Cholesky Factorization on Batches of Matrices with Fixed and Variable Sizes

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Motivation

Many scientific applications require solving a number of independent small-size problems, such as

- Astrophysics
- Quantum chemistry
- Metabolic networks
- Image and signal processing
- CFD and resulting PDEs through direct and multi-frontal solvers

Such independent problems may have the same size (batched routine) or different sizes (vbatched routine). We address both situations.

Introduction

Taking Cholesky Factorization as a case study, we consider problems of the form,

$$\texttt{xPOTRF}(A^{(1)}_{LDA_1 \times N_1}) \rightarrow L_1 L_1^\intercal$$
$$\texttt{xPOTRF}(A^{(2)}_{LDA_2 \times N_2}) \rightarrow L_2 L_2^\intercal$$
$$\dots$$
$$\texttt{xPOTRF}(A^{(k)}_{LDA_k \times N_k}) \rightarrow L_k L_k^\intercal$$

- Matrices $A^{(1)}$ through $A^{(k)}$ can have the same size or different sizes.
- Design is based on BLAS routines, which can be used for other factorizations (e.g. LU and QR)

Algorithmic Design

Factorization Loop: Blocked left-looking Cholesky factorization with small blocking size nb.

Algorithm 1: The blocked Cholesky factorization.

for $i \leftarrow 0$ **to** m **Step** nb **do**
  $\bar{m} \leftarrow m - i$;
  if $(i > 0)$ **then**
    Panel Update $C_{\bar{m} \times nb} = C_{\bar{m} \times nb} - A_{\bar{m} \times i} \times (B^T)_{i \times nb}$;
  end
  Tile Factorize $(C_1)_{nb \times nb} \leftarrow \text{Cholesky}(C_1)$ (unblocked dpotf2);
  Panel Factorize $(C_2)_{(\bar{m}-nb) \times nb} \leftarrow C_2 (C_1^T)^{-1}$ (dtrsm);
end

Two Kernel Design Approaches:

- Loop-inclusive: All factorization steps (iterations) are executed in one kernel to maximize chances of data reuse
- Loop-exclusive: Each iteration is executed in a separate kernel launch to optimize resource utilization

Design Methodology:

- Start with fixed size problems using loop-inclusive and loop-exclusive kernels
- Performance tuning across different values of nb
- Use the best performing fixed-size kernel to support variable size problems

Testing vbatched Routines

We use batches with size distributions that follow a uniform random distribution in the interval [1:N_{max}], where N_{max} can be specified by the user.

Optimization Techniques and Performance Results

1. System Setup:

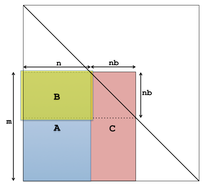
- 2 × 8-core Intel Sandy Bridge CPUs (Intel Xeon E5-2670, 2.6 GHz), 1 × Tesla K40c (745 MHz, ECC on)
- CUDA Toolkit 7.0, Intel MKL 11.3.0
- Results are shown for single and double precisions on batches of 3000 matrices

2. Key Changes to Routine Interface (in C)

- Input batches are passed as double pointer arrays
- In case of vbatched routines, matrix sizes and leading dimensions are passed as integer arrays
- Additional parameters: Batch sizes, and maximum dimension(s) across all matrices (for vbatched routines only)

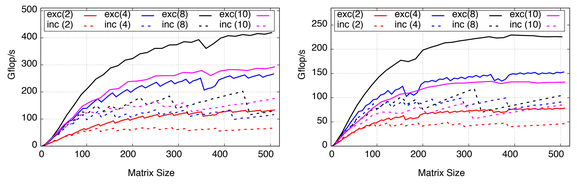
3. Symmetric Rank-k Updates

- The most dominating step (C = C - $A^T \times B$)
- We use double buffers to hide memory latency
- We also take advantage of the overlap between A and B to avoid redundant memory traffic
- Used in loop-inclusive and loop-exclusive kernels



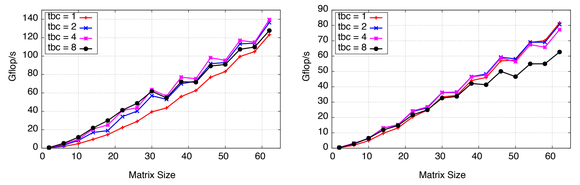
4. Performance Tuning

- Loop inclusive(inc.)/exclusive(exc.) kernels are tested against different values of nb
- Loop inclusive kernels do not utilize resources efficiently as the computation progresses, since more threads become idle



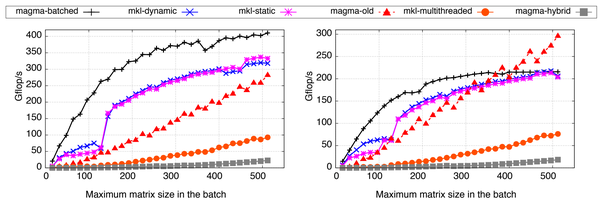
5. Thread Block (TB) Level Concurrency

- If matrices are very small, we can assign multiple matrices to a TB instead of one matrix
- Number of matrices per TB can be set dynamically during run time based on the matrix size
- Up to 2.86×/1.34× speedups in SP/DP



6. Final Fixed-size Performance

- Best competitor is a multicore CPU with dynamically unrolled OpenMP loop (one core per matrix)
- Up to 3×/2× speedups in SP/DP
- Improvement is more significant for smaller matrices



7. Adding support for vbatched factorization

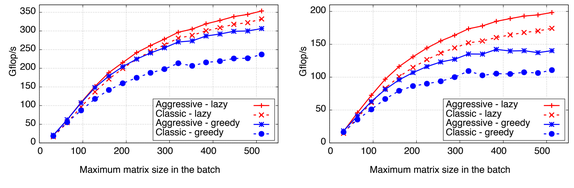
- Early Termination Scheme (ETM):
  - A vbatched kernel is always considered according to the largest matrix in the batch
  - ETMs detect and terminate threads with no work to do for smaller matrices in the batch
  - ETM-classic: can only terminate full thread blocks
  - ETM-aggressive: can also terminate idle threads in live thread blocks

8. Adding support for vbatched factorization "cont."

- Greedy vs. Lazy Scheduling
  - When should we start the factorization for smaller matrices in the batch?
  - Greedy scheduling: always start at the 0^{th}iteration.
  - Lazy scheduling: factorization of an arbitrary N×N matrix starts at iteration $\lceil \frac{N_{max}}{nb} \rceil - \lceil \frac{N}{nb} \rceil$.
  - Lazy scheduling tends to increase occupancy as the computation progresses (i.e. as the matrices gets smaller).

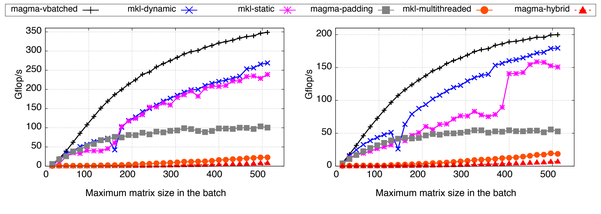
9. Impact of ETM and Scheduling Types

- With greedy scheduling, ETM-agressive is up to 50%/45% faster than ETM-classic in SP/DP
- If lazy scheduling is utilized, it improves ETM-classic by up to 87%/125% and ETM-agressive by up to 35%/90% in SP/DP



10. Final vbatched Performance

- Similarly, more performance improvement is observed in smaller matrices
- Up to 2.3×/1.88× speedups in SP/DP against the best competitor.



11. Future Directions

- Setting standard benchmarks for vbatched routines based on distributions from real applications
- Setting a standard interface for vbatched routine (e.g. like LAPACK)
- Error reporting to the user in batched routines (e.g. if the factorization succeeds except for one matrix)

References

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[3] Ahmad Abdelfattah, Azzam Haidar, Stanimire Tomov, and Jack Dongarra. Performance Tuning and Optimization of Fixed and Variable Size Batched Cholesky Factorization on GPUs. In *International Conference on Computational Science (ICCS)*, 2016. (submitted).

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