Efficient Serial and Parallel Block-Jacobi EVD/SVD Algorithms

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Outline

Our task

Compute in parallel the Singular Value Decomposition (SVD) of a complex matrix A of the size $m \times n$, $m \geq n$:

$$A = U \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^H,$$

where $U(m \times m)$ and $V(n \times n)$ are orthogonal and $\Sigma = \mathrm{diag}(\sigma_i)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$.
Numerically stable way of computation:

- one- or two-sided block-Jacobi methods;
- large degree of parallelism.

Target architecture:

- distributed memory machines (parallel supercomputers and clusters) with Message Passing Interface (MPI).

Applications

- EVD of symmetric matrices: quantum energy of atoms and molecules.
- Latent Semantic Indexing: processing and searching documents.
- Civil Engineering: eigenfrequencies and eigenmodes of buildings.

Our international partners:

- University of Electro-Communications, Tokyo, Japan
- Institute of Informatics, AS CR, Prague
- University of Salzburg, Austria
- University of Zagreb, Croatia

Recent VEGA grants

- VEGA project no. 2/004/17 “Parallel block algorithms for some canonical matrix decompositions”, 2017–2019.
- VEGA project no. 2/0015/20 “Convergence of block algorithms for canonical matrix decompositions”, 2020–2022.
- VEGA project no. 2/0001/23 “Efficient block Jacobi algorithms for the matrix EVD/SVD and their numerical properties”, 2023–2025.

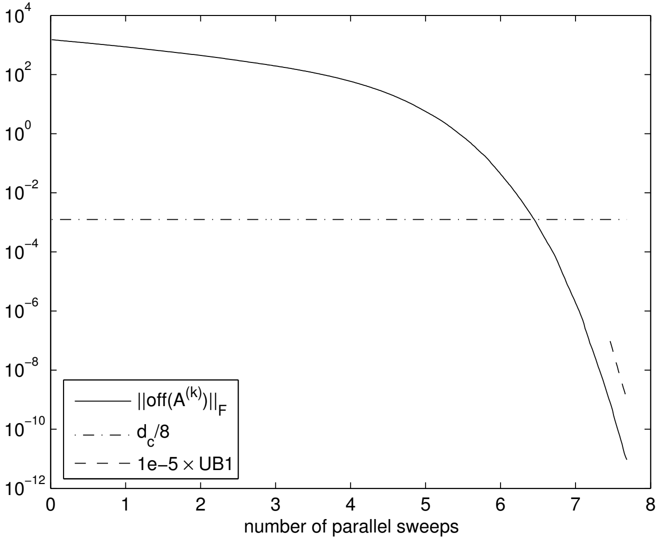
Asymptotic quadratic convergence

Having p processors, the blocking factor is $w = 2p$ and a matrix is partitioned into the $w \times w$ block structure.
Then, under some additional assumptions, there exists such an integer constant W, $w - 1 \leq W < 2w(\log w + 1)$, that after W parallel iteration steps one observes the AQC of the off-diagonal Frobenius norm of matrix A:

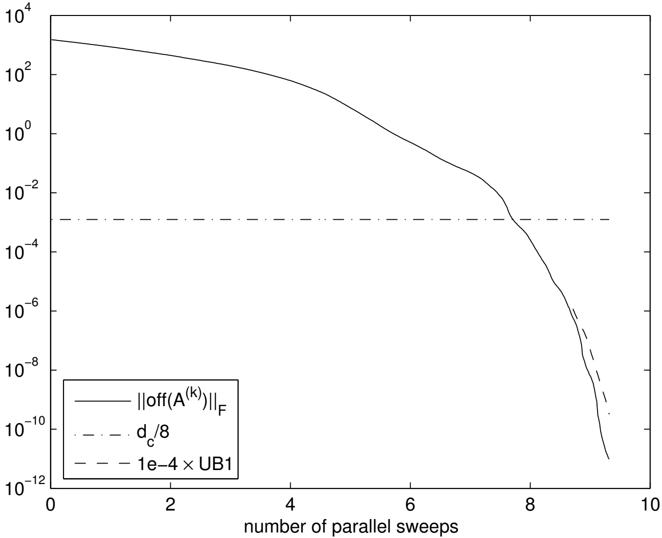
$$\|\mathrm{off}(A^{(W)})\|_F \leq \sqrt{12(w-2)}\,\frac{\|\mathrm{off}(A^{(0)})\|_F^2}{\delta},$$

where $\delta = \sqrt{2}d_c/4$ and d_c is the minimal gap between the centres of the clusters of singular values.

AQC present


10^4
10^2
10^0
10^-2
10^-4
10^-6
10^-8
10^-10
10^-12
0
1
2
3
4
5
6
7
8
number of parallel sweeps
||off(A^(k))||_F
d_c/8
1e–5 × UB1

AQC not present



Preconditioning

- Main idea: Find a ‘cheap’ orthogonal matrix matrix P such that AP will be close to $U\Sigma$ in the sense of the proximity of column vector spaces.
- First approach: Compute the EVD of the symmetric matrix $A^T A$ and use its eigenvectors W as a preconditioner: $A \to AW$, AW is the input into the block-Jacobi SVD algorithm.
- Suitable for well conditioned matrices when the condition number of $A^T A$ is not too large.
- Second approach: Compute the (partial) polar decomposition of $A = U_p H$ by the Halley iterations (cubic convergence!), then the EVD of the Hermitian factor H, and use its eigenvectors W for precond.
- Since the Gram matrix $A^T A$ is not needed at all, this approach is suitable for very ill conditioned matrices.

W based on $A^T A$, in parallel

Table: $w = 2p$, $n = 8000$, $\texttt{mode} = 3$, $\kappa(A) = 10^2$

Algorithm		p	
		10	20
PDGESVD	T [s]	934	645
PP_OSBJA	T [s]	178	98
	G+EVD+MM [s]	14+67+23	7+39+12
	Jacobi [s]	74	40
	# it	10	22

W based on $A^T A$, in parallel

Table: $w = 2p$, $n = 8000$, $\texttt{mode} = 3$, $\kappa(A) = 10^8$

Algorithm		p	
		10	20
PDGESVD	T [s]	859	499
PP_OSBJA	T [s]	408	202
	G+EVD+MM [s]	14+61+23	7+36+12
	Jacobi [s]	310	147
	# it	33	72

W based on HI, serial algorithm

- 6 iterations in the Halley algorithm are sufficient in the double precision, here we use only one iteration for the partial polar decomposition.
- 3 variants V1–V3 of serial algorithm for the partial polar decomposition were developed, they differ in the QR decomposition of a highly structured matrix of size 8000×4000 (not shown).

Table: $n = 4000$, $\texttt{mode} = 3$, $\kappa(A) = 10^{10}$

Precond. W	V1	V2	V3	Gram
$maxw$	5.4e-4	8.2e-4	1.3e-3	1.0
$iter(J)$	41	38	39	52
$T(J)$[s]	45.1	42.4	43.9	72.6
T_{tot}[s]	**65.9**	136.3	98.2	81.6

Recent publications

1 YAMAMOTO, Y., OKŠA, G., VAJTERŠIC, M., *On convergence to eigenvalues and eigenvectors in the block-Jacobi EVD algorithm with dynamic ordering*, Lin. Alg. and Its Appl. , 622 (2021) 19-45.

2 M. BEČKA, G. OKŠA, *Preconditioned Jacobi SVD algorithm outperforms PDGESVD*, In: Proc. of PPAM 2019, LNCS 12043 (2020), 555-566, Springer Nature Switzerland AG.

3 G. OKŠA, Y. YAMAMOTO, M. VAJTERŠIC, *Convergence to singular triplets in the two-sided block-Jacobi SVD algorithm with dynamic ordering*, SIAM Journal on Matrix Anal. and Appl. 43 (2022) 1238-1262.

4 G. OKŠA, M. BEČKA, *On relative accuracy of the one-sided block-Jacobi SVD algorithm*, In: Proc. of PPAM 2022, LNCS 12043 (2023), 464-475, Springer Nature Switzerland AG.