Workshop on Batched, Reproducible, and Reduced Precision BLAS

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Reference implementation and testing of batched BLAS routines

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Innovative Computing Laboratory

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Motivations

Reference implementation

- Demonstrate that the specification is implementable
- Help to improve the specification
- Provide a reliable code to validate other implementations

Testing

- Valid calling sequences
- Correctness of the computed results

Remarks

The reference implementation does not aim to be efficient

This presentation focuses on Level 3 batched BLAS routines

Outline

1. Reference implementation
2. Accuracy testing
3. Experimental results
4. Concluding remarks

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Overview of the reference implementation

1. Calling sequences with respect to the specification

$$
\begin{aligned}
\texttt{dgemm\_batch}(&\mathit{const\ enum} * transA,\ \mathit{const\ enum} * transB,\ \mathit{const\ int} * m,\\
&\mathit{const\ int} * n,\ \mathit{const\ int} * k,\ \mathit{const\ double} * alpha,\\
&\mathit{const\ double} * \mathit{const\ double} * arrayA,\ \mathit{const\ int} * lda,\\
&\mathit{const\ double} * \mathit{const\ double} * arrayB,\ \mathit{const\ int} * ldb,\\
&\mathit{const\ double} * beta,\ \mathit{double} * *arrayC,\ \mathit{const\ int} * ldc,\\
&\mathit{const\ int}\ batch\_count,\ \mathit{const\ enum}\ batch\_opts,\ \mathit{int} * info)
\end{aligned}
$$

- **batch_count**: style for the batched (**BATCH_FIXED, BATCH_VARIABLE**)
- **batch_opts**: number of sub-problems to be processed
- **info**: error handling array

Overview of the reference implementation

1. Calling sequences with respect to the specification
2. Arguments checking and error handling

Critical arguments

- Fixed size case: exit if any argument is incorrect
- Variable size case:
-
  - Exit for whole batch error (e.g. batch_count)
  - Continue for sub-problem error (e.g. matrix size)
- **Xerbla** for error handling
- Flexible error handling strategy

Overview of the reference implementation

1. Calling sequences with respect to the specification
2. Arguments checking and error handling
3. Call **reference** BLAS implementation to solve each sub-problem

```
for (iter = 0; iter < batch_count; iter++)
{
  Call a reference BLAS routine
}
```

According to the specification, the reference implementation should provide results as accurate as reference BLAS routines

Outline

Accuracy testing

Basic idea

- The quantity of interest is the relative error $err = \frac{\|C-\hat{C}\|}{\|C\|}$
- Typically we want $err \leq \tau\varepsilon$ where τ is some tolerance and ε is the machine epsilon e.g. $\varepsilon = 10^{-16}$

Remarks

- The tolerance τ is selected independently for each problem, e.g. $\tau = 10, 30, 100$ in MAGMA/LAPACK etc
- The choice of $\tau = 10, 30 \ldots$ may not be very rigorous
- Investigate a rigorous approach for small BLAS problems?

Accuracy testing

Error analysis approach

- Perform error analysis of BLAS routines [Nicholas J. Higham, 2002]
- Use the **forward/backward error bound** for accuracy testing
- $\|Forward\_Error\| \leq \|Forward\_Error\_Bound\|$ or $\|Residual\| \leq \|Backward\_Error\_Bound\|$

Remarks

- No need of intensive experiments to set a tolerance τ
- A rigorous error bound can seem pessimistic in general but meaningful for small BLAS problems

Accuracy testing

Forward error bound of GEMM

- Formula: $C = \alpha AB + \beta C_{init}$
- Forward error $\|C - \hat{C}\|_\infty$
- Forward error bound: $(N|\alpha|\|A\|_\infty\|B\|_\infty + |\beta|\|C_{init}\|_\infty)\varepsilon$

Remark

The computed solution $\hat{C}$ is acceptable if

$$\frac{\|C-\hat{C}\|_\infty}{(N|\alpha|\|A\|_\infty\|B\|_\infty+|\beta|\|C_{init}\|_\infty)\varepsilon} \leq 1$$

Accuracy testing

Backward error analysis of TRSM [Nicholas J. Higham, 2002]

Theorem: *Let the triangular systems $Tx = b$ where $T \in \mathbb{R}^{n\times n}$ is nonsingular, be solved by substitution with any ordering. Then the computed solution $\hat{x}$ satisfies $(T + \Delta T)\hat{x} = b$, $|\Delta T| \leq \gamma_n |T|$, where $\gamma_n = \frac{n\varepsilon}{1-n\varepsilon} \approx n\varepsilon$.*

Backward error bound of TRSM

- Formula: $AX = \alpha B$
- Backward error bound: $N\|A\|_\infty \|X\|_\infty \varepsilon$
- Note: TRSM's backward error bound does depend on B
- The solution $\hat{X}$ is acceptable if $\frac{\|A\hat{X} - \alpha B\|_\infty}{N\|A\|_\infty \|\hat{X}\|_\infty \varepsilon} \leq 1$

Accuracy testing: BLAS3 error bound summary

Routine	Formula	Error bound based success criteria
GEMM SYMM HEMM	$C = \alpha AB + \beta C_{init}$	$\frac{\|C - \hat{C}\|_\infty}{(N\|\alpha\|\|A\|_\infty \|B\|_\infty + \|\beta\|\|C_{init}\|_\infty)\varepsilon} \leq 1$
SYRK HERK	$C = \alpha AA^{T/H} + \beta C_{init}$	$\frac{\|C - \hat{C}\|_\infty}{(N\|\alpha\|\|A\|_\infty \|A\|_1 + \|\beta\|\|C_{init}\|_\infty)\varepsilon} \leq 1$
SYR2K HER2K	$C = \alpha AB^{T/H} + \alpha BA^{T/H} + \beta C_{init}$	$\frac{\|C - \hat{C}\|_\infty}{(N\|\alpha\|(\|A\|_\infty \|B\|_1 + \|B\|_\infty \|A\|_1) + \|\beta\|\|C_{init}\|_\infty)\varepsilon} \leq 1$
TRSM	$AX = \alpha B$	$\frac{\|AX - \alpha B\|_\infty}{N\|A\|_\infty \|X\|_\infty \varepsilon} \leq 1$

Accuracy testing: some remarks on the forward error bound

$$\frac{\|C - \hat{C}\|_\infty}{(N|\alpha|\|A\|_\infty\|B\|_\infty + |\beta|\|C_{init}\|_\infty)\varepsilon} \leq 1\,?$$

In our accuracy checking, we assume that the correct solution C of GEMM exists, what is not true in real-world applications.

$$\frac{\|C - \hat{C}\|_\infty}{(N|\alpha|\|A\|_\infty\|B\|_\infty + |\beta|\|C_{init}\|_\infty)\varepsilon} \leq 2\,?$$

- Our exact solutions: reference BLAS
- Problem: reference BLAS results have the same error bound
- Pessimistic approach: authorise twice the error bound

Outline

Some implementation details

Batched BLAS implementations tested

- **Batched_cuBLAS**: GEMM and TRSM
- **Batched_MAGMA**: GEMM, HERK, SYRK and TRSM
- **Batched_MKL**: only GEMM

Alternative to Batched on multi-core processor?

- **OMP_LOOP_MKL**: OpenMP loop over sequential MKL
- **PARALLEL_MKL**: single loop over parallel MKL

Additional details

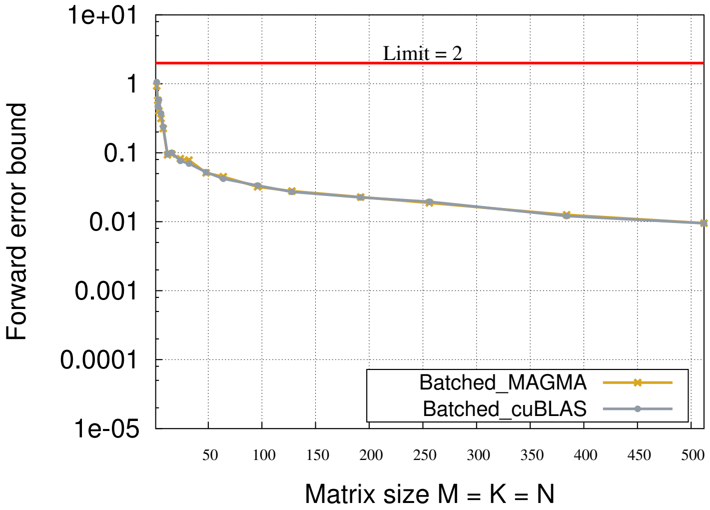
About the source code

- Programming language: C
- Precision: single, double, single complex and double complex
- Documentation: well documented (doxygen)
- First release coming soon

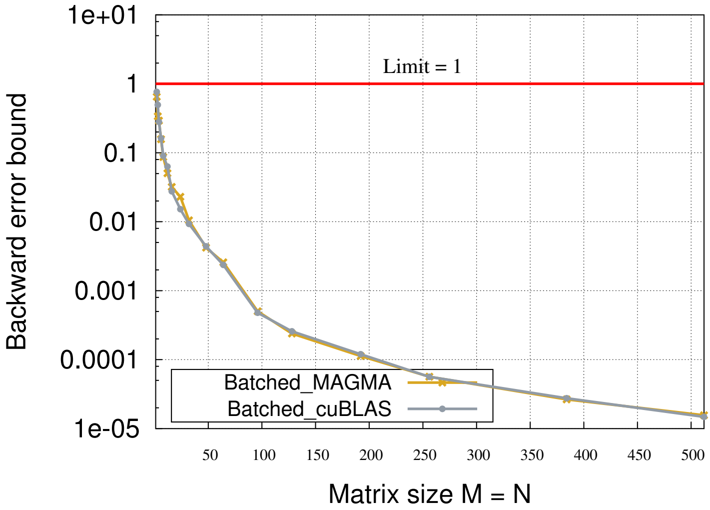
Hardware

- CPU: 2x10 Intel Xeon E5-2650 v3, 25M Cache, 2.30 GHz
- GPU: Nvidia K40c GPU with 2, 880 CUDA cores

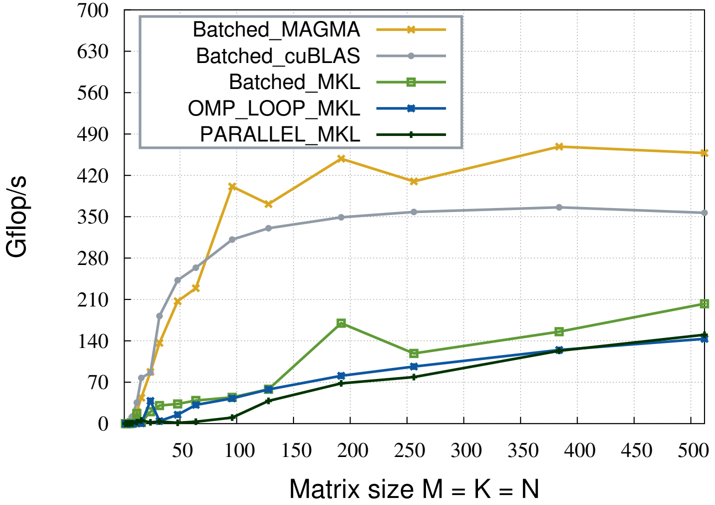
Accuracy of **1K** batched **DGEMM**



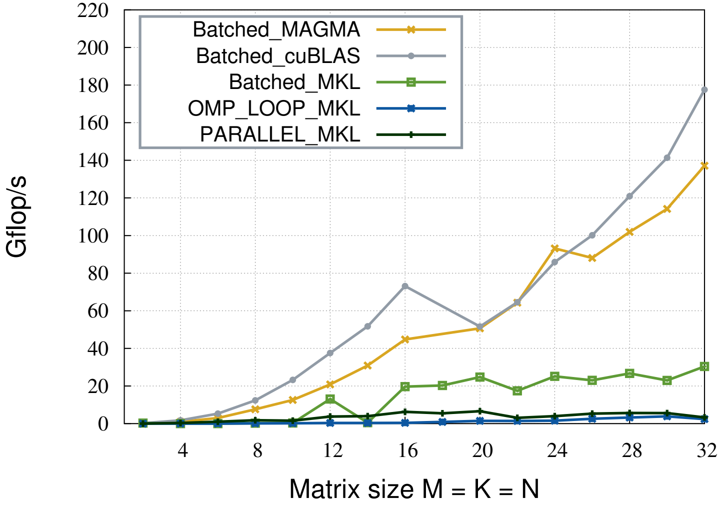
Accuracy of **1K** batched **DTRSM**



Performance of 1K batched DGEMM



Performance of **1K** batched **DGEMM**



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Concluding remarks and perspectives

Conclusion remarks

- Investigation of new accuracy checking
- Competitive performance cuBLAS/MAGMA
- MKL batched BLAS seems promising

Future work

- First release with respect to the final specification
- Extension to level 1 & 2 BLAS
- Provide fortran interface

Concluding remarks and perspectives

Conclusion remarks

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