Abstract

The standard implementation of the conjugate gradient algorithm suffers from communication bottlenecks on parallel architectures, due primarily to the two global reductions required every iteration. In this paper, we introduce several predict-and-recompute type conjugate gradient variants, which decrease the runtime per iteration by overlapping global synchronizations, and in the case of our pipelined variants, matrix vector products. Through the use of a predict-and-recompute scheme, whereby recursively updated quantities are first used as a predictor for their true values and then recomputed exactly at a later point in the iteration, our variants are observed to have convergence properties nearly as good as the standard conjugate gradient problem implementation on every problem we tested. It is also verified experimentally that our variants do indeed reduce runtime per iteration in practice, and that they scale similarly to previously studied communication hiding variants. Finally, because our variants achieve good convergence without the use of any additional input parameters, they have the potential to be used in place of the standard conjugate gradient implementation in a range of applications.

1 Introduction

The conjugate gradient algorithm (CG) is perhaps the most widely used method for solving a linear system of equations $Ax = b$, when $A \in \mathbb{C}^{n \times n}$ is Hermitian positive definite. While the low storage costs and low number of floating point operations per iteration make CG an attractive choice for solving very large sparse systems, the standard implementation of the conjugate gradient algorithm requires that nearly every computation be done sequentially. In particular, it requires two inner products and one (typically sparse) matrix vector product per iteration, none of which can occur simultaneously. Each inner product requires a costly global reduction, and the matrix vector product (even if sparse) requires local communication. The result is a communication bottleneck on parallel machines [DHMY07, AGHV12, BCD+14].

To address this bottleneck, many mathematically equivalent variants of the CG algorithm have been introduced; see for instance [Ros83, Saa85, Chr87, Meu87, Saa89, CG89b, SG06, GV14, EG16, CV17, CCV18, etc.]. Broadly speaking, these variants aim to rearrange the standard CG algorithm in such a way that communication can either be hidden behind other computations or avoided entirely. As a result, the time per iteration of these methods is reduced on parallel machines.
However, it is well known that the conjugate gradient algorithm is particularly sensitive to rounding errors, and any modification to the CG algorithm will have an effect on convergence. Specifically, both the rate of convergence (number of iterations to reach a given level of accuracy) and the maximal attainable accuracy of any CG implementation may be severely impacted by finite precision. As a result, the practical use of some of the previously mentioned variants is limited because on many problems the algorithms fail to reach an acceptable level of accuracy, or require so many more iterations to do so that the runtime is not decreased.

In this paper, we present a communication hiding variant very similar to that of Gérard Meurant in [Meu87], which requires a single global synchronization per iteration. We then introduce “pipelined” versions of this variant and of the variant introduced by which allow the matrix vector product and preconditioning step to be overlapped with all inner products. Building on an idea of Meurant in [Meu87] to use recursively computed quantities as a predictor for their true values, and then recomputing them later in the iteration, we demonstrate numerically that the convergence of our pipelined variants is comparable to the standard CG implementation. All of the algorithms introduced in this paper require exactly the same inputs as the standard CG algorithm, and therefore require no tuning by the end user.

Although we leave a roundoff error analysis of the variants introduced in this paper to later work, we provide a range of numerical experiments to support the claim that our variants improve the rate of convergence and ultimately attainable accuracy of the previously studied communication hiding variants. Moreover, because our variants appear to be numerically stable without any additional input parameters, they have the potential to be used as black box solvers wherever the standard conjugate gradient algorithm is used. Finally, we demonstrate through a strong scaling experiment that the new variants do indeed reduce the time per iteration.

Throughout this paper, we use capital Roman letters for matrices, lower case Roman letters for vectors, and lower case Greek letters for scalars. Unless otherwise stated, matrices should be assumed to be of size $n \times n$ and vectors of size $n \times 1$. The conjugate transpose of a matrix is denoted with $H$, and the inverse of the conjugate transpose denoted with $-H$. The standard Euclidean inner product and corresponding spectral/operator norm are respectively denoted $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$, and the inner product and norm induced by a positive definite matrix $B$ are denoted $\langle \cdot, \cdot \rangle_B$ and $\| \cdot \|_B$.

2 The conjugate gradient algorithm

The conjugate gradient algorithm was introduced in 1952 by Magnus Hestenes and Eduard Stiefel in [HS52], and subsequently became a popular methods for solving Hermitian positive definite linear systems. The popularity of CG is due in part to the fact (i) that it is matrix free, meaning that the algorithm never needs to access the entries of $A$ explicitly, only to be able to compute the product $v \mapsto Av$, (ii) that it requires only $\mathcal{O}(n)$ storage and floating point operations each iteration, and (iii) the development of effective preconditioners. However, as stated in the introduction, on high performance machines, CG suffers from communication bottlenecks.

The CG algorithm works by constructing a sequence of iterates $x_0, x_1, x_2, \ldots$ each meant to approximate the true solution $x^* = A^{-1}b$ of the system $Ax = b$. By construction, at step $k$,
the iterate $x_k$ minimizes the $A$-norm of the error $e_k = A^{-1}b - x_k$ over the Krylov subspace,

$$x_0 + \mathcal{K}_k(A, r_0) = x_0 + \text{span}\{r_0, Ar_0, A^2r_0, \ldots, A^{k-1}r_0\}, \quad r_0 = b - Ax_0 \quad (1)$$

**Algorithm 1** Hestenes and Stiefel Conjugate Gradient (preconditioned)

1: **procedure** HS-CG($A$, $M$, $b$, $x_0$)  
2: **initialize**()  
3: **for** $k = 1, 2, \ldots$ **do**  
4: \hspace{1em} $x_k = x_{k-1} + \alpha_{k-1}p_{k-1}$  
5: \hspace{1em} $r_k = r_{k-1} - \alpha_{k-1}s_{k-1}$, $\tilde{r}_k = M^{-1}r_k$  
6: \hspace{1em} $\nu_k = \langle \tilde{r}_k, r_k \rangle$  
7: \hspace{1em} $\beta_k = \nu_k/\nu_{k-1}$  
8: \hspace{1em} $p_k = \tilde{r}_k + \beta_k p_{k-1}$  
9: \hspace{1em} $s_k = Ap_k$  
10: \hspace{1em} $\mu_k = \langle p_k, s_k \rangle$  
11: \hspace{1em} $\alpha_k = \nu_k/\mu_k$  
12: **end for**  
13: **end procedure**  

14: **procedure** INITIALIZE  
15: \hspace{1em} $r_0 = b - Ax_0$, $\tilde{r}_0 = M^{-1}r_0$, $\nu_0 = \langle r_0, \tilde{r}_0 \rangle$, $p_0 = \tilde{r}_0$, $s_0 = Ap_0$, $\alpha_0 = \nu_0/\langle p_0, s_0 \rangle$  
16: **end procedure**

In exact arithmetic, the convergence of the conjugate gradient algorithm is well understood [Gre97b]. First, since $\mathcal{K}_j(A, r_0) \subseteq \mathcal{K}_k(A, r_0)$ for $j \leq k$, the $A$-norm of the error is non-increasing. Moreover, by applying the Cayley-Hamilton theorem, it is easy to show that the solution will be found in at most $n$ steps. In fact, the convergence of exact CG is determined entirely by the spectrum of $A$ and the size of $b$ and $x_0$ in directions of the eigenvectors of $A$, and for fixed $k$, tight bounds on the rate of convergence can be given in terms of the minimax polynomials on the set of eigenvalues. In particular, the error at step $k$ satisfies the inequality,

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq \min_{p \in \mathcal{P}_k} \left[ \max_{z \in \lambda(A)} |p(z)| \right], \quad \mathcal{P}_k = \{ p : \deg p \leq k, \ p(0) = 1 \} \quad (2)$$

where $\lambda(A)$ is the set of eigenvalues of $A$.

This can be relaxed to obtain the Chebyshev condition number bound,

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq \min_{p \in \mathcal{P}_k} \left[ \max_{z \in [\lambda_{\min}, \lambda_{\max}]} |p(z)| \right] \leq 2 \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k, \quad \kappa = \frac{\lambda_{\max}}{\lambda_{\min}} \quad (3)$$

where $\lambda_{\min}$ and $\lambda_{\max}$ are the smallest and largest eigenvalues of $A$.

### 2.1 Preconditioning

Notice that to obtain the solution $x = A^{-1}b$, we could instead solve,

$$R^{-H}AR^{-1}y = R^{-H}b \quad (4)$$

and then set $x = R^{-1}y$, where $R$ is any full rank square matrix.
Thus, if the spectrum of $R^{-H}AR^{-1}$ is “better behaved” than the spectrum of $A$, the bound in Equation 2 will be stronger and the conjugate gradient method should be expected to converge significantly faster on the preconditioned system than on the original system.

By writing out the unpreconditioned CG algorithm for the preconditioned system in Equation 4 it is easy to show that we only need to be able to evaluate the map $v \mapsto M^{-1}v$, where $M^{-1} = R^{-H}R^{-1}$. In particular, the individual factors $R^{-H}$ and $R^{-1}$ need not be known [Gre97b]. This gives the preconditioned conjugate gradient algorithm, displayed in Algorithm 1.

While using the preconditioned conjugate gradient algorithm is mathematically equivalent to applying CG to the explicitly preconditioned system in Equation 4, there are practical differences which become increasingly important when considering communication avoiding/hiding variants. For instance, notice that even for HS-CG, additional memory is required to store $\tilde{r}_k$, and since computations are done in different orders, the behaviour in finite precision can differ from the unpreconditioned versions.

Throughout this paper, we use a tilde (“$\sim$”) above a vector to indicate that, in exact arithmetic, the tilde vector is equal the preconditioner applied to the non-tilde vector; i.e. $\tilde{r}_k = M^{-1}r_k$, $\tilde{s}_k = M^{-1}s_k$, etc. With this notation in mind, the unpreconditioned version of a variant can easily be obtained by first replacing non-tilde quantities with their tilde quantities, and then removing any tildes. This is equivalent to setting $M^{-1}$ to the identity matrix and the removing any redundant expressions.

### 2.2 Communication costs

On large machines, the cost of moving data dominates the costs of floating point arithmetic. Reducing the communication costs of algorithms is important enough an endeavour that the exascale computing road map [DBM+11] places “algorithms for minimizing communications” on the recommended research agenda for upcoming numerical libraries. From the presentation of HS-CG in Algorithm 1, it is clear that the algorithm is highly sequential. Specifically, in each iteration, the preconditioning step, the first inner product, the matrix vector product, and the final inner product must occur one after the other. Thus, the communication costs for each of these steps will add to the time it takes to compute a single iteration.

**Inner products.** Each inner product requires a global synchronization of all nodes involved in the computation. This means that the next computation cannot begin until all nodes have completed their computations and the results are aggregated. Such synchronizations are typically the most expensive component of each iteration on parallel machines [DHMY07, VDGQQ08].

**Matrix vector product.** While a matrix vector product typically requires more floating point operations than a single inner product, if $A$ has an exploitable structure (i.e. $A$ is sparse, is a DFT operator, etc.) the communication costs can be much lower [VDGQQ08]. In fact, even in the extreme case that the matrix $A$ is dense, computing the matrix vector product still only requires one global synchronization, since each row of the output can be computed simultaneously and independently.

**Preconditioning.** Traditional preconditioners based on incomplete factorizations are applied through a triangular solve. While triangular solves with a sparse matrix require only $O(n)$ floating point operations, the operations are mostly sequential and inherently difficult to parallelize. For this reason, there has been a range of work on finding classes of preconditioners which can be efficiently applied on parallel machines; for an overview see [Saa03].
Table 1: Summary of costs for various conjugate gradient variants. Values in parenthesis are the additional costs for the preconditioned variants. \textit{vec. ops.}: number of vector operations (i.e. AXPYs, and inner products) per iteration. \textit{mult}: number of matrix vector products per iteration. \textit{scal}: number of inner products per iteration. \textit{time}: time spend on global reduction (GLRED) and matrix vector product/preconditioning (MV/PC). \textit{memory}: number of vectors stored.

| variant     | vec. ops. | mult. | scal. | time                  | memory |
|-------------|-----------|-------|-------|-----------------------|--------|
| HS-CG       | 5 (+0)    | 1     | 2     | 2 \cdot GLRED + MV/PC | 4 (+1) |
| CG-CG       | 6 (+0)    | 1     | 2     | GLRED + MV/PC         | 5 (+1) |
| M-CG        | 6 (+1)    | 1     | 3     | GLRED + MV/PC         | 4 (+2) |
| PR-CG       | 7 (+1)    | 1     | 4     | GLRED + MV/PC         | 4 (+2) |
| GV-CG       | 8 (+2)    | 1     | 2     | max(GLRED, MV/PC)     | 7 (+3) |
| PPR-M-CG    | 9 (+3)    | 2     | 3     | max(GLRED, MV/PC)     | 6 (+4) |
| PPR-CG      | 9 (+3)    | 2     | 4     | max(GLRED, MV/PC)     | 6 (+4) |

2.2.1 Previously considered communication reducing variants

In order to address the communication costs in the conjugate gradient algorithm, many mathematically equivalent variants have been developed. The variants presented in this paper are most closely related to communication hiding variants such as M-CG, CG-CG, and GV-CG (pipelined CG), respectively introduced by Meurant in [Meu87], Chronopoulos and Gear in [CG89b], and Gysels and Vanroose in [GV14]. These variants maintain the iteration structure of HS-CG, but rearrange the computations within an iteration so that expensive ones can occur simultaneously, effectively “hiding” communication.

While communication hiding variants are perhaps the most commonly used class of high performance conjugate gradient variants, they have some theoretical and practical shortcomings. First, even if both inner products and the matrix vector product can be overlapped, as shown in Table 1, the maximum theoretical speedup of over HS-CG is only a factor of three. In fact, for many common types of matrices, as the number of nodes is increased, the cost of the matrix vector multiplication and preconditioning will become small compared to the cost of global reductions. In this limit, the maximum theoretical speedup is only a factor of two.

Second, pipelined communication hiding methods suffer numerical problems due to the additional floating point operations required to rearrange the iteration. For example, as discussed in Section 4, there are many problems for which the final accuracy GV-CG is able to reach is orders of magnitude worse than HS-CG. There have been many approaches to improving the numerical properties of these variants. For example, residual replacement [GV14, CFYA+18] and shifts in auxiliary recurrences [CV17] have been explored as a means of improving the final accuracy of such methods. However, both strategies typically require certain parameters to selected ahead of time based on user intuition, or rely on heuristics for when/how to apply corrections.

It is also worth mentioning some other approaches to reducing communication costs in the conjugate gradient algorithm. First, it is possible to reduce the three two-term recurrences for $x_k$, $r_k$, and $p_k$ to two three-term recurrences for $x_k$ and $r_k$. However, this typically reduces the maximal accuracy, as was shown to be the case in [GS00] for one three-term formulation. Second, the Krylov subspace from Equation 1 can be expanded by $s$ dimensions.
at a time [Chr87, CG89b]. These so-called s-step methods reduce the number of global synchronization points by a factor of $O(s)$ compared to HS-CG. The communication costs and reads over the data are reduced by exploiting data locality in $A$ using a so-called “matrix powers kernel”, and by computing all inner products simultaneously using more efficient batched kernels [CG89a, Hoe10, Car15]. For a more detailed analysis of these methods we refer readers to [Car15]. Finally, there is ongoing work on deep pipelined methods [Coo18, CCV18, CCV19], which allow for multiple matrix vector products to be overlapped with a global reduction.

2.3 Considerations in finite precision

The behavior of the conjugate gradient algorithm in finite precision is often very different from the behavior in exact arithmetic. In this sense, the algorithm could be considered unstable. Unfortunately, the result is that any modification to the algorithm is likely to have a non-negligible effect on its numerical properties. In fact, poor convergence has limited the adoption of many variants of the CG algorithm meant to reduce communication costs.

In this section we highlight some of what is known about the conjugate gradient algorithm in finite precision. The goal is to give readers a sense of why finding stable high performance conjugate gradient algorithms is a difficult problem, and what tools exist to analyze such methods. For more detailed overviews of the modern analysis of Lanczos and conjugate gradient type methods in finite precision, we turn readers to [Gre97b] and [MS06].

Recall that the optimality of an iterate $x_k$ produced by the conjugate gradient method requires the orthogonality or $A$-orthogonality of certain vectors. This cannot be guaranteed in finite precision, and leads to worsened convergence. The primary effects observed are (i) a loss of maximally attainable accuracy and (ii) a delay of convergence (an increase in number of iterations to reach a given level of accuracy) [Gre97b]. Specifically, the error bound in Equation 2 may be violated. Some theory is known about both effects.

First, for variants such as HS-CG, it is observed that the updated residual $r_k$ decreases to much lower than the machine precision. As a result, an estimate of the smallest true residual attainable can be computed in terms of the residual gap $r_k - (b - Ax_k)$ [Gre97a, SvdVF94]. Such an analysis was done by Gutknecht and Strakoš in [GS00] for a three-term CG variant meant to reduce communication costs, and it was shown why the maximal accuracy of that variant was reduced. Similarly, the residual gap of pipelined conjugate gradient variants is studied in [CFYA18, CRS18]. However, for some variants, the updated residual $r_k$ may not decrease to well below machine precision, so some care must be taken when interpreting these results.

In addition to the theory about the maximal accuracy in finite precision, there is also (highly nontrivial) theory about the rate of convergence of the conjugate gradient algorithm in finite precision, due primarily to Anne Greenbaum in [Gre89]. In this paper, it was shown that for any $k$, a finite precision CG implementation will behave like exact CG applied to a larger matrix whose eigenvalues lie in small intervals about the eigenvalues of $A$, provided that (i) the updated residuals approximately satisfy the three term Lanczos recurrence, and (ii) successive residuals are approximately orthogonal. This gives a way of applying results about exact precision CG to finite precision implementations.

For instance, an immediate result is that for some small $\delta$ (depending on the machine precision and implementation), the errors of a “good” CG implementation will satisfy the
relaxation of Equation 2,
\[
\|e_k\|_A \leq \min_{p \in P_k} \left[ \max_{z \in \mathcal{L}(A)} |p(z)| \right], \quad \mathcal{L}(A) = \bigcup_{i=1}^{n} [\lambda_i - \delta, \lambda_i + \delta] \quad (5)
\]

Similarly, by relaxing Equation 5, it is clear that a "good" CG implementation will approximately satisfy the Chebyshev error bounds based on the condition number of \(A\) show in Equation 3. However, while numerical experiments suggest that some variants do satisfy these conditions [GLC19], no commonly used variants have ever been proved to satisfy these conditions.

Thus, when designing a conjugate gradient method for use in finite precision, two reasonable goals might be to keep the residual gap small, and to satisfy the conditions from [Gre89] so that the bound in Equation 5 is as strong as possible. Of course, finding variants which have these properties is not easy, and proving that variants have these properties is even harder.

3 Derivation of new variants

In this section we describe a communication hiding new variant, PR-CG, which requires only one global synchronization point per iteration. This variant is similar to M-CG, introduced by Meurant in [Meu87], and the relationship between the two algorithms is briefly discussed.

Then, in the same way that GV-CG is obtained from CG-CG, we "pipeline" PR-CG to overlap the matrix vector product with the inner products. The order in which operations are done in the pipelined version of PR-CG allows for a vector quantity to be recomputed using an additional matrix vector product, giving the pipelined predict-and-recompute variant PPR-CG. Since this matrix vector product can occur at the same time as the other matrix vector product and as the inner products, the communication costs are not increased.

Table 1 provides a comparison between some commonly used communication avoiding variants and the newly introduced variants. It should be noted that although the number of matrix vector products and inner products of PPR-M-CG and PPR-CG are increased, most of this work can be done locally, and they have the same dominant communication costs as GV-CG.

3.1 A simple communication hiding variant

Like the derivation of M-CG in [Meu87], and the variants introduced in [Joh84, Ros83, Saa85, Saa89, etc.], we derive our first communication hiding variant, PR-CG, by substituting recurrences into the inner product \(\mu_k = \langle \tilde{r}_k, r_k \rangle\). This allows us to obtain an equivalent expression for the inner product, involving quantities which are known earlier in the iteration.

To this end, we first define \(\hat{s}_k = M^{-1}s_k\) so that,
\[
\hat{r}_k = \hat{r}_{k-1} - \alpha_{k-1}\hat{s}_{k-1} \quad (6)
\]
Then, by substituting the recurrences for \( r_k \) and \( \tilde{r}_k \) we can write,
\[
\nu_k = \langle \tilde{r}_k, r_k \rangle = \langle \tilde{r}_{k-1} - \alpha_{k-1}\tilde{s}_{k-1}, r_{k-1} - \alpha_{k-1}s_{k-1} \rangle \\
= \langle \tilde{r}_{k-1}, r_{k-1} \rangle - \alpha_{k-1}\langle \tilde{r}_{k-1}, s_{k-1} \rangle \\
- \alpha_{k-1}\langle \tilde{s}_{k-1}, r_{k-1} \rangle + \alpha_{k-1}^2\langle \tilde{s}_{k-1}, s_{k-1} \rangle 
\]
(7)

Using this expression for \( \nu_k \) produces convergence which is quite good compared to HS-CG and CG-CG. However, we note that we can eliminate another inner product with no apparent effect to the convergence.\(^1\)

To do this we note that since \( M \), and therefore \( M^{-1} \), are Hermitian, that \( \langle \tilde{s}_{k-1}, r_{k-1} \rangle = \langle s_{k-1}, \tilde{r}_{k-1} \rangle \). Thus,
\[
\nu_k = \nu_k - 2\alpha_{k-1}\langle \tilde{r}_{k-1}, s_{k-1} \rangle + \alpha_{k-1}^2\langle \tilde{s}_{k-1}, s_{k-1} \rangle 
\]
(8)

Once \( s_k = Ap_k \) and \( \tilde{s}_k = M^{-1}s_k \) have been computed, we can simultaneously compute the three inner products,
\[
\mu_k = \langle p_k, s_k \rangle, \quad \delta_k = \langle \tilde{r}_k, s_k \rangle, \quad \gamma_k = \langle \tilde{s}_k, s_k \rangle 
\]
(9)

A variant using a similar expression for \( \nu_k \) was suggested in [MJC99] and briefly mentioned in [CRS+18]. However, one term of their formula for \( \nu_k \) has a sign difference from Equation 8, and no numerical tests or rounding error analysis were provided.

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**Algorithm 2 Predict-and-recompute conjugate gradient**

1: procedure PR-CG(\( A, M, b, x_0 \))
2: \hspace{1em} INITIALIZE()
3: \hspace{1em} for \( k = 1, 2, \ldots \) do
4: \hspace{2.5em} \( x_k = x_{k-1} + \alpha_{k-1}p_{k-1} \)
5: \hspace{2.5em} \( r_k = r_{k-1} - \alpha_{k-1}s_{k-1}, \tilde{r}_k = \tilde{r}_{k-1} - \alpha_{k-1}\tilde{s}_{k-1} \)
6: \hspace{2.5em} \( \nu_k = \nu_k - 2\alpha_{k-1}\delta_k + \alpha_{k-1}^2\gamma_k \)
7: \hspace{2.5em} \( \beta_k = \nu_k/\nu_{k-1} \)
8: \hspace{2.5em} \( p_k = \tilde{r}_k + \beta_k p_{k-1} \)
9: \hspace{2.5em} \( s_k = Ap_k, \tilde{s}_k = M^{-1}s_k \)
10: \hspace{2.5em} \( \mu_k = \langle p_k, s_k \rangle, \delta_k = \langle \tilde{r}_k, s_k \rangle, \gamma_k = \langle \tilde{s}_k, s_k \rangle, \nu_k = \langle \tilde{r}_k, r_k \rangle \)
11: \hspace{2.5em} \( \alpha_k = \nu_k/\mu_k \)
12: \hspace{1em} end for
13: end procedure

14: procedure INITIALIZE
15: \hspace{1em} \( r_0 = b - Ax_0, \tilde{r}_0 = M^{-1}r_0, \nu_0 = \langle r_0, \tilde{r}_0 \rangle, p_0 = \tilde{r}_0, s_0 = Ap_0, \)
16: \hspace{1em} \( s_0 = M^{-1}s_0, \alpha_0 = \nu_0/\langle p_0, s_0 \rangle, \delta_0 = \langle \tilde{r}_0, s_0 \rangle, \gamma_0 = \langle \tilde{s}_0, s_0 \rangle \)
17: end procedure

---

In the current form, the rate of convergence of this variant is improved over CG-CG, but the final accuracy is severely impacted. This phenomenon was observed in the variants suggested in [Ros83, Joh84, Saa85], all of which use similar expressions for \( \nu_k \) as M-CG, and is due to the updated value of \( \nu_k \) becoming negative. In [Meu87], it is suggested to use

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\(^1\)While using this simplified formula for \( \nu_k \) does not seem to change the convergence properties compared to using Equation 7, we have no rigorous justification for why this is the case. A short discussion is contained in Appendix Section 9.2.
the recursively updated value of $\nu_k$ as a predictor for the true value in order to update any vectors required for the algorithm to proceed, and then to recompute $\nu_k = \langle \tilde{r}_k, r_k \rangle$ at the same time as the other inner products. We observe experimentally that using this strategy effectively brings the ultimately attainable accuracy to a similar level as that of HS-CG. This algorithm, denoted PR-CG, is given in Algorithm 2.

Note that we use a prime ("\′") to distinguish the updated quantity $\nu'_k$ from the explicitly computed quantity $\nu_k$. Note further that the variant M-CG can be obtained by replacing line 6 of Algorithm 2 with the expression $\nu'_k = -\nu_{k-1} + \alpha_{k-1}^2 \gamma_{k-1}$ and skipping the computation of $\delta_k$ in line 10. Similarly, the expression $\nu_k = -\alpha_k \mu_k + \alpha_k^2 \gamma_k$ is used in [SG06]. It can easily be seen that these expressions are equivalent to Equation 8 by noticing that $\mu_k = \langle p_k, s_k \rangle = \langle \tilde{r}_k, s_k \rangle = \delta_k$ and $\alpha_k = \nu_k / \mu_k$.

### 3.2 Pipelined variants

Recall that our goal is to be able to compute the matrix vector product and inner products simultaneously. To this end, note that in both M-CG and PR-CG, we have the recurrence $p_k = \tilde{r}_k + \beta_k p_{k-1}$. Thus, defining $w_k = A \tilde{r}_k$, we can write,

$$s_k = Ap_k = A\tilde{r}_k + \beta_k Ap_{k-1} = w_k + \beta_k s_{k-1}$$  \hspace{2cm} (10)

Similarly, defining, $u_k = A\tilde{s}_k$,

$$w_k = A\tilde{r}_k = A\tilde{r}_{k-1} - \alpha_k Ap_{k-1} = w_{k-1} - \alpha_k u_{k-1}$$  \hspace{2cm} (11)

Using these recurrences allows us to compute the product $u_k = A\tilde{s}_k$ at the same time as all of the inner products.

To move the preconditioning step, we define $\tilde{w}_k = M^{-1} w_k$ so that,

$$\tilde{s}_k = M^{-1} s_k = M^{-1} w_k + \beta_k M^{-1} s_{k-1} = \tilde{w}_k + \beta_k \tilde{s}_{k-1}$$  \hspace{2cm} (12)

and define $\tilde{u}_k = M^{-1} u_k$ so that,

$$\tilde{w}_k = M^{-1} w_k = M^{-1} w_{k-1} - \alpha_k M^{-1} u_{k-1} = \tilde{w}_{k-1} - \alpha_k \tilde{u}_{k-1}$$  \hspace{2cm} (13)

### 3.2.1 Predict-and-recompute for vector updates

In this section we extend the idea to predict-and-recompute recursively updated quantities, which was first introduced by Meurant in [Meu87]. Implemented in the above form, the pipelined variants derived from M-CG and PR-CG appear to converge slightly better than GV-CG on most problems, but still suffer from delayed convergence and reduced final accuracy compared to the unpipelined versions. To address this, we observe that $w_k = A\tilde{r}_k$ and $\tilde{w}_k = M^{-1} w_k$ can be recomputed at the same time as the other matrix vector product and all inner products are being computed. Thus, in the same way we use the recursively updated value of $\nu_k$ as a predictor for the true value, we can use the recursively updated value of $w_k$ as a predictor for the true value in order to update other vector quantities, and then update the value of $w_k$ later in the iteration. Using this predict-and-recompute approach gives PPR-M-CG and PPR-CG.

Algorithm 3 shows PPR-CG, from which PPR-M-CG can be obtained by using the alternate expression $\nu'_k = -\nu_{k-1} + \alpha_{k-1}^2 \gamma_{k-1}$ in line 7. As before, we use a prime to denote predicted quantities.
We suggest that at the beginning of each iteration the scalars $\alpha$ inefficient implementation may actually increase the runtime per iteration. As with any parallel algorithm, some care must be taken at implementation time as an HS-CG, and to emphasize the mathematical equivalence of the two algorithms. However, the presentation of PPR-CG in Algorithm 3 is intended to match the derivation from HS-CG, and to emphasize the mathematical equivalence of the two algorithms. However, as with any parallel algorithm, some care must be taken at implementation time as an inefficient implementation may actually increase the runtime per iteration.

We suggest that at the beginning of each iteration the scalars $\alpha_{k-1}, \nu_k'$ and $\beta_k$ (lines 14, 7, 8) be computed. This will allow all vector updates (lines 4, 5, 6, 9, 10) to occur simultaneously. The vector updates require only local on-node communication, and therefore are assumed to be very fast. Finally, the matrix vector products/preconditioning (lines 11, 12), and inner products (line 13) can all be computed simultaneously. As a result, the dominant cost per iteration will be either the time for the global reduction associated with the inner products, or with the matrix vector products, thus giving the runtime $\max(\text{GLRED}, \text{MV/PC})$ as listed in Table 1.

The matrix vector products (and preconditioning) in lines 11 and 12 can be computed together using efficient kernels. In particular, this means that PPR-CG still requires only one pass over $A$ (and $M^{-1}$) each iteration. This is an important consideration if $A$ is too large to store in fast memory. Similarly, three of the inner products involve $s_k$, the number of passes over $s_k$ can be reduced from three to one. However, this is likely not to have a noticeable effect until the cost of reading $s_k$ from memory becomes large compared to the reduction time. Finally, there is no need to store $w_k$ and $w_k'$ as separate vectors.

![Algorithm 3: Pipelined predict-and-recompute conjugate gradient](image)

```plaintext
1: procedure PPR-CG($A$, $M$, $b$, $x_0$)
2: INITIALIZE()
3: for $k = 1, 2, \ldots$ do
4:     \quad $x_k = x_{k-1} + \alpha_{k-1}p_{k-1}$
5:     \quad $r_k = r_{k-1} - \alpha_{k-1}s_{k-1}$, \quad $\tilde{r}_k = \tilde{r}_{k-1} - \alpha_{k-1}\tilde{s}_{k-1}$
6:     \quad $w_k' = w_{k-1} - \alpha_{k-1}u_{k-1}$, \quad $\tilde{w}_k' = \tilde{w}_{k-1} - \alpha_{k-1}\tilde{u}_{k-1}$
7:     \quad $\nu_k' = \nu_{k-1} - 2\alpha_{k-1}\tilde{\delta}_{k-1} + \alpha_{k-1}^2\gamma_{k-1}$
8:     \quad $\beta_k = \nu_k'/\nu_{k-1}$
9:     \quad $p_k = \tilde{r}_k + \beta_k p_{k-1}$
10:    \quad $s_k = w_k' + \beta_k s_{k-1}$, \quad $\tilde{s}_k = \tilde{w}_k' + \beta_k \tilde{s}_{k-1}$
11:    \quad $u_k = A\tilde{s}_k$, \quad $\tilde{u}_k = M^{-1}u_k$
12:    \quad $w_k = A\tilde{r}_k$, \quad $\tilde{w}_k = M^{-1}w_k$
13:    \quad $\mu_k = \langle p_k, s_k \rangle$, \quad $\delta_k = \langle \tilde{r}_k, s_k \rangle$, \quad $\gamma_k = \langle \tilde{s}_k, s_k \rangle$, \quad $\nu_k = \langle \tilde{r}_k, r_k \rangle$
14:    \quad $\alpha_k = \nu_k/\mu_k$
15: end for
16: end procedure

17: procedure INITIALIZE
18: \quad $r_0 = b - Ax_0$, $\tilde{r}_0 = M^{-1}r_0$, $w_0 = A\tilde{r}_0$, $\tilde{w}_0 = M^{-1}w_0$, $\nu_0 = \langle r_0, \tilde{r}_0 \rangle$
19: \quad $p_0 = \tilde{r}_0$, $s_0 = Ap_0$, $\tilde{s}_0 = M^{-1}s_0$, $u_0 = A\tilde{s}_0$, $\tilde{u}_0 = M^{-1}u_0$, $\alpha_0 = \nu_0/\langle p_0, s_0 \rangle$, $\delta_0 = \langle \tilde{r}_0, s_0 \rangle$, $\gamma_0 = \langle \tilde{s}_0, s_0 \rangle$
20: end procedure
```

3.2.2 Implementation

The presentation of PPR-CG in Algorithm 3 is intended to match the derivation from HS-CG, and to emphasize the mathematical equivalence of the two algorithms. However, as with any parallel algorithm, some care must be taken at implementation time as an inefficient implementation may actually increase the runtime per iteration.
4 Numerical performance

As previously mentioned, the primary effects of finite precision on the conjugate gradient algorithm are delayed convergence and loss of accuracy. In this section we present the results of numerical experiments intended to give insight into the numerical behaviour of the variants introduced in this paper. We emphasize that while numerical experiments provide an indication that a given variant performs well in finite precision, they do not prove that this will always be the case.

We run experiments on a range of matrices from the Matrix Market [BPR+97] and outline the results in Table 2. In this table we give two summary statistics: (i) the number of iterations required to decrease the $A$-norm of the error by a factor of $10^5$, and (ii) the minimum error reached. For a given problem, these two quantities give a rough indication of the rate of convergence and ultimately attainable accuracy. Plots of convergence for all experiments appearing in Table 2 can be found online in the repository linked in Appendix Section 9.1. As done in [GV14], the right hand side $b$ is chosen so that $x^* = A^{-1}b$ has entries $1/\sqrt{n}$, and the initial guess $x_0$ is the zero vector. For most problems we selected, we run tests without a preconditioner, and then with a simple Jacobi (diagonal) preconditioner.

![Figure 1: Error $A$-norm of different variants on “difficult problems”](image)

In addition to the results in Table 2, Figure 1 shows the $A$-norm of the error at step $k$ for a few particularly difficult test problems. On such problems, finite precision CG implementations encounter a delay of convergence and/or a loss of accuracy. Two examples of problems where both effects are observed are the so-called “model problem” introduced in [Str91], and bcsstk03 from the Matrix Market. These problems are considered in [SG92, DR92, GLC19, etc.] and [WSS96, CRS+18, etc.] respectively. On many other problems, the rate of convergence of all variants is similar, but the final accuracy of certain variants is drastically reduced. One such example is s3rmq4m1, also from the Matrix Market, where the rate of convergence of all variants is initially the same, but the final accuracy of GV-CG is 8 orders of magnitude worse than HS-CG. We emphasize that these problems have been selected as they highlight the different convergence properties of the different variants. On many (perhaps most) other problems, the rate of convergence of all variants is equal until they reach their maximal accuracy.

It has previously been observed that on most problems CG-CG converges at a similar rate, and to a similar maximal accuracy, as HS-CG [GV14, GLC19]. Both M-CG and PR-CG

---

2We use a model problem, denoted model 48 8 3, of size $n = 48$ with the parameter $\rho = 0.8$ and condition number $10^3$. This value of $\rho$ clusters the eigenvalues at the lower end of the spectrum, which makes it a particularly difficult problem in finite precision. The eigenvectors are chosen uniformly at random among all unitary matrices.
Table 2: Summary statistics of convergence on problems from the matrix market. Preconditioners are applied using preconditioned variants rather than constructing an explicitly preconditioned system. Values are bold if they differ from HS-CG by more than ten percent, and dashes indicate that a method failed to reach the specified accuracy.
display this good convergence on our test problems. We do note that on problems where CG-CG encounters a delaye of convergence, such as bcsstk03, PR-CG converges more quickly.

More notably, the pipelined predict-and-recompute variants PPR-M-CG and PPR-CG show significantly better convergence than GV-CG, frequently exhibiting convergence similar to that of HS-CG. In particular, on all the problems tested, PPR-M-CG and PPR-CG converge to a final accuracy within 10 percent (on a log scale) of that of HS-CG if Jacobi preconditioning is used, and on some problems, these two variants actually converge to a better final accuracy than HS-CG.

We claim that the variants presented in this paper have a residual gap \( b - Ax_k - r_k \) depending only on local rounding errors [Car19], and satisfy the symmetric three term Lanczos recurrence to within local rounding errors, which as discussed in Section 2.3, are steps towards proving good convergence. However, to keep this paper concise, we leave the proof of these claims, and a more comprehensive roundoff error analysis to future work.

5 Parallel performance

Numerical experiments indicate that the variants presented in this paper have better convergence properties in terms of both rate of convergence and maximal accuracy, than existing communication hiding variants. However, in practice convergence speed is measured in seconds not iterations. As such, we must verify that the variants presented here actually reduce the runtime compared to the standard HS-CG implementation.

We implement PR-CG and PPR-CG in PETSc [BAA+19, BGMS97]. Unfortunately, PETSc does not natively support an efficient kernel for the simultaneous matrix product with a block of vectors, so we compute the two matrix vector products and preconditioning steps sequentially. However, this means the asymptotic runtime of our implementation of PPR-CG is \( \max(GLRED, 2 \cdot MV/PC) \) rather than \( \max(GLRED, MV/PC) \).

To account for this we add an optional parameter to our implementation to allow the “recompute” stage to be skipped (denoted PP-CG). This gives a more accurate representation of what the runtime of a good implementation of PPR-CG would be, since the cost of computing \( Ax \) and \( Ay \) together in a smart way is nearly the same as computing only \( Ax \). However, the convergence of this variant is not as good as PPR-CG, and it should not be used in practice. It should also be noted that we compute the four inner products in our pipelined methods independently. This means that some additional costs may be saved by combining the appropriate inner products as mentioned in Section 3.2.2. Thus, the performance of PPR-CG when properly implemented is expected to fall somewhere between that of PP-CG and PPR-CG.

Figure 2 shows the results of a strong scaling experiment run on the Hyak supercomputer at the University of Washington. In this experiment we solved an approximate model problem, which has diagonal entries,

\[
\lambda_1 = 1, \quad \lambda_n = \kappa, \quad \lambda_i = \lambda_1 + \left( \frac{i-1}{n-1} \right) \cdot (\kappa - 1) \cdot \rho^{n-i}, \quad i = 2, 3, \ldots, n - 1
\]

with parameters \( n = 6.5 \times 10^5, \rho = 0.95, \kappa = 10^6 \). However, in order to simulate a more expensive matrix product, we put small off diagonal entries of size \( 10^{-4} \) at all entries within the half-bandwidth \( k = 32 \) of the main diagonal. By applying Gershgorin’s circle theorem, it is clear that this matrix has eigenvalues near those of the model problem, and that in particular, the matrix is positive definite.
Figure 2: Strong scaling experiment on approximate model problem with $n = 6.5 \times 10^5$ unknowns and half bandwidth $k = 32$. *This variant is implemented suboptimally.

We run each variant for 4000 iterations without a preconditioner, resulting in residual norms on the order of $10^{-7}$ for most variants, and $10^{-4}$ for GV-CG. In order to make a fair comparison with HS-CG, we use the option `ksp.norm_type natural`. This tells PETSc to use $\nu_k$ as the measure of the error at each step, rather than computing the norm of the updated residual, which would increase the runtime of HS-CG to $3 \cdot \text{GLRED+MV/PC}$. To account for effects such as system noise and network topology, we ask for three separate allocations of nodes, and for each allocation, run three experiments on each number of MPI processes. More detailed logs of the system configuration can be found in the repository linked in Appendix Section 9.1.

As expected, the bad implementation of PP-CG takes nearly twice as long as the other variants on a single node, since the matrix vector products are the dominant cost of an iteration. However, when the number of nodes is increased and the matrix vector product becomes much cheaper, all of the communication hiding variants give roughly a two times speedup over HS-CG. Finally, there is a point between these extremes where the speedup of GV-CG and PP-CG over HS-CG is greater than two. All of these phenomena agree with the theoretical behaviours written in the time column of Table 1.

Since this is a single, small, experiment in the context of high performance computing, the results should not be taken as an indication of the scaling which will be observed on different systems or different hardware. Rather, the experiments should be taken as an indication that, even with a suboptimal implementation, pipelined predict-and-recompute methods scale similarly to the better known pipelined method GV-CG. Specifically, even our naive implementation of PPR-CG is able to decrease the runtime over HS-CG, while maintaining numerical stability. Finally, we again suggest that when using high performance conjugate gradient variants, it may be worth working with explicitly preconditioned systems to save storage (and hence communication) costs.

6 Future work

This paper opens up a few natural topics for future work, namely (i) the roundoff error analysis of PPR-CG and similar methods, (ii) the modification of PPR-CG to reduce the communication costs further, and (iii) the modification of PPR-CG to improve convergence.

First, it would be good to be able to prove that PPR-CG converges to an maximal accuracy similar to that of HS-CG. While preliminary work by Carson suggests that the improvement to the final accuracy of the predict and recompute methods (as opposed to not using predict-
and-recompute) can be explained [Car19], it remains unknown why the maximal accuracy of PPR-CG is so similar to that of HS-CG in the numerical experiments from Section 4. In fact, in many other variants we tested, using similar predict-and-recompute strategies seems to slow or even destroy convergence (for instance, recomputing the residual \( r_k = b - Ax_k \) in HS-CG at the same time as the other matrix vector product). Understanding when and why such approaches work has the potential to lead to further improvements to finite precision conjugate gradient algorithms. Thus, understanding when at what level of accuracy the breakdown occurs could be of interest.

Second, since the maximum reduction in communication costs of PPR-CG over HS-CG is only a factor of three, potential ways of further decreasing communication costs should be explored. Recently, there has been development on “deep pipelined” conjugate gradient variants where more matrix vector products are overlapped with global communication; see for instance [GV14, CCV18, CCV19, etc.]. This approach is similar to the “look ahead” strategy suggested in [Ros83].

Alternatively, it may be possible to either incorporate predict-and-recompute strategies into \( s \)-step methods, or to develop new \( s \)-step methods which are built on PR-CG. CG-CG is the \( s = 1 \) case of the \( s \)-step method from [CG89b], so it may be possible to develop an \( s \)-step method based on PR-CG, which has slightly better numerical properties than CG-CG. Finding such a method which is usable in practice would be of great practical interest.

Third, it may be possible to improve the final accuracy of PPR-CG in the cases when it is worse than HS-CG. While using a simple Jacobi preconditioner was sufficient to achieve a maximal accuracy near that of HS-CG on all the problems we tested, it is possible that there are other problems where this is not the case. In [GV14, CD14, CFYA+18, CRS+18, etc.], residual replacement is explored as a means of increasing the ultimately attainable accuracy of conjugate gradient variants. Unfortunately, residual replacement frequently leads to a further delay of convergence on problems where the rate of convergence is already slower than HS-CG. Limited numerical tests indicate that residual replacement can increase the ultimately attainable accuracy of the predict-and-recompute variants from this paper, but that it may simultaneously reduce the rate of convergence.

Finally, the predict-and-recompute variants presented here can be naturally extended to other related methods such as conjugate residual, and conjugate gradient squared.

7 Conclusion

In this paper we introduced a range of communication hiding conjugate gradient variants, each of which have better scaling properties than the standard HS-CG algorithm. These variants exhibit improved convergence compared to their analogous, previously studied, counterparts on a range of test problems. We additionally extended the predict-and-recompute idea of Meurant in order to improve the rate of convergence and final accuracy of the pipelined variants presented in this paper. The resulting pipelined predict-and-recompute variants PPR-M-CG and PPR-CG showed better convergence properties than the classic pipelined conjugate gradient variants on every numerical experiment we ran. None of our predict-and-recompute variants require the use of additional parameters in order to obtain good convergence, and therefore have the potential to be used wherever HS-CG is used. Despite these advances, there is still significant room for future work on high performance conjugate gradient variants, especially in the direction of further decreasing the communication costs.
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9 Appendix

9.1 Additional resources

A repository with the code necessary to reproduce all of the figures and results in this paper is available at https://github.com/tchen01/new_cg_variants, and released to the public domain under the MIT License. The repository also contains convergence data and plots for all the matrices listed in Table 2.

I have also written an extended introduction to this paper, intended for a broader audience, at https://chen.pw/research/publications/predict_and_recompute.html.

I am committed to facilitating the reproducibility process, and encourage questions and inquiries into the methods used in this paper. I’m more than happy to help you get my code running on your system so that you can run the experiments from this paper.

9.2 A note on other variants we studied

There are countless mathematically equivalent variants which can be derived by substituting different equivalent quantities. This section contains a discussion on some of the more “obvious” variants which for a variety of reasons do not appear in the main paper.

First, recall that we have tried alternate formulas for Equation 7. As a heuristic, we suggest that using the orthogonality of vectors to avoid computing an inner product has a larger impact than switching the ordering of vectors in an inner product induced by a positive definite matrix. This would explain why using \(\langle \tilde{s}_{k-1}, \tilde{r}_{k-1} \rangle\) in place of \(\langle \tilde{r}_{k-1}, \tilde{s}_{k-1} \rangle\) does not seem lead to a noticeable change in convergence, while using \(\langle p_k, s_k \rangle = \langle \tilde{r}_k + \beta_k p_{k-1}, s_k \rangle\) in place of either of these inner products might. However, it may be the case that when using preconditioners that introduce more rounding errors, the formula based on four inner products will produce better convergence.

On the other hand, using the \(A\)-orthogonality of \(p_k\) and \(p_{k-1}\) to interchange \(\langle p_k, s_k \rangle\) with these quantities leads to a variant which is equivalent to M-CG up to local rounding errors in computing a scalar quantity. This reduces the rate of convergence on some difficult problems, but on many problems does not change the convergence noticeably.

Next, it should be noted that the idea of predict-and-recompute does not always work. For instance, in PPR-CG, it may seem reasonable to try to recompute \(s_k = Ap_k\). However, this breaks convergence. Similarly, GV-CG by trying to update \(w_k = Ar_k\) at the same time as the matrix vector product. However, this has the effect of breaking convergence. Similarly, if the true residual in HS-CG is computed at the same time as the matrix vector product, convergence is severely slowed. Thus, predict-and-recompute approaches should not be applied haphazardly to any variant.

Finally, we note that in the derivation of CG-CG, if the formula for \(\mu_k\) is not simplified fully, that convergence is slightly improved. This comes at the cost of an additional inner product. However, using this expression in GV-CG does not appear to lead to improved convergence.

As an afterthought, we suggest that it may be possible to procedurally generate mathematically equivalent conjugate gradient variants, and then automatically check if they have improved convergence properties. Perhaps, by finding many variants which work well, the similarities between them could provide insights into necessary properties for a good finite precision conjugate gradient variant.
9.3 Previously studied communication hiding variants

While we omitted the full descriptions of the M-CG, CG-CG, and GV-CG algorithms in the main paper, we include them here for completeness. We additionally include descriptions of PP-M-CG, PPR-M-CG, and PP-CG which are described in the paper but never explicitly written.

**Algorithm 4** Meurant conjugate gradient

```plaintext
1: procedure PR-CG(A, M, b, x_0)
2:   INITIALIZE()
3:   for k = 1, 2, ... do
4:     x_k = x_{k-1} + α_{k-1}p_{k-1}
5:     r_k = r_{k-1} - α_{k-1}s_{k-1}, \tilde{r}_k = \tilde{r}_{k-1} - α_{k-1}\tilde{s}_{k-1}
6:     v'_k = -v_{k-1} + α_k^2γ_{k-1}
7:     β_k = v'_k/v_{k-1}
8:     p_k = \tilde{r}_k + β_kp_{k-1}
9:     s_k = Ap_k, \tilde{s}_k = M^{-1}s_k
10:    μ_k = \langle p_k, s_k \rangle, γ_k = \langle \tilde{s}_k, s_k \rangle, ν_k = \langle \tilde{r}_k, r_k \rangle
11:    α_k = ν_k/μ_k
12:   end for
13: end procedure
```

**Algorithm 5** Chronopoulos and Gear conjugate gradient

```plaintext
1: procedure CG-CG(A, M, b, x_0)
2:   INITIALIZE()
3:   for k = 1, 2, ... do
4:     x_k = x_{k-1} + α_{k-1}p_{k-1}
5:     r_k = r_{k-1} - α_{k-1}s_{k-1}, \tilde{r}_k = M^{-1}r_k
6:     w_k = \tilde{A}\tilde{r}_k
7:     v_k = \langle \tilde{r}_k, r_k \rangle, η_k = \langle \tilde{r}_k, w_k \rangle
8:     β_k = v_k/ν_{k-1}
9:     p_k = \tilde{r}_k + β_kp_{k-1}
10:    s_k = w_k + β_k s_{k-1}
11:    μ_k = η_k - (β_k/α_{k-1})ν_k
12:    α_k = ν_k/μ_k
13:   end for
14: end procedure
```

**Algorithm 6** PPR-M-CG

```plaintext
15: procedure INITIALIZE
16:   r_0 = b - Ax_0, \tilde{r}_0 = M^{-1}r_0, ν_0 = \langle \tilde{r}_0, r_0 \rangle, p_0 = \tilde{r}_0, s_0 = Ap_0,\n\quad \tilde{s}_0 = M^{-1}s_0, α_0 = ν_0/\langle p_0, s_0 \rangle, γ_0 = \langle \tilde{s}_0, s_0 \rangle
17: end procedure
```
Algorithm 6 Ghysels and Vanroose conjugate gradient

1: procedure GV-CG(A, M, b, x₀)
2:  INITIALIZE()
3: for k = 1, 2, \ldots do
4:  \( x_k = x_{k-1} + \alpha_k p_{k-1} \)
5:  \( r_k = r_{k-1} - \alpha_k s_{k-1} \), \( \tilde{r}_k = \tilde{r}_{k-1} - \alpha_k \tilde{s}_{k-1} \)
6:  \( w_k = w_{k-1} - \alpha_k u_{k-1} \), \( \tilde{w}_k = M^{-1} w_k \)
7:  \( \nu_k = \langle \tilde{r}_k, r_k \rangle \), \( \eta_k = \langle \tilde{r}_k, w_k \rangle \)
8:  \( t_k = A \tilde{w}_k \)
9:  \( \beta_k = \nu_k / \nu_{k-1} \)
10: \( p_k = r_k + \beta_k p_{k-1} \)
11: \( s_k = w_k + \beta_k s_{k-1} \), \( \tilde{s}_k = \tilde{w}_k + \beta_k \tilde{s}_{k-1} \)
12: \( u_k = t_k + \beta_k u_{k-1} \)
13: \( \mu_k = \eta_k - (\beta_k / \alpha_{k-1}) \nu_k \)
14: \( \alpha_k = \nu_k / \mu_k \)
15: end for
16: end procedure

Algorithm 7 Pipelined predict (and recompute) Meurant conjugate gradient

1: procedure PP-M-CG/PPR-M-CG(A, M, b, x₀)
2:  INITIALIZE()
3: for k = 1, 2, \ldots do
4:  \( x_k = x_{k-1} + \alpha_k p_{k-1} \)
5:  \( r_k = r_{k-1} - \alpha_k s_{k-1} \), \( \tilde{r}_k = \tilde{r}_{k-1} - \alpha_k \tilde{s}_{k-1} \)
6:  \( w'_k = w_{k-1} - \alpha_k u_{k-1} \), \( \tilde{w}'_k = \tilde{w}_{k-1} - \alpha_k \tilde{u}_{k-1} \)
7:  \( \nu'_k = -\nu_{k-1} + \alpha_k \gamma_{k-1} \)
8:  \( \beta'_k = \nu'_k / \nu_{k-1} \)
9:  \( p_k = r_k + \beta'_k p_{k-1} \)
10: \( s_k = w'_k + \beta'_k s_{k-1} \), \( \tilde{s}_k = \tilde{w}'_k + \beta'_k \tilde{s}_{k-1} \)
11: \( u_k = A \tilde{s}_k \), \( \tilde{u}_k = M^{-1} u_k \)
12: \( w_k = \begin{cases} \{ & \text{recompute} \\ \tilde{w}'_k & \text{otherwise} \end{cases} \)
13: \( \nu_k = \begin{cases} \{ & \text{recompute} \\ \tilde{w}'_k & \text{otherwise} \end{cases} \)
14: \( \alpha_k = \nu_k / \mu_k \)
15: end for
16: end procedure

17: procedure INITIALIZE
18: \( r_0 = b - Ax_0 \), \( \tilde{r}_0 = M^{-1} r_0 \), \( w_0 = A \tilde{r}_0 \), \( \tilde{w}_0 = M^{-1} w_0 \), \( \nu_0 = \langle r_0, \tilde{r}_0 \rangle \), \( p_0 = \tilde{r}_0 \), \( s_0 = A p_0 \), \( \tilde{s}_0 = M^{-1} s_0 \), \( u_0 = A \tilde{s}_0 \), \( \tilde{u}_0 = M^{-1} u_0 \), \( \alpha_0 = \nu_0 / p_0 \), \( \gamma_0 = (s_0, s_0) \)
19: end procedure
Algorithm 8 Pipelined predict (and recompute) conjugate gradient

1:  procedure PPR-CG($A$, $M$, $b$, $x_0$)
2:     INITIALIZE()
3:     for $k = 1, 2, \ldots$ do
4:         $x_k = x_{k-1} + \alpha_{k-1}p_{k-1}$
5:         $r_k = r_{k-1} - \alpha_{k-1}s_{k-1}$, $\tilde{r}_k = \tilde{r}_{k-1} - \alpha_{k-1}\tilde{s}_{k-1}$
6:         $w'_k = w_{k-1} - \alpha_{k-1}u_{k-1}$, $\tilde{w}'_k = \tilde{w}_{k-1} - \alpha_{k-1}\tilde{u}_{k-1}$
7:         $\nu'_k = \nu_{k-1} - 2\alpha_{k-1}\delta_{k-1} + \alpha_{k-1}^2\gamma_{k-1}$
8:         $p_k = \tilde{r}_k + \beta_k p_{k-1}$
9:         $s_k = w'_k + \beta_k s_{k-1}$, $\tilde{s}_k = \tilde{w}'_k + \beta_k \tilde{s}_{k-1}$
10:        $u_k = A\tilde{s}_k$, $\tilde{u}_k = M^{-1}u_k$
11:        $w_k = \begin{cases} A\tilde{r}_k & \text{recompute} \\ w'_k & \text{otherwise} \end{cases}$
12:        $\tilde{w}_k = \begin{cases} M^{-1}w_k & \text{recompute} \\ \tilde{w}'_k & \text{otherwise} \end{cases}$
13:        $\mu_k = \langle p_k, s_k \rangle$, $\delta_k = \langle \tilde{r}_k, s_k \rangle$, $\gamma_k = \langle \tilde{s}_k, s_k \rangle$, $\nu_k = \langle \tilde{r}_k, r_k \rangle$
14:        $\alpha_k = \nu_k / \mu_k$
15:     end for
16:  end procedure

17:  procedure INITIALIZE
18:     $r_0 = b - Ax_0$, $\tilde{r}_0 = M^{-1}r_0$, $w_0 = A\tilde{r}_0$, $\tilde{w}_0 = M^{-1}w_0$, $\nu_0 = \langle r_0, \tilde{r}_0 \rangle$
19:     $p_0 = \tilde{r}_0$, $s_0 = Ap_0$, $\tilde{s}_0 = M^{-1}s_0$, $u_0 = A\tilde{s}_0$, $\tilde{u}_0 = M^{-1}u_0$, $\alpha_0 = \nu_0 / \langle p_0, s_0 \rangle$, $\delta_0 = \langle \tilde{r}_0, s_0 \rangle$, $\gamma_0 = \langle \tilde{s}_0, s_0 \rangle$
19:  end procedure