# High Performance Batch SVD using GPUs

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## Abstract

We consider the problem of computing the singular value decomposition (SVD) on many relatively-small matrices using GPUs. This is an essential component in various scientific applications, including computational chemistry, low-rank approximations, and others. Our approach is based on the parallel one-sided Jacobi algorithm, which has a large degree of parallelism, and also heavily relies on compute-bound level-3 BLAS operations, such as matrix multiply. Our approach uses two design strategies. The first one targets very small matrices using a single GPU kernel for the entire SVD operation. The second design strategy uses a blocked version of the parallel Jacobi algorithm, which supports matrices of arbitrary dimensions. The proposed solution supports any matrix shape (square, tall-skinny, or short-wide), requires no limitations on the matrix dimensions, and delivers superior performance against state-of-the-art solutions. This work is set to be released in the MAGMA library.

## Algorithmic Background

We consider the one-sided Jacobi algorithm for solving the batch reduced SVD problem.

1) Implicitly solves $G = A^TA = V^TDV$ ($G$ is never fully explicitly computed)
2) Multiply $A \times V = U\Sigma$ ($V$ is obtained through a series of Jacobi rotations)
3) Each rotation annihilates one off-diagonal element in $G$ by solving a 2×2 symmetric eigenvalue problem
4) Several independent off-diagonal elements can be considered in parallel (parallel Jacobi)
5) We use a round-robin parallel ordering to generate independent off-diagonals
6) Block Jacobi: targets an off-diagonal block instead of one element at a time


**One-sided Jacobi Algorithm**

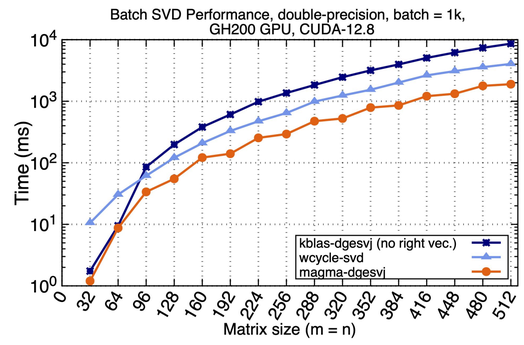
```
Function [U, Σ, V] = GESVJ(A_mxn)
    V = I
    while ( not converge ) {
        // begin Jacobi sweep
        for each pair (i, j), i < j {
            g_ii = A_i^T A_i
            g_jj = A_j^T A_j
            g_ij = A^T_i A_j
            if |g_ij| ≥ k.ϵ.sqrt(g_ii g_jj) {
                G_ij = [g_ii g_ij; g_ij g_jj]
                Solve G_ij = J^T D J
                A = A J
                V = V J
            }
        }
    }
    // Finalize values and vectors
    for i in 1:n {
        σi = ‖ai‖2
        Ui = ai / σi
    }
    // Sort Σ and reorder U and V
```

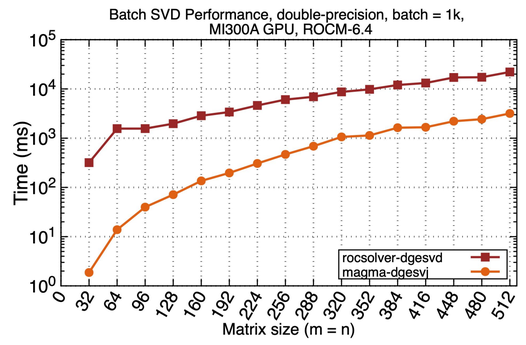
## Design Highlights

- Batch Hermitian eigensolver (HEEVJ):
  - Used to orthogonalize a batch of block-column pairs
  - Implements a two-sided Jacobi algorithm in shared memory
  - The value ***nb*** must be carefully tuned to respect the shared memory capacity
- Gram matrix computation
  - A baseline implementation require a batch Hermitian rank-k update (HERK)
  - Batch HERK is not supported in all backends: use batch GEMM instead
- Left and Right Vector Updates:
  - Baseline implementation uses batch GEMM, which dominates the execution time asymptotically (up to 67% in some cases)
  - A custom vector update kernel is developed, which delivers a **2.1*X*** speedup against the baseline updates (and more than 50% reduction in solution time, asymptotically)
- Masked Batch Operations:
  - A batch SVD solver may converge at different rates for different problems
  - The batch HEEVJ can be partially masked-off for converged problems
  - Similarly, the batch vector updates can be masked-off if the corresponding block-column pair(s) are already mutually orthogonal
  - Saves ~12% of the solution time, asymptotically

## Performance on relatively-large square problems

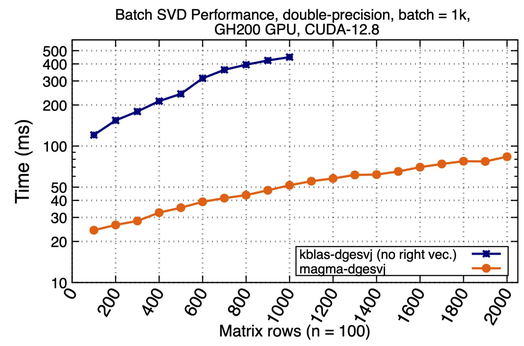
- Speedups:**1.7*X*** - **8.8*X*** against WcycleSVD, **1.1*X*** - **4.7*X*** against KBLAS, **7*X*** - **170.8*X*** against rocSOLVER
- WcycleSVD sometimes fails the orthogonality check for the left vectors

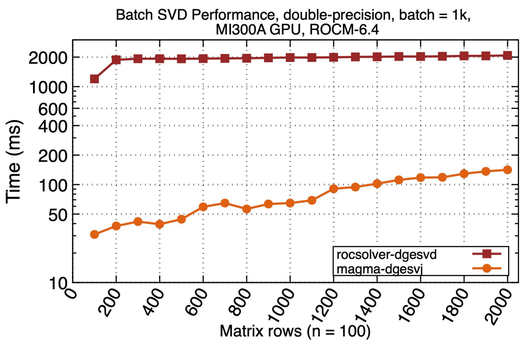



## Performance on Rectangular Shapes

- Speedups: **5*X*** - **9*X*** against KBLAS, **14.7*X*** - **49.6*X*** against rocSOLVER
- WcycleSVD did not produce accurate results in this test
- KBLAS has a limit on the number of rows, also uses a batch QR factorization as a pre-processing step




## Accuracy Requirements & Other GPU Solvers

All the following errors should be at most $\mathcal{O}(10^{-15})$

- $e_1 = \|A - U\Sigma V^T\| / (\|A\| \times max(M,N))$, $e_2 = \|I - U^TU\| / (M)$, $e_3 = \|I - VV^T\| / (N)$

| | cuSOLVER | rocSOLVER | KBLAS[1] | WcycleSVD[2] | MAGMA (this work) |
|---|---|---|---|---|---|
| **Algorithm** | Jacobi-based | Bidiagonalization + QR Algorithm | Jacobi-based | Jacobi-based | Jacobi-based |
| **Precisions** | FP32/FP64, real/complex | FP32/FP64, real/complex | FP32/FP64, real only | FP64, real only | FP32/FP64, real/complex |
| **Limitations on size** | M and N ≤ 32[1] | M ≥ N[1] | M ≥ N, M ≤ 1024[1] | M ≤ 1024[2] | None[1] |

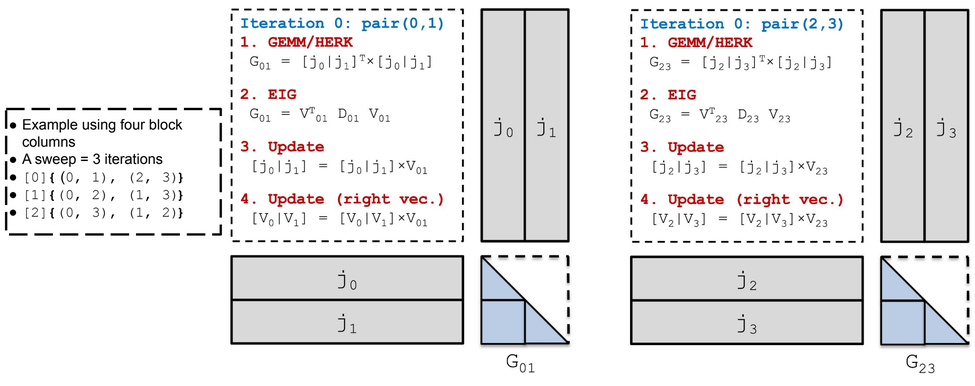
[1] All matrices must fit in GPU memory (along with any required workspace)
[2] Sometimes fails accuracy checks for supported dimensions

## Very Small Problems

- MAGMA uses a parallel scalar Jacobi algorithm that runs entirely in shared memory
- Speedups: **1.4*X*** - **2.6*X*** against KBLAS, **2.2*X*** - **33.9*X*** against cuSOLVER, **77*X*** - **514.7*X*** against rocSOLVER

## Parallel-blocked Jacobi Algorithm

- $A_{M \times N}$ is partitioned into block columns of width ***nb***
- Independent pairs of block-columns are orthogonalized




## Future Directions

- Explore performance optimizations for computing the Gram matrix
- Study the impact of the QR factorization on performance and convergence of the Jacobi method
- Extend the HEEVJ implementation to relax the constraints on the range of values for ***nb***

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