PRIMME_SVDS: A PRECONDITIONED SVD SOLVER FOR COMPUTING ACCURATELY SINGULAR TRIPLETS OF LARGE MATRICES BASED ON THE PRIMME EIGENSOLVER

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Abstract. The computation of a few singular triplets of large, sparse matrices is a challenging task, especially when the smallest magnitude singular values are needed in high accuracy. Most recent efforts try to address this problem through variations of the Lanczos bidiagonalization method, but algorithmic research is ongoing and without production level software. We develop a high quality SVD software on top of the state-of-the-art eigensolver PRIMME that can take advantage of preconditioning, and of PRIMME’s nearly-optimal methods and full functionality to compute both largest and smallest singular triplets. Accuracy and efficiency is achieved through a hybrid, two-stage meta-method, primme_svds. In the first stage, primme_svds solves the normal equations problem up to the best achievable accuracy. If further accuracy is required, the method switches automatically to an eigenvalue problem with the augmented matrix. Thus it combines the advantages of the two stages, faster convergence and accuracy, respectively. For the augmented matrix, solving the interior eigenvalue is facilitated by a proper use of the good initial guesses from the first stage and an efficient implementation of the refined projection method. We also discuss how to precondition primme_svds and to cope with some issues that arise. The method can be used with or without preconditioning, on large problems, and can be called with its full functionality from MATLAB through our MEX interface. Numerical experiments illustrate the efficiency and robustness of the method.

1. Introduction. The Singular Value Decomposition (SVD) is a ubiquitous computational kernel in science and engineering. Many applications require a few of the largest singular values of a large sparse matrix $A$ and the associated left and right singular vectors (singular triplets). These applications are from diverse areas, such as social network analysis, image processing, textual database searching, and control theory. A smaller, but increasingly important, set of applications requires a few smallest singular triplets. Examples include least square problems, determination of matrix rank, low rank approximation, and computation of pseudospectrum [1, 2, 3, 4]. Recently we have used such techniques to reduce the variance in Monte Carlo estimations of the the trace of the inverse of a large sparse matrix.

It is well known that the computation of the smallest singular triplets presents challenges both to the speed of convergence and the accuracy of iterative methods. In this paper, we mainly focus on the problem of finding the smallest singular triplets. Assume $A \in \mathbb{R}^{m \times n}$ is a large sparse matrix with full column rank and $m \geq n$. The (economy size) singular value decomposition of $A$ can be written as:

$$A = U \Sigma V^T$$

where $U = [u_1, \ldots, u_n] \in \mathbb{R}^{m \times n}$ is an orthonormal set of the left singular vectors and $V = [v_1, \ldots, v_n] \in \mathbb{R}^{n \times n}$ is the unitary matrix of the right singular vectors. $\Sigma = diag(\sigma_1, \ldots, \sigma_n) \in \mathbb{R}^{n \times n}$ contains the singular values of $A$, $\sigma_1 \leq \ldots \leq \sigma_n$. We will be looking for the smallest $k \ll n$ singular triplets $\{\sigma_i, u_i, v_i\}$, $i = 1, \ldots, k$.

There are two approaches to compute the singular triplets $\{\sigma_i, u_i, v_i\}$ by using a Hermitian eigensolver. Using MATLAB notation, the first approach seeks eigenpairs of the augmented matrix $B = [0 A^T; A 0] \in \mathbb{R}^{(m+n) \times (m+n)}$, which has eigenvalues $\pm \sigma_i$ with corresponding eigenvectors $([v_i; u_i], [-v_i; u_i])$, as well as $m - n$ zero eigenvalues $[6, 7, 8]$. The main advantage of this approach is that iterative methods can potentially

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compute the smallest singular values accurately, i.e., with residual norm close to $O(\|A\|_\text{mach})$. However, convergence of eigenvalue iterative methods is slow since it is a highly interior eigenvalue problem, and even the use of iterative refinement or inverse iteration involves a maximally indefinite matrix [5]. For restarted iterative methods convergence is even slower, irregular, and often the required eigenvalues are missed since the Rayleigh-Ritz projection method does not effectively extract the appropriate information for interior eigenvectors [29, 30, 33].

The second approach computes eigenpairs of the normal equations matrix $C = A^T A \in \mathbb{R}^{n \times n}$ which has eigenvalues $\sigma_i^2$ and associated eigenvectors $v_i$. If $\sigma_i \neq 0$, the corresponding left singular vectors are obtained as $u_i = \frac{1}{\sigma_i} A^T v_i$. $C$ is implicitly accessed through successive matrix-vector multiplications. The squaring of the singular values works in favor of this approach with Krylov methods, especially with largest singular values since their relative separations increase. Although the separations of the smallest singular values become smaller, we show in this paper that this approach still is faster than Krylov methods on $B$ because it avoids indefiniteness. On the other hand, squaring the matrix limits the accuracy at which smallest singular triplets can be obtained. Therefore, this approach is typically followed by a second stage of iterative refinement for each needed singular triplet which resolves the required accuracy [11, 12, 13]. However, this one-by-one iterative refinement does not exploit information from other singular vectors and thus is not as efficient as an eigensolver applied on $B$ with the estimates of the first stage.

The Lanczos bidiagonalization (LBD) method [1, 6] is accepted as an accurate and more efficient method for seeking singular triplets (especially smallest), and numerous variants have been proposed [22, 17, 19, 14, 15, 16, 18, 25]. LBD builds the same subspace as Lanczos on matrix $C$, but since it works on $A$ directly, it avoids the numerical problems of squaring. However, the Ritz vectors often exhibit slow, irregular convergence when the smallest singular values are clustered. To address this problem, harmonic projection [19, 14], refined projection [17], and their combinations [18] have been applied to LBD. Despite remarkable algorithmic progress, current LBD methods are still in development, with only few existing MATLAB implementations that serve mainly as a testbed for mathematical research. Moreover, we show that a two stage approach based on a well designed eigenvalue code (such as PRIMME) can be more robust and efficient for a few singular triplets. Most importantly, our approach can use preconditioning, something that is not directly possible with LBD but becomes crucial because of the difficulty of the problem even for medium matrix sizes.

The Jacobi-Davidson type SVD method, JDSVD [9, 10], is based on an inner-outer iteration and can also use preconditioning. It obtains the left and right singular vectors directly from a projection of $B$ on two subspaces and, although it avoids the numerical limitations of matrix $C$, it needs a harmonic [29, 32, 31] or a refined projection method [33, 34] to avoid the irregular convergence of the Rayleigh-Ritz method. JDSVD often has difficulty computing the smallest singular values of a rectangular matrix $A$, especially without preconditioning, due to the presence of zero eigenvalues of $B$. Also, JDSVD is only available in a MATLAB research implementation.

Recently, based on [26], an inverse free preconditioned Krylov subspace method, SVDIFP, has appeared for the singular value problem [27]. The implementation includes the robust incomplete factorization (RIF) [28] for the normal equations matrix, but other preconditioners can also be used. To circumvent the intrinsic difficulties of filtering out the zero eigenvalues of the augmented matrix $B$, the method works with the normal equations matrix $C$, but computes directly the smallest singular values
of $A$ and not the eigenvalues of $C$. Thus good numerical accuracy can be achieved but, as we show later, at the expense of efficiency. Moreover, the design of SVDIFP is based on restarting with a single vector, which is not effective when seeking more than one singular values. Finally, the SVDIFP code is only available in MATLAB.

Given the above research activity in SVD algorithms, it is surprising that there is a lack of good quality software for computing the partial SVD, especially with preconditioning. Without preconditioning, SVDPACK [20] and PROPACK [21, 22] implement variants of (block) Lanczos methods. In addition, PROPACK implements an implicitly restarted LBD. However, SVDPACK can only compute largest singular triplets while PROPACK has to leverage shift-and-invert techniques to search for smallest. SLEPc offers some limited functionality for computing the partial SVD problem of a large, sparse rectangular matrix using various eigensolvers working on $B$ or $C$ [23]. It also implements a parallel LBD method but focuses mainly on largest singular values [24]. With the growing size and difficulty of real-world problems, there is a clear need for a high quality SVD solver software that allows for additional flexibility, implements state-of-the-art methods, and allows for preconditioning.

In this paper we address this need by developing a high quality SVD software based on the state-of-the-art package PRIMME (PRReconditioned Iterative Multi-Method Eigensolver) [37]. The novelty is not on the interface but on a hybrid, two-stage method that achieves both efficiency and accuracy for both largest and smallest singular values under limited memory. In the first stage, the proposed method primme\_svds solves an extreme eigenvalue problem on $C$ up to the user required accuracy or up to the accuracy achievable by the normal equations. If further accuracy is required, primme\_svds switches to a second stage where it utilizes the eigenvectors and eigenvalues from $C$ as initial guesses to a Jacobi-Davidson method on $B$, which has been enhanced by a refined projection method. The appropriate choices for tolerances, transitions, selection of target shifts, and initial guesses are handled automatically by the method. We also discuss how to precondition primme\_svds and to cope with possible issues that can arise. Our extensive numerical experiments show that primme\_svds can be considerably more efficient than all other methods when computing a few of the smallest singular triplets, even without a preconditioner. With a good preconditioner, the primme\_svds method can be much more efficient and more robust than the JDSVD and SVDIFP methods.

In Section 2 we motivate the two stage SVD method based on the convergence of other Krylov methods to the smallest magnitude eigenvalue of $B$ and $C$. In Section 3, we develop the components of the two stage SVD method. In Section 4, we describe how to precondition primme\_svds, and how to dynamically inspect the quality of preconditioning at the two different stages. In Section 5, we present extensive experiments that corroborate our conclusions.

We denote by $\|\|\|$ the 2-norm of a vector or a matrix, by $A^T$ the transpose of $A$, by $I$ the identity matrix, $\kappa(A) = \frac{\sigma_n}{\sigma_1}$, and by $K_m(A, v) = \text{span}\{v, Av, \ldots, A^{m-1}v\}$ the m-dimensional Krylov subspace generated by $A$ and the initial vector $v$.

2. Motivation for PRIMME and a two stage strategy. We first introduce some basic iterative methods for SVD, and discuss some of the features in PRIMME that facilitate the development of a flexible SVD solver. Then, we study both the asymptotic convergence of unpreconditioned Krylov methods applied on $C$ and $B$, and the quality of the subspaces built by different methods. Even without taking into account the way we extract information from the subspaces, we arrive at the conclusion that a hybrid strategy should be preferred.
2.1. The LBD, JDSVD, and SVDIFP methods. The LBD method, [6, 7], starts with unit vectors $p_1$ and $q_1$ and after $k$ steps produces the following decomposition as a partial Lanczos bidiagonalization of $A$:

\begin{equation}
AP_k = Q_k B_k,
\end{equation}

\begin{equation}
A^T Q_k = P_k B_k^T + r_k e_k^T,
\end{equation}

where the $r_k$ is the residual vector at $k$-th step, $e_k$ is the $k$-th orthocanonical vector, $B_k = \begin{pmatrix} \alpha_1 & \beta_1 \\ & \ddots \\ & & \ddots & \beta_{k-1} \\ & & & \alpha_k \end{pmatrix} = Q_k^T A P_k$,

and $Q_k$ and $P_k$ are orthonormal bases of the Krylov subspaces $K_k(A A^T, q_1)$, and $V_k = K_k(A^T A, p_1)$ respectively. With properly chosen starting vectors, LBD produces mathematically the same space as the symmetric Lanczos method on $B$ or $C$ [18, 19].

To approximate the singular triplets of $A$, LBD solves the small singular value problem on $B_k$, and uses the corresponding Ritz approximations from $Q_k$ and $P_k$ as left and right singular vectors. To address the rapid loss of orthogonality of $P_m$ and $Q_m$ in finite precision, full [7], partial [22], or one-sided reorthogonalization [14, 18] strategies have been applied to variants of LBD. Because, all such solutions become expensive when $k$ is large, restarted LBD versions have been studied [19, 14, 17, 22].

The goal is twofold: restart with sufficient subspace information to maintain a good convergence, and identify the appropriate Ritz information to restart with. The former problem is tackled with implicit or thick restarting [38]. The latter problem is tackled with combinations of harmonic and refined projection methods. For example, IRLBA [15] uses a thick restarted block LBD with harmonic projection, while IRRHLB [18] first computes harmonic Ritz vectors, and then uses their Rayleigh quotients in a refined projection to extract refined Ritz vectors from $P_k$ and $Q_k$.

The JDSVD method [9] extends the Jacobi-Davidson method and its correction equation for singular value problems by exploiting the special structure of the augmented matrix $B$. Similarly to LBD, JDSVD computes singular values, not eigenvalues, of the projection matrix, and the left and right singular vectors from separate spaces. Because good quality approximations are important not only for restarting but also in the correction equation, various projection methods can benefit JDSVD.

We introduce only the standard choice where the test and search space are the same.

Let $U$ and $V$ be the bases of the left and right search spaces with dimension $k$. Computing a singular triplet of $H = U^T A V$ yields $(\theta, U c, V d)$ as the Ritz approximation of a corresponding singular triplet of $A$. Then JDSVD obtains new corrections $s$ and $t$ for $U$ and $V$ by solving (approximately) the following correction equation:

\begin{equation}
\begin{pmatrix} P_u & 0 \\ 0 & P_v \end{pmatrix} \begin{pmatrix} -\theta I_m & A \\ A^T & -\theta I_n \end{pmatrix} \begin{pmatrix} P_u & 0 \\ 0 & P_v \end{pmatrix} \begin{pmatrix} s \\ t \end{pmatrix} = \begin{pmatrix} A v - \theta u \\ A^T u - \theta v \end{pmatrix}
\end{equation}

where $P_v = I_n - v v^T$, $P_u = I_m - u u^T$. The left and right corrections $s, t$ are then orthogonalized against $U$ and $V$ respectively. Clearly, different Galerkin choices can be used to compute harmonic or refined singular triplets. JDSVD uses thick restarting [38, 39] with possibly extra Ritz vectors retained from the previous iteration, similarly
to the locally optimal Conjugate Gradient recurrence [35]. Most importantly, the JDSVD method can take advantage of preconditioning when solving (2.2).

The SVDIFP method [27] extends the EIGIFP method [26] by computing the smallest singular values as eigenvalues of the generalized eigenvalue problem \((C, I)\). Given the current approximation \((x_i, \rho_i = x_i^T C x_i / x_i^T x_i)\), it constructs a new approximation \(x_{i+1}\) by a projection of \((C, I)\) onto the Krylov subspace,

\[
K_m(C - \rho_i I, x_i) = \text{span}\{x_i, (C - \rho_i I)x_i, \ldots, (C - \rho_i I)^{m-1} x_i\}.
\]

The space can be preconditioned by any available preconditioner \(LDLT \approx C - \rho_i I\). To avoid the numerical problems of projecting on \(\sigma\) directly from a two sided projection of \(C\), SVDIFP computes the approximate singular values directly from a two sided projection of \(C\), similarly to the LBD.

2.2. The PRIMME eigenvalue package. Our goal is to enable practitioners to solve a variety of large, sparse singular value problems with unprecedented efficiency, robustness, and accuracy. Our methods should be able to use preconditioning because very slow convergence is a limiting factor for seeking smallest singular triplets. Moreover, large problem size suggests the use of advanced restarting techniques so that memory savings do not impede convergence. These desired functionalities are found in the PRIMME eigensolver [37], which also includes a host of additional features that can further help develop and fine-tune an efficient SVD solver.

PRIMME implements a wide variety of preconditioned eigenvalue algorithms, including the nearly optimal methods GD+k and JDQMR. Near optimality is used in the sense of achieving similar convergence to a similar method with unlimited memory (e.g., unrestarted Lanczos or unrestarted Generalized Davidson). PRIMME also allows for a dynamic choice of the best method based on runtime measurements. It also implements many techniques for improving efficiency and robustness, including block-methods and locking. Unlike Lanczos or LBD, PRIMME can use as many initial vector guesses as there are available. Also given a set of user provided shifts, PRIMME can find interior eigenvalues closest to in absolute value or on the left or right side of each of these shifts. These two features are important for our two stage SVD method because there are very good eigenvalue and eigenvector approximations from the first stage. PRIMME is a parallel, high performance implementation which has proved faster and more robust than almost any other eigensolver when seeking a small number of extreme eigenvalues of large sparse Hermitian matrices. It is natural, therefore, to build our SVD solver on top of it.

First, we need to understand whether PRIMME should be used to solve the SVD as an eigenvalue problem on \(C\) or on \(B\), and whether its convergence will be competitive to other SVD methods. The following sections address these issues.

2.3. Asymptotic convergence of Krylov methods on \(C\) and \(B\). When seeking largest singular values, it is accepted that Krylov methods on \(C\) are faster than on \(B\) [9, 19, 27, 13]. The argument is straightforward.

**Theorem 2.1.** Let \(\gamma_B = \frac{\sigma_n - \sigma_{n-1}}{\sigma_n + \sigma_{n-1}}\) and \(\gamma_C = \frac{\sigma_n^2 - \sigma_{n-1}^2}{\sigma_n^2 - \sigma_1^2}\) be the gap ratios of the largest eigenvalue of matrices \(B\) and \(C\), respectively. Then, for the largest eigenvalue, the asymptotic convergence of Lanczos on \(C\) is 2 times faster than Lanczos on \(B\).

**Proof.** The asymptotic convergence rate is the square root of the gap ratio. Then:

\[
\gamma_C = \left(\frac{(\sigma_n - \sigma_{n-1})(\sigma_n + \sigma_{n-1})}{(\sigma_n + \sigma_{n-1})(\sigma_n^2 - \sigma_1^2)}\right)^2 = \gamma_B \frac{(\sigma_n + \sigma_{n-1})^2}{(\sigma_n^2 - \sigma_1^2)} > \gamma_B \frac{4\sigma_{n-1}^2}{(\sigma_{n-1} - \sigma_1^2)} = \frac{4\gamma_B}{1 - (\frac{\sigma_{n-1}}{\sigma_n})^2}.
\]
Therefore, for \( \sigma_1 \approx 0 \), the asymptotic convergence rate \( \sqrt{\gamma C} > 2\sqrt{\gamma B} \). In the less interesting case \( \sigma_1 \to \sigma_{n-1} \), Lanczos on \( C \) is arbitrarily faster than on \( B \). \( \square \)

For smallest singular values the literature is less clear, although methods that work on \( C \) have been avoided for numerical reasons. In previous experiments we have observed much faster convergence with approaches on \( C \) than on \( B \) [41]. To obtain some intuition, we perform a basic asymptotic convergence analysis of Krylov methods working on \( C \) or on \( B \) trying to compute the smallest magnitude eigenvalue.

**Lemma 2.2.** Let the union of two intervals: \( K = [-a,b] \cup [c,d], -b < 0 < c, \) and \( p_k(x) \) the optimal degree-\( k \) polynomial that is as small as possible on \( K \) and \( p_k(0) = 1 \). Let \( \epsilon_k = \max_{x \in K} |p_k(x)| \), and \( \rho = \lim_{k \to \infty} \epsilon_k^{1/k} \). Then asymptotically:

\[
\rho \simeq 1 - \sqrt{\frac{bc}{da}}.
\]

**Proof.** This is an application of Theorem 5 in [40]. \( \square \)

This \( \rho \) translates to an upper bound for the asymptotic convergence rate of any Krylov solver applied to an indefinite matrix whose spectrum lies in the interval \( K \). Thus it can also be used for the convergence rate to the smallest positive eigenvalue of the augmented matrix \( B \). Assume \( \sigma_1 \) is a simple eigenvalue of \( B \) and thus \( \sigma_2^1 \) is a simple eigenvalue of \( C \). Define its gap ratio in \( C \) as, \( \gamma = \frac{\sigma_2^1 - \sigma_1}{\sigma_n - \sigma_1} \), and assume \( \gamma \ll 1 \).

**Theorem 2.3.** Consider the spectrum of the matrix \( B - \sigma_1 I \), which lies (except for the zero eigenvalue) in the two intervals: \( K = [-\sigma_n - \sigma_1, -2\sigma_1] \cup [\sigma_2 - \sigma_1, \sigma_n - \sigma_1] \). The asymptotic convergence rate for any Krylov solver that finds \( \sigma_1 \) is bounded by:

\[
\rho = 1 - \sqrt{\gamma \frac{2\sigma_1}{\sigma_2 + \sigma_1} \frac{\sigma_2^2 - \sigma_1^2}{\sigma_n^2 - \sigma_1^2}}.
\]

**Proof.** Clearly, the optimal polynomial \( p_k(x) \) of Lemma 2.2 is the best polynomial for finding \( \sigma_1 \). Applying the Lemma for the specific bounds for this interval we get:

\[
\frac{bc}{ad} = \frac{2\sigma_1 (\sigma_2 - \sigma_1)}{(\sigma_n + \sigma_1)(\sigma_n - \sigma_1)} = \frac{2\sigma_1}{\sigma_2 + \sigma_1} \frac{\sigma_2^2 - \sigma_1^2}{\sigma_n^2 - \sigma_1^2} = \frac{2\sigma_1}{\sigma_2 + \sigma_1} \frac{\sigma_2^2 - \sigma_1^2}{\sigma_n - \sigma_2} \frac{\sigma_n^2 - \sigma_2^2}{\sigma_n - \sigma_1}.
\]

\( \square \)

**Lemma 2.4.** The bound of the asymptotic convergence rate to \( \sigma_2^1 \) of Lanczos on \( C \) is approximately: \( \rho = 1 - 2\sqrt{\gamma} \).

**Proof.** The bound on the rate of convergence of Lanczos for \( \sigma_2^1 \) is approximated as \( e^{-2\sqrt{\gamma}} \) [5, p. 280]. Taking the first order approximation from Taylor series around 0, we obtain \( e^{-2\sqrt{\gamma}} = 1 - 2\sqrt{\gamma} + O(\gamma) \). \( \square \)

**Theorem 2.5.** A Krylov method on \( C \) that computes \( \sigma_2^1 \) has always faster asymptotic convergence rate than a Krylov method on \( B \) that finds \( \sigma_1 \), by a factor of

\[
\tau = \frac{1 - \sqrt{\gamma \frac{2\sigma_1}{\sigma_2 + \sigma_1} \frac{\sigma_2^2 - \sigma_1^2}{\sigma_n^2 - \sigma_1^2}}}{1 - 2\sqrt{\gamma}}.
\]

**Proof.** For the method on \( C \) to be faster it must hold \( \tau > 1 \) or \( \frac{2\sigma_1}{\sigma_2 + \sigma_1} \frac{\sigma_2^2 - \sigma_1^2}{\sigma_n^2 - \sigma_1^2} < 4 \). Basic manipulations lead to the condition \( (4 - 2\frac{\sigma_2^2 - \sigma_1^2}{\sigma_n^2 - \sigma_1^2})\sigma_1 > = -4\sigma_2 \). Since \( \frac{\sigma_2^2 - \sigma_1^2}{\sigma_n^2 - \sigma_1^2} < 1 \) and all \( \sigma_i > 0 \), the above condition always holds. \( \square \)
First, we observe that if $\sigma_1$ is very close to 0, the normal equations approach becomes arbitrarily faster than the augmented one, as long as $\sigma_2$ remains bounded away from 0. Second, it is not hard to see that $\tau = 1 + O(\sqrt{\sigma_2 - \sigma_1})$, which means that the two approaches become similar with highly clustered eigenvalues. In that case, however, using a block method would increase the gap ratios and the gains from the approach on $C$ would be larger again.

Most importantly, the above asymptotic convergence rates reflect optimal methods applied to $C$ and $B$, and an extraction of the best information from the subspaces. While for extremal eigenvalues near-optimal methods, such as those in PRIMME, coupled with the Rayleigh Ritz procedure can deliver this convergence, for interior problems practical Krylov methods have a hard time achieving this convergence and extracting the best eigenvectors from the subspace. Therefore, we expect in practice the normal equations to be significantly faster than any approach based on $B$.

2.4. Comparison of subspaces from LBD, JDSVD and an eigenmethod.
We extend the discussion on Lanczos to include the two native SVD methods. The relative differences between their convergence can be inferred by studying the subspace they build. A higher dimensional Krylov subspace implies faster convergence, if we assume eigenvector approximations can be extracted effectively from the subspace. We compare LBD, JDSVD, and Lanczos (or equivalently unpreconditioned GD) working on $C$ and on $B$.

Suppose $u_1, v_1$ are left and right initial guesses. After $k$ iterations ($2k$ matvecs), Lanczos working on the normal equations matrix $C$ builds:

\[ V_k = K_k(A^T A, v_1). \]

The LBD method builds both left and right Krylov spaces [14]:

\[ U_k = K_k(A A^T, A v_1), \quad V_k = K_k(A^T A, v_1). \]

The JDSVD method also builds two subspaces, each being a direct sum of two Krylov spaces of half the dimension [9]:

\[ U_k = K_{k/2}(A A^T, u_1) \oplus K_{k/2}(A A^T, A v_1), \quad V_k = K_{k/2}(A^T A, v_1) \oplus K_{k/2}(A^T A, A^T u_1) \]

Lanczos working on $B$ builds $K_k(B, [v_1; u_1])$ which does not correspond exactly to the spaces above in general. In the special case of $u_1 = 0$, the subspace is given below:

\[ \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} 0 \\ K_{k/2}(A^T A, v_1) \end{pmatrix} \oplus \begin{pmatrix} K_{k/2}(A A^T, v_1) \\ 0 \end{pmatrix}. \]

Clearly, Lanczos (or GD) working on $C$ and LBD build the same Krylov subspace for right singular vectors. The LBD method also builds the Krylov subspace for left singular vectors, and while that helps generate the bidiagonal projection, it does not improve convergence of LBD over Lanczos on $C$. On the other hand, Lanczos (or GD) on $B$ and JDSVD may generate a $k$ vector subspace, but this comes from a direct sum of Krylov spaces of $k/2$ dimension. Thus, they are expected to take twice the number of iterations of LBD in the worst case. The JDSVD subspace can also be richer than that of Lanczos on $B$ because JDSVD handles the left and right search spaces independently for arbitrary initial guesses.

Figure 2.1(a) demonstrates the relative convergence behavior of these unrestarted methods seeking the smallest singular value of a sample matrix. Only the outer
iteration of JDSVD is used (inner iterations = 1). The results agree with the above analysis. The convergence speed of LBD is the same as GD on C. JDSVD is slower than LBD or GD but faster than GD on B which is about twice as slow as LBD.

In practice, however, memory and computational requirements necessitate the restarting of these methods. Because LBD, JDSVD, and GD on B extract interior spectral information from the subspaces, critical directions may be dropped during restarting, causing significant convergence slow downs and irregular behavior. The use of harmonic or refined Ritz projections during restart help ameliorate this problem up to a point. However, the problem is still an interior one. In contrast, GD+1 (one of the nearly optimal methods in PRIMME) on C should see a far smaller effect on its convergence. This is because first, it solves an extreme eigenvalue problem, where the Rayleigh-Ritz projection results in optimal eigenvalue convergence, and second, it combines thick restarting with the locally optimal conjugate gradient directions to keep appropriate information during restart [38, 35].

Figure 2.1(b) reflects the above. Once restarting is used, GD+k is faster than any other method. The only disadvantage is the limited accuracy because of the squared conditioning of C. Therefore, a natural idea is to apply another phase to refine the accuracy until user requirements are satisfied. Instead of iterative refinement, we claim that a second stage eigensolver on B is more efficient.

3. Developing the two stage strategy. We develop primme_svds, a two-stage SVD meta-method that uses the suite of methods in PRIMME to first get a fast solution of the eigenvalue problem on C to the best accuracy possible, and then resolve the remaining accuracy with a PRIMME eigensolver on B. We discuss and automate issues of accuracy, convergence tolerance, initial guesses, interior eigenvalues of B, and how to apply preconditioning.

3.1. The first stage of primme_svds. Although an eigensolver on C can be much faster than other methods, the residual norms of the eigenvalues involve $\|C\| = \|A\|^2$. Thus achieving the required numerical accuracy may not be possible.

Let $(\sigma, u, v)$ be a targeted singular triplet of $A$ and $(\tilde{\sigma}, \tilde{v})$ the approximating Ritz
pair from an eigenmethod working on $C$. Using the approximation $\tilde{u} = A\tilde{v}/\tilde{\sigma}$, we can write the following four residuals:

\begin{equation}
    r_v = A\tilde{v} - \tilde{\sigma}\tilde{u}, \quad r_u = A^T\tilde{u} - \tilde{\sigma}\tilde{v}, \quad r_C = C\tilde{v} - \tilde{\sigma}^2\tilde{v}, \quad r_B = B\begin{bmatrix} \tilde{v} \\ \tilde{u} \end{bmatrix} - \tilde{\sigma}\begin{bmatrix} \tilde{v} \\ \tilde{u} \end{bmatrix}.
\end{equation}

Typically a singular triplet is considered converged when $\|r_v\|$ and $\|r_u\|$ are less than a given tolerance. Since our eigenvalue methods work on $C$ and $B$ we need to relate the above quantities. First, it is easy to see that $r_C = A^T(A\tilde{v}) - \tilde{\sigma}^2\tilde{v} = \tilde{\sigma}A^T\tilde{u} - \tilde{\sigma}^2\tilde{v} = \tilde{\sigma}r_u$. To relate to the norm of the residual of the second stage note that $\|r_B\|^2 = (\|r_v\|^2 + \|r_u\|^2)/(|\|\tilde{v}\|^2 + \|\tilde{u}\|^2)$. If the Ritz vector is normalized, $\|\tilde{v}\| = 1$, we also obtain $\|\tilde{u}\| = \|A\tilde{v}/\tilde{\sigma}\| = 1$ and $r_v = 0$. Bringing it all together (see also [41, 27]),

\begin{equation}
    \|r_u\| = \frac{\|r_C\|}{\tilde{\sigma}} = \|r_B\|\sqrt{2}.
\end{equation}

Given a user requirement $\|r_u\| < \delta \|A\|$, the normal equations and the augmented methods should be stopped when $r_C < \delta \tilde{\sigma} \|A\|$ and $r_B < \delta \|A\|/\sqrt{2}$ respectively. PRIMME’s stopping criterion is $\|r_C\| < \delta_c \|C\|$, so we must provide $\delta_c = \delta \tilde{\sigma}/\|A\|$. In floating point arithmetic this may not be achievable since $\|r_C\|$ can only be guaranteed to achieve $O(\|C\|\epsilon_{mach})$ [5]. Thus, the criterion for the normal equations becomes,

\begin{equation}
    \delta_C = \max(\delta \tilde{\sigma}/\|A\|, \epsilon_{mach}).
\end{equation}

As $\tilde{\sigma}$ is not known a priori, we modify slightly the PRIMME stopping criterion.

First, note that for the largest $\sigma_n$, $\delta_C = \delta$ and thus full residual accuracy is achievable with the normal equations. Since $\tilde{\sigma} \approx \sqrt{\tilde{\sigma}^2 - \tilde{\sigma}^2}$ based on the Bauer-Fike bound, $|\tilde{\sigma}^2 - \tilde{\sigma}^2| \approx |\sigma - \tilde{\sigma}|(2\tilde{\sigma}) \leq \|r_C\| < \delta_C \|A\|^2 = \tilde{\sigma}\delta \|A\|$ and thus $|\sigma - \tilde{\sigma}| \leq \delta \|A\|/2$ so the singular values are as accurate as can be expected.

This does not hold for smaller, and in particular the smallest few, eigenvalues. Thus, if the user requires $\delta < \|A\|\epsilon_{mach}/\tilde{\sigma}$, primme svds first makes full use of the first stage and then switches to the second stage working on $B$ to resolve the remaining accuracy of $O(\tilde{\sigma}/\|A\|) < \kappa(A)^{-1}$. For not too ill conditioned matrices, most of the time is then spent on the more efficient first stage.

A second, more subtle issue involves the accuracy of the Ritz vectors from $C$ which are used as initial guesses to $B$. We have observed that even though their residual norms are below the desired tolerance, the convergence of the interior eigenvalues in $B$ is sometimes (but not often) irregular, with long plateaus, and might not be able to reach machine precision. This occurs when the eigenvalues are highly clustered. On the other hand, it does not occur when only one eigenvalue is sought, which implies that it has to do with the sensitivity of interior eigenvalues to the nearby eigenvectors that we pass as initial guesses [30]. Therefore, before we start stage two, we perform a complete Rayleigh Ritz procedure with the converged eigenvectors of $C$. Providing the new Ritz vectors as initial guesses completely cures this problem.

To understand the problem as well as the solution, consider the decomposition of the smallest Ritz vector $\tilde{u}_1$ on the exact eigenvectors of $C$, $\tilde{u}_1 = c_1 u_1 + \sum_{i=2}^n c_i u_i$. On exit from the first stage, its residual satisfies $\|r_{\tilde{u}_1}\| < \|C\|\delta_C$, and from Bauer-Fike it also holds, $\sqrt{1-c_1^2} < \|C\|\delta_C$ and $c_i \leq \|C\|\delta_C$. Therefore, if we omit second and higher order terms, the Rayleigh quotient and the residual of $\tilde{u}_1$ can be written as:

\begin{equation}
    \mu = \frac{\tilde{u}_1^T A\tilde{u}_1}{\tilde{u}_1^T u_1} = \lambda_1 + \sum_{i=2}^n \frac{c_i}{c_1}^2 \lambda_i, \quad r_{\tilde{u}_1} = A\tilde{u}_1 - \mu\tilde{u}_1 \approx \sum_{i=2}^n c_i (\lambda_i - \lambda_1) u_i.
\end{equation}
As a result of the convergence behavior of iterative methods, the \( c_i \) tend to be larger for nearby eigenpairs, and fall drastically as \( i \) increases. Then, from (3.4), the accuracy of \( \mu \) is dominated by nearby \( (c_i/c_1)^2 \). The post-processing Rayleigh-Ritz uses the \( k \) nearby converged Ritz vectors, recomputes the projection with less floating point errors, and rearranges the directions to produce smaller \( c_i, i = 2, \ldots, k \), and thus better Ritz values. Of course, the additional Rayleigh-Ritz cannot improve the residual norms without the incorporation of new information in the basis. Even in floating point arithmetic, the improvements are minimal. This is evident also in (3.4) where \( r_{\tilde{u}_1} \) depends on the \( c_i \) linearly, so the effect of improving the nearby \( c_i \) is small. Figure 3.1 shows these effects on a matrix that presented the original problem.

In the second stage, the improvements on \( c_i \) translate to a starting search space of better quality, and thus better Ritz (or harmonic Ritz) pairs for the interior eigenvalue problem. The original PRIMME implementation includes a verification phase which checks if any converged eigenpairs have become slightly unconverged. If so, then it performs another Rayleigh-Ritz procedure on the restarted basis and repeats the algorithm. Therefore, it is only a minor modification to, based on a user input, force another Rayleigh-Ritz procedure before PRIMME exits. Algorithm 1 shows how the specific functionality needed for the first stage is given to PRIMME.

**Algorithm 1** Dynamic threshold adjusting and additional Rayleigh-Ritz in the first stage of primme_svd

1. Every iteration, PRIMME checks convergence based on an external function that obtains the current largest and targeted Ritz value \( \tilde{\sigma}_n \) and \( \tilde{\sigma}_i \)
2. if (target == largest or (target == smallest and \( \tilde{\sigma}_i < 1.0 \)) then
3.   adjust PRIMME’s \( \delta_C = \max (\delta_{\text{user}} \tilde{\sigma}_i/\tilde{\sigma}_n, \epsilon_{\text{mach}}) \)
4. else
5.   adjust PRIMME’s \( \delta_C = \max (\delta_{\text{user}}/\tilde{\sigma}_n, \epsilon_{\text{mach}}) \)
6. end if
7. If requested, perform Rayleigh-Ritz on the returned vector basis

---

**Fig. 3.1.** The cosine of angles \( (c_i = \tilde{u}_i^T u_i, i = 2, \ldots, 19) \) between the smallest exact eigenvectors and the smallest Ritz vector before and after pre-processing. The table compares the accuracy of the Rayleigh quotient and the residual norm for \( \tilde{u}_1 \) before and post-processing for matrix jagmesh8.
3.2. The second stage of primme_svds. We argue that solving an eigenvalue problem on matrix $B$ with an approximate eigenspace as initial guess is a better approach than iterative refinement [12, 13] for the following reasons. First, with iterative refinement, eigenvectors are improved one by one without any synergy from the nearby subspace information. In contrast, a good quality eigensolver, such as those in PRIMME, provides global convergence to all desired pairs. Second, an inner-outer eigensolver such as JDQMR stops the inner linear solver dynamically and near-optimally to avoid exiting too early (which increases the number of outer iterations) or iterating too long (which increases the number of inner iterations). We are not familiar with similar implementations for iterative refinement. Third, iterative refinement for clustered interior eigenvalues may not be able to converge to the desired high accuracy due to the lack of proper deflation strategies [43], both at the linear solver and at the outer iteration. Naturally, a well designed eigensolver that employs locking and blocking techniques is more robust to address these problems. Finally, we point out that the correction equation of the Jacobi-Davidson method applied on $B^T$,

$$(I - w w^T)(B^T - \mu I)(I - w w^T)i = \tilde{\sigma}w - B^Tw,$$

where $w^T = [u^Tv^T]$ is equivalent to the iterative refinement proposed in [12] ([9]). Therefore, JDQMR enjoys the benefits of both eigensolvers and iterative refinement.

PRIMME inserts any available initial guesses to its search space and if the guesses are less than the minimum restart size, fills the rest of the positions with a Lanczos space from a random vector to guard against extremely bad guesses. Because this is not true for the second stage, we have modified the Lanczos space to start from the first blocked targeted eigenvalue. Because of irregular convergence of interior eigenvalue problems, sometimes eigenvector approximations that were introduced initially in the search space but have not been targeted yet may degrade in quality or even be displaced. For this reason, when an eigenvector converges and is locked out of the search space, we re-introduce the initial guess of the next vector to be targeted. This resulted in significant improvement in robustness and often in convergence speed.

PRIMME provides remarkable flexibility for seeking interior eigenvalues. It accepts multiple shifts and provides three different ways to select an interior Ritz value: closest in absolute value to each shift (primme\_closest\_abs), or left or on the right of each shift. Because of the very good accuracy of eigenvalue approximations from $C$, the primme\_closest\_abs option is more effective at selecting the proper Ritz value during the outer iterations. More importantly, with such accurate shifts, the correction equation in JDQMR often returns the exact correction to the eigenvector after the solution of only one linear system. In the case of ill-conditioned matrices, where the shifts from the first stage are less accurate, GD+k may be preferable for the second stage because it provides better global convergence to nearby eigenvalues. However, it is computationally more expensive per iteration than JDQMR [37].

For interior eigenvalues, the Rayleigh-Ritz procedure does not have the same optimality as for extreme eigenvalues, causing the convergence to be irregular. In the GD+k method with sufficiently large search space, such problems are transient and do not affect the convergence and overall speed of the method. This is why PRIMME only implemented the Rayleigh-Ritz method originally. In the second stage of primme_svds, the availability of accurate initial guesses and shifts calls for the JDQMR method. For this method, spurious Ritz values can cause Ritz vectors to fail to converge [34]. The effect can be detrimental also during restart where major eigenvector components may be discarded and need to be recovered [29, 30, 31]. The problem is accentuated in the maximally indefinite case of SVD problems.
We addressed this problem by extending PRIMME’s functionality to include the refined projection that minimizes the residual \( \|BVy - \tilde{\sigma}Vy\| \) over the search space \( V \) and for a given \( \tilde{\sigma} \) [33, 34]. Because the shifts \( \tilde{\sigma} \) are very accurate, a harmonic Ritz procedure is not necessary, and the refined one is expected to give the best approximation for the targeted eigenpair. Our refined projection method is similar to the one in [10] and [29] that produces refined Ritz vectors for all the required eigenvectors (not just the closest to \( \tilde{\sigma} \)). Since \( \tilde{\sigma} \) remains constant, there is no need to perform a QR factorization of \( BV - \tilde{\sigma}V \) at every step. Instead, as part of Gram-Schmidt, we add one more column to the orthonormal matrix \( Q \) and to the matrix \( R \).

A full QR factorization is only needed at restart. Then, following [34], we compute the refined Ritz vectors by solving the small SVD problem with \( R \), and replace the targeted Ritz value with the Rayleigh quotient of the first refined Ritz vector.

Algorithm 2 PRIMME enhancements and special algorithmic choices needed for the second stage of primme_svds

```
1: Initial shifts \( \tilde{\sigma}_i \), initial vectors \([\tilde{v}_i; A\tilde{v}_i/\tilde{\sigma}_i], i = 1, ..., k qr.full = 1\)
2: Build an orthonormal basis \( V \) of \([K_{m-k}(B, \tilde{v}_1), \tilde{v}_i] \). Set \( t \) as the Lanczos residual
3: while all \( k \) eigenvalues have not converged do
4:   Orthonormalize \( t \) against \((v_i)_{i=1}^{m-1} \). Update \( v_m = t, w_m = Bv_m, H_{:,m} = VTw_m \)
5:   if \( qr.full == 1 \) then
6:      \( W - \tilde{\sigma}_1V = QR, \; qr.full = 0 \)
7:   else
8:      During orthogonalization perform one-column QR updating
9:   end if
10:  Compute eigendecomposition \( H = S\Theta S^T \) with \( \theta_j \) ordered by closeness to \( \tilde{\sigma}_1 \)
11:  Compute SVD decomposition of \( R = U\Sigma S^T \), Rayleigh quotient \( \theta_1 = s_1^T H s_1 \)
12:  If \( (\sigma_i, [v_i; u_i]) \) converged, lock, and re-introduce \([\tilde{v}_{i+1}; A\tilde{v}_{i+1}/\tilde{\sigma}_{i+1}] \) into \( V \)
13:  If restarting, set \( qr.full = 1 \)
14:  Obtain the next vector \( t = Prec(r) \) (typically with JDQMR)
15: end while
```

Solving the small SVD problem for only one shift per iteration reduces the cost of the refined procedure considerably, making it similar to the cost of computing the Ritz vectors. However, the quality of other refined Ritz vectors reduces with the distance of their Rayleigh quotient from \( \tilde{\sigma} \), so they may not be as effective in a block algorithm. Nevertheless, these approximations have the desirable property of monotonic convergence as claimed in [10, 29] and also observed in our experiments. This added robustness for JDQMR more than justifies the small additional cost. Algorithm 2 shows all these second stage changes in the context of PRIMME.

### 3.3. Outline of the implementation.

We first developed PRIMME MEX, a MATLAB interface for PRIMME. This exposes the full functionality of PRIMME to a broader class of users, who can now take advantage of MATLAB’s built-in matrix times block-of-vectors operators and preconditioners. Its user interface is similar to MATLAB `eigs` allowing it to be called not only by non-expert users but also by experts that can adjust over 30 parameters. The meta-method `primes_svds` was then implemented as a MATLAB function on top of PRIMME MEX. This allowed flexibility for algorithmically tuning the two stages. Many of the enhancements, such as the refined projection method or a user provided stopping criterion, were implemented directly in PRIMME and will be part of its next release, which will also include a
native C implementation of primme_{svds}.

Algorithm 3 primme_{svds}: a hybrid two stage method for SVD

1: Set up the problem and call PRIMME through the PRIMME_MEX function
   Use enhancements of Algorithm 1.
2: if (target == smallest) then
3:   Form shifts and initial guesses for $B$ from the approximations of $C$
4:   Call PRIMME for interior eigenvalues of $B$ through PRIMME_MEX function.
   Use enhancements of Algorithm 2.
5: end if
6: Return converged desired singular triplets to user

Algorithm 3 summarizes the primme_{svds} without considering preconditioning. At a minimum, users must provide the input matrix $A$, or function pointers that perform matrix-vector operations with $A$ and $A^T$, or directly with $B$ and/or $C$. Then, primme_{svds} sets up the matrix-vector functions for PRIMME. By default, the first stage uses the PRIMME DYNAMIC method to decide between GD+k and JDQMR, and the second stage uses JDQMR. But users can set different eigenmethods for each stage just as they can tune any of PRIMME’s parameters. We form the initial guesses for the second stage as $[\tilde{v}_i, \tilde{u}_i]$, where $(\tilde{\sigma}_i^2, \tilde{v}_i)$ are the approximate eigenpairs from $C$, and $\tilde{u}_i = \frac{1}{\tilde{\sigma}_i} A^T \tilde{v}_i$. When the singular value is extremely small or even zero, the first stage provides low or no accuracy to $\tilde{u}_i$. In this extreme case, it is better to choose $\tilde{u}_i$ as a random vector and orthogonalize it to other left singular vectors computed after the first stage. For tiny and highly clustered singular values, we suggest that the first stage uses locking and block methods that are both available in PRIMME.

4. Preconditioning in primme_{svds}. The shift-and-invert technique is sometimes thought of as a form of preconditioning. If a direct factorization of the matrix $A, C$ or $B$ is possible, this is often the method of choice for highly indefinite or highly clustered extreme eigenproblems. For smallest singular values, the MATLAB svds relies solely on shift and invert ARPACK [46] using the LU factorization of $B$. PROPACK follows a similar strategy on $C$, but uses QR factorization. However, as pointed out in [27], for rectangular matrices svds often converges to the zero eigenvalues of $B$ rather than the smallest singular value. Our method can also be used in shift-and-invert mode, assuming the user provides the inverted operator as a matrix-vector. For large matrices, however, preconditioners become a necessary alternative.

JDSVD accepts a preconditioner for a square matrix $A$ or, if $A$ is rectangular, leverages a preconditioner for $B - \tau I$ [9]. SVDFF is combined with the robust incomplete factorization (RIF) method [28] to provide a preconditioner directly for $C - \tau I$ [27]. The advantage is that it works seamlessly for both square and rectangular matrices, but RIF may not be the best choice of preconditioner.

primme_{svds} accepts any user-provided preconditioning operator. In the most general form, any preconditioner directly for $C$ or $B$ can be used. When $M \approx A$ is available (e.g., the incomplete LU factorization of a square matrix), primme_{svds} forms $M^{-1}M^{-T}$ and $[0, M^{-1}; M^{-T}, 0]$ as the preconditioning operators for PRIMME for the different stages. Moreover, if a preconditioner such as RIF is given $M \approx C^{-1}$, we can build preconditioners for the second stage as $[0, AM; MA^T, 0]$. It is not clear in general how to form a preconditioner for $C$ from a preconditioner of $B$. 

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4.1. A dynamic two stage method with preconditioning. The analysis in Sections 2.3 and 2.4 holds for Krylov methods but it is less meaningful with preconditioners. Clearly, if two different preconditioners are provided for $C$ and $B$ their relative strengths are not known by primme_svds. But we have also noticed cases where the first stage benefits less than the second stage when a less powerful preconditioner $M$ for $A$ is used to form preconditioners for both $C$ and $B$. If $M$ is ill-conditioned but its near-kernel space does not correspond well to that of $A$, it may work for $B$, but taking $M^TM$ produces an unstable preconditioner for $C$ [42]. On the other hand, with a sufficiently good preconditioner, both methods enjoy similar benefits on convergence. If the relative strengths of the provided preconditioner are known, users can choose the two-stage approach or only one of the stages (e.g., the second one). For the general case, we present a method that, based on runtime measurements, switches dynamically between the normal equations and the augmented approach to identify the most effective one for the given preconditioning. This is shown in Algorithm 4.

To estimate the convergence of the two approaches, we run a set of initial tests alternating between running on $C$ and on $B$. Because JDQMR relies on good initial guesses which are not available initially, the dynamic algorithm uses only the GD+k method. Once the algorithm decides on the approach, other PRIMME methods can be used as specified by the user. Without loss of generality, we only consider GD+k for our dynamic primme_svds experiments. The approximations obtained from one run are passed as initial guesses to the next run.

We estimate the convergence rate by measuring the average reduction per iteration of the residual norm. To be able to capture the convergence at different phases of the iterative method, we must switch between the two approaches several times. However, switching too frequently incurs a lot of overhead (rebuilding the initial basis, performing extra Rayleigh-Ritz procedures, and possibly convergence loss from restarting the search space). Switching too infrequently may be wasteful when the preconditioner for $C$ does not work well. Thus, we control the maximum number of iterations for the next GD+k run, $maxIter$. This number is always larger than $initIter$ which is a reasonably small number, i.e., 50. If the same approach is chosen in two successive runs, $maxIter$ doubles. If the approach should be switched, $maxIter$ is reduced more aggressively for the next run (Step 12) to avoid wasting too much time on the wrong approach. On the other hand, if one eigenvalue converges in the initial tests or at least two eigenvalues converge later, we stop the dynamic switching and choose the currently faster approach. If the faster approach is on the normal equations, a two-stage method might be necessary to get to full accuracy. Although two or three switches typically suffice to distinguish between approaches, we also limit the number of switches.

5. Numerical experiments. Our first two experiments use diagonal matrices to demonstrate the principle of the two stage method and that the method can compute artificially clustered tiny singular values to full accuracy. Then, we conduct an extensive set of experiments for finding the smallest singular values of several matrices. Large singular values are also computed under the shift-invert setting. The matrix set is chosen to overlap with those in other papers in the literature. We compare against several state-of-the-art SVD methods: JDSVD [9, 10], SVDIFP [27], IRRHLB [18], IRLBA [14], and MATLAB’s svds. First, we compute a few of the smallest singular triplets on both square and rectangular matrices without a preconditioner. Then we show a performance comparison between the two stage primme_svds method and its dynamic version with different quality of preconditioners. Subsequently, we demon-
Algorithm 4 Dynamic switching between stages for preconditioned primme\textunderscore svds

1: Set $\text{initIter}$, $\text{maxSwitch}$
2: $\text{numSwitch} = \text{numConverged} = j = 0$, $\text{maxIter} = \text{initIter}$, Undecided = true
3: Run $\text{initIter}$ iterations of GD+k on $C$ and on $B$ and collect initial average convergence rate of both approaches.
4: while ($\text{numSwitch} < \text{maxSwitch}$ and Undecided) do
5: Choose estimated faster approach ($C$ or $B$) for next call
6: if ($\text{numSwitch} == 0$ and $\text{numConverged} > 0$) or $\text{numConverged} > 1$ then
7: undecided = false (Choose faster approach and no more switching)
8: else
9: if Same approach is chosen again then
10: $j = j + 1$; $\text{maxIter} = \text{initIter} \times 2^j$
11: else if Different approach is chosen then
12: $j = \text{floor}(j/2)$; $\text{maxIter} = \text{initIter} \times 2^j$
13: end if
14: end if
15: $\text{numSwitch} = \text{numSwitch} + 1$
16: Call PRIMME with $\text{maxIter}$ and current chosen approach
17: end while
18: if All desired singular triplets are found on $B$ then
19: Return final singular triplets to users
20: else if All desired singular triplets are found on $C$ then
21: Return resulting singular triplets to augmented approach
22: else if Faster approach is on $C$ then
23: Proceed with the two-stage approach
24: else if Faster approach is on $B$ then
25: Continue only with the augmented approach
26: end if

strate that primme\textunderscore svds provides faster convergence with a good preconditioner compared with JDSVD and SVDIFP. We also show that primme\textunderscore svds achieves better performance than svds and SVDIFP using shift-and-invert. Finally, we present some numerical results on a real-world problem.

All computations are carried out on a DELL dual socket with Intel Xeon processors at 2.93GHz for a total of 16 cores and 50 GB of memory running the SUSE Linux operating system. We use MATLAB 2013a with machine precision $\epsilon = 2.2 \times 10^{-16}$ and PRIMME is linked to the BLAS and LAPACK libraries available in MATLAB. Our stopping criterion is for the left and right residuals to satisfy,

\begin{equation}
\sqrt{\|r_u\|^2 + \|r_v\|^2} < \|A\|\delta_{\text{user}}.
\end{equation}

For JDSVD we use the refined projection method as it performed best in our experiments, which is also consistent with [9]. We choose the default for all parameters except for setting ‘krylov = 0’ to avoid occasional convergence problems for smallest singular values. SVDIFP is a recent method and its MATLAB implementation is still under development. Its maximum number of inner iterations can be chosen as fixed or adaptive. We run with both choices and report the best result. Also, we use singular triplet residuals as the stopping criterion for SVDIFP instead of the default residual of the normal equations. For IRLBA and IRRHLB, we choose all default parameters as suggested in the code.
All methods start with the same initial guess, \texttt{ones(min(m,n),1)}, except for matrix lshp3025 for which a random guess is necessary. We set the maximum number of restarts to 5000 for IRRHLB and IRLBA and to 10000 for JDSVD and primme\_svds. Since SVDIFP can only set a maximum number of iterations for each targeted singular triplet, we report that SVDIFP cannot converge to all desired singular values if its overall number of matrix-vector operations is larger than \((\text{maxBasisSize} - k) \times 5000\). For primme\_svds, we set \text{maxBasisSize}=35, \text{minRestartSize}=21 and experiment with two \(\delta\) tolerances, 1e-8 and 1e-14. For \(\delta = 1\text{e-8}\), primme\_svds does not need to enter the second stage for any of our tests. Since the numbers of matrix-vector products with \(A\) and \(A^T\) are the same, the tables report as “MV” the number of products with \(A\) only. “Sec” is the run time in seconds, and “–” means the method cannot converge to all desired singular values or that the code breaks down. For the first stage of primme\_svds we use the GD\_Olsen\_PlusK method. For the second stage, we run experiments with both GD\_PlusK and JDQMR. Since our implementation is mainly in C, we focus on comparing the number of matrix-vector operations as the primary measurement of the performance. However, we also report execution times which is relevant since matrix-vector, preconditioner, and all BLAS/LAPACK operations are performed by the MATLAB libraries.

5.1. Primme\_svds for clustered tiny singular values. We illustrate first how our two-stage method works in a seamless manner. We consider a diagonal matrix \(A = \text{diag}([1:10,1000:100:1\text{e}6])\) and the preconditioner \(M = A + \text{rand}(1,10000) \times 1\text{e}4\). In Figure 5.1, the green and black lines show the convergence behaviors of PRIMME on \(B\) and \(C\) respectively. Indeed, the convergence on \(B\) is very slow due to a highly indefinite problem while the accuracy on \(C\) is limited and stagnates when reaching its limit. The two stage primme\_svds combines the benefits of the two methods, and determines the smallest singular efficiently and accurately as the magenta line shows.

![Fig. 5.1. An example to show how two stage of primme\_svds works seamlessly for seeking smallest singular values accurately](image)

Next we show how primme\_svds can determine several clustered tiny singular
values. Consider the matrix $A = \text{diag}(\{1e-14, 1e-12, 1e-8:1e-8:4e-8, 1e-3:1e-3:1\})$ with identity matrix as a preconditioner. Although locking may be able to determine clustered or multiple singular values, we increase robustness by using a block size of two in PRIMME, for the first stage only. We set the user tolerance $\delta_{\text{user}} = 1e-15$ to examine the ultimate accuracy of primme svds. As shown in Table 5.1, primme svds is capable of computing all the desired clustered, tiny singular values accurately.

### Table 5.1

| Singular values | true value | primme svds | residuals |
|-----------------|------------|-------------|-----------|
| $\sigma_1$      | 1e-14      | 9.952750930151887E-15 | 4.9E-16   |
| $\sigma_2$      | 1e-12      | 1.000014102726476E-12 | 8.9E-16   |
| $\sigma_3$      | 1e-8       | 1.0000000003582006E-08 | 6.5E-16   |
| $\sigma_4$      | 2e-8       | 2.0000000002073312E-08 | 9.2E-16   |
| $\sigma_5$      | 3e-8       | 3.000000000893043E-08 | 9.0E-16   |
| $\sigma_6$      | 4e-8       | 4.000000000192591E-08 | 9.2E-16   |
| $\sigma_7$      | 1e-3       | 1.000000000000025E-03 | 9.7E-16   |
| $\sigma_8$      | 2e-3       | 1.999999999999956E-03 | 8.1E-16   |
| $\sigma_9$      | 3e-3       | 2.999999999999997E-03 | 9.1E-16   |
| $\sigma_{10}$   | 4e-3       | 3.999999999999958E-03 | 9.8E-16   |

### 5.2. Without preconditioning.

We compare two variants of primme svds with four methods, JDSVD, SVDIFP, IRRHLB, and IRLBA on both square and rectangular matrices without preconditioning. Since a good preconditioner is usually not easy to obtain for SVD problems, it is important to examine the effectiveness of a method in this case. We compute the $k = 1, 3, 5, 10$ smallest singular triplets. In order to speed up convergence, $k + 3$ eigenvalues are computed when $k$ desired eigenvalues are required in svds. A similar strategy is applied to IRRHLB and IRLBA. For primme svds, we found this is not necessary.

We select six square and six rectangular matrices from other research papers [18, 27] and the University of Florida Sparse Matrix Collections [45]. Table 5.2 lists these matrices along with some of their basic properties. Among them, the matrices pde2961, dw2048, well1850 and lp_ganges have relative larger gap ratios and smaller condition number, and thereby are easy ones. Matrices fidap4, jagmesh8, wang3, deter4, and plldb are hard cases, and matrices lshp3025, ch, and lp_bul2 are very hard ones. We expect all methods to perform well for solving easy problems. Harder problems tend to magnify the difference between methods.

Tables 5.3, 5.4, 5.5 and 5.6 show that primme svds variants converge faster and more robustly than all other methods on both square and rectangular matrices. Specifically, table 5.3 shows that for moderate accuracy the normal equations solved with a PRIMME method are significantly faster. For instance, primme svds is generally at least two or three times faster than other methods when solving hard problems for any number of smallest singular values. When solving easy problems, primme svds is still several times faster than JDSVD, SVDIFF, and IRLBA. IRRHLB can be competitive with our method only when seeking 10 singular values on easy cases. This is typical behavior of the Lanczos method when looking for a large number eigenvalues [36]. The superiority of primme svds is achieved as a result of the near-optimal properties of the eigenmethods in PRIMME [35]. We have noticed that even for moderate accuracy, JDSVD, SVDIFF, IRRHLB and IRLBA are all challenged by hard problems, where they are often inefficient or even fail to converge to all desired singular values.
Table 5.2
Properties of the test square and rectangular matrices, where $\gamma_m(k) = \min_{i=1}^k (\text{gap}(\sigma_i))$, and $\text{gap}(\sigma_i) = \min_{j \neq i} |\sigma_i - \sigma_j|$

| Matrix         | pde2961 | dw2048 | fidap4 | jagmesh8 | wang3 | lshp3025 |
|----------------|---------|--------|--------|----------|-------|----------|
| order          | 2961    | 2048   | 1601   | 1141     | 26064 | 3025     |
| $\text{nnz}(A)$| 14585   | 10114  | 31387  | 7465     | 77168 | 120833   |
| $\kappa(\|A\|_2)$| 9.5e2   | 5.3e3  | 5.2e3  | 5.9e4    | 1.1e4 | 2.2e5    |
| $\gamma_m(1)$  | 8.2e-3  | 2.6e-3 | 1.5e-3 | 1.7e-3   | 7.4e-5| 1.8e-3   |
| $\gamma_m(3)$  | 2.4e-3  | 2.9e-4 | 2.5e-4 | 1.6e-3   | 1.9e-5| 9.1e-4   |
| $\gamma_m(5)$  | 2.4e-3  | 2.9e-4 | 2.5e-4 | 4.8e-5   | 1.9e-5| 1.8e-4   |
| $\gamma_m(10)$ | 7.0e-4  | 1.6e-4 | 2.5e-4 | 4.8e-5   | 6.6e-6| 2.2e-5   |

| Matrix         | well1850 | lp_ganges | deter4 | plddb | ch | lp_bn12 |
|----------------|----------|-----------|--------|-------|----|--------|
| rows $m$:      | 1850     | 1309      | 3235   | 3049  | 3700| 2324   |
| cols $n$:      | 712      | 1706      | 9133   | 5069  | 8291| 4486   |
| $\text{nnz}(A)$| 8755     | 6937      | 19231  | 10839 | 24102| 14996  |
| $\kappa(\|A\|_2)$| 1.1e2   | 2.1e4     | 3.7e2  | 1.2e4 | 2.8e3| 7.8e3  |
| $\gamma_m(1)$  | 3.0e-3  | 1.1e-1    | 1.1e-1 | 4.2e-3 | 1.6e-3| 7.1e-3 |
| $\gamma_m(3)$  | 3.0e-3  | 4.5e-2    | 3.1e-4 | 5.1e-5 | 7.7e-4| 4.8e-3 |
| $\gamma_m(5)$  | 3.0e-3  | 2.4e-3    | 8.9e-5 | 5.1e-5 | 3.6e-4| 1.1e-3 |
| $\gamma_m(10)$ | 2.6e-3  | 8.0e-5    | 8.9e-5 | 2.0e-5 | 4.0e-5| 1.1e-3 |

Table 5.4 shows smaller differences between methods, reflecting the slower convergence of the augmented method in stage two. We see that the two variants of primme_svd have comparable number of matrix-vector operations, but the JDQMR one typically requires less time if the matrix is sparse enough [35]. For computing 10 eigenpairs, IRRHLB shows a small edge in the number of iterations for two easy cases. However, primme_svd method never misses eigenvalues, is consistently much faster than all other methods, and significantly faster than IRRHLB in the hard cases. Note the slow convergence of JDSVD, since it relies on the augmented matrix to produce all the required accuracy. SVDIFP is also not competitive, partly due to its inefficient restarting strategy. Clearly, demanding higher accuracy for the hard problems does not help the rest of the methods. Note that because of PRIMME’s high quality implementation, not only does primme_svd enjoy better robustness but it is also ten times faster than IRRHLB for the cases where IRRHLB takes fewer MVs.

Tables 5.5 and 5.6 show that the advantage of primme_svd is even more significant on rectangular matrices. For example, except for the two easy problems well1850 and lp_ganges, primme_svd is often five or ten times faster than the other methods. The reason is two-fold. First, primme_svd works on $C$ with dimension $\min(m, n)$, which saves memory and computational costs. SVDIFP also shares this advantage. Second, PRIMME’s advanced restarting techniques exploits the convergence optimality of exterior eigenvalues of the matrix $C$. Interestingly, JDQMR converges much faster than GD+k on some hard problems such as plddb, ch and lp_bn12 in table 5.6. The reason is the availability of excellent shifts from the first stage. We conclude that primme_svd is the fastest method and sometimes the only method that converges for hard problems without preconditioning.

5.3. With preconditioning. What is remarkable from the previous Tables 5.3 to 5.6 is the difficulty of solving for the smallest singular values, even for small matri-
ces. Preconditioning is a prerequisite for addressing larger, practical problems, which limits our choice to primme_svds, JDSVD and SVDIFP.

We first compare our two stage method and our dynamic two-stage method for two different quality preconditioners. We choose \( M = LU \), the factorization obtained from MATLAB’s ILU function on a square matrix \( A \) with parameters ‘type=ilutp’, ‘thresh=1.0’, and varying ‘droptol=1e-2’ or ‘droptol=1e-3’. Given these two \( M \), we form the preconditioners for primme_svds as \( M^{-1}M^{-T} \) and \( [0 M^{-1}; M^{-T} 0] \). Without loss of generality, primme_svds chooses GD+k eigenmethod for the underlying eigensolver PRIMME. We seek ten smallest singular values with tolerance 1e-14.

As shown in Table 5.7, both variants of primme_svds can solve the problems effectively with a good preconditioner (‘droptol=1e-3’). In this case, the static two stage method is always better than the dynamic one because of the overhead incurred by switching between the two methods. On the other hand, when using the preconditioner with ‘droptol=1e-2’, the two stage primme_svds is slower than the dynamic in some cases, and in the case of lshp3025, much slower. The reason is the inefficiency of the preconditioner in the normal equations. Our dynamic primme_svds can detect the convergence rate difference and choose the faster method to accomplish the remaining computations. Of course, if this issue is known beforehand, users can bypass the dynamic heuristic and call directly the second stage.

Next, we compare the two stage primme_svds with JDSVD and SVDIFP when a good quality of preconditioner is available. Except for preconditioning, all other parameters remain as before. For the first preconditioner we use MATLAB’s ILU on a square matrix \( A \). For the second preconditioner we use the RIF MEX function provided in [27] on a rectangular matrix with ‘droptol=1e-3’. The resulting RIF factors \( LDL^T \approx A^T A \), where \( D \) is diagonal matrix with 0 and 1 elements, are used to construct the pseudoinverses \( M^{-1} = L^{-T}L^{-1}A^T \) and \( M^{-T} = AL^{-T}L^{-1} \) for preconditioning the second stage of primme_svds and JDSVD. In the SVDIFP code, there is an input parameter ‘COLAMD’ which computes approximate column minimum degree permutation to obtain sparser LU factors. This technique can be applied to other methods but some modifications are needed. Therefore, we disable this parameter in the SVDIFP code. For the JDSVD code, we try both enabling and disabling the initial Krylov subspace and report the best result.

Tables 5.8 and 5.9 show that a good preconditioner makes the problems tractable, with all three methods solving the problems effectively. Still, in most cases primme_svds provides much faster convergence and execution time on both square and rectangular matrices. We see that when seeking one smallest singular value with high accuracy, JDSVD takes less iterations for one square matrix (wang3), and SVDIFP is competitive in two rectangular cases (plddb and lp_ban2). This is because these cases require very few iterations, and the first stage of primme_svds forces a Rayleigh-Ritz with 21 extra matrix-vector operations. This robust step is not necessary for this quality of preconditioning. If we are allowed to tune some of its parameters (as we did with JDSVD and SVDIFP) primme_svds does require fewer iterations even in these cases.

5.4. With the shift and invert technique. Shift and invert is also applicable to PRIMME and primme_svds. Moreover, because it turns the eigenvalues closest to the shift to a largest eigenvalue problem, there is no need for the second stage. SVDIFP can utilize shift and invert operator as a preconditioner. Therefore, we report results on primme_svds, SVDIFP, and svds. svds, uses shift and invert operator on the augmented matrix \( B \). For primme_svds and SVDIFP we use two different factorizations, an LU and a QR factorization of the matrix \( A \). Since svds uses a
basis size of 40 for seeking 10 smallest singular values, we give the same basis size to primme_svdps and SVDIFP. Also, we disable the ‘COLAMD’ option in SVDIFP. For SVDIFP the shifts are all zeros, for svds we give a shift of 1e-8, and there is no need of shifts for primme_svdps due to an extreme eigenvalue problem. We have instrumented the MATLAB native svds code to return the number of iterations. To facilitate comparisons, we include the LU and QR factorization times in the running times of all methods, but also report them separately. The tolerance is $\delta = 1e-10$, and primme_svdps uses the DYNAMIC method that switches between GD+k and JDQMR to optimize performance.

Table 5.10 shows that primme_svdps is faster than svds both in convergence and execution time, partly because it works on C which is smaller in size and allows for faster convergence. primme_svdps is much faster than SVDIFP due to its more efficient restarting strategy, and also because an inverted operator may not be as effective when used as a preconditioner. Note that svds does not work well on rectangular matrices because $B$ becomes singular and cannot be inverted, and if instead a small shift is used, it finds the zero eigenvalues of $B$ first.

5.5. With real-world problems. We use primme_svdps, SVDIFP, and JDSVD to compute the smallest singular triplet of matrices of order larger than 1 million. Some information on these matrices appears in Table 5.11. We apply the two-stage primme_svdps(JDQMR) on all test matrices except thermal2, which is solved by dynamic preconditioning primme_svdps. The preconditioners are applied similar to our previous experiments with the exception that ILU uses ‘thresh=0.1’, and ‘udiag=1’. The tolerance is $\delta = 1e-12$. The symbol ‘*’ means the method returns results that either did not satisfy the desired accuracy or did not converge to the smallest singular triplet.

Table 5.12 shows the results without or with various preconditioners. Debr is a numerically singular square matrix. primme_svdps is capable of resolving this more efficiently than JDSVD, while SVDIFP returns early when it detects that it is not likely to converge to the desired accuracy for left singular vector [27]. All methods easily solve problem cage14 with ILU(0), but primme_svdps is much faster. Thermal2 is an ill-conditioned matrix, whose preconditioner turns out to be less effective for $C$ than for $B$. Therefore, SVDIFP has much slower convergence than JDSVD. Thanks to the dynamic scheme, primme_svdps recognizes this deficiency and converges without too many additional iterations, and with the same execution time as JDSVD. However, if we had prior knowledge about the preconditioner’s performance, running only at the second stage gives almost exactly the same matrix-vectors as JDSVD and much lower time. Reducing further the overhead of the dynamic heuristic is part of our current research. JDSVD often fails to converge to the smallest singular value for rectangular matrices since it has difficulty to distinguish them from zero eigenvalues of $B$, as shown in the cases sls and Rucci1. For matrix sls, SVDIFP misconverges to the wrong singular triplet while primme_svdps is successful in finding the correct one. SVDIFP and primme_svdps have similar performance for solving problem Rucci1. In summary, primme_svdps is far more robust and more efficient than either of the other two methods for large problems.

6. Conclusion. Based on the state-of-the-art eigensolver PRIMME, we have developed a full functionality, high quality SVD solver for a few smallest or largest singular values of a large matrix. The key is a two stage meta-method, primme_svdps, that in the first stage solves the normal equations as a fast way to get sufficiently accurate approximations, and if further accuracy is needed, solves an interior eigen-
value problem from the augmented matrix. In addition, we have presented several enhancements to the PRIMME eigensolver that allow for an efficient computation of the interior eigenproblem. We have motivated the merit of this approach theoretically, and confirmed its performance through an extensive set of experiments. primme svds improves on convergence and robustness over other state-of-the-art singular value methods, but most importantly it is based on a highly optimized production software that allows its use, with or without preconditioning, in large real world problems. Currently, primme svds is available in MATLAB through the MEX interface, and we are planning to release it in the near future. A native C implementation of primme svds as part of PRIMME is planned next.

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Table 5.3

Seeking 1, 3, 5, and 10 smallest singular triplets of square matrices with user tolerance $1e^{-8}$. The primme\_svds method has two variants: primme\_svds(GD+k) uses GD+k eigenmethod while primme\_svds(JDQMR) uses JDQMR eigenmethod respectively in the second stage.

| $k$ | Method              | $\delta = 1e^{-8}$ Matrix: pde2961 |          | dw2048 |          | fidap4 |          |
|-----|---------------------|------------------------------------|----------|--------|----------|--------|----------|
| 1   | primme\_svds(1st stage only) | 2165  1.8                        | 1766  1.2                         | 4750  3.2                         |        |         |
| 1   | JDSDV               | 2460  4.8                        | 3840  3.1                         | 4379  3.8                         |        |         |
| 1   | SVDIFP              | 3433  7.9                        | 2520  2.7                         | 11572 13.3                        |        |         |
| 1   | IRRHLB              | 3755  44.6                       | 3228  35.1                        | 8839  97.9                        |        |         |
| 1   | IRLBA               | 12292 8.7                        | 7684  3.3                         | 47332 20.3                        |        |         |
| 3   | primme\_svds(1st stage only) | 2643  2.2                        | 2135  1.5                         | 5661  3.8                         |        |         |
| 3   | JDSDV               | 7195  8.3                        | 5776  4.8                         | 14334 12.7                        |        |         |
| 3   | SVDIFP              | 11466 29.6                       | 12123 14.7                        | 26285 28.7                        |        |         |
| 3   | IRRHLB              | 3718  44.6                       | 3225  36.1                        | 14303 156.2                       |        |         |
| 3   | IRLBA               | 14676 9.9                        | 7656  4.1                         | 69456 38.5                        |        |         |
| 5   | primme\_svds(1st stage only) | 3118  2.6                        | 2431  1.7                         | 6890  5.4                         |        |         |
| 5   | JDSDV               | 2460  12.2                       | 7514  8.1                         | 16270 16.3                        |        |         |
| 5   | SVDIFP              | 17272 46.4                       | 17564 21.8                        | 45560 51.8                        |        |         |
| 5   | IRRHLB              | 4301  53.8                       | 2978  34.6                        | 13184 152.5                       |        |         |
| 5   | IRLBA               | 10759 7.7                        | 6083  3.4                         | 60207 34.3                        |        |         |
| 10  | primme\_svds(1st stage only) | 4894  4.2                        | 3912  2.8                         | 10087 6.8                         |        |         |
| 10  | JDSDV               | 2460  20.8                       | 11683 10.4                        | 20934 19.7                        |        |         |
| 10  | SVDIFP              | 12343 8.2                        | 28996 36.6                        | 97653 115.7                       |        |         |
| 10  | IRRHLB              | 14676 6.8                        | 5482  3.3                         | 38946 18.4                        |        |         |
| 10  | IRLBA               | 8786  6.8                        | 5482  3.3                         | 38946 18.4                        |        |         |

| $k$ | Method          | $\delta = 1e^{-8}$ Matrix: jagmesh8 |          | wang3 |          | lshp3025 |          |
|-----|-----------------|------------------------------------|----------|--------|----------|----------|----------|
| 1   | primme\_svds(1st stage only) | 5472  2.9                        | 6579  40.1                       | 11312 10.4                       |        |         |
| 1   | JDSDV           | 12343 8.2                       | 11353 83.8                       | 37225 40.9                       |        |         |
| 1   | SVDIFP          | 20223 16.3                       | 14063 228.1                      | 27413 73.0                       |        |         |
| 1   | IRRHLB          | 30105 317.7                      | 19689 632.1                      | 46845 565.8                      |        |         |
| 1   | IRLBA           | - -                             | - -                             | - -                             |        |         |
| 3   | primme\_svds(1st stage only) | 5915  3.2                        | 7589  58.3                       | 12250 10.9                       |        |         |
| 3   | JDSDV           | 13861 8.7                       | 17865 127.3                      | 50282 57.5                       |        |         |
| 3   | SVDIFP          | 146224 123                      | 48696 1090                      | 15352 518.0                      |        |         |
| 3   | IRRHLB          | 25497 27.1                      | 19001 619.5                      | 42201 518.4                      |        |         |
| 3   | IRLBA           | 139266 48.6                      | 129876 577.2                     | - -                             |        |         |
| 5   | primme\_svds(1st stage only) | 6679  3.7                        | 8673  68.7                       | 14126 12.5                       |        |         |
| 5   | JDSDV           | 18173 12.8                       | 22441 157.3                      | 66034 80.9                       |        |         |
| 5   | SVDIFP          | - -                             | 68774 1671                      | 146336 569.2                     |        |         |
| 5   | IRRHLB          | 18314 197.8                      | 17963 570                        | 93239 1186.6                     |        |         |
| 5   | IRLBA           | 85043 29.9                      | 82551 359.1                      | - -                             |        |         |
| 10  | primme\_svds(1st stage only) | 8861  4.8                        | 19445 154.2                      | 19755 18.7                       |        |         |
| 10  | JDSDV           | 21209 14.7                       | - -                             | 86780 115.6                      |        |         |
| 10  | SVDIFP          | - -                             | - -                             | - -                             |        |         |
| 10  | IRRHLB          | 52043 608.1                      | 16975 537                        | - -                             |        |         |
| 10  | IRLBA           | 43798 15.1                      | 52490 250.7                      | - -                             |        |         |
Table 5.4

Seeking 1, 3, 5, and 10 smallest singular triplets of square matrices with user tolerance 1e-14. The primme svds method has two variants: primme svds(GD+k) uses GD+k eigenmethod while primme svds(JDQMR) uses JDQMR eigenmethod respectively in the second stage.

### δ = 1e-14 Matrix: pde2961 dw2048 fidap4

| k | Method               | MV    | MV    | MV    |
|---|----------------------|-------|-------|-------|
| 1 | primme svds(GD+k)    | 2986  | 2.7   | 2421  | 1.9   |
|   | JDSVD                | 6106  | 7.6   | 5061  | 4.5   |
|   | SVDFP                | 5992  | 14.0  | 5241  | 5.6   |
|   | IRRHLB               | 6328  | 75.5  | 4561  | 50.9  |
|   | IRLBA                | 21700 | 15.3  | 7684  | 3.3   |
| 3 | primme svds(GD+k)    | 4243  | 6.1   | 3679  | 3.7   |
|   | JDSVD                | 10517 | 11.6  | 8911  | 7.1   |
|   | SVDFP                | 20613 | 49.6  | 23290 | 27.6  |
|   | IRRHLB               | 6241  | 77.0  | 4193  | 49.1  |
|   | IRLBA                | 24906 | 21.4  | 7684  | 3.3   |
| 5 | primme svds(GD+k)    | 5579  | 7.1   | 4776  | 3.7   |
|   | JDSVD                | 14554 | 19.1  | 12266 | 11.7  |
|   | SVDFP                | 31506 | 77.0  | 33117 | 39.9  |
|   | IRRHLB               | 6218  | 79.2  | 4193  | 49.1  |
|   | IRLBA                | 16629 | 13.7  | 9763  | 5.5   |
| 10| primme svds(GD+k)    | 9337  | 12.1  | 8069  | 7.9   |
|   | JDSVD                | 13608 | 9.6   | 16457 | 105.4 |
|   | SVDFP                | 73847 | –     | –     | –     |
|   | IRRHLB               | 6371  | 86.8  | 4589  | 58.6  |
|   | IRLBA                | 12497 | 12    | 7796  | 4.8   |

### δ = 1e-14 Matrix: jagmesh8 wang3 lshp3025

| k | Method               | MV    | MV    | MV    |
|---|----------------------|-------|-------|-------|
| 1 | primme svds(GD+k)    | 7080  | 5.0   | 9160  | 74.8  |
|   | JDSVD                | 13608 | 9.6   | 16457 | 105.4 |
|   | SVDFP                | 31506 | 77.0  | 33117 | 39.9  |
|   | IRRHLB               | 43869 | 466.5 | 27470 | 1003  |
|   | IRLBA                | 43869 | 466.5 | 27470 | 1003  |
| 3 | primme svds(GD+k)    | 8859  | 5.7   | 14184 | 179.7 |
|   | JDSVD                | 17029 | 11.0  | 41900 | 387   |
|   | SVDFP                | 31506 | 77.0  | 33117 | 39.9  |
|   | IRRHLB               | 31210 | 330.1 | 29035 | –     |
|   | IRLBA                | 31210 | 330.1 | 29035 | –     |
| 5 | primme svds(GD+k)    | 11569 | 7.5   | 21396 | 302.7 |
|   | JDSVD                | 22573 | 15.2  | 57454 | 441.4 |
|   | SVDFP                | 23498 | 331.4 | 22985 | 730.1 |
|   | IRRHLB               | 12441 | 53.6  | –     | –     |
|   | IRLBA                | 12441 | 53.6  | –     | –     |
| 10| primme svds(GD+k)    | 17344 | 10.8  | 37898 | 480.7 |
|   | JDSVD                | 29613 | 21.0  | 91290 | 871.9 |
|   | SVDFP                | 23498 | 331.4 | 22985 | 730.1 |
|   | IRRHLB               | 55673 | 820.4 | 43309 | 1679.4|
|   | IRLBA                | 59595 | 27.4  | –     | –     |
Seeking 1, 3, 5, and 10 smallest singular triplets of rectangular matrices with user tolerance 1e-8. The `primme_svd` method has two variants: `primme_svd(GD+k)` uses GD+k eigenmethod while `primme_svd(JDQMR)` uses JDQMR eigenmethod respectively in the second stage.

| $k$ | Method | $\delta = 1e-8$ | Matrix: | well11850 | lp_ganges | deter4 |
|-----|--------|-----------------|---------|-----------|-----------|--------|
|     |        | MV | Sec | MV | Sec | MV | Sec |
| 1   | `primme_svd(1st stage only)` | 519 | 0.4 | 233 | 0.2 | 235 | 0.2 |
| 1   | JDSVD  | 1563 | 3.3 | 771 | 0.7 | 670 | 1.5 |
| 1   | SVDIFP | 1352 | 1.4 | 403 | 0.5 | 330 | 1.4 |
| 1   | IRRHLB | 872 | 8.7 | 345 | 3.4 | 500 | 6.6 |
| 1   | IRLBA  | 1060 | 0.5 | 260 | 0.2 | 292 | 0.4 |
| 3   | `primme_svd(1st stage only)` | 584 | 0.4 | 242 | 0.3 | 1943 | 2.0 |
| 3   | JDSVD  | 2773 | 2.4 | 7052 | 7.1 | - | - |
| 3   | SVDIFP | 2779 | 2.7 | 990 | 1.1 | 6794 | 29.2 |
| 3   | IRRHLB | 847 | 8.5 | 325 | 3.3 | 11896 | 170.1 |
| 3   | IRLBA  | 816 | 0.4 | 246 | 0.2 | 17616 | 17.7 |
| 5   | `primme_svd(1st stage only)` | 668 | 0.5 | 536 | 0.7 | 2853 | 3.1 |
| 5   | JDSVD  | 4203 | 3.5 | 15533 | 16.1 | - | - |
| 5   | SVDIFP | 4169 | 4.1 | 1979 | 2.2 | 21725 | 99.1 |
| 5   | IRRHLB | 872 | 9.3 | 926 | 10.3 | 12644 | 187 |
| 5   | IRLBA  | 931 | 0.5 | 802 | 0.5 | 25515 | 26.3 |
| 10  | `primme_svd(1st stage only)` | 956 | 0.7 | 1036 | 0.9 | 4240 | 4.3 |
| 10  | JDSVD  | 85053 | 73.3 | - | - | - | - |
| 10  | SVDIFP | 7279 | 7.2 | 9213 | 10.1 | 28303 | 132.3 |
| 10  | IRRHLB | 827 | 10.0 | 2851 | 34.7 | - | - |
| 10  | IRLBA  | 788 | 0.4 | 890 | 0.5 | 42038 | 44.3 |

| $\delta = 1e-8$ | Matrix: | plpdb | ch | lp_bnl2 |
|-----------------|---------|-------|----|--------|
| $k$             | Method  | MV | Sec | MV | Sec | MV | Sec |
| 1               | `primme_svd(1st stage only)` | 2513 | 2.4 | 10408 | 19.3 | 16581 | 12.2 |
| 1               | JDSVD  | 11100 | 16.2 | 74592 | 139.1 | 69576 | 94.2 |
| 1               | SVDIFP | 6097 | 18.2 | 15843 | 60.9 | 18653 | 34.9 |
| 1               | IRRHLB | 23161 | 290.4 | - | - | - | - |
| 1               | IRLBA  | 31684 | 21.1 | 21700 | 22.4 | - | - |
| 3               | `primme_svd(1st stage only)` | 2457 | 3.3 | 21071 | 31.8 | 20023 | 15.0 |
| 3               | JDSVD  | 13531 | 20.0 | - | - | 101696 | 135.9 |
| 3               | SVDIFP | 19934 | 60.7 | 31431 | 127.4 | 55302 | 119 |
| 3               | IRRHLB | 23032 | 293.3 | - | - | - | - |
| 3               | IRLBA  | 16836 | 11.1 | - | - | - | - |
| 5               | `primme_svd(1st stage only)` | 2607 | 2.7 | 27342 | 34.6 | 25387 | 19.0 |
| 5               | JDSVD  | 17832 | 27.3 | - | - | - | - |
| 5               | SVDIFP | 22565 | 68.7 | 49137 | 215.3 | 96769 | 197.2 |
| 5               | IRRHLB | 20015 | 261.5 | - | - | - | - |
| 5               | IRLBA  | 13755 | 10.4 | - | - | - | - |
| 10              | `primme_svd(1st stage only)` | 3355 | 3.3 | 36820 | 43.0 | 36420 | 26.9 |
| 10              | JDSVD  | 55100 | 100.4 | - | - | - | - |
| 10              | SVDIFP | 40019 | 125.8 | - | - | - | - |
| 10              | IRRHLB | 14907 | 210.2 | - | - | - | - |
| 10              | IRLBA  | 8617 | 7.4 | - | - | - | - |
Seeking 1, 3, 5, and 10 smallest singular triplets of rectangular matrices with user tolerance 1e-14. The primme\textsubscript{svds} method has two variants: primme\textsubscript{svds}(GD+k) uses GD+k eigenmethod while primme\textsubscript{svds}(JDQMR) uses JDQMR eigenmethod respectively in the second stage.

| δ = 1e-14 Matrix: | well1850 | lp\_ganges | deter4 |
|-------------------|-----------|------------|--------|
| k Method | MV | Sec | MV | Sec | MV | Sec |
| 1 primme\textsubscript{svds}(GD+k) | 637 | 0.4 | 546 | 0.5 | 455 | 0.6 |
| 1 primme\textsubscript{svds}(JDQMR) | 638 | 0.4 | 512 | 0.3 | 448 | 0.4 |
| 1 JDSVD | 1838 | 1.9 | 1002 | 0.9 | 9351 | 18.3 |
| 1 SVDIFP | 2306 | 2.3 | 697 | 0.8 | 514 | 2.4 |
| 1 IRRHLB | 1368 | 13.8 | 500 | 5.1 | 1213 | 17.0 |
| 1 IRLBA | 1700 | 0.7 | 356 | 0.2 | 548 | 0.5 |
| 3 primme\textsubscript{svds}(GD+k) | 894 | 0.5 | 506 | 0.4 | 3356 | 3.4 |
| 3 primme\textsubscript{svds}(JDQMR) | 883 | 0.5 | 505 | 0.3 | 3319 | 2.9 |
| 3 JDSVD | 71259 | 57.3 | 4357 | 3.9 | – | – |
| 3 SVDIFP | 5016 | 5.0 | 1540 | 1.7 | 13383 | 58.8 |
| 3 IRRHLB | 1137 | 12.3 | 528 | 5.5 | – | – |
| 3 IRLBA | 1206 | 0.6 | 396 | 0.2 | 33426 | 27.2 |
| 5 primme\textsubscript{svds}(GD+k) | 1158 | 0.7 | 1065 | 0.8 | 5097 | 5.0 |
| 5 primme\textsubscript{svds}(JDQMR) | 1147 | 0.6 | 1039 | 0.7 | 5064 | 4.5 |
| 5 JDSVD | 7250 | 7.0 | 15302 | 13.5 | – | – |
| 5 SVDIFP | 1196 | 12.9 | 1493 | 16.4 | 17342 | 257.5 |
| 5 IRRHLB | 1378 | 0.5 | 1268 | 0.5 | 45445 | 38.9 |
| 5 IRLBA | 1368 | 13.8 | 528 | 5.5 | – | – |
| 10 primme\textsubscript{svds}(GD+k) | 1846 | 1.0 | 2044 | 1.4 | 9644 | 9.7 |
| 10 primme\textsubscript{svds}(JDQMR) | 1839 | 1.0 | 1976 | 1.1 | 9437 | 8.3 |
| 10 JDSVD | – | – | 15302 | 13.5 | – | – |
| 10 SVDIFP | 1137 | 12.3 | 4435 | 53.5 | – | – |
| 10 IRRHLB | 1378 | 0.5 | 1268 | 0.5 | 66861 | 57.5 |
| 10 IRLBA | 1368 | 13.8 | 528 | 5.5 | – | – |

| δ = 1e-14 Matrix: | plddb | ch | lp\_bn12 |
|-------------------|--------|----|--------|
| k Method | MV | Sec | MV | Sec | MV | Sec |
| 1 primme\textsubscript{svds}(GD+k) | 3994 | 3.8 | 24937 | 42.5 | 25549 | 25.0 |
| 1 primme\textsubscript{svds}(JDQMR) | 3355 | 2.6 | 16606 | 15.0 | 20564 | 14.5 |
| 1 JDSVD | 72964 | 99.9 | – | – | 89420 | 113.7 |
| 1 SVDIFP | 12995 | 38.7 | 20993 | 80 | 34769 | 68.2 |
| 1 IRRHLB | 32957 | 41.8 | – | – | – | – |
| 1 IRLBA | 63236 | 39.3 | 52484 | 43.1 | – | – |
| 3 primme\textsubscript{svds}(GD+k) | 8213 | 12.9 | 81205 | 184.5 | 92755 | 138.1 |
| 3 primme\textsubscript{svds}(JDQMR) | 4119 | 3.1 | 32604 | 30.0 | 30688 | 21.8 |
| 3 JDSVD | – | – | – | – | – | – |
| 3 SVDIFP | 47169 | 134.8 | 58073 | 240 | – | – |
| 3 IRRHLB | 27556 | 356.1 | – | – | – | – |
| 3 IRLBA | 26016 | 17.0 | – | – | – | – |
| 5 primme\textsubscript{svds}(GD+k) | 13145 | 22.5 | 115175 | 266 | 84784 | 113.9 |
| 5 primme\textsubscript{svds}(JDQMR) | 5216 | 3.8 | 44269 | 41.1 | 40641 | 28.8 |
| 5 JDSVD | – | – | – | – | – | – |
| 5 SVDIFP | 57706 | 176.5 | – | – | – | – |
| 5 IRRHLB | 27332 | 360.2 | – | – | – | – |
| 5 IRLBA | 23891 | 16.3 | – | – | – | – |
| 10 primme\textsubscript{svds}(GD+k) | 14591 | 23.3 | – | – | – | – |
| 10 primme\textsubscript{svds}(JDQMR) | 7633 | 5.6 | 74120 | 67.5 | 68111 | 47.8 |
| 10 JDSVD | – | – | – | – | – | – |
| 10 SVDIFP | 92668 | 288.2 | – | – | – | – |
| 10 IRRHLB | 17811 | 208.8 | – | – | – | – |
| 10 IRLBA | 11913 | 8.7 | – | – | – | – |
Table 5.7
Comparing two preconditioning methods for seeking ten smallest singular triplets. Primme$_{svds}$(two stage) is the two stage Primme$_{svds}$ we proposed before while Primme$_{svds}$(dynamic) is the dynamic switching approach between the normal equations approach and the augmented approach.

| $\delta = 1e^{-14}$ | Matrix:          | Primme$_{svds}$(two stage) | Primme$_{svds}$(dynamic) |
|---------------------|-----------------|----------------------------|--------------------------|
|                      | pde2961 dw2048  | MV Sec 0.4 MV Sec 0.7 MV Sec 1.3 | MV Sec 0.4 MV Sec 0.7 MV Sec 1.4 |
| 1e-3 dynamic        | 216 0.4 211 0.7 210 1.3 | 242 0.4 283 0.7 286 1.4 |
| 1e-2 dynamic        | 258 0.5 673 1.6 813 3.2 | 307 0.5 668 1.5 1043 3.7 |

| $\delta = 1e^{-14}$ | Matrix: jagmesh8 wang3 lshp3025 | Primme$_{svds}$(two stage) | Primme$_{svds}$(dynamic) |
|---------------------|---------------------------------|----------------------------|--------------------------|
|                      | MV Sec 0.5 MV Sec 5.5 MV Sec 3.0 | MV Sec 0.6 MV Sec 5.5 MV Sec 3.6 |
| 1e-3 dynamic        | 163 0.5 306 5.5 209 3.0 | 223 0.6 396 5.5 273 3.6 |
| 1e-2 dynamic        | 990 3.1 736 8.9 7631 132.4 | 547 1.6 1038 9.6 698 10.1 |

Table 5.8
Seeking smallest singular triplet with ILU, $\delta = 1e^{-3}$. The Primme$_{svds}$ method has two variants: Primme$_{svds}$(GD+k) uses GD+k eigenmethod while Primme$_{svds}$(JDQMR) uses JDQMR eigenmethod respectively in the second stage. We report the time for generating the preconditioner and running each method separately.

| $\delta = 1e^{-8}$ | Matrix: fidap4 jagmesh8 wang3 lshp3025 | ILU Time: | Primme$_{svds}$(1st stage only) | JDSVD | SVDIFP |
|---------------------|---------------------------------|----------|--------------------------------|-------|--------|
|                      | MV Sec 0.1 MV Sec 0.1 MV Sec 2.8 MV Sec 0.1 |
| 1                   | Primme$_{svds}$(1st stage only) | 15 0.1 13 0.1 46 2.5 19 0.3 |
| 1                   | JDSVD                           | 67 0.7 34 0.3 45 2.0 56 1.5 |
| 1                   | SVDIFP                          | 58 0.4 51 0.2 132 5.7 82 1.7 |
| 10                  | Primme$_{svds}$(1st stage only) | 117 0.6 91 0.2 185 2.5 122 1.7 |
| 10                  | JDSVD                           | 342 3.1 287 1.4 320 15.7 364 10.5 |
| 10                  | SVDIFP                          | 691 3.0 561 1.2 1179 29.1 1187 21.9 |

| $\delta = 1e^{-14}$ | Matrix: fidap4 jagmesh8 wang3 lshp3025 | ILU Time: | Primme$_{svds}$(GD+k) | Primme$_{svds}$(JDQMR) | JDSVD | SVDIFP |
|---------------------|---------------------------------|----------|---------------------|------------------------|-------|--------|
|                      | MV Sec 0.1 MV Sec 0.1 MV Sec 2.8 MV Sec 0.1 |
| 1                   | Primme$_{svds}$(GD+k)           | 62 0.6 52 0.1 102 1.8 66 0.5 |
| 1                   | Primme$_{svds}$(JDQMR)          | 64 0.3 55 0.1 106 1.1 68 0.5 |
| 1                   | JDSVD                           | 78 1.5 45 0.3 67 3.0 79 1.2 |
| 1                   | SVDIFP                          | 98 0.6 100 0.3 235 8.3 159 2.3 |
| 10                  | Primme$_{svds}$(GD+k)           | 210 1.3 163 0.5 306 5.5 209 3.0 |
| 10                  | Primme$_{svds}$(JDQMR)          | 251 1.2 215 0.5 402 5.0 265 3.5 |
| 10                  | JDSVD                           | 573 5.5 408 1.9 518 14.6 606 26.9 |
| 10                  | SVDIFP                          | 1152 5.4 981 1.9 1991 51.4 1897 29.1 |
Table 5.9
Seeking smallest singular triplet with RIF, droptol = 1e-3. The primme_svd method
has two variants: primme_svd(GD+k), denoted as p(GD+k), uses GD+k eigenmethod while
primme_svd(JDQMR), denoted as p(JDQMR), uses JDQMR eigenmethod respectively in the second
stage. We report the time for generating the preconditioner and running each method separately.

| $\delta$ = 1e-8 Matrix: | fidap4 | jagmesh8 | lshp3025 | deter4 | plldb | lp_bnl2 |
|-------------------------|--------|----------|----------|--------|-------|--------|
| $k$ | Method | MV | Sec | MV | Sec | MV | Sec | MV | Sec | MV | Sec |
| 1 | primme_svd | 291 | 0.4 | 119 | 0.1 | 295 | 0.6 | 27 | 0.2 | 10 | 0.1 | 15 | 0.1 |
| 1 | JDSVD | 1720 | 8.9 | 1311 | 3.6 | 2674 | 21.7 | 122 | 3.8 | 67 | 0.3 | 89 | 0.5 |
| 1 | SVDFPF | 513 | 1.4 | 622 | 0.9 | 732 | 5.3 | 142 | 2.1 | 29 | 0.1 | 49 | 0.1 |
| 10 | primme_svd | 1224 | 1.8 | 307 | 0.5 | 784 | 2.8 | 405 | 2.4 | 52 | 0.1 | 74 | 0.1 |
| 10 | JDSVD | 8131 | 39.5 | 2356 | 5.7 | – | – | – | – | – | – | – | – |
| 10 | SVDFPF | 4359 | 10.3 | 3118 | 4.2 | 5308 | 40.8 | 2278 | 45.4 | 300 | 1.0 | 453 | 1.0 |

Table 5.10
Seeking 10 smallest singular triplets using shift and invert technique. LU(A) and QR(A) are
the time for LU factorization and QR factorization on the matrix $A$ respectively. We report the
time of each method including their running time and associated factorization time.

| $\delta$ = 1e-10 Matrix: | fidap4 | jagmesh8 | lshp3025 | deter4 | plldb | lp_bnl2 |
|-------------------------|--------|----------|----------|--------|-------|--------|
| $k$ | Method | MV | Sec | MV | Sec | MV | Sec | MV | Sec | MV | Sec |
| 1 | p(GD+k) | 521 | 1.0 | 207 | 0.3 | 466 | 1.5 | 82 | 0.5 | 45 | 0.1 | 66 | 0.1 |
| 1 | p(JDQMR) | 544 | 1.0 | 229 | 0.2 | 514 | 1.5 | 87 | 0.4 | 45 | 0.1 | 69 | 0.1 |
| 1 | JDSVD | 2037 | 10.5 | 1410 | 3.6 | 3004 | 24.5 | 188 | 5.5 | 122 | 0.5 | 134 | 0.6 |
| 1 | SVDFPF | 843 | 2.1 | 990 | 1.3 | 1394 | 8.5 | 221 | 4.3 | 48 | 0.1 | 63 | 0.1 |
| 10 | p(GD+k) | 2074 | 3.2 | 562 | 0.8 | 1364 | 4.8 | 769 | 2.5 | 152 | 0.5 | 192 | 0.5 |
| 10 | p(JDQMR) | 2604 | 4.9 | 641 | 0.9 | 1616 | 7.0 | 877 | 5.3 | 247 | 0.5 | 242 | 0.5 |
| 10 | JDSVD | – | – | 12057 | 28.2 | – | – | – | – | – | – | – | – |
| 10 | SVDFPF | 7470 | 15.1 | 5024 | 6.1 | 9999 | 83 | 3705 | 45.4 | 748 | 1.0 | 862 | 1.0 |

Table 5.11
Basic information of some real-world test matrices.

| Matrix | debr | cage14 | thermal2 | sls | Rucci1 |
|--------|------|--------|----------|-----|-------|
| rows $m$: | 1048576 | 1505785 | 1228045 | 1748122 | 1977885 |
| cols $n$: | 1048576 | 1505785 | 1228045 | 62729 | 109900 |
| nnz(A) | 4194298 | 27130349 | 8580313 | 6804304 | 7791168 |
| $\sigma_1$ | 1.11E+20 | 9.52E-02 | 1.61E-06 | 9.99E-03 | 1.04E-03 |
| $\kappa(A)$ | 3.6E+20 | 1.01E+1 | 7.48E+6 | 1.30E+3 | 6.74E+3 |
| Application | undirected | directed | thermal | Least | Least |
| | graph | graph | Sqaures | Sqaures | Sqaures |
| Preconditioner | No | ILU(0) | ILU(1e-3) | RIF(1e-3) | RIF(1e-3) |
Table 5.12

Seeking the smallest singular triplet for real world problems. We report the time of each method including their running time and associated factorization time (PRtime) separately.

| Matrix | PRtime | PRtime | PRtime | PRtime | PRtime | PRtime |
|--------|--------|--------|--------|--------|--------|--------|
| debr   | 539    | 84.3   | 3e-12  | 403*   | 245.7* | 2.0e-01|
| cage14 | 2e0    | 19     | 11     | 4e-13  | 33     | 28     | 5.9e-13|
| thermal2 | 3.69e+03 | 419     | 506     | 7e-12 | -      | -      | 4.4e-09|
| sls    | 3.29e3 | 1779   | 170    | 1e-09  | 408*   | 328*   | 1.1e-09|
| Rucci1 | 6.92e4 | 4728   | 1087   | 7e-12  | 4649   | 6464   | 5.8e-12|

\( \delta = 1e-12 \)