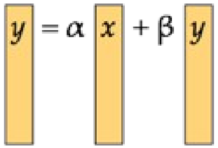
Dense Numerical Linear Algebra with MAGMA

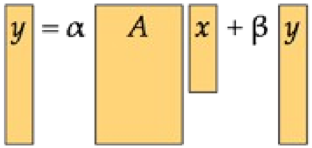
Piotr Luszczek

Basic Linear Algebra Subroutines

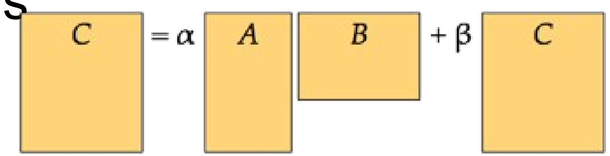
- Level 1 BLAS - vector operations
  - O(n) data and flops
  - Memory bound:
    - O(1) flops per memory access
    - ~ 2 Gflop/s on Skylake (not per core)

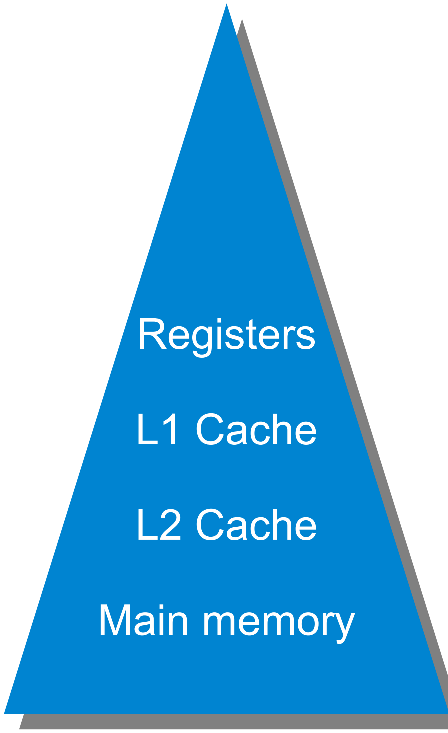


- Level 2 BLAS - matrix-vector operations
  - O(n^2) data and flops
  - Memory bound:
    - O(1) flops per memory access
    - ~ 4 Gflop/s on Skylake (not per core)



- Level 3 BLAS - matrix-matrix operations
  - O(n^2) data, O(n^3) flops
  - Surface-to-volume effect
  - Compute bound:
    - O(n) flops per memory access
    - As high as 80 Gflop/s per core on Skylake





Innovative Computing Laboratory’s Libraries

- MAGMA
  - Matrix Algebra for GPUs and Multicore Architectures
- PLASMA
  - Parallel Linear Algebra Software for Multicore Architectures
- SLATE
  - Scalable Linear Algebra Targeting Exascale

Academic Collaborations

ICL UT

MANCHESTER 1824
The University of Manchester

Berkeley
UNIVERSITY OF CALIFORNIA

University of Colorado Denver

Inria informatics mathematics

KAUST

Funding / Licensing

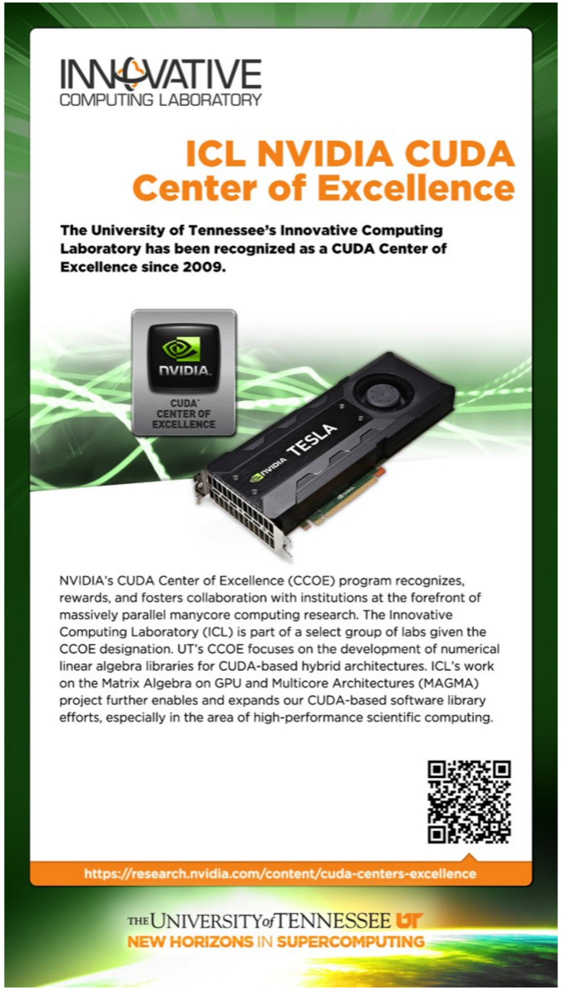
National Science Foundation

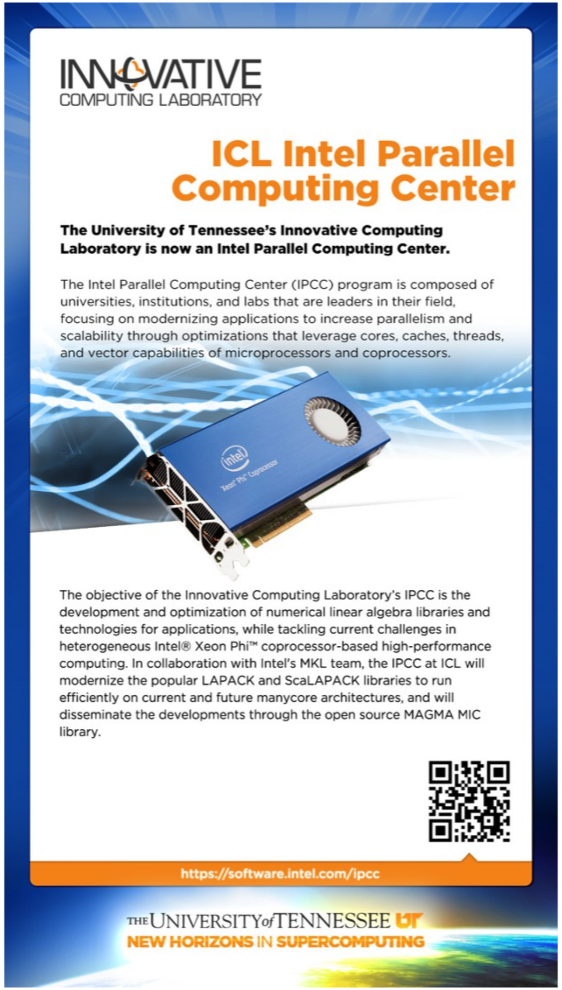
U.S. DEPARTMENT OF ENERGY

Modified BSD License

en.wikipedia.org/wiki/BSD_licenses

Industry Collaborations





MathWorks®

AMD

Microsoft®

FUJITSU

Software Projects - Legacy

netlib.org

LAPACK	dense linear algebra (serial)
ScaLAPACK	dense linear algebra (distributed memory)
BLAS	Basic Linear Algebra Subroutines
CBLAS	BLAS C API
LAPACKE	LAPACK C API

legacy software
and reference implementations

Software Projects – Multicores and Accelerators

www.netlib.org

- LAPACK
- ScaLAPACK
- BLAS
- CBLAS
- LAPACKE

icl.utk.edu/research

PLASMA	dense linear algebra (multicore)
MAGMA	dense linear algebra (accelerators)
SLATE	dense linear algebra (distributed memory + accelerators)

new software for multicore and accelerators

Software Projects - Runtimes

www.netlib.org

LAPACK

ScaLAPACK

BLAS

CBLAS

LAPACKE

icl.utk.edu/research

PLASMA

MAGMA

SLATE

QUARK

PaRSEC

scheduling (multicore)

scheduling (distributed memory)

dynamic runtime schedulers

Software Projects – New Runtimes

netlib.org

icl.utk.edu/research

LAPACK

PLASMA

MAGMA

OpenMP

scheduling
(multicore)

ScaLAPACK

SLATE

PaRSEC

scheduling
(distributed memory)

**dynamic
runtime
schedulers**

LAPACKE

LAPACK++

`https://bitbucket.org/icl/lapackpp`

CBLAS

BLAS

BLAS++

`https://bitbucket.org/icl/blaspp`

Software Projects - HPC

www.netlib.org

- LAPACK
- ScaLAPACK
- BLAS
- CBLAS
- LAPACKE

icl.utk.edu/research

High Performance LINPACK Benchmark (dense)	HPL
High Performance Conjugate Gradient (sparse)	HPCG
HPC Challenge (composite)	HPCC
Performance API	PAPI

benchmarks and performance tools

BLAS Naming Scheme and Level 1 Examples

- One or two letter data type
  - I = integer (e.g., index)
  - s = single (float)
  - d = double
  - c = single-complex
  - z = double-complex
- Two letter matrix type (BLAS 2, 3)
  - ge = general nonsymmetric
  - sy = symmetric ($A = A^T$)
  - he = complex Hermitian ($A = A^H$)
  - tr = triangular (L or U)
  - Also banded and packed formats
- Two or more letter function, e.g.
  - mv = matrix-vector product
  - mm = matrix-matrix product

- BLAS 1 examples
  - sdot result = $x^T y$ (single)
  - ddot result = $x^T y$ (double)
  - cdotc result = $x^H y$ (single-complex)
  - cdotu result = $x^T y$ (single-complex)
  - zdotc result = $x^H y$ (double/complex)
  - zdotu result = $x^T y$ (double/complex)
  - _axpy $y = \alpha x + y$
  - _scal $y = \alpha y$
  - _copy $y = x$
  - _swap $x \leftrightarrow y$
  - _nrm2 $||x||_2$
  - _asum $\Sigma|x|$
  - i_amax arg max $|x|$
  - _rot Apply Given's rotation

BLAS Naming Scheme and Levels 2 and 3 Examples

- One or two letter data type
  - I = integer (e.g., index)
  - s = single (float)
  - d = double
  - c = single-complex
  - z = double-complex
- Two letter matrix type (BLAS 2, 3)
  - ge = general non-symmetric
  - sy = symmetric ($A = A^T$)
  - he = complex Hermitian ($A = A^H$)
  - tr = triangular (L or U)
  - Also banded and packed formats
- Two or more letter function, e.g.
  - mv = matrix-vector product
  - mm = matrix-matrix product

- BLAS 2 examples
  - _gemv $y = Ax + y$, A general
  - _symv $y = Ax + y$, A symmetric
  - _hemv $y = Ax + y$, A Hermitian
  - _ger $C = xy^T + C$, C general
  - _syr $C = xx^T + C$, C symmetric
  - _her $C = xx^H + C$, C Hermitian
  - _trmv $x = Ax$, A triangular
  - _trsvsolve $Ax = b$, A triangular
- BLAS 3 examples
  - _gemm $C = AB + C$ all matrices general
  - _symm $C = AB + C$ A symmetric
  - _hemm $C = AB + C$ A Hermitian
  - _syrk $C = AA^T + C$, C symmetric
  - _herk $C = AA^H + C$, C Hermitian
  - _trmm $X = AX$, A triangular
  - _trsm solve $AX = B$, A triangular

Dense Linear Algebra Problems

- linear systems of equations $AX = B$
- linear least squares $min \| B - AX \|_2$
- singular value decomposition (SVD) $A = U\Sigma V^T$
- eigenvalue value problems (EVP) $Ax = \lambda x$

- dense (square, rectangular)
- band

Data Types

dgesv

Example	Precision	Description	C type
zgesv	z	double precision complex	double _Complex
cgesv	c	single precision complex	float _Complex
dgesv	d	double precision real	double
sgesv	s	single precision real	float

Data Types – Mixed Precision

dsgesv

Precision	Description	Example
dz	double-complex input, double precision result	cblas_dznrm2
sc	single-complex input, single precision result	cblas_scnrm2
zc	mixed-precision algorithm (double-complex/single-complex)	zcgesv
ds	mixed-precision algorithm (double/single)	dsgesv

Matrix Types

dgesv

Precision	Description
ge	general
sy	symmetric
he	Hermitian
po	positive definite
tr	triangular
or	orthogonal
un	unitary

Precision	Description
gb	general band
sb	symmetric band
hb	Hermitian band
pb	positive definite band

Driver Routines

Precision	Description	
_gesv	$AX = B$	A is general (nonsymmetric)
_posv	$AX = B$	A is symmetric/Hermitian positive definite
_sysv/_hesv	$AX = B$	A is symmetric/Hermitian indefinite
_gels	$AX = B$	A is rectangular

Precision	Description	
_geev	$Ax = \lambda x$	A is general
_syev/_heev	$Ax = \lambda x$	A is symmetric/Hermitian
syevd/heevd	$Ax = \lambda x$	A is symmetric/Hermitian, divide and conquer
sygvd/_hegvd	$Ax = \lambda Bx$	A is symmetric/Hermitian
_gesvd	$A = U\Sigma V^T$	A is general
_gesdd	$A = U\Sigma V^T$	A is general, divide and conquer

Computational Routines

Name	Description
_getrf, _potrf, _sytrf	triangular factorization (LU, Cholesky, LDL^T)
_getrs, _potrs, _sytrs	triangular solve (forward, backward substitution)
_getri, _potri, _sytri	triangular inverse

Name	Description
_geqrf, _gelqf	QR, LQ factorizations
_ormqr, _ormlq	multiply by Q (real)
_unmqr, _unmlq	multiply by Q (complex)
_orgqr, _orglq	generate Q (real)
_ungqr, _unglq	generate Q (complex)

Auxiliary Routines

Name	Description
_geadd	add two matrices
_laset	set entries to a constant
_lacpy	copy a matrix
_lascal	scale a matrix
_lange	compute a norm

LAPACK Working Notes

http://www.netlib.org/lapack/lawns/

lawn05 [pdf]
Provisional Contents
by C. Bischof, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, and D. Sorensen ANL, MCS-TM-38, September 1988

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Guidelines for the Design of Symmetric Eigenroutines, SVD, and Iterative Refinement and Condition Estimation for Linear Systems by J. Demmel, J. Du Croz, S. Hammarling, and D. Sorensen ANL, MCS-TM-111, March 1988

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Computing Small Singular Values of Bidiagonal Matrices with Guaranteed High Relative Accuracy by J. Demmel and W. Kahan ANL, MCS-TM-110, February 1988

lawn02 [pdf] Block Reduction of Matrices to Condensed Forms for Eigenvalue Computations by J. Dongarra, S. Hammarling, and D. Sorensen ANL, MCS-TM-99, September 1987

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Prospectus for the Development of a Linear Algebra Library for High-Performance Computers by J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, and D. Sorensen ANL, MCS-TM-97, September 1987 Last updated 2016-11-18 17:33:01 PST

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The Bidiagonal Singular Value Decomposition and Hamiltonian Mechanics by P. Deift, J. Demmel, L.-C. Li, and C. Tomei ANL, MCS-TM-133, August 1989.

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Installing and Testing the Initial Release of LAPACK --Unix and Non-Unix Versions by E. Anderson and J. Dongarra ANL, MCS-TM-130, May 1989.

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A Test Matrix Generation Suite by J. Demmel and A. McKenney ANL, MCS-P69-0389, March 1989.

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On a Block Implementation of Hessenberg Multishift QR Iteration by Z. Bai and J. Demmel ANL, MCS-TM-127, January 1989.

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Computing Accurate Eigensystems of Scaled Diagonally Dominant Matrices by J. Barlow and J. Demmel ANL, MCS-TM-126, December 1988.

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Tools to Aid in the Analysis of Memory Access Patterns for FORTRAN Programs by O. Brewer, J. Dongarra, and D. Sorensen ANL, MCS-TM-120, June 1988

Open Source Stack

LAPACK
LAPACKE
BLAS
CBLAS

http://www.netlib.org/lapack/
http://www.netlib.org/lapack/lapack-3.6.1.tgz
https://github.com/Reference-LAPACK/lapack
includes: LAPACKE, BLAS, CBLAS – reference implementations

ATLAS

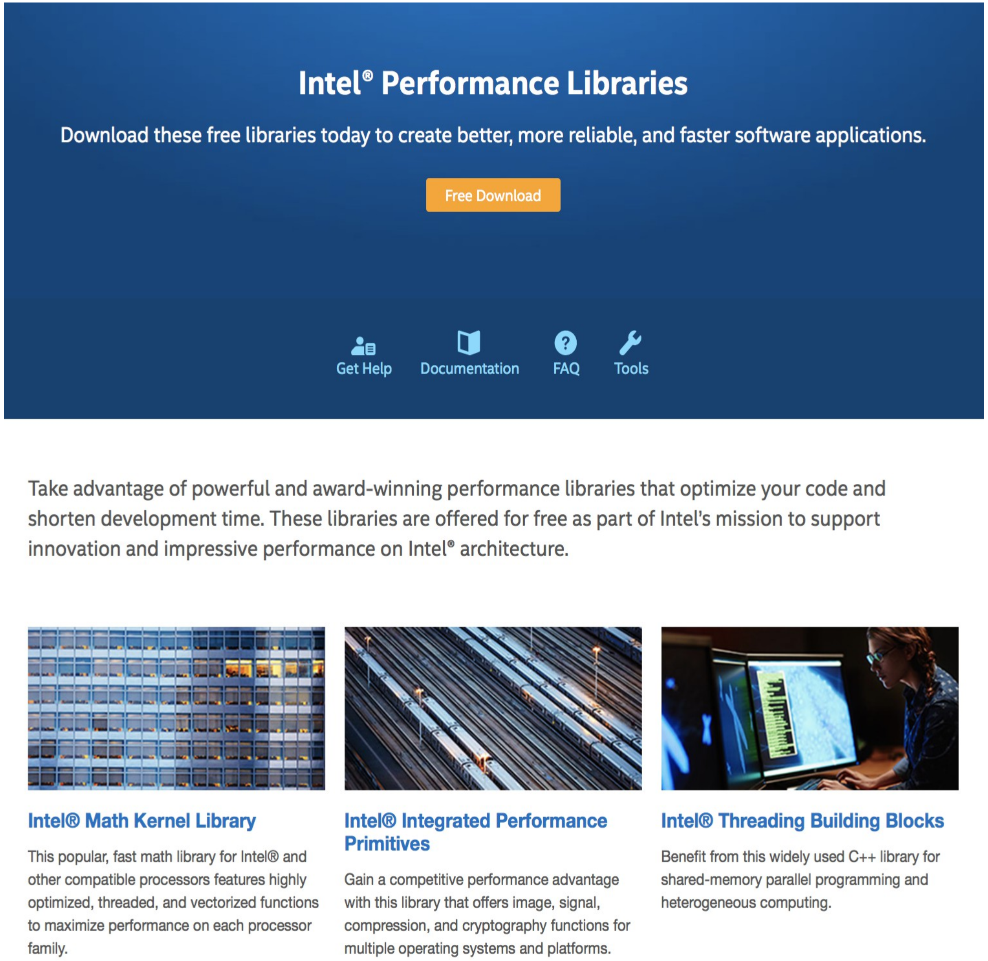
http://math-atlas.sourceforge.net

OpenBLAS

http://www.openblas.net
https://github.com/xianyi/OpenBLAS

Intel Stack for Numerical Linear Algebra

- Intel Threading Building Blocks
- Intel Integrated Performance Primitives
- Intel Data Analytics Acceleration Library
- Intel Math Kernel Library
  - LAPACK
  - LAPACKE
  - BLAS
  - CBLAS
- Royalty free
  - Some sources available

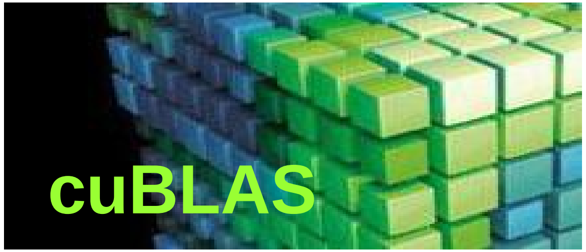


NVIDIA Software Stack

MAGMA

https://developer.nvidia.com/gpu-accelerated-libraries

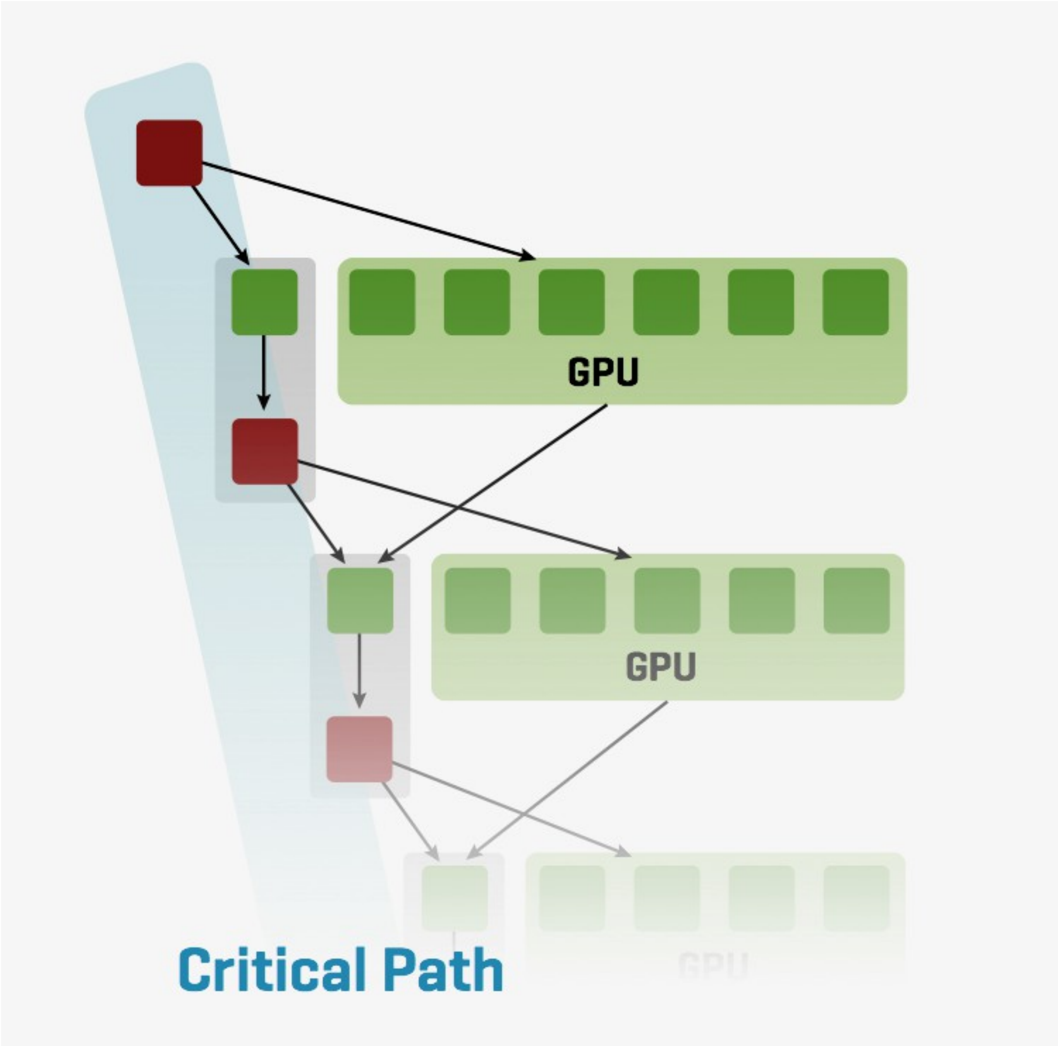
http://icl.cs.utk.edu/magma/software/



https://developer.nvidia.com/cuda-downloads

- cuBLAS – single GPU BLAS
- cuBLAS-XT – multi-GPU “OOC” BLAS
- NVBLAS – “auto acceleration” API for cuBLAS-XT

MAGMA



- dense linear algebra for accelerators
  - NVIDIA using CUDA
  - AMD using OpenCL
  - Intel Xeon Phi
- hybrid, CPU-GPU implementations
  - single-GPU
  - multi-GPU
  - OO-GPU-memory
- managing data transfers
- some batched routines
- some sparse solvers

MAGMA Overview

NVIDIA
GPU
CENTER OF EXCELLENCE

NVIDIA's GPU Center of Excellence Program recognizes universities expanding the frontier of massively parallel computing using CUDA.

Intel Parallel Computing Center

The objective of the Innovative Computing Laboratory's IPCC is the development and optimization of numerical linear algebra libraries and technologies for applications, while tackling current challenges in heterogeneous Intel® Xeon Phi™ coprocessor-based High Performance Computing.

AMD

Long-term collaboration and support on the development of clMAGMA, the OpenCL™ port of MAGMA.

FEATURES AND SUPPORT

- **MAGMA** 2.2 FOR **CUDA**
- **clMAGMA** 1.4 FOR **OpenCL**
- **MAGMA MIC** 1.4 FOR **Intel Xeon Phi**

CUDA	OpenCL	Intel Xeon Phi	
●	●	●	Linear system solvers
●	●	●	Eigenvalue problem solvers
●	●		Auxiliary BLAS
●			Batched LA
●		●	Sparse LA
●	●	●	CPU Interface
●	●	●	GPU Interface
●	●	●	Multiple precision support
●			Non-GPU-resident factorizations
●	●	●	Multicore and multi-GPU support
●	●	●	LAPACK testing
●	●	●	Linux
●	●		Windows
●	●		Mac OS

MAGMA User Outreach

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

→ User Forum

→ Documentation

MAGMA Routines for LU Solver

Suffix	Example	Description
<empty>	magma_dgesv	hybrid CPU/GPU routine – matrix in CPU memory
_m	magma_dgesv_m	hybrid CPU/multi-GPU routine – matrix in CPU memory
_gpu	magma_dgesv_gpu	hybrid CPU/GPU routine – matrix in GPU memory
_mgpu	magma_dgesv_mgpu	hybrid CPU/multi-GPU routine – matrix distributed across GPU memories

MAGMA Memory Allocation

Name	Description
magma_malloc_cpu	allocate CPU memory
magma_malloc_pinned	allocate pinned CPU memory
magma_malloc	allocate GPU memory
magma_free_cpu	free CPU memory
magma_free_pinned	free pinned CPU memory
magma_free	free GPU memory

MAGMA Data Transfers

Name	Description
setmatrix	send matrix to GPU
setvector	send vector to GPU
getmatrix	get matrix from GPU
getvector	get vector from GPU

Calling MAGMA LU Factorization

```
info = LAPACKE_dgetrf   (layout, m, n, hA,   lda, ipiv);
       // A in CPU memory
       magma_dgetrf     (        m, n, hA,   lda, ipiv, &info);
       // A in CPU memory
       magma_dgetrf_m   (ngpu,   m, n, hA,   lda, ipiv, &info);
       // A in GPU memory
       magma_dgetrf_gpu (        m, n, dA,   lda, ipiv, &info);
       // A in GPU memories
       magma_dgetrf_mgpu(ngpu,   m, n, dA[], lda, ipiv, &info);
```

MAGMA: initialize, compute, finalize

```
magma_init();

magma_dgetrf(m, n, hA, lda, ipiv, &info);

magma_finalize();
```

```
magma_init();

magma_dgetrf_m(ngpu, m, n, hA, lda, ipiv, &info);

magma_finalize();
```

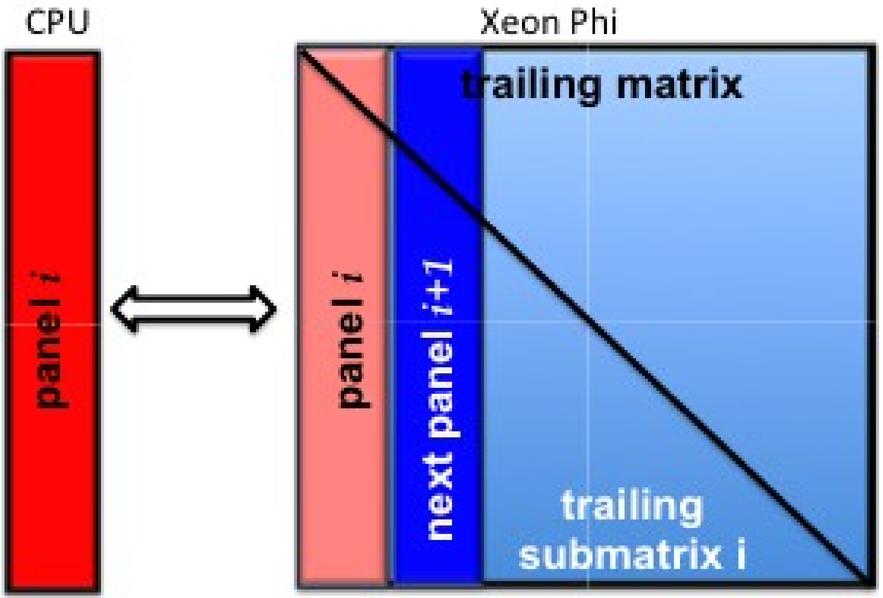
MAGMA Queues

```
magma_init();
magma_queue_create(device, &queue);
magma_zsetmatrix(m, n, h_A, lda, d_A, ldda, queue);


magma_zgetrf_gpu(m, n, d_A, ldda, ipiv, &info);


magma_zgetmatrix(m, n, d_A, ldda, h_A, lda, queue);
magma_queue_destroy(queue);
magma_finalize();
```

Multi-GPU Interface

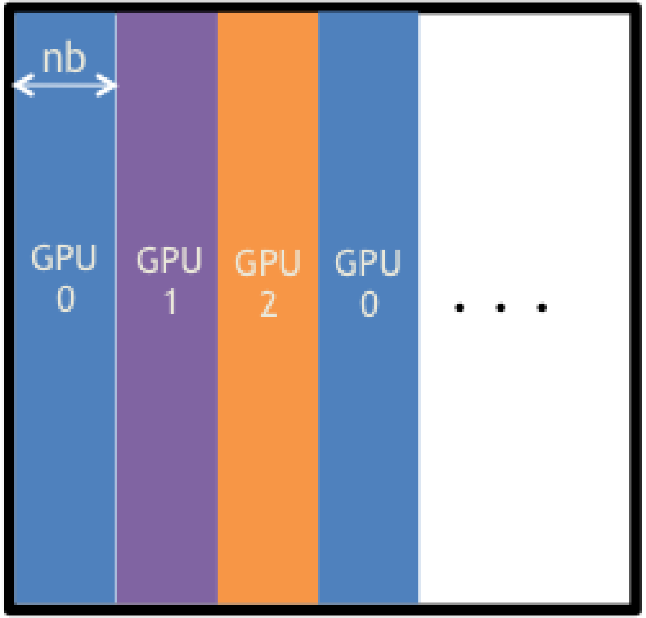
```
magma_init();

nb = magma_get_zgetrf_nb(m, n);

magma_queue_create(device, &queue);

magma_zsetmatrix_1D_col_bcyclic(m, n, h_A, lda, d_lA, ldda,

ngpu, nb, queues);

magma_zgetrf_mgpu(ngpu, M, N, d_lA, ldda, ipiv, &info);

magma_zgetmatrix_1D_col_bcyclic(m, n, d_lA, ldda, h_A, lda,

ngpu, nb, queues);

magma_queue_destroy(queue);

magma_finalize();
```

MAGMA Factorization Algorithms



- panel factorization on multicore
- trailing submatrix update on GPU/Phi
- concurrent operation
- lookahead
- hidden communication

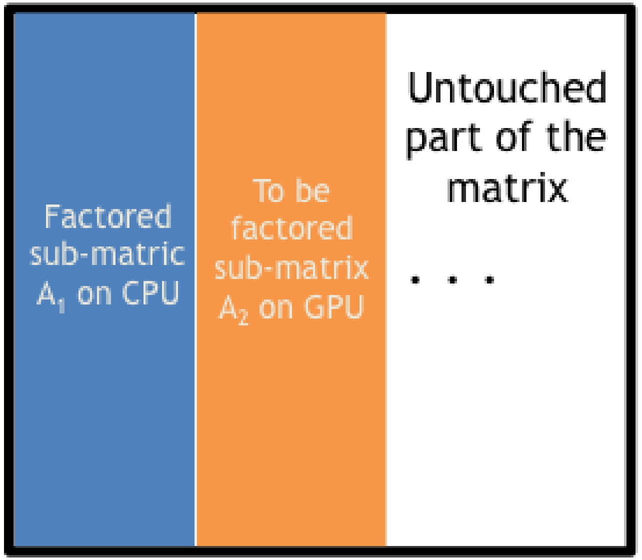
MAGMA Multi-GPU



- 1D block-cyclic distribution
- panel on CPUs
- updates on GPUs
- lookahead

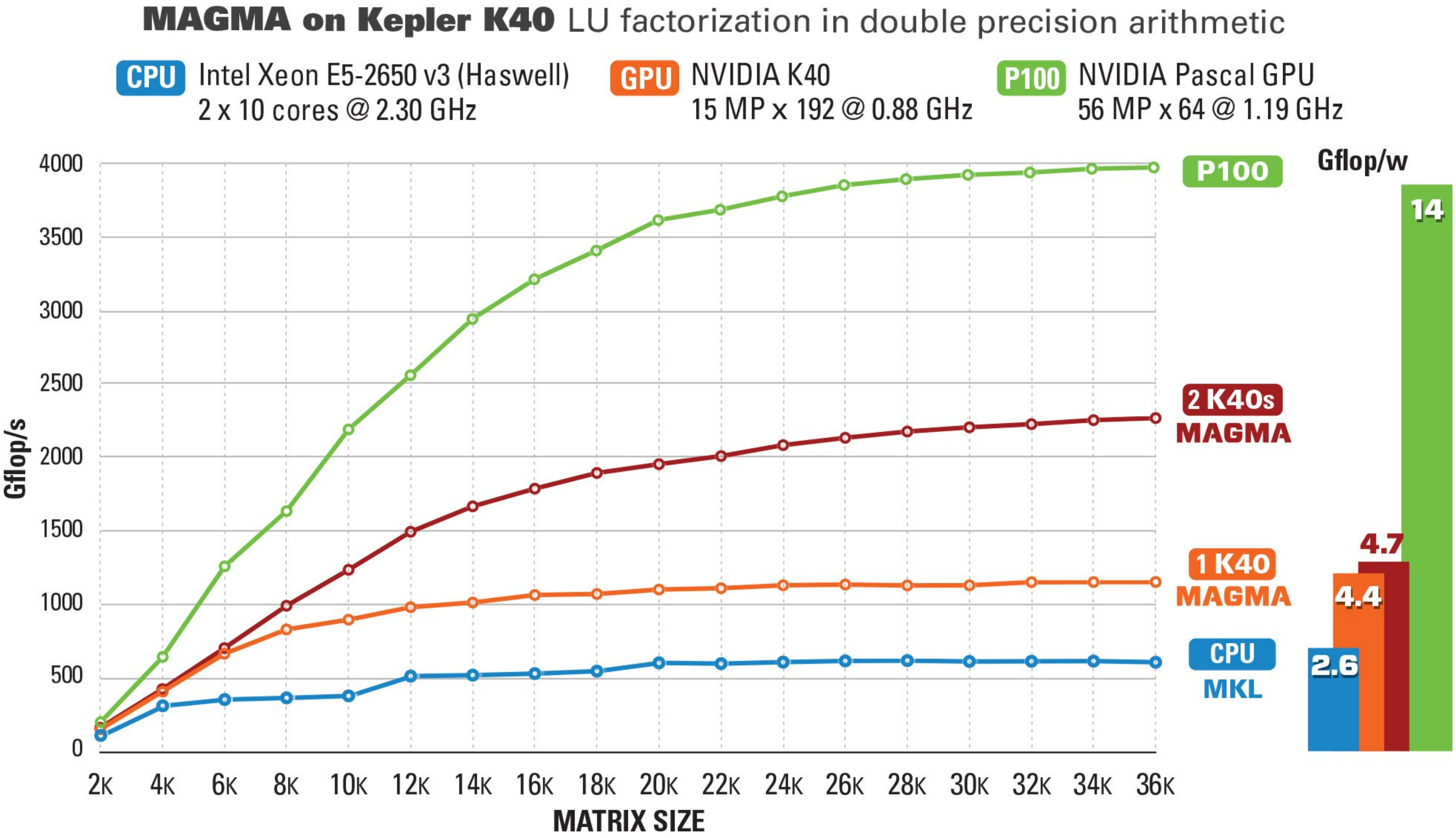
MAGMA External-Memory Computing

- perform left-looking factorization on a submatrix that fits in the GPU memory
- the rest of the matrix stays on the CPU

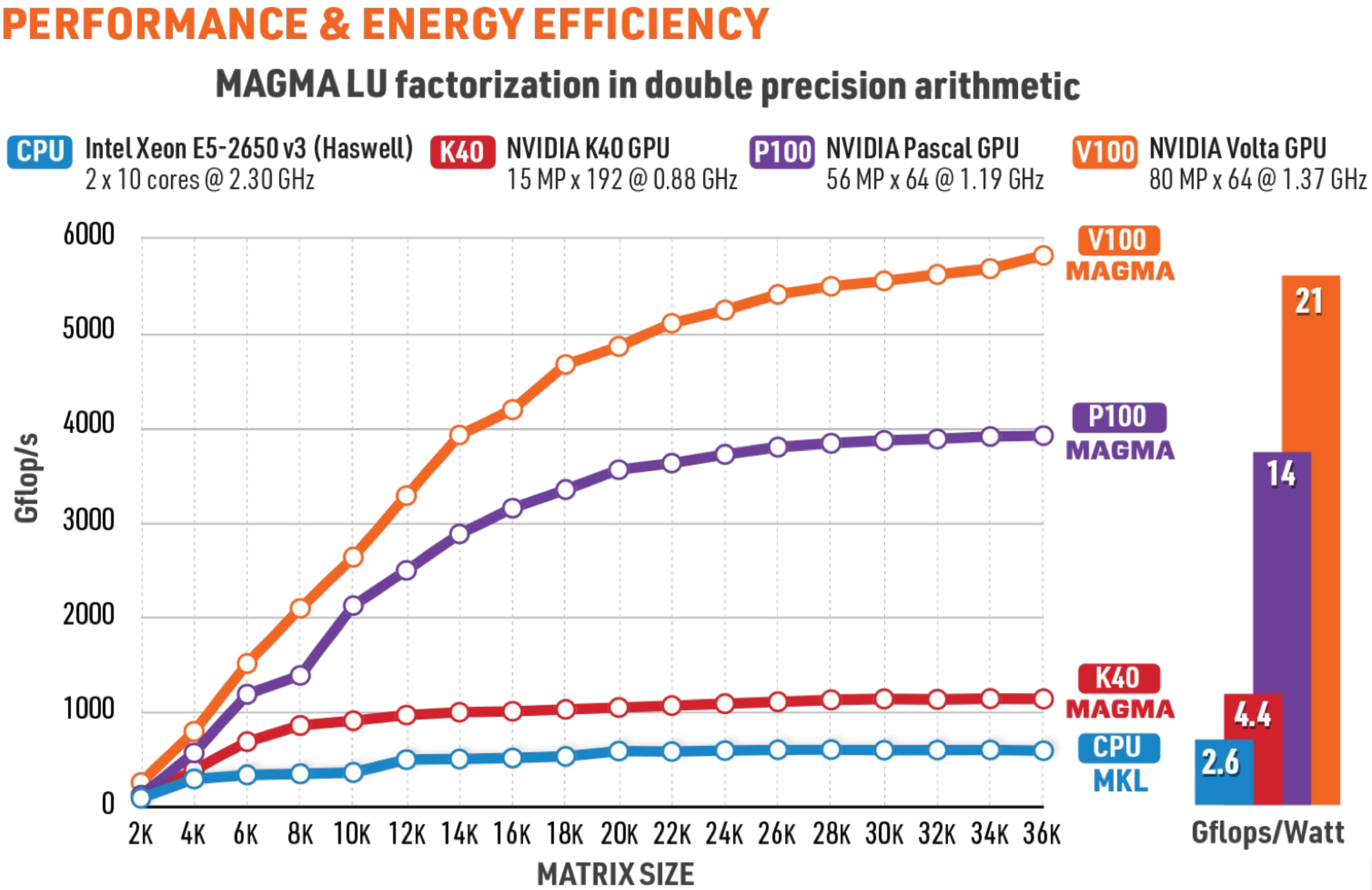


- copy A2 to the GPU
- update A2 using A1
- factor the updated A2
- return A2 to the CPU

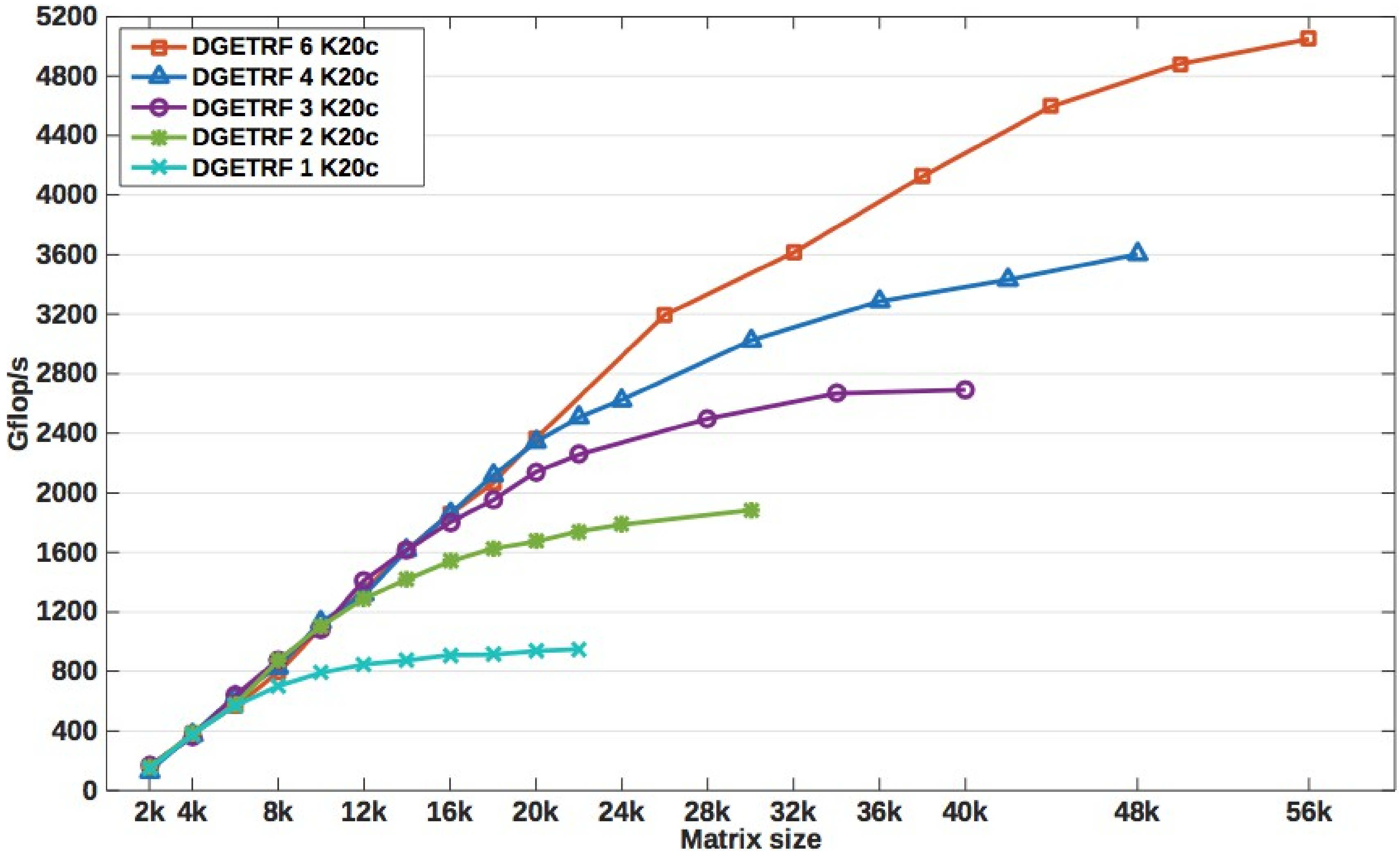
MAGMA Performance – LU Factorization



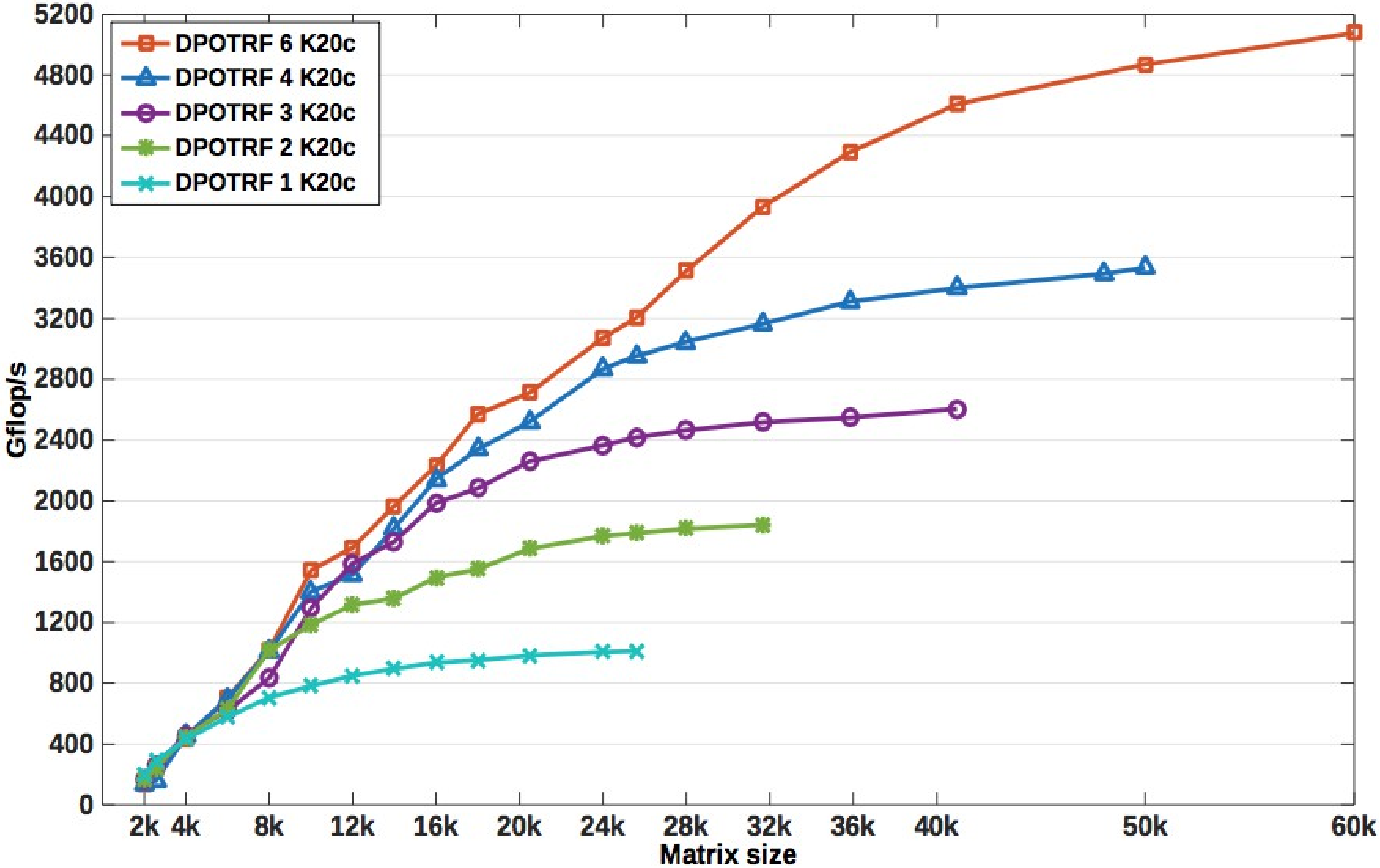
MAGMA Performance on NVIDIA Volta



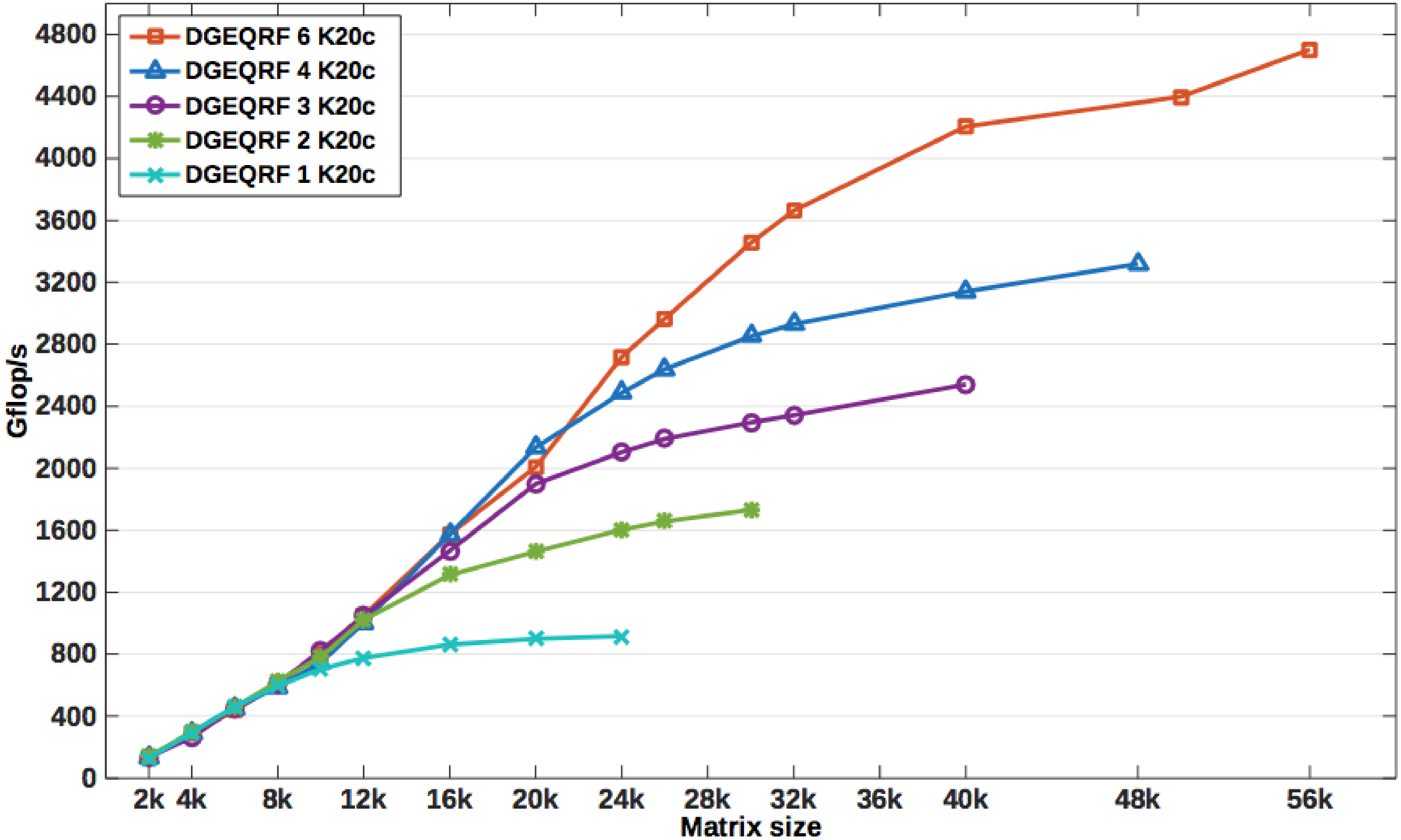
MAGMA Performance – DGETRF on Kepler K20c



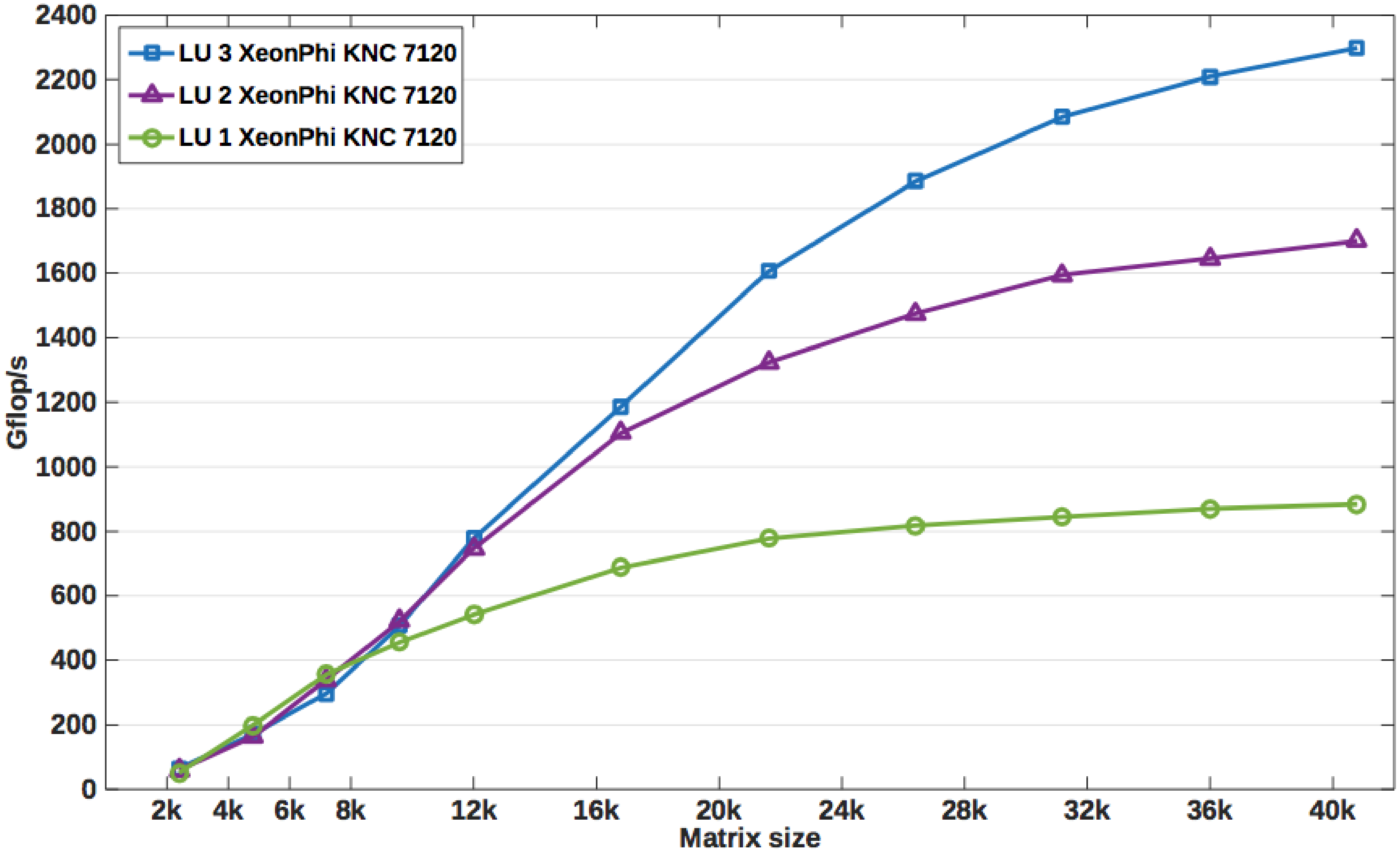
MAGMA Performance – DPOTRF on Kepler K20c



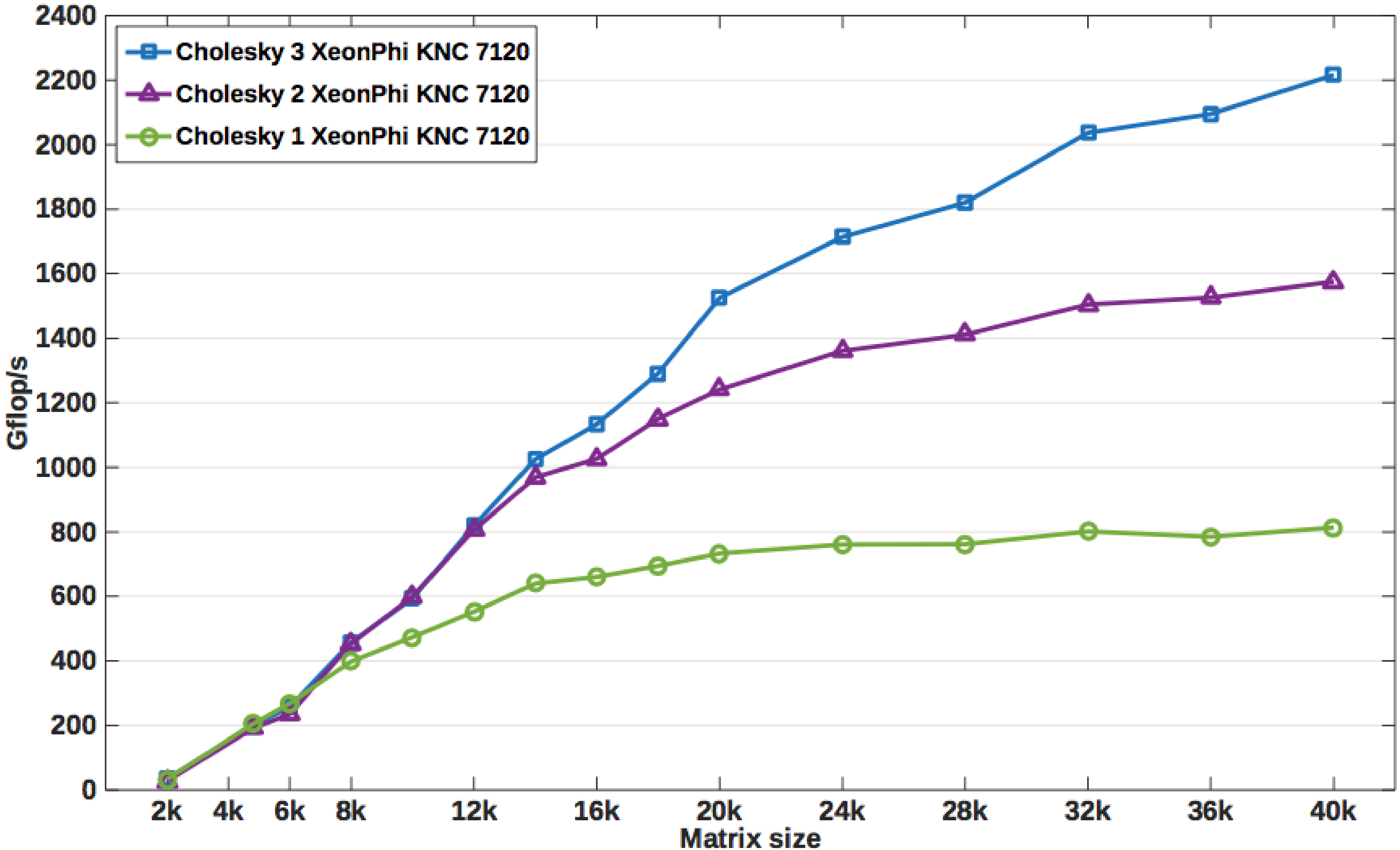
MAGMA Performance – DGEQRF on Kepler K20c



MAGMA Performance – DGETRF on Intel Xeon Phi KNC



MAGMA Performance – DPOTRF on Intel Xeon Phi KNC



MAGMA Performance – DGEQRF on Intel Xeon Phi KNC