# MAGMA Library

version 0.2

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-- MAGMA (version 0.2) --

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## Chapter 1

## The MAGMA Library

The goal of the Matrix Algebra on GPU and Multicore Architectures (MAGMA) project is to create a new generation of linear algebra libraries that achieve the fastest possible time to an accurate solution on hybrid/heterogeneous architectures, starting with current multicore+multiGPU systems. To address the complex challenges stemming from these systems' heterogeneity, massive parallelism, and gap in compute power vs CPU-GPU communication speeds, MAGMA's research is based on the idea that optimal software solutions will themselves have to hybridize, combining the strengths of different algorithms within a single framework. Building on this idea, the goal is to design linear algebra algorithms and frameworks for hybrid multicore and multiGPU systems that can enable applications to fully exploit the power that each of the hybrid components offers.

Designed to be similar to LAPACK in functionality, data storage, and interface, the MAGMA library will allow scientists to effortlessly port their LAPACK-relying software components and to take advantage of the new hybrid architectures

MAGMA version 0.2 is a release intended for a single GPU – see the specifications in Section 3.1. MAGMA (version 0.2) includes the one-sided matrix factorizations and solvers based on them, including mixed-precision iterative refinement solvers. The factorizations are provided in all 4 precisions – single, double, single complex, and double complex. For each function there are 2 LAPACK-style interfaces. The first one, referred to as CPU interface, takes the input and produces the result in the CPU's memory. The second, referred to as GPU interface, takes the input and produces the result in the GPU's memory. Work is in progress on the two-sided factorizations and eigen-solvers based on them. Included is the reduction to upper Hessenberg form in single and double precision. Included is also MAGMA BLAS, a complementary to CUBLAS subset of CUDA BLAS that are crucial for the performance of MAGMA routines. MAGMA uses standard data layout (column major) and

can be used as a complement to LAPACK to accelerate the functions currently provided.

The algorithm names are derived by the corresponding LAPACK names, prefixed by magma\_, and for the case of the GPU interface suffixed by \_gpu.

MAGMA version 0.1 included the LU, QR, and Cholesky factorizations in real arithmetic (single and double) for both CPU and GPU interfaces [4]. The following list gives the additions that are now available in MAGMA version 0.2:

- Complex arithmetic (single and double) LU, QR, and Cholesky factorizations for both CPU and GPU interfaces;
- LQ and QL factorizations in real arithmetic (single);
- Linear solvers based on LU, QR, and Cholesky in real arithmetic (single and double);
- Mixed-precision, iterative refinement solvers based on LU, QR, and Cholesky in real arithmetic;
- Reduction to upper Hessenberg form in real arithmetic (single and double)
- MAGMA BLAS in real arithmetic (single and double), including gemm and trsm.

A reference performance is given in Chapter 4.

#### 1.1 One-sided matrix factorizations

We use hybrid algorithms where the computation is split between the GPU and and the CPU. In general for the one-sided factorizations, the panels are factored on the CPU and the trailing sub-matrix updates on the GPU. Look-ahead techniques are used to overlap the CPU and GPU work (and some communications). Figure 1.1 illustrates this by quantifying the CPU-GPU overlap for the case of QR in single precision arithmetic.

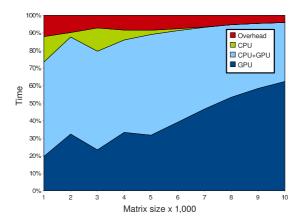


Figure 1.1: Time breakdown for the hybrid QR from MAGMA in single precision arithmetic on GTX280 GPU and Intel Xeon 2.33GHz CPU.

In both the CPU and GPU interfaces the matrix to be factored resides on the GPU memory, and CPU-GPU transfers are associated only with the panels. The resulting matrix is accumulated (on the CPU or GPU according to the interface) along the computation, as a byproduct of the algorithm, vs sending the the entire matrix when needed. In the CPU interface, the original transfer of the matrix to the GPU is overlapped with the factorization of the first panel. In this sense the CPU and GPU interfaces, although similar, are not derivatives of each other as they have different communication patterns.

Besides this common approach, the different algorithms have specific optimizations motivated by the GPU architecture [3, 5].

#### 1.1.1 Function magma\_sgetrf

SGETRF computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges.

The factorization has the form  $% \left( 1\right) =\left( 1\right) \left( 1\right)$ 

A = P \* L \* U

where P is a permutation matrix, L is lower triangular with unit diagonal elements (lower trapezoidal if m > n), and U is upper triangular (upper trapezoidal if m < n).

This is the right-looking Level 3 BLAS version of the algorithm.

- N (input) INTEGER

  The number of columns of the matrix A. N >= 0.
- A (input/output) REAL array, dimension (LDA,N)
  On entry, the M-by-N matrix to be factored.
  On exit, the factors L and U from the factorization
  A = P\*L\*U; the unit diagonal elements of L are not stored.
  Higher performance is achieved if A is in pinned memory,
  e.g. allocated using cudaMallocHost.
- IPIV (output) INTEGER array, dimension  $(\min(M,N))$ The pivot indices; for 1 <= i <=  $\min(M,N)$ , row i of the matrix was interchanged with row IPIV(i).
- WORK (workspace/output) REAL array, dimension >= N\*NB, where NB can be obtained through magma\_get\_sgetrf\_nb(M). Higher performance is achieved if WORK is in pinned memory, e.g. allocated using cudaMallocHost.
- DA (workspace) REAL array on the GPU, dimension  $(\max(M, N) + k1)^2 + (M + k2)*NB + 2*NB^2,$  where NB can be obtained through magma\_get\_sgetrf\_nb(M). k1 < 32 and k2 < 32 are such that  $(\max(M, N) + k1)%32 = 0 \text{ and } (M+k2)%32 = 0.$
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, U(i,i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and division by zero will occur if it is used to solve a system of equations.

#### 1.1.2 Function magma\_sgeqrf

SGEQRF computes a QR factorization of a real M-by-N matrix A: A = Q \* R.

- M (input) INTEGER

  The number of rows of the matrix A.  $M \ge 0$ .
- N (input) INTEGER The number of columns of the matrix A. N >= 0.
- A (input/output) REAL array, dimension (LDA,N)
  On entry, the M-by-N matrix A.
  On exit, the elements on and above the diagonal of the array contain the min(M,N)-by-N upper trapezoidal matrix R (R is upper triangular if m >= n); the elements below the diagonal, with the array TAU, represent the orthogonal matrix Q as a product of min(m,n) elementary reflectors.
  Higher performance is achieved if A is in pinned memory, e.g. allocated using cudaMallocHost.
- TAU (output) REAL array, dimension  $(\min(M,N))$ The scalar factors of the elementary reflectors.
- WORK (workspace/output) REAL array, dimension (MAX(1,LWORK))
  On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
  Higher performance is achieved if WORK is in pinned memory,
  e.g. allocated using cudaMallocHost.
- LWORK (input) INTEGER

  The dimension of the array WORK. LWORK >= N\*NB,

  where NB can be obtained through magma\_get\_sgeqrf\_nb(M).

If LWORK = -1, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued.

- DA (workspace) REAL array on the GPU, dimension N\*(M + NB), where NB can be obtained through magma\_get\_sgeqrf\_nb(M). (size to be reduced in upcoming versions).

The matrix Q is represented as a product of elementary reflectors Q = H(1) H(2) . . . H(k), where k = min(m,n). Each H(i) has the form H(i) = I - tau \* v \* v'

where tau is a real scalar, and v is a real vector with v(1:i-1) = 0 and v(i) = 1; v(i+1:m) is stored on exit in A(i+1:m,i), and tau in TAU(i).

#### 1.1.3 Function magma\_spotrf

int magma\_spotrf(char \*uplo, int \*n, float \*a, int \*lda, float \*work, int \*info)

SPOTRF computes the Cholesky factorization of a real symmetric positive definite matrix A.

The factorization has the form A = U\*\*T \* U, if UPLO = 'U', or A = L \* L\*\*T, if UPLO = 'L',

where U is an upper triangular matrix and L is lower triangular.

This is the block version of the algorithm, calling Level 3 BLAS.

- UPLO (input) CHARACTER\*1
  - = 'U': Upper triangle of A is stored;
  - = 'L': Lower triangle of A is stored.
- (input) INTEGER

The order of the matrix A.  $N \ge 0$ .

(input/output) REAL array, dimension (LDA,N) On entry, the symmetric matrix A. If UPLO = 'U', the leading N-by-N upper triangular part of A contains the upper triangular part of the matrix A, and the strictly lower triangular part of A is not referenced. If UPLO = 'L', the leading N-by-N lower triangular part of A contains the lower triangular part of the matrix A, and the strictly upper triangular part of A is not referenced.

> On exit, if INFO = 0, the factor U or L from the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T. Higher performance is achieved if A is in pinned memory, e.g. allocated using cudaMallocHost.

- LDA (input) INTEGER The leading dimension of the array A. LDA  $\geq \max(1,N)$ .
- WORK (workspace) REAL array on the GPU, dimension (N, N)  $\,$ (size to be reduced in upcoming versions).
- INFO (output) INTEGER

  - = 0: successful exit < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, the leading minor of order i is not positive definite, and the factorization could not be  $% \left( 1\right) =\left( 1\right) \left( 1\right)$ completed.

#### 1.1.4 Function magma\_sgetrf\_gpu

SGETRF computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges.

The factorization has the form  $% \left( 1\right) =\left( 1\right) \left( 1\right)$ 

A = P \* L \* U

where P is a permutation matrix, L is lower triangular with unit diagonal elements (lower trapezoidal if m > n), and U is upper triangular (upper trapezoidal if m < n).

This is the right-looking Level 3 BLAS version of the algorithm.

- N (input) INTEGER

  The number of columns of the matrix A. N >= 0.
- A (input/output) REAL array on the GPU, dimension (LDA,N) where LDA >=  $\max(M, N)+k1$ , k1<32 such that  $(\max(M, N)+k1)\%32==0$ . The memory pointed by A should be at least  $(\max(M, N) + k1)^2 + (M + k2)*NB + 2*NB^2$  where k2 < 32 such that (M + k2) %32 == 0.

On entry, the M-by-N matrix to be factored. On exit, the factors L and U from the factorization A = P\*L\*U; the unit diagonal elements of L are not stored. The rest of A is considered work space and is changed.

- IPIV (output) INTEGER array, dimension  $(\min(M,N))$ The pivot indices; for 1 <= i <=  $\min(M,N)$ , row i of the matrix was interchanged with row IPIV(i).
- WORK (workspace/output) REAL array, dimension >= N\*NB, where NB can be obtained through magma\_get\_sgetrf\_nb(M). Higher performance is achieved if WORK is in pinned memory, e.g. allocated using cudaMallocHost.
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, U(i,i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and division by zero will occur if it is used to solve a system of equations.

#### 1.1.5 Function magma\_sgeqrf\_gpu

SGEQRF computes a QR factorization of a real M-by-N matrix A: A = Q \* R.

- M (input) INTEGER The number of rows of the matrix A.  $M \ge 0$ .
- A (input/output) REAL array on the GPU, dimension (LDA,N)
  On entry, the M-by-N matrix A.
  On exit, the elements on and above the diagonal of the array contain the min(M,N)-by-N upper trapezoidal matrix R (R is upper triangular if m >= n); the elements below the diagonal, with the array TAU, represent the orthogonal matrix Q as a product of min(m,n) elementary reflectors.
- LDA (input) INTEGER  $\mbox{The leading dimension of the array A. LDA} >= \mbox{max(1,M)}.$
- TAU (output) REAL array, dimension  $(\min(M,N))$ The scalar factors of the elementary reflectors (see Further Details).
- WORK (workspace/output) REAL array, dimension (MAX(1,LWORK))
  On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
  Higher performance is achieved if WORK is in pinned memory,
  e.g. allocated using cudaMallocHost.

If LWORK = -1, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued.

- DWORK (workspace) REAL array on the GPU, dimension N\*NB, where NB can be obtained through magma\_get\_sgeqrf\_nb(M).

The matrix Q is represented as a product of elementary reflectors Q = H(1) H(2) . . . H(k), where k = min(m,n). Each H(i) has the form

H(i) = I - tau \* v \* v'

where tau is a real scalar, and v is a real vector with v(1:i-1) = 0 and v(i) = 1; v(i+1:m) is stored on exit in A(i+1:m,i), and tau in TAU(i).

#### 1.1.6 Function magma\_spotrf\_gpu

SPOTRF computes the Cholesky factorization of a real symmetric positive definite matrix  ${\tt A}.$ 

The factorization has the form  $A = U**T * U, \quad \text{if UPLO} = `U', \quad \text{or} \\ A = L * L**T, \quad \text{if UPLO} = `L', \\$ 

where  ${\tt U}$  is an upper triangular matrix and  ${\tt L}$  is lower triangular.

This is the block version of the algorithm, calling Level 3 BLAS.

- UPLO (input) CHARACTER\*1
  - = 'U': Upper triangle of A is stored;
  - = 'L': Lower triangle of A is stored.
- A (input/output) REAL array on the GPU, dimension (LDA,N)
  On entry, the symmetric matrix A. If UPLO = 'U', the leading
  N-by-N upper triangular part of A contains the upper
  triangular part of the matrix A, and the strictly lower
  triangular part of A is not referenced. If UPLO = 'L', the
  leading N-by-N lower triangular part of A contains the lower
  triangular part of the matrix A, and the strictly upper
  triangular part of A is not referenced.

On exit, if INFO = 0, the factor U or L from the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T.

- WORK (workspace) REAL array, dimension at least (nb, nb)
  where nb can be obtained through magma\_get\_spotrf\_nb(\*n)
  Work array allocated with cudaMallocHost.
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, the leading minor of order i is not positive definite, and the factorization could not be completed.

#### 1.1.7 Function magma\_dgetrf

<code>DGETRF</code> computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges.

The factorization has the form  $% \left( 1\right) =\left( 1\right) \left( 1\right)$ 

A = P \* L \* U

where P is a permutation matrix, L is lower triangular with unit diagonal elements (lower trapezoidal if m > n), and U is upper triangular (upper trapezoidal if m < n).

This is the right-looking Level 3 BLAS version of the algorithm.

- M (input) INTEGER The number of rows of the matrix A. M  $\geq$  0.
- N (input) INTEGER

  The number of columns of the matrix A. N >= 0.
- A (input/output) DOUBLE array, dimension (LDA,N)
  On entry, the M-by-N matrix to be factored.
  On exit, the factors L and U from the factorization
  A = P\*L\*U; the unit diagonal elements of L are not stored.
  Higher performance is achieved if A is in pinned memory,
  e.g. allocated using cudaMallocHost.
- IPIV (output) INTEGER array, dimension  $(\min(M,N))$ The pivot indices; for 1 <= i <=  $\min(M,N)$ , row i of the matrix was interchanged with row IPIV(i).
- WORK (workspace/output) DOUBLE array, dimension >= N\*NB, where NB can be obtained through magma\_get\_sgetrf\_nb(M). Higher performance is achieved if WORK is in pinned memory, e.g. allocated using cudaMallocHost.
- DA (workspace) DOUBLE array on the GPU, dimension  $(\max(M, N) + k1)^2 + (M + k2)*NB + 2*NB^2,$  where NB can be obtained through magma\_get\_sgetrf\_nb(M). k1 < 32 and k2 < 32 are such that  $(\max(M, N) + k1)%32 = 0 \text{ and } (M+k2)%32 = 0.$
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, U(i,i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and division by zero will occur if it is used to solve a system of equations.

#### 1.1.8 Function magma\_dgeqrf

- M (input) INTEGER
  The number of rows of the matrix A. M >= 0.
- N (input) INTEGER The number of columns of the matrix A. N >= 0.
- A (input/output) DOUBLE array, dimension (LDA,N)
  On entry, the M-by-N matrix A.
  On exit, the elements on and above the diagonal of the array contain the min(M,N)-by-N upper trapezoidal matrix R (R is upper triangular if m >= n); the elements below the diagonal, with the array TAU, represent the orthogonal matrix Q as a product of min(m,n) elementary reflectors.
  Higher performance is achieved if A is in pinned memory, e.g. allocated using cudaMallocHost.
- TAU (output) DOUBLE array, dimension  $(\min(M,N))$ The scalar factors of the elementary reflectors.
- WORK (workspace/output) DOUBLE array, dimension (MAX(1,LWORK))
  On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
  Higher performance is achieved if WORK is in pinned memory,
  e.g. allocated using cudaMallocHost.
- - If LWORK = -1, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued.
- DA (workspace) DOUBLE array on the GPU, dimension N\*(M + NB), where NB can be obtained through magma\_get\_dgeqrf\_nb(M). (size to be reduced in upcoming versions).

The matrix Q is represented as a product of elementary reflectors Q = H(1) H(2) . . . H(k), where k =  $\min(m,n)$ . Each H(i) has the form H(i) = I - tau \* v \* v' where tau is a real scalar, and v is a real vector with v(1:i-1) = 0 and

where tau is a real scalar, and v is a real vector with v(1:i-1) = 0 and v(i) = 1; v(i+1:m) is stored on exit in A(i+1:m,i), and tau in TAU(i).

#### Function magma\_dpotrf 1.1.9

int magma\_dpotrf(char \*uplo, int \*n, double \*a, int \*lda, double \*work, int \*info)

DPOTRF computes the Cholesky factorization of a real symmetric positive definite matrix A.

The factorization has the form A = U\*\*T \* U, if UPLO = 'U', or A = L \* L\*\*T, if UPLO = 'L', where U is an upper triangular matrix and L is lower triangular.

This is the block version of the algorithm, calling Level 3 BLAS.

- UPLO (input) CHARACTER\*1 = 'U': Upper triangle of A is stored; = 'L': Lower triangle of A is stored.
- (input) INTEGER The order of the matrix A.  $N \ge 0$ .
- (input/output) DOUBLE array, dimension (LDA,N) On entry, the symmetric matrix A. If UPLO = 'U', the leading N-by-N upper triangular part of A contains the upper triangular part of the matrix A, and the strictly lower triangular part of A is not referenced. If UPLO = 'L', the leading N-by-N lower triangular part of A contains the lower triangular part of the matrix A, and the strictly upper triangular part of A is not referenced.

On exit, if INFO = 0, the factor U or L from the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T. Higher performance is achieved if A is in pinned memory, e.g. allocated using cudaMallocHost.

- LDA (input) INTEGER The leading dimension of the array A. LDA  $\geq \max(1,N)$ .
- WORK (workspace) DOUBLE array on the GPU, dimension (N, N)  $\,$ (size to be reduced in upcoming versions).
- INFO (output) INTEGER

  - = 0: successful exit < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, the leading minor of order i is not positive definite, and the factorization could not be completed.

#### 1.1.10 Function magma\_dgetrf\_gpu

<code>DGETRF</code> computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges.

The factorization has the form  $% \left( 1\right) =\left( 1\right) \left( 1\right)$ 

A = P \* L \* U

where P is a permutation matrix, L is lower triangular with unit diagonal elements (lower trapezoidal if m > n), and U is upper triangular (upper trapezoidal if m < n).

This is the right-looking Level 3 BLAS version of the algorithm.

- N (input) INTEGER

  The number of columns of the matrix A.  $N \ge 0$ .
- A (input/output) DOUBLE array on the GPU, dimension (LDA,N) where LDA >=  $\max(M, N)+k1$ , k1<32 such that  $(\max(M, N)+k1)\%32==0$ . The memory pointed by A should be at least  $(\max(M, N) + k1)^2 + (M + k2)*NB + 2*NB^2$  where k2 < 32 such that (M + k2) %32 == 0.

On entry, the M-by-N matrix to be factored. On exit, the factors L and U from the factorization A = P\*L\*U; the unit diagonal elements of L are not stored. The rest of A is considered work space and is changed.

- $\begin{array}{lll} \mbox{IPIV} & \mbox{(output) INTEGER array, dimension } (\mbox{min}(M,N)) \\ & \mbox{The pivot indices; for 1 <= i <= min(M,N), row i of the matrix was interchanged with row IPIV(i).} \\ \end{array}$
- WORK (workspace/output) DOUBLE array, dimension >= N\*NB,
   where NB can be obtained through magma\_get\_dgetrf\_nb(M).
   Higher performance is achieved if WORK is in pinned memory,
   e.g. allocated using cudaMallocHost.
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, U(i,i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and division by zero will occur if it is used to solve a system of equations.

#### 1.1.11 Function magma\_dgeqrf\_gpu

int magma\_dgeqrf\_gpu(int \*m, int \*n, double \*a, int \*lda, double \*tau, double \*work, int \*lwork, double \*dwork, int \*info )

DGEQRF computes a QR factorization of a real M-by-N matrix A: A = Q \* R.

- (input) INTEGER The number of rows of the matrix A. M >= 0.
- (input) INTEGER The number of columns of the matrix A.  $N \ge 0$ .
- (input/output) DOUBLE array on the GPU, dimension (LDA,N) On entry, the M-by-N matrix A. On exit, the elements on and above the diagonal of the array contain the  $\min(M,N)$ -by-N upper trapezoidal matrix R (R is upper triangular if m  $\geq$ = n); the elements below the diagonal, with the array TAU, represent the orthogonal matrix Q as a product of min(m,n) elementary reflectors.
- T.DA (input) INTEGER The leading dimension of the array A. LDA  $>= \max(1,M)$ .
- TAU (output) DOUBLE array, dimension (min(M,N)) The scalar factors of the elementary reflectors.
- WORK (workspace/output) DOUBLE array, dimension (MAX(1,LWORK)) On exit, if INFO = 0, WORK(1) returns the optimal LWORK. Higher performance is achieved if WORK is in pinned memory, e.g. allocated using cudaMallocHost.
- LWORK (input) INTEGER The dimension of the array WORK. LWORK >= (M+N)\*NB, where NB can be obtained through magma\_get\_dgeqrf\_nb(M).

If LWORK = -1, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued.

- DWORK (workspace) DOUBLE array on the GPU, dimension N\*NB, where NB can be obtained through magma\_get\_dgeqrf\_nb(M).
- INFO (output) INTEGER = 0: successful exit < 0: if INFO = -i, the i-th argument had an illegal value

The matrix Q is represented as a product of elementary reflectors Q = H(1) H(2) . . . H(k), where k = min(m,n).Each H(i) has the form

H(i) = I - tau \* v \* v'

where tau is a real scalar, and v is a real vector with v(1:i-1) = 0 and v(i) = 1; v(i+1:m) is stored on exit in A(i+1:m,i), and tau in TAU(i).

## 1.1.12 Function magma\_dpotrf\_gpu

DPOTRF computes the Cholesky factorization of a real symmetric positive definite matrix  ${\tt A}.$ 

The factorization has the form A = U\*\*T \* U, if UPLO = 'U', or A = L \* L\*\*T, if UPLO = 'L',

where  ${\tt U}$  is an upper triangular matrix and  ${\tt L}$  is lower triangular.

This is the block version of the algorithm, calling Level 3 BLAS.

- UPLO (input) CHARACTER\*1
  - = 'U': Upper triangle of A is stored; = 'L': Lower triangle of A is stored.
- N (input) INTEGER The order of the matrix A. N >= 0.
- A (input/output) DOUBLE array on the GPU, dimension (LDA,N)
  On entry, the symmetric matrix A. If UPLO = 'U', the leading
  N-by-N upper triangular part of A contains the upper
  triangular part of the matrix A, and the strictly lower
  triangular part of A is not referenced. If UPLO = 'L', the
  leading N-by-N lower triangular part of A contains the lower
  triangular part of the matrix A, and the strictly upper
  triangular part of A is not referenced.

On exit, if INFO = 0, the factor U or L from the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T.

- WORK (workspace) DOUBLE array, dimension at least (nb, nb) where nb can be obtained through magma\_get\_dpotrf\_nb(\*n) Work array allocated with cudaMallocHost.
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, the leading minor of order i is not positive definite, and the factorization could not be completed.

#### 1.1.13 Function magma\_cgetrf

CGETRF computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges.

The factorization has the form  $% \left( 1\right) =\left( 1\right) \left( 1\right)$ 

A = P \* L \* U

where P is a permutation matrix, L is lower triangular with unit diagonal elements (lower trapezoidal if m > n), and U is upper triangular (upper trapezoidal if m < n).

This is the right-looking Level 3 BLAS version of the algorithm.

- M (input) INTEGER The number of rows of the matrix A. M >= 0.
- N (input) INTEGER The number of columns of the matrix A. N >= 0.
- A (input/output) COMPLEX array, dimension (LDA,N)
  On entry, the M-by-N matrix to be factored.
  On exit, the factors L and U from the factorization
  A = P\*L\*U; the unit diagonal elements of L are not stored.
  Higher performance is achieved if A is in pinned memory,
  e.g. allocated using cudaMallocHost.
- IPIV (output) INTEGER array, dimension  $(\min(M,N))$ The pivot indices; for 1 <= i <=  $\min(M,N)$ , row i of the matrix was interchanged with row IPIV(i).
- WORK (workspace/output) COMPLEX array, dimension >= N\*NB, where NB can be obtained through magma\_get\_cgetrf\_nb(M). Higher performance is achieved if WORK is in pinned memory, e.g. allocated using cudaMallocHost.
- DA (workspace) COMPLEX array on the GPU, dimension  $(\max(M, N) + k1)^2 + (M + k2)*NB + 2*NB^2,$  where NB can be obtained through magma\_get\_cgetrf\_nb(M). k1 < 32 and k2 < 32 are such that  $(\max(M, N) + k1)%32 = 0 \text{ and } (M+k2)%32 = 0.$
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, U(i,i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and division by zero will occur if it is used to solve a system of equations.

#### 1.1.14 Function magma\_cgeqrf

H(i) = I - tau \* v \* v'

```
int magma_cgeqrf(int *m, int *n, float2 *a, int *lda, float2 *tau,
                float2 *work, int *lwork, float2 *da, int *info )
   CGEQRF computes a QR factorization of a complex M-by-N matrix A: A = Q * R.
            (input) INTEGER
           The number of rows of the matrix A. M >= 0.
            (input) INTEGER
           The number of columns of the matrix A. N \ge 0.
            (input/output) COMPLEX array, dimension (LDA,N)
           On entry, the M-by-N matrix A.
           On exit, the elements on and above the diagonal of the array
           contain the \min(M,N)-by-N upper trapezoidal matrix R (R is
           upper triangular if m \geq= n); the elements below the diagonal,
           with the array TAU, represent the orthogonal matrix Q as a
           product of min(m,n) elementary reflectors.
           Higher performance is achieved if A is in pinned memory,
           e.g. allocated using cudaMallocHost.
   LDA
           (input) INTEGER
           The leading dimension of the array A. LDA \geq \max(1,M).
   TAU
            (output) COMPLEX array, dimension (min(M,N))
           The scalar factors of the elementary reflectors.
   WORK
           (workspace/output) COMPLEX array, dimension (MAX(1,LWORK))
           On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
           Higher performance is achieved if WORK is in pinned memory,
           e.g. allocated using cudaMallocHost.
   LWORK
           (input) INTEGER
           The dimension of the array WORK. LWORK >= N*NB,
           where NB can be obtained through magma_get_cgeqrf_nb(M).
           If LWORK = -1, then a workspace query is assumed; the routine
           only calculates the optimal size of the WORK array, returns
           this value as the first entry of the WORK array, and no error
           message related to LWORK is issued.
            (workspace) COMPLEX array on the GPU, dimension N*(M + NB),
   DA
           where NB can be obtained through magma_get_cgeqrf_nb(M).
           (size to be reduced in upcoming versions).
   INFO
           (output) INTEGER
           = 0: successful exit
           < 0: if INFO = -i, the i-th argument had an illegal value
   The matrix Q is represented as a product of elementary reflectors
      Q = H(1) H(2) \dots H(k), where k = min(m,n).
   Each H(i) has the form
```

where tau is a complex scalar, and v is a complex vector with v(1:i-1) = 0 and v(i) = 1; v(i+1:m) is stored on exit in A(i+1:m,i), and tau in TAU(i).

#### 1.1.15 Function magma\_cpotrf

int magma\_cpotrf(char \*uplo, int \*n, float2 \*a, int \*lda, float2 \*work, int \*info)

CPOTRF computes the Cholesky factorization of a complex Hermitian positive definite matrix A.

The factorization has the form A = U\*\*T \* U, if UPLO = 'U', or A = L \* L\*\*T, if UPLO = 'L',

where U is an upper triangular matrix and L is lower triangular.

This is the block version of the algorithm, calling Level 3 BLAS.

- UPLO (input) CHARACTER\*1 = 'U': Upper triangle of A is stored; = 'L': Lower triangle of A is stored.
- (input) INTEGER The order of the matrix A.  $N \ge 0$ .
- (input/output) COMPLEX array, dimension (LDA,N) On entry, the symmetric matrix A. If UPLO = 'U', the leading N-by-N upper triangular part of A contains the upper triangular part of the matrix A, and the strictly lower triangular part of A is not referenced. If UPLO = 'L', the leading N-by-N lower triangular part of A contains the lower triangular part of the matrix A, and the strictly upper triangular part of A is not referenced.

On exit, if INFO = 0, the factor U or L from the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T. Higher performance is achieved if A is in pinned memory, e.g. allocated using cudaMallocHost.

- LDA (input) INTEGER The leading dimension of the array A. LDA  $\geq \max(1,N)$ .
- WORK (workspace) COMPLEX array on the GPU, dimension (N, N)  $\,$ (size to be reduced in upcoming versions).
- INFO (output) INTEGER

  - = 0: successful exit < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, the leading minor of order i is not positive definite, and the factorization could not be  $% \left( 1\right) =\left( 1\right) \left( 1\right)$ completed.

#### 1.1.16 Function magma\_cgetrf\_gpu

CGETRF computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges.

The factorization has the form  $% \left( 1\right) =\left( 1\right) \left( 1\right)$ 

A = P \* L \* U

where P is a permutation matrix, L is lower triangular with unit diagonal elements (lower trapezoidal if m > n), and U is upper triangular (upper trapezoidal if m < n).

This is the right-looking Level 3 BLAS version of the algorithm.

- N (input) INTEGER

  The number of columns of the matrix A. N >= 0.
- A (input/output) COMPLEX array on the GPU, dimension (LDA,N) where LDA >=  $\max(M, N)+k1$ , k1<32 such that  $(\max(M, N)+k1)\%32==0$ . The memory pointed by A should be at least  $(\max(M, N) + k1)^2 + (M + k2)*NB + 2*NB^2$  where k2 < 32 such that (M + k2) %32 == 0.

On entry, the M-by-N matrix to be factored. On exit, the factors L and U from the factorization A = P\*L\*U; the unit diagonal elements of L are not stored. The rest of A is considered work space and is changed.

- IPIV (output) INTEGER array, dimension  $(\min(M,N))$ The pivot indices; for 1 <= i <=  $\min(M,N)$ , row i of the matrix was interchanged with row IPIV(i).
- WORK (workspace/output) COMPLEX array, dimension >= N\*NB, where NB can be obtained through magma\_get\_cgetrf\_nb(M). Higher performance is achieved if WORK is in pinned memory, e.g. allocated using cudaMallocHost.
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, U(i,i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and division by zero will occur if it is used to solve a system of equations.

#### 1.1.17 Function magma\_cgeqrf\_gpu

```
int magma_cgeqrf_gpu(int *m, int *n, float2 *a, int *lda, float2 *tau,
                     float2 *work, int *lwork, float2 *dwork, int *info )
    CGEQRF computes a QR factorization of a complex M-by-N matrix A: A = Q * R.
            (input) INTEGER
            The number of rows of the matrix A. M >= 0.
            (input) INTEGER
            The number of columns of the matrix A. N \ge 0.
            (input/output) COMPLEX array on the GPU, dimension (LDA,N)
            On entry, the M-by-N matrix A.
            On exit, the elements on and above the diagonal of the array
            contain the \min(M,N)-by-N upper trapezoidal matrix R (R is
            upper triangular if m \geq= n); the elements below the diagonal,
            with the array TAU, represent the orthogonal matrix Q as a
            product of min(m,n) elementary reflectors.
   T.DA
            (input) INTEGER
            The leading dimension of the array A. LDA >= \max(1,M).
    TAU
            (output) COMPLEX array, dimension (min(M,N))
            The scalar factors of the elementary reflectors (see Further
            Details).
    WORK
            (workspace/output) COMPLEX array, dimension (MAX(1,LWORK))
            On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
            Higher performance is achieved if WORK is in pinned memory,
            e.g. allocated using cudaMallocHost.
   L.WOR.K
            (input) INTEGER
            The dimension of the array WORK. LWORK >= (M+N)*NB,
            where NB can be obtained through magma\_get\_cgeqrf\_nb(M).
            If LWORK = -1, then a workspace query is assumed; the routine
            only calculates the optimal size of the WORK array, returns
            this value as the first entry of the WORK array, and no error
            message related to LWORK is issued.
    DWORK
            (workspace) COMPLEX array on the GPU, dimension N*NB,
            where \overline{\text{NB}} can be obtained through \overline{\text{magma\_get\_cgeqrf\_nb(M)}}.
    INFO
            (output) INTEGER
            = 0: successful exit
< 0: if INFO = -i, the i-th argument had an illegal value</pre>
    The matrix {\bf Q} is represented as a product of elementary reflectors
       Q = H(1) H(2) \dots H(k), where k = min(m,n).
    Each H(i) has the form
      H(i) = I - tau * v * v'
```

where tau is a complex scalar, and v is a complex vector with v(1:i-1) = 0 and v(i) = 1; v(i+1:m) is stored on exit in A(i+1:m,i), and tau in TAU(i).

## 1.1.18 Function magma\_cpotrf\_gpu

CPOTRF computes the Cholesky factorization of a complex Hermitian positive definite matrix  ${\tt A}\xspace.$ 

The factorization has the form

A = U\*\*T \* U, if UPLO = 'U', or

A = L \* L\*\*T, if UPLO = 'L',

where  ${\tt U}$  is an upper triangular matrix and  ${\tt L}$  is lower triangular.

This is the block version of the algorithm, calling Level 3 BLAS.

- UPLO (input) CHARACTER\*1
  = 'U': Upper triangle of A is stored;
  = 'L': Lower triangle of A is stored.
- N (input) INTEGER The order of the matrix A. N >= 0.
- A (input/output) COMPLEX array on the GPU, dimension (LDA,N)
  On entry, the symmetric matrix A. If UPLO = 'U', the leading
  N-by-N upper triangular part of A contains the upper
  triangular part of the matrix A, and the strictly lower
  triangular part of A is not referenced. If UPLO = 'L', the
  leading N-by-N lower triangular part of A contains the lower
  triangular part of the matrix A, and the strictly upper
  triangular part of A is not referenced.

On exit, if INFO = 0, the factor U or L from the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T.

- WORK (workspace) COMPLEX array, dimension at least (nb, nb) where nb can be obtained through magma\_get\_cpotrf\_nb(\*n) Work array allocated with cudaMallocHost.
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, the leading minor of order i is not positive definite, and the factorization could not be completed.

#### 1.1.19 Function magma\_zgetrf

ZGETRF computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges.

The factorization has the form  $% \left( 1\right) =\left( 1\right) \left( 1\right)$ 

A = P \* L \* U

where P is a permutation matrix, L is lower triangular with unit diagonal elements (lower trapezoidal if m > n), and U is upper triangular (upper trapezoidal if m < n).

This is the right-looking Level 3 BLAS version of the algorithm.

- M (input) INTEGER The number of rows of the matrix A. M  $\geq$  0.
- N (input) INTEGER

  The number of columns of the matrix A. N >= 0.
- A (input/output) DOUBLE COMPLEX array, dimension (LDA,N)
  On entry, the M-by-N matrix to be factored.
  On exit, the factors L and U from the factorization
  A = P\*L\*U; the unit diagonal elements of L are not stored.
  Higher performance is achieved if A is in pinned memory,
  e.g. allocated using cudaMallocHost.
- IPIV (output) INTEGER array, dimension  $(\min(M,N))$ The pivot indices; for 1 <= i <=  $\min(M,N)$ , row i of the matrix was interchanged with row IPIV(i).
- WORK (workspace/output) DOUBLE COMPLEX array, dimension >= N\*NB, where NB can be obtained through magma\_get\_cgetrf\_nb(M).

  Higher performance is achieved if WORK is in pinned memory, e.g. allocated using cudaMallocHost.
- DA (workspace) DOUBLE COMPLEX array on the GPU, dimension  $(\max(M, N) + k1)^2 + (M + k2)*NB + 2*NB^2,$  where NB can be obtained through magma\_get\_cgetrf\_nb(M). k1 < 32 and k2 < 32 are such that  $(\max(M, N) + k1)%32 = 0 \text{ and } (M+k2)%32 = 0.$
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, U(i,i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and division by zero will occur if it is used to solve a system of equations.

## 1.1.20 Function magma\_zgeqrf

```
int magma_zgeqrf(int *m, int *n, double2 *a, int *lda, double2 *tau,
                double2 *work, int *lwork, double2 *da, int *info )
   ZGEQRF computes a QR factorization of a complex M-by-N matrix A: A = Q * R.
            (input) INTEGER
           The number of rows of the matrix A. M >= 0.
            (input) INTEGER
           The number of columns of the matrix A. N \ge 0.
            (input/output) DOUBLE COMPLEX array, dimension (LDA,N)
           On entry, the M-by-N matrix A.
           On exit, the elements on and above the diagonal of the array
           contain the \min(M,N)-by-N upper trapezoidal matrix R (R is
           upper triangular if m \geq= n); the elements below the diagonal,
           with the array TAU, represent the orthogonal matrix Q as a
           product of min(m,n) elementary reflectors.
           Higher performance is achieved if A is in pinned memory,
           e.g. allocated using cudaMallocHost.
   LDA
           (input) INTEGER
           The leading dimension of the array A. LDA \geq \max(1,M).
   TAU
            (output) DOUBLE COMPLEX array, dimension (min(M,N))
           The scalar factors of the elementary reflectors.
           (workspace/output) DOUBLE COMPLEX array, dimension (MAX(1,LWORK))
   WORK
           On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
   Higher performance is achieved if WORK is in pinned memory,
           e.g. allocated using cudaMallocHost.
   LWORK
           (input) INTEGER
           The dimension of the array WORK. LWORK >= N*NB,
           where NB can be obtained through magma_get_zgeqrf_nb(M).
           If LWORK = -1, then a workspace query is assumed; the routine
           only calculates the optimal size of the WORK array, returns
           this value as the first entry of the WORK array, and no error
           message related to LWORK is issued.
            (workspace) DOUBLE COMPLEX array on the GPU, dimension N*(M + NB),
   DA
           where NB can be obtained through magma_get_zgeqrf_nb(M).
           (size to be reduced in upcoming versions).
   INFO
           (output) INTEGER
           = 0: successful exit
           < 0: if INFO = -i, the i-th argument had an illegal value
   The matrix Q is represented as a product of elementary reflectors
      Q = H(1) H(2) \dots H(k), where k = min(m,n).
   Each H(i) has the form
      H(i) = I - tau * v * v'
   where tau is a complex scalar, and v is a complex vector with v(1:i-1) = 0 and
   v(i) = 1; v(i+1:m) is stored on exit in A(i+1:m,i), and tau in TAU(i).
```

#### 1.1.21 Function magma\_zpotrf

ZPOTRF computes the Cholesky factorization of a complex Hermitian positive definite matrix  ${\tt A}\mbox{.}$ 

The factorization has the form  $A = U**T * U, \quad \text{if UPLO = 'U', or} \\ A = L * L**T, \quad \text{if UPLO = 'L',} \\ \text{where U is an upper triangular matrix and L is lower triangular.}$ 

This is the block version of the algorithm, calling Level 3 BLAS.

- UPLO (input) CHARACTER\*1
  = 'U': Upper triangle of A is stored;
  = 'L': Lower triangle of A is stored.
- N (input) INTEGER The order of the matrix A. N >= 0.
- A (input/output) DOUBLE COMPLEX array, dimension (LDA,N)
  On entry, the symmetric matrix A. If UPLO = 'U', the leading
  N-by-N upper triangular part of A contains the upper
  triangular part of the matrix A, and the strictly lower
  triangular part of A is not referenced. If UPLO = 'L', the
  leading N-by-N lower triangular part of A contains the lower
  triangular part of the matrix A, and the strictly upper
  triangular part of A is not referenced.

On exit, if INFO = 0, the factor U or L from the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T. Higher performance is achieved if A is in pinned memory, e.g. allocated using cudaMallocHost.

- LDA (input) INTEGER

  The leading dimension of the array A. LDA  $\geq$  max(1,N).
- WORK (workspace) DOUBLE COMPLEX array on the GPU, dimension (N, N) (size to be reduced in upcoming versions).
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, the leading minor of order i is not positive definite, and the factorization could not be completed.

#### 1.1.22 Function magma\_zgetrf\_gpu

ZGETRF computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges.

The factorization has the form

A = P \* L \* U

where P is a permutation matrix, L is lower triangular with unit diagonal elements (lower trapezoidal if m > n), and U is upper triangular (upper trapezoidal if m < n).

This is the right-looking Level 3 BLAS version of the algorithm.

- N (input) INTEGER

  The number of columns of the matrix A. N >= 0.
- A (input/output) DOUBLE COMPLEX array on the GPU, dimension (LDA,N) where LDA >=  $\max(M, N)+k1$ , k1<32 such that  $(\max(M, N)+k1)\%32==0$ . The memory pointed by A should be at least  $(\max(M, N) + k1)^2 + (M + k2)*NB + 2*NB^2$  where k2 < 32 such that (M + k2) %32 == 0.

On entry, the M-by-N matrix to be factored. On exit, the factors L and U from the factorization A = P\*L\*U; the unit diagonal elements of L are not stored. The rest of A is considered work space and is changed.

- IPIV (output) INTEGER array, dimension  $(\min(M,N))$ The pivot indices; for 1 <= i <=  $\min(M,N)$ , row i of the matrix was interchanged with row IPIV(i).
- WORK (workspace/output) DOUBLE COMPLEX array, dimension >= N\*NB, where NB can be obtained through magma\_get\_zgetrf\_nb(M).

  Higher performance is achieved if WORK is in pinned memory, e.g. allocated using cudaMallocHost.
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, U(i,i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and division by zero will occur if it is used to solve a system of equations.

#### 1.1.23 Function magma\_zgeqrf\_gpu

```
int magma_zgeqrf_gpu(int *m, int *n, double2 *a, int *lda, double2 *tau,
                    double2 *work, int *lwork, double2 *dwork, int *info )
   ZGEQRF computes a QR factorization of a complex M-by-N matrix A: A = Q * R.
            (input) INTEGER
           The number of rows of the matrix A. M >= 0.
            (input) INTEGER
           The number of columns of the matrix A. N \ge 0.
            (input/output) DOUBLE COMPLEX array on the GPU, dimension (LDA,N)
           On entry, the M-by-N matrix A.
           On exit, the elements on and above the diagonal of the array
           contain the \min(M,N)-by-N upper trapezoidal matrix R (R is
           upper triangular if m \geq= n); the elements below the diagonal,
            with the array TAU, represent the orthogonal matrix Q as a
           product of min(m,n) elementary reflectors.
   T.DA
            (input) INTEGER
           The leading dimension of the array A. LDA >= \max(1,M).
   TAU
           (output) DOUBLE COMPLEX array, dimension (min(M,N))
           The scalar factors of the elementary reflectors.
   WORK
           (workspace/output) DOUBLE COMPLEX array, dimension (MAX(1,LWORK))
           On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
           Higher performance is achieved if WORK is in pinned memory,
           e.g. allocated using cudaMallocHost.
   LWORK
           (input) INTEGER
           The dimension of the array WORK. LWORK >= (M+N)*NB,
           where NB can be obtained through magma_get_zgeqrf_nb(M).
           If LWORK = -1, then a workspace query is assumed; the routine
           only calculates the optimal size of the WORK array, returns
           this value as the first entry of the WORK array, and no error
           message related to LWORK is issued.
   DWORK
           (workspace) DOUBLE COMPLEX array on the GPU, dimension N*NB,
           where NB can be obtained through magma_get_zgeqrf_nb(M).
   INFO
           (output) INTEGER
           = 0: successful exit
           < 0: if INFO = -i, the i-th argument had an illegal value
   The matrix Q is represented as a product of elementary reflectors
      Q = H(1) H(2) . . . H(k), where k = min(m,n).
   Each H(i) has the form
      H(i) = I - tau * v * v'
   where tau is a complex scalar, and v is a complex vector with v(1:i-1) = 0 and
```

v(i) = 1; v(i+1:m) is stored on exit in A(i+1:m,i), and tau in TAU(i).

## 1.1.24 Function magma\_zpotrf\_gpu

ZPOTRF computes the Cholesky factorization of a complex Hermitian positive definite matrix  ${\tt A}\xspace.$ 

The factorization has the form  $A = U**T * U, \quad \text{if UPLO = 'U', or} \\ A = L * L**T, \quad \text{if UPLO = 'L',} \\ \text{where U is an upper triangular matrix and L is lower triangular.}$ 

This is the block version of the algorithm, calling Level 3 BLAS.

- UPLO (input) CHARACTER\*1
  = 'U': Upper triangle of A is stored;
  = 'L': Lower triangle of A is stored.
- N (input) INTEGER The order of the matrix A. N >= 0.
- (input/output) DOUBLE COMPLEX array on the GPU, dimension (LDA,N)
  On entry, the symmetric matrix A. If UPLO = 'U', the leading
  N-by-N upper triangular part of A contains the upper
  triangular part of the matrix A, and the strictly lower
  triangular part of A is not referenced. If UPLO = 'L', the
  leading N-by-N lower triangular part of A contains the lower
  triangular part of the matrix A, and the strictly upper
  triangular part of A is not referenced.

On exit, if INFO = 0, the factor U or L from the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T.

- WORK (workspace) DOUBLE COMPLEX array, dimension at least (nb, nb) where nb can be obtained through magma\_get\_zpotrf\_nb(\*n) Work array allocated with cudaMallocHost.
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, the leading minor of order i is not positive definite, and the factorization could not be completed.

## 1.1.25 Function magma\_sgeqlf

```
int magma_sgeqlf(int *m, int *n, float *a, int *lda,
                 float *tau, float *work, int *lwork, float *da, int *info)
    SGEQLF computes a QL factorization of a real M-by-N matrix A: A = Q * L.
            (input) INTEGER
            The number of rows of the matrix A. M \ge 0.
            (input) INTEGER
            The number of columns of the matrix A. N \ge 0.
            (input/output) REAL array, dimension (LDA,N)
            On entry, the M-by-N matrix A.
            On exit, if m \ge n, the lower triangle of the subarray
            A(m-n+1:m,1:n) contains the N-by-N lower triangular matrix L;
            if m \leq n, the elements on and below the (n-m)-th superdiagonal
            contain the M-by-N lower trapezoidal matrix L; the remaining
            elements, with the array TAU, represent the orthogonal matrix {\bf Q}
            as a product of elementary reflectors.
            Higher performance is achieved if A is in pinned memory,
            e.g. allocated using cudaMallocHost.
    LDA
            (input) INTEGER
            The leading dimension of the array A. LDA >= \max(1,M).
    TAU
            (output) REAL array, dimension (\min(M,N))
            The scalar factors of the elementary reflectors.
    WORK
            (workspace/output) REAL array, dimension (MAX(1,LWORK))
            On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
            Higher performance is achieved if WORK is in pinned memory, e.g.
            allocated using cudaMallocHost.
    LWORK
            (input) INTEGER
            The dimension of the array WORK. LWORK \geq \max(1,N).
            For optimum performance LWORK >= N*NB, where NB is the
            optimal blocksize. If LWORK = -1, then a workspace query is
            assumed; the routine only calculates the optimal size of the WORK
            array, returns this value as the first entry of the WORK array,
            and no error message related to LWORK is issued.
            (workspace) REAL array on the GPU, dimension N*(M + NB),
    DA
            where NB can be obtained through magma_get_sgeqlf_nb(M).
            (size to be reduced in upcoming versions).
    INFO
            (output) INTEGER
            = 0: successful exit
< 0: if INFO = -i, the i-th argument had an illegal value
    The matrix {\bf Q} is represented as a product of elementary reflectors
       Q = H(k) . . . H(2) H(1), where k = min(m,n).
    Each H(i) has the form
      H(i) = I - tau * v * v'
    where tau is a real scalar, and v is a real vector with
    v(m-k+i+1:m) = 0 and v(m-k+i) = 1; v(1:m-k+i-1) is stored on exit in
    A(1:m-k+i-1,n-k+i), and tau in TAU(i).
```

#### 1.1.26 Function magma\_sgelqf

```
int magma_sgelqf(int *m, int *n, float *a, int *lda, float *tau,
                                                      float *work, int *lwork, float *da, int *info)
            SGELQF computes an LQ factorization of a real M-by-N matrix A: A = L * Q.
                                      (input) INTEGER
                                      The number of rows of the matrix A. M >= 0.
                                      (input) INTEGER
                                      The number of columns of the matrix A. N \ge 0.
                                      (input/output) REAL array, dimension (LDA,N)
                                      On entry, the M-by-N matrix A.
                                      On exit, the elements on and below the diagonal of the array
                                      contain the m-by-min(m,n) lower trapezoidal matrix L (L is
                                      lower triangular if m \le n; the elements above the diagonal,
                                      with the array TAU, represent the orthogonal matrix Q as a
                                      product of elementary reflectors.
                                      Higher performance is achieved if A is in pinned memory, e.g.
                                      allocated using cudaMallocHost.
            LDA
                                      (input) INTEGER
                                      The leading dimension of the array A. LDA \geq \max(1,M).
            TAU
                                      (output) REAL array, dimension (min(M,N))
                                      The scalar factors of the elementary reflectors.
            WORK
                                      (workspace/output) REAL array, dimension (MAX(1,LWORK))
                                      On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
                                      Higher performance is achieved if WORK is in pinned memory, e.g.
                                      allocated using cudaMallocHost.
            LWORK
                                      (input) INTEGER
                                      The dimension of the array WORK. LWORK \geq \max(1,M).
                                      For optimum performance LWORK >= M*NB, where NB is the optimal
                                      blocksize. If LWORK = -1, then a workspace query is assumed; the
                                      routine only calculates the optimal size of the WORK array, returns % \left( 1\right) =\left( 1\right) \left( 1\right)
                                      this value as the first entry of the WORK array, and no error
                                      message is issued.
            DΑ
                                      (workspace) REAL array on the GPU, dimension M*(N + NB),
                                      where NB can be obtained through magma_get_sgeqrf_nb(M).
                                      (size to be reduced in upcoming versions).
            INFO
                                      (output) INTEGER
                                      = 0: successful exit
                                      < 0: if INFO = -i, the i-th argument had an illegal value
            The matrix Q is represented as a product of elementary reflectors
                     Q = H(k) . . . H(2) H(1), where k = min(m,n).
            Each H(i) has the form
                     H(i) = I - tau * v * v'
            where tau is a real scalar, and v is a real vector with
            v(1:i-1) = 0 and v(i) = 1; v(i+1:n) is stored on exit in A(i,i+1:n),
            and tau in TAU(i).
```

#### 1.2 Linear solvers

Provided are solvers in real arithmetic, both single and double precision, based on the LU, QR, and Cholesky factorizations. To solve

$$Ax = b$$

the matrix A is first factored, and second, the resulting factors are used in solving the original problem. A general recommendation is to use LU for general  $n \times n$  matrices, Cholesky for symmetric and positive definite  $n \times n$  matrices, and QR for solving least squares problems

$$min ||Ax - b||$$

for general  $m \times n$ ,  $m \ge n$  matrices.

The solvers are provided in the more critical GPU interface. Indeed, if a user has used the CPU interface for the matrix factorization, it would be often faster to do the solving step directly on the CPU using LAPACK with optimized CPU BLAS – the solving step is a bandwidth limited (Level 2 BLAS) operation and currently CPU's bus is of higher bandwidth than the bandwidth of the CPU-GPU connection (i.e. the time to solve on the CPU would be faster than just transferring the entire matrix to the GPU).

Although the solution step has  $O(n) \times$  less floating point operations than the factorization, it is still very important to optimize it. Solving a triangular system of equations can be very slow because the computation is bandwidth limited and naturally not parallel. Various approaches have been proposed in the past. We use an approach where diagonal blocks of A are explicitly inverted and used in a block algorithm. This results in a numerically stable algorithm, especially when used with triangular matrices coming from numerically stable factorization algorithms (e.g. as in LAPACK and as implemented here in MAGMA), of high performance, e.g. often exceeding  $100 \times$  the performance of the corresponding CUBLAS implementations.

To take advantage of the fact that GPU's single precision is currently of much higher performance than the double precision (theoretically  $\approx 10\times$ ), MAGMA version 0.2 provides a second set of solvers, based on the mixed precision iterative refinement technique. The solvers are based again on correspondingly the LU, QR, and Cholesky factorizations, and are designed to solve linear problems in double precision accuracy but at a speed that is characteristic for the much faster single precision computations. The idea is to use single precision for the bulk of the computation, namely the factorization step, and than use that factorization as a preconditioner in a simple iterative refinement process in double precision arithmetic. This often results in the desired high performance and high accuracy solvers.

#### 1.2.1 Function magma\_sgetrs\_gpu

```
int magma_sgetrs_gpu(char *trans , int n, int nrhs, float *a , int lda,
                    int *ipiv, float *b, int ldb, int *info, float *hwork)
   Solves a system of linear equations
     A * X = B or A' * X = B
   with a general N-by-N matrix A using the LU factorization computed by SGETRF_GPU.
   TRANS
           (input) CHARACTER*1
           Specifies the form of the system of equations:
           = 'N': A * X = B (No transpose)
           = 'T': A'* X = B (Transpose)
           = 'C': A'* X = B (Conjugate transpose = Transpose)
           (input) INTEGER
           The order of the matrix A. N >= 0.
   NRHS
           (input) INTEGER
           The number of right hand sides, i.e., the number of columns
           of the matrix B. NRHS >= 0.
           (input) REAL array on the GPU, dimension (LDA, \mathbb{N})
           The factors L and U from the factorization A = P*L*U as computed
           by SGETRF_GPU.
   LDA
           (input) INTEGER
           The leading dimension of the array A. LDA \geq \max(1,N).
   IPIV
           (input) INTEGER array, dimension (N)
           The pivot indices from SGETRF; for 1<=i<=N, row i of the
           matrix was interchanged with row IPIV(i).
           (input/output) REAL array on the GPU, dimension (LDB,NRHS)
   В
           On entry, the right hand side matrix B.
           On exit, the solution matrix X.
   LDB
           (input) INTEGER
           The leading dimension of the array B. LDB >= \max(1,N).
   INFO
           (output) INTEGER
           = 0: successful exit
           < 0: if INFO = -i, the i-th argument had an illegal value
   HWORK
           (workspace) REAL array, dimension N*NRHS
```

#### 1.2.2 Function magma\_sgeqrs\_gpu

```
int magma_sgeqrs_gpu(int *m, int *n, int *nrhs,
                     float *a, int *lda, float *tau, float *c, int *ldc,
                     float *work, int *lwork, float *td, int *info)
   Solves the least squares problem
          min || A*X - C ||
   using the QR factorization A = Q*R computed by SGEQRF_GPU2.
            (input) INTEGER
            The number of rows of the matrix A. M \ge 0.
            (input) INTEGER
            The number of columns of the matrix A. M >= N >= 0.
    NRHS
            (input) INTEGER
            The number of columns of the matrix C. NRHS >= 0.
            (input) REAL array on the GPU, dimension (LDA,N)
            The i-th column must contain the vector which defines the
            elementary reflector H(i), for i = 1, 2, ..., n, as returned by
            {\tt SGEQRF\_GPU2} in the first n columns of its array argument A.
   LDA
            (input) INTEGER
            The leading dimension of the array A, LDA \geq M.
            (input) REAL array, dimension (N) \,
   TAU
            TAU(i) must contain the scalar factor of the elementary
            reflector H(i), as returned by MAGMA_SGEQRF_GPU2.
            (input/output) REAL array on the GPU, dimension (LDC,NRHS)
            On entry, the M-by-NRHS matrix C.
            On exit, the N-by-NRHS solution matrix {\tt X}.
   LDC
            (input) INTEGER
            The leading dimension of the array C.\ LDC >= M.
    WOR.K
            (workspace/output) REAL array, dimension (LWORK)
            On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
            (input) INTEGER
    LWORK
            The dimension of the array WORK, LWORK \geq \max(1, NRHS).
            For optimum performance LWORK >= (M-N+NB+2*NRHS)*NB, where NB is
            the blocksize given by magma_get_sgeqrf_nb(\ M\ ).
            If LWORK = -1, then a workspace query is assumed; the routine
            only calculates the optimal size of the WORK array, returns
            this value as the first entry of the WORK array.
    TD
            (input) REAL array that is the output (the 9th argument)
            of magma_sgeqrf_gpu2.
    INFO
            (output) INTEGER
            = 0: successful exit
            < 0: if INFO = -i, the i-th argument had an illegal value
```

#### 1.2.3 Function magma\_spotrs\_gpu

int magma\_spotrs\_gpu(char \*UPLO, int N , int NRHS, float \*A , int LDA, float \*B, int LDB, int \*INFO)

Solves a system of linear equations A\*X = B with a symmetric positive definite matrix A using the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T computed by SPOTRF\_GPU.

- UPLO (input) CHARACTER\*1
  = 'U': Upper triangle of A is stored;
  = 'L': Lower triangle of A is stored.
- N (input) INTEGER The order of the matrix A. N >= 0.
- NRHS (input) INTEGER 
  The number of right hand sides, i.e., the number of columns of the matrix B. NRHS >= 0.
- A (input) REAL array on the GPU, dimension (LDA,N) The triangular factor U or L from the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T, as computed by SPOTRF.
- LDA (input) INTEGER  $\mbox{The leading dimension of the array A. LDA} >= \mbox{max(1,N)}.$
- B (input/output) REAL array on the GPU, dimension (LDB,NRHS)
  On entry, the right hand side matrix B.
  On exit, the solution matrix X.

#### 1.2.4 Function magma\_dgetrs\_gpu

```
int magma_dgetrs_gpu(char *trans , int n, int nrhs, double *a , int lda,
                    int *ipiv, double *b, int ldb, int *info, double *hwork)
   Solves a system of linear equations
     A * X = B or A' * X = B
   with a general N-by-N matrix A using the LU factorization computed by SGETRF_GPU.
   TRANS
           (input) CHARACTER*1
           Specifies the form of the system of equations:
           = 'N': A * X = B (No transpose)
           = 'T': A'* X = B (Transpose)
           = 'C': A'* X = B (Conjugate transpose = Transpose)
           (input) INTEGER
           The order of the matrix A. N >= 0.
   NRHS
            (input) INTEGER
           The number of right hand sides, i.e., the number of columns
           of the matrix B. NRHS >= 0.
           (input) DOUBLE array on the GPU, dimension (LDA,N) \,
           The factors L and U from the factorization A = P*L*U as computed
           by SGETRF_GPU.
   LDA
           (input) INTEGER
           The leading dimension of the array A. LDA \geq \max(1,N).
   IPIV
           (input) INTEGER array, dimension (N)
           The pivot indices from SGETRF; for 1<=i<=N, row i of the
           matrix was interchanged with row IPIV(i).
           (input/output) DOUBLE array on the GPU, dimension (LDB,NRHS) \,
   В
           On entry, the right hand side matrix B.
           On exit, the solution matrix X.
   LDB
            (input) INTEGER
           The leading dimension of the array B. LDB >= \max(1,N).
   INFO
           (output) INTEGER
           = 0: successful exit
           < 0: if INFO = -i, the i-th argument had an illegal value
           (workspace) DOUBLE array, dimension N*NRHS
   HWORK
```

#### 1.2.5 Function magma\_dgeqrs\_gpu

```
int magma_dgeqrs_gpu(int *m, int *n, int *nrhs,
                     double *a, int *lda, double *tau, double *c, int *ldc,
                     double *work, int *lwork, double *td, int *info)
    Solves the least squares problem
          min || A*X - C ||
   using the QR factorization A = Q*R computed by SGEQRF_GPU2.
            (input) INTEGER
            The number of rows of the matrix A. M \ge 0.
            (input) INTEGER
            The number of columns of the matrix A. M >= N >= 0.
    NRHS
            (input) INTEGER
            The number of columns of the matrix C. NRHS >= 0.
            (input) DOUBLE array on the GPU, dimension (LDA,N)
            The i-th column must contain the vector which defines the
            elementary reflector H(i), for i = 1, 2, ..., n, as returned by
            {\tt SGEQRF\_GPU2} in the first n columns of its array argument A.
   LDA
            (input) INTEGER
            The leading dimension of the array A, LDA \gt= M.
            (input) DOUBLE array, dimension (N)
   TAU
            TAU(i) must contain the scalar factor of the elementary
            reflector H(i), as returned by MAGMA_DGEQRF_GPU2.
            (input/output) DOUBLE array on the GPU, dimension (LDC,NRHS)
            On entry, the M-by-NRHS matrix C.
            On exit, the N-by-NRHS solution matrix {\tt X}.
   LDC
            (input) INTEGER
            The leading dimension of the array C.\ LDC >= M.
    WOR.K
            (workspace/output) DOUBLE array, dimension (LWORK)
            On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
            (input) INTEGER
    LWORK
            The dimension of the array WORK, LWORK \geq \max(1, NRHS).
            For optimum performance LWORK >= (M-N+NB+2*NRHS)*NB, where NB is
            the blocksize given by magma_get_sgeqrf_nb(\ M\ ).
            If LWORK = -1, then a workspace query is assumed; the routine
            only calculates the optimal size of the WORK array, returns
            this value as the first entry of the WORK array.
    TD
            (input) DOUBLE array that is the output (the 9th argument)
            of magma_dgeqrf_gpu2.
    INFO
            (output) INTEGER
            = 0: successful exit
            < 0: if INFO = -i, the i-th argument had an illegal value
```

#### 1.2.6 Function magma\_dpotrs\_gpu

int magma\_dpotrs\_gpu(char \*UPLO, int N , int NRHS, double \*A , int LDA, double \*B, int LDB, int \*INFO)

Solves a system of linear equations A\*X = B with a symmetric positive definite matrix A using the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T computed by SPOTRF\_GPU.

- UPLO (input) CHARACTER\*1
  = 'U': Upper triangle of A is stored;
  = 'L': Lower triangle of A is stored.
- NRHS (input) INTEGER 
  The number of right hand sides, i.e., the number of columns of the matrix B. NRHS >= 0.
- A (input) DOUBLE array on the GPU, dimension (LDA,N) The triangular factor U or L from the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T, as computed by SPOTRF.
- LDA (input) INTEGER  $\mbox{The leading dimension of the array A. LDA} >= \mbox{max(1,N)}.$
- B (input/output) DOUBLE array on the GPU, dimension (LDB,NRHS)
  On entry, the right hand side matrix B.
  On exit, the solution matrix X.

#### 1.2.7 Function magma\_dsgesv\_gpu

Computes the solution to a real system of linear equations A \* X = B, where A is an N-by-N matrix and X and B are N-by-NRHS matrices.

DSGESV first attempts to factorize the matrix in SINGLE PRECISION and use this factorization within an iterative refinement procedure to produce a solution with DOUBLE PRECISION normwise backward error quality (see below). If the approach fails the method switches to a DOUBLE PRECISION factorization and solve.

The iterative refinement is not going to be a winning strategy if the ratio SINGLE PRECISION performance over DOUBLE PRECISION performance is too small. A reasonable strategy should take the number of right-hand sides and the size of the matrix into account. This might be done with a call to ILAENV in the future. Up to now, we always try iterative refinement.

The iterative refinement process is stopped if

ITER > ITERMAX

or for all the RHS we have:

RNRM < SQRT(N)\*XNRM\*ANRM\*EPS\*BWDMAX

where

- o ITER is the number of the current iteration in the iterative refinement process
- o RNRM is the infinity-norm of the residual
- o  ${\tt XNRM}$  is the infinity-norm of the solution
- o ANRM is the infinity-operator-norm of the matrix  ${\tt A}$
- o EPS is the machine epsilon returned by DLAMCH('Epsilon') The value ITERMAX and BWDMAX are fixed to 30 and 1.0D+00 respectively.
- N (input) INTEGER

  The number of linear equations, i.e., the order of the matrix A.  $N \ge 0$ .
- NRHS (input) INTEGER

  The number of right hand sides, i.e., the number of columns of the matrix B. NRHS >= 0.
- (input or input/output) DOUBLE PRECISION array, dimension (LDA,N)
  On entry, the N-by-N coefficient matrix A.
  On exit, if iterative refinement has been successfully used
  (INFO.EQ.O and ITER.GE.O, see description below), A is
  unchanged. If double precision factorization has been used
  (INFO.EQ.O and ITER.LT.O, see description below), then the
  array A contains the factors L and U from the factorization
  A = P\*L\*U; the unit diagonal elements of L are not stored.

row i of the matrix was interchanged with row IPIV(i). Corresponds either to the single precision factorization (if INFO.EQ.O and ITER.GE.O) or the double precision factorization (if INFO.EQ.O and ITER.LT.O).

- B (input) DOUBLE PRECISION array, dimension (LDB,NRHS) The N-by-NRHS right hand side matrix B.
- LDB (input) INTEGER

  The leading dimension of the array B. LDB >= max(1,N).
- X (output) DOUBLE PRECISION array, dimension (LDX,NRHS) If INFO = 0, the N-by-NRHS solution matrix X.
- WORK (workspace) DOUBLE PRECISION array, dimension (N\*NRHS)
  This array is used to hold the residual vectors.
- SWORK (workspace) REAL array, dimension (N\*(N+NRHS))

  This array is used to store the single precision matrix and the right-hand sides or solutions in single precision.
- ITER (output) INTEGER
  - < 0: iterative refinement has failed, double precision factorization has been performed
    - -1 : the routine fell back to full precision for implementation- or machine-specific reasons
    - -2 : narrowing the precision induced an overflow, the routine fell back to full precision
    - -3 : failure of SGETRF
    - $\mbox{-31:}$  stop the iterative refinement after the 30th iterations
  - > 0: iterative refinement has been successfully used.
    Returns the number of iterations
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, U(i,i) computed in DOUBLE PRECISION is exactly zero. The factorization has been completed, but the factor U is exactly singular, so the solution could not be computed.
- H\_SWORK (workspace) REAL array, dimension at least (nb, nb)
   where nb can be obtained through magma\_get\_sgetrf\_nb(\*n)
   Work array allocated with cudaMallocHost.
- H\_WORK (workspace) DOUBLE array, dimension at least (nb, nb)
   where nb can be obtained through magma\_get\_dgetrf\_nb(\*n)
   Work array allocated with cudaMallocHost.
- DIPIV (output) INTEGER array on the GPU, dimension (min(M,N))
   The pivot indices; for 1 <= i <= min(M,N), row i of the
   matrix was moved to row IPIV(i).</pre>

#### 1.2.8 Function magma\_dsgeqrsv\_gpu

int magma\_dsgeqrsv\_gpu(int M, int N, int NRHS, double \*A, int LDA, double \*B,
 int LDB, double \*X,int LDX, double \*WORK, float \*SWORK,
 int \*ITER, int \*INFO, float \*tau, int lwork, float \*h\_work,
 float \*d\_work, double \*tau\_d, int lwork\_d, double \*h\_work\_d,
 double \*d\_work\_d)

DSGEQRSV solves the least squares problem min || A\*X - B ||, where A is an M-by-N matrix and X and B are M-by-NRHS matrices.

DSGEQRSV first attempts to factorize the matrix in SINGLE PRECISION and use this factorization within an iterative refinement procedure to produce a solution with DOUBLE PRECISION norm-wise backward error quality (see below). If the approach fails the method switches to a DOUBLE PRECISION factorization and solve.

The iterative refinement is not going to be a winning strategy if the ratio SINGLE PRECISION performance over DOUBLE PRECISION performance is too small. A reasonable strategy should take the number of right-hand sides and the size of the matrix into account. This might be done with a call to ILAENV in the future. Up to now, we always try iterative refinement.

The iterative refinement process is stopped if

ITER > ITERMAX

or for all the RHS we have:

RNRM < SQRT(N)\*XNRM\*ANRM\*EPS\*BWDMAX

where

- o ITER is the number of the current iteration in the iterative refinement process
- o RNRM is the infinity-norm of the residual  $% \left( 1\right) =\left( 1\right) +\left( 1\right)$
- o  ${\tt XNRM}$  is the infinity-norm of the solution
- o ANRM is the infinity-operator-norm of the matrix  $\boldsymbol{A}$
- o EPS is the machine epsilon returned by DLAMCH('Epsilon') The value ITERMAX and BWDMAX are fixed to 30 and 1.0D+00 respectively.
- M (input) INTEGER

  The number of rows of the matrix A.  $M \ge 0$ .
- NRHS (input) INTEGER

  The number of right hand sides, i.e., the number of columns of the matrix B. NRHS >= 0.
- (input or input/output) DOUBLE PRECISION array, dimension (LDA,N)
  On entry, the M-by-N coefficient matrix A.
  On exit, if iterative refinement has been successfully used
  (INFO.EQ.O and ITER.GE.O, see description below), A is
  unchanged. If double precision factorization has been used
  (INFO.EQ.O and ITER.LT.O, see description below), then the
  array A contains the QR factorization of A as returned by
  function DGEQRF\_GPU2.
- LDA (input) INTEGER

The leading dimension of the array A. LDA  $\Rightarrow$  max(1,M).

- B (input) DOUBLE PRECISION array, dimension (LDB,NRHS)
  The M-by-NRHS right hand side matrix B.
- LDB (input) INTEGER

  The leading dimension of the array B. LDB >= max(1,M).
- X (output) DOUBLE PRECISION array, dimension (LDX,NRHS)
  If INFO = 0, the N-by-NRHS solution matrix X.
- WORK (workspace) DOUBLE PRECISION array, dimension (N\*NRHS) This array is used to hold the residual vectors.
- SWORK (workspace) REAL array, dimension (M\*(N+NRHS))

  This array is used to store the single precision matrix and the right-hand sides or solutions in single precision.
- ITER (output) INTEGER
  - $\!<\!$  0: iterative refinement has failed, double precision factorization has been performed
    - -1: the routine fell back to full precision for implementation- or machine-specific reasons
    - -2 : narrowing the precision induced an overflow, the routine fell back to full precision
    - -3 : failure of SGETRF
    - -31: stop the iterative refinement after the 30th iterations
  - > 0: iterative refinement has been successfully used. Returns the number of iterations
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
- TAU (output) REAL array, dimension (N)
  On exit, TAU(i) contains the scalar factor of the elementary reflector H(i), as returned by magma\_sgeqrf\_gpu2.
- LWORK (input) INTEGER  $\label{eq:local_theory} \mbox{The dimension of the array $H_WORK$. LWORK >= $(M+N+NB)*NB$, } \\ \mbox{where $NB$ can be obtained through magma_get_sgeqrf_nb(M)}.$
- H\_WORK (workspace/output) REAL array, dimension (MAX(1,LWORK))
  Higher performance is achieved if H\_WORK is in pinned memory, e.g.
  allocated using cudaMallocHost.
- D\_WORK (workspace/output) REAL array on the GPU, dimension 2\*N\*NB,
   where NB can be obtained through magma\_get\_sgeqrf\_nb(M).
   It starts with NB\*NB blocks that store the triangular T
   matrices, followed by the NB\*NB blocks of the diagonal
   inverses for the R matrix.
- TAU\_D (output) DOUBLE REAL array, dimension (N)

On exit, if the matrix had to be factored in double precision, TAU(i) contains the scalar factor of the elementary reflector H(i), as returned by magma\_dgeqrf\_gpu2.

- H\_WORK\_D (workspace/output) DOUBLE REAL array, dimension (MAX(1,LWORK\_D)) This memory is unattached if the iterative refinement worked, otherwise it is used as workspace to factor the matrix in double precision. Higher performance is achieved if H\_WORK\_D is in pinned memory, e.g. allocated using cudaMallocHost.
- D\_WORK\_D (workspace/output) DOUBLE REAL array on the GPU, dimension 2\*N\*NB, where NB can be obtained through magma\_get\_dgeqrf\_nb(M).

  This memory is unattached if the iterative refinement worked, otherwise it is used as workspace to factor the matrix in double precision. It starts with NB\*NB blocks that store the triangular T matrices, followed by the NB\*NB blocks of the diagonal inverses for the R matrix.

#### 1.2.9 Function magma\_dsposv\_gpu

DSPOSV computes the solution to a real system of linear equations A \* X = B.

where A is an N-by-N symmetric positive definite matrix and X and B are N-by-NRHS matrices.

DSPOSV first attempts to factorize the matrix in SINGLE PRECISION and use this factorization within an iterative refinement procedure to produce a solution with DOUBLE PRECISION norm-wise backward error quality (see below). If the approach fails the method switches to a DOUBLE PRECISION factorization and solve.

The iterative refinement is not going to be a winning strategy if the ratio SINGLE PRECISION performance over DOUBLE PRECISION performance is too small. A reasonable strategy should take the number of right-hand sides and the size of the matrix into account. This might be done with a call to ILAENV in the future. Up to now, we always try iterative refinement.

The iterative refinement process is stopped if  $\ensuremath{\mbox{ITER}}\xspace > \ensuremath{\mbox{ITERMAX}}\xspace$ 

or for all the RHS we have:

RNRM < SQRT(N)\*XNRM\*ANRM\*EPS\*BWDMAX

where

- o ITER is the number of the current iteration in the iterative refinement process
- o  ${\tt RNRM}$  is the infinity-norm of the residual
- o  ${\tt XNRM}$  is the infinity-norm of the solution
- o ANRM is the infinity-operator-norm of the matrix  $\boldsymbol{A}$
- o EPS is the machine epsilon returned by DLAMCH('Epsilon')
  The value ITERMAX and BWDMAX are fixed to 30 and 1.0D+00 respectively.

UPLO (input) CHARACTER

- = 'U': Upper triangle of A is stored;
- = 'L': Lower triangle of A is stored.
- N (input) INTEGER

The number of linear equations, i.e., the order of the matrix A.  $\, N \, > = \, 0 \, . \,$ 

NRHS (input) INTEGER

The number of right hand sides, i.e., the number of columns of the matrix B. NRHS >= 0.

A (input or input/output) DOUBLE PRECISION array, dimension (LDA,N)

On entry, the symmetric matrix A. If UPLO = 'U', the leading N-by-N upper triangular part of A contains the upper triangular part of the matrix A, and the strictly lower triangular part of A is not referenced. If UPLO = 'L', the leading N-by-N lower triangular part of A contains the lower triangular part of the matrix A, and the strictly upper triangular part of A is not referenced.

On exit, if iterative refinement has been successfully used (INFO.EQ.O and ITER.GE.O, see description below), then A is unchanged, if double precision factorization has been used (INFO.EQ.O and ITER.LT.O, see description below), then the array A contains the factor U or L from the Cholesky factorization A = U\*\*T\*U or A = L\*L\*\*T.

- B (input) DOUBLE PRECISION array, dimension (LDB,NRHS) The N-by-NRHS right hand side matrix B.
- LDB (input) INTEGER

  The leading dimension of the array B. LDB >= max(1,N).
- X (output) DOUBLE PRECISION array, dimension (LDX,NRHS) If INFO = 0, the N-by-NRHS solution matrix X.

- SWORK (workspace) REAL array, dimension (N\*(N+NRHS))

  This array is used to use the single precision matrix and the right-hand sides or solutions in single precision.
- ITER (output) INTEGER
  - < 0: iterative refinement has failed, double precision factorization has been performed
    - -1: the routine fell back to full precision for implementation- or machine-specific reasons
    - -2 : narrowing the precision induced an overflow, the routine fell back to full precision
    - -3 : failure of SPOTRF
    - -31: stop the iterative refinement after the 30th iterations
  - > 0: iterative refinement has been successfully used. Returns the number of iterations
- INFO (output) INTEGER
  - = 0: successful exit
  - < 0: if INFO = -i, the i-th argument had an illegal value
  - > 0: if INFO = i, the leading minor of order i of (DOUBLE PRECISION) A is not positive definite, so the factorization could not be completed, and the solution has not been computed.

1.3 Two-sided matrix factorizations

#### 1.3.1 Function magma\_sgehrd

DGEHRD reduces a real general matrix A to upper Hessenberg form H by an orthogonal similarity transformation: Q'\* A \* Q = H .

- ILO (input) INTEGER
  IHI (input) INTEGER
  - It is assumed that A is already upper triangular in rows and columns 1:ILO-1 and IHI+1:N. ILO and IHI are normally set by a previous call to DGEBAL; otherwise they should be set to 1 and N respectively. See Further Details.

    1 <= ILO <= IHI <= N, if N > 0; ILO=1 and IHI=0, if N=0.
- A (input/output) SINGLE PRECISION array, dimension (LDA,N)
  On entry, the N-by-N general matrix to be reduced.
  On exit, the upper triangle and the first subdiagonal of A are overwritten with the upper Hessenberg matrix H, and the elements below the first subdiagonal, with the array TAU, represent the orthogonal matrix Q as a product of elementary reflectors. See Further Details.
- TAU (output) SINGLE PRECISION array, dimension (N-1)
  The scalar factors of the elementary reflectors (see Further Details). Elements 1:ILO-1 and IHI:N-1 of TAU are set to zero.
- WORK (workspace/output) SINGLE PRECISION array, dimension (LWORK)
  On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
- LWORK (input) INTEGER
   The length of the array WORK. LWORK >= max(1,N).
   For optimum performance LWORK >= N\*NB, where NB is the optimal blocksize.

If LWORK = -1, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued by XERBLA.

- DA (workspace) SINGLE array on the GPU, dimension N\*N + 2\*N\*NB + NB\*NB, where NB can be obtained through magma\_get\_sgehrd\_nb(N).
- INFO (output) INTEGER
  = 0: successful exit
  < 0: if INFO = -i, the i-th argument had an illegal value.</pre>

Further Details

The matrix  ${\tt Q}$  is represented as a product of (ihi-ilo) elementary reflectors

```
Q = H(ilo) H(ilo+1) . . . H(ihi-1).
```

Each H(i) has the form

```
H(i) = I - tau * v * v'
```

where tau is a real scalar, and v is a real vector with v(1:i) = 0, v(i+1) = 1 and v(ihi+1:n) = 0; v(i+2:ihi) is stored on exit in A(i+2:ihi,i), and tau in TAU(i).

The contents of A are illustrated by the following example, with n = 7, ilo = 2 and ihi = 6:

```
on entry,
                         on exit,
( a
                   a )
                         (aahh
                                          h a)
   a a
          a
             a
                a
                                       h
                   a )
                                             a )
    a a a
             a
                a
(
                   a )
                         (
                              h
                                 h
                                    h
                                       h
                                          h
                                              h )
    a
       a
          a
             a
                a
                              v2 h
(
    a
       a
          a
             a
                a
                    a )
                         (
                                     h
                                       h
                                           h
                                              h )
(
                   a )
                              v2 v3 h h h
                                              h )
    a
       a
          a
             a
                a
                              v2 v3 v4 h
(
                   a )
                         (
                                              h )
             а
                a
                    a )
                                              a )
```

where a denotes an element of the original matrix A, h denotes a modified element of the upper Hessenberg matrix H, and vi denotes an element of the vector defining H(i).

This implementation follows the algorithm and notations described in

S. Tomov and J. Dongarra, "Accelerating the reduction to upper Hessenberg form through hybrid GPU-based computing," University of Tennessee Computer Science Technical Report, UT-CS-09-642 (also LAPACK Working Note 219), May 24, 2009.

#### 1.3.2 Function magma\_dgehrd

DGEHRD reduces a real general matrix A to upper Hessenberg form H by an orthogonal similarity transformation: Q'\* A \* Q = H .

- ILO (input) INTEGER
  IHI (input) INTEGER
  - It is assumed that A is already upper triangular in rows and columns 1:ILO-1 and IHI+1:N. ILO and IHI are normally set by a previous call to DGEBAL; otherwise they should be set to 1 and N respectively. See Further Details.

    1 <= ILO <= IHI <= N, if N > 0; ILO-1 and IHI-0, if N=0.
- A (input/output) DOUBLE PRECISION array, dimension (LDA,N)
  On entry, the N-by-N general matrix to be reduced.
  On exit, the upper triangle and the first subdiagonal of A are overwritten with the upper Hessenberg matrix H, and the elements below the first subdiagonal, with the array TAU, represent the orthogonal matrix Q as a product of elementary reflectors. See Further Details.
- TAU (output) DOUBLE PRECISION array, dimension (N-1)
  The scalar factors of the elementary reflectors (see Further Details). Elements 1:ILO-1 and IHI:N-1 of TAU are set to zero.
- WORK (workspace/output) DOUBLE PRECISION array, dimension (LWORK)
  On exit, if INFO = 0, WORK(1) returns the optimal LWORK.
- LWORK (input) INTEGER
   The length of the array WORK. LWORK >= max(1,N).
   For optimum performance LWORK >= N\*NB, where NB is the optimal blocksize.

If LWORK = -1, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued by XERBLA.

- DA (workspace) DOUBLE array on the GPU, dimension N\*N + 2\*N\*NB + NB\*NB, where NB can be obtained through magma\_get\_dgehrd\_nb(N).
- INFO (output) INTEGER
  = 0: successful exit
  < 0: if INFO = -i, the i-th argument had an illegal value.</pre>

Further Details

The matrix  ${\tt Q}$  is represented as a product of (ihi-ilo) elementary reflectors

```
Q = H(ilo) H(ilo+1) . . . H(ihi-1).
```

Each H(i) has the form

```
H(i) = I - tau * v * v'
```

where tau is a real scalar, and v is a real vector with v(1:i) = 0, v(i+1) = 1 and v(ihi+1:n) = 0; v(i+2:ihi) is stored on exit in A(i+2:ihi,i), and tau in TAU(i).

The contents of A are illustrated by the following example, with n = 7, ilo = 2 and ihi = 6:

```
on entry,
                         on exit,
                         (aahh
( a
                   a )
                                          h a)
   a a
         a
             a
                a
                                       h
                   a )
                                             a )
    a a a
             a
               a
(
                   a )
                         (
                              h
                                 h
                                    h
                                       h
                                          h
                                             h )
    a
       a
          a
             a
                a
                              v2 h
(
    a
       a
          a
             a
                a
                   a )
                         (
                                    h
                                       h
                                          h
                                             h )
(
                   a )
                              v2 v3 h h h
                                             h )
    a
       a
          a
             a
                a
                              v2 v3 v4 h h
(
                   a )
                         (
                                             h )
             а
                a
                   a )
                                              a )
```

where a denotes an element of the original matrix A, h denotes a modified element of the upper Hessenberg matrix H, and vi denotes an element of the vector defining H(i).

This implementation follows the algorithm and notations described in

S. Tomov and J. Dongarra, "Accelerating the reduction to upper Hessenberg form through hybrid GPU-based computing," University of Tennessee Computer Science Technical Report, UT-CS-09-642 (also LAPACK Working Note 219), May 24, 2009.

# Chapter 2

# The MAGMA BLAS Library

## 2.1 Matrix-Matrix Multiplication

#### 2.1.1 Function magmablasSgemm

```
int magmablasSgemm(char TRANSA, char TRANSB, int m , int n, int k, float alpha,
                    const float *A, int lda, const float *B, int ldb, float beta,
                    float *C, int ldc)
   SGEMM performs one of the matrix-matrix operations
      C := alpha*op(A)*op(B) + beta*C,
   where op(X) is one of
      op(X) = X \quad or \quad op(X) = X',
   alpha and beta are scalars, and A, B and C are matrices, with op( A )
   an m by k matrix, op(B) a k by n matrix and C an m by n matrix.
   TRANSA - CHARACTER*1.
            On entry, TRANSA specifies the form of op( A ) to be used in
            the matrix multiplication as follows:
               TRANSA = 'N' or 'n', op( A ) = A.

TRANSA = 'T' or 't', op( A ) = A'.
               TRANSA = 'C' or 'c', op( A ) = A'.
            Unchanged on exit.
   TRANSB - CHARACTER*1.
            On entry, TRANSB specifies the form of op( B ) to be used in
            the matrix multiplication as follows:
               TRANSB = 'N' or 'n', op(B) = B.
               TRANSB = 'T' or 't', op(B) = B'.
TRANSB = 'C' or 'c', op(B) = B'.
            Unchanged on exit.
            On entry, {\tt M} specifies the number of rows of the matrix {\tt op}({\tt A}) and of
            the matrix C. M must be at least zero.
            Unchanged on exit.
          - INTEGER.
            On entry, N specifies the number of columns of the matrix op(B) and
            the number of columns of the matrix {\tt C.}\ {\tt N} must be at least zero.
            Unchanged on exit.
   K
          - INTEGER.
            On entry, K specifies the number of columns of the matrix op(A) and
            the number of rows of the matrix op( B ). K must be at least zero.
            Unchanged on exit.
   ALPHA - SINGLE PRECISION.
            On entry, ALPHA specifies the scalar alpha.
            Unchanged on exit.
          - SINGLE PRECISION array of DIMENSION (LDA, ka), where ka is k when
            {\tt TRANSA} = 'N' or 'n', and is m otherwise. Before entry with {\tt TRANSA}
            = 'N' or 'n', the leading m by k part of the array A must contain
            the matrix A, otherwise the leading k by m part of the array A
            must contain the matrix A.
            Unchanged on exit.
   LDA
          - INTEGER.
            On entry, LDA specifies the first dimension of A as declared
            in the calling (sub) program. When TRANSA = 'N' or 'n' then
```

LDA must be at least  $\mbox{ max( 1, m ), otherwise }$  LDA must be at least  $\mbox{ max( 1, k ).}$  Unchanged on exit.

B - SINGLE PRECISION array of DIMENSION (LDB, kb), where kb is n when TRANSB = 'N' or 'n', and is k otherwise.

Before entry with TRANSB = 'N' or 'n', the leading k by n part of the array B must contain the matrix B, otherwise the leading n by k part of the array B must contain the matrix B.

Unchanged on exit.

#### LDB - INTEGER

On entry, LDB specifies the first dimension of B as declared in the calling (sub) program. When TRANSB = 'N' or 'n' then LDB must be at least max(1, k), otherwise LDB must be at least max(1, n). Unchanged on exit.

#### BETA - SINGLE PRECISION.

On entry, BETA specifies the scalar beta. When BETA is supplied as zero then C need not be set on input. Unchanged on exit.

C - SINGLE PRECISION array of DIMENSION ( LDC, n ).

Before entry, the leading m by n part of the array C must contain the matrix C, except when beta is zero, in which case C need not be set on entry.

On exit, the array C is overwritten by the m by n matrix ( alpha\*op( A )\*op( B ) + beta\*C ).

#### LDC - INTEGER.

On entry, LDC specifies the first dimension of C as declared in the calling (sub) program. LDC must be at least max( 1, m ). Unchanged on exit.

#### 2.1.2 Function magmablasDgemm

```
int magmablasDgemm(char TRANSA, char TRANSB, int m, int n, int k, double alpha,
                     const double *A, int lda, const double *B, int ldb,
                     double beta, double *C, int ldc)
    {\tt DGEMM}\ \ {\tt performs} one of the matrix-matrix operations
      C := alpha*op(A)*op(B) + beta*C,
    where op(X) is one of
      op(X) = X \quad or \quad op(X) = X',
    alpha and beta are scalars, and A, B and C are matrices, with op( A )
    an m by k matrix, op( B ) a \, k by n matrix and \, C an m by n matrix.
    TRANSA - CHARACTER*1.
              On entry, TRANSA specifies the form of op( A ) to be used in
              the matrix multiplication as follows:
                 TRANSA = 'N' or 'n', op( A ) = A.

TRANSA = 'T' or 't', op( A ) = A'.

TRANSA = 'C' or 'c', op( A ) = A'.
              Unchanged on exit.
    TRANSB - CHARACTER*1.
              On entry, TRANSB specifies the form of op( B ) to be used in
              the matrix multiplication as follows:
                 TRANSB = 'N' or 'n', op( B ) = B.
                 TRANSB = 'T' or 't', op( B ) = B'.
TRANSB = 'C' or 'c', op( B ) = B'.
              Unchanged on exit.
              On entry, M specifies the number of rows of the matrix
              op( A ) and of the matrix C. M must be at least zero.
              Unchanged on exit.
            - INTEGER.
              On entry, N specifies the number of columns of the matrix
              op( B ) and the number of columns of the matrix C. N must be
              at least zero.
              Unchanged on exit.
            - INTEGER.
    K
              On entry, \, K \, specifies \, the number of columns of the matrix \,
              op( A ) and the number of rows of the matrix op( B ). K must
              be at least zero.
              Unchanged on exit.
    ALPHA - DOUBLE PRECISION.
              On entry, ALPHA specifies the scalar alpha.
              Unchanged on exit.
            - DOUBLE PRECISION array of DIMENSION ( LDA, ka ), where ka is
              k when TRANSA = 'N' or 'n', and is m otherwise. Before entry with TRANSA = 'N' or 'n', the leading m by k
              part of the array A must contain the matrix A, otherwise
              the leading \, k by m \, part of the array \, A \, must contain \, the
              matrix A.
              Unchanged on exit.
```

#### LDA - INTEGER.

On entry, LDA specifies the first dimension of A as declared in the calling (sub) program. When TRANSA = 'N' or 'n' then LDA must be at least max( 1, m ), otherwise LDA must be at least max( 1, k ). Unchanged on exit.

B - DOUBLE PRECISION array of DIMENSION ( LDB, kb ), where kb is n when TRANSB = 'N' or 'n', and is k otherwise.

Before entry with TRANSB = 'N' or 'n', the leading k by n part of the array B must contain the matrix B, otherwise the leading n by k part of the array B must contain the matrix B.

Unchanged on exit.

#### LDB - INTEGER.

On entry, LDB specifies the first dimension of B as declared in the calling (sub) program. When TRANSB = 'N' or 'n' then LDB must be at least max(1, k), otherwise LDB must be at least max(1, n). Unchanged on exit.

#### BETA - DOUBLE PRECISION.

On entry, BETA specifies the scalar beta. When BETA is supplied as zero then C need not be set on input. Unchanged on exit.

C - DOUBLE PRECISION array of DIMENSION ( LDC, n ).

Before entry, the leading m by n part of the array C must contain the matrix C, except when beta is zero, in which case C need not be set on entry.

On exit, the array C is overwritten by the m by n matrix ( alpha\*op( A )\*op( B ) + beta\*C ).

#### LDC - INTEGER.

On entry, LDC specifies the first dimension of C as declared in the calling (sub) program. LDC must be at least max( 1, m ). Unchanged on exit.

## 2.2 Matrix-Vector Multiplication

### ${\bf 2.2.1} \quad {\bf Function \ magma\_smemv}$

## ${\bf 2.2.2 \quad Function \; magma\_dgemv}$

2.3 Symmetric Matrix-Vector multiplication

#### 2.3.1 Function magma\_ssymv

```
int magma_ssymv(char uplo, int m, float alpha, float *A, int lda, float *X,
                 int incx, float beta, float *Y, int incy)
    SSYMV performs the matrix-vector operation
      y := alpha*A*x + beta*y,
    where alpha and beta are scalars, x and y are n element vectors and
    A is an n by n symmetric matrix.
    UPLO
             CHARACTER*1.
             On entry, UPLO specifies whether the upper or lower triangular
             part of the array A is to be referenced as follows:
                UPLO = 'U' or 'u' Only the upper triangular part of A
                                     is to be referenced.
                UPLO = 'L' or 'l' Only the lower triangular part of A
                                     is to be referenced.
             Unchanged on exit.
             INTEGER.
    N
             On entry, N specifies the order of the matrix A.
             \ensuremath{\text{N}} must be at least zero.
             Unchanged on exit.
    ALPHA
             REAL.
             On entry, ALPHA specifies the scalar alpha.
             Unchanged on exit.
             REAL array of DIMENSION ( LDA, n ).
             Before entry with UPLO = 'U' or 'u', the leading n by n
             upper triangular part of the array A must contain the upper
             triangular part of the symmetric matrix and the strictly
             lower triangular part of {\tt A} is not referenced.
             Before entry with UPLO = 'L' or 'l', the leading n by n
             lower triangular part of the array \mbox{\mbox{\bf A}} must contain the lower
             triangular part of the symmetric matrix and the strictly
             upper triangular part of A is not referenced.
             Unchanged on exit.
             INTEGER.
    LDA
             On entry, LDA specifies the first dimension of {\tt A} as declared
             in the calling (sub) program. LDA must be at least
             max( 1, n ).
             Unchanged on exit.
             REAL array of dimension at least
    Х
             (1 + (n - 1)*abs(INCX)).
             Before entry, the incremented array \boldsymbol{X} must contain the n
             element vector x.
             Unchanged on exit.
    TNCX
             INTEGER.
             On entry, INCX specifies the increment for the elements of
             X. INCX must not be zero.
             Unchanged on exit.
    BETA
             REAL.
```

On entry, BETA specifies the scalar beta. When BETA is supplied as zero then Y need not be set on input. Unchanged on exit.

Y REAL array of dimension at least
(1 + (n - 1)\*abs(INCY)).

Before entry, the incremented array Y must contain the n
element vector y. On exit, Y is overwritten by the updated
vector y.

#### INCY INTEGER.

On entry, INCY specifies the increment for the elements of Y. INCY must not be zero. Unchanged on exit.

#### 2.3.2 Function magma\_dsymv

DSYMV performs the matrix-vector operation y := alpha\*A\*x + beta\*y, where alpha and beta are scalars, x and y are n element vectors and A is an n by n symmetric matrix.

#### UPLO CHARACTER\*1.

On entry, UPLO specifies whether the upper or lower triangular part of the array A is to be referenced as follows:

Unchanged on exit.

#### N INTEGER.

On entry, N specifies the order of the matrix A. N must be at least zero. Unchanged on exit.

#### ALPHA DOUBLE PRECISION.

On entry, ALPHA specifies the scalar alpha. Unchanged on exit.

A DOUBLE PRECISION array of DIMENSION (LDA, n).
Before entry with UPLO = 'U' or 'u', the leading n by n
upper triangular part of the array A must contain the upper
triangular part of the symmetric matrix and the strictly
lower triangular part of A is not referenced.
Before entry with UPLO = 'L' or 'l', the leading n by n
lower triangular part of the array A must contain the lower
triangular part of the symmetric matrix and the strictly
upper triangular part of A is not referenced.
Unchanged on exit.

#### LDA INTEGER.

On entry, LDA specifies the first dimension of A as declared in the calling (sub) program. LDA must be at least max( 1, n ). Unchanged on exit.

X DOUBLE PRECISION array of dimension at least
 (1 + (n - 1)\*abs(INCX)).
Before entry, the incremented array X must contain the n
 element vector x.
Unchanged on exit.

#### INCX INTEGER.

On entry, INCX specifies the increment for the elements of X. INCX must not be zero. Unchanged on exit.

#### BETA DOUBLE PRECISION.

On entry, BETA specifies the scalar beta. When BETA is supplied as zero then Y need not be set on input. Unchanged on exit.

Y DOUBLE PRECISION array of dimension at least
(1 + (n - 1)\*abs(INCY)).

Before entry, the incremented array Y must contain the n
element vector y. On exit, Y is overwritten by the updated
vector y.

#### INCY INTEGER.

On entry, INCY specifies the increment for the elements of  $\Upsilon.$  INCY must not be zero. Unchanged on exit.

## 2.4 Triangular Matrix Solvers

#### 2.4.1 Function magma\_strsm

```
int magmablas_strsm(char side, char uplo, char tran, char diag, int M, int N, float alpha, float* A, int lda, float* b, int ldb)
```

```
STRSM solves one of the matrix equations on GPU
op(A)*X = alpha*B, or X*op(A) = alpha*B,
where alpha is a scalar, X and B are m by n matrices, A is a unit, or
non-unit, upper or lower triangular matrix and op(A) is one of
op(A) = A or op(A) = A'.
```

The solution matrix X overwrites B.

To extract more parallelism and performance, the diagonal blocks of A of size 32x32 are explicitly inverted. When M or N is not a multiple of the current blocking size (32 for now), cublasStrsm is called instead.

#### side CHARACTER\*1.

On entry, side specifies whether op(  ${\tt A}$  ) appears on the left or right of  ${\tt X}$  as follows:

```
side = 'L' or 'l' op( A )*X = alpha*B.
side = 'R' or 'r' X*op(A) = alpha*B.
```

Unchanged on exit.

#### uplo CHARACTER\*1.

On entry, uplo specifies whether the matrix  ${\tt A}$  is an upper or lower triangular matrix as follows:

```
uplo = 'U' or 'u' A is an upper triangular matrix.
uplo = 'L' or 'l' A is a lower triangular matrix.
Unchanged on exit.
```

#### tran CHARACTER\*1.

On entry, tran specifies the form of op(  ${\tt A}$  ) to be used in the matrix multiplication as follows:

```
tran = 'N' or 'n' op( A ) = A.
tran = 'T' or 't' op( A ) = A'.
tran = 'C' or 'c' op( A ) = A'.
Unchanged on exit.
```

#### diag CHARACTER\*1.

On entry, diag specifies whether or not A is unit triangular as follows:

#### m INTEGER.

On entry,  ${\tt m}$  specifies the number of rows of B.  ${\tt m}$  must be at least zero. Unchanged on exit.

#### n INTEGER.

On entry, n specifies the number of columns of B. n must be at least zero.

Unchanged on exit.

#### alpha REAL.

On entry, alpha specifies the scalar alpha. When alpha is

zero then  $\mbox{\ A}$  is not referenced and  $\mbox{\ B}$  need not be set before entry.

Unchanged on exit.

A REAL array of DIMENSION (lda, k), where k is m when side = 'L' or 'l' and is n when side = 'R' or 'r'.

Before entry with uplo = 'U' or 'u', the leading k by k upper triangular part of the array A must contain the upper triangular matrix and the strictly lower triangular part of A is not referenced.

Before entry with uplo = 'L' or 'l', the leading k by k lower triangular part of the array A must contain the lower triangular matrix and the strictly upper triangular part of A is not referenced.

Note that when diag = 'U' or 'u', the diagonal elements of A are not referenced either, but are assumed to be unity. Unchanged on exit.

#### lda INTEGER.

On entry, lda specifies the first dimension of A as declared in the calling (sub) program. When side = 'L' or 'l' then lda must be at least max( 1, m ), when side = 'R' or 'r' then lda must be at least max( 1, n ). Unchanged on exit.

b REAL array of DIMENSION (ldb, n). Before entry, the leading m by n part of the array B must contain the right-hand side matrix B, and on exit is overwritten by the solution matrix X.

#### ldb INTEGER.

On entry, ldb specifies the first dimension of B as declared in the calling (sub) program. ldb must be at least max( 1, m ). Unchanged on exit.

#### 2.4.2 Function magma\_dtrsm

```
int magmablas_dtrsm(char side, char uplo, char tran, char diag, int M, int N, double alpha, double* A, int lda, double* b, int ldb)
```

```
DTRSM solves one of the matrix equations on GPU
   op(A)*X = alpha*B,   or   X*op(A) = alpha*B,
where alpha is a scalar, X and B are m by n matrices, A is a unit, or
non-unit, upper or lower triangular matrix and op(A) is one of
   op(A) = A   or   op(A) = A'.
The matrix X is overwritten on B.
```

To extract more parallelism and performance, the diagonal blocks of A of size 32x32 are explicitly inverted. When M or N is not a multiple of the current blocking size (32 for now), cublasStrsm is called instead.

#### uplo CHARACTER\*1.

On entry, uplo specifies whether the matrix  ${\tt A}$  is an upper or lower triangular matrix as follows:

```
uplo = 'U' or 'u' A is an upper triangular matrix.
uplo = 'L' or 'l' A is a lower triangular matrix.
Unchanged on exit.
```

#### tran CHARACTER\*1.

On entry, tran specifies the form of op(  ${\tt A}$  ) to be used in the matrix multiplication as follows:

```
tran = 'N' or 'n' op( A ) = A.
tran = 'T' or 't' op( A ) = A'.
tran = 'C' or 'c' op( A ) = A'.
Unchanged on exit.
```

#### diag CHARACTER\*1.

On entry, diag specifies whether or not  ${\tt A}$  is unit triangular as follows:

```
diag = 'U' or 'u' A is assumed to be unit triangular. diag = 'N' or 'n' A is not assumed to be unit triangular.
```

Unchanged on exit.

#### m INTEGER.

On entry,  ${\tt m}$  specifies the number of rows of B.  ${\tt m}$  must be at least zero. Unchanged on exit.

#### n INTEGER.

On entry, n specifies the number of columns of B. n must be at least zero.

Unchanged on exit.

#### alpha DOUBLE PRECISION.

On entry, alpha specifies the scalar alpha. When alpha is

zero then  $\mbox{\ A}$  is not referenced and  $\mbox{\ B}$  need not be set before entry.

Unchanged on exit.

A DOUBLE PRECISION array of DIMENSION (lda, k), where k is m when side = 'L' or 'l' and is n when side = 'R' or 'r'.

Before entry with uplo = 'U' or 'u', the leading k by k upper triangular part of the array A must contain the upper triangular matrix and the dtrictly lower triangular part of A is not referenced.

Before entry with uplo = 'L' or 'l', the leading k by k lower triangular part of the array A must contain the lower triangular matrix and the dtrictly upper triangular part of A is not referenced.

Note that when diag = 'U' or 'u', the diagonal elements of A are not referenced either, but are assumed to be unity. Unchanged on exit.

#### lda INTEGER.

On entry, lda specifies the first dimension of A as declared in the calling (sub) program. When side = 'L' or 'l' then lda must be at least max( 1, m ), when side = 'R' or 'r' then lda must be at least max( 1, n ). Unchanged on exit.

b DOUBLE PRECISION array of DIMENSION (ldb, n). Before entry, the leading m by n part of the array B must contain the right-hand side matrix B, and on exit is overwritten by the solution matrix X.

#### ldb INTEGER.

On entry, ldb specifies the first dimension of B as declared in the calling (sub) program. ldb must be at least max( 1, m ). Unchanged on exit.

## Chapter 3

## Use

### 3.1 Hardware specifications

MAGMA version 0.2 is intended for a single CUDA enabled NVIDIA GPU and it's host. CUDA enabled GPUs are for example the GeForce 8 Series, the Tesla GPUs, and some Quadro GPUs [2]. MAGMA's double precision routines can be used on CUDA enabled GPUs that support double precision arithmetic. These are for example the GeForce 200 Series and the Tesla solutions. The host can be any shared memory multiprocessor for which LAPACK is suitable. One host core is required and multiple can be used through multicore LAPACK implementation.

### 3.2 Software specifications

MAGMA version 0.2 is a Linux release that requires

- the CUDA driver and CUDA toolkit <sup>1</sup>;
- CPU BLAS and LAPACK.

MAGMA users do not have to know CUDA in order to use the library. A testing directory gives examples on how to use every function (see Section 3.3). Applications can use the CPU interface without any significant change to the application – LAPACK calls have to be prefixed with magma\_ and a workspace argument (for the GPU memory) has to be added (shown in the examples).

<sup>&</sup>lt;sup>1</sup>freely available from NVIDIA http://www.nvidia.com/object/cuda\_get.html

### 3.3 Examples and testing

Directory magma/testing has drivers that test and show how to use every function of this distribution. Below is an example showing the output of the sgetrf driver.

> ./testing\_sgetrf

Using device 0: GeForce GTX 280

Usage:

testing\_sgetrf -N 1024

N	CPU GFlop/s	GPU GFlop/s	PA-LU   / (  A  *N)
1024 2048 3072 4032 5184 6016 7040 8064	33.26 52.29 64.03 80.60 86.65 91.66 96.02 99.88	42.77 96.06 146.33 195.44 224.92 240.33 255.51 267.17	1.861593e-09 1.722339e-09 1.411851e-09 1.371482e-09 1.332554e-09 1.331916e-09 1.306940e-09
9088 10112	101.18 104.38	276.59 284.30	1.549758e-09 1.661756e-09

Performance and accuracy for particular values of the matrix size can also be tested. Note that performance is slower for matrix sizes that are not divisible by the block size of the corresponding algorithm. The block sizes will be auto-tuned in future releases. Currently, the user can change them through file <code>get\_nb.cpp</code> to manually tune the performance for specific hardware and software settings. The issue for matrix sizes not divisible by the block size will be addressed in future MAGMA releases (currently due to CUBLAS being slower for those cases).

> ./testing\_sgetrf -N 1026
Using device 0: GeForce GTX 280

N	CPU GFlop/s	GPU GFlop/s	PA-LU   / (  A  *N)
=====			=======================================
1026	32.93	41.09	1.834303e-09

## Chapter 4

## Performance

Here we give the reference performance results using MAGMA version 0.2 in the following hardware and software configuration:

GPU: NVIDIA GeForce GTX 280;

CPU: Intel Xeon dual socket quad-core @ 2.33 GHz;

GPU BLAS: CUBLAS 2.3;

CPU BLAS: MKL 10.0;

Compiler: gcc 4.1.2;

Tuning: Hand tuned (and hard coded).

Note that this release is hand tuned for this particular configuration. Different configurations may require different tuning in which case there would be a negative impact on the performance. Future releases will be auto-tuned using an empirically-based approach [1]. A handle to user tuning is given in file

testing/get\_nb.cpp
through functions

magma\_get\_{function name}\_nb

which, based on a matrix size, return a block size to be used by the corresponding function. Optimal sizes (for the functions in this distribution) would be a multiple of 32.

### 4.1 Single precision one-sided factorizations

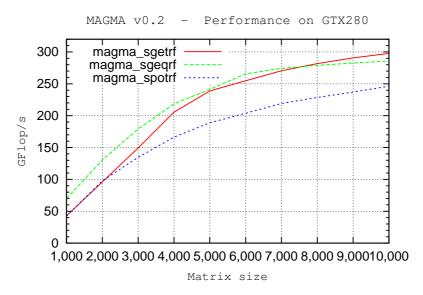


Figure 4.1: Performance of the **CPU interface** one-sided factorizations.

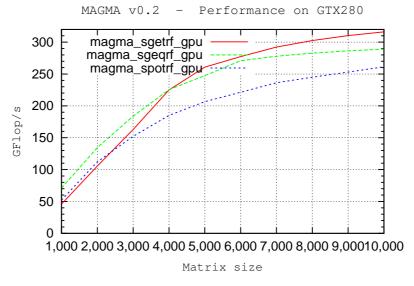


Figure 4.2: Performance of the GPU interface one-sided factorizations.

### 4.2 Double precision one-sided factorizations

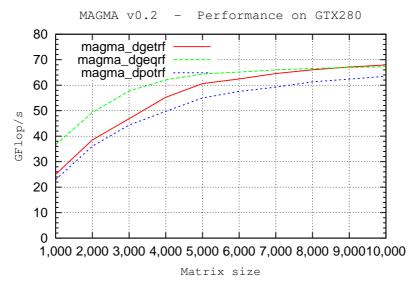


Figure 4.3: Performance of the CPU interface one-sided factorizations.

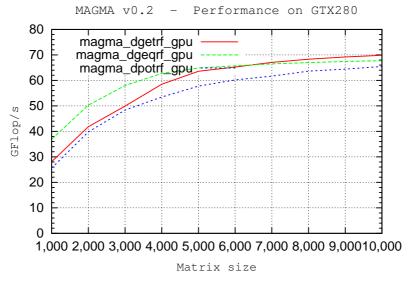


Figure 4.4: Performance of the GPU interface one-sided factorizations.

### 4.3 Single complex one-sided factorizations

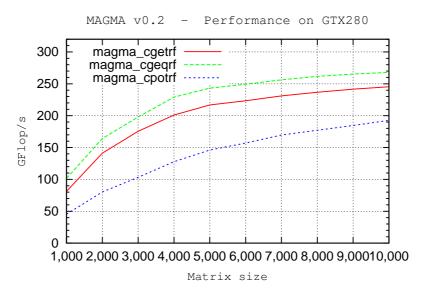


Figure 4.5: Performance of the CPU interface one-sided factorizations.

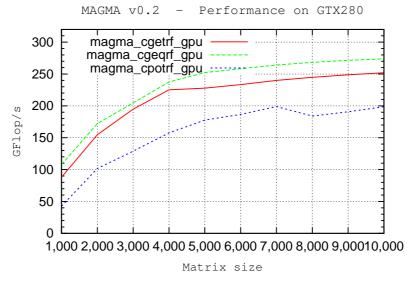


Figure 4.6: Performance of the GPU interface one-sided factorizations.

### 4.4 Double complex one-sided factorizations

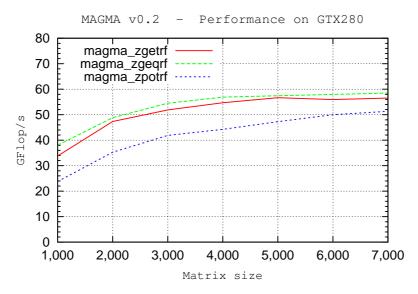


Figure 4.7: Performance of the CPU interface one-sided factorizations.

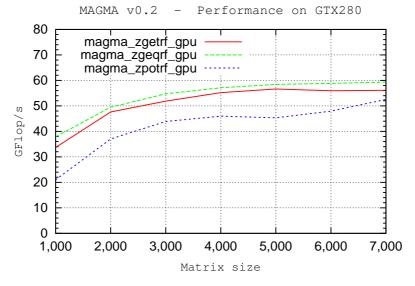


Figure 4.8: Performance of the **GPU** interface one-sided factorizations.

### 4.5 LU-based linear solvers

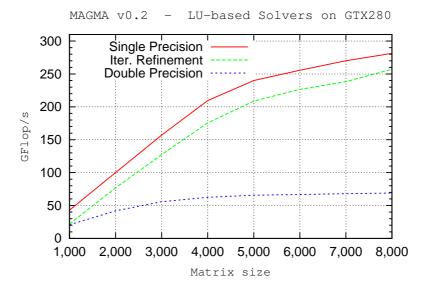


Figure 4.9: Performance of LU-based linear solvers.

## 4.6 QR-based least squares solvers

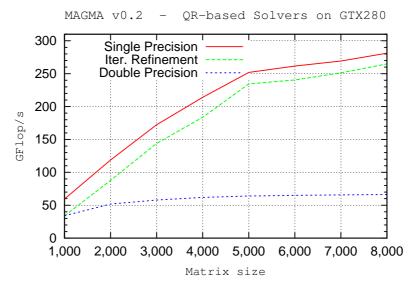


Figure 4.10: Performance of QR-based least squares solvers.

## 4.7 Cholesky-based linear solvers

MAGMA v0.2 - Cholesky-based Solvers on GTX280

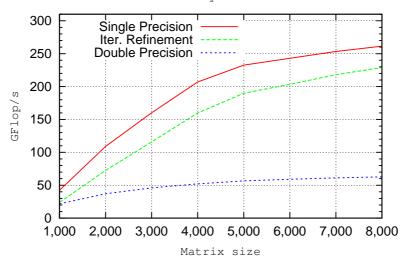


Figure 4.11: Performance of Cholesky-based linear solvers.

# Acknowledgments

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# Bibliography

- [1] Yinan Li, Jack Dongarra, and Stanimire Tomov, A note on auto-tuning GEMM for GPUs., Lecture Notes in Computer Science, vol. 5544, Springer, 2009.
- [2] NVIDIA, NVIDIA CUDA Programming Guide, 6/07/2008, Version 2.0.
- [3] S. Tomov, J. Dongarra, and M. Baboulin, *Towards dense linear algebra for hybrid GPU accelerated manycore systems.*, Tech. report, LAPACK Working Note 210, October 2008.
- [4] S. Tomov, J. Dongarra, V. Volkov, and J. Demmel, MAGMA Library version 0.1, http://icl.cs.utk.edu/magma, 08/2009.
- [5] V. Volkov and J. Demmel, Benchmarking GPUs to tune dense linear algebra, SC '08: Proceedings of the 2008 ACM/IEEE conference on Supercomputing (Piscataway, NJ, USA), IEEE Press, 2008, pp. 1–11.