

Pipelined, Flexible Krylov Subspace Methods

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September 16, 2016

Abstract

We present variants of the Conjugate Gradient (CG), Conjugate Residual (CR), and Generalized Minimal Residual (GMRES) methods which are both *pipelined* and *flexible*. These allow computation of inner products and norms to be overlapped with operator and nonlinear or nondeterministic preconditioner application. The methods are hence aimed at hiding network latencies and synchronizations which can become computational bottlenecks in Krylov methods on extreme-scale systems or in the strong-scaling limit. The new variants are not arithmetically equivalent to their base flexible Krylov methods, but are chosen to be similarly performant in a realistic use case, the application of strong nonlinear preconditioners to large problems which require many Krylov iterations. We provide scalable implementations of our methods as contributions to the PETSC package and demonstrate their effectiveness with practical examples derived from models of mantle convection and lithospheric dynamics with heterogeneous viscosity structure. These represent challenging problems where multiscale nonlinear preconditioners are required for the current state-of-the-art algorithms, and are hence amenable to acceleration with our new techniques. Large-scale tests are performed in the strong-scaling regime on a contemporary leadership supercomputer, where speedups approaching, and even exceeding $2\times$ can be observed. We conclude by analyzing our new methods with a performance model targeted at future exascale machines.

1 Introduction

The current High Performance Computing (HPC) paradigm involves computation on larger and larger clusters of individual compute nodes connected through a network. Since single-core performance has plateaued, increased parallelism is used to increase total performance. As systems scale in this way, new performance bottlenecks emerge in algorithms popularized before massive parallelism became relevant. While peak compute power is abundant on modern high performance clusters, utilizing them at full capacity requires modifications to many well established algorithms. We investigate modifications to flexible Krylov subspace methods to better exploit computational resources available from modern clusters. As parallelism increases, collective operations are more likely to become computational bottlenecks. For instance, distributed dot products can become performance limiting due to network latency exposed by synchronized all-to-all communication. Similar concerns apply to hypothetical future machines and to current machines in the strong-scaling limit, when small amounts of local work expose bottlenecks in collective operations. One approach to mitigate these bottlenecks is to overlap these collective operations with local work, hiding the latency. This is a non-trivial task due to data dependencies which forbid arbitrary rearrangements of operations.

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1.1 Pipelining Flexible Krylov Subspace Methods

A classical way to use a system with independent hardware resources at higher efficiency is to *pipeline*. Broadly, this technique can accelerate throughput of a repeated multi-stage process when different stages require different resources. Concurrent work is performed on multiple iterations of the process, overlapped such that multiple resources are used simultaneously. This induces latency as the pipeline is filled as well as other overheads related to rearranging an algorithm and allowing simultaneous progress on multiple tasks.

We consider pipelining a particular class of algorithms, namely Krylov subspace methods for the solution of large, sparse, linear systems $Ax = b$ [34, 39]. Recent research has provided algorithms which loosen data dependencies in these algorithms, allowing communication- and computation-oriented resources to operate concurrently [12, 13, 23].

Krylov subspace methods for scientific applications are typically preconditioned [40]. This is essential for scalability in many cases. For instance, when the operator A is a discretized elliptic operator, a multilevel preconditioner [38] is required for algorithmic scalability. Preconditioners are often not available as assembled matrices. They commonly involve nested approximate solves, an important case being the application of another Krylov method [28]. The application of a nested Krylov method to a given tolerance and/or iteration count is a nonlinear operation; the optimal polynomial chosen at each iteration depends on A , b , and x_0 . This requires the ‘outer’ Krylov method to be *flexible*, able to operate with a nonlinear preconditioner. Flexible Krylov methods do not involve Krylov subspaces but approximations to them. In comparison with their non-flexible counterparts, flexible Krylov methods typically have higher storage requirements, as they cannot exploit the structure of true Krylov spaces.

In this work, we explore, analyze, and implement Krylov methods which are both pipelined and flexible. As shown in §5-7, promising applications of the new methods presented here involve preconditioners with nested inexact solves used over many Krylov iterations. For the overlap of reductions to be useful, systems must involve large numbers of nodes, or one must be in a strong-scaling regime where the time for a global reduction is comparable to the time spent performing local and neighbor-wise work, or when local processing times are very variable.

Our methods are applicable to the solution of any system of linear equations, but are expected to be useful when the number of processing units is large, relative to the local problem size, and when strong, complex, nonlinear (or even nondeterministic) preconditioners are applied to systems difficult enough to require enough Krylov iterations to amortize the overhead of filling a pipeline. Thus, for the examples presented in §6, we focus on applications in geophysics, in particular on mantle convection and lithospheric dynamics with heterogeneous viscosity structure. These represent challenging problems, where strong multiscale nonlinear preconditioners are typically required for acceptable convergence.

Nonlinear preconditioning is still an active area of research, and newly developed nonlinear methods [6] may provide additional use cases for the methods presented here. The advent of non-deterministic and randomized preconditioning techniques, promising for use with hybrid or heterogeneous clusters featuring accelerators, may provide future use cases for algorithms of the type presented here; these allow overlap of communication and computation and also loosen synchronization requirements, crucial when local processing times have heavy-tailed distributions [30].

1.2 Notation and Algorithmic Presentation

We use similar notation to analyze variants of the Conjugate Gradient (CG), Conjugate Residual (CR), and Generalized Minimal Residual (GMRES) methods, as described in Tables 1 and 2. This allows similar presentation of the methods, despite the fact that CG and CR methods are written as left preconditioned, while flexible GMRES methods are right preconditioned. Operators are denoted by capital letters, vectors by lowercase Latin letters, and scalars by Greek letters. Algorithms are presented using 0-based iteration counts. For readability and analysis, main iteration loops are arranged such that variables indexed by the current index are updated. Convergence tests and optimizations related to initialization, elimination of intermediates, and loop ordering are omitted for readability; the interested reader is referred to §5 where full open-source implementations are discussed. We adopt the following coloring scheme for operations involving

vectors. Scalar or ‘no operation’ operations are not colored.

- **Green** denotes an algorithmic step which is “local”, meaning that no internode communication is required in a typical parallel implementation.
- **Orange** denotes an algorithmic step which operates “neighbor-wise”, only involving communication between $O(1)$ neighboring nodes interspersed with local work. Sparse matrix-vector multiplication typically falls into this category.
- **Red** denotes an algorithmic step which is “global”, involving global communication, exposing the full latency of the network. These operations, which include computing vector dot products and norms, can become the computational bottleneck in massively parallel systems.
- **Purple** is used for preconditioner application, which may be local (e.g. applying a Jacobi preconditioner), neighbor-wise (e.g. applying a sparse approximate inverse), or global (e.g. applying a nested Krylov method).

Algorithm line numbers corresponding to local, neighbor-wise, global, and preconditioning operations are also marked with a dash(-), plus(+), bullet(•), and asterisk(*), respectively.

1.3 Contributions

- We present pipelined variants of flexible methods, allowing for inexact and variable preconditioning. (§2-4)
- We provide open-source, scalable implementations of three solvers as contributions to the PETSC package. (§5)
- We provide analysis of a novel modification of a “naive” pipelining which gives unacceptable convergence behavior in typical applications. This leads to useful, pipelined variants of the Flexible CG (FCG) and Generalized CR (GCR) methods. (§2.2)
- We demonstrate the use of the methods with applications to solving linear systems from challenging problems in lithospheric dynamics (§6), and with performance models to extrapolate to exascale (§7).

2 Pipelined Flexible Conjugate Gradient Methods

Notation We base the notation used in this section, collected in Table 1, on standard notation for Conjugate Gradient methods and its pipelined variant [13].

2.1 Review of Conjugate Gradient Methods

2.1.1 The Method of Conjugate Directions

A general class of methods known as *conjugate direction (CD) methods* [11, 19] have been investigated to compute (approximate) numerical solutions to the linear system $Ax = b$, where $A = A^H$ and A is positive definite. Presume one has a set of A -orthogonal (“conjugate”) vectors $\{p_j\}, j = 0, \dots, n - 1$ available, that is a set of n vectors with the property $\langle p_j, p_k \rangle_A = \langle p_j, Ap_k \rangle = 0$ when $j \neq k$. At each step of the algorithm, the conjugate directions method computes an approximate solution x_i with the property that $\|x - x_i\|_A^2$ is minimal for $x_i - x_0 \in \text{span}(p_0, \dots, p_{i-1})$. The resulting process is described in Algorithm 1. Due to the unspecified nature of the A -orthogonal directions $\{p_j\}$, it includes a wide range of algorithms, including Gaussian elimination and the family of Conjugate Gradient methods which are the main subject of this section.

| | |
|---------------|---|
| A | linear operator |
| M^{-1} | linear, symmetric positive definite, left preconditioner |
| B | nonlinear left preconditioner |
| x | true solution vector $A^{-1}b$ |
| x_i | approximate solution vector at iteration $i = 0, 1, \dots$ |
| e_i | error $x - x_i$ at iteration i |
| r_i | residual $b - Ax_i = Ae_i$ at iteration i |
| u_i | preconditioned residual $B(r_i)$ or $M^{-1}r_i$ |
| \tilde{u}_i | approximation to u_i , exact for a linear preconditioner |
| w_i | pipelining intermediate Au_i or $A\tilde{u}_i$ |
| m_i | pipelining intermediate $B(w_i)$ or $M^{-1}w_i$ |
| n_i | pipelining intermediate Am_i |
| p_i | search direction or basis vector |
| s_i | transformed search direction Ap_i |
| q_i | pipelining intermediate $B(s_i)$ or $M^{-1}s_i$ |
| z_i | pipelining intermediate Aq_i |
| α_i | scalar weight in solution and residual update |
| β_i | scalar weight in computation of new search direction or basis vector |
| η_i | squared norm $\langle Ap_i, p_i \rangle = \ p_i\ _A^2$ |
| δ_i | squared norm $\langle Au_i, u_i \rangle = \ u_i\ _A^2$ |
| γ_i | L_2 -inner product involving preconditioned or unpreconditioned residuals depending on the method under consideration ($\langle r_i, r_i \rangle$, $\langle u_i, u_i \rangle$, or $\langle u_i, r_i \rangle$) |

Table 1: Notation for Conjugate Gradient and related methods

We note an important property of all CD methods. By the minimization property, we have

$$e_i \perp_A \text{span}(p_0, \dots, p_{i-1}) \iff r_i \perp \text{span}(p_0, \dots, p_{i-1}). \quad (1)$$

That is, the residual is orthogonal to the previously explored space in the standard norm ¹.

The directions p_j need not be specified before the algorithm begins; they can be computed as needed, based on the progress of the algorithm.

Algorithm 1 Conjugate Directions [19]

```

1: function CD( $A, b, x_0, p_0, \dots, p_{n-1}$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
- 3:    $p_0 \leftarrow r_0$ 
+ 4:    $s_0 \leftarrow Ap_0$ 
• 5:    $\gamma_0 \leftarrow \langle p_0, r_0 \rangle$ 
• 6:    $\eta_0 \leftarrow \langle p_0, s_0 \rangle$ 
7:    $\alpha_0 \leftarrow \gamma_0 / \eta_0$ 
8:   for  $i = 1, 2, \dots, n$  do
- 9:      $x_i \leftarrow x_{i-1} + \alpha_{i-1} p_{i-1}$ 
-10:     $r_i \leftarrow r_{i-1} - \alpha_{i-1} s_{i-1}$ 
•11:     $\gamma_i \leftarrow \langle p_i, r_i \rangle$ 
+12:     $s_i \leftarrow Ap_i$ 
•13:     $\eta_i \leftarrow \langle s_i, p_i \rangle$ 
14:     $\alpha_i \leftarrow \gamma_i / \eta_i$ 

```

2.1.2 Flexible Conjugate Gradient Methods

To ensure rapid convergence of the CD algorithm, it is desirable at each iteration for the new search direction p_i to be well-aligned with the remaining error $e_i = x - x_i$. As the true error is unknown, one available option is the residual $r_i = Ae_i$, A -orthogonalized against the other search directions.

¹Other norms may be used, as described by Hestenes [18].

Algorithm 2 Flexible Conjugate Gradients [31]

```
1: function FCG( $A, B, b, x_0$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
* 3:    $u_0 \leftarrow B(r_0)$ 
- 4:    $p_0 \leftarrow u_0$ 
+ 5:    $s_0 \leftarrow Ap_0$ 
• 6:    $\gamma_0 \leftarrow \langle u_0, r_0 \rangle$ 
• 7:    $\eta_0 \leftarrow \langle p_0, s_0 \rangle$ 
8:    $\alpha_0 \leftarrow \gamma_0 / \eta_0$ 
9:   for  $i = 1, 2, \dots$  do
-10:     $x_i \leftarrow x_{i-1} + \alpha_{i-1} p_{i-1}$ 
-11:     $r_i \leftarrow r_{i-1} - \alpha_{i-1} s_{i-1}$ 
*12:     $u_i \leftarrow B(r_i)$ 
•13:     $\gamma_i \leftarrow \langle u_i, r_i \rangle$ 
14:    for  $k = i - \nu_i, \dots, i - 1$  do
•15:      $\beta_{i,k} \leftarrow \frac{-1}{\eta_k} \langle u_i, s_k \rangle$ 
-16:     $p_i \leftarrow u_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k} p_k$ 
+17:     $s_i \leftarrow Ap_i$ 
•18:     $\eta_i \leftarrow \langle p_i, s_i \rangle$ 
19:     $\alpha_i \leftarrow \gamma_i / \eta_i$ 
```

Algorithm 3 Preconditioned Conjugate Gradients [18]

```
1: function PCG( $A, M^{-1}, b, x_0$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
* 3:    $u_0 \leftarrow M^{-1} r_0$ 
- 4:    $p_0 \leftarrow u_0$ 
+ 5:    $s_0 \leftarrow Ap_0$ 
• 6:    $\gamma_0 \leftarrow \langle u_0, r_0 \rangle$ 
• 7:    $\eta_0 \leftarrow \langle s_0, p_0 \rangle$ 
8:    $\alpha_0 \leftarrow \gamma_0 / \eta_0$ 
9:   for  $i = 1, 2, \dots$  do
-10:     $x_i \leftarrow x_{i-1} + \alpha_{i-1} p_{i-1}$ 
-11:     $r_i \leftarrow r_{i-1} - \alpha_{i-1} s_{i-1}$ 
*12:     $u_i \leftarrow M^{-1} r_i$ 
•13:     $\gamma_i \leftarrow \langle u_i, r_i \rangle$ 
14:
15:     $\beta_i \leftarrow \gamma_i / \gamma_{i-1}$ 
-16:     $p_i \leftarrow u_i + \beta_i p_{i-1}$ 
+17:     $s_i \leftarrow Ap_i$ 
•18:     $\eta_i \leftarrow \langle s_i, p_i \rangle$ 
19:     $\alpha_i \leftarrow \gamma_i / \eta_i$ 
```

The residual can be seen as a transformed error or as a gradient descent direction for the function $\frac{1}{2} \|x\|_A^2 - \langle b, x \rangle$, a minimizer of which is a solution of $Ax = b$. Preconditioning can be seen as an attempt to obtain a direction better aligned with e_i by instead A -orthogonalizing $u_i \doteq B(r_i) = B(Ae_i)$ against the previous search directions p_0, \dots, p_{i-1} . If B is an approximate inverse of A , it is effective by this criterion, and many preconditioners are motivated as such.

The process just described, found in Algorithm 2, describes the Flexible Conjugate Gradient (FCG) method [31], with complete orthogonalization, i.e., the new search direction is found by A -orthogonalizing the residual against all previous directions in every iteration. Full A -orthogonalization requires potentially excessive memory usage and computation. Hence, it is a common approach to only A -orthogonalize against a number ν_i of previous directions. Note however that only for full orthogonalization ($\nu_i = i$) is a true A -orthogonal basis computed by the Gram-Schmidt process in lines 14–16 of Algorithm 2, defining a CD method in the strict sense.

One can observe from Algorithm 2 that no overlapping of reductions and operator or preconditioner application is possible; the dot products depend on the immediately preceding computations.

2.1.3 Preconditioned Conjugate Gradients

Let $\mathcal{K}^j(A, b)$ represent the j th Krylov subspace $\text{span}(b, Ab, \dots, A^{j-1}b)$. If B is a linear operator $B(v) \equiv M^{-1}v$, then line 15 of Algorithm 2 evaluates to zero for all but the most recent previous direction, and the search directions lie in Krylov subspaces $\mathcal{K}^i(M^{-1}A, M^{-1}b)$. We thus recover the Preconditioned Conjugate Gradient Method [14, 18, 37] shown in Algorithm 3. Again, communication and computation cannot be overlapped using the algorithm as written, and in a parallel implementation, two reductions must be performed per iteration.

2.1.4 Pipelined Preconditioned Conjugate Gradients

Any rearrangement of the PCG algorithm beyond trivial options must appeal to a notion of algorithmic equivalence more general than producing identical floating-point results. These notions include algebraic rearrangements, which typically do not produce the same iterates in finite precision arithmetic, but which are equivalent in exact arithmetic. One such operation is to rearrange the CG algorithm to involve a single reduction, requiring less communication and synchronization overhead on parallel systems. This was done by Chronopoulos and Gear [8], as described in Algorithm 4. The rearrangement is also particularly important in the context of implementing efficient Krylov methods for current hybrid systems involving high throughput coprocessors for which kernel fusion is beneficial [32].

This rearrangement is possible because CG relies on the geometric structure induced by interpreting symmetric positive definite operators as inner products. Noting that η_i is defined as the squared A -norm of p_i and that p_i is constructed by A -orthogonalizing u_i with respect to p_{i-1} , one can use the Pythagorean Theorem to write

$$\eta_i = \|p_i\|_A^2 = \|u_i + \beta p_{i-1}\|_A^2 = \|u_i\|_A^2 - |\beta_i|^2 \|p_{i-1}\|_A^2 = \|u_i\|_A^2 - |\beta_i|^2 \eta_{i-1}$$

where terms involving products of directions at different iteration numbers are zero because of the A -orthogonality of p_i and p_{i-1} . The quantity $\delta_i \doteq \|u_i\|_A^2 = \langle u_i, Au_i \rangle$ does not depend on p_i and can thus be computed at the same time as γ_i . The quantity $w_i \doteq Au_i$ needs to be computed, which apparently adds another matrix multiply to the overall iteration. However, a second type of structure, namely linear structure, can be exploited to reuse this computation and remove the existing matrix multiply with a recurrence relation

$$s_i = Ap_i = Au_i + \beta_i Ap_{i-1} = w_i + \beta_i s_{i-1}. \quad (2)$$

These rearrangements require additional storage (one extra vector w in this case) and floating point computations and come with potential numerical penalties as the computed norm could become negative (“norm breakdown”) in finite precision arithmetic. These breakdowns are most easily handled through algorithm restarts. Also, errors can accumulate in recursively computed variables.

As η_i is only used to calculate α_i , one can avoid computing it and update α_i directly as

$$\alpha_i = \frac{\gamma_i}{\eta_i} = \frac{\gamma_i}{(\delta_i - |\beta_i|^2 \eta_{i-1})} = \frac{\gamma_i}{\delta_i - \left(\frac{\gamma_i}{\gamma_{i-1}}\right)^2 \left(\frac{\gamma_{i-1}}{\alpha_{i-1}}\right)} = \frac{\gamma_i}{\delta_i - \beta_i \frac{\gamma_i}{\alpha_{i-1}}}.$$

This recurrence is more concise, but we retain explicit computation of η_i in the algorithms as presented here to allow for an easier comparison.

The Chronopoulos-Gear CG method cannot overlap the preconditioner and sparse matrix multiply with the reductions, so some further rearrangement is desirable to allow concurrent use of computational resources. Ghysels and Vanroose [13] developed a further variant of the Chronopoulos-Gear algorithm to accomplish this, as described in Algorithm 5. The algorithm takes advantage of multiple “unrollings” using the linear structure of the variable updates, as in (2). For example, since the computation of $u_i = M^{-1}r_i$ on line 20 of Algorithm 4 blocks the subsequent inner product involving u_i , one can use the identity

$$u_i = M^{-1}r_i = M^{-1}r_{i-1} - \alpha_{i-1}M^{-1}s_i = u_{i-1} - \alpha_{i-1}q_i \quad (3)$$

which shifts the application of M^{-1} from r_i to s_i , to compute a new variable $q_i \doteq M^{-1}s_i$. Similarly, q_i is rewritten until computation, for m_i in Algorithm 5, can be overlapped with the dot products in the previous iteration. The identity in (3) relies on the linearity of M^{-1} . This rearrangement allows for more concurrent use of computational resources at the cost of storing more vectors, performing more floating point operations, and reducing numerical stability [13]. Examples as well as a performance model [12, 13] show performance gains on current and future parallel systems.

The Pipelined Conjugate Gradient method as presented in Algorithm 5 requires storing 10 vectors compared to 6 for PCG and 7 for CGCG.

Algorithm 4 Chronopoulos-Gear Conjugate Gradients [8]

```

1: function CGCG( $A, M^{-1}, b, x_0$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
* 3:    $u_0 \leftarrow M^{-1}r_0$ 
+ 4:    $w_0 \leftarrow Au_0$ 
5:
6:
• 7:    $\gamma_0 \leftarrow \langle u_0, r_0 \rangle$ 
• 8:    $\delta_0 \leftarrow \langle u_0, w_0 \rangle$ 
9:    $\eta_0 \leftarrow \delta_0$ 
-10:   $p_0 \leftarrow u_0$ 
-11:   $s_0 \leftarrow w_0$ 
12:
13:
14:   $\alpha_0 \leftarrow \gamma_0 / \eta_0$ 
15:  for  $i = 1, 2, \dots$  do
-16:     $x_i \leftarrow x_{i-1} + \alpha_{i-1}p_{i-1}$ 
-17:     $r_i \leftarrow r_{i-1} - \alpha_{i-1}s_{i-1}$ 
18:
19:
*20:    $u_i \leftarrow M^{-1}r_i$ 
+21:    $w_i \leftarrow Au_i$ 
•22:    $\delta_i \leftarrow \langle u_i, w_i \rangle$ 
•23:    $\gamma_i \leftarrow \langle u_i, r_i \rangle$ 
24:    $\beta_i \leftarrow \gamma_i / \gamma_{i-1}$ 
25:    $\eta_i \leftarrow \delta_i - |\beta_i|^2 \eta_{i-1}$ 
26:    $\alpha_i \leftarrow \gamma_i / \eta_i$ 
-27:    $p_i \leftarrow u_i + \beta_i p_{i-1}$ 
-28:    $s_i \leftarrow w_i + \beta_i s_{i-1}$ 
29:
30:

```

Algorithm 5 Pipelined Conjugate Gradients [13]

```

1: function PIPECG( $A, M^{-1}, b, x_0$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
* 3:    $u_0 \leftarrow M^{-1}r_0$ 
+ 4:    $w_0 \leftarrow Au_0$ 
* 5:    $m_0 \leftarrow M^{-1}w_0$ 
+ 6:    $n_0 \leftarrow Am_0$ 
• 7:    $\gamma_0 \leftarrow \langle u_0, r_0 \rangle$ 
• 8:    $\delta_0 \leftarrow \langle u_0, w_0 \rangle$ 
9:    $\eta_0 \leftarrow \delta_0$ 
-10:   $p_0 \leftarrow u_0$ 
-11:   $s_0 \leftarrow w_0$ 
-12:   $q_0 \leftarrow m_0$ 
-13:   $z_0 \leftarrow n_0$ 
14:   $\alpha_0 \leftarrow \gamma_0 / \eta_0$ 
15:  for  $i = 1, 2, \dots$  do
-16:     $x_i \leftarrow x_{i-1} + \alpha_{i-1}p_{i-1}$ 
-17:     $r_i \leftarrow r_{i-1} - \alpha_{i-1}s_{i-1}$ 
-18:     $u_i \leftarrow u_{i-1} - \alpha_{i-1}q_{i-1}$ 
-19:     $w_i \leftarrow w_{i-1} - \alpha_{i-1}z_{i-1}$ 
*20:    $m_i \leftarrow M^{-1}w_i$ 
+21:    $n_i \leftarrow Am_i$ 
•22:    $\gamma_i \leftarrow \langle u_i, r_i \rangle$ 
•23:    $\delta_i \leftarrow \langle u_i, w_i \rangle$ 
24:    $\beta_i \leftarrow \gamma_i / \gamma_{i-1}$ 
25:    $\eta_i \leftarrow \delta_i - |\beta_i|^2 \eta_{i-1}$ 
26:    $\alpha_i \leftarrow \gamma_i / \eta_i$ 
-27:    $p_i \leftarrow u_i + \beta_i p_{i-1}$ 
-28:    $s_i \leftarrow w_i + \beta_i s_{i-1}$ 
-29:    $q_i \leftarrow m_i + \beta_i q_{i-1}$ 
-30:    $z_i \leftarrow n_i + \beta_i z_{i-1}$ 

```

2.2 Pipelined Flexible Conjugate Gradient Methods

The FCG algorithm can be modified in the same manner used to produce the Chronopoulos-Gear CG algorithm. This does not involve any assumption of linearity of B , so the new single reduction FCG algorithm described in Algorithm 6 is equivalent to FCG in exact arithmetic, for an arbitrary preconditioner.

Algorithm 6 Single Reduction Flexible Conjugate Gradients

```

1: function CGFCG( $A, B, b, x_0$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
* 3:    $u_0 \leftarrow B(r_0)$ 
+ 4:    $w_0 \leftarrow Ap_0$ 
• 5:    $\gamma_0 \leftarrow \langle u_0, r_0 \rangle$ 
• 6:    $\delta_0 \leftarrow \langle u_0, w_0 \rangle$ 
- 7:    $p_0 \leftarrow u_0$ 
- 8:    $s_0 \leftarrow w_0$ 
9:    $\eta_0 \leftarrow \delta_0$ 
10:   $\alpha_0 \leftarrow \gamma_0 / \eta_0$ 
11:  for  $i = 1, 2, \dots$  do
-12:     $x_i \leftarrow x_{i-1} + \alpha_{i-1} p_{i-1}$ 
-13:     $r_i \leftarrow r_{i-1} - \alpha_{i-1} s_{i-1}$ 
*14:     $u_i \leftarrow B(r_i)$ 
+15:     $w_i \leftarrow Au_i$ 
•16:     $\gamma_i \leftarrow \langle u_i, r_i \rangle$ 
17:    for  $k = i - \nu_i, \dots, i - 1$  do
18:       $\beta_{i,k} \leftarrow \frac{-1}{\eta_k} \langle u_i, s_k \rangle$ 
•19:     $\delta_i \leftarrow \langle u_i, w_i \rangle$ 
-20:     $p_i \leftarrow u_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k} p_k$ 
-21:     $s_i \leftarrow w_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k} s_k$ 
22:     $\eta_i \leftarrow \delta_i - \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}^2 \eta_k$ 
23:     $\alpha_i \leftarrow \gamma_i / \eta_i$ 

```

One can now attempt to pipeline FCG in the same manner as pipelined variants of CG are obtained - this leads to the variant described in Algorithm 7. The quantity \tilde{u} is used to reinforce the idea that the preconditioned search directions differ in general from those computed by FCG.

A variant analogous to Gropp's asynchronous CG [16] could also be defined. We do so for the corresponding method based on conjugate residuals in §3.2.

2.2.1 Issues with Naive Pipelining and Variable Preconditioning

Convergence of Algorithm 7 typically stagnates for nonlinear preconditioners B . In cases where the preconditioner has an associated “noise level” or tolerance which characterizes its variability, stagnation is typically observed at a relative error comparable to this quantity. This is illustrated in Figure 1, plotting convergence for a diagonal system with a preconditioner which simply adds Gaussian noise to the residual.

Analysis of preconditioned conjugate gradient methods typically makes use of the preconditioner as an inner product. The CG method can be seen as a Ritz-Galerkin approach to a Krylov subspace method where approximations in successive Krylov subspaces are chosen to satisfy the condition that the resulting residual is orthogonal to the Krylov subspace [39, §4.1]. Choosing a different definition of orthogonality, based on the metric induced by M^{-1} , produces the PCG method. This is equivalent to the notion of simply replacing the L_2 inner product with a different inner product, wherever it appears in the algorithm. This freedom to choose norms was recognized soon after the development of the CG method [18]. In terms of the PCG,

Algorithm 7 Pipelined FCG (Naive)

```
1: function PIPEFCG?( $A, B, b, x_0$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
* 3:    $\tilde{u}_0 \leftarrow B(r_0)$ 
- 4:    $p_0 \leftarrow \tilde{u}_0$ 
+ 5:    $w_0 \leftarrow Ap_0$ 
* 6:    $m_0 \leftarrow B(w_0)$ 
+ 7:    $n_0 \leftarrow Am_0$ 
• 8:    $\gamma_0 \leftarrow \langle \tilde{u}_0, r_0 \rangle$ 
• 9:    $\delta_0 \leftarrow \langle \tilde{u}_0, w_0 \rangle$ 
-10:   $s_0 \leftarrow w_0$ 
-11:   $q_0 \leftarrow m_0$ 
-12:   $z_0 \leftarrow n_0$ 
13:   $\eta_0 \leftarrow \delta_0$ 
14:   $\alpha_0 \leftarrow \gamma_0/\eta_0$ 
15:  for  $i = 1, 2, \dots$  do
-16:     $x_i \leftarrow x_{i-1} + \alpha_{i-1}p_{i-1}$ 
-17:     $r_i \leftarrow r_{i-1} - \alpha_{i-1}s_{i-1}$ 
-18:     $\tilde{u}_i \leftarrow \tilde{u}_{i-1} - \alpha_{i-1}q_{i-1}$ 
-19:     $w_i \leftarrow w_{i-1} - \alpha_{i-1}z_{i-1}$ 
•20:     $\gamma_i \leftarrow \langle \tilde{u}_i, r_i \rangle$ 
21:    for  $k = i - \nu_i, \dots, i - 1$  do
•22:       $\beta_{i,k} \leftarrow \frac{-1}{\eta_k} \langle \tilde{u}_i, s_k \rangle$ 
•23:     $\delta_i \leftarrow \langle \tilde{u}_i, w_i \rangle$ 
*24:     $\mathbf{m}_i \leftarrow \mathbf{B}(\mathbf{w}_i)$ 
+25:     $n_i \leftarrow Am_i$ 
-26:     $p_i \leftarrow \tilde{u}_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}p_k$ 
-27:     $s_i \leftarrow w_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}s_k$ 
-28:     $q_i \leftarrow m_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}q_k$ 
-29:     $z_i \leftarrow n_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}z_k$ 
30:     $\eta_i \leftarrow \delta_i - \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}^2 \eta_k$ 
31:     $\alpha_i \leftarrow \gamma_i/\eta_i$ 
```

Algorithm 8 Pipelined FCG

```
1: function PIPEFCG( $A, B, b, x_0$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
* 3:    $\tilde{u}_0 \leftarrow B(r_0)$ 
- 4:    $p_0 \leftarrow \tilde{u}_0$ 
+ 5:    $w_0 \leftarrow Ap_0$ 
* 6:    $m_0 \leftarrow B(w_0)$ 
+ 7:    $n_0 \leftarrow Am_0$ 
• 8:    $\gamma_0 \leftarrow \langle u_0, r_0 \rangle$ 
• 9:    $\delta_0 \leftarrow \langle u_0, w_0 \rangle$ 
-10:   $s_0 \leftarrow w_0$ 
-11:   $q_0 \leftarrow m_0$ 
-12:   $z_0 \leftarrow n_0$ 
13:   $\eta_0 \leftarrow \delta_0$ 
14:   $\alpha_0 \leftarrow \gamma_0/\eta_0$ 
15:  for  $i = 1, 2, \dots$  do
-16:     $x_i \leftarrow x_{i-1} + \alpha_{i-1}p_{i-1}$ 
-17:     $r_i \leftarrow r_{i-1} - \alpha_{i-1}s_{i-1}$ 
-18:     $\tilde{u}_i \leftarrow \tilde{u}_{i-1} - \alpha_{i-1}q_{i-1}$ 
-19:     $w_i \leftarrow w_{i-1} - \alpha_{i-1}z_{i-1}$ 
•20:     $\gamma_i \leftarrow \langle \tilde{u}_i, r_i \rangle$ 
21:    for  $k = i - \nu_i, \dots, i - 1$  do
•22:       $\beta_{i,k} \leftarrow \frac{-1}{\eta_k} \langle \tilde{u}_i, s_k \rangle$ 
•23:     $\delta_i \leftarrow \langle \tilde{u}_i, w_i \rangle$ 
*24:     $\mathbf{m}_i \leftarrow \tilde{\mathbf{u}}_i + \mathbf{B}(\mathbf{w}_i - \mathbf{r}_i)$ 
+25:     $n_i \leftarrow Am_i$ 
-26:     $p_i \leftarrow \tilde{u}_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}p_k$ 
-27:     $s_i \leftarrow w_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}s_k$ 
-28:     $q_i \leftarrow m_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}q_k$ 
-29:     $z_i \leftarrow n_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}z_k$ 
30:     $\eta_i \leftarrow \delta_i - \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}^2 \eta_k$ 
31:     $\alpha_i \leftarrow \gamma_i/\eta_i$ 
```

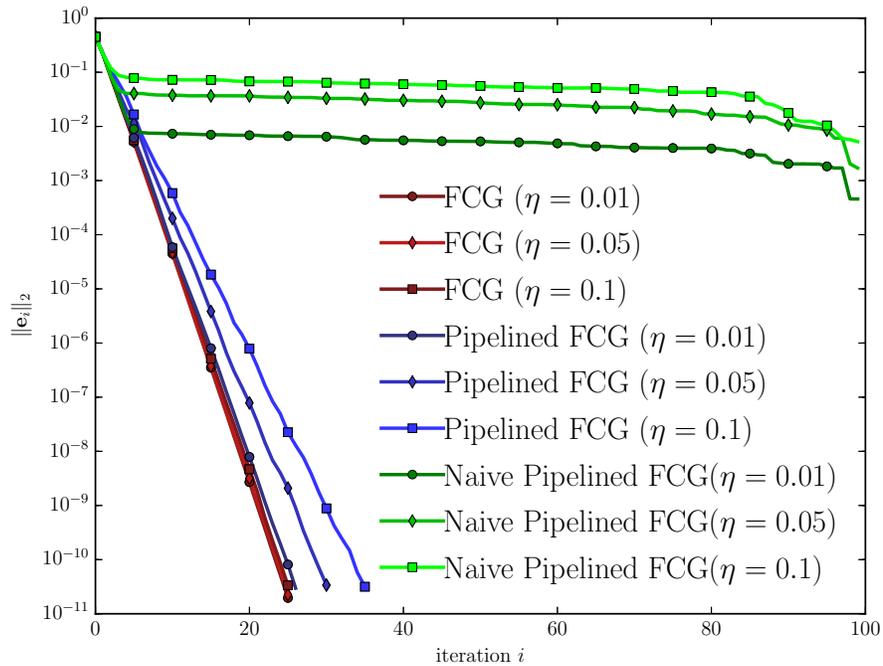


Figure 1: A toy diagonal system, $n = 100$, with condition number 5, equally-spaced eigenvalues, and $b = \mathbb{1}/\sqrt{n}$, solved with FCG, naively pipelined FCG (Algorithm 7), and our PIPEFCG (Algorithm 8). The pathological preconditioner B adds Gaussian noise of magnitude $\eta\|r\|$ to the residual r . $\nu_{\max} = n$. Note that convergence for the naively pipelined algorithm stagnates at a relative error of approximately η .

Algorithm 3,

$$\gamma_i = \langle r_i, r_i \rangle_{M^{-1}} = \langle u_i, r_i \rangle. \quad (4)$$

Here, the nonlinearity of the preconditioner precludes direct use of this idea. We opt to consider B in a more general sense of a preconditioner, as an approximate inverse to A . Specifically, noting that $Ae_i = r_i$, we shall later require that $\|B(r_i) - e_i\|/\|e_i\|$ is controlled.

Naively replacing the linear preconditioner M^{-1} in (3) with a nonlinear one, we obtain the unrolling used in Algorithm 7,

$$u_i = B(r_i) \approx B(r_{i-1}) - B(\alpha_{i-1}s_i) \approx u_{i-1} - \alpha_{i-1}q_i, \quad (5)$$

which is inexact even in exact arithmetic. This unrolling is not a priori unacceptable, as FCG is designed to cope with varying and inexact preconditioning, and the rearrangement amounts to a different nonlinear preconditioner, albeit one derived using intuition from the linear case. However, unlike the unrolling (3) the above leads to an accumulation of errors in the preconditioned residual \tilde{u}_i , with respect to $u_i = B(r_i)$. This invalidates the equivalence (4), which PCG structurally relies on for projecting out search directions from the residual.

Note that when introducing a nonlinear preconditioner with FCG² the basis vectors p_j remain A -orthogonal with this rearrangement, yet the residuals r_i , which are M^{-1} -orthogonal when $B(v) \equiv M^{-1}v$, are now orthogonal with respect to an equivalent linear operator \hat{B} , using Notay's concept and notation of an *equivalent linear operator* [31]. This operator is defined by the relations $u_i = B(r_i) = \hat{B}r_i$, depends on b and x_0 , and is unique except in degenerate cases. It seems to be the case that the equivalent linear operator \hat{B} implicitly defined (Cf. (3)) by the update on line 18 of Algorithm 7 is unbounded as $i \rightarrow \infty$, mapping residuals of arbitrarily small magnitude to preconditioned residuals of the same order, making it an unacceptable approximation for any given linear operator M^{-1} bounded as $n \rightarrow \infty$.

Thus, it will be useful to distinguish between the equivalent linear operators as induced by the base and pipelined methods, \hat{B} and $\tilde{\hat{B}}$, respectively. The operator $\tilde{\hat{B}}$ is defined by the relations $\tilde{u}_i = \tilde{\hat{B}}r_i$. The quantities α_i , in a CD method like FCG, are chosen to minimize $\|x - (x_{i+1} + \alpha_{i-1}u_i)\|_A$. However, in the pipelined variant, the effective update is $x_i \leftarrow x_{i-1} + \alpha_{i-1}\tilde{u}_i$. Thus, deviation from the base method induced by pipelining can of course be characterized by the difference between u and \tilde{u} , or equivalently the difference between $\tilde{\hat{B}}$ and \hat{B} . The advantage of this second view is that it suggests a repair procedure. Namely, one should respect the already-defined part of \hat{B} as much as possible when computing \tilde{u} , hence partially defining $\tilde{\hat{B}}$. One approach is to note that the operation of the equivalent linear operator in direction r_i has already been defined, so one can project this direction out of the quantity which B is applied to. Thus, the algorithm can be modified to compute the vector

$$m_i \leftarrow \theta_i \tilde{u}_{i-1} + B(w_{i-1} - \theta_i r_{i-1}), \quad \theta_i \doteq \frac{\langle r, w \rangle}{\|r\|^2} \quad (6)$$

Indeed, numerical experiments show that this modification can restore convergence in some cases. This modification is, unfortunately, not useful as it stands for the purposes of improving the naive pipelined FCG algorithm, as it requires additional blocking reductions. A natural question, however, is how one might estimate θ_i . One useful property is that as the preconditioner approaches A^{-1} , θ_i approaches 1 for all i . This motivates the choice of $\theta_i \equiv 1$ as at least an “unbiased” approximation.

2.2.2 Faithful Preconditioners

To be more precise, we restrict our attention to a subclass of nonlinear preconditioners.

Definition 2.1 *A family of functions $B_n : \mathbb{C}^n \mapsto \mathbb{C}^n$, $n = 1, 2, \dots$ represents a faithful preconditioner with respect to a family of linear operators $A_n \in L(\mathbb{C}^n, \mathbb{C}^n)$ if $B_n(A_n(\cdot)) - I_n(\cdot)$ is a uniformly bounded sequence of operators, with respect to the standard norm on \mathbb{C}^n . That is, there exists $c \in \mathbb{R}$ such that*

$$\|B_n(A_n v) - v\| < c\|v\| \quad \forall v \in \mathbb{C}^n \setminus \{0\}, \quad \forall n \in \{1, 2, \dots\}$$

²We assume $\nu_i = i$, that is complete orthogonalization, for all of the analysis in this section.

Remark 2.2 We will typically abuse notation and omit the dependence on n .

Remark 2.3 Applied to the special case where $v = e_i \doteq x - x_i$, the error in a particular iteration of a Krylov method, noting that $B(Ae_i) = B(r_i) = u_i$, the condition above implies that

$$\|u_i - e_i\| < c\|e_i\|,$$

which is to say that the preconditioned residual is a uniformly accurate approximation to the error.

Remark 2.4 The class of Sparse Approximate Inverse preconditioners are a special case of faithful preconditioners, if the approximation quality is uniform in the problem size.

To compute θ_i in (6) requires additional inner products, so instead we seek to cheaply estimate it. Note that θ_i minimizes the distance $\|w_i - \theta_i r_i\|$. If we assume our preconditioner to be faithful with a small constant, so that the operator $AB(\cdot) - I(\cdot)$ is bounded with a small constant, then $\theta_i \equiv 1$ is a reasonable estimate, as $\|w - r\|/\|r\| = \|AB(r) - r\|/\|r\|$ is then small.

Note that $\theta_i \equiv 0$ corresponds to the naive unrolling as in (5).

2.2.3 Defining an Improved Pipelined Flexible Conjugate Gradient Algorithm

In a modified version of the naive pipelined Flexible Conjugate Gradients, Algorithm 7, we take advantage of the estimate $\theta_i \equiv 1$ to mitigate the observed stagnation of convergence.

Motivated by the considerations above, we observe great improvements employing the approximation

$$\tilde{u}_i = B(r_i) = B(r_{i-1} - \alpha_{i-1}Ap_{i-1}) \approx (1 - \alpha_{i-1})B(r_{i-1}) - \alpha_{i-1}B(Ap_{i-1} - r_{i-1}) \quad (7)$$

instead of the recurrence relation (5). This leads to a replacement of the algorithmic step $m_i \leftarrow B(w_i)$ in line 24 of Algorithm 7 by

$$m_i \leftarrow \tilde{u}_i + B(w_i - r_i). \quad (8)$$

For a linear preconditioner these are equivalent in exact arithmetic.

We proceed to show that this can be interpreted in terms of improved control of the accumulation of perturbations in \tilde{u}_i with respect to $B(r_i)$, assuming the preconditioner is sufficiently faithful.

Note that $w_i = A\tilde{u}_i$ in exact arithmetic and rewrite (8) as

$$m_i \leftarrow \tilde{u}_i + B(A\tilde{u}_i - r_i) = \tilde{u}_i + B(A(\tilde{u}_i - e_i)).$$

With $q_i = m_i + \sum_k \beta_k q_k$ we write out the recurrence relation

$$\begin{aligned} \tilde{u}_i &= \tilde{u}_{i-1} - \alpha_{i-1} \left(\tilde{u}_{i-1} + B(A(\tilde{u}_{i-1} - e_{i-1})) + \sum_k \beta_k q_k \right) \\ &= (1 - \alpha_{i-1})\tilde{u}_{i-1} - \alpha_{i-1} \left(B(A(\tilde{u}_{i-1} - e_{i-1})) + \sum_k \beta_k q_k \right). \end{aligned}$$

Rearranging terms we obtain

$$\tilde{u}_i = \underbrace{\left[(1 - \alpha_{i-1})\tilde{u}_{i-1} - \alpha_{i-1} \sum_k \beta_k q_k \right]}_{\text{I}} - \underbrace{\left[\alpha_{i-1} B(A(\tilde{u}_{i-1} - e_{i-1})) \right]}_{\text{II}}, \quad (9)$$

where Term II is affected by the nonlinear preconditioner but Term I is not. Using Definition 2.1 and Remark 2.3 we rewrite II as

$$\alpha_{i-1} B(A(\tilde{u}_{i-1} - e_{i-1})) = \alpha_{i-1} \tilde{I}(\tilde{u}_{i-1} - e_{i-1}) \approx \alpha_{i-1} (\tilde{u}_{i-1} - e_{i-1}),$$

with the operator \tilde{I} close to the identity operator using the notion of a faithful preconditioner. Comparing magnitudes of I and this approximation of II we expect that

$$\|(1 - \alpha_{i-1})\tilde{u}_{i-1} - \alpha_{i-1} \sum_k \beta_k q_k\| > \|\alpha_{i-1}(\tilde{u}_{i-1} - e_{i-1})\| \quad (10)$$

as a faithful preconditioner transforms the residual such that it is similar to the true error e . If instead we use $B(w)$ as in the naive Algorithm 7, then

$$\tilde{u}_i = \underbrace{\tilde{u}_{i-1} - \alpha_{i-1} \sum_k \beta_k q_k}_{\text{III}} - \underbrace{B(A\tilde{u}_{i-1})}_{\text{IV}}.$$

Following the same line of arguments we obtain that $B(A\tilde{u}_{i-1}) = \tilde{I}(\tilde{u}_{i-1}) \approx \tilde{u}_{i-1}$. Hence, Terms III and IV are of similar magnitude. While for the modified formulation the application of a nonlinear preconditioner leads to small perturbations of the preconditioned residual and consequently of the next search directions, this does not hold true for the naive formulation. Through recurrence of the preconditioned residual the accumulation of perturbations eventually leads to effectively random search directions and stagnation of convergence. This is observed in Figure 1, Once the “noise level” of the preconditioner is reached, convergence stagnates.

By employing the modification to the computation of the quantity m , analyzed in the previous section, we arrive at a useful pipelined variant of the FCG method, Algorithm 8.

Remark 2.5 *Algorithm 8 satisfies several desiderata:*

- *In exact arithmetic, with a linear preconditioner, it is equivalent to CG and FCG.*
- *As $B \rightarrow A^{-1}$, the operator becomes increasingly “faithful”, hence the algorithm approaches the behavior of FCG.*
- *No new reductions are introduced.*
- *A single reduction phase per iteration is used, which can be overlapped with application of the operator and preconditioner.*

The pipelined Flexible Conjugate Gradient method requires storing $(4\nu_{\max} + 11)$ vectors, compared to $(\nu_{\max} + 6)$ vectors for FCG (Algorithm 2) and $(2\nu_{\max} + 7)$ for Single Reduction FCG (Algorithm 6).

3 Pipelined Generalized Conjugate Residuals Methods

The Conjugate Residual family of Krylov subspace methods is applicable to systems with a Hermitian but not necessarily positive definite operator. While CG methods enforce A -conjugacy of search directions and minimize $\|e\|_A$, CR methods construct $A^H A$ -orthogonal search directions. In some derivations of the method, such as in Saad’s textbook [34], iterates minimize $\|e_i\|_{A^H A} = \|r_i\|$ over a Krylov subspace, which puts these methods in close relation to MINRES [39, §6.4] and GMRES [33, 35]. However, in some other derivations [25], these methods are described as minimizing $\|e\|_A$, as does CG. Here, we consider methods of the first kind, that is minimal-residual methods.

3.1 Review of Conjugate Residuals Methods

There is also an ambiguity regarding the terminology within the related flexible Krylov subspace methods. We note that the Generalized Conjugate Residual (GCR) method [10], which this section is concerned with, is closely related to FCG. However, despite its name, the GCR method is less closely related to Axelsson’s Generalized Conjugate Gradients (GCG) method [2, 1]. While FCG and GCR both employ a multi term

Algorithm 9 Generalized CR

```

1: function GCR( $A, B, b, x_0$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
* 3:    $u_0 \leftarrow B(r_0)$ 
- 4:    $p_0 \leftarrow u_0$ 
+ 5:    $s_0 \leftarrow Ap_0$ 
• 6:    $\gamma_0 \leftarrow \langle u_0, s_0 \rangle$ 
• 7:    $\eta_0 \leftarrow \langle s_0, s_0 \rangle$ 
8:    $\alpha_0 \leftarrow \gamma_0/\eta_0$ 
9:   for  $i = 1, 2, \dots$  do
-10:      $x_i \leftarrow x_{i-1} + \alpha_{i-1}p_{i-1}$ 
-11:      $r_i \leftarrow r_{i-1} - \alpha_{i-1}s_{i-1}$ 
*12:     $u_i \leftarrow B(r_i)$ 
13:    for  $k = i - \nu_i, \dots, i - 1$  do
•14:       $\beta_{i,k} \leftarrow \frac{-1}{\eta_k} \langle Au_i, s_k \rangle$ 
-15:     $p_i \leftarrow u_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}p_k$ 
+16:     $s_i \leftarrow Ap_i$ 
•17:     $\gamma_i \leftarrow \langle u_i, s_i \rangle$ 
•18:     $\eta_i \leftarrow \langle s_i, s_i \rangle$ 
19:     $\alpha_i \leftarrow \gamma_i/\eta_i$ 

```

Algorithm 10 Preconditioned CR

```

1: function PCR( $A, M^{-1}, b, x_0$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
* 3:    $u_0 \leftarrow M^{-1}r_0$ 
- 4:    $p_0 \leftarrow u_0$ 
+ 5:    $s_0 \leftarrow Ap_0$ 
• 6:    $\gamma_0 \leftarrow \langle u_0, s_0 \rangle$ 
• 7:    $\eta_0 \leftarrow \langle s_0, s_0 \rangle$ 
8:    $\alpha_0 \leftarrow \gamma_0/\eta_0$ 
9:   for  $i = 1, 2, \dots$  do
-10:      $x_i \leftarrow x_{i-1} + \alpha_{i-1}p_{i-1}$ 
-11:      $r_i \leftarrow r_{i-1} - \alpha_{i-1}s_{i-1}$ 
*12:     $u_i \leftarrow M^{-1}r_i$ 
•13:     $\gamma_i \leftarrow \langle u_i, s_i \rangle$ 
14:     $\beta_i \leftarrow \gamma_i/\gamma_{i-1}$ 
-15:     $p_i \leftarrow u_i + \beta_i p_{i-1}$ 
+16:     $s_i \leftarrow Ap_i$ 
17:
•18:     $\eta_i \leftarrow \langle s_i, s_i \rangle$ 
19:     $\alpha_i \leftarrow \gamma_i/\eta_i$ 

```

Gram-Schmidt orthogonalization of new search directions against previous ones, GCG additionally applies old directions in the update of the solution and residual vectors.

As in the preceding section, we describe the flexible method (GCR) and proceed to show its reduction to Preconditioned CR (PCR) for constant preconditioners and extension to pipelined CR [13]. We introduce pipelined GCR in §3.2.

The GCR method is shown in Algorithm 9. From a comparison of the GCR and FCG Algorithms 9 and 2 it is straightforward to see that they employ $A^H A$ - and A -inner products, respectively. As in Sec 2.1.3, we recover the non-flexible (or non-generalized) Preconditioned Conjugate Residuals method by restricting to linear preconditioners. In this case all β_k but one are zero, giving Algorithm 10.

3.2 Pipelined Generalized Conjugate Residual Methods

GCR and PCR do not allow any overlapping of global reductions in their standard formulation. Reformulating the algorithms using the Chronopoulos-Gear trick and introducing unrollings and pipelining intermediates leads to two pipelined GCR variants shown in algorithms 11 and 12. These employ the same modification to the computation of m_i as discussed in §2.2.3.

In Algorithm 11 the quantity w_i is computed by performing the sparse matrix-vector product Au_i in line 15, whereas in Algorithm 12 w is a recurred quantity. Note that the overlapping properties of the variants are different as in Algorithm 11 the application of the preconditioner overlaps the reductions while in Algorithm 12 a sparse matrix-vector product also contributes to the overlapping. The performance of both variants is modeled in §7. The suitability of one or the other algorithm depends on the cluster architecture, in particular the speed of the connecting network, and the available memory. Algorithm 12 has a larger memory footprint due to the storage of the extra intermediate variable z and its history of length ν_i .

The original GCR method [10] as presented in Algorithm 9 requires a total of $(2\nu_{\max} + 7)$ vectors to be stored. The pipelined variants of Algorithms 11 and 12 require $(\nu_{\max} + 2)$ and $(2\nu_{\max} + 4)$ additional vectors to be stored.

Algorithm 11 Pipelined GCR

```
1: function PIPEGCR( $A, B, b, x_0$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
* 3:    $\tilde{u}_0 \leftarrow B(r_0)$ 
- 4:    $p_0 \leftarrow u_0$ 
+ 5:    $s_0 \leftarrow Ap_0$ 
* 6:    $q_0 \leftarrow B(s_0)$ 
7:
• 8:    $\gamma_0 \leftarrow \langle r_0, Ar_0 \rangle$ 
• 9:    $\eta_0 \leftarrow \|s_0\|$ 
10:   $\alpha_0 \leftarrow \gamma_0/\eta_0$ 
11:  for  $i = 1, 2, \dots$  do
-12:     $x_i \leftarrow x_{i-1} + \alpha_{i-1}p_{i-1}$ 
-13:     $r_i \leftarrow r_{i-1} - \alpha_{i-1}s_{i-1}$ 
-14:     $u_i \leftarrow \tilde{u}_{i-1} - \alpha_{i-1}q_{i-1}$ 
+15:     $w_i \leftarrow Au_i$ 
*16:     $m_i \leftarrow B(w_i - r_i) + \tilde{u}_i$ 
17:
•18:     $\gamma_i \leftarrow \langle r_i, w_i \rangle$ 
•19:     $\delta_i \leftarrow \langle w_i, w_i \rangle$ 
20:    for  $k = i - \nu_i, \dots, i - 1$  do
•21:       $\beta_{i,k} \leftarrow \frac{-1}{\eta_k} \langle w_i, s_k \rangle$ 
-22:     $p_i \leftarrow \tilde{u}_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}p_k$ 
-23:     $s_i \leftarrow w_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}s_k$ 
-24:     $q_i \leftarrow m_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}q_k$ 
25:
26:     $\eta_i \leftarrow \delta_i - \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}^2 \eta_k$ 
27:     $\alpha_i \leftarrow \gamma_i/\eta_i$ 
```

Algorithm 12 Pipelined GCR (w unrolled)

```
1: function PIPEGCR_w( $A, B, b, x_0$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
* 3:    $\tilde{u}_0 \leftarrow B(r_0)$ 
- 4:    $p_0 \leftarrow \tilde{u}_0$ 
+ 5:    $s_0 \leftarrow Ap_0$ 
* 6:    $q_0 \leftarrow B(s_0)$ 
+ 7:    $z_0 \leftarrow Aq_0$ 
• 8:    $\gamma_0 \leftarrow \langle r_0, Ar_0 \rangle$ 
• 9:    $\eta_0 \leftarrow \|s_0\|$ 
10:   $\alpha_0 \leftarrow \gamma_0/\eta_0$ 
11:  for  $i = 1, 2, \dots$  do
-12:     $x_i \leftarrow x_{i-1} + \alpha_{i-1}p_{i-1}$ 
-13:     $r_i \leftarrow r_{i-1} - \alpha_{i-1}s_{i-1}$ 
-14:     $u_i \leftarrow \tilde{u}_{i-1} - \alpha_{i-1}q_{i-1}$ 
-15:     $w_i \leftarrow w_{i-1} - \alpha_{i-1}z_{i-1}$ 
*16:     $m_i \leftarrow B(w_i - r_i) + \tilde{u}_i$ 
+17:     $n_i \leftarrow Am_i$ 
•18:     $\gamma_i \leftarrow \langle r_i, w_i \rangle$ 
•19:     $\delta_i \leftarrow \langle w_i, w_i \rangle$ 
20:    for  $k = i - \nu_i, \dots, i - 1$  do
•21:       $\beta_{i,k} \leftarrow \frac{-1}{\eta_k} \langle w_i, s_k \rangle$ 
-22:     $p_i \leftarrow \tilde{u}_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}p_k$ 
-23:     $s_i \leftarrow w_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}s_k$ 
-24:     $q_i \leftarrow m_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}q_k$ 
-25:     $z_i \leftarrow n_i + \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}z_k$ 
26:     $\eta_i \leftarrow \delta_i - \sum_{k=i-\nu_i}^{i-1} \beta_{i,k}^2 \eta_k$ 
27:     $\alpha_i \leftarrow \gamma_i/\eta_i$ 
```

4 Pipelined Flexible GMRES Methods

GMRES methods use explicitly-orthonormalized basis vectors and as such do not rely on the same identities which were so easily disturbed by algorithmic rearrangement in the FCG and GCR cases above. Thus, deriving a usable pipelined FGMRES method is a relatively straightforward extension of pipelined GMRES, as predicted with the introduction of that method [12].

4.1 Notation

We base our notation in Table 2 on standard notation for GMRES methods and pipelined GMRES. It is distinct from the notation used for CG and its variants because Flexible GMRES methods naturally use right preconditioning. The symbols p_i , r_i , e_i , A , B , and M^{-1} have identical meaning to those in Table 1.

| | |
|---------------|---|
| u_i | preconditioned basis vector $B(p_i)$ or $M^{-1}p_i$ |
| \tilde{u} | approximation to u_i , exact if B is linear |
| z_i | transformed and preconditioned basis vector Au_i or $A\tilde{u}_i$ |
| \bar{z}_i | preconditioned, transformed and shifted basis vector $Au_i - \sigma_i p_i$ or $A\tilde{u}_i - \sigma_i p_i$ |
| \tilde{q}_i | pipelining intermediate $B(\bar{z}_i)$ |
| \tilde{w}_i | pipelining intermediate $A\tilde{q}_i$ |

Table 2: Notation for GMRES and related methods

4.2 Review of the Flexible GMRES Method

The Flexible GMRES

(FGMRES) method [33] modifies the GMRES method [35] to admit variable right preconditioning. It accomplishes this by finding approximate solutions x_i with $x_i - x_0$ having minimal residual 2-norm $\|b - Ax_i\|_2$ in the subspace $\text{span}(b, u_1, \dots, u_{i-1})$, where $u_i \doteq B(p_i)$ and p_i is formed by orthonormalizing $z_{i-1} \doteq Au_{i-1} = AB(p_{i-1})$ with p_0, \dots, p_{i-1} ³. This Arnoldi process can be summarized as $AU = PH$, where P is a matrix with i th column p_i , U is a matrix with i th column u_i , and H is an upper Hessenberg matrix. Let P be a matrix with i th column p_i . If $B = M^{-1}$ for some fixed linear operator, GMRES is recovered: the solution is found in the Krylov space $\mathcal{K}^i(AM^{-1}, b)$ and the relation $AU = AM^{-1}P = PH$ is available to avoid the need to explicitly store the vectors u_i . Algorithm 13 describes the FGMRES method. Replacing line 15 with

$$x \leftarrow x_0 + M^{-1}Py$$

in the case of a linear preconditioner recovers the right preconditioned GMRES algorithm. The FGMRES method may be preferable even for a constant preconditioner if this additional application of the preconditioner (“unwinding”) is expensive and the required additional memory is available. Restarting and convergence checks (including on-the-fly QR decomposition of H and happy breakdown checks) are not included for simplicity. Similarly, checks for the (rare in practice) possibility that the Hessenberg matrix H is singular are omitted.

4.3 Review of the Pipelined GMRES Method

The GMRES algorithm can be pipelined with the strategy outlined by Ghysels and Vanroose [12]. They observe that at the cost of degraded numerical stability, GMRES can be modified to only involve one global reduction (l^1 -GMRES in their nomenclature). This parallels the modification of preconditioned CG (Algorithm 3) to derive Chronopoulos-Gear CG (Algorithm 4). They use the identity $p_i = Ap_{i-1} - \sum_{k=1}^{i-1} \langle Ap_{i-1}, p_k \rangle p_k$ and note that if $z_i \doteq Ap_{i-1}$ is already available, this update can be performed while $Az_i = A^2 p_{i-1}$ is being computed. Using the now available value of p_i , one can (locally) compute $z_{i+1} \doteq Ap_i$.

³For improved numerical stability, the same subspace can be spanned by orthogonalizing $\bar{z}_{i-1} \doteq Au_{i-1} - \sigma_i p_{i-1}$ [12].

Algorithm 13 Flexible GMRES [33]

```
1: function FGMRES( $A, B, b, x_0, m$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
• 3:    $p_0 \leftarrow r_0 / \|r_0\|_2$ 
* 4:    $u_0 \leftarrow B(p_0)$ 
+ 5:    $z_0 \leftarrow Au_0$ 
6:   for  $i = 1, \dots, m$  do
7:     for  $j = 0, \dots, i - 1$  do
• 8:        $h_{j, i-1} \leftarrow \langle p_j, z_{i-1} \rangle$ 
- 9:        $\bar{p} \leftarrow z_{i-1} - \sum_{k=0}^{i-1} p_k h_{k, i-1}$ 
•10:       $h_{i, i-1} \leftarrow \|\bar{p}\|_2$ 
-11:      $p_i \leftarrow \bar{p} / h_{i, i-1}$ 
*12:      $u_i \leftarrow B(p_i)$ 
+13:      $z_i \leftarrow Au_i$ 
-14:    $y \leftarrow \operatorname{argmin} \|H_{m+1, m} y - \|r_0\|_2 e_0\|_2$ 
-15:    $x \leftarrow x_0 + Uy$ 
```

4.4 Pipelining the Flexible GMRES Method

The same procedure used to pipeline GMRES can also be used to produce a single-reduction variant of FGMRES, as shown in Algorithm 14, and a pipelined version of FGMRES, shown in Algorithm 15.

This algorithm can suffer “norm breakdown” requiring a restart and refilling of the pipeline. Tuning of the shift parameters can help avoid this. We allow for a distinct shift σ_i to be used at each iteration, but note that if this value is constant, the expression on line 22 of Algorithm 15 simplifies to

$$\bar{z}_i \leftarrow (\bar{w}_{i-1} - \sum_{k=0}^{i-1} h_{k, i-1} \bar{z}_k) / h_{i, i-1} \quad (11)$$

A practical choice, and the one we use in our implementations discussed in § 5-6, is to set σ_i to a constant value which approximates the largest eigenvalue of the preconditioned operator.

In exact arithmetic, the iterates produced by Algorithm 15 are not equivalent to the FGMRES algorithm because of the approximation in computing \tilde{u}_i on line 21. Recall that $u_i \doteq B(p_i) = B((v_i - \sum_{k=1}^{i-1} h_{k, i-1} p_k) / h_{i, i-1})$. If B were linear, then the approximation \tilde{u}_i on line 21 would be arithmetically equivalent. PIPEFGMRES requires storage of $4m + 2$ vectors, as opposed to $2m + 2$ for FGMRES and CGFGMRES.

5 Implementation

As a practical consequence of our choice of pipelined algorithms which are not arithmetically equivalent to their base flexible methods, useful preconditioners for the base solver, for a given problem, will not necessarily translate to be effective solvers with the pipelined variant. In particular, for the Pipelined FCG and GCR methods, the preconditioner must be compatible with the approximation $\theta_i \equiv 1$, as described in §2.2.1. Thus, experimentation is required, as it is in general when choosing preconditioners for complex systems where canonical solutions or analysis tools are not available.

To allow for this experimentation to be performed easily, and to allow for usage in highly distributed settings by way of MPI, we implement the PIPEFCG (Alg. 8), PIPEGCR (Alg. 11), PIPEGCR_w (Alg. 12), and PIPEFGMRES (Alg. 15) algorithms within the KSP class in PETSC [3, 4]. The implementations are identified as KSPPIPEFCG, KSPPIPEGCR, and KSPPIPEFGMRES⁴.

⁴See bitbucket.org/pascgeopc/petsc for current information.

Algorithm 14 Single Reduction FGMRES

```
1: function CGFGMRES( $A, B, b, x_0, m$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
• 3:    $p_0 \leftarrow r_0 / \|r_0\|_2$ 
* 4:    $u_0 \leftarrow B(p_0)$ 
+ 5:    $\bar{z}_0 \leftarrow Au_0 - \sigma_0 p_0$ 
6:   for  $i = 1, \dots, m$  do
7:     for  $j = 0, \dots, i - 2$  do
• 8:        $\bar{h}_{j,i-1} \leftarrow \langle p_j, \bar{z}_{i-1} \rangle$ 
9:        $h_{j,j-1} \leftarrow \bar{h}_{j,i-1}$ 
•10:       $\bar{h}_{i-1,i-1} \leftarrow \langle p_{i-1}, \bar{z}_{i-1} \rangle$ 
11:       $h_{i-1,i-1} \leftarrow \bar{h}_{i-1,i-1} + \sigma_{i-1}$ 
•12:       $t \leftarrow \|\bar{z}_{i-1}\|_2^2 - \sum_{k=0}^{i-1} \bar{h}_{k,i-1}^2$ 
13:      if  $t < 0$  then
14:        BREAKDOWN
15:         $\bar{h}_{i,i-1} \leftarrow \sqrt{t}$ 
16:         $h_{i,i-1} \leftarrow \bar{h}_{i,i-1}$ 
17:        if  $i = m$  then break
-18:       $p_i \leftarrow (\bar{z}_{i-1} - \sum_{k=0}^{i-1} \bar{h}_{k,i-1} p_k) / \bar{h}_{i,i-1}$ 
*19:       $u_i \leftarrow B(p_i)$ 
+20:       $\bar{z}_i \leftarrow Au_i - \sigma_i p_i$ 
-21:       $y \leftarrow \operatorname{argmin} \|H_{m+1,m} y - \|r_0\|_2 e_0\|_2$ 
-22:       $x \leftarrow x_0 + Uy$ 
```

An important practical point is that although many residual norms may be used to monitor convergence, only the natural norm for the CG- and CR-based solvers may be used without introducing extra computations and reductions. Similarly, the right preconditioned residual norm for PIPEFGMRES should be used when performance is important. Other norms can and should be used to assess convergence behavior.

All of the pipelined algorithms may suffer from norm breakdown, although in practice this is typically only observed near convergence. Our implementations detect norm breakdown and respond by restarting the algorithm, flushing the pipeline in the process.

Remark 5.1 (Truncation strategies for FCG and GCR methods) *In [31] Notay proposes a truncation-restart technique for determining the number of old directions ν_i to be used in the current iteration i as $\nu_i = \max(1, \operatorname{mod}(i, \nu_{\max} + 1))$. With this technique after every restart there are two consecutive iterations using only the respective last search direction. Consequently, the first two steps after a restart are actually standard CG iterations. In our implementations we implement the rule $\nu_i = \operatorname{mod}(i, \nu_{\max}) + 1$. This employs $n + 1$ directions in the n th iteration after a restart. If $\nu_{\max} = 1$ we recover the IPCG algorithm as analyzed by Golub and Ye [15]. We also provide a standard truncation procedure, $\nu_i = \min(i, \nu_{\max})$.*

Remark 5.2 (Shift parameters for KSPPIPEFGMRES) *Our implementation only covers the constant- σ case, as discussed in §4.4.*

Remark 5.3 (Scaling) *We observe that scaling the system matrix A is often essential to allow for a faithful preconditioner (and see the survey by Wathen [40] for an exposition on scenarios which may otherwise profit from diagonal scaling). This is due to the fact that an effective preconditioner for A may not be faithful, as we have defined it in Definition 2.1. Indeed, a Krylov method will typically converge rapidly when the preconditioned operator has a small number of tight clusters of eigenvalues, a property which is not affected by scaling of the preconditioner or operator. Operators close to the identity frequently exhibit this property, but this property is neither necessary nor sufficient.*

Algorithm 15 Single-stage Pipelined FGMRES

```

1: function PIPEFGMRES( $A, B, b, x_0, m$ )
+ 2:    $r_0 \leftarrow b - Ax_0$ 
• 3:    $p_0 \leftarrow r_0 / \|r_0\|_2$ 
* 4:    $u_0 \leftarrow B(p_0)$ 
+ 5:    $\bar{z}_0 \leftarrow Au_0 - \sigma_0 p_0$ 
* 6:    $\bar{q}_0 \leftarrow B(\bar{z}_0)$ 
+ 7:    $\bar{w}_0 \leftarrow Aq_0$ 
8:   for  $i = 1, \dots, m$  do
9:     for  $j = 0, \dots, i - 2$  do
•10:       $\bar{h}_{j,i-1} \leftarrow \langle p_j, \bar{z}_{i-1} \rangle$ 
11:       $h_{j,j-1} \leftarrow \bar{h}_{j,i-1}$ 
•12:       $\bar{h}_{i-1,i-1} \leftarrow \langle p_{i-1}, \bar{z}_{i-1} \rangle$ 
13:       $h_{i-1,i-1} \leftarrow \bar{h}_{i-1,i-1} + \sigma_{i-1}$ 
•14:       $t \leftarrow \|\bar{z}_{i-1}\|_2^2 - \sum_{k=0}^{i-1} \bar{h}_{k,i-1}^2$ 
15:      if  $t < 0$  then
16:        BREAKDOWN
17:         $\bar{h}_{i,i-1} \leftarrow \sqrt{t}$ 
18:         $h_{i,i-1} \leftarrow \bar{h}_{i,i-1}$ 
19:        if  $i = m$  then break
-20:        $p_i \leftarrow (\bar{z}_{i-1} - \sum_{k=0}^{i-1} \bar{h}_{k,i-1} p_k) / \bar{h}_{i,i-1}$ 
-21:        $\tilde{u}_i \leftarrow (\bar{q}_{i-1} - \sum_{k=0}^{i-1} u_k \bar{h}_{k,i-1}) / \bar{h}_{i,i-1}$ 
-22:        $\bar{z}_i \leftarrow (\bar{w}_{i-1} - \sum_{k=0}^{i-1} (\bar{z}_k + \sigma_k p_k) \bar{h}_{k,i-1}) / \bar{h}_{i,i-1} - \sigma_i p_i$ 
*23:        $\bar{q}_i \leftarrow B(\bar{z}_i)$ 
+24:        $\bar{w}_i \leftarrow A\bar{q}_i$ 
-25:    $y \leftarrow \operatorname{argmin} \|H_{m+1,m} y - \|r_0\|_2 e_0\|_2$ 
-26:    $x \leftarrow x_0 + \tilde{U}y$ 

```

▷ see (11)

6 Numerical Experiments

6.1 Blocking and Non-Blocking Reductions

The MPI-3 standard [29] provides an API for asynchronous operations which *may* allow for overlap of communication and computation, as required by the algorithms described in this paper. This is still an active area of software development [5, 21, 41]. The latency involved in a global reduction on a given massively parallel machine is difficult to characterize, particularly if only using a portion of the nodes, and performance models are not always predictive [22]. It should be noted that the only reliably reproducible quantity when testing message passing routines on complex machines is the *minimum* time required for an operation, in the limit of a large number of tests, though of course users are more affected by typical or average times [17].

Here and in the following tests, we report a variety of data and statistics to allow for *interpretability* [20] of our experiments, even in the absence of access to the specific hardware and software environment available to the authors at the time of this writing. Note that the performance model discussed in §7 can also provide additional insight into the performance characteristics of the new solvers.

In order to assess the potential time savings and performance enhancements by using pipelined versus non-pipelined preconditioned Krylov solvers, empirical data are presented, comparing the time to execute `MPI_Allreduce` and `MPI_Iallreduce` [29]. The reductions are paired with identical computational work local to each rank, consisting of arbitrary floating point operations on individual elements of a small local array. In the former case we get the combined time of the sequence of local work and the blocking reduction while in the latter case, we time the sequence of starting the reduction, doing the local work and finishing with `MPI_Wait`. The reduction size is 32 double values. Table 3 lists the timing results for Piz Daint, a Cray XC30 cluster at the Swiss National Supercomputing Center (CSCS). The machine includes 5272 nodes, each with an 8-core Intel Xeon E5-2670 CPU, 32 GiB DDR3-1600 RAM, and Aries routing and communications ASIC. The cluster features the Dragonfly network topology [24]. As a reference we also include timings for performing the reduction and the local work only. We used five warmup rounds and 50 trial runs. The timings presented are the minimum and maximum times across ranks averaged over the trial runs.

It can be confirmed that `MPI_Iallreduce` functionality is in place. While the time for performing the local work and a blocking reduction just exceeds the cumulative time for the individual operations, the reduction time is hidden when using non-blocking reductions. From the min/max values we also see that usually timing is consistent across the communicator sizes we considered.

Table 3 is also instructive to understand when a performance gain can be expected by using a pipelined solver as these methods require computing and updating of additional intermediate variables.

| #Ranks | 256 | 1024 | 2048 | 4096 | 8192 | 16384 | 24576 | 32768 |
|-----------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Reduction only | 0.188 | 0.577 | 0.613 | 0.670 | 0.787 | 0.843 | 0.918 | 0.894 |
| | 0.198 | 0.588 | 0.622 | 0.689 | 0.821 | 0.876 | 0.956 | 0.929 |
| Local work only | 4.88 | 4.88 | 4.88 | 4.87 | 4.88 | 4.88 | 4.88 | 4.88 |
| | 4.95 | 4.95 | 4.97 | 4.97 | 4.98 | 5.68 | 5.67 | 5.68 |
| + blocking red. | 5.56 | 5.75 | 5.81 | 5.89 | 6.03 | 6.12 | 6.13 | 6.13 |
| | 5.57 | 5.76 | 5.83 | 5.90 | 6.05 | 6.14 | 6.15 | 6.15 |
| + non-bl. red. | 4.90 | 4.88 | 4.90 | 4.89 | 4.93 | 5.65 | 5.64 | 5.66 |
| | 4.98 | 4.98 | 4.99 | 4.99 | 4.98 | 5.71 | 5.69 | 5.71 |

Table 3: Timing for blocking and non-blocking reductions in milliseconds. We report both the min (upper rows) and max (lower rows) CPU time over all ranks within the MPI communicator. The times for the non-blocking reductions with local work have to be compared to the maximum times of the local work only as the reduction can terminate only once all ranks finish with the local work.

6.2 3D Strong-Scaled Coarse Grid Solver Example

A key motivation for the development of pipelined Krylov methods for use on current supercomputers is the scenario in which the amount of local work per iteration in a Krylov method is very low, hence requiring time comparable to that consumed by reductions. This is the case when attempting to strong-scale past the point of the current reduction bottleneck. The same situation arises when a Krylov method is employed as a coarse-grid solver within a multigrid hierarchy.

In the Piz Daint environment described in §6.1, we use Cray CLE 5.2.40 and Cray-MPICH 7.2.2, a PETSC development branch based on PETSC 3.6 `maint`⁵, and a PTATIN3D [26] development branch. This allows us to evaluate our solvers with real application software to solve the variable viscosity Stokes equations using $Q_2 - P_1^{\text{disc}}$ mixed finite elements.

We examine a 3D “viscous sinker” scenario with a spherical inclusion of higher (1.2×) density and viscosity (100×) in a cubic domain. This is a useful test case for challenging Stokes flow problems, as it presents a tunable, non-grid-aligned viscosity contrast. Tests correspond to a highly-distributed coarse grid solve, or an extreme strong-scaling. The former case is a particularly interesting potential application of our methods, as it allows some adjustment of the grid size to balance communication and computation to be overlapped. 4096 MPI ranks on 1024 nodes each hold a single Q_2 finite element, for 16^3 elements and 107,811 degrees of freedom. The resulting linear systems are solved with the new KSPFCG and KSPPIPEFCG solvers to a relative tolerance of 10^{-8} in the natural residual norm. In each case, $\nu_{\text{max}} = 30$ and standard truncation is employed. FCG and PIPEFCG are compared for two nonlinear preconditioners. 60 tests were run for each of the two solves in each test, 10 at a time per batch job. The first run is considered warmup and is reported separately. Sets of three batch jobs were submitted at a time.

6.2.1 Block Jacobi Preconditioner

A per-rank block Jacobi preconditioner is employed, performing 5 iterations of Jacobi-preconditioned CG on each block. Figure 2 shows the residual norm convergence behavior as a function of the iteration count (left) and CPU time (right) for a typical experiment. Despite the increase in iterations required for convergence when using PIPEFCG, the time to solution is $\sim 2\times$ faster compared to FCG. Table 4 collects statistical variations obtained from multiple runs (indicated via the “Samples” column). The “First solve” column indicates whether the solve was the first call to PETSC’s `KSPSolve` routine after defining the system; successive solves were run with no intermediate calls apart from those used for timing. Note the relatively large variability in timings. Interestingly, the maximum speedup per iteration can *exceed* $2\times$. While this might initially seem impossible to accomplish with an algorithm which aims to overlap two processes, it should be noted that there is also some benefit to be gained in relaxing the synchronization required, beneficial in the presence of heavy-tailed distributions of local processing times. For more, see the recent work by Knepley et al. [30].

| Solver | First solve | Samples | Its. | Time / Krylov Iteration [s] | | |
|---------|-------------|---------|------|-----------------------------|----------|----------|
| | | | | Mean (Std. Dev.) | Min. | Max. |
| FCG | yes | 6 | 454 | 6.38E-04 (1.38E-04) | 4.48E-04 | 7.89E-04 |
| PIPEFCG | yes | 6 | 540 | 4.21E-04 (7.20E-05) | 3.31E-04 | 5.41E-04 |
| FCG | no | 54 | 454 | 5.58E-04 (1.11E-04) | 3.73E-04 | 9.13E-04 |
| PIPEFCG | no | 54 | 540 | 2.45E-04 (3.15E-05) | 1.94E-04 | 3.73E-04 |

Table 4: Statistics for multiple runs of the PTATIN3D viscous sinker system with a block Jacobi preconditioner.

⁵commit 2c5c660747c89d9a265191735ba48020b7a0dd72 at <https://bitbucket.org/petsc/petsc>

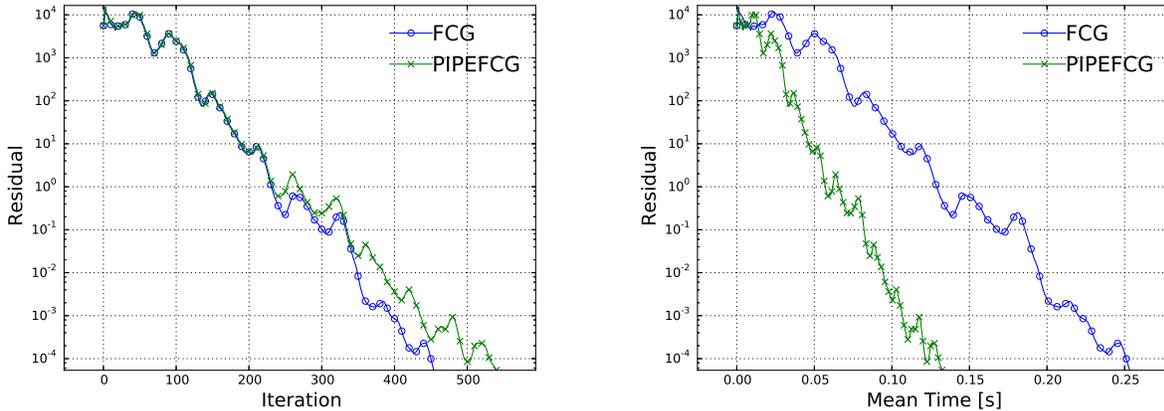


Figure 2: Convergence behavior for the viscous sinker system using block Jacobi preconditioning.

6.2.2 RASM-1 Preconditioner

A rank-wise RASM-1 [7] preconditioner is used, with 5 iterations of Jacobi-preconditioned CG as a subdomain solver. Figure 3 shows the residual norm convergence behavior as a function of the iteration count (left) and mean CPU time (right) for a typical experiment. Note that, as expected, choosing a more faithful preconditioner allows recovery of comparable convergence behavior between the pipelined and base method. Here, the speedup is not as pronounced as in the previous example, as the problem size was tuned as an example of a coarse grid solve with respect to the block Jacobi preconditioner. This example shows that speedup is practically achievable even given nested MPI calls defining neighbor-wise communication patterns in the preconditioner. Table 5 presents statistics of the multiple solves performed.

| Solver | First solve | Samples | Its. | Time / Krylov Iteration [s] | | |
|---------|-------------|---------|------|-----------------------------|----------|----------|
| | | | | Mean (Std. Dev.) | Min. | Max. |
| FCG | yes | 6 | 191 | 1.28E-03 (1.28E-04) | 1.11E-03 | 1.41E-03 |
| PIPEFCG | yes | 6 | 195 | 1.21E-03 (1.18E-04) | 1.10E-03 | 1.36E-03 |
| FCG | no | 54 | 191 | 1.16E-03 (1.48E-04) | 9.08E-04 | 1.55E-03 |
| PIPEFCG | no | 54 | 195 | 8.85E-04 (9.89E-05) | 6.99E-04 | 1.10E-03 |

Table 5: Statistics for multiple runs of the pTATIN3D viscous sinker system with restricted ASM-1 preconditioner.

6.3 2D Stokes Flow Test

As a relevant yet still comparatively simple test case of a full solve, we ran extensive tests using a PETSC tutorial⁶, which solves the incompressible, variable viscosity Stokes equation in two spatial dimensions. The discretization employs $Q_1 - Q_1$ elements, stabilized with Bochev’s polynomial projection method [9] and free slip boundary conditions on all sides. The viscosity structure is a circular viscous sinker, with density contrast giving a buoyant force and a viscosity contrast of $25\times$. All tests run on 4096 MPI ranks on 1024 nodes of Piz Daint. We experiment with all three new solvers as subsolvers within an upper-triangular block

⁶www.mcs.anl.gov/petsc/petsc-current/src/ksp/ksp/examples/tutorials/ex43.c.html

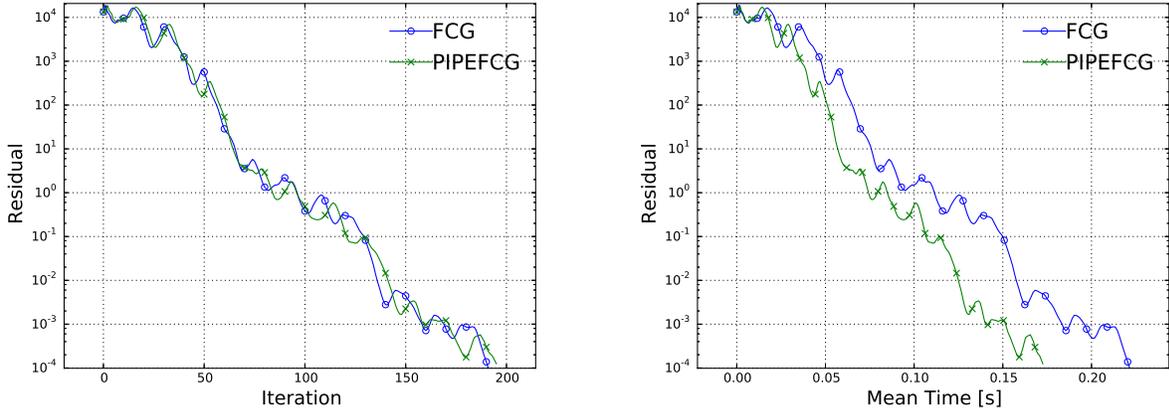


Figure 3: Convergence behavior for the viscous sinker system using RASM-1 preconditioning

preconditioner. The discrete Stokes problem is of the form

$$\begin{bmatrix} K & G \\ D & C \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}$$

which is right preconditioned with

$$B = \begin{bmatrix} \hat{K} & G \\ 0 & \hat{S} \end{bmatrix}^{-1},$$

where \hat{S} is a Jacobi preconditioner derived from the pressure mass matrix scaled by the local (element-wise) inverse of the viscosity and \hat{K} is an inexact flexible pipelined Krylov solve applied to the viscous block of the Stokes system, preconditioned with a rank-wise block Jacobi preconditioner with 5 iterations of Jacobi-preconditioned CG as subsolves. The convergence criterion is that the unpreconditioned norm of an outer FGMRES method is reduced by a factor of 10^6 . Inner solves are limited to 100 iterations. As they best exploit the structure of the suboperator, we would expect FCG and PIPEFCG to be more performant. Table 6 shows the resulting timings. We see significant speedup in all cases as the reduction bottlenecks in the base solvers are overcome. In the case where Conjugate Residuals are employed as inner solvers, we observe variability in the number of iterations to convergence, due to the degradation in conditioning arising from use of the $A^H A$ -inner product.

| Inner Solver | Outer Its. | Solve Time [s] | | |
|--------------|------------|------------------|------|-------|
| | | Mean (Std. Dev.) | Min. | Max. |
| FCG | 8 | 3.80 (0.29) | 3.47 | 4.37 |
| PIPEFCG | 8 | 1.80 (0.18) | 1.52 | 2.03 |
| GCR | 18–23 | 10.02 (1.51) | 8.26 | 12.76 |
| PIPEGCR | 12–16 | 3.08 (0.46) | 2.59 | 4.01 |
| FGMRES | 19 | 6.70 (0.53) | 6.10 | 7.71 |
| PIPEFGMRES | 19 | 5.04 (0.27) | 4.73 | 5.65 |

Table 6: Statistics for 9 runs of a 2D Stokes flow problem with an upper block triangular preconditioner employing various inner solvers, as described in §6.3 .

7 Performance Model and Extrapolation to Exascale

We describe performance models to predict the performance of our methods at exascale. For ease of comparison we consider the same hypothetical exaflop machine used to analyze pipelined GMRES [12], based on a 2010 report [36]. The specifications of the hypothetical machine are listed in Table 7. Rank-local computation times are obtained by counting flops and multiplying by t_c . This makes the significant assumption that any give computation can attain the peak flop rate of the machine, without being memory bandwidth limited.

| Property | Symbol | Value |
|-------------------------------------|-----------------|------------------|
| Nodes | P_n | 2^{20} |
| Cores per node | C_n | 2^{10} |
| Compute cores | $P_c = P_n C_n$ | 2^{30} |
| Word size | w | 32 B |
| Machine node interconnect bandwidth | BW | 100 GB/s |
| Tree radix | r | 8 |
| Per word transfer time | t_w | w/BW |
| Latency (startup) time | t_s | 1 μs |
| Time per flop | t_c | $2^{30}/10^{18}$ |

Table 7: Properties of a hypothesized exascale machine.

Global Reductions Dot products are typically computed with a reduction tree of height $\lceil \log_r(P_n) \rceil$ with r the tree radix. Present day networks make use of a hierarchy of interconnects where more closely located nodes, e.g. in a cabinet, are connected through a tree with a high effective radix. A job scheduler typically assigns compute nodes, giving the user limited influence on the specific compute nodes used. Our performance model makes the simplifying assumption of a tree radix $r = 8$ for the entire machine [12, 36].

In order to obtain an expression for the global reduction communication time $T_{\text{red,comm}}$ we assume the model $t_s + mt_w$ consisting of a constant latency or startup time t_s and a message size dependent part involving the number of words m and the time t_w required to exchange a word. We neglect time for intranode communication leading to the cost of $2\lceil \log_r(P_n) \rceil(t_s + mt_w)$ for a reduction and subsequent broadcast across the entire machine. In the context of pipelined methods global reduction costs include only the excess time (if any) which is not overlapped by other work.

Global reductions also involve floating point operations, accounted for in the computation time $T_{\text{red,calc}}$. Adding up the partial reduction results across the reduction tree leads to $\lceil \log_r(P_n) \rceil$ flops along the longest path. While this is the maximum number of flops performed by one process only, all other processes wait for this summation to finish. This might appear to be an insignificant contribution to the overall computational cost but can become non-negligible in the strong scaling limit.

Sparse Matrix-Vector Products (SpMV) The cost of a sparse matrix-vector multiplication also includes both communication and computation. The system matrix is assumed to represent a stencil based approximation of the underlying partial differential equations, with n_{nz} non-zero entries per row. For a standard second order finite difference discretization in three dimensional space, e.g., $n_{\text{nz}} = 7$. Denoting by $N = N_x N_y N_z$ the total problem size and by $n_{\text{loc}} = N/P_c$ the portion local to a process we obtain the compute costs $T_{\text{SpMV,calc}} = 2n_{\text{nz}}n_{\text{loc}}t_c$. Neighbor communication costs are $T_{\text{SpMV,comm}} = 6(t_s + (N/P_n)^{2/3}t_w)$ and can mostly be overlapped. Consequently, the SpMV cost function is $T_{\text{SpMV}} = \max(T_{\text{SpMV,calc}}, T_{\text{SpMV,comm}})$.

Preconditioner Application We augment the model with the application of a preconditioner. We model the performance of the RASM preconditioner used in §6, defining T_{PC} to account for 5 CG-Jacobi iterations on subdomains overlapping by one degree of freedom, and an internode communication step with the same pattern as a SpMV. We note that scalable multigrid preconditioners may also be designed which

| Method | Operation | Communication time cost function |
|--------|--|--|
| RED | for $k = 1..w : \beta_k \leftarrow \langle p, u_k \rangle$ | $T_{\text{red,comm}}(w) = 2\lceil \log_r(P_n) \rceil (t_s + wt_w)$ |
| SpMV | $s \leftarrow Ap$ | $T_{\text{SpMV,comm}} = 6(t_s + (N/P_n)^{2/3}t_w)$ |

Table 8: Communication time cost functions for fundamental operations with n_{loc} as defined above, n_{nz} the number of nonzero entries per row, and w the number of values (words) to be broadcast.

do not involve any reductions [27] and thus could be attractive for extreme scale solves. Nested pipelined Krylov methods could be used as coarse grid solvers within these preconditioners.

Total Cost per Iteration The total cost of one iteration comprises the time for performing flops, T_{calc} , involving the cost of sparse matrix-vector products, T_{SpMV} , the time for applying the preconditioner, T_{PC} , and fundamental operations listed in Table 9 as well as the (excess of the) reduction communication time $T_{\text{red,comm}}$. We do not take into account fused operations and vector units to establish an easier comparison with previous work [12].

The cost per iteration for flexible methods depends on the number of previous directions to orthogonalize against and hence on the truncation strategy and the iteration count. In our model we use a factor representing an average number of previous directions being used in the Gram-Schmidt orthogonalization as $\nu_{\text{avg}} = k_{\text{avg}} \cdot \nu_{\text{max}}$. Operations involving scalar values only are not taken into account. This leads to the models for the single iteration cost functions listed in Table 10.

| Method | Operation | Compute time cost function |
|--------|---------------------------------------|--|
| AXPY | $x \leftarrow x + \alpha p$ | $T_{\text{AXPY}} = t(n_{\text{loc}}(\text{mlt}) + n_{\text{loc}}(\text{add})) = 2n_{\text{loc}}t_c$ |
| MAXPY | $p \leftarrow u + \sum_m \beta_m p_m$ | $T_{\text{MAXPY}}(m) = t(mn_{\text{loc}}(\text{mlt}) + (m-1)n_{\text{loc}}(\text{add}) + n_{\text{loc}}(\text{add})) = 2mn_{\text{loc}}t_c$ |
| RED | $\langle r, u \rangle$ | $T_{\text{red,calc}} = t(n_{\text{loc}}(\text{mlt}) + (n_{\text{loc}} - 1)(\text{add}) + \lceil \log_r(P_n) \rceil (\text{add})) \approx (2n_{\text{loc}} + \lceil \log_r(P_n) \rceil)t_c$ |

Table 9: Compute time cost functions for fundamental operations with $n_{\text{loc}} = N/P_c$ denoting the vector size local to the process.

Problem and Solver Specifications For evaluating the cost functions, we consider a strong scaling experiment (cf. [12]) with a total problem size $N = 2000^3$, $n_{\text{nz}} = 7$ non-zero entries per row and evaluate for a varying number of node counts. For PIPEFCG and PIPEGCR we assume $\nu_{\text{max}} = 30$ and $k_{\text{avg}} = 0.8$; for PIPEFGMRES we assume a restart parameter of 30.

Evaluation In Figure 4 we show a comparison of the anticipated performance of all solvers for this problem. Eventually all methods are limited by latency time but the graphs indicate that the pipelined methods scale up to the 10^6 nodes of the assumed exascale machine while their standard counterparts level off about one order of magnitude earlier. The performance crossover regarding pipelined vs. non-pipelined methods for this particular example occurs around $8 \cdot 10^4$ nodes. The example of PIPEGCR vs. PIPEGCR_w clearly shows the effect of trading local work load for better overlapping. Note how PIPEGCR (explicit computation of w , overlapping by preconditioner application) performs slightly better at lower node counts while PIPEGCR_w (recurrence of w , additional AXPY and MAXPY, overlapping by preconditioner and SpMV) shows a more significant gain in efficiency for larger numbers of nodes.

Figure 5 shows a breakdown of the anticipated total iteration time for FCG and PIPEFCG. For the test case considered here the model predicts that global reductions will be entirely overlapped up to approximately $5 \cdot 10^5$ nodes.

| Krylov method | Total cost |
|----------------------|---|
| FCG | $T_{\text{calc}} = 2T_{\text{AXPY}} + T_{\text{MAXPY}}(\nu_{\text{avg}}) + (\nu_{\text{avg}} + 2)T_{\text{red,calc}} + T_{\text{SpMV}} + T_{\text{PC}}$ $T_{\text{red}} = T_{\text{red,comm}}(\nu_{\text{avg}} + 1) + T_{\text{red,comm}}(1)$ |
| PIPEFCG | $T_{\text{calc}} = 4T_{\text{AXPY}} + 4T_{\text{MAXPY}}(\nu_{\text{avg}}) + (\nu_{\text{avg}} + 2)T_{\text{red,calc}} + T_{\text{SpMV}}$ $+ T_{\text{PC}} + 2nt_c$ $T_{\text{red}} = \max(0, T_{\text{red,comm}}(\nu_{\text{avg}} + 2) - [T_{\text{SpMV}} + T_{\text{PC}} + 2nt_c])$ |
| GCR | $T_{\text{calc}} = 2T_{\text{AXPY}} + T_{\text{MAXPY}}(\nu_{\text{avg}}) + (\nu_{\text{avg}} + 2)T_{\text{red,calc}} + T_{\text{SpMV}} + T_{\text{PC}}$ $T_{\text{red}} = T_{\text{red,comm}}(\nu_{\text{avg}}) + T_{\text{red,comm}}(2)$ |
| PIPEGCR | $T_{\text{calc}} = 3T_{\text{AXPY}} + 3T_{\text{MAXPY}}(\nu_{\text{avg}}) + (\nu_{\text{avg}} + 2)T_{\text{red,calc}} + T_{\text{SpMV}}$ $+ T_{\text{PC}} + 2nt_c$ $T_{\text{red}} = \max(0, T_{\text{red,comm}}(\nu_{\text{avg}} + 2) - [T_{\text{PC}} + 2nt_c])$ |
| PIPEGCR _w | $T_{\text{calc}} = 4T_{\text{AXPY}} + 4T_{\text{MAXPY}}(\nu_{\text{avg}}) + (\nu_{\text{avg}} + 2)T_{\text{red,calc}} + T_{\text{SpMV}}$ $+ T_{\text{PC}} + 2nt_c$ $T_{\text{red}} = \max(0, T_{\text{red,comm}}(\nu_{\text{avg}} + 2) - [T_{\text{SpMV}} + T_{\text{PC}} + 2nt_c])$ |
| FGMRES | $T_{\text{calc}} = T_{\text{MAXPY}}(\nu_{\text{avg}}) + t_c n + (\nu_{\text{avg}} + 1)T_{\text{red,calc}} + T_{\text{SpMV}} + T_{\text{PC}}$ $T_{\text{red}} = T_{\text{red,comm}}(\nu_{\text{avg}}) + T_{\text{red,comm}}(1)$ |
| PIPEFGMRES | $T_{\text{calc}} = \nu_{\text{avg}}T_{\text{AXPY}} + 3T_{\text{MAXPY}}(\nu_{\text{avg}}) + (\nu_{\text{avg}} + 5)t_c n + (\nu_{\text{avg}} + 2)T_{\text{red,calc}}$ $+ T_{\text{SpMV}} + T_{\text{PC}}$ $T_{\text{red}} = \max(0, T_{\text{red,comm}}(\nu_{\text{avg}} + 2) - [T_{\text{SpMV}} + T_{\text{PC}}])$ |

Table 10: Performance models for standard and pipelined methods for the truncation strategy. Again, $n = N/P_c$, $\nu_{\text{avg}} = k_{\text{avg}} \cdot \nu_{\text{max}}$, where k_{avg} corresponds to a factor accounting for the average number of previous search directions being used. If the number of iterations required is $\gg \nu_{\text{max}}$, this factor approaches one for a standard truncation strategy. Communication time for multiple reductions is fused whenever possible. GMRES-type models do not include the time for manipulating the Hessenberg matrix.

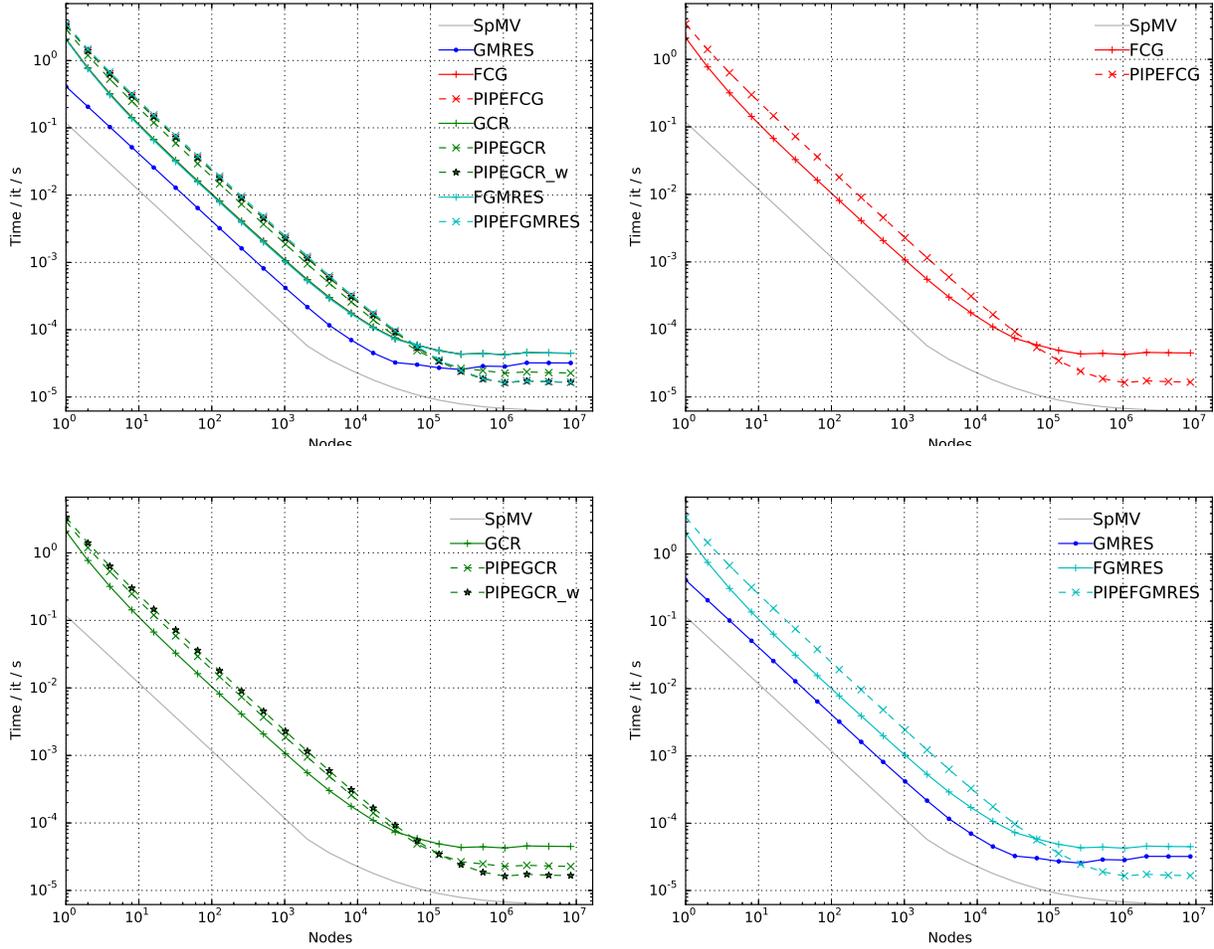


Figure 4: Evaluation of the performance models of Table 10 for predicting iteration times on the hypothesized exascale machine of Table 7. The top left panel includes all methods and the others compare FCG-, GCR- and GMRES-type methods. All graphs include the time for performing a SpMV operation as a reference. The number of nodes scales beyond the 1M nodes of the assumed machine to better visualize the leveling at high node counts. While all methods are eventually limited by latency time the pipelined methods outperform their standard counterparts on high node counts.

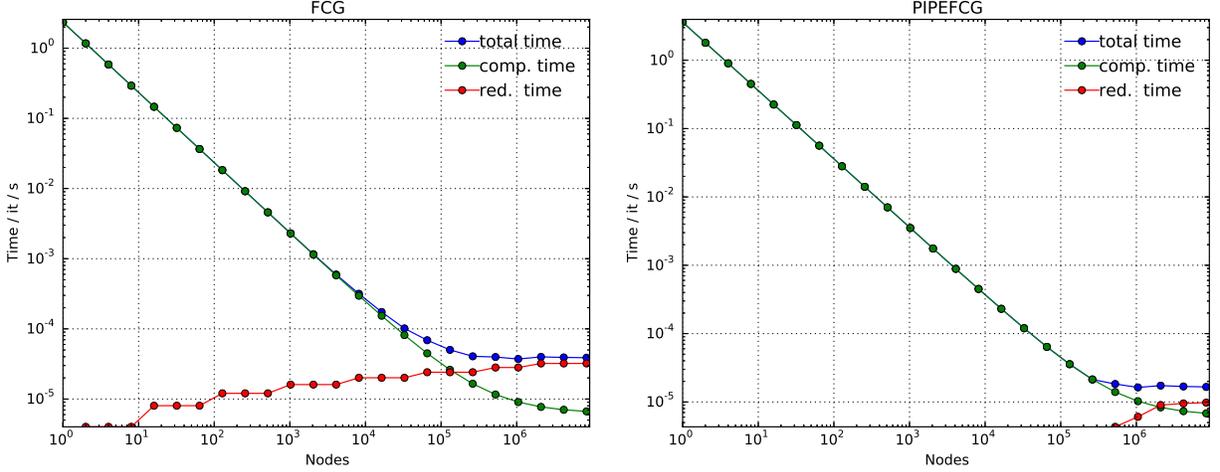


Figure 5: Breakdown of the total iteration time into computation and reduction time for FCG and PIPEFCG. For the test case considered it is anticipated that the reductions will be entirely overlapped up to approximately $5 \cdot 10^5$ nodes for the pipelined method.

Sensitivity to Parameters The performance models are insensitive to the specific value of most of the parameters when chosen within reasonable bounds. Among the insensitive parameters are the interconnect bandwidth, word size, the tree radix and assumptions such as ignoring fused AXPY operations. It may appear unintuitive that the interconnect bandwidth is not a sensitive parameter, but latency is dominant in the communication time model.

The models are most obviously sensitive to the latency time but also to the number of cores per node as more or less cores per node implies a different number of nodes for obtaining exaflop performance. Another sensitive parameter is the total problem size N . A mild dependency of the average fill factor k_{avg} and the maximum number of previous direction ν_{max} as well as the number of non-zero entries n_{nz} per row is observed. Varying any of these values does not cause a change of the general shape of the curves but rather induces a shift of the crossover point.

For the hypothesized exascale machine a latency time of $1\mu\text{s}$ is assumed, significantly lower than times observed on current systems including Piz Daint as in Table 3. Consequently, pipelined Krylov methods can lead to significant performance improvements for much smaller numbers of nodes on current systems, as confirmed by the tests in §6.

8 Conclusions and Outlook

Bottlenecks related to global communication and synchronization are increasingly common in high performance computing, as parallelism and hybridism are used to increase peak performance. Traditional algorithms can often be improved with this consideration in mind. Given the increasing relative impact of latency and synchronization required with global all-to-all communication patterns, it becomes increasingly attractive to tailor algorithms to mitigate these costs. This requires introducing additional costs in terms of memory footprint, local computational work, memory traffic, numerical stability, and allowing asynchronous operations.

We introduce variants of the FCG, GCR and FGMRES flexible Krylov methods, allowing overlap of global reductions with other work through operation pipelining. The base methods are amongst the most commonly used flexible Krylov methods for Hermitian positive definite, Hermitian, and general operators, respectively. Future work includes extending and implementing the approaches here for other useful Krylov methods. A crucial consideration in this process, as demonstrated here, is the effect of allowing algorithmic

rearrangements which modify the effective preconditioner. Naive rearrangement is not always effective, and effective rearrangements may impose conditions on the class of useful preconditioners beyond those common in previous Krylov methods. We propose and analyze an approach to provide methods which are increasingly effective for stronger preconditioners.

The proposed methods are shown to be effective on a current leadership supercomputing platform with a fast network, where speedups could exceed $2\times$, challenging common assumptions that pipelined Krylov methods are only effective at future machine scales, and that the speedup of single-stage pipelining is limited to $2\times$. Additionally, we develop analytic models for anticipating performance on future exascale systems.

All methods have been implemented in the PETSC package and are available open-source.

Deeper Pipelining The same rearrangements used in the single-stage pipelined methods described here could be pursued to allow a reduction to overlap more than one iteration’s worth of other work. This has been explored for the GMRES method [12]. Our focus has been on the “faithful” preconditioners discussed above, which require a substantial amount of work to apply and thus would likely not benefit from further pipelining. Additionally, numerical instability becomes more of a concern with deeper pipelining—in the case of GMRES, norm breakdown becomes more common—and we anticipate that the required stabilization for nonlinear preconditioners would also be non-trivial. Investigation of deeper pipelining is of course of interest from a mathematical point of view, but it is unclear whether exascale systems will be developed exhibiting the extreme reduction latency required to justify overlapping inner products with multiple nonlinear preconditioner applications. From a practical point of view, current MPI implementations do not prioritize operations like multiple overlapping reductions, which makes the testing of these methods problematic.

Outlook The methods described in this paper are expected to become more and more relevant as non-deterministic, randomized, nested, highly-distributed, and nonlinear preconditioning techniques come into greater usage. These trends are encouraged by an increasing level of parallelism, hybridism, and hierarchy in computational machinery, as well as intense research into randomized, finely-grained parallel, and asynchronous techniques for approximate and exact solvers.

Acknowledgments

We acknowledge financial support from the Swiss University Conference and the Swiss Council of Federal Institutes of Technology through the Platform for Advanced Scientific Computing (PASC) program.

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