QR Decomposition on GPUs in Multiple Double Precision

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Outline

problem statement

Given a linear system $A\mathbf{x} = \mathbf{b}$,
compute the least squares solution $\mathbf{x}$.

The least squares solution minimizes $\|\mathbf{b} - Ax\|_2^2$.

Two steps with the QR decomposition:

1. Compute the Householder QR factorization: $A = QR$.

   The blocked Householder QR [Bischof & Van Loan, 1987] is rich in matrix-matrix multiplications.

2. Solve the upper triangular system $R\mathbf{x} = Q^T\mathbf{b}$.

   Formulas in [Heller, 1978] are applied recursively in a parallel triangular matrix inversion [Nasri & Mahjoub, 2001].

Problem:
Can acceleration by Graphics Processing Units (GPUs) compensate the cost overhead caused by multiple double precision?

error analysis of a lower triangular block Toeplitz solver

joint with Simon Telen and Marc Van Barel, in the CASC 2020 proceedings

Solving $(A_0 + A_1 t + A_2 t^2 + \cdots + A_i t^i)(x_0 + x_1 t + x_2 t^2 + \cdots + x_i t^i)$
$= (b_0 + b_1 t + b_2 t^2 + \cdots + b_i t^i)$
leads to a lower triangular block system:

$$\left[\begin{array}{ccccc} A_0 & & & & \\ A_1 & A_0 & & & \\ A_2 & A_1 & A_0 & & \\ \vdots & \vdots & \vdots & \ddots & \\ A_i & A_{i-1} & A_{i-2} & \cdots & A_0 \end{array}\right] \left[\begin{array}{c} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_i \end{array}\right] = \left[\begin{array}{c} b_0 \\ b_1 \\ b_2 \\ \vdots \\ b_i \end{array}\right].$$

Let κ be the condition number of A_0. Let $\|A_0\| = \|x_0\| = 1$, $\|x_i\| \approx \rho^i$.
In our context, $\rho \approx 1/R$, where R is the convergence radius.

If $\|A_i\| \approx \rho^i$, then $\dfrac{\|\Delta x_i\|}{\|x_i\|} \approx \kappa^{i+1} \epsilon_{\rm mach}$, and accuracy is lost.

With multiple double precision, a small $\epsilon_{\rm mach}$ gives accurate results.

multiple double precision — error free transformations

```
Computing the 2-norm of a vector of dimension 64
of random complex numbers on the unit circle equals 8.
Observe the second double of the multiple double 2-norm.

double double : 8.00000000000000E+00 - 6.47112461314111E-32
  quad double : 8.00000000000000E+00 + 3.20475411419393E-65
  octo double : 8.00000000000000E+00 - 9.72609915198313E-129
```

- QDlib by Y. Hida, X. S. Li, and D. H. Bailey.
  Algorithms for quad-double precision floating point arithmetic.
  In the *Proceedings of the 15th IEEE Symposium on Computer Arithmetic*, pages 155–162, 2001.
- CAMPARY by M. Joldes, J.-M. Muller, V. Popescu, and W. Tucker.
  CAMPARY: Cuda Multiple Precision Arithmetic Library and Applications.
  In *Mathematical Software – ICMS 2016, the 5th International Conference on Mathematical Software*, pages 232–240, Springer-Verlag, 2016.

cost overhead of multiple double precision

	double double: 37.7x				
	$+$	$-$	$*$	$/$	Σ
add	8	12			20
mul	5	9	9		23
div	33	18	16	3	70
	quad double: 439.3x				
	$+$	$-$	$*$	$/$	Σ
add	35	54			89
mul	99	164	73		336
div	266	510	112	5	893
	octo double: 2379.0x				
	$+$	$-$	$*$	$/$	Σ
add	95	174			269
mul	529	954	259		1742
div	1599	3070	448	9	5126

alternatives and related work

- T. Nakayama and D. Takahashi. Implementation of multiple-precision floating-point arithmetic library for GPU computing. In *Proc. 23rd IASTED International Conference on Parallel and Distributed Computing and Systems (PDCS 2011)*, pages 343–349. ACTA Press, 2011.
- K. Isupov and V. Knyazkov. Multiple-precision matrix-vector multiplication on graphics processing units. *Program Systems: Theory and Applications* 11(3): 62–84, 2020.
  - The double double arithmetic of CAMPARY performs best for the problem of matrix-vector multiplication.
  - Concerning quad double precision, *“the CAMPARY library is faster than our implementation; however as the precision increases the execution time of CAMPARY also increases significantly.”*

Graphics Processing Units (GPUs)

- Data parallel algorithms execute the same Single Instruction on Multiple Data elements (SIMD).
- Memory bandwidth of GPUs is typically ten times higher than the memory bandwidth of CPUs.

Definition (CGMA ratio)

The *Compute to Global Memory Access (CGMA) ratio* is the number of floating-point calculations performed by a kernel for each access to the global memory.

- The NVIDIA K20C, P100, and V100 are capable of teraflop performance in double precision.

five different NVIDIA GPUs

NVIDIA GPU	CUDA	#MP	#cores/MP	#cores	GHz
Tesla C2050	2.0	14	32	448	1.15
Kepler K20C	3.5	13	192	2496	0.71
Pascal P100	6.0	56	64	3584	1.33
Volta V100	7.0	80	64	5120	1.91
GeForce RTX 2080	7.5	46	64	2944	1.10

The double precision peak performance of the P100 is 4.7 TFLOPS. At 7.9 TFLOPS, the V100 is 1.68 times faster than the P100.

To evaluate the algorithms, compare the ratios of the wall clock times on the P100 over V100 with the factor 1.68.

For every kernel, the number of arithmetical operations is accumulated. The total number of double precision operations is computed using the cost overhead multipliers.

customized software

The code for the arithmetical operations generated by the CAMPARY software was customized for each precision.

- Instead of representing a quad double by an array of four doubles, all arithmetical operations work on four separate variables, one for each double.
  By this customization an array of quad doubles is stored as four separate arrays of doubles and a matrix of quad doubles is represented by four matrices of doubles.
- The `double2` and `double4` types of the CUDA SDK work for double double and quad double, but not for the more general multiple double arithmetic.
- QDlib provides definitions for the square roots and various other useful functions for double double and quad double arithmetic. Those definitions are extended to octo double precision.

computational algebraic geometry

The lower triangular block Toeplitz matrix originates
from the application of Newton's method
to compute power series developments of algebraic curves.

Power series are a symbolic-numeric way to solve polynomial systems.

With S. Telen, M. Van Barel: A Robust Numerical Path Tracking Algorithm for Polynomial Homotopy Continuation.
SIAM Journal on Scientific Computing 42(6):A3610–A3637, 2020.

Two computational tasks for polynomial homotopy continuation:

1. evaluation and differentiation of polynomials,
2. solving linear systems.

Both tasks are suitable for acceleration with graphics processing units.

the blocked Householder QR

Consider a $3m$-by-$3n$ tiled matrix, $m \geq n$:

$$A = \left[\begin{array}{c|c|c} & \multicolumn{2}{c}{A_{1,2}} \\ \cline{2-3} A_{1,1} & A_{2,2} & A_{2,3} \\ \cline{3-3} & & A_{3,3} \end{array} \right], \qquad \begin{array}{l} A_{1,1} \text{ is } 3m\text{-by-}n, \\ A_{1,2} \text{ is } m\text{-by-}2n,\ A_{2,3} \text{ is } m\text{-by-}n, \\ A_{2,2} \text{ is } 2m\text{-by-}n,\ A_{3,3} \text{ is } m\text{-by-}n. \end{array}$$

The Householder transformations are accumulated in an orthogonal $3m$-by-$3m$ matrix Q.

The upper triangular reduction R of A is written in the matrix A.

Early GPU implementations:

- Baboulin, Dongarra, and Tomov, TR UT-CS-08-200, 2008
- Kerr, Campbell, and Richards, GPGPU'09 conference
- Volkov and Demmel, Conference on Supercomputing, 2008

evolution of Q and R, I is the identity matrix

$$
\begin{array}{rcl}
A,\ Q & = & \left[\begin{array}{c|c} A_{1,1} & \begin{array}{c} A_{1,2} \\ \hline \begin{array}{c|c} A_{2,2} & \begin{array}{c} A_{2,3} \\ \hline A_{3,3} \end{array} \end{array} \end{array} \end{array}\right], \quad \left[\begin{array}{c|c|c} I & & \\ & I & \\ & & I \end{array}\right] \\[1em]
& \rightarrow & \left[\begin{array}{c|c} R_{1,1} & \begin{array}{c} R_{1,2} \\ \hline \begin{array}{c|c} A_{2,2} & \begin{array}{c} A_{2,3} \\ \hline A_{3,3} \end{array} \end{array} \end{array} \end{array}\right], \quad \left[\begin{array}{c|c|c} Q_1 & I & \\ & & I \end{array}\right] \\[1em]
& \rightarrow & \left[\begin{array}{c|c} R_{1,1} & \begin{array}{c} R_{1,2} \\ \hline \begin{array}{c|c} R_{2,2} & \begin{array}{c} R_{2,3} \\ \hline A_{3,3} \end{array} \end{array} \end{array} \end{array}\right], \quad \left[\begin{array}{c|c|c} Q_1 & Q_2 & \\ & & I \end{array}\right] \\[1em]
& \rightarrow & \left[\begin{array}{c|c} R_{1,1} & \begin{array}{c} R_{1,2} \\ \hline \begin{array}{c|c} R_{2,2} & \begin{array}{c} R_{2,3} \\ \hline R_{3,3} \end{array} \end{array} \end{array} \end{array}\right], \quad \left[\begin{array}{c|c|c} Q_1 & Q_2 & Q_3 \end{array}\right].
\end{array}
$$

Householder Reflectors

The Householder reflector P is represented by a vector $\mathbf{v}$:

$$P = I - \beta \mathbf{v}\mathbf{v}^T, \quad \beta = 2/\mathbf{v}^T\mathbf{v}, \quad P\mathbf{x} = \|\mathbf{x}\|_2 \mathbf{e}_1,$$

where $\mathbf{x}$ is the current column and $\mathbf{e}_1 = (1, 0, \ldots, 0)^T$.

The Householder matrices are aggregated in an orthogonal matrix

$$P_{WY} = I + WY^T,$$

where Y stores the Householder vectors in a trapezoidal shape.
W is defined by the Householder vectors and the corresponding βs.

With this WY representation, the updates to Q and R are

$$\begin{array}{rcl} Q & = & Q + Q \star W \star Y^T, \\ R & = & R + Y \star W^T \star C, \end{array}$$

which involve many matrix-matrix products.

four stages, several kernels

Algorithm 2: BLOCKED ACCELERATED HOUSEHOLDER QR.

Input : N is the number of tiles,
n is the size of each tile,
M is the number of rows, $M \geq Nn$,
A is an M-by-Nn matrix.

Output : Q is an orthogonal M-by-M matrix,
R is an M-by-Nn matrix, $A = QR$.

For k from 1 to N do

1. Compute Householder vectors for one tile, reduce $R_{k,k}$.
2. Define Y, compute W and $Y \star W^T$.
3. Add $Q \star YW^T$ to update Q.
4. If $k < N$, add $YW^T \star C$ to update R.

Householder QR is cubic in the dimension

The code is written for multiple double precision.

Thanks to the high Compute to Global Memory Access ratios of multiple double precision, entries of a matrix can be loaded directly into the registers of a kernel (bypassing shared memory).

The computation cost is proportional to M^3, for $M = Nn$.
The hope is to reduce the cost by a factor of M.

data staging

A matrix A of multiple doubles is stored as $[A_1, A_2, \ldots, A_m]$,

- A_1 holds the most significant doubles of A,
- A_m holds the least significant doubles of A.

Similarly, $\mathbf{b}$ is an array of m arrays $[\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_m]$,
sorted in the order of significance.

In complex data, real and imaginary parts are stored separately.

The main advantages of this representation are twofold:

1. facilitates staggered application of multiple double arithmetic,
2. benefits efficient memory coalescing,
   as adjacent threads in one block of threads read/write adjacent data in memory, avoiding bank conflicts.

experimental setup

About the input matrices:

- Random numbers are generated for the input matrices.
- Condition numbers of random triangular matrices almost surely grow exponentially [Viswanath & Trefethen, 1998].
- In the standalone tests, the upper triangular matrices are the Us of an LU factorization of a random matrix, computed by the host.

Two input parameters are set for every run:

- The size of each tile is the number of threads in a block.
  The tile size is a multiple of 32.
- The number of tiles equals the number of blocks.
  As the V100 has 80 streaming multiprocessors,
  the number of tiles is at least 80.

5 GPUs on 8×128, double double, milliseconds, Gigaflops

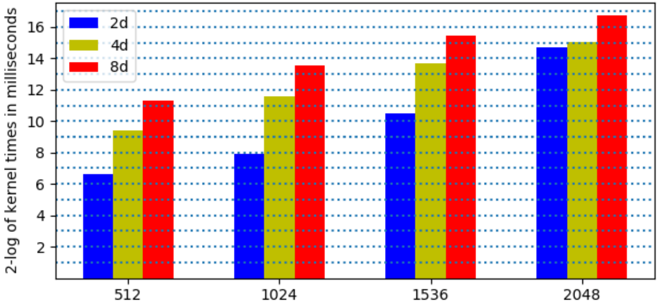
stage in	Linux on the host				Windows
Algorithm 2	C2050	K20C	P100	V100	RTX 2080
β, v	35.5	43.8	21.4	16.2	26.2
$\beta R^T \star v$	418.8	897.8	89.6	76.6	389.7
update R	107.0	107.6	23.0	15.2	47.5
compute W	1357.8	1631.8	349.2	222.4	1298.4
$Y \star W^T$	100.0	50.3	9.7	6.6	153.5
$Q \star WY^T$	790.9	423.9	77.2	52.1	1228.8
$YWT \star C$	6068.5	2345.2	141.2	61.6	822.6
$Q + QWY$	2.4	1.6	0.4	0.4	0.7
$R + YWTC$	7.4	4.2	0.7	0.5	0.8
all kernels	8888.3	5506.1	712.4	451.5	3968.2
wall clock	9083.0	5682.0	826.0	568.0	4700.0
kernel flops	115.8	187.0	1445.3	2280.4	259.5
wall flops	113.4	181.2	1247.2	1812.7	219.1

2-logarithms of times on the V100 in 3 precisions

For increasing dimensions,
we expect the time to be multiplied by 8 when the dimension doubles.

Increasing precision, multipliers are 11.7 (2d to 4d) and 5.4 (4d to 8d).

$512 = 4 \times 128$, $1024 = 8 \times 128$, $1536 = 12 \times 128$, $2048 = 16 \times 128$

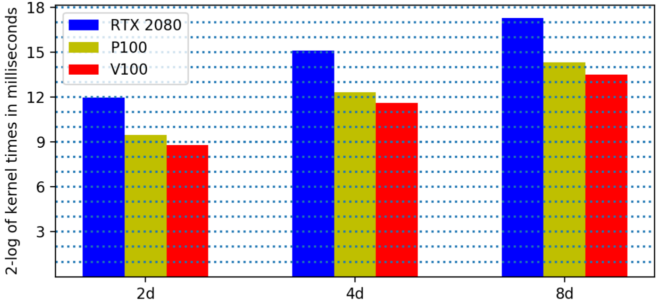


The performance drops at 2048 in double double precision.

2-logarithms of times on 3 GPUs in 3 precisions

Increasing precision, multipliers are 11.7 (2d to 4d) and 5.4 (4d to 8d).

On 8 tiles for size 128:



The observed cost overhead factors are less than the multipliers.
The heights of the bars follow a regular pattern.

least squares on the V100 in 4 precisions, 8×128

BS = Back Substitution, times in milliseconds, flops unit is Gigaflops.

stage	1d	2d	4d	8d
QR kernel time	157.9	451.1	3020.6	11924.5
QR wall time	204.0	566.0	3203.0	12244.0
BS kernel time	2.0	4.0	28.0	114.5
BS wall time	4.0	7.0	35.0	127.0
QR kernel flops	303.4	2282.2	3369.8	4041.4
QR wall flops	235.1	1819.6	3177.8	3936.1
BS kernel flops	8.1	89.8	127.9	149.1
BS wall flops	4.2	49.8	102.9	134.5
total kernel flops	299.6	2262.9	3340.0	4004.4
total wall flops	230.8	1797.3	3144.7	3897.0

Teraflop performance is attained already in double double precision.

conclusions

Taking 439, the average number of double operations in the tallies of the operational counts for quad double arithmetic, as the scaling factor, teraflop performance on a GPU can be viewed as 2.2 gigaflops on a single threaded computation.

Using this interpretation, the experiments show that GPU acceleration does compensate the cost overhead of quad double arithmetic.

In any case, the observed cost overhead ratios in going from double double to quad double are less than the ratios predicted by the operational count tallies, thanks to the high CGMA ratios.

The good performance on problems of dimension 1,024 in quad double precision observed on many GPUs should be encouraging to consider the use of multiple double arithmetic in scientific applications.

All code is available under the GPL-3.0 license at
`https://github.com/janverschelde/PHCpack/src/GPU/Matrices`