The communication-hiding pipelined BiCGStab method for the efficient parallel solution of large unsymmetric linear systems

S. Cools\textsuperscript{a}, W. Vanroose\textsuperscript{a}

\textsuperscript{a}Applied Mathematics Research Group, Department of Mathematics and Computer Science, University of Antwerp, Middelheimlaan 1, B-2020 Antwerp, Belgium. Contact: siegfried.cools@uantwerp.be, wim.vanroose@uantwerp.be

Abstract

A High Performance Computing alternative to traditional Krylov methods, pipelined Krylov solvers offer better scalability in the strong scaling limit compared to standard Krylov methods for large and sparse linear systems. The traditional synchronization bottleneck is mitigated by overlapping time-consuming global communication phases with local computations in the algorithm. This paper describes a general framework for deriving the pipelined variant of any Krylov algorithm. The proposed framework was implicitly used to derive the pipelined Conjugate Gradient (p-CG) method in \textit{Hiding global synchronization latency in the preconditioned Conjugate Gradient algorithm} by P. Ghysels and W. Vanroose, Parallel Computing, 40(7):224–238, 2014. The pipelining framework is subsequently illustrated by formulating a pipelined version of the BiCGStab method for the solution of large unsymmetric linear systems on parallel hardware. A residual replacement strategy is proposed to account for the possible loss of attainable accuracy and robustness by the pipelined BiCGStab method. It is shown that the pipelined algorithm improves scalability on distributed memory machines, leading to significant speedups compared to standard preconditioned BiCGStab.

Keywords: Parallelization, Global communication, Latency hiding, Krylov subspace methods, Bi-Conjugate Gradients Stabilized, Residual replacement

1. Introduction

At present, Krylov subspace methods fulfill the role of standard linear algebra solution methods in many high-performance computing (HPC) applications where large and sparse linear systems need to be solved. The Conjugate Gradient (CG) method \cite{1} can be considered as the earliest member of this well-known class of iterative solvers. However, the CG method is restricted to the solution of symmetric and positive definite (SPD) systems. Several variants of the CG method have been proposed that allow for the solution of more general classes of unsymmetric and indefinite linear systems. These include e.g. the Bi-Conjugate Gradient (BiCG) method \cite{2}, the Conjugate Gradient Squared (CGS) method \cite{3}, and the widely used BiCGStab method which was introduced as a smoother converging version of the aforementioned methods by H.A. Van der Vorst in 1992 \cite{4}.

Motivated by the vast numbers of processors in contemporary petascale and future exascale HPC hardware, research on the scalability of Krylov methods on massively parallel hardware has become increasingly prominent over the last years. The practical importance of Krylov methods for solving sparse linear systems is reflected in the High Performance Conjugate Gradients (HPCG) benchmark used for ranking HPC systems introduced in 2013 \cite{5, 6}. This new ranking is based on sparse matrix-vector computations and data access patterns, rather than the dense matrix algebra used in the traditional High Performance LINPACK (HPL) benchmark.

Krylov algorithms are build from three basic components, namely: \textit{sparse matrix-vector products} (SPMV) $Ax$, \textit{dot-products} (DOT-PROD) $(x,y)$ or inner products between two vectors, and \textit{AXPY} operations $x \leftarrow ax + y$ that combine scalar multiplication $ax$ and vector addition $x + y$. Single-node Krylov solver performance is dominated by the computation of the SPMV, which has the highest floating-point operation (FLOP) count of the algorithmic components. However, the main bottleneck...
for efficient parallelization is typically not the easy-to-parallelize SPMV application, but the dot-product computation that requires a global reduction over all processors. Global synchronization phases cause severe communication overhead on large parallel machines, and are thus effectively the most time-consuming component of Krylov algorithms for large scale linear systems.

A significant amount of research has been devoted to the reduction and elimination of the synchronization bottlenecks in Krylov methods over the last decades. The idea of reducing the number of global communication phases and hiding the communication latency in Krylov methods on parallel computer architectures was first presented by Chronopoulos and Gear in [5] and further elaborated in a variety of papers, among which [9, 2, 17]. Yang et al. [39, 38, 37] proposed the so-called improved versions of the standard BiCG, BiCGStab and CGS algorithms, which reduce the number of global reductions to only one per iteration. Furthermore, the work on s-step Krylov methods [4, 7, 6] allows to reduce the total number of global synchronization points by a factor of s.

In addition to avoiding communication by reducing the number of global synchronization points, research on hiding global communication latency by overlapping communication and computations was performed by Demmel et al. [12], De Sturler et al. [10] and Ghysels et al. [21, 22]. The latter introduces the class of pipelined Krylov subspace methods, which in addition to removing costly global synchronization points (communication-avoiding), aim at overlapping the remaining global communication phases by the SPMV and the preconditioner application (communication-hiding). In this way idle core time is minimized by performing useful computations simultaneously to the time-consuming global communication phases, cf. [15].

The current paper aims to extend the work on pipelined Krylov methods by proposing a high-level framework for formulating a pipelined variant of any Krylov subspace method. The paper is structured as follows. Section 2 introduces a general framework for the derivation of a pipelined method starting from the original Krylov algorithm. Section 3 illustrates the use of this framework by deriving the new pipelined BiCGStab (p-BiCGStab) method. The inclusion of a preconditioner - which is conveniently simple for pipelined Krylov solvers - is also discussed in this section. Experimental results with the p-BiCGStab method on a wide range of problems proposed in Section 4 validate the mathematical equivalence between the traditional and pipelined methods. A residual replacement strategy is proposed to improve the numerical accuracy and robustness of the pipelined BiCGStab solver when required. Section 5 compares the parallel performance of the traditional and pipelined BiCGStab methods on a moderately-sized cluster and comments on the numerical accuracy of p-BiCGStab. Finally, conclusions are formulated in Section 6.

2. General framework for deriving a pipelined Krylov algorithm

This section provides the outline of a generic work plan for deriving the pipelined version of any traditional Krylov method. The framework is based on the two main properties of the ‘pipelining’
Algorithm 2 CA-Krylov method

| Step 2: Hiding communication | Algorithm 2 CA-Krylov method |
|-------------------------------|-----------------------------|
| 1(a) identification          | function \textsc{ca-krylov}(A, b, x_0) |
| 1(b) recurrences             | 2: ... |
| 1(c) reformulation           | 3: for $i = 0, \ldots$ do |
| 1(d) new SPMVs               | 4: ... |
| (S2)                          | 5: \texttt{compute} SPMVs ($A \ast \cdot$) |
| (R1)                          | 6: ... |
| (S3)                          | 7: \texttt{compute} DOT-PRODS ($\cdot, \cdot$) |
| (R1)                          | 8: ... |
| (R1)                          | 9: ... |
| (R1)                          | 10: end for |
| (S3)                          | 11: end function |

Technique: avoiding communication, achieved by reducing the number of global reductions where possible, and hiding communication by overlapping local computational work such as AXPYS or SPMVs with the global communication required for the composition of dot-products. The below framework was implicitly used in the derivation of existing pipelined algorithms, such as the pipelined p-CG and p-CR methods in [22], as well as the $l^1$-GMRES algorithm proposed in [21].

2.1. Step 1: Avoiding communication

The primary goal in the first step is the merging of global reduction phases (DOT-PRODS) to reduce the number of global synchronization points, and hence, the overall time spent in communication. Algorithm 1 shows a schematic illustration of the original Krylov algorithm (left) and indicates the operations that are performed in Step 1 (right) to obtain the communication-avoiding Krylov method presented in Algorithm 2 (left). The following successive sequence of steps (a) to (d) may be repeated any number of times to merge multiple global reduction phases if required.

(a) Identify two global reduction phases, denoted by (R1) (the chronologically first phase) and (R2) (the subsequent reduction phase), that are candidates for merging.

(b) Introduce a recurrence for the SPMV computation (S1) that is computed in between the global reductions (R1) and (R2). This is done by substituting the SPMV vector by its respective recurrence, which is computed before (S1). Define new SPMV variables where needed and compute these SPMVs directly below their corresponding recursive vector definitions, see (S2).

(c) Use the new recursive vector characterizations defined in (b) to reformulate the dot-products of the (R2) reduction phase independently of any intermediate variables that are computed between the reduction phases (R1) and (R2).

(d) Move the (R2) global reduction phase upward to merge it with the (R1) global reduction into a single global communication phase.

Note that for preconditioned Krylov methods the SPMV phases (S1) and (S2) may also include the (right) preconditioner application, which is typically computed just before the SPMV in the (pipelined) Krylov algorithm. This is illustrated in Section 3.

2.2. Step 2: Hiding communication

The aim of the second step is the simultaneous execution (overlapping) of the global reduction communication phases with independent local SPMV computations to hide communication time behind useful computations and hence minimize worker idling. Step 2 is illustrated in Algorithm 2. Starting from the communication-avoiding Krylov method that is represented schematically by Algorithm 2 (left), the operations (a)-(d) in Step 2 required to obtain the pipelined Krylov method are indicated (right), which ultimately leads to Algorithm 3.
Algorithm 3 Pipelined Krylov method

1: function PIPE-KRYLOV\( (A, b, x_0) \)
2:     ... 
3:     for \( i = 0, \ldots \) do
4:         ... 
5:         compute DOT-PRODS \( (\cdot, \cdot) \) \hspace{1cm} \text{(R1)}
6:         compute SPMV\( s \) \( (A \ast \cdot) \) \hspace{1cm} \text{overlapping} \hspace{1cm} \text{(S3)}
7:         ... 
8:     end for
9: end function

(a) Following Step 1, each SPMV phase (S2) is followed by a corresponding global reduction phase (R1). These SPMV/DOT-PROD pairs are possibly separated by intermediate AXPY operations.
(b) Introduce a recurrence for the SPMV vector in (S2) through substitution by its recursive characterization, which is computed before (S2). Define new SPMV variables where needed (S3).
(c) Use the new recursive definition obtained in (b) to reformulate the dot-products of the (R1) reduction phase independently of the new SPMV variables that are computed in (S3).
(d) Insert the new SPMV variables (S3) defined in (b) right after the global reduction phase (R1). These SPMV computations can now be overlapped with the global synchronization (R1), since they do not use the results computed in the (R1) global reduction phase.

The resulting pipelined algorithm is shown in Algorithm 3. The proposed framework allows for the derivation of a pipelined Krylov method with a length-one pipeline, similar to the p-CG and p-CR methods described in [22]. A general framework for derivation of methods with longer pipeline lengths, cf. the p-GMRES\( (l) \) method described in [21], is currently work in progress.

3. Derivation of the pipelined BiCGStab algorithm

3.1. The standard BiCGStab algorithm

The traditional Biconjugate Gradient Stabilized method (BiCGStab), shown in Algorithm 4, was developed as a fast and smoothly converging variant of the BiCG and CGS methods [35]. It presently serves as the standard workhorse Krylov method for the iterative solution of nonsymmetric linear systems \( Ax = b \), where \( A \) is a general real or complex matrix with generic spectral properties, be it positive definite, positive or negative semidefinite, or indefinite.

Algorithm 4 performs two SPMV applications (lines 4 and 8) and a total of 4 recursive vector updates (lines 7, 11, 12 and 15) in each iteration. When implemented on a parallel machine, the AXPYs used to compute the recurrences are fully local operations, requiring no communication between individual workers. The SPMV\( s \) can be considered semi-local operations, since only limited communication between neighboring workers is required for boundary elements. In the particular cases of stencil application or the application of the banded sparse matrix structure that typically results from the discretization of PDEs, data locality can be exploited to ensure limited communication is required for computing the SPMV. Hence, the SPMV\( s \) operations are considered to be primarily compute-bound.

The traditional BiCGStab algorithm additionally features three global reduction steps to compute the dot-products required in the calculation of the scalar variables \( \alpha_i \) (line 5-6), \( \omega_i \) (line 9-10) and \( \beta_i \) (line 13-14). On a parallel machine, these dot-products require global communication among all workers to assemble the locally computed dot-product fractions and redistribute the final scalar result to all workers. This global communication is commonly performed through a 2-by-2 reduction tree, which requires \( O(\log_2(P)) \) time (cf. [21]), where \( P \) is the number of processors in the machine. Hence, the dot-product computations are communication-bound, and form the main bottleneck for efficient parallel execution of the BiCGStab method.
Algorithm 4 Standard BiCGStab

1: function bicgstab($A$, $b$, $x_0$)
2: \[ r_0 := b - Ax_0; \quad p_0 := r_0 \]
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: $q_i := r_i - \alpha_is_i$
8: $y_i := Ap_i$
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

3.2. Avoiding global communication: towards CA-BiCGStab

Starting from the original BiCGStab Algorithm 4 first the number of global communication phases is reduced. To this aim the dot-products for the computation of $\alpha_i$ (line 5-6) are merged with the computation of $\beta_i$ (line 13-14). Rewriting the intermediate spmv $s_i = Ap_i$ by using the recurrence for $p_i$ on line 15, we obtain:

\[
s_i := Ap_i = A(r_i + \beta_{i-1}(p_{i-1} - \omega_{i-1} s_{i-1}))
= w_i + \beta_{i-1}(s_{i-1} - \omega_{i-1} z_{i-1}),
\]

where we use that $s_{i-1} = Ap_{i-1}$, and the auxiliary variables $w_i := Ar_i$ and $z_i := As_i$ are defined. Subsequently, the new recurrence for $s_i$ is applied to rewrite the dot-product $(r_0, s_i)$ (line 5-6), so that $\alpha_i$ becomes independent of the intermediate variables $s_i$ and $p_{i+1}$, i.e.

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

Hence, by substituting (2), the new expression for $\alpha_i$ becomes

\[
\alpha_i := \frac{(r_0, r_i)}{(r_0, w_i) + \beta_{i-1}(r_0, s_{i-1}) - \beta_{i-1}\omega_{i-1}(r_0, z_{i-1})},
\]

which requires the dot-products $(r_0, w_i)$, $(r_0, s_{i-1})$ and $(r_0, z_{i-1})$, but does no longer use the dot-product $(r_0, s_i)$. Since $\alpha_i$ is now independent of the intermediate variables $s_i$ and $p_{i+1}$, it can be moved upward and merged with the global reduction required to compute $\beta_i$ (line 13-14). Note that the spmv $y_i = Ap_i$ (line 8) can also be replaced by a recursion by using the new variables $w_i = Ar_i$ and $z_i = As_i$.

\[
y_i := Ap_i = A(r_i - \alpha_is_i) = w_i - \alpha_iz_i,
\]

such that the total number of spmvs to be computed is two, similar to the original BiCGStab algorithm. After a minor reordering of operations, this leads to the communication-avoiding version of the BiCGStab method shown in Algorithm 5.

Although the total number of dot-products in Algorithm 5 is two higher than in the original BiCGStab algorithm, the number of global reduction phases was reduced from three in Algorithm 4 to only two in Algorithm 5. The first global reduction phase in Algorithm 5 (line 9) is unaltered compared to Algorithm 4 (line 9). In the second global reduction the dot-products $(r_0, r_{i+1})$, $(r_0, w_{i+1})$,
Algorithm 5 Communication-avoiding BiCGStab

```plaintext
1: function CA-BiCGStab(A, b, x0)
2:     r0 := b - Ax0; w0 := Ar0; α0 := (r0, r0) / (r0, w0); β1 := 0
3: for i = 0, ..., do
4:     pi := ri + βi-1 (pi-1 - ωi-1 si-1)
5:     si := wi + βi-1 (si-1 - ωi-1 zi-1)
6:     zi := Asi
7:     qi := ri - αi si
8:     yi := wi - αi zi
9:     compute (qi, yi) ; (yi, yi)
10:    ωi := (qi, yi) / (yi, yi)
11:    xi+1 := xi + αip + ωiqi
12:    r_i+1 := qi - ωiyi
13:    w_i+1 := Ar_i+1
14:    compute (r0, r_i+1) ; (r0, w_i+1) ; (r0, s_i) ; (r0, z_i)
15:    βi := (αi/ωi) (r0, r_i+1) / (r0, ri)
16:    αi+1 := (r0, r_i+1) / ((r0, w_i+1) + βi (r0, s_i) - βiωi (r0, z_i))
17: end for
18: end function
```

$(r_0, s_i)$ and $(r_0, z_i)$ are communicated simultaneously. This uses slightly more memory bandwidth\(^1\) but leads to only one global synchronization point to compute both $\alpha_{i+1}$ and $\beta_i$ in Algorithm 5 (line 14), compared to two global synchronizations in Algorithm 4 (lines 5 and 13).

Note that the expression $[7]$ for $\alpha_{i+1}$ can alternatively be rewritten as

$$\alpha_{i+1} := \frac{1}{\omega_i} + \frac{(r_0, w_i+1)}{(r_0, r_i+1)} - \beta_i \omega_i \frac{(r_0, z_i)}{(r_0, r_i+1)}^{-1}.$$  

(5)

The above expression for $\alpha_{i+1}$ is equivalent to $[8]$ in exact arithmetic, but employs only three dot-products instead of four, resulting in a more elegant expression for $\alpha_{i+1}$. However, since the number of global reductions remains unaffected by this operation, replacing the expression for $\alpha_{i+1}$ by $[5]$ has no effect on communication time. Moreover, numerical experiments in finite precision arithmetic have shown that expression $[9]$ results in a more robust variant of the BiCGStab algorithm, in particular when combined with a residual replacement strategy, see Section 4.

3.3. Hiding global communication: towards p-BiCGStab

Following Step 1, the modified BiCGStab Algorithm 5 now features two spmv operations (lines 6 and 13), which are each followed by a global reduction step (lines 9-10 and 14-15). The first spmv-global reduction pair (lines 6 and 9) is separated by intermediate axpy operations. Starting from this algorithm, we now aim at formulating a communication-hiding version of BiCGStab by moving the spmv operations below the global reduction phases.

The spmv $z_i := As_i$ is rewritten using the recurrence for $s_i$ (Algorithm 5, line 5) derived in (1):

$$z_i := As_i = A (w_i + \beta_i-1 (s_{i-1} - \omega_i-1 zi-1))$$

$$= t_i + \beta_i-1 (zi-1 - \omega_i-1 vi-1),$$

(6)

where we use that $z_{i-1} := As_{i-1}$, and two new auxiliary variables are defined as the spmvs $t_i := Aw_i$ and $v_i := Az_i$. In a similar way the second spmv $w_{i+1} := Ar_{i+1}$ can be rewritten as a recurrence

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\(^1\)The extra bandwidth usage for performing multiple dot-product communications in the same global synchronization is negligible, since communication is limited to scalars only.
Algorithm 6 Pipelined BiCGStab

1: function PIPE-BICGSTAB($A$, $b$, $x_0$) 
2: $r_0 := b - Ax_0$; $w_0 := Ar_0$; $t_0 := Aw_0$; $\alpha_0 := (r_0, r_0) / (r_0, w_0)$; $\beta_1 := 0$
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: $z_i := t_i + \beta_{i-1} (z_{i-1} - \omega_{i-1} v_{i-1})$
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: $w_{i+1} := y_i - \omega_i (t_i - \alpha_i v_i)$
13: $r_{i+1} := q_i - \omega_i y_i$
14: $t_{i+1} := r_{i+1} + \omega_i q_i$
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

using the recursive definition of $r_{i+1} = q_i - \omega_i y_i = r_i - \alpha_i s_i - \omega_i (w_i - \alpha_i z_i)$ (lines 7, 8 and 12). We obtain

$$w_{i+1} := Ar_{i+1} = A (q_i - \omega_i (w_i - \alpha_i z_i))$$

$$= y_i - \omega_i (t_i - \alpha_i v_i),$$

where we again use the definitions $w_i = Ar_i$, $z_i = As_i$, $t_i = Aw_i$ and $v_i = Az_i$. Next, the dot-products are reformulated such that they are independent of the corresponding newly defined SPMVs. For the first global reduction on line 9 in Algorithm 5 this implies $q_i$ and $y_i$ should be independent of $v_i$, which is clearly the case, and for the second global reduction on line 14, the variables $r_{i+1}$, $w_{i+1}$, $s_i$ and $z_i$ are required to be independent of $t_{i+1}$, which is also trivially satisfied. Hence, the SPMV $v_i = Az_i$ can be computed below the first global reduction phase (line 9), and the second new SPMV $t_{i+1} = Aw_{i+1}$ is moved below the corresponding second global reduction (line 14). This results in the pipelined BiCGStab method shown in Algorithm 6.

Mathematically, i.e. in exact arithmetic, Algorithm 6 is equivalent to standard BiCGStab. Moreover, similar to Algorithm 5 the pipelined BiCGStab Algorithm 6 features only two global communication phases, yet it additionally allows for a communication-hiding strategy. After local computation of the dot-product contributions has been executed on each worker, each global reduction (lines 9 and 15) can be overlapped with the computation of the corresponding SPMV (lines 11 and 18), which hides (part of) the communication latency behind the SPMV computations. In the remainder of this work Algorithm 6 shall be referred to as unpreconditioned pipelined BiCGStab.

Note that in finite precision arithmetic, the pipelined BiCGStab method may display different convergence behavior compared to standard BiCGStab due to the different way rounding errors are handled by the algorithm. Notably, pipelined BiCGStab features 8 lines of recursive vector operations, whereas traditional BiCGStab has only 4 lines with vector recurrences. The authors refer to the extensive literature 25 29 23 11 24 25 54 25 43 27 and their own related work 8 for a more elaborate discussion of the number of AXPYs and their influence on the propagation of rounding errors in the solution throughout both standard and pipelined Krylov methods. The p-BiCGStab residuals may deviate slightly from their original counterparts. Moreover, the maximal attainable accuracy of the method may be affected by the reordering of the algorithm by the pipelining approach. This is illustrated in Section 4, where countermeasures to the accuracy loss are proposed.
### Table 1: Specifications of different unpreconditioned BiCGStab variations. Columns \textit{glred} and \textit{spmv} list the number of global reduction phases and \textit{spmv}s respectively. The "\textit{*}"-symbol for p-BiCGStab indicates that \textit{spmv}s are overlapped with global reductions. Column \textit{Flops} shows the number of flops ($\times N$) required to compute \textit{axpy}s and dot-products. The \textit{Time} column has the time spent in global all-reduce communications (\textit{glreds}) and \textit{spmv}s. Memory counts the total number of vectors that need to be kept in memory.

| Method     | glred | spmv | Flops (\textit{axpy} + \textit{dot-prod}) | Time (\textit{glred} + \textit{spmv}) | Memory |
|------------|-------|------|------------------------------------------|---------------------------------------|--------|
| BiCGStab   | 3     | 2    | 20                                       | 3 glred + 2 \textit{spmv}            | 7      |
| p-BiCGStab | 2     | 2*   | 38                                       | 2 max(glred, \textit{spmv})          | 11     |

#### 3.4. Pipelined BiCGStab vs. Improved BiCGStab

We briefly comment on the communication-avoiding and -hiding framework applied to BiCGStab above. The derivation of the pipelined method, Algorithm 6, is essentially but one of many possible ways to obtain a more efficient parallel variant of the BiCGStab algorithm. Indeed, by performing the recursive substitutions and re-orderings of the algorithm in a different manner, other parallel algorithms that are mathematically equivalent to standard BiCGStab but feature improved global communication properties may be derived.

In particular, it is possible to reduce the number of global reductions even further after obtaining Algorithm 5 in Section 3.2. This can be achieved by merging the global reduction required to compute $\omega_i$ on line 9 in Algorithm 5 with the global reduction for $\alpha_i$ and $\beta_i$ on line 14. The resulting algorithm comprises only one global reduction step per iteration. This algorithm has been proposed by Yang & Brent in 2002 as the Improved BiCGStab method (IBiCGStab) [38]. Since only one global reduction step (avoiding) but no \textit{spmv} overlap (hiding) is performed, the IBiCGStab method performs well on setups with a very heavy communication-to-computation ratio.

We refer to Table 1 for a comparison between the unpreconditioned IBiCGStab and p-BiCGStab algorithms. The \textit{Flops} and Memory requirements for both methods are largely comparable. Only the two main time-consuming components (global reductions and \textit{spmv}s) are taken into account for the \textit{Time} estimates; the \textit{axpy} operations are neglected. In the ideal scenario for pipelined methods where the \textit{spmv} computation perfectly overlaps the communication time of one global reduction, the IBiCGStab method achieves a speed-up of approximately $1.5 \times$ compared to standard BiCGStab, whereas the p-BiCGStab method is theoretically able to attain a speed-up factor of $2.5 \times$.

Note that it is possible to combine the communication-avoiding strategy of the IBiCGStab method with a communication-hiding strategy, resulting in a single global reduction phase that is overlapped by all \textit{spmv}s. This results in a hybrid pipelined IBiCGStab algorithm that features only one \textit{spmv}-overlapped global all-reduce communication phase. Starting from the IBiCGStab algorithm, additional recurrences for auxiliary variables can indeed be introduced to merge all \textit{spmv}s into one block that directly follows the global reduction phase. However, to reorganize the algorithm to such a state, a large number of auxiliary \textit{axpy}s is required. Furthermore, this reorganization is not possible without the introduction of an additional \textit{spmv}, increasing the total number of \textit{spmv}s from two to three. This is an undesirable feature, i.e. the reduction of global communication latency should not come at the expense of a significantly increased computational cost. More importantly, the stability of the algorithm is threatened by the large number of extra operations, leading to very low attainable accuracy. We therefore do not expound on the details of this method here, and denote Algorithm 6 as the pipelined version of the BiCGStab algorithm in this paper.

#### 3.5. Preconditioned pipelined BiCGStab

A right-preconditioned system $AM^{-1}y = b$ with $Mx = y$ is considered, where $M$ is the preconditioning operator. The derivation of the pipelined BiCGStab algorithm can easily be extended to the preconditioned BiCGStab method shown in Algorithm 7. The preconditioned algorithm differs only slightly from unpreconditioned BiCGStab: lines 4 and 9 are added to implement the preconditioner, and the solution update in line 13 now uses the preconditioned direction vectors; the remaining
Algorithm 7 Preconditioned BiCGStab

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

expressions in Algorithm 7 are identical to the ones in Algorithm 4. The preconditioned variables in the algorithms are denoted by their respective variable with a hat-symbol, e.g. $\hat{p}_i = M^{-1}p_i$ and $\hat{q}_i = M^{-1}q_i$. The preconditioned pipelined BiCGStab method is derived starting from Algorithm 7 following a framework that is comparable to the derivation of unpreconditioned pipelined algorithm. However, in this case the preconditioned variables $\hat{p}_i$ (line 4) and $\hat{q}_i$ (line 9) are also reformulated as recurrence relations where required, similar to the reformulation of the spmv for $s_i$ (line 5) and $y_i$ (line 8), see below.

First, the number of global communication phases is reduced by joining the global reductions required to compute $\alpha_i$ and $\beta_i$ together into one global reduction phase, similar to the unpreconditioned case. To this aim, we rewrite the variables $\hat{p}_i$ and $s_i$ in the first preconditioned spmv (line 4-5) as recurrences, i.e.

$$\hat{p}_i := M^{-1}p_i = M^{-1}(r_i + \beta_{i-1}(p_{i-1} - \omega_{i-1}s_{i-1}))$$
$$= \hat{r}_i + \beta_{i-1}(\hat{p}_{i-1} - \omega_{i-1}\hat{s}_{i-1}),$$

where the new variables $\hat{r}_i := M^{-1}r_i$ and $\hat{s}_i := M^{-1}s_i$ are defined, and furthermore we write

$$s_i := Ap_i = A(\hat{r}_i + \beta_{i-1}(\hat{p}_{i-1} - \omega_{i-1}\hat{s}_{i-1}))$$
$$= w_i + \beta_{i-1}(s_{i-1} - \omega_{i-1}z_{i-1}),$$

where $\hat{p}_i$ is substituted by the recurrence (8), and the variables $w_i := A\hat{r}_i = AM^{-1}r_i$ and $z_i := A\hat{s}_i = AM^{-1}s_i$ are introduced. Furthermore, using the above definitions, the variables $\hat{q}_i$ and $y_i$ in the second preconditioned spmv (line 9-10) are rewritten as recurrence relations, yielding for $\hat{q}_i := M^{-1}q_i$

$$\hat{q}_i := M^{-1}q_i = M^{-1}(r_i - \alpha_i s_i) = \hat{r}_i - \alpha_i \hat{s}_i,$$

and for the variable $y_i = A\hat{q}_i$ the recurrence

$$y_i := A\hat{q}_i = A(\hat{r}_i - \alpha_i \hat{s}_i) = w_i - \alpha_i z_i.$$  

Observe how the recurrences (9) and (11) for $s_i$ and $y_i$ respectively are identical to their counterparts (1) and (3) in the unpreconditioned case. Consequently, definition (3) for $\alpha_i$ can now again be used.
Algorithm 8 Preconditioned Pipelined BiCGStab

1: function p-pipe-bicgstab($A$, $M^{-1}$, $b$, $x_0$)
2: $r_0 := b - Ax_0$; $\hat{r}_0 := M^{-1}r_0$; $w_0 := Ax_0$; $\hat{w}_0 := M^{-1}w_0$
3: $t_0 := Ax_0$; $\alpha_0 := (r_0, r_0) / (r_0, w_0)$; $\beta_0 := 0$
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: end for
13: compute $(q_i, y_i) ; (y_i, y_i)$
14: $\omega_i := (q_i, y_i) / (y_i, y_i)$
15: overlap $\hat{z}_i := M^{-1}z_i$
16: overlap $u_i := A\hat{z}_i$
17: $x_{i+1} := x_i + \alpha_i \hat{p}_i + \omega_i \hat{q}_i$
18: $r_{i+1} := q_i - \omega_i y_i$
19: $\hat{r}_{i+1} := \hat{q}_i - \omega_i (\hat{w}_i - \alpha_i \hat{z}_i)$
20: $w_{i+1} := y_i - \omega_i (t_i - \alpha_i u_i)$
21: compute $(r_0, r_{i+1}) ; (r_0, w_{i+1}) ; (r_0, s_i) ; (r_0, z_i)$
22: $\beta_i := (\alpha_i / \omega_i) (r_0, r_{i+1}) / (r_0, r_i)$
23: $\alpha_{i+1} := (r_0, r_{i+1}) / (r_0, w_{i+1}) + \beta_i (r_0, s_i) - \beta_i \omega_i (r_0, z_i)$
24: overlap $\hat{w}_{i+1} := M^{-1}w_{i+1}$
25: overlap $t_{i+1} := A\hat{w}_{i+1}$
26: end function

This expression does not depend on the variables $p_{i+1}$, $\hat{p}_i$ and $s_i$. The global reduction for $\alpha_i$ can thus be moved upward and merged with the global reduction for $\beta_i$. Hence, the number of global reductions is reduced from three to two at the cost of two additional recursive vector operations, resulting in a communication-avoiding preconditioned BiCGStab algorithm.

We subsequently focus on hiding the global communication phases behind the preconditioned SPMVs, which allows both the preconditioner application and the SPMV itself to be overlapped with the global reduction. The two preconditioned SPMVs that compute $s_i = M^{-1}s_i$, $z_i = A\hat{s}_i$ and $\hat{r}_{i+1} = M^{-1}r_{i+1}$, $w_{i+1} = A\hat{w}_{i+1}$ are rewritten, such that the SPMVs can be placed below the corresponding global reduction phases. This is achieved by introducing recurrences and auxiliary variables as follows:

$$
\hat{s}_i := M^{-1}s_i = M^{-1}(w_i + \beta_{i-1} (s_{i-1} - \omega_{i-1} z_{i-1}))
= \hat{w}_i + \beta_{i-1} (\hat{s}_{i-1} - \omega_{i-1} \hat{z}_{i-1}), \quad (12)
$$

where $\hat{w}_i := M^{-1}w_i$ and $\hat{z}_i := M^{-1}z_i$ are introduced, and

$$
z_i := A\hat{s}_i = A(\hat{w}_i + \beta_{i-1} (\hat{s}_{i-1} - \omega_{i-1} \hat{z}_{i-1}))
= t_i + \beta_{i-1} (z_{i-1} - \omega_{i-1} v_{i-1}), \quad (13)
$$

where $t_i := A\hat{w}_i$ and $v_i := A\hat{z}_i$ are defined. Additionally, using these new definitions, the following recurrences for $\hat{r}_{i+1}$ and $w_{i+1}$ can be derived

$$
\hat{r}_{i+1} := M^{-1}r_{i+1} = M^{-1}(q_i - \omega_i (w_i - \alpha_i z_i))
= \hat{q}_i - \omega_i (\hat{w}_i - \alpha_i \hat{z}_i), \quad (14)
$$

10
and

\[ w_{i+1} := A\hat{r}_{i+1} = A(\hat{q}_i - \omega_i (\hat{w}_i - \alpha_i \hat{z}_i)) = y_i - \omega_i (t_i - \alpha_i v_i). \]  

(15)

After moving the preconditioned \( \text{spmv}\)s \( \hat{w}_i := M^{-1}w_i, t_i := A\hat{w}_i \) and \( \hat{z}_i := M^{-1}z_i, v_i := Az_i \) below the dot-product computations of which they are independent, and following a minor reordering of operations, the above recurrences result in Algorithm 8. This algorithm is denoted as preconditioned pipelined BiCGStab.

Note that Algorithm 8 can alternatively be derived directly from the unpreconditioned pipelined BiCGStab Algorithm 6 by adding the proper preconditioned variables. This includes recursively computing \( \hat{p}_i := M^{-1}p_i \) (line 5), \( \hat{s}_i := M^{-1}s_i \) (line 7), \( \hat{q}_i := M^{-1}q_i \) (line 10) and \( \hat{r}_{i+1} := M^{-1}r_{i+1} \) (line 18), whose recurrences can be derived directly from the corresponding unpreconditioned variables, and defining the preconditioned variables \( \hat{z}_i := M^{-1}z_i \) (line 14) and \( \hat{w}_{i+1} := M^{-1}w_{i+1} \) (line 23), which are computed explicitly just before their respective \( \text{spmv}\)s.

Similar to the unpreconditioned case, the preconditioned pipelined BiCGStab Algorithm 8 allows for the overlap of the two \( \text{spmv}\) operations (lines 15 and 24) with the above global reduction phases (lines 12-13 and 20-21-22). In addition, due to the consecutive application of the preconditioner \( M^{-1} \) (lines 14 and 23) and the operator \( A \), the global reductions also overlap with preconditioning. Depending on the preconditioner choice, this possibly results in a much better hiding of global communication when the application of \( A \) is not sufficient to cover the global reduction time frame. For good parallel performance the preconditioner application should be compute-bound, requiring only limited communication between neighboring processors.

4. Numerical results

In this section a variety of numerical experiments is reported to benchmark the convergence of the pipelined BiCGStab method. Results comparing BiCGStab and p-BiCGStab on a wide range of matrices from applications are presented in Section 4.1. Additionally, a residual replacement strategy is presented in Section 4.2 to increase the maximal attainable accuracy and robustness of the pipelined method.

4.1. Pipelined BiCGStab benchmark on Matrix Market problems

Numerical results on a wide range of different linear systems are presented. Table 2 lists a collection of matrices from Matrix Market\(^*\) with their respective condition number \( \kappa \), number of rows \( N \) and total number of nonzero elements \( \#nnz \). A linear system with exact solution \( \hat{x}_i = 1/\sqrt{N} \) and right-hand side \( b = Ax \) is solved for each of these matrices. The system is solved using both standard BiCGStab, Algorithm 7 and the new pipelined BiCGStab variant, Algorithm 8. The initial guess is the all-zero vector \( x_0 = 0 \) for both methods. An Incomplete LU factorization preconditioner is included to reduce the number of Krylov iterations where possible. The relative stopping criterion on the recursive residual is \( ||r_i||_2 / ||r_0||_2 \leq 10^{-6} \).

Table 2 lists the number of iterations required to reach the stopping criterion as well as the final true residual norm \( ||r_i||_2 = ||b - Ax_i||_2 \) for both methods. The preset relative residual tolerance of \( 10^{-6} \) is achievable by p-BiCGStab in a comparable number of iterations with respect to standard BiCGStab. Averaged over all matrices, 3.5% less iterations are required by the pipelined BiCGStab algorithm.

Additionally, Table 2 shows that the final residual norms attained by BiCGStab and p-BiCGStab are comparable, but the final residuals are in general not exactly identical. This discrepancy is due to the different way rounding errors are treated by both algorithms in finite precision arithmetic. Hence, although BiCGStab and p-BiCGStab are mathematically equivalent algorithms, differences in convergence behavior may be observed in practice due to finite precision computations.

\(^*\)http://math.nist.gov/MatrixMarket/
Table 2: Collection of matrices from Matrix Market with condition number $\kappa(A)$, number of rows/columns $N$ and total number of nonzeros $\#nnz$. A linear system with right-hand side $b = Ax$ where $x = 1/\sqrt{N}$ is solved with each of these matrices with the presented BiCGStab and pipelined BiCGStab algorithms. The initial guess is all-zero $x_0 = 0$. An Incomplete LU preconditioner with zero fill-in (ILU0) is included where applicable. The number of iterations required to reach a relative residual tolerance of $1e-6$, i.e. $\|r_i\|_2/\|r_0\|_2 \leq 10^{-6}$, is shown along with the corresponding true residual norm $\|r_i\|_2 = \|b - Ax_i\|_2$.

![Image of the table]

Fig. 1 illustrates the convergence histories corresponding to a few randomly selected Matrix Market problems listed in Table 2. The per-iteration residual norms for BiCGStab and p-BiCGStab on the 1138_bus (top-left), bcsstk18 (top-right), bwm2000 (bottom-left) and sherman3 (bottom-right) matrices are shown, all with ILU0 preconditioner except the bwm2000 problem. The relative residual tolerance of $10^{-6}$ used as stopping criterion in Table 2 is marked by the dashed black line. Note that a stagnation of the true residual (solid colored lines) does not necessarily imply stagnation of the recursive residual (dotted colored lines). The latter may continue to decrease although the solution no longer improves with additional iterations [24].

The convergence behavior of the standard and pipelined BiCGStab methods is comparable. However, as pointed out above, small differences in convergence may arise as a result of different rounding errors in the algorithm, cf. [24, 25, 34, 33, 27, 8], causing the residuals to level off sooner. Although in practice the loss of maximal attainable accuracy for pipelined methods is only several orders of magnitude typical, this effect may be problematic when a very high precision on the solution is required, from a numerical point of view the behavior of the traditional and pipelined methods is largely identical.

4.2. Improving accuracy: the residual replacement strategy

Some applications may demand a significantly higher accuracy on the solution than imposed by the relatively mild stopping criterion $\|r_i\|_2/\|r_0\|_2 \leq 10^{-6}$ that was used in Section 4.1. Table 3 shows the maximal attainable accuracy (true residual norm $\|r_i\|_2 = \|b - Ax_i\|_2$) and corresponding number of iterations for the BiCGStab and p-BiCGStab algorithms on the Matrix Market problem selection. The pipelined BiCGStab method is unable to reach the same maximal accuracy as standard BiCGStab. This is a known issue related to pipelined Krylov methods, see [22, 8].

Several orders of magnitude are typically lost when switching to the pipelined algorithm. This accuracy loss is caused by the increased number of axpy operations in the pipelined Algorithm 7 which features 11 vector recurrence operations, compared to only 4 recurrences in the standard preconditioned BiCGStab Algorithm 6. The additional recurrence relations are prone to introducing rounding errors in the algorithm, cf. [24, 25, 34, 33, 27, 8], causing the residuals to level off sooner.

Although in practice the loss of maximal attainable accuracy for pipelined methods is only problematic when a very high precision on the solution is required, from a numerical point of view it...
is nonetheless important to address this issue. Therefore, countermeasures in the form of a residual replacement strategy \cite{30, 24, 36, 31, 3} are introduced to negate the effect of propagating rounding errors introduced by the additional recurrences in the pipelined method. The residual replacement technique resets the residuals $r_i$ and $\hat{r}_i$, as well as the auxiliary variables $w_i$, $s_i$, $\hat{s}_i$ and $z_i$, to their true values every $k$ iterations, i.e.

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

This induces an extra computational cost of 4 $spmv$s and 2 preconditioner applications every $k$ iterations. However, it is typically sufficient to perform only a small number of residual replacement steps to improve the maximal attainable accuracy, as indicated by the average $\#nrr$ percentage displayed in the bottom right corner of Table 3. Hence, the replacement period $k$ is often chosen large, limiting the computational overhead of performing the residual replacements. In Section 5 it is shown that the extra $spmv$ cost is negligible compared to the global cost of the method. The pipelined BiCGStab method with residual replacement is denoted as p-BiCGStab-rr, in short.

---

3The replacement period parameter $k$ is chosen manually for the matrices in Table 3 based on an ad hoc estimation of the total number of BiCGStab iterations. Note that a different choice of this parameter could lead to either significantly slower or faster convergence of the p-BiCGStab-rr algorithm.
Table 3: Collection of matrices from Matrix Market. See Table 2 for specifications. A linear system
with right-hand side $b = Ax$ where $x = 1/\sqrt{N}$ is solved with each of these matrices with the standard
BiCGStab, p-BiCGStab and p-BiCGStab-rr algorithms. The initial guess is all-zero $x_0 = 0$. An Incomplete
LU preconditioner with zero fill-in (ILU(0)) is included where applicable. The number of iterations required
to reach the maximal attainable accuracy on the residual is given, along with the corresponding true
residuals, the residual replacement strategy resolves these robustness issues, and Figure 2 shows a
this unwanted behavior. By periodically resetting the residual and auxiliary variables to their true
values, the residual replacement strategy resolves these robustness issues, and Figure 2 shows a

Table 3: Collection of matrices from Matrix Market. See Table 2 for specifications. A linear system
with right-hand side $b = Ax$ where $x = 1/\sqrt{N}$ is solved with each of these matrices with the standard
BiCGStab, p-BiCGStab and p-BiCGStab-rr algorithms. The initial guess is all-zero $x_0 = 0$. An Incomplete
LU preconditioner with zero fill-in (ILU(0)) is included where applicable. The number of iterations required
to reach the maximal attainable accuracy on the residual is given, along with the corresponding true residual

| Matrix   | $\|r_0\|_2$ | BiCGStab iter | $\|r_i\|_2$ | p-BiCGStab iter | $\|r_i\|_2$ | p-BiCGStab-rr iter | $\|r_i\|_2$ | k | #nrr |
|----------|-------------|---------------|-------------|----------------|-------------|---------------------|-------------|---|------|
| 1138_bus | 4.3e+01     | 123 1.8e-11   | 130 4.0e-09 | 120 3.5e-12    | 35 3        |                     |             |   |      |
| add32    | 8.0e-03     | 46 7.8e-18    | 42 5.0e-16  | 51 5.7e-18     | 10 2       |                     |             |   |      |
| bcsctk14 | 2.1e+09     | 559 7.3e-06   | 444 6.6e-01 | 522 3.8e-03    | 200 2      |                     |             |   |      |
| bcsctk18 | 2.6e+09     | 523 4.8e-06   | 450 1.1e-01 | 725 2.8e-05    | 50 7       |                     |             |   |      |
| bcsctk26 | 3.5e+09     | 414 1.1e-05   | 216 5.7e-01 | 475 8.6e-04    | 30 6       |                     |             |   |      |
| bcsctm25 | 6.9e+07     | - 3.2e+00     | - 3.8e+00  | - 4.6e+00      | 1000 9     |                     |             |   |      |
| bfw782a  | 3.2e-01     | 117 9.5e-14   | 106 5.1e-13 | 133 2.6e-15    | 20 4       |                     |             |   |      |
| bwnm2000 | 1.1e+03     | 1735 2.5e-09  | 1621 1.4e-05 | 2231 3.8e-08  | 500 3      |                     |             |   |      |
| c deed   | 5.8e-01     | 151 8.1e-14   | 147 2.0e-11 | 159 2.1e-15    | 10 13      |                     |             |   |      |
| fdpad014 | 2.7e+06     | - 4.3e-03     | - 9.7e-03  | - 4.3e-03      | 50 3       |                     |             |   |      |
| fs_260_3 | 1.6e+07     | 1979 1.2e-05  | 1039 5.1e-02 | 4590 1.1e-05  | 900 3      |                     |             |   |      |
| jagmesh9 | 6.8e+00     | 6230 2.4e-14  | 3582 5.8e-09 | 9751 1.1e-11  | 500 13     |                     |             |   |      |
| jpwz99i  | 3.8e-01     | 53 1.3e-14    | 54 1.8e-12 | 63 2.5e-15     | 10 4       |                     |             |   |      |
| orncz_1  | 4.8e+00     | 51 4.0e-11    | 52 3.7e-09  | 56 5.9e-12     | 10 3       |                     |             |   |      |
| pde2961  | 2.9e-01     | 50 4.5e-15    | 48 3.4e-13 | 52 1.4e-15     | 10 3       |                     |             |   |      |
| rdnl3200 | 1.0e+01     | 178 3.7e-08   | 167 9.9e-08 | 181 3.4e-08    | 100 1      |                     |             |   |      |
| sblqo4m2 | 6.8e-01     | - 1.0e-05     | - 1.4e-05 | - 1.3e-05      | 1000 9     |                     |             |   |      |
| sayr4    | 3.1e-03     | 52 4.0e-12    | 43 7.5e-11 | 46 3.8e-12     | 10 4       |                     |             |   |      |
| sherman3 | 1.8e+01     | 111 2.5e-11   | 100 2.8e-07 | 128 6.2e-11    | 20 4       |                     |             |   |      |
| stamodel | 7.9e+00     | - 5.1e-06     | - 3.1e-06 | - 4.5e-06      | 1000 9     |                     |             |   |      |
| utm5940  | 3.6e-01     | 256 3.0e-12   | 248 4.3e-08 | 395 2.9e-11    | 100 3      |                     |             |   |      |

Average iter deviation wrt BiCGStab
Average #nrr wrt p-BiCGStab-rr iter

By resetting the residual to its true value every k-th iteration, any build-up rounding errors are
effectively killed. With the periodic elimination of rounding errors the algorithm is able to attain
the same maximal accuracy as standard BiCGStab, see the p-BiCGStab-rr residual norms in Table
However, the introduction of the residual replacement step alters the p-BiCGStab convergence
behavior, resulting in an increase in iterations required to attain the maximum precision on the
solution for some problems. This phenomenon is also illustrated in Figure 2, where the convergence
histories of the BiCGStab and p-BiCGStab methods on four selected matrices are shown up to a
high accuracy.

Table 3 indicates an average reduction of iterations by 11.0% for p-BiCGStab compared to
standard BiCGStab over all listed matrices. These iteration numbers are however related to the lower
maximal attainable accuracy of p-BiCGStab, and in general do not imply p-BiCGStab converges
faster than the original BiCGStab method, cf. Figure 2. For the p-BiCGStab-rr method an average
increase in iterations of 22.1% is observed. Indeed, for some problems such as 1138_bus, fa760_3
and utm5940 a significant increase in iterations and convergence irregularity is observed, see also the
residual histories in Figure 2. Yet, final residuals displayed in Table 3 show that a high accuracy
on the solution can be achieved by use of the residual replacement strategy when required by
the application. The associated increase in iterations implies a trade-off between speedup and
accuracy that should be kept in mind when using the p-BiCGStab-rr method.

Figure 2 illustrates an additional beneficial effect of the residual replacement strategy on the
pipelined BiCGStab method. The convergence history of the p-BiCGStab method is generally
comparable (albeit not identical) to the BiCGStab residuals, up to the stagnation point where
p-BiCGStab attains maximal accuracy. However, it is observed that after some iterations the p-
BiCGStab true residuals $|b - Ax|$ again start to increase. Standard BiCGStab does not display this
unexpected behavior. By periodically resetting the residual and auxiliary variables to their true
values, the residual replacement strategy resolves these robustness issues, and Figure 2 shows a

stagnation of the p-BiCGStab-rr residual similar to standard BiCGStab after maximal accuracy is attained.

5. Parallel performance results

In this section we illustrate the parallel performance of the pipelined BiCGStab method, Algorithm 8. The scaling and accuracy experiments in this section are performed on a small cluster with 20 compute nodes, consisting of two 6-core Intel Xeon X5660 Nehalem 2.80 GHz processors each (12 cores per node), for a total of 240 cores. Nodes are connected by 4 × QDR InfiniBand technology, providing 32 Gb/s of point-to-point bandwidth for message passing and I/O. Since each node consists of 12 cores, we use 12 MPI processes per node to fully exploit parallelism on the machine. The MPI library used for this experiment is MPICH-3.1.3. Note that the environment variables MPICH_ASYNC_PROGRESS=1 and MPICH_MAX_THREAD_SAFETY=multiple are set to ensure optimal parallelism.

http://www.mpich.org/
Figure 3: **Parallel test problem 1.** Strong scaling experiment on up to 20 nodes (240 cores). Top left: Average time per iteration ($\log_{10}$ scale) as function of the number of nodes ($\log_2$ scale). Top right: Speedup (per iteration) over standard BiCGStab on a single node as function of the number of nodes. Bottom left: Total CPU time as function of the number of nodes. Bottom right: Absolute speedup over standard BiCGStab on a single node as function of the number of nodes. All methods were set to converge to a relative residual tolerance of $10^{-6}$, which was reached in 205 (min.) to 282 (max.) iterations. The $p$-BiCGStab-rr algorithm performs a replacement step every 100 iterations.

**Parallel test problem 1.** The pipelined BiCGStab Algorithm was implemented in the open-source PETSc library, version 3.6.2, as a direct modification of the $\texttt{fbcgs}$ implementation found in the PETSc Krylov solvers folder. The first benchmark problem is a 2D PDE-type model defined by the unsymmetric 5-point stencil

$$A_{1\times 1} = \begin{pmatrix} -1 & 4 & -\varepsilon \\ -\varepsilon \\ -\varepsilon \end{pmatrix}, \quad \varepsilon = 1 - 0.001.$$

(PTP1)

The right-hand side $b = A_{1\times 1} \hat{x}$ is constructed using the exact solution $\hat{x} = 1$. The operator is a modification of the 2D Poisson PDE stencil discretized using second order finite difference approximations on a uniform grid, which is available in the PETSc distribution as example 2 in the Krylov solvers folder. Note that this unsymmetric model problem, although academic, is non-trivial from an iterative solver perspective, since a large number of eigenvalues of the system operator are located close to zero. The number of grid points is set to 1.000 per spatial dimension, resulting in a total of one million unknowns. In the following experiments no preconditioner is included.
Figure 4: **Parallel test problem 1.** Accuracy experiment on 20 nodes (240 cores). Left: True residual as function of iterations. Right: True residual as function of total time spent by the algorithm. Maximal number of iterations is 2000 for all methods. The p-BiCGStab-rr algorithm performs a replacement step every 100 iterations (max. 10 replacements steps).

Figure 3 (top left) shows the average time per iteration required to solve the problem up to the relative residual tolerance of $10^{-6}$ as a function of the number of nodes. The pipelined BiCGStab method (green) starts to outperform standard BiCGStab (blue) when the number of nodes exceeds four. Figure 3 (top right) shows the same data, reformulated as speedup over standard 1-node BiCGStab. The p-BiCGStab method scales well up to 20 nodes. The bottom row in Figure 3 shows the non-averaged total time (left) and absolute speedup in function of the number of nodes (right), which display similar scaling behavior, albeit slightly less smooth due to the varying number of iterations between individual runs. The maximum speedup on 20 nodes over standard BiCGStab on a single node is $7.89 \times$ (computed on averaged timings). In contrast, the standard BiCGStab method stops scaling at around 8 nodes, obtaining a speedup of only $3.30 \times$ on 20 nodes. Hence, pipelined BiCGStab attains a net speedup (per iteration) of $2.39 \times$ compared to standard CG when both are executed on 20 nodes, which approximates the theoretically optimal speedup of $2.5 \times$, cf. Section 3.4. The absolute (non-averaged) speedup factor of p-BiCGStab (270 iterations) over standard BiCGStab (254 iterations) on 20 nodes is $2.25 \times$. Performance results for the p-BiCGStab-rr method are similar to those of p-BiCGStab. The small computational overhead from the residual replacement steps does not affect strong scaling.

Figure 4 shows the accuracy of the solution in function of the number of iterations (left) and in function of the total computational time (right) for the BiCGStab and p-BiCGStab algorithms on the 2D unsymmetric benchmark problem on a 20 node setup. Standard BiCGStab attains a maximal accuracy on the solution corresponding to a residual 2-norm of $5.8e-12$ in 4.0 seconds. The pipelined variant is significantly faster, attaining a residual norm of $1.7e-9$ in only 1.2 seconds. However, for the pipelined method a higher accuracy is only obtainable by including the residual replacement strategy. The p-BiCGStab-rr method is able to attain a residual norm of $2.5e-12$ in 1.5 seconds, which is significantly faster than standard BiCGStab for a comparable accuracy.

**Parallel test problem 2.** The second benchmark problem used to assess parallel performance is a Helmholtz-type PDE model given by the 5-point stencil

$$A_2^{sf} = \begin{pmatrix} -1 & -1 \\ -1 & 1 \\ -1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \text{(PTP2)}$$

and a right-hand side $b = A_2\hat{x}$, where again $\hat{x} = 1$. This operator can be considered as a 2D Poisson operator shifted by a diagonal matrix that relates to the Helmholtz wave number. It is
Table 4: **Parallel test problem 2.** Reference table showing the number of iterations required to attain the relative residual tolerance of 1e-6, corresponding to a true residual norm $\|r_i\| = \|b - Ax_i\| \leq 3.0 \text{e-3}$, as a function of the number of nodes.

| nodes | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  |
|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| BiCGStab | 1563 | 1885 | 1879 | 1875 | 1710 | 1852 | 1780 | 1555 | 1641 | 1909 |
| p-BiCGStab | 1807 | 1611 | 1779 | 1787 | 1673 | 1547 | 1668 | 1773 | 1640 | 1673 |
| p-BiCGStab-rr | 1857 | 1788 | 1728 | 1570 | 1677 | 1721 | 1688 | 1283 | 1884 | 1718 |

| nodes | 11  | 12  | 13  | 14  | 15  | 16  | 17  | 18  | 19  | 20  |
|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| BiCGStab | 1805 | 1175 | 1717 | 1766 | 1722 | 1651 | 2050 | 1778 | 1670 |
| p-BiCGStab | 1936 | 1811 | 1629 | 1642 | 1849 | 1843 | 1726 | 1796 | 1713 | 1870 |
| p-BiCGStab-rr | 1845 | 1628 | 1562 | 1581 | 1650 | 1647 | 1889 | 1750 | 1701 | 2112 |

highly indefinite and notably hard to solve using iterative methods, see [19] and references therein. The one million unknowns system $A_2x = b$ is solved using unpreconditioned BiCGStab, Algorithm 4, and its pipelined variant, Algorithm 6.

Figure 5 shows the timing (left) and speedup (right) results for the indefinite test problem on one up to 20 nodes. The averaged speedup graph (top right) for p-BiCGStab is largely comparable to the results for Parallel test problem 1, showing good scaling on up to 20 nodes with a per-iteration speedup of $7.52 \times$ (non-averaged: $6.29 \times$) compared to 1-node BiCGStab. Total timings are slightly more oscillating due to the significant differences in iterations between individual runs, see Table 4. The total time spent by the p-BiCGStab algorithm on 20 nodes is 9.8 s. (for 1670 iterations), whereas the p-BiCGStab algorithm requires only 4.6 s. (for 1870 iterations) to attain the same accuracy. Hence, pipelining results in a net speedup factor of $2.23 \times$ on 20 nodes for this model problem.

6. Conclusions

In this work we have proposed a general framework for the derivation of a pipelined variant of any given Krylov method. Applications include the reformulation of several widely used Krylov methods such as the Conjugate Gradients method (CG) for symmetric and positive definite linear systems and the Bi-Conjugate Gradients Stabilized method (BiCGStab) for the solution of general unsymmetric and/or indefinite systems.

The pipelining framework consists of two main steps. In the first step, denoted as communication-avoiding, or CA in short, the standard Krylov algorithm is rewritten into a mathematically equivalent algorithm that has fewer global synchronization points than the original algorithm. This is achieved by combining the global reduction phases of different dot-products scattered across the algorithm into one global communication phase. The second step, called communication-hiding, subsequently reformulates the algorithm such that the remaining global reduction phases are overlapped by the sparse matrix-vector product and preconditioner (when applicable). In this way, the typical communication bottleneck is mitigated by ‘hiding’ communication time behind useful computational work. Note that, contrary to the so-called $s$-step methods [5, 4, 7, 3], the combination of pipelined methods and preconditioning is straightforward. However, to ensure optimal scaling the chosen preconditioner should preferably require only limited global communication.

The pipelined algorithms (partially) circumvent the traditional global synchronization bottleneck and, as a consequence, offer better scalability in the strong scaling limit for computing solutions to large and sparse linear systems on massively parallel hardware. The current high-level framework can be used to derive a length-one pipelined version of any traditional Krylov method. Research on a general framework for the derivation of length-$l$ pipelined methods is left as future work.

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5 Note that most standard preconditioners based on e.g. incomplete LU factorization, multigrid methods or domain decomposition methods that are available in PETSc do not improve convergence for this problem. The authors are aware of the existence of specialized preconditioning techniques for Helmholtz-type problems, as proposed in e.g. [15, 16]; however, a discussion on the effectiveness of these preconditioners is beyond the scope of this work.
Figure 5: **Parallel test problem 2.** Strong scaling experiment on up to 20 nodes (240 cores). **Top left:** Average time per iteration (log10 scale) as function of the number of nodes (log2 scale). **Top right:** Speedup (per iteration) over standard BiCGStab on a single node as function of the number of nodes. **Bottom left:** Total CPU time as function of the number of nodes. **Bottom right:** Absolute speedup over standard BiCGStab on a single node as function of the number of nodes. All methods were set to converge to a relative residual tolerance of $10^{-6}$, which was reached in 1283 (min.) to 2112 (max.) iterations. The p-BiCGStab-rr algorithm performs a replacement step every 100 iterations (max. 10 replacements steps).

To illustrate the methodology, the pipelining framework is successfully applied to the BiCGStab method for the solution of large and sparse unsymmetric linear systems. The pipelined BiCGStab method (p-BiCGStab) reduces the number of global synchronization points from three to two, and overlaps the remaining global reduction phases with computational work. This induces a theoretical speed-up of up to 250% over traditional BiCGStab on a large number of nodes.

Numerical experiments on a moderately sized cluster show that the p-BiCGStab method displays significantly increased parallel performance and improved strong scaling compared to standard BiCGStab on an increasing number of computational nodes. In practice a speedup of 2.0 to 2.5× over the traditional BiCGStab method can be expected when both are executed on the same number of parallel processors.

Finally, the experimental results point out two minor numerical drawbacks that originate from reordering the BiCGStab algorithm into a pipelined version. In the extremely small residual regime, a loss of maximal attainable accuracy can be expected, which is a typical phenomenon related to pipelined methods [22, 5]. Furthermore, due to the introduction of additional AXPY operations by the pipelining framework, the p-BiCGStab algorithm is typically less robust with respect to numerical...
ropounding errors compared to the standard algorithm. Indeed, residuals cannot be guaranteed to remain at the same level after attaining the maximal attainable accuracy, which is a highly unwanted feature. Both of these numerical issues are simultaneously resolved by including a residual replacement strategy in the pipelined method. Indeed, through a periodical reset of the residual and auxiliary variables to their true values by explicitly computing the corresponding SPMVs, it is shown that both robustness and attainable accuracy can be restored to the original BiCGStab method’s level if required, at the cost of an added computational cost.

7. Acknowledgments

This work is funded by the EXA2CT European Project on Exascale Algorithms and Advanced Computational Techniques, which receives funding from the EU’s Seventh Framework Programme (FP7/2007-2013) under grant agreement no. 610741. Additionally, S.C. is funded by the Research Foundation Flanders (FWO). The authors are grateful to Pieter Ghysels and Bram Reps for their useful insights on the topic.

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