Matrix Algebra on GPU and Multicore Architectures (MAGMA)

PART II : Hands-on training

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Outline

- Install MAGMA
- Using MAGMA
  - Documentation, naming conventions, and functionality
- Solving a linear system of equations
  $Ax = b$
- Solving an eigenvalue problem
  $Ax = \lambda x$
- DGEMM example
- Writing a hybrid algorithm

Install MAGMA

- **Get MAGMA 1.4**
  > wget http://icl.cs.utk.edu/projectsfiles/magma/downloads/magma-1.4.0.tar.gz
- **Unpack the library**
  > tar zxvf magma-1.4.0.tar.gz
- **Prerequisites: LAPACK, BLAS, and CUDA toolkit**
  > module load cudatoolkit intel
- **Modify 'make.inc' (where are CUDA & LAPACK, and for what GPU)**

  See examples in make.inc.{mkl-gcc | mkl-icc | mkl-ilp64 | mkl-shared | acml | atlas | goto | shared},
  > cp make.inc.mkl-gcc make.inc

  and modify make.inc by setting GPU_TARGET, MKLROOT, and CUDADIR, e.g.,

  ```
  GPU_TARGET ?= Kepler
  MKLROOT    =  $(INTEL_PATH)/mkl
  CUDADIR    =  $(CRAY_CUDATOOLKIT_DIR)
  ```
- **Create libmagma.a in 'lib' and testing drivers in 'testing'**
  > make
- **For more information on installation, read file 'README'**

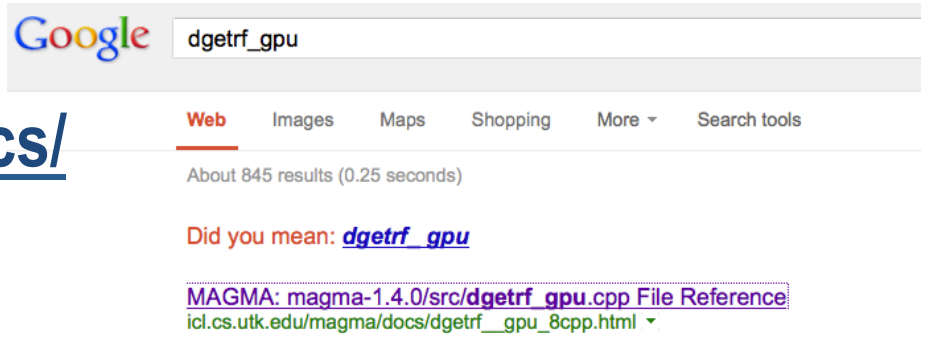
Using MAGMA

- **Support is provided through the MAGMA user forum**
  http://icl.cs.utk.edu/magma/forum/viewforum.php?f=2

NaN errors with dpotrf and dpotrf_gpu by fletchjp » Tue Dec 28, 2010 7:08 pm	9	3095	by fletchjp Thu Sep 12, 2013 12:03 pm
GMRES on magma by nitinb60 » Sun Aug 12, 2012 8:15 pm	4	1064	by fletchjp Thu Sep 12, 2013 11:02 am
Help please with choice of forums by fletchjp » Sat Apr 13, 2013 2:44 pm	4	1628	by fletchjp Thu Sep 12, 2013 10:42 am
the error when I compile magma1.4.0 in vs2010 by Eva Joo » Mon Sep 09, 2013 4:57 am	2	62	by Eva Joo Thu Sep 12, 2013 4:54 am
Undefined reference to cuda functions within libmagma by Matt Phillips » Mon Sep 09, 2013 10:40 pm	1	63	by Matt Phillips Mon Sep 09, 2013 11:17 pm
crash testing strsv, using OpenBLAS by Matt Phillips » Thu Sep 05, 2013 9:15 pm	0	101	by Matt Phillips Thu Sep 05, 2013 9:15 pm
MAGMA Installation: CLAPACK reference BLAS problem by psrivas2 » Tue Sep 03, 2013 4:07 am	0	84	by psrivas2 Tue Sep 03, 2013 4:07 am
Running MAGMA across several GPUs on several nodes by hsahasra » Tue Aug 13, 2013 1:32 pm	1	310	by mgates3 Fri Aug 30, 2013 3:48 pm
magma_init/finalize missing in fortran interface by stachon » Wed Aug 28, 2013 4:02 am	1	116	by mgates3 Fri Aug 30, 2013 2:13 pm
Error: BLAS/LAPACK routine 'magma_' gave error code -7 by christianHEL » Thu Aug 22, 2013 2:37 pm	2	197	by christianHEL Fri Aug 23, 2013 3:50 pm
Problems testing dsyevd with magma-1.4.0 by dougrabson » Thu Aug 15, 2013 5:44 am	1	173	by mgates3 Wed Aug 21, 2013 2:35 pm

Using MAGMA

- **Doxygen documentation**
  http://icl.cs.utk.edu/magma/docs/



Using MAGMA

- **Naming conventions (e.g., magma_dgesv_gpu)**
  - Prefix **magma_** or **magmablas_**
  - Followed by precision
    s single, **d** double, **c** single complex, or **z** double complex
    ds mixed double-single, or **zc** double complex-single complex
  - Matrix type
    general **sy**mmetric **he**rmetian **po**sitive definite
    orthogonal **un**itary **tr**iangular
  - Operation
    sv solve **ev** eigenvalue problem
    trf triangular factorization **gv** generalized eigenvalue
  - Suffix **_gpu** if input and output are on the GPU memory

Using MAGMA

- **MAGMA functionality**
  http://icl.cs.utk.edu/graphics/posters/files/SC12-MAGMA.pdf

GE	– General
SPD/HPD	– Symmetric/Hermitian Positive Definite
TR	– Triangular
D & C	– Divide & Conquer
B & I IT	– Bisection & Inverse Iteration
MP	– Mixed-precision Iterative Refinement
Naming Convention: magma_{routine name}[_gpu]	

DRIVER ROUTINES IN MAGMA 1.3

	MATRIX	OPERATION	ROUTINE	INTERFACES CPU	INTERFACES GPU
LINEAR EQUATIONS	GE	Solve using LU	{sdcz}gesv	✓	✓
		Solve using MP	{zc,ds}gesv		✓
	SPD/HPD	Solve using Cholesky	{sdcz}posv	✓	✓
		Solve using MP	{zc,ds}posv		✓
LLS	GE	Solve LLS using QR	{sdcz}geqrs		✓
		Solve using MP	{zc,ds}geqrsv		✓
STANDARD EVP	GE	Compute e-values, optionally e-vectors	{sdcz}geev	✓	
	SY/HE	Computes all e-values, optionally e-vectors	{sd}syevd	✓	✓
			{cz}heevd	✓	✓
		Range (D&C)	{cz}heevdx		✓
		Range (B & I It.)	{cz}heevx	✓	✓
		Range (MRRR)	{cz}heevr	✓	✓
STAND. SVP	GE	Compute SVD, optionally s-vectors	{sdcz}gesvd	✓	
				✓	
GENERALIZED EVP	SPD/HPD	Compute all e-values, optionally e-vectors	{sd}sygvd	✓	
			{cz}hegvd	✓	
		Range (D&C)	{cz}hegvdx	✓	
		Range (B & I It.)	{cz}hegvx	✓	
		Range (MRRR)	{cz}hegvr	✓	

COMPUTATIONAL ROUTINES IN MAGMA 1.3

	MATRIX	OPERATION	ROUTINE	INTERFACES CPU	INTERFACES GPU
LINEAR EQUATIONS	GE	LU	{sdcz}getrf	✓	✓
		Solve	{sdcz}getrs		✓
		Invert	{sdcz}getri		✓
	SPD/HPD	Cholesky	{sdcz}potrf	✓	✓
		Solve	{sdcz}potrs		✓
		Invert	{sdcz}potri		✓
	TR	Invert	{sdcz}trtri	✓	
ORTHOGONAL FACTORIZATIONS	GE	QR	{sdcz}geqrf	✓	
		QR w/ pivoting	{sdcz}geqp3		✓
		Generate Q	{sd}orgqr	✓	✓
			{cz}ungqr	✓	✓
		Multiply matrix by Q	{sd}ormqr	✓	✓
			{cz}unmqr	✓	✓
		LQ factorization	{sdcz}gelqf	✓	✓
		QL factorization	{sdcz}geqlf	✓	
		Multiply matrix by Q	{sd}ormql	✓	✓
			{cz}unmql	✓	✓
STANDARD EVP	GE	Hessenberg reduction	{sdcz}gehrd	✓	
		Generate Q	{sd}orghr	✓	
			{cz}unghr	✓	
	SY/HE	Tridiagonalization	{sd}sytrd	✓	
			{cz}hetrd	✓	
		Generate Q	{sd}orgtr		✓
			{cz}ungtr		✓
		Multiply by Q	{sd}ormtr	✓	✓
			{cz}unmtr	✓	✓
SVD	GE	Bidiagonalization	{sdcz}gebrd	✓	
GENER-ALIZED EVP	SPD/HPD	Reduction to standard form	{sd}sygst	✓	✓
			{cz}hegst	✓	✓

Examples / Exercises

- **Solving a linear system of equations**

$$Ax = b$$

```
#include "magma.h"
#include "magma_lapack.h"
…

magma_init();
cublasInit();
…
double *hA, *hB;                                                    // A is a typical array on the CPU
magma_malloc_pinned((void **)&hA,  lda * N * sizeof(double));       // A can be allocated in pinned memory
magma_malloc_cpu(     (void **)&hB, nrhs* M *sizeof(double));
…
init_matrix(M, N, hA, lda);
…
magma_dgetrf( M, N, hA, lda, ipiv, &info);                          // LU factorization (using CPU+GPU)
lapackf77_dgetrs( MagmaNoTransStr, &N, &nrhs,                       // Solve on CPU with LAPACK
                  hA, &lda, ipiv, hB, &ldb, &info );
```

Alternatively, there is a direct MAGMA function to solve:
see **testing_dgesv.cpp** and **testing_dgetrf.cpp**

Examples / Exercises

- **Solving an eigenvalue problem**

$$Ax = \lambda x$$

```
#include "magma.h”
#include "magma_lapack.h”
…

magma_init();
cublasInit();
…
double *hA;                                                          // A is a typical array on the CPU
magma_malloc_pinned((void **)&hA,  lda * N * sizeof(double));     // A can be allocated in pinned memory
…
init_matrix(M, N, hA, lda);
…
magma_dsyevd( opts.jobz, opts.uplo,
                        N, hA, lda, w1,
                        h_work, lwork,
                        iwork, liwork, &info );
```

see **testing_dsyevd.cpp**

Examples / Exercises

- **DGEMM example**

```
salloc -N1 --gres=gpu:1 --time=00:30:00
module load cudatoolkit intel
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/apps/dom/intel/composer_xe_2013/mkl/lib/intel64/
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/apps/opcode/CUDA-5.0/lib64
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/apps/dom/intel/composer_xe_2013.1.117/compiler/lib/intel64/

aprun -n1 -N1 -e  OMP_NUM_THREADS=16 -d16 ./testing_dgemm -l –c

MAGMA 1.4.0 , capability 3.0
device 0: Tesla K20X, 732.0 MHz clock, 5759.6 MB memory, capability 3.5

Usage: ./testing_dgemm [options] [-h|--help]

transA = N, transB = N
    M      N      K   MAGMA Gflop/s (ms)  CUBLAS Gflop/s (ms)   CPU Gflop/s (ms)  MAGMA error  CUBLAS error
==========================================================================================================
1088   1088   1088    612.88 (   4.20)       969.12 (   2.66)        3.13 ( 823.44)       6.92e-15       6.92e-15
2112   2112   2112    667.85 (  28.21)      1100.09 (  17.13)        6.79 (2775.89)       8.12e-15       7.95e-15
3136   3136   3136    675.16 (  91.36)      1144.59 (  53.89)       11.14 (5538.38)       1.13e-14       1.13e-14
…
```

see file **testing_dgemm.cpp, sgemm.pdf, dgemm_fermi.cu**, and directory **testing**

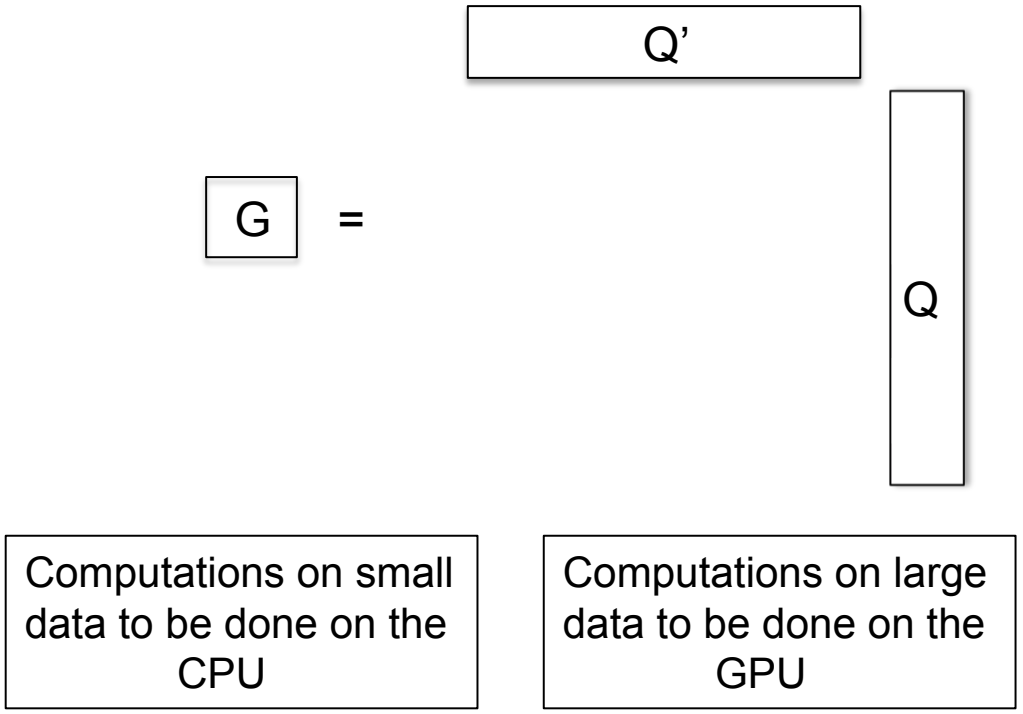
Examples / Exercises

- **Writing a hybrid algorithm**

  Develop a hybrid CPU-GPU algorithm for this Matlab code

```
function [Q,R] = chol_qr_it(A)
    i=0;
    cn = 200;
    Q = A;
    G = Q'*Q;
    n = size(A,2);
    R = eye(n);

    while cn > 100, i = i + 1
        [u,s,v]=svd(G);
        [q,r]=qr(sqrt(s)*v');
        R = r * R;
        cn = sqrt(cond(s));
        Q = Q * inv(r);
        if cn>100
            G = Q'*Q;
        end;
    end;
return
```



Examples / Exercises

- **Writing a hybrid algorithm**

  Develop a hybrid CPU-GPU algorithm for this Matlab code

```
function [Q,R] = chol_qr_it(A)
   i=0;
   cn = 200;
   Q = A;
   G = Q'*Q;                                   cublasSgemm( ... );       // G = Q' *Q (GPU computation)
   n = size(A,2);
   R = eye(n);

   while cn > 100, i = i + 1                   cublasGetVector( ... );   // G -> work (send the result G to the CPU)
       [u,s,v]=svd(G);                         sgesvd_( ... );           //  svd G on the CPU
       [q,r]=qr(sqrt(s)*v');                   sgeqrf_( ... );           //  QR on the CPU
       R = r * R;
       cn = sqrt(cond(s));                     cublasSetVector( ... );   // send r back to the the GPU)
       Q = Q * inv(r);                         cublasStrsm( ... );        // Triangular matrix solve on the GPU
       if cn>100
          G = Q'*Q;
       end;
   end;
return
```

see **testing_dgegqr_gpu.cpp** and **dgegqr_gpu.cpp**

Contributions

The MAGMA program style follows the general guidelines for Sca/LAPACK in terms of interfaces, copyrights and licensing, citing the authors of the software, and documentation:
http://www.netlib.org/lapack-dev/lapack-coding/program-style.html

- Routine Naming and Design
- Language, source formatting, timing, and testing
- See file '**ContributorsGuige.txt**'

Collaborators and Support

Microsoft

MAGMA team

http://icl.cs.utk.edu/magma

PLASMA team

http://icl.cs.utk.edu/plasma

Collaborating partners

University of Tennessee, Knoxville
University of California, Berkeley
University of Colorado, Denver
INRIA, France (StarPU team)
KAUST, Saudi Arabia

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