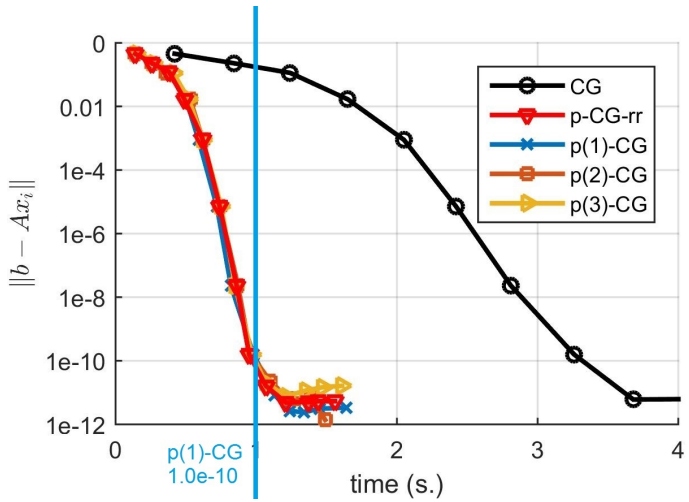
Stabilized p(l)-CG:

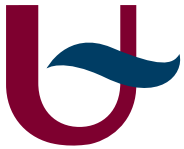
$$v_{j+1} = (Av_j - \gamma_j v_j - \delta_{j-1} v_{j-1}) / \delta_j$$

Attainable accuracy is improved for all pipeline lengths l, but extra SpMV increases computation time

$\Rightarrow$ trade-off between numerical stability and performance

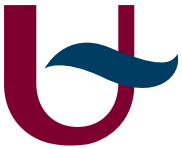






Wrap-up of this talk

- Pipelined Krylov subspace methods are a promising approach to reduce synchronization cost in linear solvers for large-scale problems
  - By adding *auxiliary variables* and recurrences it is possible to *hide* communication latency behind computational kernels
  - *Deep pipelines* allow to hide global reductions behind multiple SpMV's
  - *Asynchronous implementation*: dot-products can take multiple iterations to complete, 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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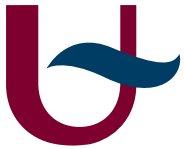
- Finite precision behavior of communication reducing and hiding algorithms should be carefully monitored!
  - *Rounding error analysis* allows to explain observed loss of attainable accuracy
  - *Residual replacement* -type techniques can be applied to improve numerical stability, but at a (slight) increase in computational cost



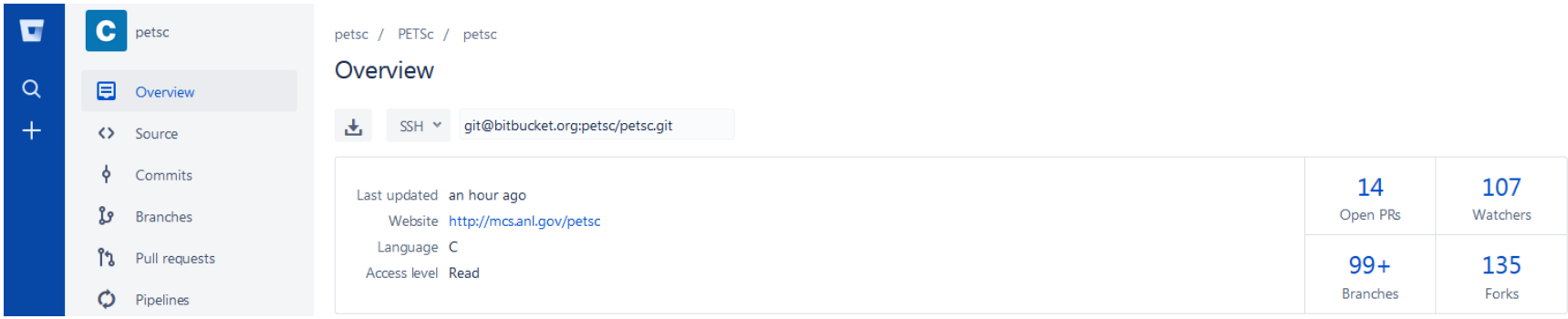
Related work

- Work in progress (not covered in this talk):
  - Impact of *hard faults* & *soft-errors* on pipelined Krylov subspace methods (INRIA Bordeaux)
  - Resilience of pipelined Krylov subspace methods to *system noise* (UChicago/ETHZ/Rice/UIllinois)
  - *Pipelined Lanczos* for eigenvalue calculation in graph partitioning algorithms (UAntwerp/LBNL)
  - *Pipelined Blocked* Krylov subspace methods for systems with multiple rhs (UAntwerp/INRIA Bordeaux)
  - *Communication avoiding/hiding LOBPCG* for eigenvalue calculations (UAntwerp/LBNL)

- Many interesting open problems and challenges remain as we push toward exascale-level computing!

Contributions to PETSc

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



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

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We are soliciting for feedback from your applications!

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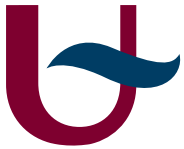

Thank you!

siegfried.cools@uantwerp.be

https://www.uantwerpen.be/en/staff/siegfried-cools

Publications

- 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. C48C71, 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.
- S. Cools, W. Vanroose, *The communication-hiding pipelined BiCGStab method for the parallel solution of large unsymmetric linear systems.* Parallel Computing, 65, pp. 1-20, Elsevier, 2017.
- J. Cornelis, S. Cools, W. Vanroose, *The communication-hiding Conjugate Gradient method with deep pipelines.* Submitted to SIAM J. Sci. Comput., 2018, Preprint available at arXiv:1801.04728.
- S. Cools, *Numerical stability analysis of the class of communication hiding pipelined Conjugate Gradient methods.* Submitted to SIAM J. Sci. Comput., 2018, Preprint available at arXiv:1804.02962.