Randomization Algorithm to Compute Low-Rank Approximation

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Outline

- Background
- Algorithm and Math Model
- Project Scheme
- Performance Results
- Motivation and Application of Randomized Approximation
- Future Work

Background-General SVD

$A = U\sum V^T$

$U = [u_1 u_2, \ldots, u_M] \in R_M \times R_M$

$V = [v_1 v_2, \ldots, v_N] \in R_N \times R_N$

$\Sigma = \mathrm{diag}(\sigma 1, \ldots, \sigma \nu) = U^T A V$, $\Sigma \in R_M \times R_N$, $\nu = \min\{M, N\}$, $\sigma 1 \geq \sigma 2 \geq \ldots \geq \sigma \nu \geq 0$.

Background-General SVD

Example: $A=U\Sigma V^T$

A

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 2 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{U} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{\Sigma} = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{V}^* = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \sqrt{0.2} & 0 & 0 & 0 & \sqrt{0.8} \\ 0 & 0 & 0 & 1 & 0 \\ -\sqrt{0.8} & 0 & 0 & 0 & \sqrt{0.2} \end{bmatrix}$$

$$\mathbf{U}\mathbf{U}^\mathbf{T} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \mathbf{I}_4$$

$$\mathbf{V}\mathbf{V}^\mathbf{T} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} = \mathbf{I}_5$$

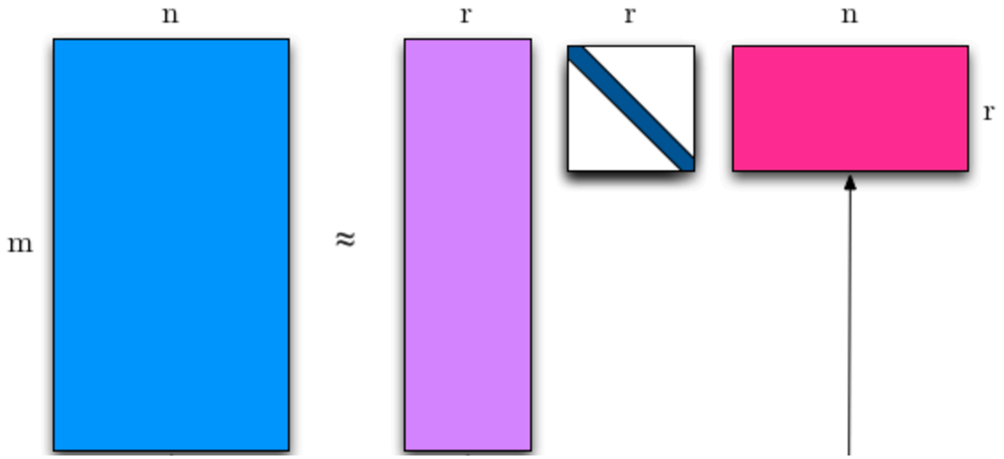
Background

- Low-Rank SVD Approximation

$A = U_k \Sigma_k V_k^t$

Σ_k: largest k singular values of A

large matrix in image processing



- LAPACK/MAGMA/CUBLAS-XT software framework

Algorithm--Power iteration

Matlab Code “svd_rand./” SVD approximation

```
function [u,s,v] = svd_rand(A, k, l, max_iters)
q = randn(n,k+l);
[q,r] = qr(q,0);
   for iter=1:(max_iters-1)
      p = A*q;
      q = A'*p;
      [q,r] = qr(q,0);
   end
 p = A*q;
   [p,b] = qr(p,0);
end
[x,s,y] = svd(b);
```

u_k = p*x(:,1:k);

s = s(1:k,1:k);

v_k= q*y(:,1:k);

Algorithm and Math Model

- Input: mxn matrix A, int k,

1. Draw a random nx(k+l) matrix Ω.
2. Compute QR of $(AA^T)^q A \Omega$
3. and SVD:
4. Truncate SVD $Q^T A = \hat{U}\hat{\Sigma}\hat{V}^T$

$$\hat{U}_k \hat{\Sigma}_k \hat{V}_k^T$$

- Output:

$$B = (Q\hat{U}_k)\hat{\Sigma}_k \hat{V}_k^T$$

QR needs done carefully for numerical accuracy.

Algorithm is old one when q = 0; but q = 1 far more accurate.

Should converge faster when singular values do not decay very fast.

Thm [Limited Warranty] (Halko/Martinsson/Tropp, 2011)

$$\|A - B\|_2 = O(\sigma_{k+1}) > \sigma_{k+1}$$

with failure probability $5p^{-p}$

Computational Cost

LAPACK SVD: M*N*N floating point operations (FLOPS)

randomization algorithm: {2*[2*M*(K+L)*N]*max_iterations} FLOPS

M*N*N>{2*[2*M*(K+L)*N]*max_iterations}

N>4*(K+L)*max_iterations

P=A*Q/ Q=A^T*P: 2*N*M*K FLOPS

Matrix	Size
A	M-by-N
Q	N-by-(K+L)
P	M-by-(K+L)
B	(K+L)-by-(K+L)
X	(K+L)-by-(K+L)
Y^T	(K+L)-by-(K+L)
SI	(K+L)-by-1
S	K-by-1
u_k	M-by-K
v_k	N-by-K

QR Decomposition

Consider the decomposition of

$$A = \begin{pmatrix} 12 & -51 & 4 \\ 6 & 167 & -68 \\ -4 & 24 & -41 \end{pmatrix}.$$

Recall that an orthonormal matrix Q has the property

$$Q^T Q = I.$$

Then, we can calculate Q by means of Gram–Schmidt as follows:

$$U = (\mathbf{u}_1 \quad \mathbf{u}_2 \quad \mathbf{u}_3) = \begin{pmatrix} 12 & -69 & -58/5 \\ 6 & 158 & 6/5 \\ -4 & 30 & -33 \end{pmatrix};$$

$$Q = \left(\frac{\mathbf{u}_1}{\|\mathbf{u}_1\|} \quad \frac{\mathbf{u}_2}{\|\mathbf{u}_2\|} \quad \frac{\mathbf{u}_3}{\|\mathbf{u}_3\|} \right) = \begin{pmatrix} 6/7 & -69/175 & -58/175 \\ 3/7 & 158/175 & 6/175 \\ -2/7 & 6/35 & -33/35 \end{pmatrix}.$$

[q,r] = qr(q,0);
q=q*r

In linear algebra, a **QR decomposition** (also called a **QR factorization**) of a matrix is a **decomposition** of a matrix A into a product A = **QR** of an orthogonal matrix Q and an upper triangular matrix R.

Thus, we have

$$Q^T A = Q^T Q R = R;$$

$$R = Q^T A = \begin{pmatrix} 14 & 21 & -14 \\ 0 & 175 & -70 \\ 0 & 0 & 35 \end{pmatrix}.$$

Optimization of the algorithm Cholesky QR

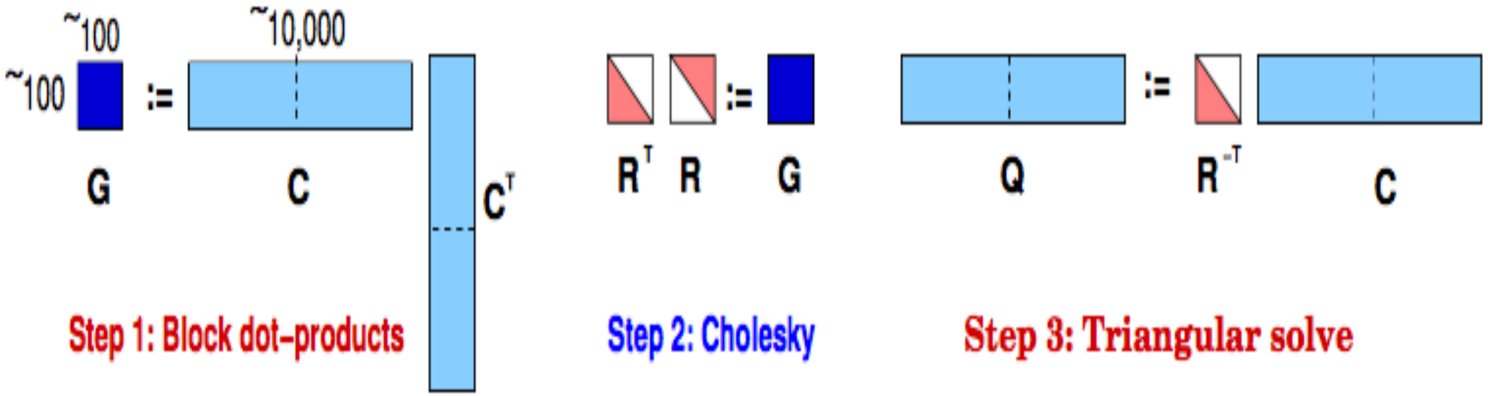
efficiency (Gflops/s): giga-flops per second: 10^9 flops per second

algorithm of Cholesky QR Decomposition:

(1) $G=C^TC$

(2) $G=R^TR$

(3) $Q=CR^{-1}$



Optimization of the algorithm Cholesky QR

(1)G=C^TC

(2)G=R^TR

(3) Q=CR⁻¹

- suppose C is an m $\times$ n matrix with linearly independent columns
- the matrix G = C^TC is positive definite

every positive definite matrix G $\in$ Rn$\times$n can be factored as G= R^TR where R is upper triangular with positive diagonal elements

- complexity of computing R is $(1/3)n^3$ flops
- R is called the Cholesky factor of G

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} R_{11} & 0 & 0 \\ R_{12} & R_{22} & 0 \\ R_{13} & R_{23} & R_{33} \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} & R_{13} \\ 0 & R_{22} & R_{23} \\ 0 & 0 & R_{33} \end{bmatrix}$$

$$= \begin{bmatrix} 5 & 0 & 0 \\ 3 & 3 & 0 \\ -1 & 1 & 3 \end{bmatrix} \begin{bmatrix} 5 & 3 & -1 \\ 0 & 3 & 1 \\ 0 & 0 & 3 \end{bmatrix}$$

Optimization of the algorithm Cholesky QR

EXAMPLE

$$B = \begin{bmatrix} 3 & -6 \\ 4 & -8 \\ 0 & 1 \end{bmatrix}, \qquad A = B^T B = \begin{bmatrix} 25 & -50 \\ -50 & 101 \end{bmatrix}$$

1. Cholesky factorization:

$$A = \begin{bmatrix} 5 & 0 \\ -10 & 1 \end{bmatrix} \begin{bmatrix} 5 & -10 \\ 0 & 1 \end{bmatrix}$$

2. QR factorization

$$B = \begin{bmatrix} 3 & -6 \\ 4 & -8 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 3/5 & 0 \\ 4/5 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 5 & -10 \\ 0 & 1 \end{bmatrix}$$

Optimization of the algorithm

```
[han123@comet-33-02 testing]$ ./testing_dgesvd_rand --range 10000,2000,20 -l --niter 1 -c
% MAGMA 2.2.0 svn compiled for CUDA capability >= 3.0, 32-bit magma_int_t, 64-bit pointer.
% CUDA runtime 7000, driver 8000. OpenMP threads 1. MKL 11.3.3, MKL threads 1.
% device 0: Tesla P100-PCIE-16GB, 405.0 MHz clock, 16276.2 MiB memory, capability 6.0
% Wed Jul 26 07:35:06 2017
% Usage: ./testing_dgesvd_rand [options] [-h|--help]

 Error is ||A - Uk*Sk*Vk^T||_2, L=K, performs 1 iterations

%   M     N     K      LAPACK time (s)    Randomized time (s)      LAPACK error         Randomized error
%                                         CPU, GPU, NGR, UMA                            CPU, GPU, NGR, UMA
%===================================================================================================================

Intel MKL ERROR: Parameter 5 was incorrect on entry to DGEQRF.
  QR(Q)     : 5.31e-04 second,   24.27Gflop/s
  Gemm(Q)   : 8.73e-04 second, 3665.15Gflop/s
  Gemm(P)   : 1.27e-03 second, 1256.96Gflop/s
  QR(P)     : 3.13e-04 second,  103.37Gflop/s
  SVD       : 5.89e-04
  GEMM(X)   : 9.80e-05 second,  163.28Gflop/s
  GEMM(Y)   : 4.60e-05 second,   69.54Gflop/s
  GET-SET   : 1.88e-02
  laset     : 0.00e+00
  lacpy     : 0.00e+00
  ungqr     : 0.00e+00
    Total   : 2.26e-02
simpleCUBLASXT test running..
10000  2000    20     13.28            0.19, 0.03, 0.15, 4.01      4.09e+01       4.15e+01,4.15e+01,4.15e+
01,4.15e+01      (S[20]=4.09e+01)
[han123@comet-33-02 testing]$ make testing_dgesvd_rand
```

Project Scheme

1. Implementing the randomized algorithm using LAPACK on CPU

2. Implementing the randomized algorithm using MAGMA on GPU

3. Implementing the out-of-memory randomized algorithm on GPU

-manual pipelining.

-UMA

-CUBLAS-XT

4. set up tester to compare performances

Out-of-Memory GPU Implementation

Device: Tesla K80, 823.5 MHz clock, 11439.9 MiB memory, capability 3.7

1 MiB = 2^{20} bytes = 1024 kibibytes = 1048576bytes

11439.9Mib$*$1048576=1.1996e+10 bytes

Sqrt(12e9/8)=3.8730e+04

Out-of-Memory GPU Implementation manual pipelining

P=A*Q

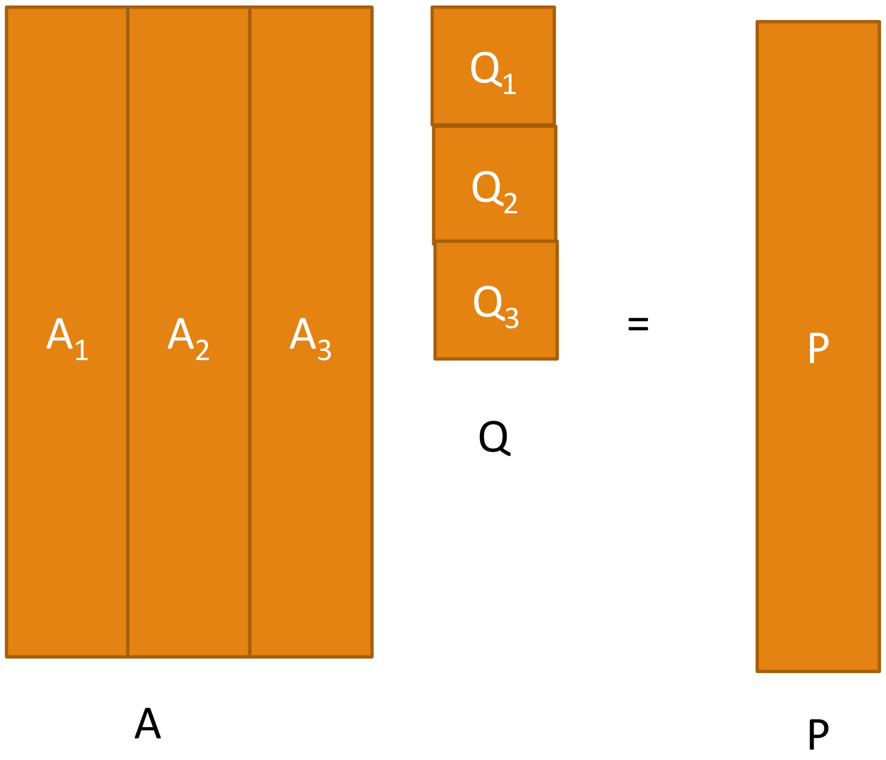
P=0;

For k=1,2,3…..

set (A_k to dA);

$P=P+A_kQ_k$;

end



Out-of-Memory GPU Implementation manual pipelining

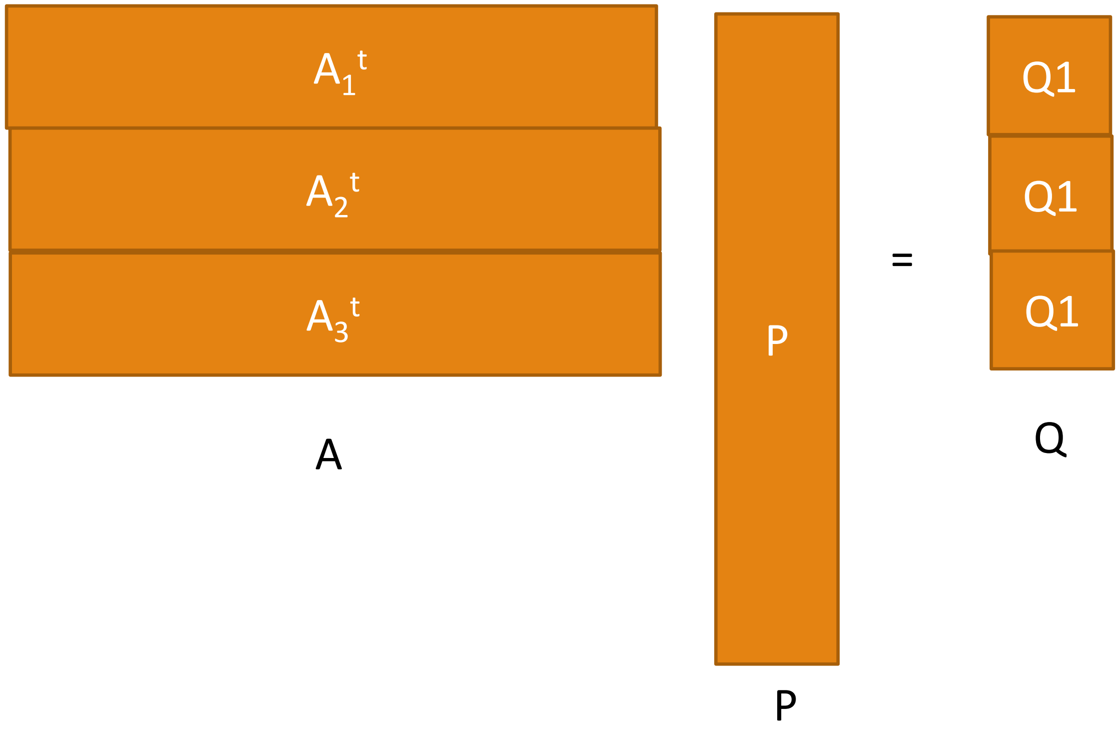
$Q=A^t*P$

For k=1,2,3…..

set (A_k to dA);

$Q_k=A_k^tP$;

end



Out-of-Memory GPU Implementation manual pipelining

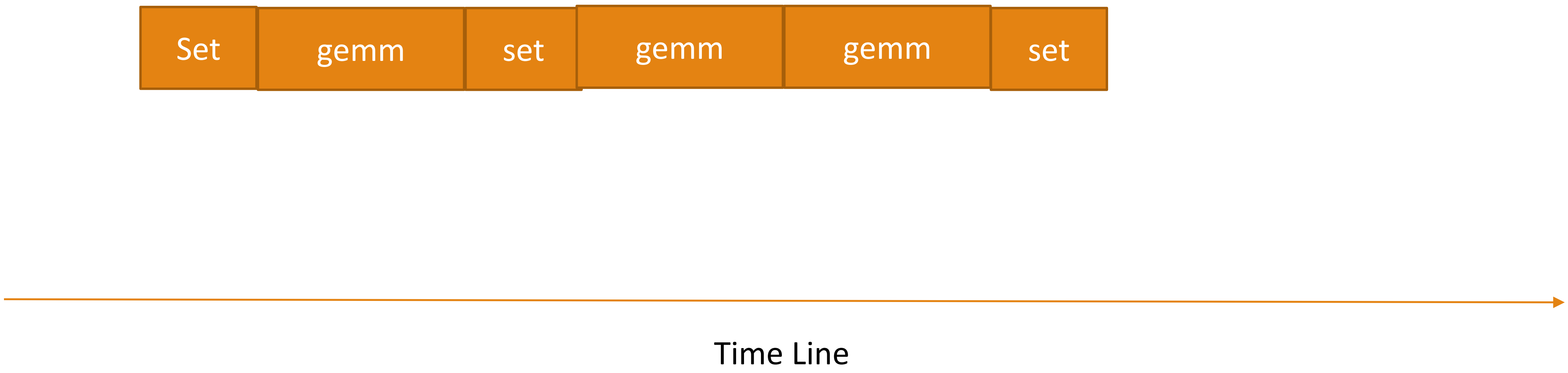
NB: the number of rows of A_i

calling *cudaMemGetInfo()*

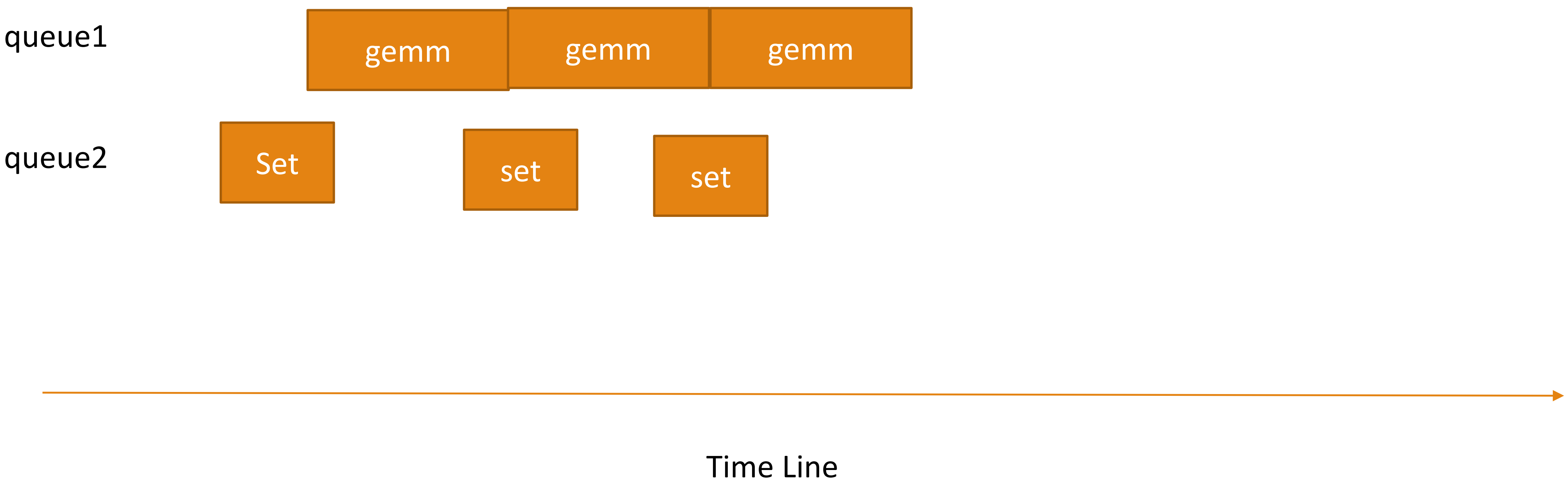
*NB = (0.8 * (freeMem/sizeof (magmaDoubleComplex)))/ (N * num_queues);*

NB = MAX (1, MIN (MIN (N, KL), NB));

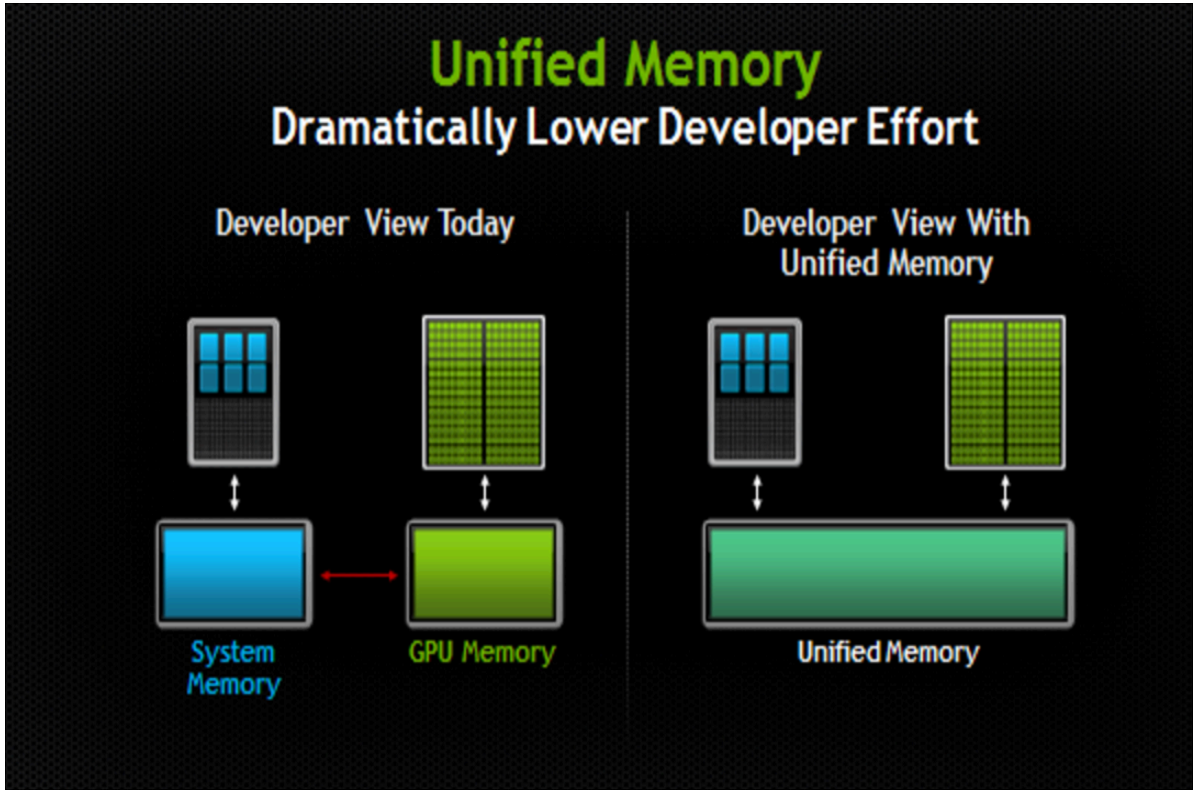
Out-of-Memory GPU Implementation manual pipelining



Out-of-Memory GPU Implementation manual pipelining



Out-of-Memory GPU Implementation UMA

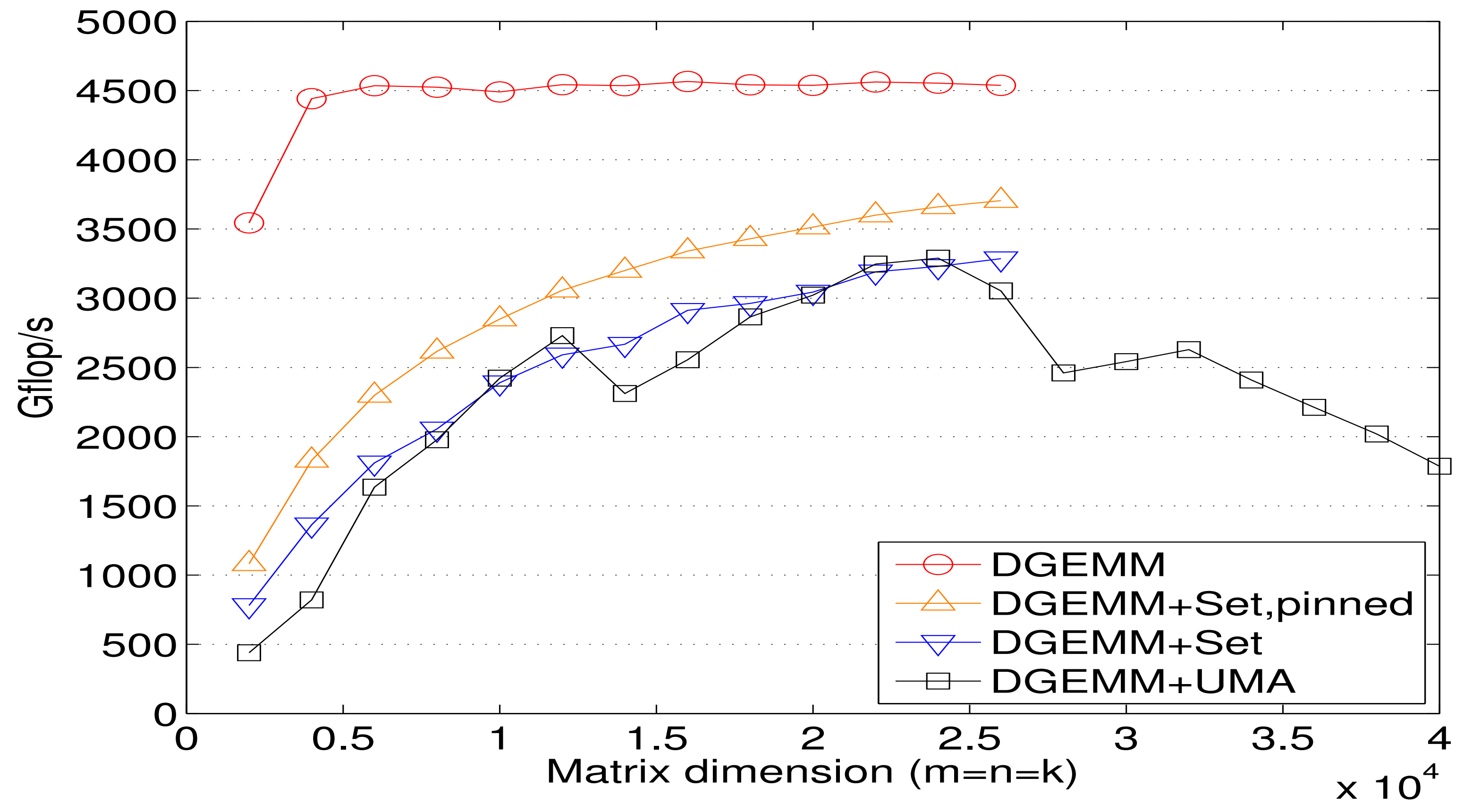


UMA

Unified Memory Access.

Unified Memory creates a pool of managed memory that is shared between the CPU and GPU.

Out-of-Memory GPU Implementation UMA



Out-of-Memory GPU Implementation CUBLAS-XT

- NVIDIA cuBLAS library : a fast GPU-accelerated implementation of the standard basic linear algebra subroutines (BLAS).

- accept arrays on CPU and break up the matrix on CPU into blocks and perform data transfer and computations on GPU.

- multiple GPUs on the same node

Performance Results

‘zgesvd_rand_cpu.cpp ’: CPU

‘zgesvd_rand.cpp’:in-core on GPU

‘zgesvd_rand_m.cpp’ : out-of-core using manual pipelining

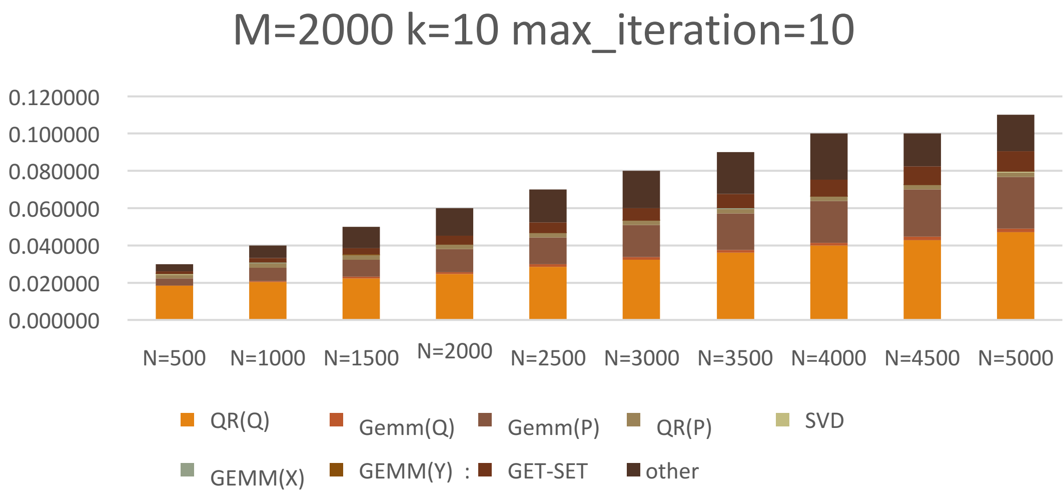
‘zgesvd_rand_uma.cpp’: out-of-core using UMA&CUBLAS.

Performance Results

Name	Steps
QR(Q)	[q,r] = qr(q,0);
Gemm(Q)	q = A'*p
Gemm(P)	p = A*q;
QR(P)	[p,b] = qr(p,0)
SVD	[x,s,y] = svd(b)
Gemm(X)	u = p*x(:,1:k)
Gemm(Y)	v = q*y(:,1:k)
GET-SET	setmatrix and getmatrix

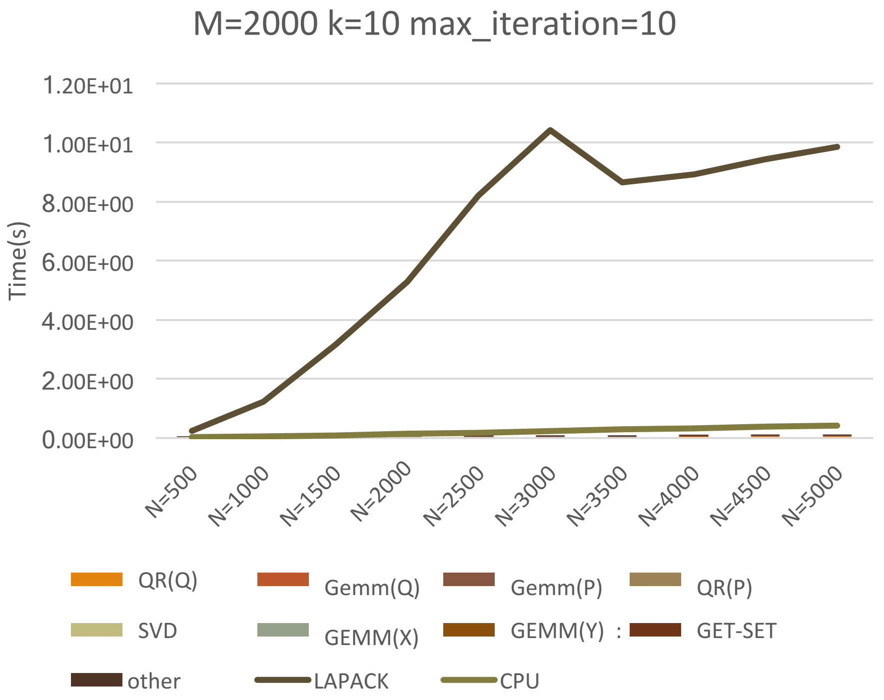
Comparison 1: M=2000, k=10, max_iteration=10 change N

GPU	QR(Q)	Gemm(Q)	Gemm(P)	QR(P)	SVD	GEMM(X)	GEMM(Y) :	GET-SET	other
N=500	0.018300	0.000316	0.003510	0.002270	0.000132	0.000038	0.000025	0.001410	0.004000
N=1000	0.020200	0.000565	0.007440	0.002290	0.000147	0.000038	0.000025	0.002500	0.006800
N=1500	0.022500	0.000705	0.009240	0.002310	0.000146	0.000038	0.000028	0.003580	0.011400
N=2000	0.024800	0.000928	0.012300	0.002250	0.000153	0.000038	0.000028	0.004690	0.014800
N=2500	0.028600	0.001100	0.014600	0.002220	0.000149	0.000039	0.000030	0.005730	0.017500
N=3000	0.032400	0.001290	0.017200	0.002220	0.000149	0.000039	0.000034	0.006820	0.019900
N=3500	0.035900	0.001470	0.020000	0.002230	0.000146	0.000038	0.000037	0.007860	0.022300
N=4000	0.039800	0.001680	0.022400	0.002240	0.000145	0.000038	0.000037	0.008930	0.024800
N=4500	0.042900	0.001860	0.025300	0.002260	0.000152	0.000037	0.000039	0.010000	0.017400
N=5000	0.047000	0.002060	0.027800	0.002340	0.000177	0.000038	0.000041	0.011100	0.019400



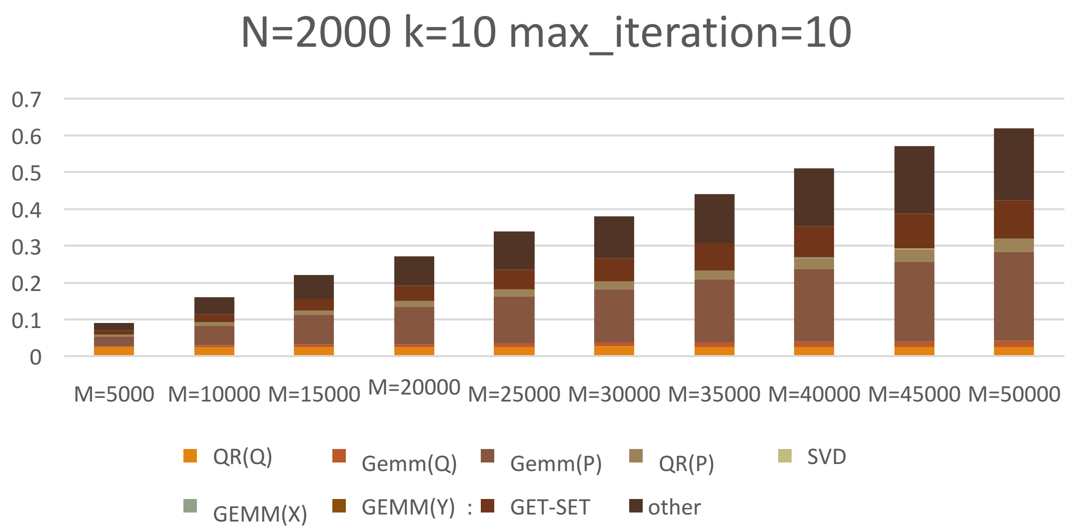
Comparison 1: M=2000, k=10, max_iteration=10 change N

	LAPACK	CPU	GPU
N=500	0.24	0.03	0.030001
N=1000	1.23	0.06	0.040005
N=1500	3.16	0.09	0.049947
N=2000	5.3	0.14	0.059987
N=2500	8.21	0.19	0.069968
N=3000	10.42	0.24	0.080052
N=3500	8.64	0.29	0.089981
N=4000	8.93	0.33	0.100070
N=4500	9.42	0.38	0.099948
N=5000	9.84	0.42	0.109956



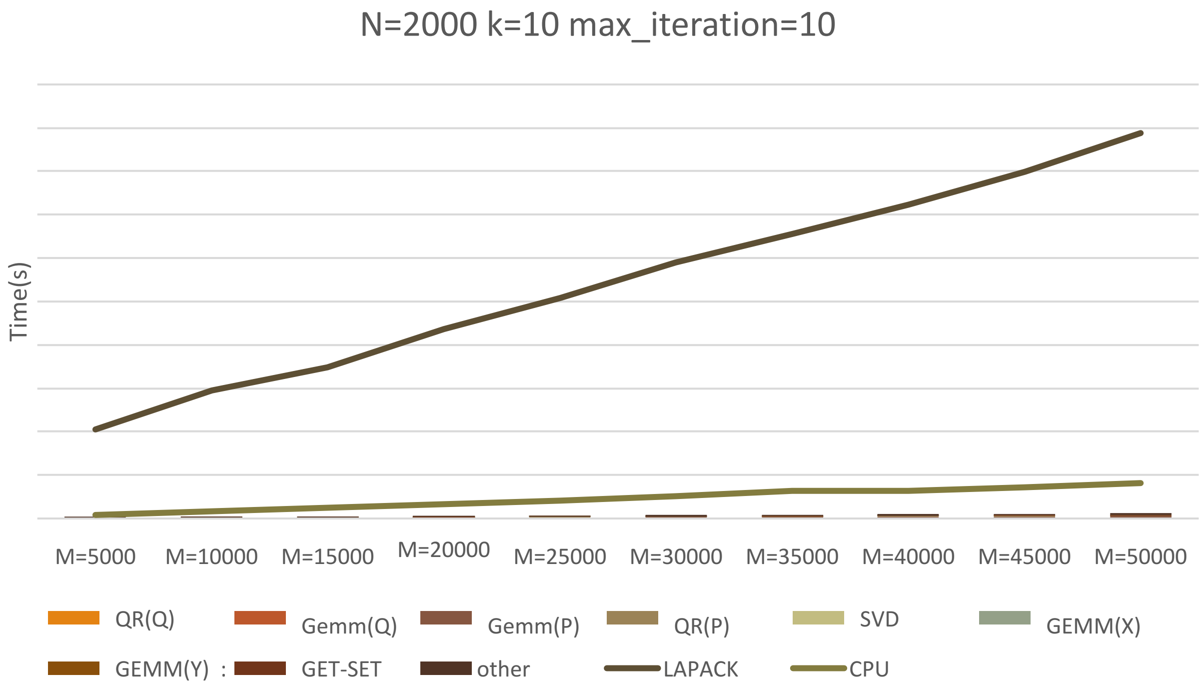
Comparison 2: N=2000, k=10, max_iteration=10 change M

GPU	QR(Q)	Gemm(Q)	Gemm(P)	QR(P)	SVD	GEMM(X)	GEMM(Y) :	GET-SET	other
M=5000	0.0245	0.00206	0.0279	0.00456	1.24e-04	0.000051	0.0000279	0.011	0.0198
M=10000	0.025	0.00402	0.0542	0.00825	0.000149	0.000127	0.0000331	0.0216	0.047
M=15000	0.0251	0.00608	0.0807	0.0114	0.000123	0.00015	0.0000329	0.0319	0.064
M=20000	0.0246	0.00725	0.103	0.0149	0.000134	0.000155	0.0000391	0.0423	0.078
M=25000	0.0247	0.00917	0.129	0.0186	0.000125	0.000179	0.000031	0.0529	0.105
M=30000	0.0262	0.0101	0.145	0.0221	0.000149	0.000183	0.000031	0.0631	0.114
M=35000	0.0248	0.012	0.171	0.0254	0.000166	0.000206	0.00003	0.0737	0.133
M=40000	0.0256	0.0137	0.198	0.0303	0.000161	0.000221	0.00003	0.0844	0.158
M=45000	0.0245	0.0155	0.218	0.0339	0.000174	0.00025	0.00003	0.0946	0.183
M=50000	0.0252	0.0174	0.24	0.0367	0.00016	0.000247	0.00003	0.105	0.195



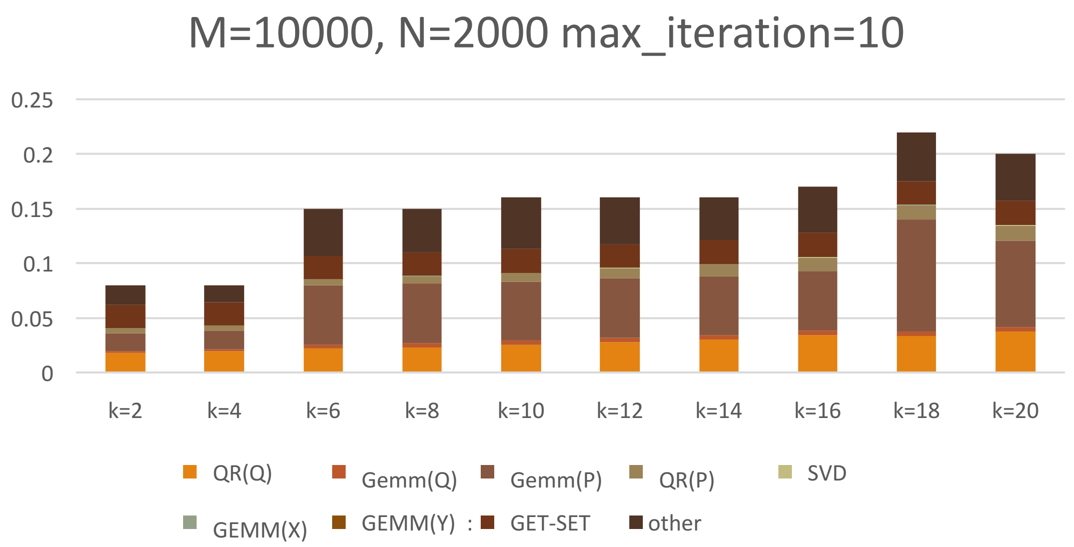
Comparison 2: N=2000, k=10, max_iteration=10 change M

	LAPACK	CPU	GPU
M=5000	10.26	0.41	0.0898989
M=10000	14.71	0.85	0.1603791
M=15000	17.43	1.24	0.2194859
M=20000	21.78	1.66	0.2703781
M=25000	25.45	2.1	0.339705
M=30000	29.47	2.52	0.380863
M=35000	32.82	3.15	0.440302
M=40000	36.15	3.2	0.510412
M=45000	39.98	3.62	0.569954
M=50000	44.4	4.08	0.619737



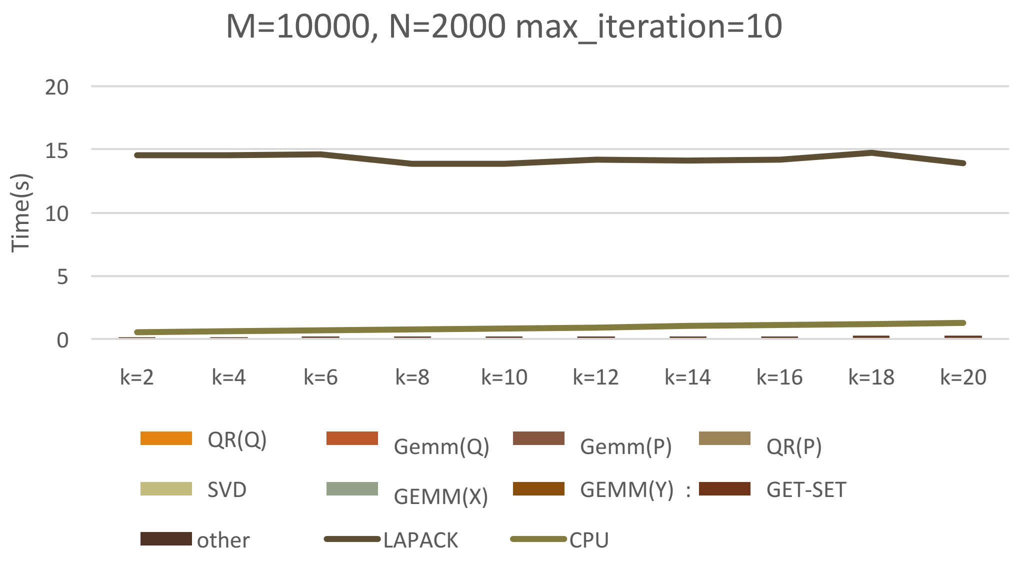
Comparison 3: M=10000, N=2000, max_iteration=10 change k

	QR(Q)	Gemm(Q)	Gemm(P)	QR(P)	SVD	GEMM(X)	GEMM(Y) :	GET-SET	other
k=2	0.0179	0.00128	0.0169	0.0042	0.0000372	0.000042	0.0000188	0.0212	0.0184
k=4	0.0197	0.00131	0.0169	0.00513	0.000073	0.000046	0.0000219	0.0213	0.0155
k=6	0.0221	0.00348	0.054	0.00573	0.000067	0.000047	0.0000219	0.0214	0.043
k=8	0.0231	0.00398	0.054	0.00699	0.000093	0.000112	0.000031	0.0215	0.04
k=10	0.0251	0.00401	0.0541	0.00792	0.00012	0.000133	0.0000329	0.0215	0.047
k=12	0.0278	0.00401	0.0542	0.00942	0.000163	0.000109	0.000047	0.0215	0.043
k=14	0.0299	0.00402	0.0543	0.0108	0.000214	0.000121	0.0000501	0.0215	0.039
k=16	0.034	0.00403	0.0544	0.0128	0.000275	0.00012	0.0000498	0.0217	0.043
k=18	0.0334	0.00368	0.103	0.0127	0.000465	0.000123	0.0000532	0.0216	0.045
k=20	0.0375	0.0036	0.0789	0.0144	0.000582	0.000119	0.0000498	0.0216	0.043



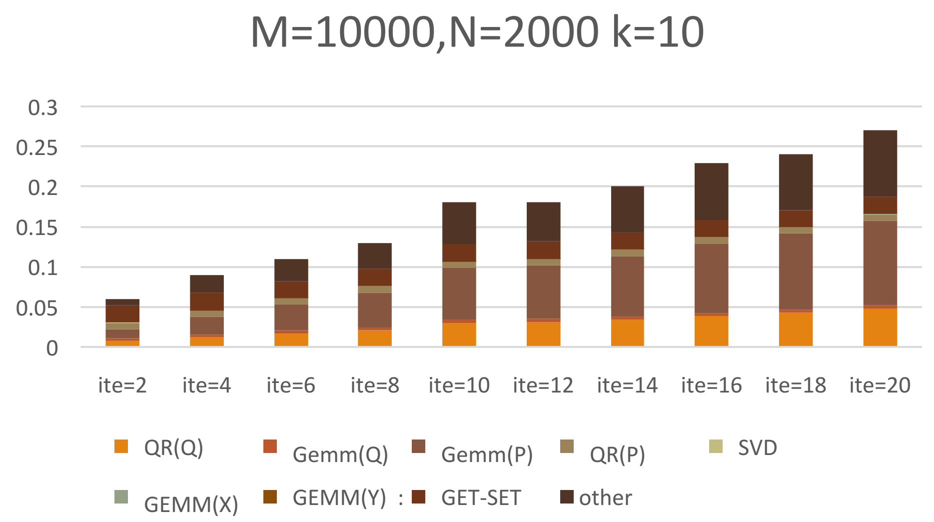
Comparison 3: M=10000, N=2000, max_iteration=10 change k

	LAPACK	CPU	GPU
k=2	14.55	0.53	0.079978
k=4	14.55	0.61	0.0799809
k=6	14.59	0.69	0.1498459
k=8	13.86	0.78	0.149806
k=10	13.86	0.85	0.1599159
k=12	14.19	0.92	0.160249
k=14	14.14	1	0.1599051
k=16	14.21	1.11	0.1703748
k=18	14.73	1.19	0.2200212
k=20	13.91	1.27	0.1997508



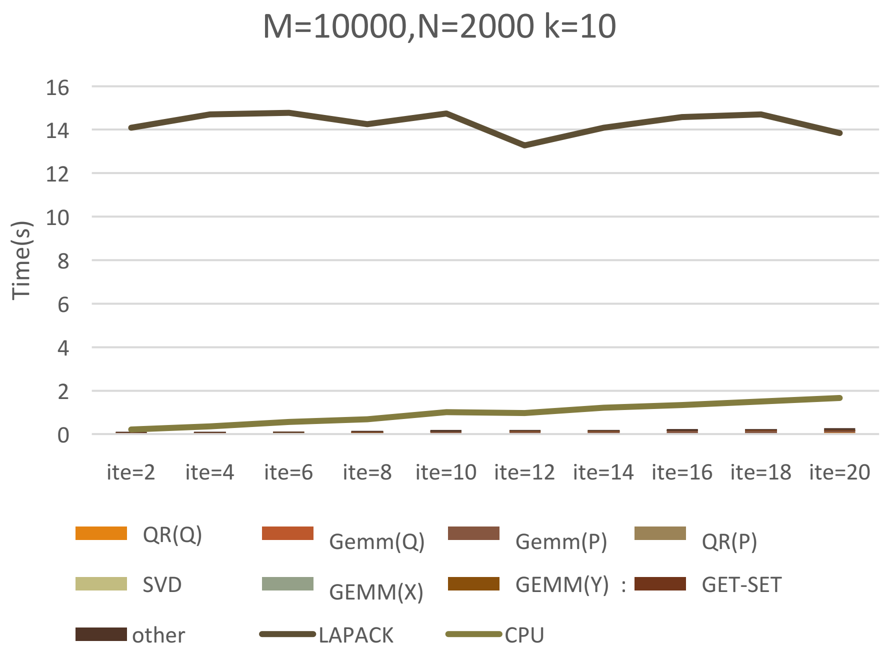
Comparison 4: M=10000,N=2000 k=10 change max_iteration

	QR(Q)	Gemm(Q)	Gemm(P)	QR(P)	SVD	GEMM(X)	GEMM(Y) :	GET-SET	other
ite=2	0.00737	0.00401	0.0109	0.008	0.000129	0.000126	0.0000331	0.0215	0.008
ite=4	0.0118	0.00402	0.0216	0.00792	0.000124	0.000127	0.0000319	0.0215	0.0228
ite=6	0.0163	0.00402	0.0324	0.0079	0.000123	0.000134	0.0000372	0.0214	0.0276
ite=8	0.0206	0.004	0.0433	0.00794	0.000121	0.000125	0.0000319	0.0215	0.0323
ite=10	0.0296	0.00402	0.0649	0.00796	0.000122	0.000128	0.0000331	0.0215	0.052
ite=12	0.0311	0.00409	0.0661	0.00851	0.000148	0.000133	0.0000319	0.0214	0.049
ite=14	0.0337	0.00401	0.0757	0.00788	0.000131	0.000127	0.0000329	0.0215	0.057
ite=16	0.0382	0.00403	0.0865	0.00819	0.000124	0.00012	0.000031	0.0214	0.071
ite=18	0.0429	0.0036	0.0948	0.00786	0.000129	0.000128	0.0000319	0.0215	0.069
ite=20	0.0478	0.00359	0.106	0.00795	0.000131	0.000125	0.000031	0.0215	0.083



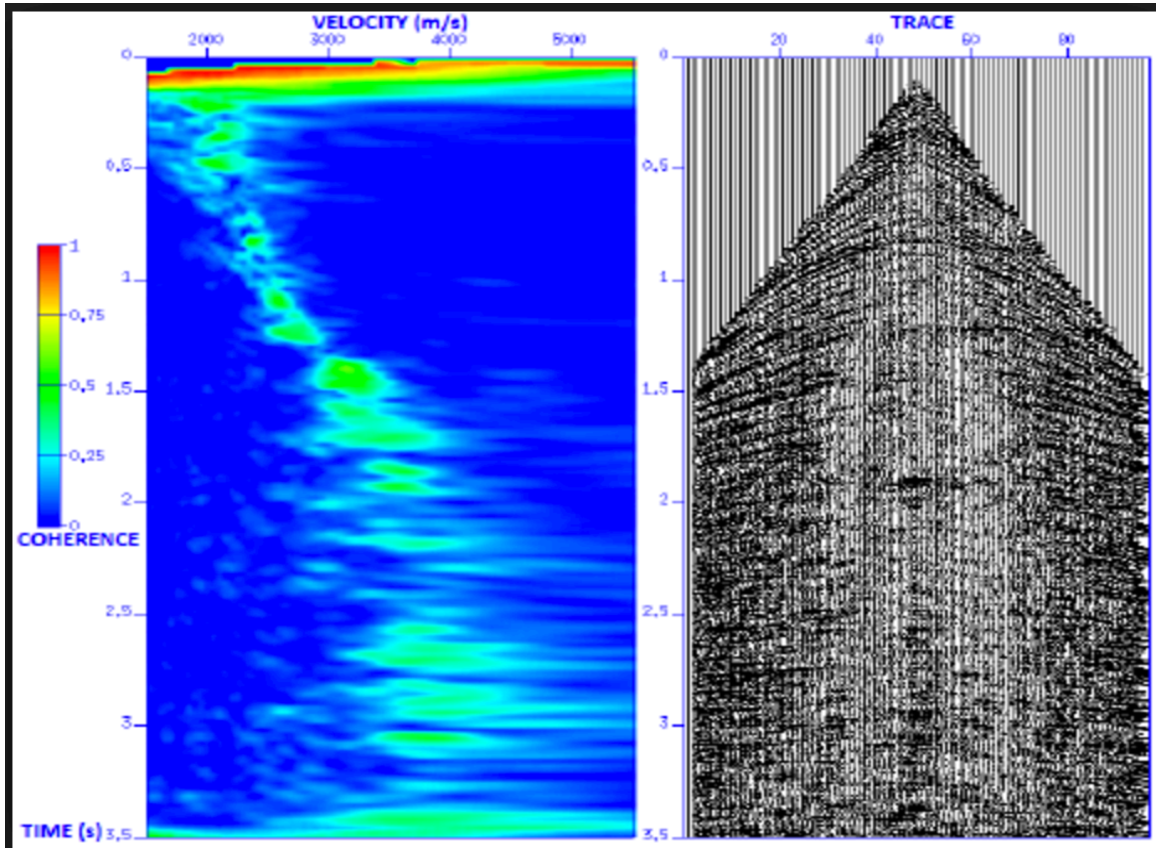
Comparison 4: M=10000,N=2000, k=10 change max_iteration

	LAPACK	CPU	GPU
ite=2	14.1	0.21	0.0600681
ite=4	14.72	0.37	0.0899229
ite=6	14.78	0.54	0.1099142
ite=8	14.27	0.69	0.1299179
ite=10	14.73	1.01	0.1802631
ite=12	13.28	0.97	0.1805129
ite=14	14.11	1.21	0.2000809
ite=16	14.57	1.33	0.229595
ite=18	14.72	1.49	0.2399489
ite=20	13.85	1.66	0.270127



Motivation and Application

- Latent Semantic Indexing (LSI)
- Genetic clustering
- subspace tracking
- image processing



Future Work

multiple GPU: CUBLAS-XT

randomized sampling and updating methods

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