Mixed-precision orthogonalization process
Performance on multicore CPUs with GPUs

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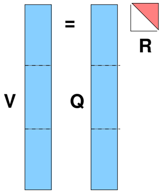
SIAM Conference on Applied Linear Algebra
Atalanta, U.S.A., 10-28-2015

TSQR: Tall-Skinny QR

orthogonalizes a set of dense columns vectors V (m-by-n, $m \gg n$),



where Q is a set of orthogonal vectors, and R is upper triangular.

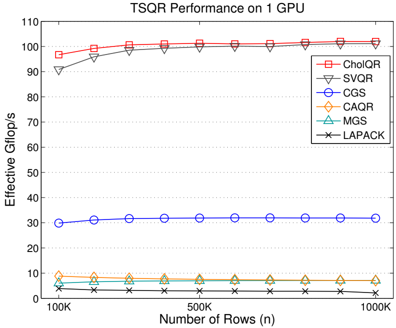
- important computational kernels:
  - 1st part of this talk: $n = O(10)$
    "Communication-avoiding" Krylov ($n = s$)
  - 2nd part of this talk: $n = O(100)$
    Random sampling for low-rank matrix approximation ($n = k + \ell$)

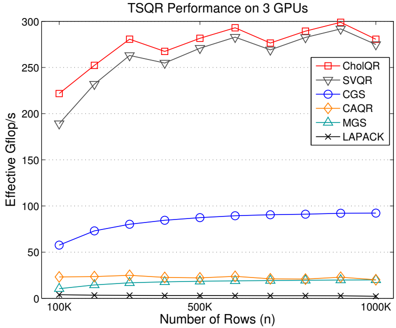
TSQR Algorithms

Many ways to compute *TSQR*:

- Householder QR (with $O(s)$ reductions)
  - Householder transform each column based on BLAS-1,2 xGEQR2
- Modified Gram-Schmidt (with $O(s)$ reductions)
  - ortho each column against each column based on BLAS-2,1 xGEMV, xDOT
- Classical Gram-Schmidt (with $O(s)$ reductions)
  - ortho each column against prev columns based on BLAS-2,1 xGEMV, xDOT
- Cholesky QR (or SVQR) (with $O(1)$ reductions)
  - ortho all columns against prev columns based on BLAS-3 xGEMM, xTRSM
- CAQR (with $O(1)$ reductions)
  - ortho all columns against prev columns based on tree-reduction BLAS-1,2 xGEQR2

TSQR Performance (16-core SandyBridge with three M2090 Fermi, $s = 30$)





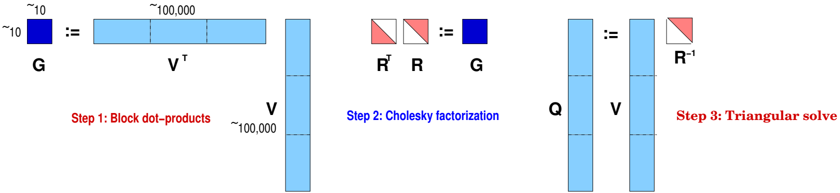
- CholQR shows superior performance based on BLAS-3
- performance depends more on intra-comm (BLAS performance) than on inter-comm.
- it scales well over 3 GPUs.

CholQR factorization for *TSQR* [A. Stathopoulos and K. Wu. 2002]

Step 1 Gram-matrix formation $G := V^T V$ ($\frac{1}{2} ns^2$ ops on GPUs).

Step 2 Cholesky factorization $R^T R := G$ ($\frac{1}{6} s^3$ ops on CPUs).

Step 3 Backward-substitution $Q := VR^{-1}$ ($\frac{1}{2} ns^2$ ops on GPUs).



- Most of flops using BLAS-3.
- Only a pair of global communication (reduction+broadcast).

TSQR Stability:

- trade-off between performance and stability
  - CholQR performs most of computation using BLAS-3.
  - Condition number of Gram matrix G is square of A.

	$\|I - Q^T Q\|$	# flops, GPU kernel	# GPU-CPU comm.
MGS	$O(\epsilon\kappa(V))$	$2ns^2$, BLAS-1 xDOT	$O(s^2)$
CGS	$O(\epsilon\kappa(V)^{s-1})$	$2ns^2$, BLAS-2 xGEMV	$O(s)$
CholQR	$O(\epsilon\kappa(V)^2)$	$2ns^2$, BLAS-3 xGEMM	$O(1)$
SVQR	$O(\epsilon\kappa(V)^2)$	$2ns^2$, BLAS-3 xGEMM	$O(1)$
CAQR	$O(\epsilon)$	$4ns^2$, BLAS-1,2 xGEQR2	$O(1)$

- it often requires reorthogonalization
- it could fail if $\kappa(V) > \epsilon^{-1/2}$.

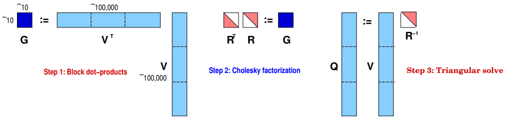
Mixed Precision CholQR

- Remove "square" in error bound by selectively using "doubled" precision:

  Step 1 Gram-matrix formation $G := V^T V$ (V in double)
  doubled-precision on GPUs.

  Step 2 Cholesky factorization $R^T R := G$
  doubled-precision on CPUs.

  Step 3 Backward-substitution $Q := VR^{-1}$
  working-precision on GPUs.



→ orthogonality error depends linearly on $\kappa(V)$ (more details in SISC paper, submitted)
$\|I - Q^T Q\| \leq O(\epsilon\kappa(V) + (\epsilon\kappa(V))^2)$ and $\|Q\| \leq 1 + O(\epsilon\kappa(V))$

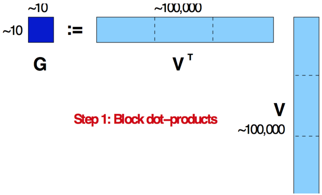
→ may require software-emulated arithmetics for doubled-precision
e.g., for working double, double-double to emumerate quadruple precision
computation increases by $8.5\times$ [Y. Hida, X. Li, and D. Bailey, '00], but
communication-bounded, $\frac{1+n}{2}$ flops per read
read V in double, only volume doubles to form G

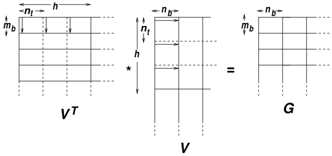
Batched GPU kernels for block inner-products

"batched" xGEMM/xSYRK kernel

1. thread block to compute partial block product
2. local reduction to compute partial Gram matrix
3. global all reduce to form final Gram matrix

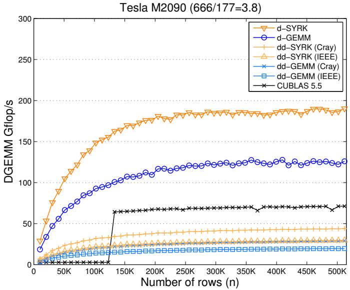
brute-force tune for dimension and precision on GPU
(by Tim Dong)

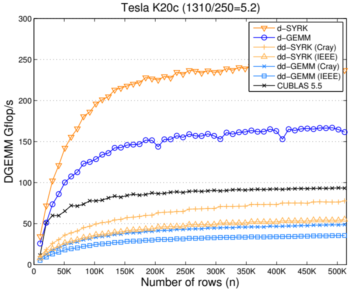




Block inner-products in double-double vs. double precision

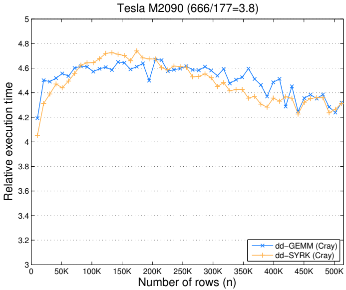
- optimized batched xGEMM kernel for block inner-product, $n = O(10^5), s = O(10)$.
  - 1.7× speedups over CUBLAS 5.5 for d-precision.
    30% of the peak based on memory bandwidth
  - 16× more ops for dd-precision (Cray).
    - input matrix in d-precision, compute intermediate results in dd-precision

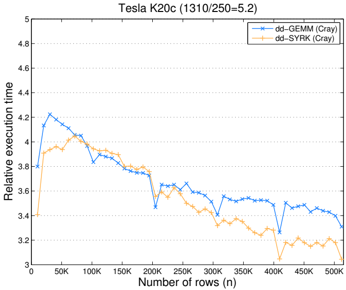




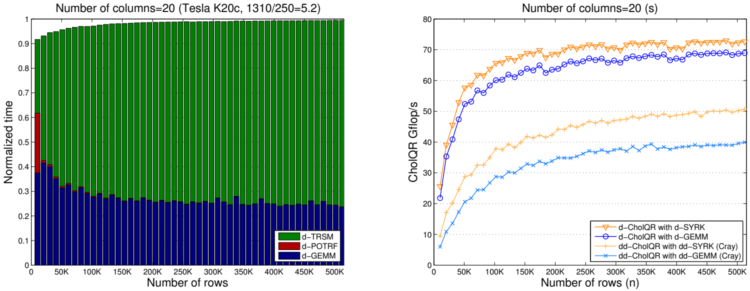
Block inner-products in double vs. double-double precision

- optimized batched xGEMM kernel for block inner-product, $n = O(10^5), s = O(10)$.
  - 1.7× speedups over CUBLAS 5.5 for d-precision.
  - 16× more ops for dd-precision (Cray).
  - memory-bound operation.
    → 4.5× or 3.5× slower on Fermi or Kepler.





Mixed Precision CholQR Performance



- only about 30% of d-CholQR in d-GEMM.
- dd-CholQR 8.5× ops, but 1.7× slower than d-CholQR
  - dd-CholQR may be competitive with 2×d-CholQR
    d- or dd-CholQR could fail if $\kappa(V) > \epsilon^{-1/2}$ or $> \epsilon^{-1}$
- CA-Krylov performance can be improved
  - reduced orthogonalization time, larger step size, or faster convergence

Extension to orthogonalize many columns

- Motivation: random sampling of large sparse matrix, $n = O(100)$
- CholQR performs $\frac{1+n}{2}$ flops on each numerical value read.
- As n increases,

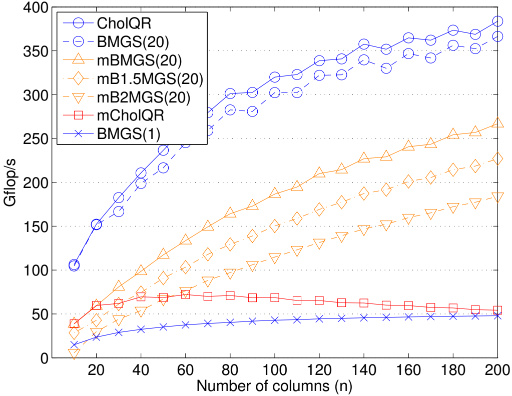
  - it becomes more compute-bound

  - mixed-precision CholQR becomes slower
- Use mixed-precision CholQR within block MGS

  - BMBS and then CholQR
    same bound by using mCholQR+CholQR
    with comp. overhead of $\frac{8.5}{n_t}\times$

  - restarted CA-Krlov to orthogonalize s vectors of m vectors at a time

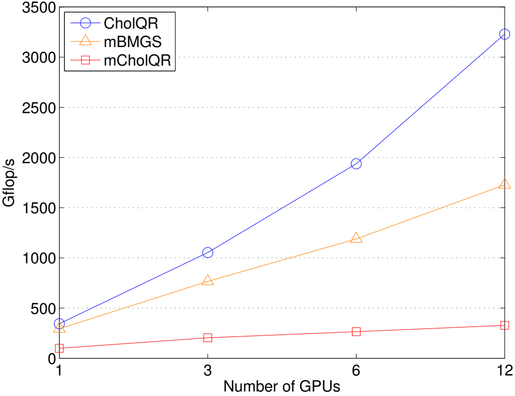
Performance of BMGS: $m = 100,000$ on one GPU



with $n = 200$,

- mCholQR was 7.1× slower than CholQR (with 8.5× ops)
- mB1.5MGS was 1.7× slower than CholQR (with 1.8× ops) and was 4.1× faster than mCholQR

Performance of BMGS: $(m, n) = (500,000,200)$ on multiple GPUs



compared to CholQR,

- B1.5MGS communicates $n_t \times$ more
- mCholQR has greater bottleneck with ddPOTRF

Final Remarks

- Mixed-precision CholQR
  - performs 8.5× more computation
  - reduces 2× more words, $O(n^2)$ with $n \ll m$
  - was 1.4× slower when $n = O(10)$
  - was 7.1× slower when $n = O(100)$
  - smaller overhead if supported by hardware (e.g., single)
- BMGS combined with dd-CholQR + d-CholQR
  - performs $\frac{8.5}{n_t}\times$ more computation, where n_t is number of block columns
  - was 1.7× slower when $n = O(100)$
  - communicates $n_t\times$ more often

Current Work

- Numerical studies and theoretical bounds
- CAQR based on batched QR
  [J. Demmel, L. Grigori, M. Hoemmen, J. Langou, 2012]

Thank you!!