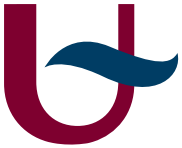


Hiding Global Reduction Latency in Pipelined Krylov Methods

On Parallel Performance and Numerical Stability of the Pipelined Conjugate Gradient and BiCGStab Algorithms for Solving Large Scale Linear Systems

PARCO 2017, Savoia Hotel Regency, Bologna, Italy, September 12-15, 2017

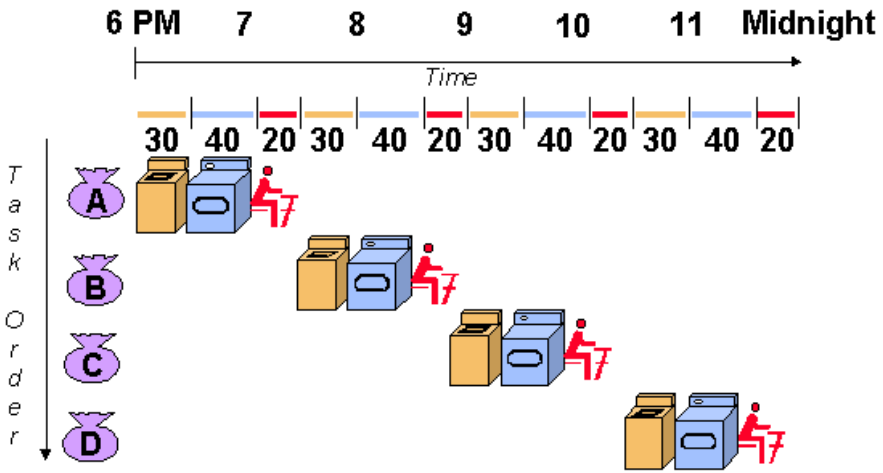
University of Antwerp* [BE], LBNL‡ [US], INRIA Bordeaux† [FR]

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

Contact: siegfried.cools@uantwerp.be

Universiteit Antwerpen

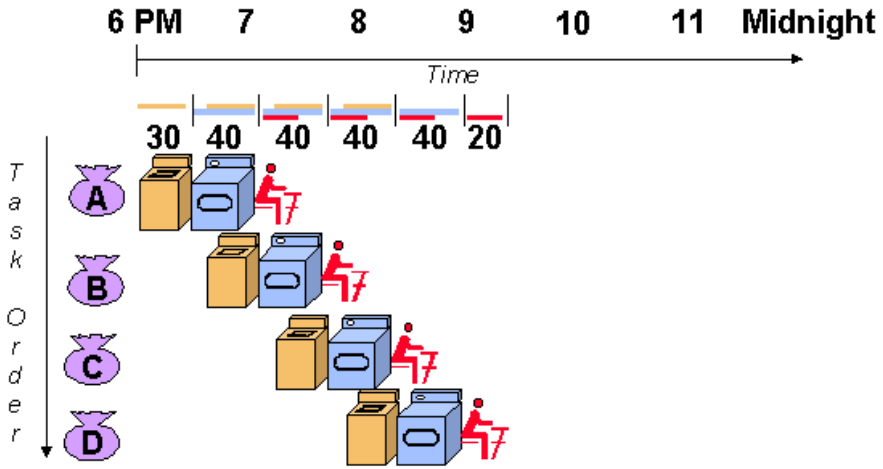
What are we working on?



Classical Krylov subspace method

Washing, *drying* *and* *ironing*
in classical 'Laundry method'

vs.



Pipelined Krylov subspace method

Latency hiding of global *drying*
in pipelined 'Laundry method'

Our benefactors

Work initiated under:

EXascale Algorithms and Advanced Computational Techniques

`http://exa2ct.eu/`

EU FP7 Project - Horizon 2020 - Ran from 2013 to 2016

Fellowship 12H4617N
(2016-2019)

Observation: increasing gap between computation and communication costs

- Floating point performance steadily increases
- Network latencies only go down marginally
- Memory latencies decline slowly
- Avoid communication:
  trade communication for computations
- Hide communication:
  overlap communication with computations

General idea

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

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

- minimize an error measure over expanding Krylov subspace $\mathcal{K}_i(A, r_0)$
- usually in combination with sparse linear algebra/stencil application
- three building blocks:
  i. dot-product
  ii. SpMV
  iii. axpy

E.g. Conjugate Gradients

Algorithm 1 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: $s_i := Ap_i$
5: $\alpha_i := (r_i, r_i) \,/\, (s_i, p_i)$
6: $x_{i+1} := x_i + \alpha_i p_i$
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**

dot-pr
SpMV
axpy

Classical CG

Algorithm 1 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: $s_i := Ap_i$
5: $\alpha_i := (r_i, r_i) / (s_i, p_i)$
6: $x_{i+1} := x_i + \alpha_i p_i$
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**

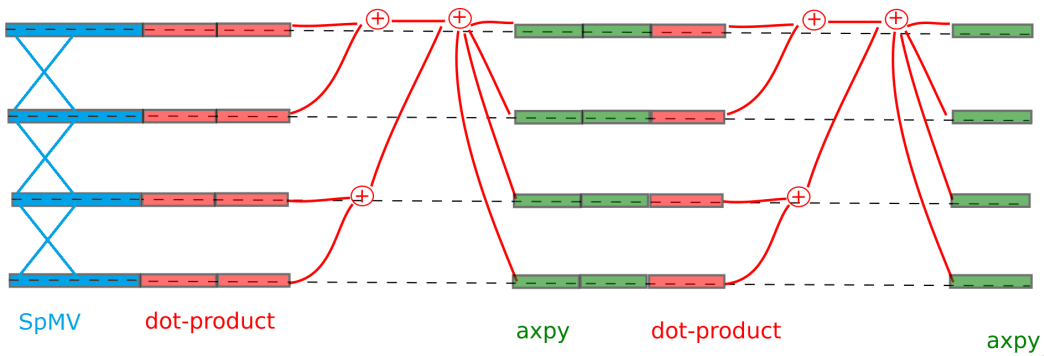
dot-pr
SpMV
axpy

Hestenes & Stiefel (1952)

i. 3 dot-products
- 2 global reduction phases
- latency dominated
- scales as $log_2(\#partitions)$

ii. 1 SpMV
- scales well (minor commun.)
- non-overlapping (sequential to dot-product)

iii. 3 axpy's
- recurrences (vector operations)
- perfectly scalable (no commun.)



Pipelined CG

Algorithm 3 Pipelined CG

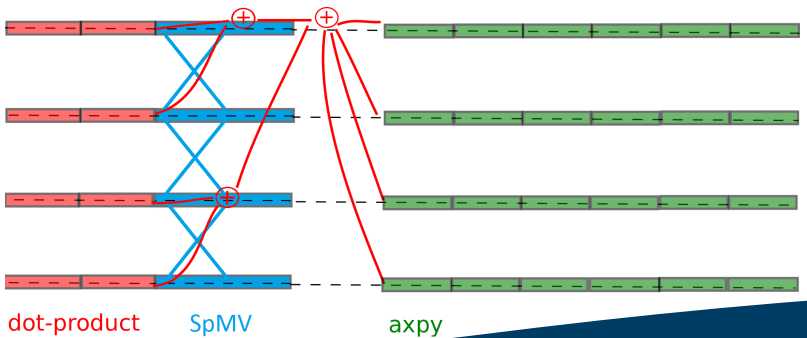
1: **procedure** PIPE-CG(A, b, x_0)
2: $r_0 := b - Ax_0$; $w_0 := Ar_0$
3: **for** $i = 0, \ldots$ **do**
4: $\gamma_i := (r_i, r_i)$
5: $\delta := (w_i, r_i)$
6: $q_i := Aw_i$
7: **if** $i > 0$ **then**
8: $\beta_i := \gamma_i/\gamma_{i-1}$; $\alpha_i := (\delta/\gamma_i - \beta_i/\alpha_{i-1})^{-1}$
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: $p_i := r_i + \beta_i p_{i-1}$
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**

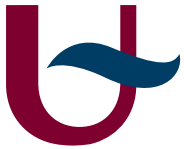
dot-pr
SpMV
axpy

Ghysels & Vanroose (2013)

Re-organized version of classical CG for improved parallel performance

- equivalent to CG in exact arithmetic
- Communication avoiding: dot-products are grouped in one global reduction phase (line 4+5)
- Communication hiding: overlap global commun. (line 4+5) with computations (SpMV, line 6)
- 3 extra recurrences for $s_i = Ap_i$, $w_i = Ar_i$, $z_i = As_i$ (line 12+13+17)





BiCGStab

Algorithm 4 Standard BiCGStab

1: **function** BICGSTAB(A, b, x_0)
2: $r_0 := b - Ax_0$; $p_0 := r_0$
3: **for** $i = 0, \ldots$ **do**
4: $s_i := Ap_i$
5: **compute** (r_0, s_i)
6: $\alpha_i := (r_0, r_i) \,/\, (r_0, s_i)$
7: $q_i := r_i - \alpha_i s_i$
8: $y_i := Aq_i$
9: **compute** (q_i, y_i) ; (y_i, y_i)
10: $\omega_i := (q_i, y_i) \,/\, (y_i, y_i)$
11: $x_{i+1} := x_i + \alpha_i p_i + \omega_i q_i$
12: $r_{i+1} := q_i - \omega_i y_i$
13: **compute** (r_0, r_{i+1})
14: $\beta_i := (\alpha_i/\omega_i)\,(r_0, r_{i+1}) \,/\, (r_0, r_i)$
15: $p_{i+1} := r_{i+1} + \beta_i\,(p_i - \omega_i s_i)$
16: **end for**
17: **end function**

dot-prod
SpMV
axpy

Traditional BiCGStab:

(non-preconditioned)

Global communication

- 3 global reduction phases

Local communication

- 2 SpMVs

No communication

- 4 recurrences

General two-step framework for deriving pipelined Krylov methods:

Step 1. Avoiding communication: merge global reductions

Step 2. Hiding communication: overlap SpMVs & global reductions

Step 1. Avoiding communication

Algorithm 4 Standard BiCGStab

1: **function** BICGSTAB(A, b, x_0)
2: $r_0 := b - Ax_0$; $p_0 := r_0$
3: **for** $i = 0, \ldots$ **do**
4: $s_i := Ap_i$
5: **compute** (r_0, s_i)
6: $\alpha_i := (r_0, r_i) \,/\, (r_0, s_i)$
7: $q_i := r_i - \alpha_i s_i$
8: $y_i := Aq_i$
9: **compute** (q_i, y_i) ; (y_i, y_i)
10: $\omega_i := (q_i, y_i) \,/\, (y_i, y_i)$
11: $x_{i+1} := x_i + \alpha_i p_i + \omega_i q_i$
12: $r_{i+1} := q_i - \omega_i y_i$
13: **compute** (r_0, r_{i+1})
14: $\beta_i := (\alpha_i/\omega_i)\,(r_0, r_{i+1}) \,/\, (r_0, r_i)$
15: $p_{i+1} := r_{i+1} + \beta_i\,(p_i - \omega_i s_i)$
16: **end for**
17: **end function**

dot-prod
SpMV
axpy

(a) *Identify* two global comm. phases for merger (lines 5-6 & 13-14)

(b) *Rewrite* SpMV as recurrence:

$$s_i = Ap_i = w_i + \beta_{i-1}\,(s_{i-1} - \omega_{i-1} z_{i-1})\,,$$

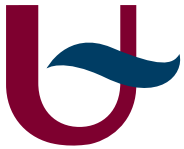
define $w_i := Ar_i$, $z_i := As_i$ and note that $y_i := w_i - \alpha_i z_i$

(c) *Rewrite* dot-product using (b):

$$(r_0, s_i) = (r_0, w_i + \beta_{i-1}\,(s_{i-1} - \omega_{i-1} z_{i-1}))\,,$$

independent of interlying variables

(d) *Move* dot-product (lines 5-6) upward and merge with existing global comm. phase (lines 13-14)



CA-BiCGStab

Algorithm 5 Communication avoiding BiCGStab

1: **function** CA-BICGSTAB(A, b, x_0)
2: $r_0 := b - Ax_0$; $w_0 := Ar_0$; $\alpha_0 := (r_0, r_0) \,/\, (r_0, w_0)$; $\beta_{-1} := 0$
3: **for** $i = 0, \ldots$ **do**
4: $p_i := r_i + \beta_{i-1} (p_{i-1} - \omega_{i-1} s_{i-1})$
5: $s_i := w_i + \beta_{i-1} (s_{i-1} - \omega_{i-1} z_{i-1})$
6: $z_i := As_i$
7: $q_i := r_i - \alpha_i s_i$ **dot-prod**
8: $y_i := w_i - \alpha_i z_i$ **SpMV**
9: **compute** (q_i, y_i) ; (y_i, y_i) **axpy**
10: $\omega_i := (q_i, y_i) \,/\, (y_i, y_i)$
11: $x_{i+1} := x_i + \alpha_i p_i + \omega_i q_i$
12: $r_{i+1} := q_i - \omega_i y_i$
13: $w_{i+1} := Ar_{i+1}$
14: **compute** (r_0, r_{i+1}) ; (r_0, w_{i+1}) ; (r_0, s_i) ; (r_0, z_i)
15: $\beta_i := (\alpha_i / \omega_i) \, (r_0, r_{i+1}) \,/\, (r_0, r_i)$
16: $\alpha_{i+1} := (r_0, r_{i+1}) \,/\, ((r_0, w_{i+1}) + \beta_i (r_0, s_i) - \beta_i \omega_i (r_0, z_i))$
17: **end for**
18: **end function**

Communication-avoiding BiCGStab:
(non-preconditioned)

Global communication

- 2 global red. phases (vs. 3)

Local communication

- 2 SpMVs

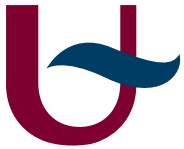
No communication

- 6 recurrences (vs. 4)

Status after Step 1:

number of global comm. phases reduced from 3 to 2, at the cost of 2 axpys

Note: further reduction from 2 to 1 global comm. phase possible, but not recommended (see later).



Step 2. Hiding communication

Algorithm 5 Communication avoiding BiCGStab

1: **function** CA-BICGSTAB(A, b, x_0)
2: $r_0 := b - Ax_0$; $w_0 := Ar_0$; $\alpha_0 := (r_0, r_0) \,/\, (r_0, w_0)$; $\beta_{-1} := 0$
3: **for** $i = 0, \ldots$ **do**
4: $p_i := r_i + \beta_{i-1} (p_{i-1} - \omega_{i-1} s_{i-1})$
5: $s_i := w_i + \beta_{i-1} (s_{i-1} - \omega_{i-1} z_{i-1})$
6: $z_i := As_i$
7: $q_i := r_i - \alpha_i s_i$ **dot-prod**
8: $y_i := w_i - \alpha_i z_i$ **SpMV**
9: **compute** (q_i, y_i) ; (y_i, y_i) **axpy**
10: $\omega_i := (q_i, y_i) \,/\, (y_i, y_i)$
11: $x_{i+1} := x_i + \alpha_i p_i + \omega_i q_i$
12: $r_{i+1} := q_i - \omega_i y_i$
13: $w_{i+1} := Ar_{i+1}$
14: **compute** (r_0, r_{i+1}) ; (r_0, w_{i+1}) ; (r_0, s_i) ; (r_0, z_i)
15: $\beta_i := (\alpha_i / \omega_i) \, (r_0, r_{i+1}) \,/\, (r_0, r_i)$
16: $\alpha_{i+1} := (r_0, r_{i+1}) \,/\, ((r_0, w_{i+1}) + \beta_i (r_0, s_i) - \beta_i \omega_i (r_0, z_i))$
17: **end for**
18: **end function**

(a) *Identify* SpMV / global reduction pairs (lines 6 & 9 and 13 & 14)

(b) *Rewrite* SpMVs as recurrences:

$$z_i := As_i = t_i + \beta_{i-1} (z_{i-1} - \omega_{i-1} v_{i-1}),$$
$$w_{i+1} := Ar_{i+1} = y_i - \omega_i (t_i - \alpha_i v_i),$$

define $t_i := Aw_i$, $v_i := Az_i$

(c) *Check* SpMV / global reduction pairwise dependencies:

- line 9 independent of v_i? **yes**
- line 14 indep. of t_{i+1}? **yes**

(d) *Insert* new SpMVs *below* corresponding global comm. phases

pipe-BiCGStab

Algorithm 6 Pipelined BiCGStab

1: **function** PIPE-BICGSTAB(A, b, x_0)
2: $r_0 := b - Ax_0$; $w_0 := Ar_0$; $t_0 := Aw_0$;
3: **for** $i = 0, \ldots$ **do**
4: $p_i := r_i + \beta_{i-1}(p_{i-1} - \omega_{i-1}s_{i-1})$
5: $s_i := w_i + \beta_{i-1}(s_{i-1} - \omega_{i-1}z_{i-1})$
6: $z_i := t_i + \beta_{i-1}(z_{i-1} - \omega_{i-1}v_{i-1})$
7: $q_i := r_i - \alpha_i s_i$
8: $y_i := w_i - \alpha_i z_i$
9: **compute** (q_i, y_i) ; (y_i, y_i)
10: $\omega_i := (q_i, y_i) / (y_i, y_i)$
11: **overlap** $v_i := Az_i$
12: $x_{i+1} := x_i + \alpha_i p_i + \omega_i q_i$
13: $r_{i+1} := q_i - \omega_i y_i$
14: $w_{i+1} := y_i - \omega_i (t_i - \alpha_i v_i)$
15: **compute** (r_0, r_{i+1}) ; (r_0, w_{i+1}) ; (r_0, s_i) ; (r_0, z_i)
16: $\beta_i := (\alpha_i/\omega_i)(r_0, r_{i+1}) / (r_0, r_i)$
17: $\alpha_{i+1} := (r_0, r_{i+1}) / ((r_0, w_{i+1}) + \beta_i (r_0, s_i) - \beta_i\omega_i (r_0, z_i))$
18: **overlap** $t_{i+1} := Aw_{i+1}$
19: **end for**
20: **end function**

dot-prod
SpMV
axpy

Pipelined BiCGStab:

(non-preconditioned)

Global communication

- 2 global red. phases (vs. 3)

Local communication

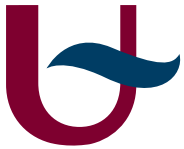
- 2 overlapping SpMVs

No communication

- 8 recurrences (vs. 4)

Status after Step 2:

both global comm. phases are overlapped with SpMV computations ('hidden'), at the cost of 4 additional axpys compared to standard BiCGStab



Bi-Conjugate Gradients Stabilized

Preconditioned pipe-BiCGStab

Algorithm 8 Preconditioned Pipelined BiCGStab

1: **function** P-PIPE-BICGSTAB(A, M^{-1}, b, x_0)
2: $r_0 := b - Ax_0$; $\hat{r}_0 := M^{-1}r_0$; $w_0 := A\hat{r}_0$; $\hat{w}_0 := M^{-1}w_0$
3: $t_0 := A\hat{w}_0$; $\alpha_0 := (r_0, r_0) \,/\, (r_0, w_0)$; $\beta_{-1} := 0$
4: **for** $i = 0, \ldots$ **do**
5: $\hat{p}_i := \hat{r}_i + \beta_{i-1}(\hat{p}_{i-1} - \omega_{i-1}\hat{s}_{i-1})$
6: $s_i := w_i + \beta_{i-1}(s_{i-1} - \omega_{i-1}z_{i-1})$
7: $\hat{s}_i := \hat{w}_i + \beta_{i-1}(\hat{s}_{i-1} - \omega_{i-1}\hat{z}_{i-1})$
8: $z_i := t_i + \beta_{i-1}(z_{i-1} - \omega_{i-1}v_{i-1})$
9: $q_i := r_i - \alpha_i s_i$
10: $\hat{q}_i := \hat{r}_i - \alpha_i \hat{s}_i$
11: $y_i := w_i - \alpha_i z_i$
12: **compute** (q_i, y_i) ; (y_i, y_i)
13: $\omega_i := (q_i, y_i) \,/\, (y_i, y_i)$
14: **overlap** $\hat{z}_i := M^{-1}z_i$
15: **overlap** $v_i := A\hat{z}_i$
16: $x_{i+1} := x_i + \alpha_i\hat{p}_i + \omega_i\hat{q}_i$
17: $r_{i+1} := q_i - \omega_i y_i$
18: $\hat{r}_{i+1} := \hat{q}_i - \omega_i(\hat{w}_i - \alpha_i\hat{z}_i)$
19: $w_{i+1} := y_i - \omega_i(t_i - \alpha_i v_i)$
20: **compute** (r_0, r_{i+1}) ; (r_0, w_{i+1}) ; (r_0, s_i) ; (r_0, z_i)
21: $\beta_i := (\alpha_i/\omega_i)\,(r_0, r_{i+1}) \,/\, (r_0, r_i)$
22: $\alpha_{i+1} := (r_0, r_{i+1}) \,/\, ((r_0, w_{i+1}) + \beta_i(r_0, s_i) - \beta_i\omega_i(r_0, z_i))$
23: **overlap** $\hat{w}_{i+1} := M^{-1}w_{i+1}$
24: **overlap** $t_{i+1} := A\hat{w}_{i+1}$
25: **end for**
26: **end function**

dot-prod
SpMV
axpy

Like for any pipelined method, including a preconditioner is - in theory - easy.

Pipelined BiCGStab:

(preconditioned)

Global communication

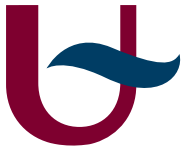
- 2 global red. phases (vs. 3)

Local communication

- 2 overlapping Prec + SpMVs

No communication

- 11 recurrences (vs. 4)



Pipe-BiCGStab vs. IBiCGStab vs. s-step CA-BiCGStab

	GLRED	SPMV	Flops (AXPY + DOT-PROD)	Time (GLRED + SPMV)	Memory
BiCGStab	3	2	20	3 GLRED + 2 SPMV	7
IBiCGStab	1	2	30	1 GLRED + 2 SPMV	10
p-BiCGStab	2	2*	38	2 max(GLRED, SPMV)	11
s-step CA-BiCGStab	$1/s$	4	$32s$+45	$1/s$ GLRED + 4 SPMV	$4s$+5

Theoretical speed-up factors over classical BiCGStab:

	pipe-BiCGStab C., Vanroose, 2017	IBiCGStab Yang & Brent, 2002	CA-BiCGStab Carson, 2015
if time(GLRED) $\approx$ time(SPMV)	$\times$ 2.5	$\times$ 1.67	$\times$ 1.25
if time(GLRED) $\gg$ time(SPMV)	$\times$ 1.5	$\times$ 3.0	$\times$ $3s$

Is algorithm with 1 GLRED overlapped with all SPMVs possible? Yes; however...

- no. axpys is much larger $\rightarrow$ algorithm robustness decreases (rounding errors)
- one extra SpMV required per iteration

Other pipelined Krylov methods

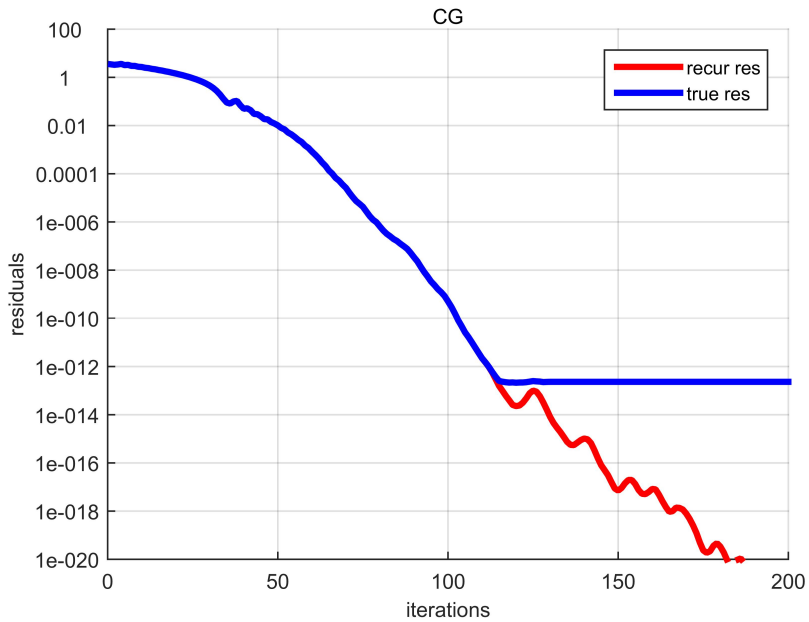
- Pipelined GMRES — Ghysels et al. (2013)

$$V_{i-\ell+1} = [v_0, v_1, \ldots, v_{i-\ell}]$$
$$Z_{i+1} = [z_0, z_1, \ldots, z_{i-\ell}, \underbrace{z_{i-\ell+1}, \ldots, z_i}_{\ell}]$$

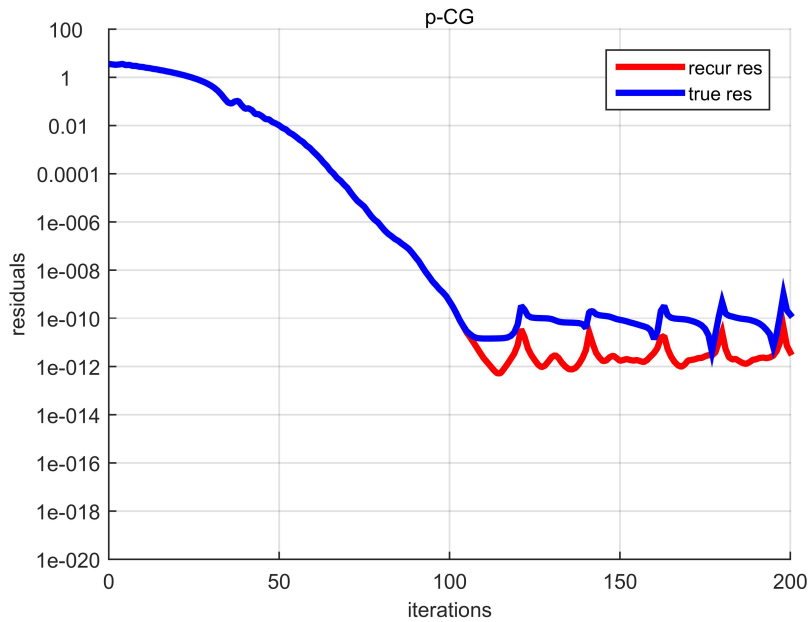
  - compute ℓ new basis vectors for Krylov subspace (SpMVs) during global communication (dot-products), orthogonalize after ℓ iterations.
  - deeper/variable pipelining possible: p(ℓ)-GMRES
- Pipelined CG — Ghysels et al. (2014)
  - deeper pipelining also possible: p(ℓ)-CG
- Pipelined BiCGStab — C., Vanroose (2017)
  - non-symmetric operators
- Preconditioned pipelined variants are available
  - prec-pipe-CG / prec-pipe-GMRES / prec-pipe-BiCGStab
- Augmented/deflated/hybrid *s*-step pipelined methods are available — Yamazaki et al. (2017)

Rounding error propagation

Classical CG



Pipelined CG



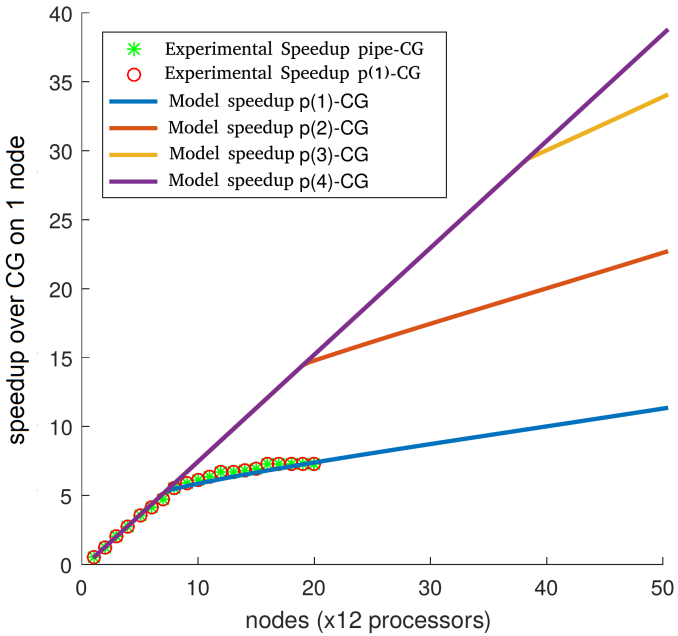
Observation: pipe-CG loses max. attainable accuracy compared to classical CG

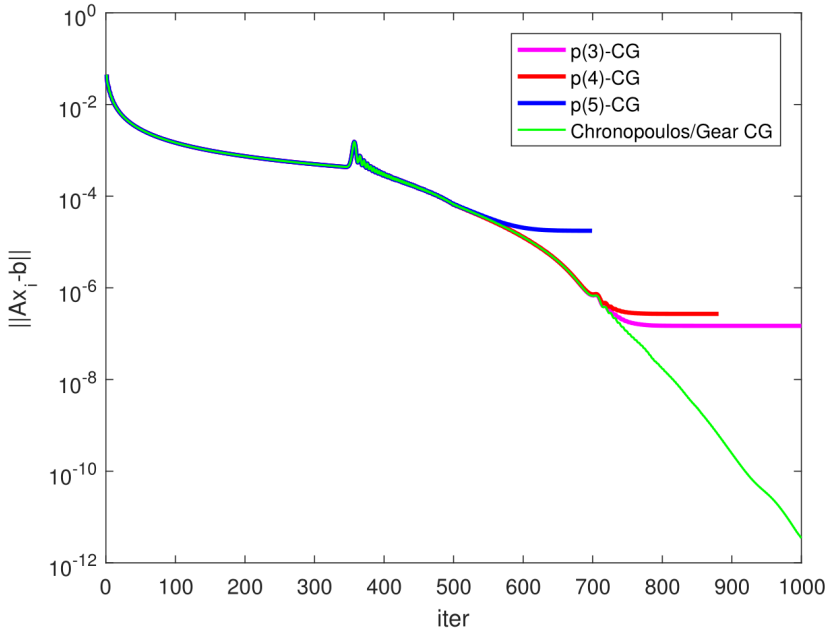
- Model problem: small 2D Laplacian with 2,500 unknowns
- Loss of attainable accuracy is more pronounced for larger systems/longer pipelines

Rounding error propagation

Pipe(ℓ)-CG: length ℓ pipeline

J. Cornelis, MaTh (2017)





Observation: pipe-CG loses max. attainable accuracy compared to classical CG

- Model problem: medium-sized 2D Laplacian with 250,000 unknowns
- Loss of attainable accuracy is more pronounced for larger systems/longer pipelines

Rounding error propagation in CG

Rounding errors due to recursive definition of residual (and auxiliary variables)

$$\begin{aligned} \bar{p}_{i+1} &= \bar{u}_{i+1} + \bar{\beta}_{i+1}\bar{p}_i + \delta_i^p, \\ \bar{x}_{i+1} &= \bar{x}_i + \bar{\alpha}_i\bar{p}_i + \delta_i^x, \\ \bar{r}_{i+1} &= \bar{r}_i - \bar{\alpha}_i A\bar{p}_i + \delta_i^r, \end{aligned}$$

which deviates from the true residual $b - A\bar{x}_i$ in finite precision arithmetics

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

After i iterations:

$$f_{i+1} = f_0 - \sum_{j=0}^{i} \left(A\delta_j^x + \delta_j^r\right).$$

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

Greenbaum (1997), Gutknecht & Strakos (2000)

Rounding errors in pipe-CG

Observation: *rounding error propagation in pipe-CG may be much more dramatic due to additional recurrence relations that all induce rounding errors.*

$$\bar{x}_{i+1} = \bar{x}_i + \bar{\alpha}_i \bar{p}_i + \delta_i^x, \qquad \bar{s}_i = \bar{w}_i + \bar{\beta}_i \bar{s}_{i-1} + \delta_i^s,$$
$$\bar{r}_{i+1} = \bar{r}_i - \bar{\alpha}_i \bar{s}_i + \delta_i^r, \qquad \bar{w}_{i+1} = \bar{w}_i - \bar{\alpha}_i \bar{z}_i + \delta_i^w,$$
$$\bar{p}_i = \bar{u}_i + \bar{\beta}_i \bar{p}_{i-1} + \delta_i^p, \qquad \bar{z}_i = A\bar{m}_i + \bar{\beta}_i \bar{z}_{i-1} + \delta_i^z,$$

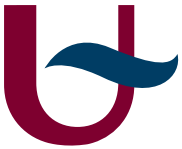
Residual gap is **coupled** with the gaps on the other auxiliary variables:

$$f_i = (b - A\bar{x}_i) - \bar{r}_i, \quad g_i = A\bar{p}_i - \bar{s}_i, \quad h_i = A\bar{u}_i - \bar{w}_i, \quad j_i = A\bar{q}_i - \bar{z}_i$$

$$\begin{bmatrix} f_{i+1} \\ g_i \\ h_{i+1} \\ j_i \end{bmatrix} = \begin{bmatrix} 1 & -\bar{\alpha}_i\bar{\beta}_i & -\bar{\alpha}_i & 0 \\ 0 & \bar{\beta}_i & 1 & 0 \\ 0 & 0 & 1 & -\bar{\alpha}_i\bar{\beta}_i \\ 0 & 0 & 0 & \bar{\beta}_i \end{bmatrix} \begin{bmatrix} f_i \\ g_{i-1} \\ h_i \\ j_{i-1} \end{bmatrix} + \begin{bmatrix} -A\delta_i^x - \delta_i^r - \bar{\alpha}_i\left(A\delta_i^p - \delta_i^s\right) \\ A\delta_i^p - \delta_i^s \\ A\delta_i^u - \delta_i^w - \bar{\alpha}_i\left(A\delta_i^q - \delta_i^z\right) \\ A\delta_i^q - \delta_i^z \end{bmatrix}.$$

Amplification of local rounding errors possible, depending on α_i's and β_i's.

C. & Vanroose (2017)



Rounding error model for CG

Error bounds: Local rounding errors $A\delta_i^x + \delta_i^r$ can be bounded by

$$\begin{aligned} \|A\delta_i^x + \delta_i^r\| &\leq \left(\|A\| \, \|\bar{x}_i\| + (\mu\sqrt{n} + 4) \, |\bar{\alpha}_i| \, \|A\| \, \|\bar{p}_i\| + \|\bar{r}_i\|\right) \epsilon \\ &:= e_i^f \, \epsilon. \qquad (\epsilon = \text{machine precision}) \end{aligned}$$

In practice:

- *characterizes extreme case rounding error effects*
- *often largely overestimates the actual errors*

Error estimates: Local rounding errors can be approximated as

$$\|A\delta_i^x + \delta_i^r\| \approx \sqrt{e_i^f \, \epsilon}$$

In practice:

- *additional norm computations required*
- *include in existing global reduction phase to avoid overhead*

Pipe-CG with automated residual replacement

Explicitly replace $\bar{r}_i$, $\bar{s}_i$, $\bar{w}_i$ and $\bar{z}_i$ by their true values in selected iterations:

$$\bar{r}_{i+1} = \mathrm{fl}(b - A\bar{x}_{i+1}), \qquad \bar{w}_{i+1} = \mathrm{fl}(A\bar{u}_{i+1}),$$
$$\bar{s}_i = \mathrm{fl}(A\bar{p}_i), \qquad \bar{z}_i = \mathrm{fl}(A\bar{q}_i).$$

Residual replacement criterion:

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

with $\tau = \sqrt{\epsilon}$.

- Sleijpen & Van der Vorst 1996
- Tong & Ye, 1999
- Van der Vorst & Ye, 2000

Estimate of gap $\|f_i\|$ can be computed at runtime (without additional overhead), so fully automated replacement strategy is established for pipe-CG.

Numerical results: attainable accuracy

MatrixMarket collection: convergence tests on all non-diagonal SPD matrices

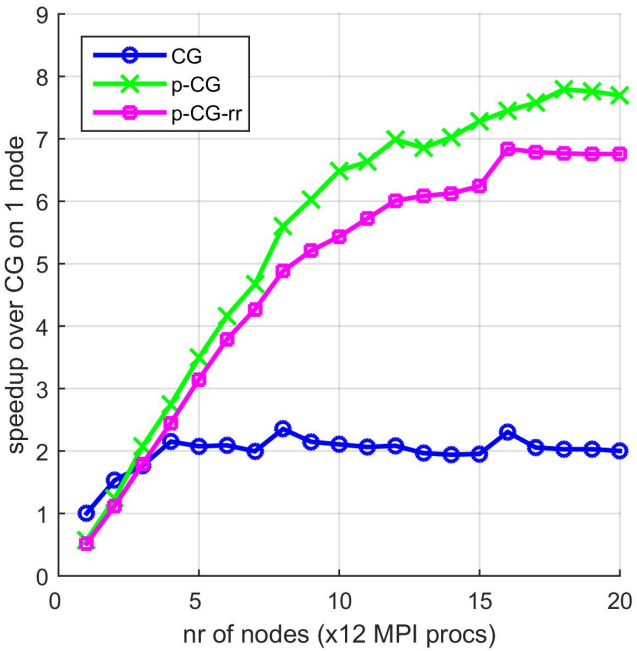
Matrix	Prec	$\kappa(A)$	n	$\#nnz$	CG		CG-CG		p-CG		p-CG-rr		
					iter	relres	iter	relres	iter	relres	iter	relres	rr
bcsstk14	JAC	1.3e+10	1806	63,454	650	7.6e-16	658	7.1e-16	506	5.2e-12	658	5.2e-16	9
bcsstk15	JAC	8.0e+09	3948	117,816	772	3.7e-15	785	3.5e-15	646	2.3e-11	974	4.0e-15	10
bcsstk16	JAC	65	4884	290,378	298	3.5e-15	300	4.0e-15	261	8.7e-12	301	2.1e-15	4
bcsstk17	JAC	65	10,974	428,650	3547	1.0e-14	3428	1.7e-14	2913	2.8e-09	4508	1.2e-14	54
bcsstk18	JAC	65	11,948	149,090	2299	2.2e-15	2294	2.1e-15	1590	2.9e-11	2400	1.5e-15	50
bcsstk27	JAC	7.7e+04	1224	56,126	345	3.2e-15	345	4.0e-15	295	8.0e-12	342	2.7e-15	6
gr_30_30	-	3.8e+02	900	7744	56	2.7e-15	55	3.1e-15	52	2.0e-13	61	3.0e-15	2
nos1	*ICC	2.5e+07	237	1017	301	1.3e-14	338	1.2e-14	337	2.6e-10	968	1.9e-14	21
nos2	*ICC	6.3e+09	957	4137	3180	8.3e-14	3292	1.1e-13	2656	1.2e-07	4429	2.7e-11	113
nos3	ICC	7.3e+04	960	15,844	64	1.0e-14	63	1.1e-14	59	1.0e-12	61	2.5e-14	3
nos4	ICC	2.7e+03	100	594	31	1.9e-15	31	1.9e-15	29	4.0e-14	33	1.3e-15	2
nos5	ICC	2.9e+04	468	5172	63	3.2e-16	64	3.4e-16	58	4.3e-14	65	2.3e-16	2
nos6	ICC	8.0e+06	675	3255	34	5.1e-15	35	6.2e-15	31	5.5e-11	33	1.0e-14	2
nos7	ICC	4.1e+09	729	4617	29	4.0e-14	31	2.8e-14	29	4.5e-14	29	3.0e-14	3
s1rmq4m1	ICC	1.8e+06	5489	262,411	122	4.3e-15	122	4.6e-15	114	5.5e-12	135	3.7e-15	6
s1rmt3m1	ICC	2.5e+06	5489	217,651	229	9.3e-15	228	8.7e-15	213	2.2e-11	240	1.7e-14	9
s2rmq4m1	*ICC	1.8e+08	5489	263,351	370	6.7e-15	387	7.3e-15	333	2.7e-10	349	2.5e-13	25
s2rmt3m1	ICC	2.5e+08	5489	217,681	285	8.7e-15	283	1.0e-14	250	7.3e-10	425	8.7e-15	17
s3dkq4m2	*ICC	1.9e+11	90,449	2,455,670	-	1.9e-08	-	2.1e-08	-	2.8e-07	-	5.6e-08	199
s3dkt3m2	*ICC	3.6e+11	90,449	1,921,955	-	2.9e-07	-	2.9e-07	-	3.5e-07	-	2.9e-07	252
s3rmq4m1	*ICC	1.8e+10	5489	262,943	1651	1.5e-14	1789	1.6e-14	1716	2.6e-08	1602	5.3e-10	154
s3rmt3m1	*ICC	2.5e+10	5489	217,669	2282	2.7e-14	2559	2.9e-14	2709	9.3e-08	3448	8.0e-10	149
s3rmt3m3	*ICC	2.4e+10	5357	207,123	2862	3.3e-14	2798	3.4e-14	3378	2.0e-07	2556	7.1e-11	248

Column 'relres' indicates the maximal attainable accuracy.

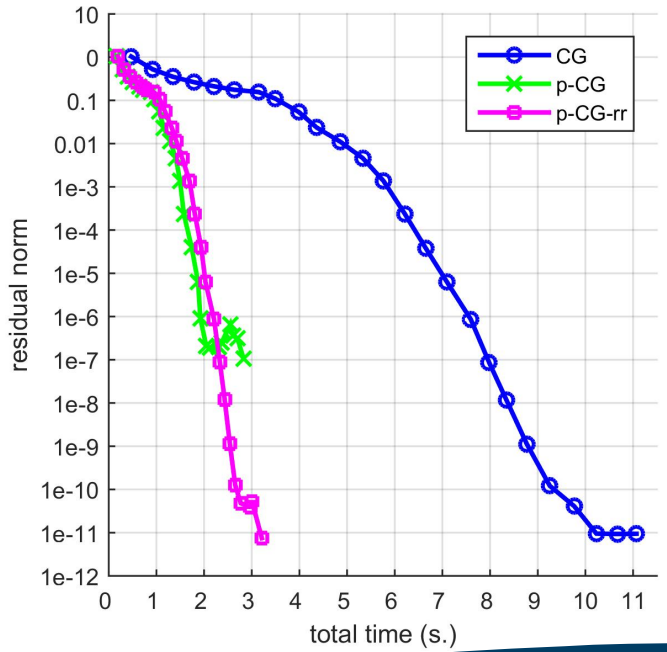
Numerical results: strong scaling

- 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)



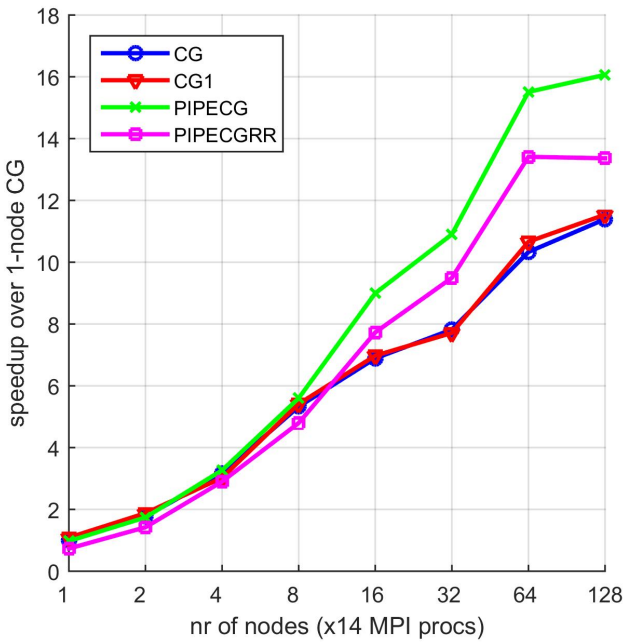
Accuracy i.f.o. total time spent (240 cores)



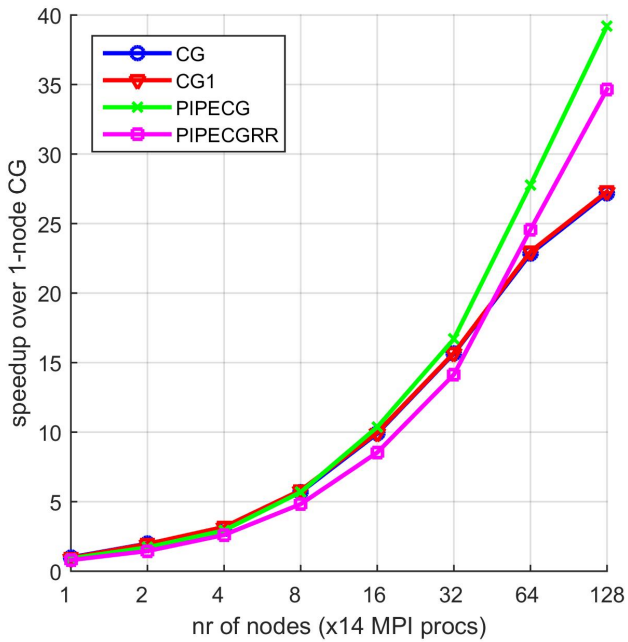
Numerical results: strong scaling

- PETSc implementation using MPICH-3.3a2 communication
- Benchmark problem: 3D ice sheet flow, $150 \times 150 \times 100$ / $500 \times 500 \times 50$ Q1 FE
- System specs: 128 nodes, two 14-core Intel Xeon E5-2680v4 2.4GHz CPUs/node

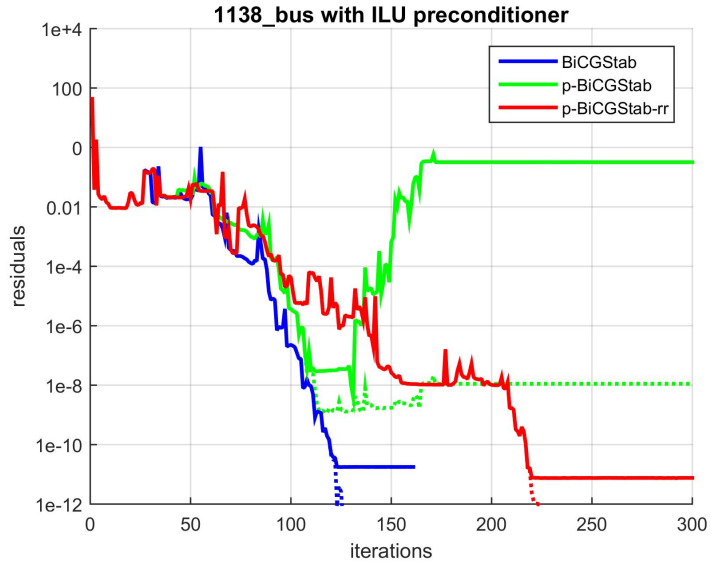
Speedup over single-node CG (2,250,000 unk)

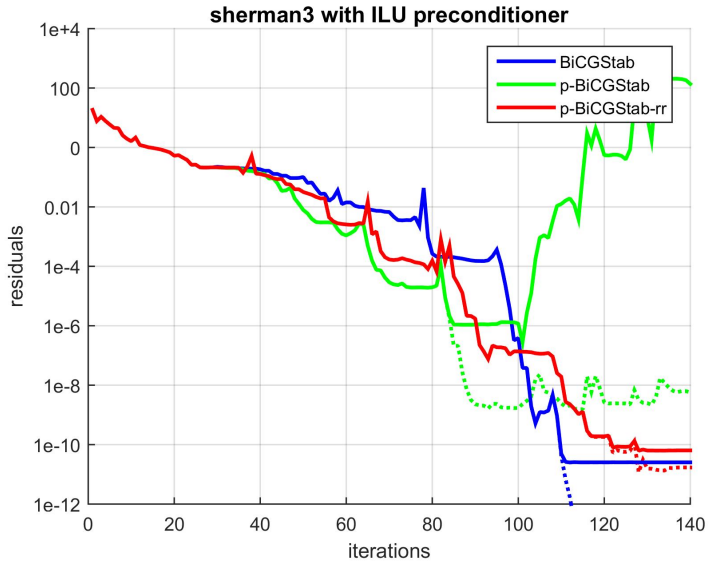


Speedup over single-node CG (12,500,000 unk)



Numerical results: attainable accuracy





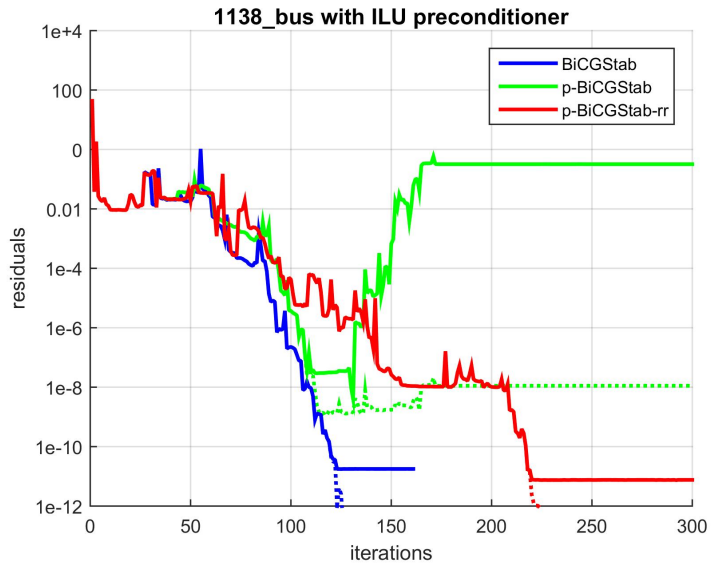
Residual replacement in i-th iteration:

$$r_i := b - Ax_i, \quad \hat{r}_i := M^{-1} r_i, \quad w_i := A\hat{r}_i, \quad s_i := A\hat{p}_i, \quad \hat{s}_i := M^{-1} s_i, \quad z_i := A\hat{s}_i.$$

- $\oplus$ increased maximal attainable accuracy: comparable to BiCGStab level
- $\oplus$ increased robustness: resets accumulated rounding errors
- $\ominus$ delay of convergence: increased number of iterations possible

Strakos & Tichy, 2002

Numerical results: attainable accuracy



Multi-term auxiliary recurrences

$\Downarrow$

Local error propagation matrix

$$\begin{bmatrix} 1 & -\bar{\alpha}_i\bar{\beta}_i & -\bar{\alpha}_i - \bar{\omega}_i & \bar{\alpha}_i\bar{\beta}_i(\bar{\omega}_i + \bar{\omega}_{i-1}) \\ 0 & \bar{\beta}_i & 1 & -\bar{\beta}_i\bar{\omega}_{i-1} \\ 0 & 0 & 1 & -\bar{\alpha}_i\bar{\beta}_i \\ 0 & 0 & 0 & \bar{\beta}_i \end{bmatrix}$$

Residual replacement in i-th iteration:

$$r_i := b - Ax_i, \quad \hat{r}_i := M^{-1}r_i, \quad w_i := A\hat{r}_i, \quad s_i := A\hat{p}_i, \quad \hat{s}_i := M^{-1}s_i, \quad z_i := A\hat{s}_i.$$

- $\oplus$ increased maximal attainable accuracy: comparable to BiCGStab level
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Strakos & Tichy, 2002

Numerical results: strong scaling

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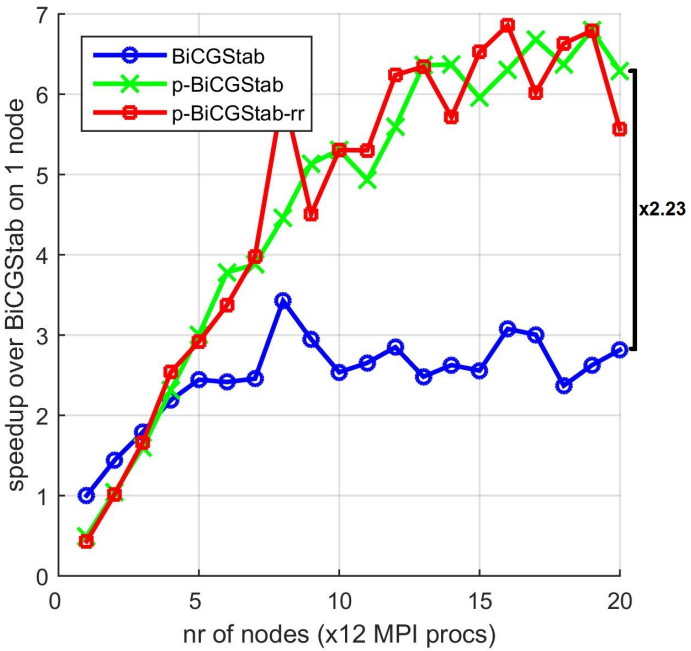
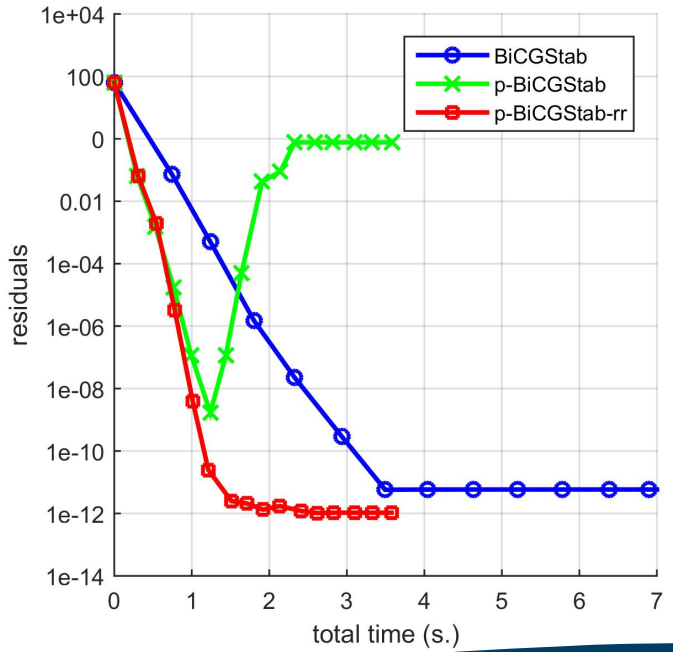
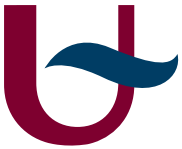
- Benchmark problem 2: 2D indefinite Helmholtz model, 1,000,000 unknowns
- System specs: 20 nodes, two 6-core Intel Xeon X5660 Nehalem 2.8GHz CPUs/node

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



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





Overview

In this talk

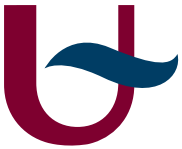
Pipelined Conjugate Gradients: rounding error analysis

- pipe-CG is much more sensitive to rounding errors than standard CG
- rounding error model allows for real-time countermeasures: pipe-CG-rr

Pipelined BiCGStab: numerical stability

- pipe-BiCGStab for non-symmetric operators (alternative to pipe-GMRES)

- P. Ghysels, W. Vanroose, *Hiding global synchronization latency in the preconditioned Conjugate Gradient algorithm*, Parallel Computing, 40, 2013.
- H.A. Van der Vorst, Q. Ye, *Residual Replacement strategies for Krylov Subspace iterative methods for Convergence of the True Residuals*, 22(3), SIAM J. Sci. Comput., 2000.
- E. Carson, J. Demmel, *A Residual Replacement Strategy for Improving the Maximum Attainable Accuracy of s-Step Krylov Methods*, SIAM J. Mat. Anal. Appl., 35(1), 2014.
- S. Cools, W. Vanroose, *Analyzing the effect of local rounding error propagation on the maximal attainable accuracy of the pipelined Conjugate Gradients method*, submitted, SIAM J. Mat. Anal. Appl., 2017.
- 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, 2017.



Work in progress

Related work

Stabilized shifted pipelined CG *

- introduce shift σ in auxiliary variables: $s_i = (A - \sigma)p_i$, $w_i = (A - \sigma)s_i$
- stabilizing effect on rounding error propagation for the right shift choice

Deep pipelines: pipe(ℓ)-GMRES & pipe(ℓ)-CG

- useful when time(GLRED) is much larger than time(SPMV+PREC)
- further reduced numerical stability

Soft error detection **with INRIA Bordeaux**

- rounding error model allows separation rounding errors vs. soft errors
- detect-and-correct strategy improves soft error resilience

Pipelined Lanczos **with L. Berkeley Lab**

- communication-hiding iterative algorithm for approximation of eigenpairs
- Nested Dissection: graph partitioning using Fiedler vector of adjacency matrix

* S. Cools, W. Vanroose, *Numerically Stable Variants of the Communication-hiding Pipelined Conjugate Gradients Algorithm for the Parallel Solution of Large Scale Symmetric Linear Systems*, Technical Report, `https://arxiv.org/abs/1706.05988`, 2017.

Thank you for your attention!

Q: *What is the difference between pipelined and s-step Krylov methods?*

Carson, Knight, Demmel, 2013

A: Global communication is hidden vs. avoided
A: Off-the-shelf preconditioning possible vs. specialized preconditioning required

Q: *Is the code available online?*

A: Pipe-CG, pipe-CG-rr, gropp-CG, pipe-GMRES and pipe-BiCGStab are included in the current PETSc version, available at `https://www.mcs.anl.gov/petsc/`.
A: The inclusion of pipe(ℓ)-CG and pipe(ℓ)-GMRES in PETSc is work in progress.