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Packed storage extension for ScaLAPACK*

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Abstract

We describe a new extension to ScaLAPACK [2] for computing with symmetric (Hermitian) matrices stored in a packed form. The new code is built upon the ScaLAPACK routines for full dense storage for a high degree of software reuse. The original ScaLAPACK stores a symmetric matrix as a full matrix but accesses only the lower or upper triangular part. The new code enables more efficient use of memory by storing only the lower or upper triangular part of a symmetric (Hermitian) matrix. The packed storage scheme distributes the matrix by block column panels. Within each panel, the matrix is stored as a regular ScaLAPACK matrix. This storage arrangement simplifies the subroutine interface and code reuse. Routines PxPPTRF/PxPPTRS implement the Cholesky factorization and solution for symmetric (Hermitian) linear systems in packed storage. Routines PxSPEV/PxSPEVX (PxHPEV/PxHPEVX) implement the computation of eigenvalues and eigenvectors for symmetric (Hermitian) matrices in packed storage. Routines PxSPGVX (PxHPGVX) implement the expert driver for the generalized eigenvalue problem for symmetric (Hermitian) matrices in packed storage. Routines PFxSPGVX/PFxSPEVX (PFxHPGVX/PFxHPEVX) uses the packed storage and perform out-of-core computation of eigenvectors. Performance results on the Intel Paragon suggest that the packed storage scheme incurs only a small time overhead over the full storage scheme.

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1 Introduction

This paper describes a new extension to ScaLAPACK [2] for computing with symmetric (Hermitian) matrices stored in a packed form. ScaLAPACK is an acronym for Scalable Linear Algebra PACKage, or Scalable LAPACK. ScaLAPACK is a library of high-performance linear algebra routines for distributed-memory message-passing MIMD (Multiple Instruction Multiple Data) computers and networks of workstations. Capability of ScaLAPACK is described in the ScaLAPACK Users' Guide [2].

The new code is built upon the ScaLAPACK routines for full dense storage for maximum portability. The original ScaLAPACK stores a symmetric matrix as a full matrix but accesses only the lower or upper triangular part. This design allows the reuse of Level 3 PBLAS (Parallel Basic Linear Algebra Subroutines) [3] without modification. However, almost half of the storage is holding redundant information. The new code enables more efficient use of memory by storing the submatrix blocks associated with only the lower or upper triangular part of a symmetric (Hermitian) matrix.

Although current computers have unprecedented storage and computation speed, they are also called upon to tackle ever larger problems. Let $N \times N$ be the largest symmetric (Hermitian) problem that can be stored in memory, then a larger approximately $\sqrt{2}N \times \sqrt{2}N$ symmetric matrix can be stored in the same memory using the packed storage scheme. Linear solution of symmetric (Hermitian) matrices by Cholesky factorization and computing eigenvalues and eigenvectors by the QR algorithm both have $O(N^3)$ complexities. With an $O(N^3)$ complexity, the runtime for solving the larger problem will be approximately $\sqrt{2}^3 \approx 2.8$ times longer.

A symmetric eigensolver for packed storage is adapted for use with out-of-core algorithms for solving large eigenvalue problems. The initial stage in the classical algorithm for finding eigenvalues and eigenvectors is to first reduce the original symmetric matrix into a tridiagonal matrix by orthogonal similarity Householder transformations. The original matrix is overwritten by these Householder transformations. One of the key steps is the frequent need for computing a matrix-vector multiply. An out-of-core algorithm that stores the symmetric matrix on disk would be highly inefficient since the matrix must be read in from disk for each matrix-vector multiply operation. A solution suggested by Ken Stanley is to hold in memory the symmetric matrix in packed storage and store the eigenvectors on disk. This approach would require $O(N^2/2)$ memory for the symmetric matrix in packed storage instead of $O(2N^2)$ memory for holding the symmetric matrix and eigenvectors in full storage, and would allow larger problems to be solved using the same limited amount of memory.

We have developed prototype codes PxPPTRF/PxPPTRS for Cholesky factorization and solution, and simple driver routines PxSPEV (PxHPEV) for finding eigenvalues and optionally eigenvectors of symmetric (Hermitian) matrices in packed storage. Expert drivers for symmetric (Hermitian) matrices PxSPGVX (PxHPGVX) and generalized eigenvalue problems PxSPGVX (PxHPGVX) are also available as prototype code. The out-of-core drivers [4] PFxSPGVX/PFxSPEVX (PFxHPGVX/PFxHPEVX) are based on the packed storage eigenvalue routines but stores the eigenvectors on disk. The names for the new routines follow the convention used in LAPACK [1] of using a 'P' to represent packed storage. Thus 'SY' ('HE') represents a symmetric (Hermitian) matrix and 'SP' ('HP') represents a symmetric (Hermitian)

tion) matrix in packed storage; similarly, 'PO' denotes a symmetric positive definite matrix and 'PP' denotes the symmetric positive definite matrix in packed storage.

Section 2 describes the layout of the packed storage scheme. Section 3 shows by a simple example how other ScaLAPACK routines can be modified for use with packed matrices. Section 4 summarizes the performance of PDPPTRF/PDPPTRS, PDSPEV, PDSPEVX, PDSPGVX, PFDSPEVX and PFDSPGVX on the Intel Paragon. Finally, Section 5 contains the summary.

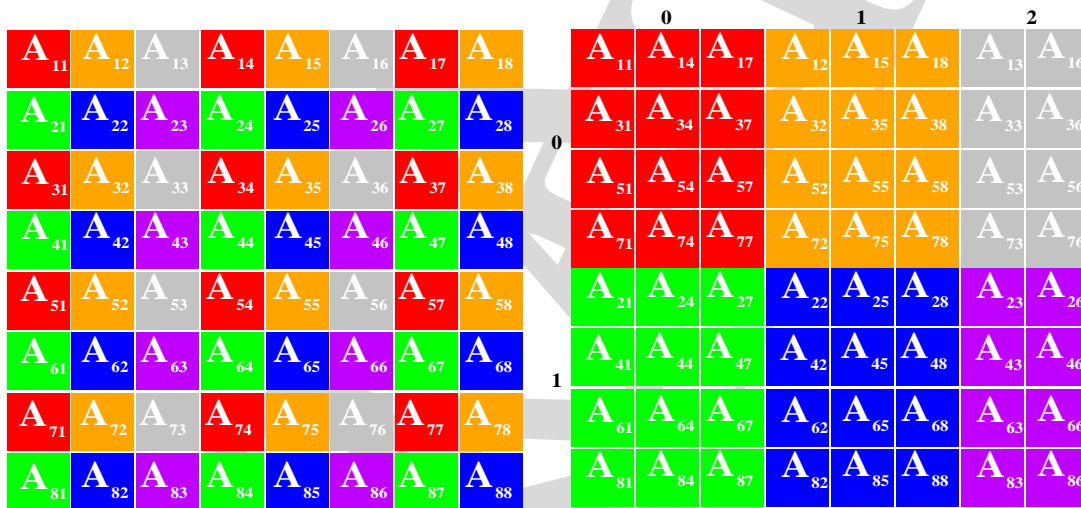
2 Data layout for packed storage

ScaLAPACK principally uses a two-dimensional block-cyclic data distribution (see Figure 1) for full dense in-core matrices [2, Chapter 4]. This distribution has the desirable properties of good load balancing where the computation is spread reasonably evenly among the processes, and can make use of highly efficient level 3 BLAS (Basic Linear Algebra Subroutines) at the process level. Each colored rectangle represents an $mb \times nb$ submatrix. Matrix entry (i, j) is mapped to matrix block $(ib, jb) = (1 + \lfloor (i-1)/mb \rfloor, 1 + \lfloor (j-1)/nb \rfloor)$ and is assigned to process $(p, q) = (\text{mod}(ib-1, P_r), \text{mod}(jb-1, P_c))$ on a $P_r \times P_c$ process grid. Thus the first entry $(1, 1)$ is mapped to process $(0, 0)$ and entry $(1 + mb, 1 + nb)$ is mapped to process $(1, 1)$.

The packed storage scheme resembles the ScaLAPACK two-dimensional block-cyclic data distribution but physically stores only the lower (or upper) *blocks*. For example, on a 2×3 process grid as shown in Figure 1, if only the lower blocks are stored, then process $(0, 0)$ holds blocks $A_{11}, A_{31}, A_{51}, A_{71}, A_{54}, A_{74}, A_{77}$. Process $(0, 2)$ holds blocks A_{33}, A_{53}, A_{73} and A_{76} . Similarly process $(1, 1)$ holds blocks $A_{22}, A_{42}, A_{62}, A_{82}$ and A_{65}, A_{85} plus A_{88} . We note that each block in the packed storage scheme is assigned to the *same* process as in the fully two-dimensional block-cyclic data distribution. Moreover, each block column or panel in the packed storage scheme may be considered a full ScaLAPACK matrix distributed across only one process column. This treatment of a block column panel as a particular ScaLAPACK submatrix is a key characteristic to the reuse of ScaLAPACK and PBLAS library components.

If we consider the 'local' view in process $(0, 0)$, the first block column panel consists of A_{11}, A_{31}, A_{51} and A_{71} . This panel is stored in memory as a $4 * mb \times nb$ Fortran column-major matrix. The second block column panel consists of blocks A_{54} and A_{74} . It is stored in local memory as a $2 * mb \times nb$ Fortran column-major matrix. The first entry of the second panel follows the last entry of the first panel in memory, i.e. the first entry in block A_{54} follows the last entry in block A_{71} . Note that the entire diagonal block A_{11} is stored, even though only the lower triangular part is accessed. This incurs a small price in extra storage but greatly simplifies reuse of ScaLAPACK components.

2-DIMENSIONAL BLOCK CYCLIC DISTRIBUTION



Global (left) and distributed (right) views of matrix

Figure 1: Two-dimensional block-cyclic distribution.

3 Examples in the use of packed storage matrix

Here we illustrate by examples the reuse of ScaLAPACK library components for matrices stored in packed form. The key idea is the treatment of each block column or panel as a regular ScaLAPACK matrix distributed across a process column. The routine DESCINITT is provided to simplify the manipulation of indices by initializing a new matrix descriptor for a block column panel. The routine interface can be described using Fortran 90 syntax as

```
SUBROUTINE DESCINITT(UPLO, IA, JA, DESCA, IAP, JAP, LOFFSET, DESCAP)
  CHARACTER, INTENT(IN) :: UPLO
  INTEGER, INTENT(IN) :: IA, JA, DESCA(:)
  INTEGER, INTENT(OUT) :: IAP, JAP, LOFFSET, DESCAP(:)
END SUBROUTINE DESCINITT
```

For example, access to the global entry $A(IA, JA)$ in full storage is obtained by the ScaLAPACK routine

```
CALL PDELGET( SCOPE, TOP, ALPHA, A, IA, JA, DESCA )
```

The corresponding code to access the lower triangular entry in packed storage would be

```
CALL DESCINITT( 'Lower', IA, JA, DESCA, IAP, JAP, LOFFSET, DESCAP )
CALL PDELGET( SCOPE, TOP, ALPHA, A(LOFFSET), IAP, JAP, DESCAP )
```

The routine DESCINITT generates a new matrix descriptor DESCAP that corresponds to the block column panel with new indices (IAP, JAP) relative to the new descriptor. It will also produce the correct value for LOFFSET to adjust for the beginning of the column panel.

Another more complicated example (see Figure 2) is computing the largest absolute value ($\max(|A(I, J)|)$) in a packed matrix. This is similar to computing with the NORM='M' option in PDLANSY for the full storage,

```
ANRM = PDLANSY( 'M', UPLO, N, A, 1, 1, DESCA, WORK )
```

The new code reuses ScaLAPACK PDLANSY and PDLANGE for computing the maximum entry in each block column panel.

The code traverses each block column (line 4) and calls DESCINITT to establish the appropriate matrix descriptor. It calls PDLANSY (line 11) to find the largest value in the diagonal block. Routine PDLANGE (line 19) computes the largest value in the remaining off-diagonal rectangular block. Although essentially the same computation is performed, the packed version has higher overhead in making several separate calls to PDLANSY and PDLANGE. Moreover, the granularity of the algorithm is limited by the width of the column panel ($NB=DESCA(NB_)$).

```

1  N = DESCA(N_)           ! Number of columns in matrix A
2  NB = DESCA(NB_)         ! Width of each block column
3  ANRM = ZERO
4  DO JA=1,N,NB
5      JB = MIN( NB, N-JA+1 )
6      IA = JA
7      CALL DESCINITT('Lower',IA,JA,DESCA,IAP,JAP,LOFFSET,DESCAP)
8      !
9      ! Handle diagonal block
10     !
11     ANRM2 = PDLANSY('M','Lower',JB,A(LOFFSET),IAP,JAP,DESCAP,WORK)
12     ANRM = MAX( ANRM, ANRM2 )
13     !
14     ! Handle off-diagonal rectangular block
15     ! Use Lower triangular part
16     !
17     IA = IA + JB
18     IF (IA .LE. N) THEN
19         ANRM2 = PDLANGE('M',N-IA+1,JB,A(LOFFSET),IAP+JB,JAP,DESCAP,WORK)
20         ANRM = MAX( ANRM, ANRM2 )
21     ENDIF
22 ENDDO

```

Figure 2: Example code to illustrate the reuse of ScaLAPACK components for matrices stored in packed storage.

4 Numerical experiments

We have developed the following prototype codes: P_xPPTRF/P_xPPTRS for Cholesky factorization and solution, simple driver P_xSPEV (P_xHPEV) routines for finding eigenvalues and eigenvectors of symmetric (Hermitian) matrices stored in packed form, expert drivers for symmetric (Hermitian) matrices P_xSPEVX/P_xHPEVX and generalized eigenvalue problems P_xSPGVX/P_xHPGVX. Out-of-core drivers [4] PF_xSPGVX/PF_xSPEVX (PF_xHPGVX/PF_xHPEVX) are based on the packed storage eigenvalue routines but stores the eigenvectors on disk.

We have compared the performance of the new routines in packed storage with ScaLAPACK routines in full storage. The goal is to demonstrate that the new version with packed storage has little or no overhead cost over the existing routines for full storage. The new routines have higher overhead in index calculations and have algorithm granularity limited by the width of the block column panel. However, the packed storage may have better data locality and cache reuse.

The tests were performed on the XPS/35 Intel Paragon at the Center for Computational Sciences at the Oak Ridge National Laboratory. The XPS/35 has 512 GP nodes arranged in a 16×32 rectangular mesh. Each GP node has 32MBytes of memory. The runs were performed in a time-shared multi-user (non-dedicated) environment using a $P_r \times P_c$ logical process grid. Matrix block $mb = nb = 50$ was used for all tests. Results for upper case (UPLD='U') and lower case (UPLD='L') are very similar so results for only the lower case are presented. The latest version of PBLAS (version 2.0 alpha) was compiled with '-O3 -Mvect -Knoieee'[†] and linked with '-lkmath', the highly optimized CLASSPACK serial BLAS library. The new version of PBLAS incorporates automatic algorithmic blocking with block size set to 50[‡]. The PBLAS version 2.0 alpha release is still undergoing performance tuning.

Table 1 summarizes the times for the Cholesky factorization PDPOTRF for full storage and PDPPTRF for packed storage. The relative increase in runtime with packed storage over full storage is also displayed in the table. Routines PDPPTRS and PDPOTRS are used to solve the factored system with 50 and 1000 (NRHS) right-hand vectors. For the cases considered, the times for factorization by PDPPTRF with packed storage is comparable (at most two seconds difference) to times taken by PDPOTRF with full storage. Solution times for a narrow right-hand matrix (NRHS=50) show PDPPTRS for packed storage to be slower than PDPOTRS for full storage for large problems ($N \geq 2000$). The difference is about 3 seconds. Solution times for a wide right-hand matrix (NRHS=1000) show PDPPTRS for packed storage to be competitive with PDPPTRS. Routine PDPPTRS is slightly faster than PDPOTRS for cases $N = 1000$ and $N = 4000$, whereas for $N = 2000$, PDPPTRS is slower by 36%.

Table 2 summarizes the execution times for the symmetric eigensolvers PDSYEV with full storage and PDSPEV with packed storage. The computations were performed with JOBZ='N' to find all eigenvalues or with JOBZ='V' to find all eigenvectors and eigenvalues. Routine PDSPEV for packed storage incurs at most a 11% increase over PDSYEV for full storage in finding eigenvalues only. On closer examination and profiling, we find part of the extra time is incurred in a routine to perform a matrix vector multiply operation where the matrix is stored in packed storage. Performance of DSYMV and DGEMV for the packed

[†]Option -Knoieee turns off software emulation of IEEE arithmetic in divisions or operations on denormalized numbers to use the faster (but slightly less accurate) hardware units.

[‡]value return by routine PILAENV in PBLAS.

version may be limited by the width of the block column panel and by the block column by block column nature of the algorithm. When both eigenvectors and eigenvalues are required, PDSPEV compares favorably with PDSYEV for full storage.

Table 3 summarizes the execution times for the expert drivers for the symmetric eigensolvers. Although the expert driver is capable of finding specific clusters of eigenvalues, all eigenvalues (RANGE= ' ALL ') are requested. The routine PDSPEVX performs reorthogonalization of eigenvectors when there is sufficient temporary workspace. This reorthogonalization can cause the higher run times for finding all eigenvectors over the simple driver PDSYEV. In these runs, reorthogonalization is turned off by setting ORFAC=0 and ABSTOL=0. Performance analysis of PDSYEVX is described in [2, Chapter 5] and [5]. When only eigenvalues are requested (JOBZ= ' N '), PDSPEVX for packed storage is slower than PDSYEVX for full storage by 5 to 9 seconds. For longer running computation when both eigenvectors and eigenvalues are requested (JOBZ= ' V '), PDSPEVX for packed storage is comparable to PDSYEVX for full storage.

Table 4 summarizes the times for the generalized symmetric eigensolvers PDSPGVX with packed storage and PDSYGVX with full storage for finding all eigenvalues with RANGE= ' ALL ' . The input parameter IBTYPE describes the type of problem to be solved:

$$\text{IBTYPE} = \begin{cases} 1 & \text{solve } Ax = \lambda Bx, \\ 2 & \text{solve } ABx = \lambda x, \\ 3 & \text{solve } BAx = \lambda x. \end{cases} \quad (1)$$

The problem is reduced to canonical form by first performing a Cholesky factorization on B ($B = LL^H$ or $U^H U$) and then overwriting A with

$$\text{IBTYPE} = \begin{cases} 1 & A \leftarrow U^{-H} A U^{-1} \text{ or } L^{-1} A L^{-H}, \\ 2 \text{ or } 3 & A \leftarrow U A U^H \text{ or } L^H A L. \end{cases} \quad (2)$$

For the cases IBTYPE=2 and IBTYPE=3, the packed version incurs a significant extra overhead compared to the version for full storage. The in-place conversion of matrix A to canonical form (2) may require access to block rows in matrix A or B . Since the packed storage is stored in a column panel oriented manner, traversal *across* block rows will be less efficient than traversal *down* columns.

Table 5 summarizes the times for the out-of-core eigensolvers PFDSPEVX with RANGE= ' ALL ' . Routine PFDSPEVX is based on the packed storage PDSPEVX to compute groups of the eigenvectors using RANGE= ' Interval ' and store them to disk. The results suggest the out-of-core version PFDSPEVX is almost competitive with PDSYEVX.

Table 6 summarizes the times for the out-of-core eigensolver PFDSPGVX that calls PFDSPEVX to compute subsets of the eigenvectors. ScaLAPACK routine PDSYGVX calls PDSYEVX for the computation of eigenvectors, and performs a modification of eigenvectors by Cholesky factors of B . Unlike PDSYGVX, routine PFDSPGVX calls a routine similar to PFDSPEVX but also computes the modification of eigenvectors by B before they are stored to disk. If PFDSPEVX were used, there would be unnecessary input/output overhead to bring eigenvectors from disk to be modified by B and then write the vectors back out. However, even with this arrangement, the out-of-core packed routines still impose a significant overhead. For the

$P_r \times P_c$	N	NRHS=50			NRHS=1000		
		PDPOTRF	PDPPTRF	change	PDPOTRS	PDPPTRS	change
8×8	1000	2.3s	0.9s	-63%	1.6s	1.5s	-1%
8×8	2000	2.5s	2.9s	14%	1.3s	2.2s	73%
8×8	4000	14.7s	13.9s	-5%	3.9s	7.6s	93%
10×10	1000	2.3s	0.8s	-63%	1.9s	1.6s	-20%
10×10	2000	2.0s	2.5s	21%	1.3s	2.1s	68%
10×10	4000	11.3s	10.8s	-4%	4.1s	6.8s	67%

Table 1: Performance (in seconds) of Cholesky factorizations and solves.

$P_r \times P_c$	N	JOBZ	PDSYEV	PDSPEV	Change
8×8	1000	N	25.3s	27.6s	9%
8×8	2000	N	81.4s	90.5s	11%
8×8	4000	N	317.0s	341.1s	8%
10×10	1000	N	25.4s	27.7s	9%
10×10	2000	N	79.0s	87.8s	11%
10×10	4000	N	304.2s	321.6s	6%
8×8	1000	V	64.6s	62.8s	-3%
8×8	2000	V	239.6s	226.8s	-5%
8×8	4000	V	1336.1s	1342.3s	0%
10×10	1000	V	65.3s	62.3s	-5%
10×10	2000	V	217.4s	221.7s	2%
10×10	4000	V	866.4s	843.2s	-3%

Table 2: Performance (in seconds) of simple drivers for symmetric eigensolvers.

large problem $N=6000$, PDSYGVX did not complete in a reasonable amount of time due to excessive paging whereas PFDSPGVX completes in about 1500s since PFDSPGVX require only $O(N^2)$ instead of $O(3N^2)$ amount of memory.

5 Summary

The overall results suggest that for a reasonably large block size ($nb = 50$), the packed storage incurs only a small time overhead over the full storage routines. The difference may be as large as 20 seconds for short runs that complete in about a minute and approximately extra 10% overhead for larger problems. In some cases, the packed storage may even yield slightly better performance due to better data locality and cache reuse. The generalized eigensolver with IBTYPE=2 or IBTYPE=3 may require traversal across block rows and this leads to higher overhead (about 30% – 50%) for packed storage over full storage. The out-of-core generalized eigensolver incurs substantial time overhead (about 60% – 70%). A more efficient version is under development.

The design of the packed storage data layout to be a dense ScaLAPACK matrix in each block column panel also facilitates the reuse of PBLAS and ScaLAPACK library components for good performance.

$P_r \times P_c$	N	JOBZ	PDSYEVX	PDSPEVX	Change
8×8	1000	N	11.7s	15.2s	29%
8×8	2000	N	36.4s	44.9s	23%
8×8	4000	N	137.6s	157.2s	14%
8×8	1000	V	14.8s	18.2s	23%
8×8	2000	V	49.2s	57.8s	17%
8×8	4000	V	222.3s	228.1s	3%
10×10	1000	N	10.8s	14.3s	33%
10×10	2000	N	30.5s	38.8s	27%
10×10	4000	N	107.6s	126.6s	18%
10×10	1000	V	13.0s	16.6s	28%
10×10	2000	V	40.1s	48.4s	21%
10×10	4000	V	172.0s	176.9s	3%

Table 3: Performance (in seconds) of expert drivers for symmetric eigensolvers.

$P_r \times P_c$	N	IBTYPE	JOBZ	PDSYGVX	PDSPGVX	Change
8×8	500	1	N	9s	8s	-11%
8×8	1000	1	N	15s	21s	34%
8×8	2000	1	N	54s	70s	30%
8×8	500	2	N	6s	7s	15%
8×8	1000	2	N	15s	21s	38%
8×8	2000	2	N	48s	75s	55%
8×8	500	3	N	5s	7s	31%
8×8	1000	3	N	15s	21s	39%
8×8	2000	3	N	48s	75s	55%
10×10	500	1	N	10s	8s	-16%
10×10	1000	1	N	14s	20s	39%
10×10	2000	1	N	47s	62s	32%
10×10	500	2	N	6s	7s	14%
10×10	1000	2	N	13s	19s	41%
10×10	2000	2	N	40s	65s	62%
10×10	500	3	N	5s	7s	36%
10×10	1000	3	N	13s	19s	44%
10×10	2000	3	N	40s	65s	61%
8×8	500	1	V	12s	10s	-19%
8×8	1000	1	V	21s	25s	18%
8×8	2000	1	V	76s	89s	16%
8×8	500	2	V	7s	8s	25%
8×8	1000	2	V	19s	25s	33%
8×8	2000	2	V	66s	94s	42%
8×8	500	3	V	6s	8s	29%
8×8	1000	3	V	18s	25s	34%
8×8	2000	3	V	65s	93s	44%
10×10	500	1	V	13s	10s	-25%
10×10	1000	1	V	18s	23s	27%
10×10	2000	1	V	64s	76s	19%
10×10	500	2	V	6s	8s	28%
10×10	1000	2	V	16s	22s	38%
10×10	2000	2	V	53s	79s	49%
10×10	500	3	V	6s	8s	34%
10×10	1000	3	V	16s	22s	39%
10×10	2000	3	V	52s	78s	51%

Table 4: Performance (in seconds) of expert drivers for generalized eigensolvers.

$P_r \times P_c$	N	JOBZ	PDSYEVX	PFDSPEVX	Change
8×8	1000	V	21	21	-1%
8×8	2000	V	55	63	15%
8×8	4000	V	220	260	18%
8×8	6000	V	1123	1056	-6%

Table 5: Performance (in seconds) of expert drivers for out-of-core symmetric eigensolvers.

$P_r \times P_c$	N	IBTYPE	JOBZ	PDSYGVX	PFDSPGVX	Change
8×8	1000	1	V	21s	37s	77%
8×8	2000	1	V	73s	99s	35%
8×8	4000	1	V	336s	444s	32%
8×8	6000	1	V	N/A ^a	1511s	N/A
8×8	1000	2	V	19s	27s	43%
8×8	2000	2	V	66s	98s	49%
8×8	4000	2	V	296s	487s	64%
8×8	6000	2	V	N/A	1503s	N/A
8×8	1000	3	V	19s	27s	42%
8×8	2000	3	V	65s	100s	54%
8×8	4000	3	V	292s	487s	67%
8×8	6000	3	V	N/A	1500s	N/A

Table 6: Performance (in seconds) of expert drivers for out-of-core generalized eigensolvers.

^aDid not complete due to excessive paging.

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