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'**

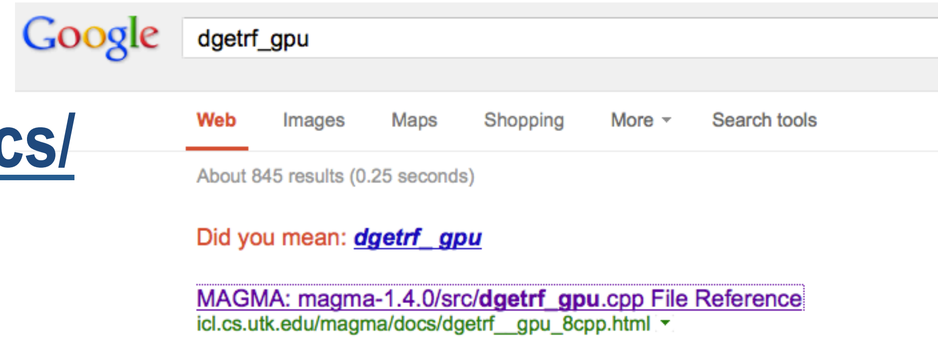
Using MAGMA

- **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
qrf	QR factorization		

  - Suffix _**gpu** if input and output are on the GPU memory
    (no suffix indicates CPU interface – use GPUs to accelerate where input and output are on the CPU)

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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,	{sdcz}geev	✓	
		optionally e-vectors			
	SY/HE	Computes all e-values,	{sd}syevd	✓	✓
		optionally e-vectors	{cz}heevd	✓	✓
		Range (D&C)	{cz}heevdx		✓
		Range (B & I It.)	{cz}heevx	✓	✓
		Range (MRRR)	{cz}heevr	✓	✓
STAND. SVP	GE	Compute SVD,	{sdcz}gesvd	✓	
		optionally s-vectors		✓	
GENERALIZED EVP	SPD/HPD	Compute all e-values,	{sd}sygvd	✓	
		optionally e-vectors	{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	{sd}sygst	✓	✓
		form	{cz}hegst	✓	✓

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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**

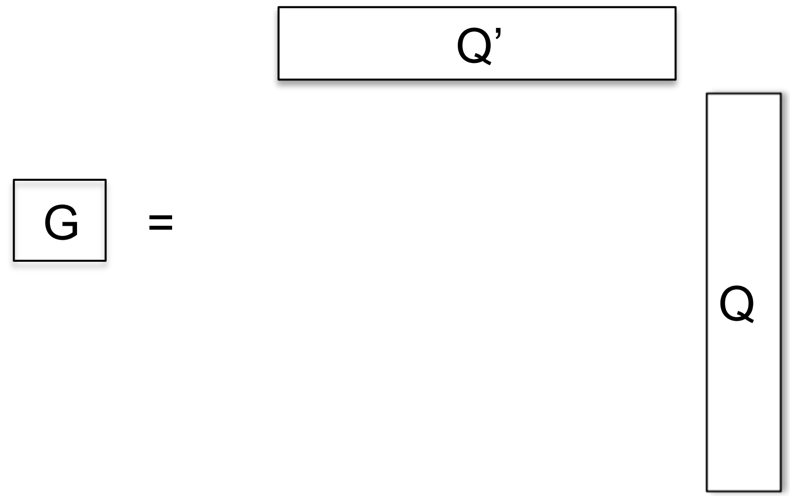
Examples / Exercises

- **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
```



Computations on small data to be done on the CPU

Computations on large data to be done on the GPU

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
  - Use BLAS
  - Develop in double complex; other precisions are generated
  - Machine parameters are determined at **magma_init** (as needed for tuning)
  - Block sizes are provided by **extern "C" int magma_get_ROUTINE_nb(int m)**, i.e., not by ilaenv
- Language, source formatting, timing, and testing
  - Written in C/C++; wrappers for Fortran are supported
- See file **'ContributorsGuige.txt'**

Collaborators and Support

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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