UT College of Engineering Tutorial

Accelerating Linear Algebra on Heterogeneous Architectures of Multicore and GPUs using MAGMA and DPLASMA and StarPU Schedulers

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Outline

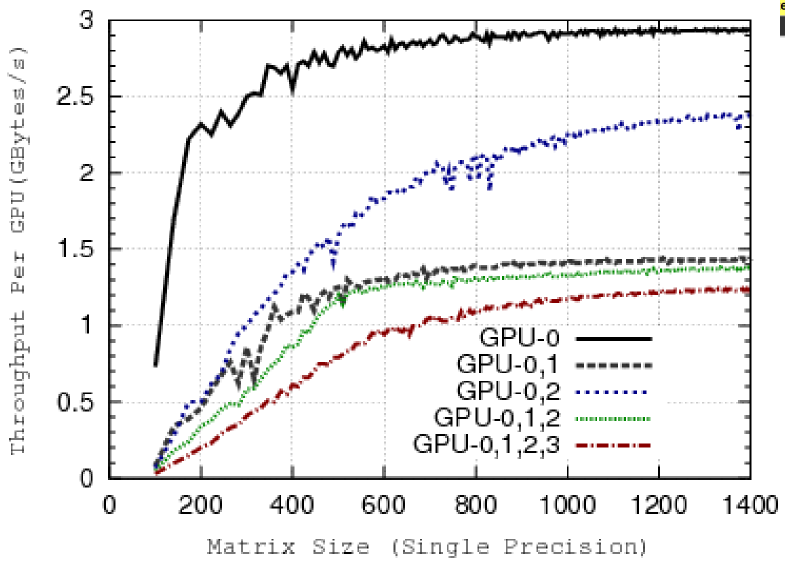
- **Linear Algebra for Multicore and GPUs**
    - **The MAGMA project**
    - **The *Hybridization Methodology* of MAGMA – enabling task-based parallelism**
- **DPLASMA**
- **StarPU**

Challenges

- Increase in parallelism
  Tesla C2050 (Fermi): 448 CUDA cores @1.15 GHz
  SP peak is 1075 GFlop/s, DP peak is 515 Gflop/s

- Increase in communication cost [vs computation]
  Processor speed improves ~59% / year
  memory bandwidth by only 23%

- Heterogeneity



Matrix Algebra on GPU and Multicore Architectures (MAGMA)

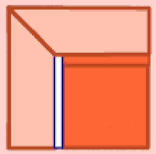
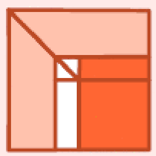
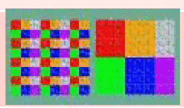
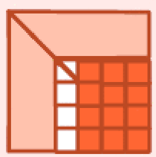
- **MAGMA**: **a new generation linear algebra (LA) libraries** to achieve the fastest possible time to an accurate solution **on hybrid/heterogeneous architectures**, starting with current multicore+MultiGPU systems
  Homepage: **http://icl.cs.utk.edu/magma/**

- **MAGMA & LAPACK**
  - **MAGMA** - based on LAPACK and extended for hybrid systems (multi-GPUs + multicore systems);
  - **MAGMA** - designed to be similar to LAPACK in functionality, data storage and interface, in order to allow scientists to effortlessly port any of their LAPACK-relying software components to take advantage of the new architectures
  - **MAGMA** - to leverage years of experience in developing open source LA software packages and systems like LAPACK, ScaLAPACK, BLAS, ATLAS as well as the newest LA developments (e.g. communication avoiding algorithms) and experiences on homogeneous multicores (e.g. PLASMA)

- **Support**
  - NSF, Microsoft, NVIDIA [now **CUDA Center of Excellence at UTK** on the development of **Linear Algebra Libraries for CUDA-based Hybrid Architectures**]

- **MAGMA developers**
  - University of Tennessee, **Knoxville**; University of California, **Berkeley**; University of Colorado, **Denver**

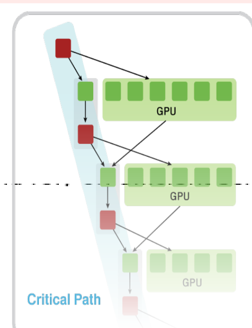
A New Generation of Algorithms

Software/Algorithms follow hardware evolution in time		
LINPACK (70's) (Vector operations)		Rely on - Level-1 BLAS operations
LAPACK (80's) (Blocking, cache friendly)		Rely on - Level-3 BLAS operations
ScaLAPACK (90's) (Distributed Memory)		Rely on - PBLAS Mess Passing
PLASMA (00's) New Algorithms (many-core friendly)		Rely on - a DAG/scheduler - block data layout - some extra kernels

"**delayed update**" to organize successive Level 2 BLAS as a single Level 3 BLAS

Localized (over tiles) elementary **transformations**

MAGMA
Hybrid Algorithms
(heterogeneity friendly)

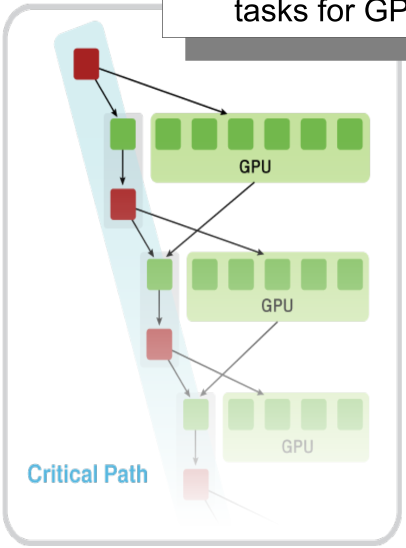


Rely on
- hybrid scheduler (of DAGs)
- hybrid kernels
  (for nested parallelism)
- existing software infrastructure

Hybridization methodology

- MAGMA uses **HYBRIDIZATION** methodology based on
  - Representing linear algebra algorithms as collections of **TASKS** and **DATA DEPENDANCIES** among them
  - Properly **SCHEDULING** the tasks' execution over the multicore and the GPU hardware components
- Successfully applied to fundamental linear algebra algorithms
  - One and two-sided factorizations and slvers
  - Iterative linear and eigen-solvers
- Faster, cheaper, better ?
  - High-level
  - Leveraging prior developments
  - Exceeding in performance (and sometimes accuracy) homogeneous solutions

Hybrid CPU+GPU algorithms
(small tasks for multicores and large tasks for GPUs)



MAGMA Status

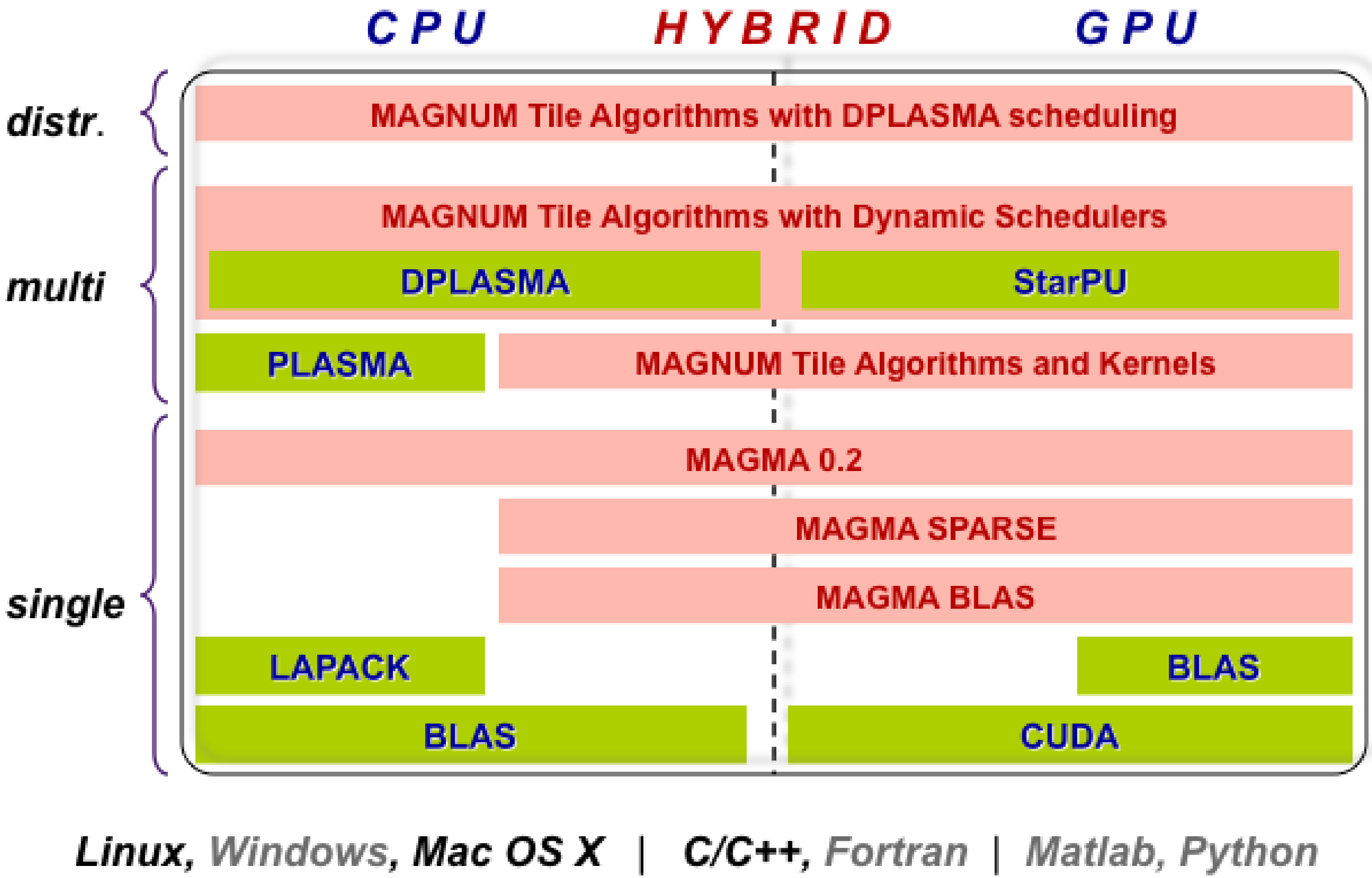
MAGMA 0.2

- **LU, QR, Cholesky (S, C, D, Z)**
- **Linear solvers**
  - In working precision, based on LU, QR, and Cholesky
  - Mixed-precision iterative refinement
- **CPU and GPU interfaces**
- **Two-sided factorizations**
  - Reduction to upper Hessenberg form for the general eigenvalue problem
- **MAGMA BLAS**
  - Routines critical for MAGMA (GEMM, SYRK, TRSM, GEMV, SYMV, etc.)

Unreleased

- **Bidiagonal two-sided reduction for SVD**
- **Tridiagonal two-sided for the symmetric eigenvalue problem**
- **Divide & Conquer for the symmetric eigenvalue problem**
- **GEMM for FERMI**
- **Cholesky and QR for multiGPUs on MAGNUM tiles**
  - Hybrid kernels (building blocks) for tile algorithms (e.g., dynamically scheduled)
- **GMRES and PCG**

MAGMA Software Stack



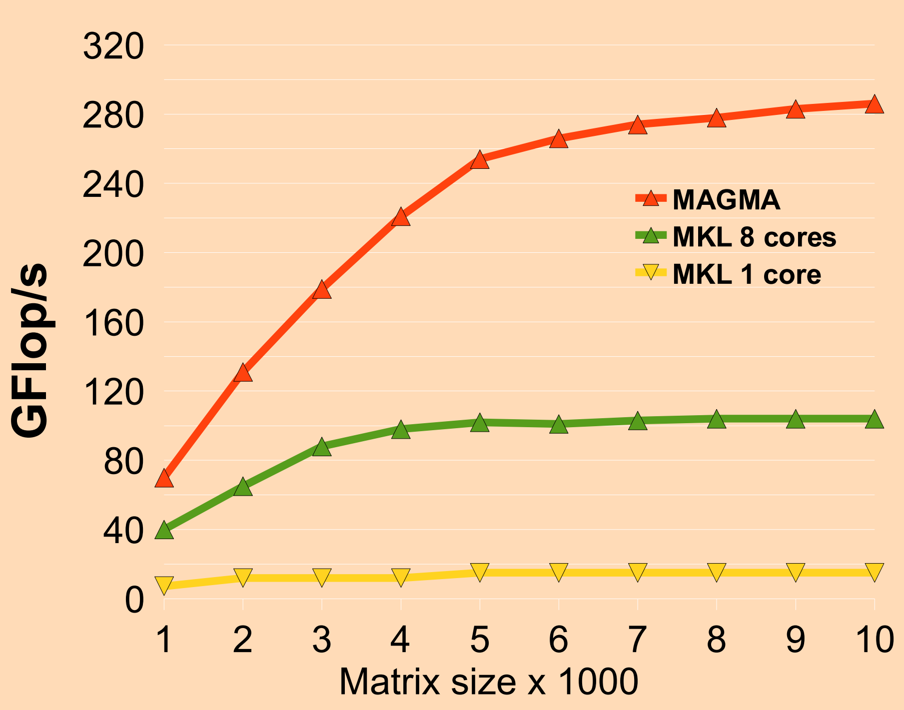
Statically Scheduled **One-Sided Factorizations** (LU, QR, and Cholesky)

- Hybridization
  - Panels (Level 2 BLAS) are factored on CPU using LAPACK
  - Trailing matrix updates (Level 3 BLAS) are done on the GPU using “look-ahead”
- Note
  - Panels are memory bound but are only $O(N^2)$ flops and can be overlapped with the $O(N^3)$ flops of the updates
  - In effect, the GPU is used only for the high-performance Level 3 BLAS updates, i.e., no low performance Level 2 BLAS is scheduled on the GPU

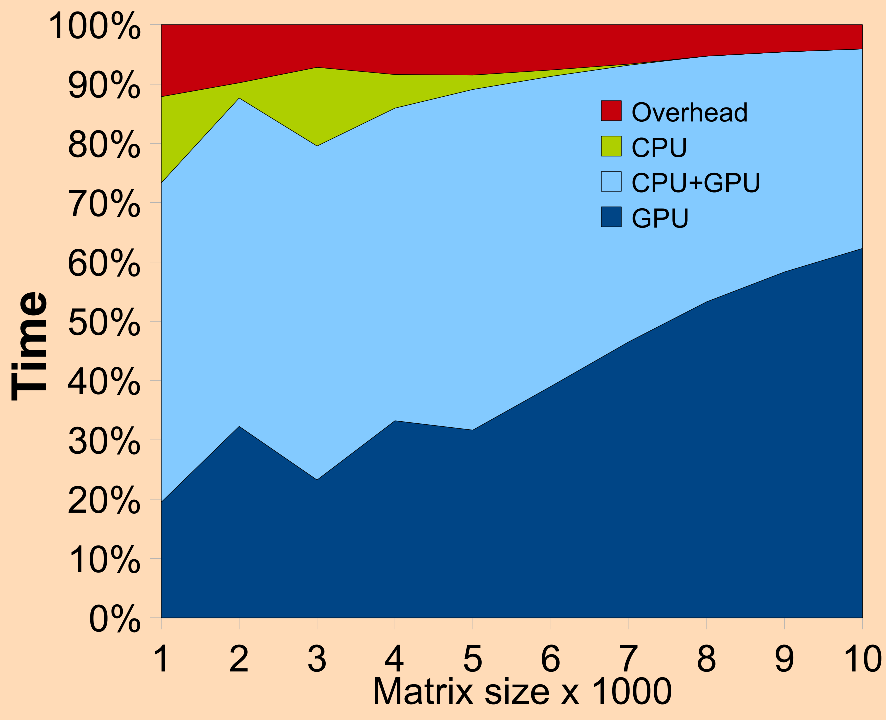
Performance of the one-sided statically scheduled hybrid factorizations

QR factorization in single precision arithmetic, CPU interface

Performance of MAGMA *vs* MKL



MAGMA QR time breakdown



GPU : NVIDIA GeForce GTX 280 (240 cores @ 1.30GHz)
CPU : Intel Xeon dual socket quad-core (8 cores @2.33 GHz)

GPU BLAS : CUBLAS 2.2, sgemm peak: 375 GFlop/s
CPU BLAS : MKL 10.0 , sgemm peak: 128 GFlop/s

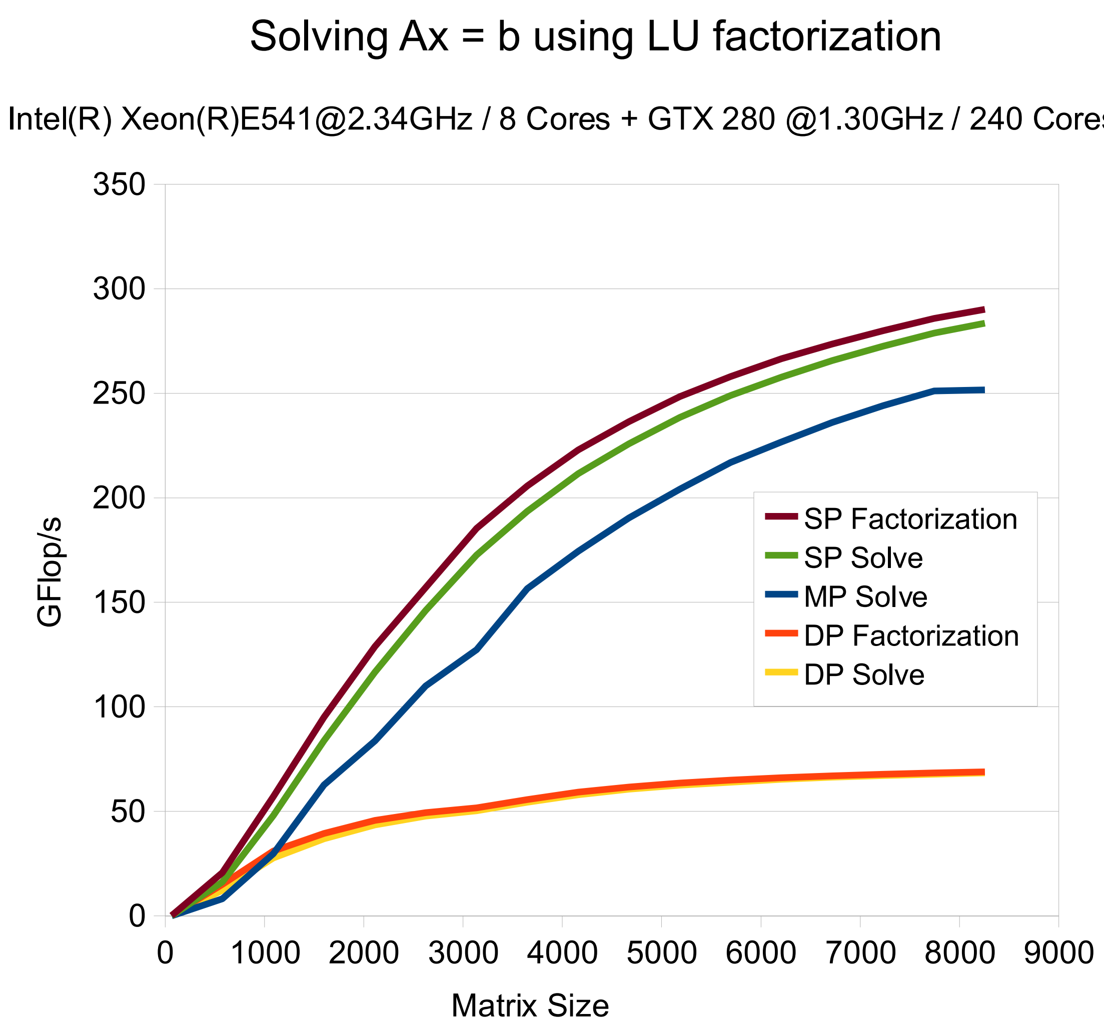
[for more performance data, see **http://icl.cs.utk.edu/magma**]

A look into MAGMA

- MAGMA homepage
  http://icl.cs.utk.edu/magma/

- An example using the Cholesky factorization
  CPU interface: http://www.cs.utk.edu/~tomov/magma/spotrf.cpp
  GPU interface: http://www.cs.utk.edu/~tomov/magma/spotrf_gpu.cpp

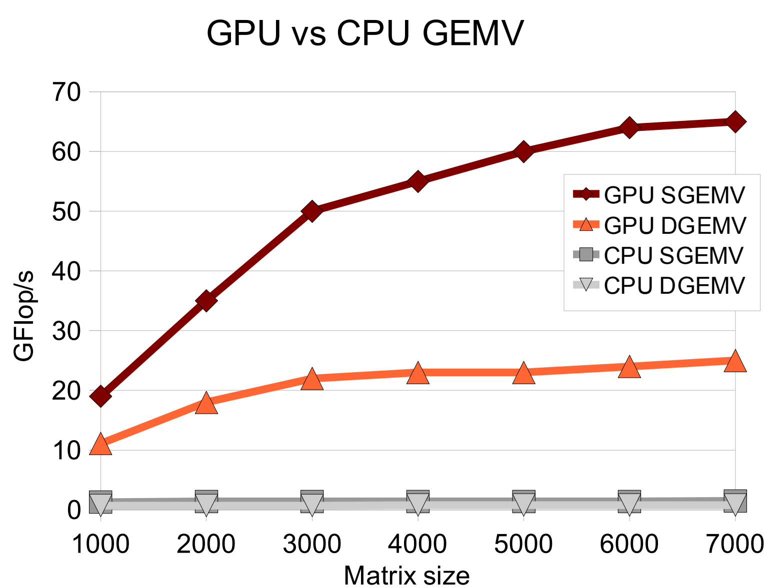
Linear Solvers



- **Direct solvers**
  - Factor and do triangular solves in the same, working precision
- **Mixed Precision Iterative Refinement**
  - Factor in single (i.e. the bulk of the computation in fast arithmetic) and use it as preconditioner in simple double precision iteration, e.g.
    $x_{i+1} = x_i + (LU_{SP})^{-1} P (b - A x_i)$

Two-sided matrix factorizations

- Used in singular-value and eigen-value problems
- LAPACK-based two-sided factorizations are rich in Level 2 BLAS and therefore can not be properly accelerated on multicore CPUs
- We developed hybrid algorithms exploring GPUs' high bandwidth

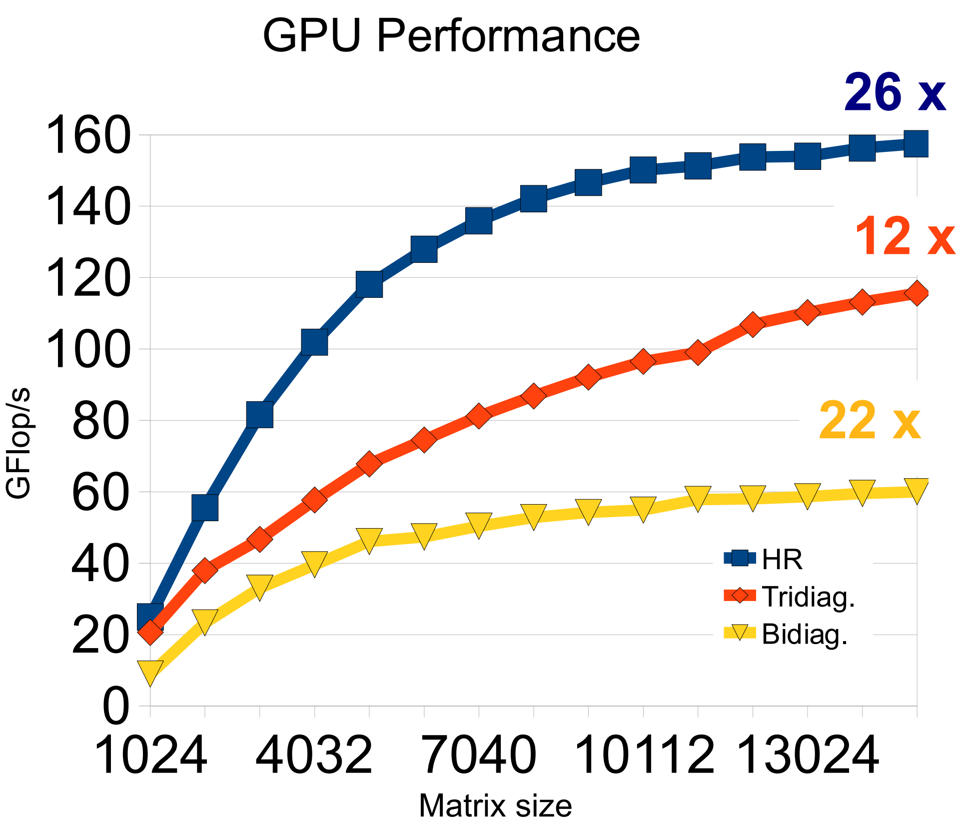


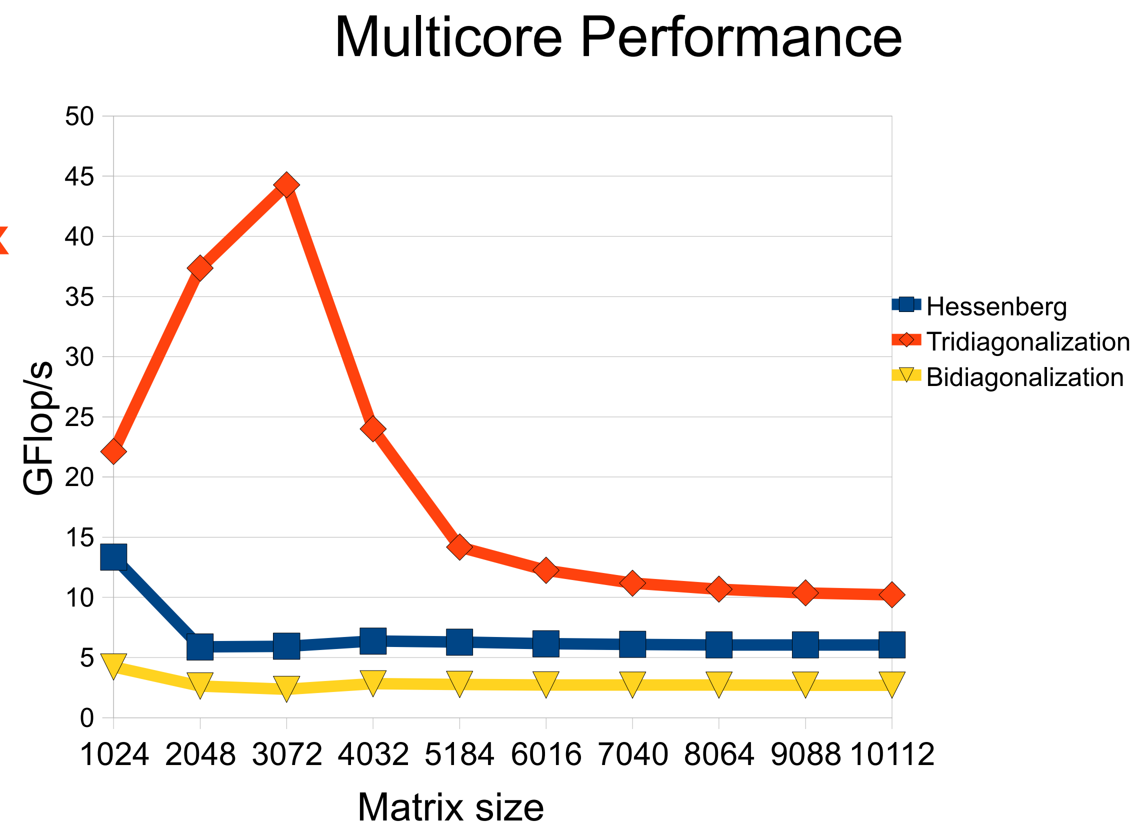
GPU: GTX280 (240 cores @ 1.30GHz, 141 GB/s)
CPU: 2 x 4 cores Intel Xeon @ 2.33GHz, 10.4 GB/s)

High-performance CUDA kernels were developed for various matrix-vector products
[e.g., **ssymv** reaching up to **102 Gflop/s** for the symmetric eigenvalue problem]

Two-sided factorizations

(performance in single precision arithmetic)





GPU : NVIDIA GeForce GTX 280 (240 cores @ 1.30GHz)
CPU : Intel Xeon dual socket quad-core (8 cores @2.33 GHz)

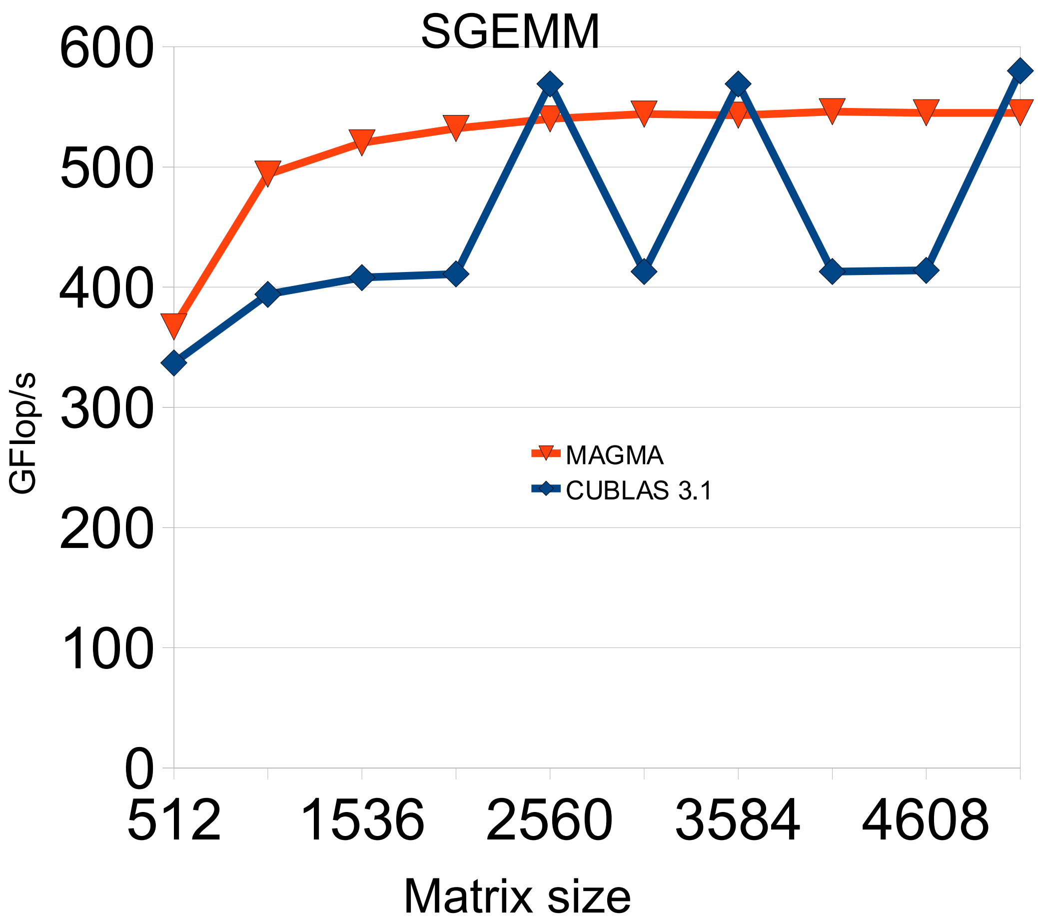
GPU BLAS : CUBLAS 2.3, dgemm peak: 75 GFlop/s
CPU BLAS : MKL 10.0 , dgemm peak: 65 GFlop/s

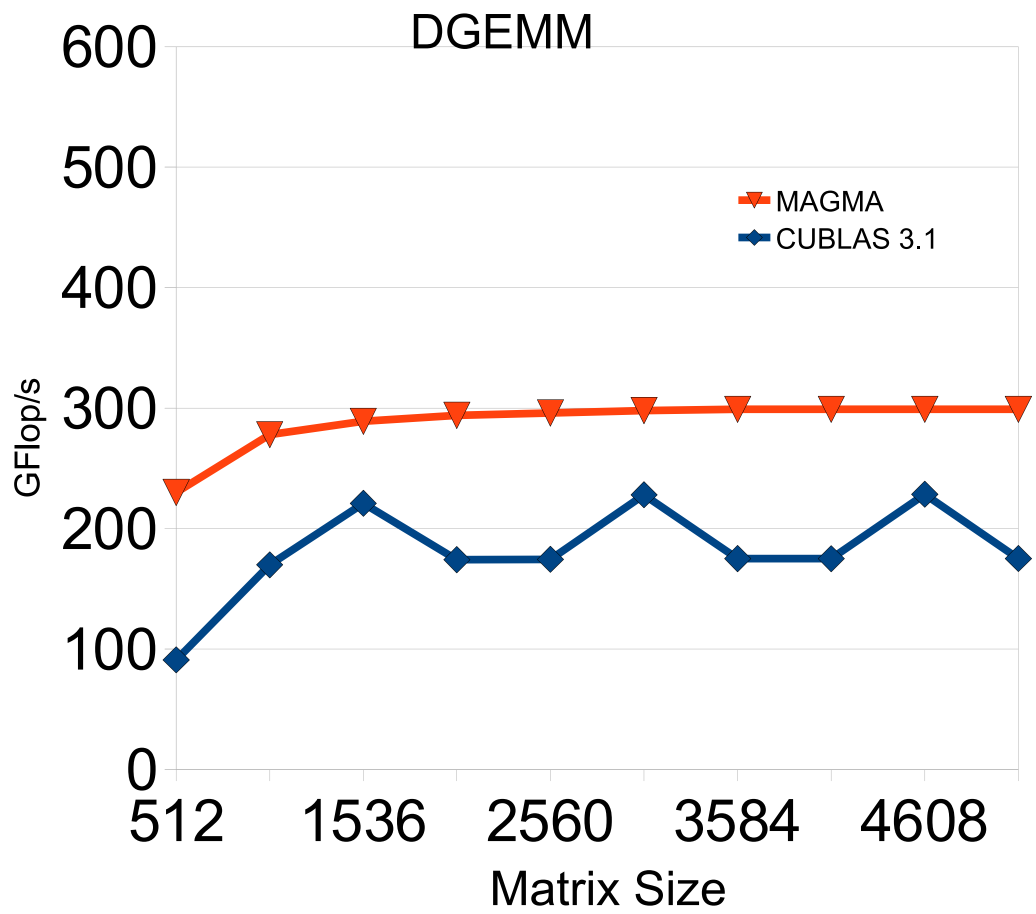
FERMI

- What has changed regarding MAGMA algorithms?
  - MAGMA is coded on high-level, extracting its performance from the performance of low-level kernels, i.e.,
    everything works for FERMI and nothing has changed on high-level
  - We have relied on being able to develop the low-level kernels needed of very high-performance
    as GPUs become more complex, this has become more difficult
  - **Auto-tuning has become more important**

GEMM for FERMI

(Tesla C2050: 448 CUDA cores @ 1.15GHz, theoretical SP peak is 1.03 Tflop/s, DP peak 515 GFlop/s)



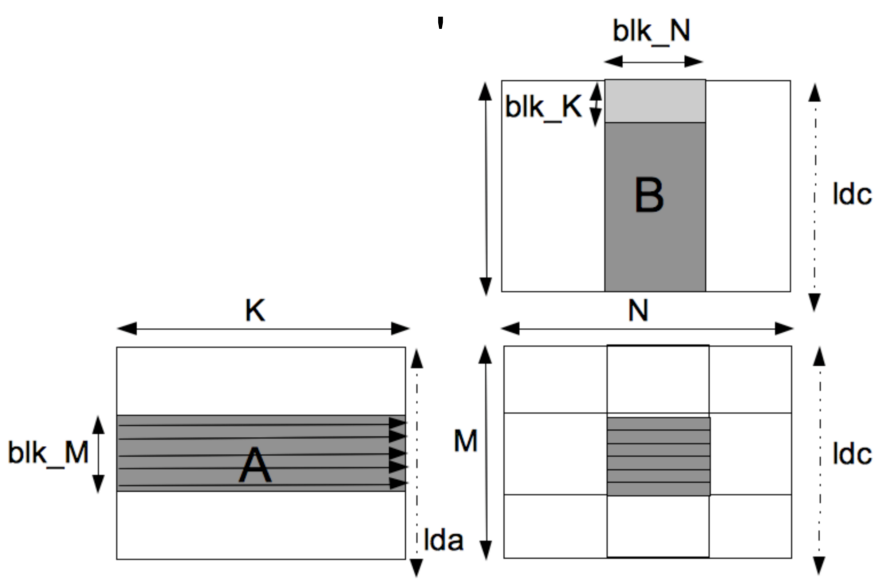


- Kernels have to be **redesigned** and **auto-tuned** for Fermi, e.g., inner-most blocking sizes have to be increased; add register blocking, etc.
- May even need to be written in **assembly**

Auto-tuning GEMM on Fermi GPUs

Previous generation GPUs

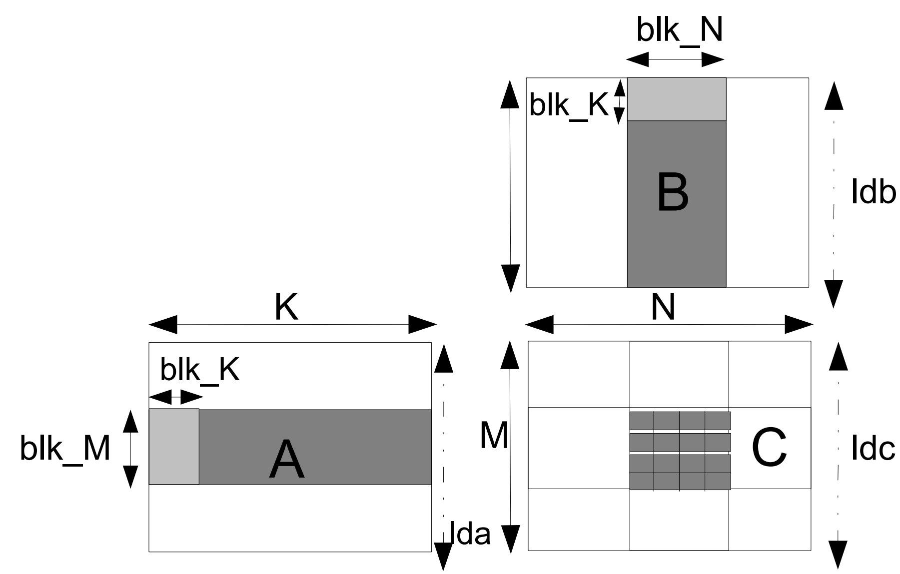
[parametrize kernel by V. Volkov, UC Berkeley]



- A thread block computes a block of matrix C
- Each thread computes a row of the block submatrix of C
- Part of matrix B is loaded into shared memory and computations are done in terms of axpy

Fermi

[search space extended by R. Nath, UTK]



- Increase blocking size and add register blocking
- Each thread computes a sub-block of submatrix of C
- Parts of both A and B are first loaded into shared memory and each thread loads corresponding values into registers to do register-blocked computation

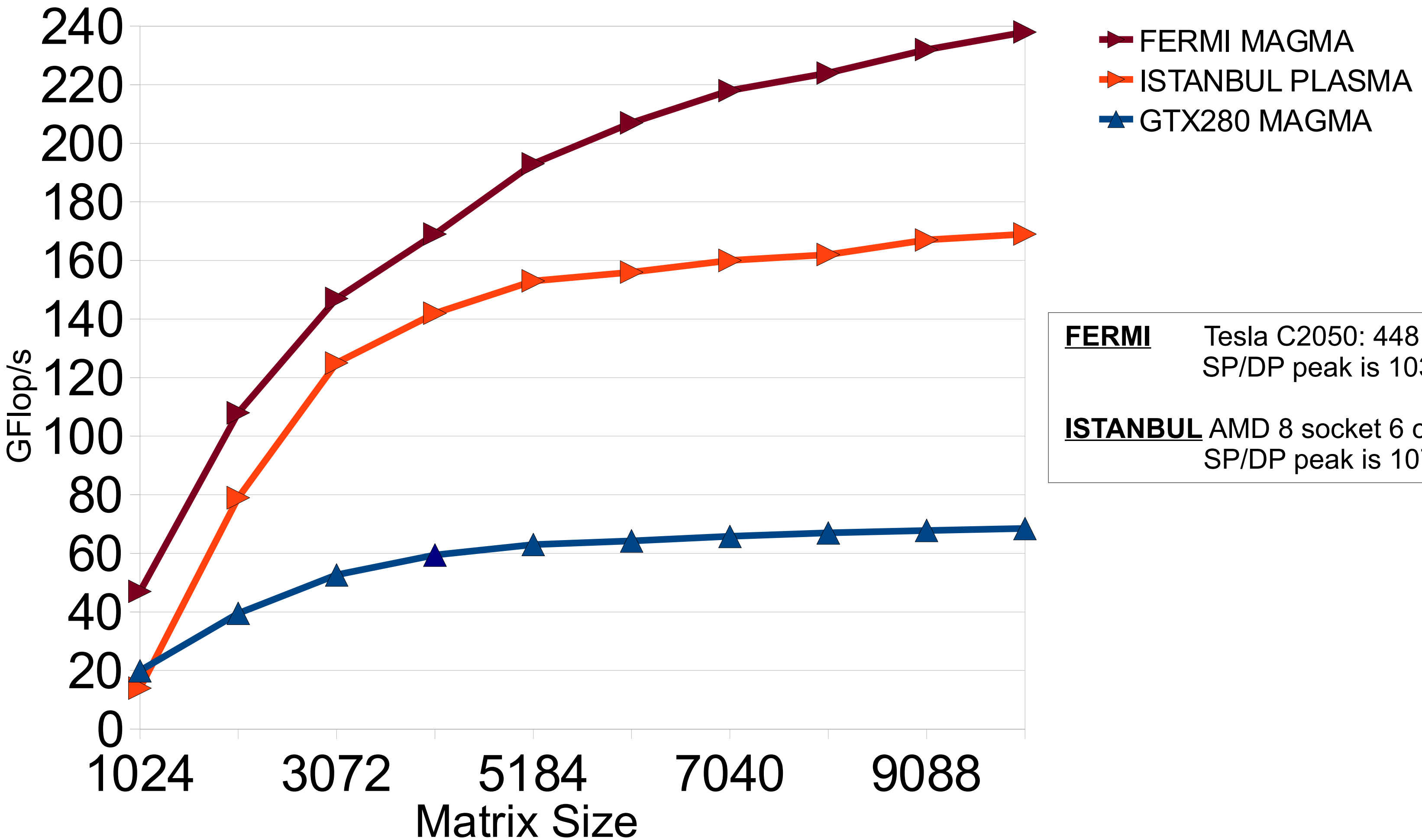
A look into MAGMA BLAS

- MAGMA BLAS DGEMM for Fermi

  http://www.cs.utk.edu/~tomov/magma/fermi_dgemm.cu

  Note: This is just one version, produced by
  a code generator, exploring the search
  space described on the previous slide

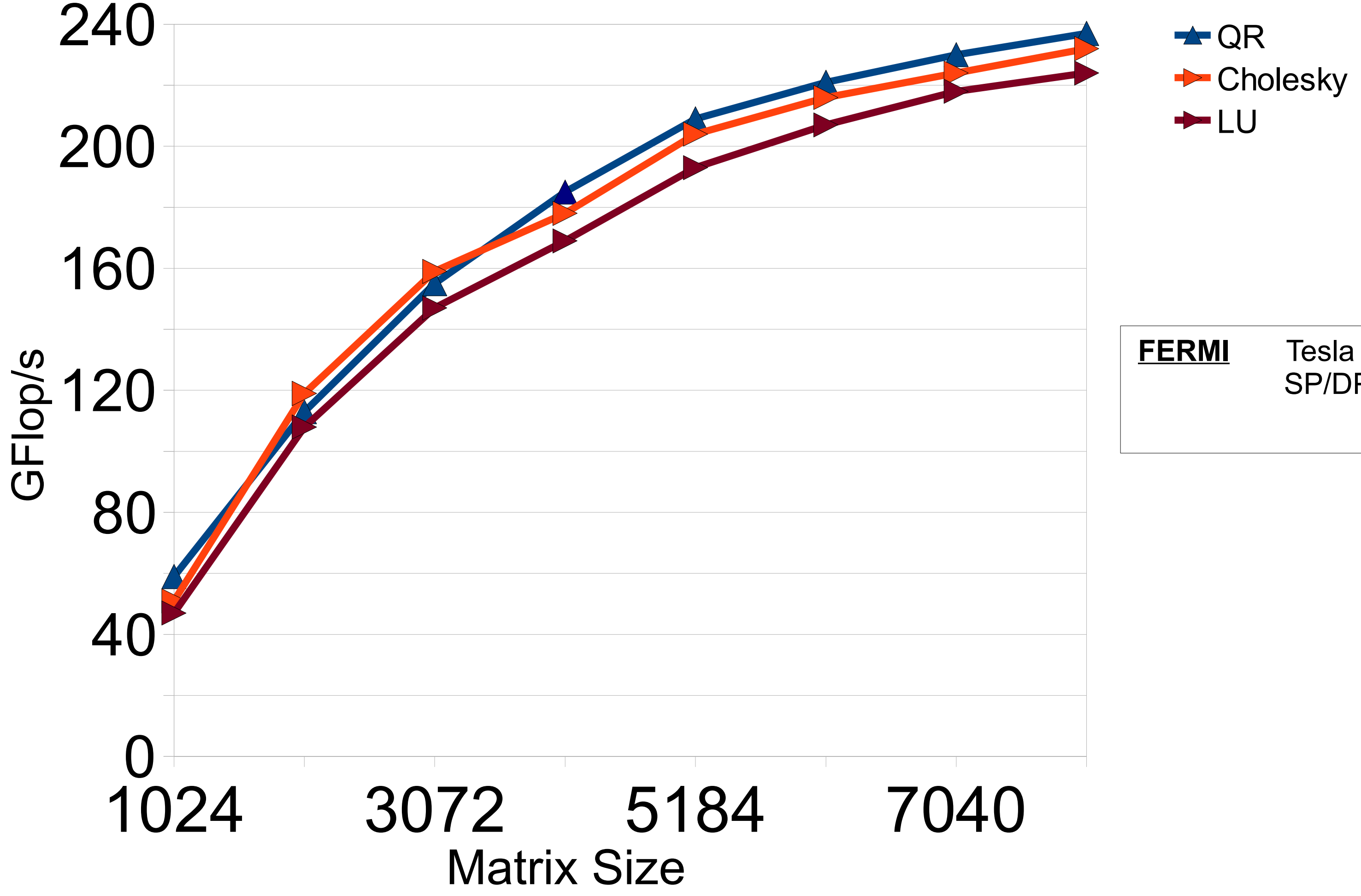
LU factorization in double precision



FERMI Tesla C2050: 448 CUDA cores @ 1.15GHz
SP/DP peak is 1030 / 515 GFlop/s

ISTANBUL AMD 8 socket 6 core (48 cores) @2.8GHz
SP/DP peak is 1075 / 538 GFlop/s

LU, Cholesky, and QR on Fermi in DP



FERMI Tesla C2050: 448 CUDA cores @ 1.15GHz
SP/DP peak is 1030 / 515 GFlop/s

MultiGPU and Multicore

MAGNUM tiles

- Tasks are **hybrid**, **GPU BLAS-based**, or **multicore** kernels

Scheduling:

- Using **PLASMA** with customized extensions to reduce communication and w/ hybrid MAGMA kernels
  - Demonstrated scalability for one-sided factorizations
  - Highly optimized, used as benchmark to compare with dynamic schedulers
    [e.g., performance on 4 C1060 GPUs for Cholesky is up to 1200 Gflop/s, for QR is up to 830 Gflop/s in SP]
- Using **StarPU** to schedule hybrid, GPU and multicore kernels (from PLASMA and MAGMA)
  http://runtime.bordeaux.inria.fr/StarPU/
- Using the **DPLASMA** scheduler

Rectangular tiles

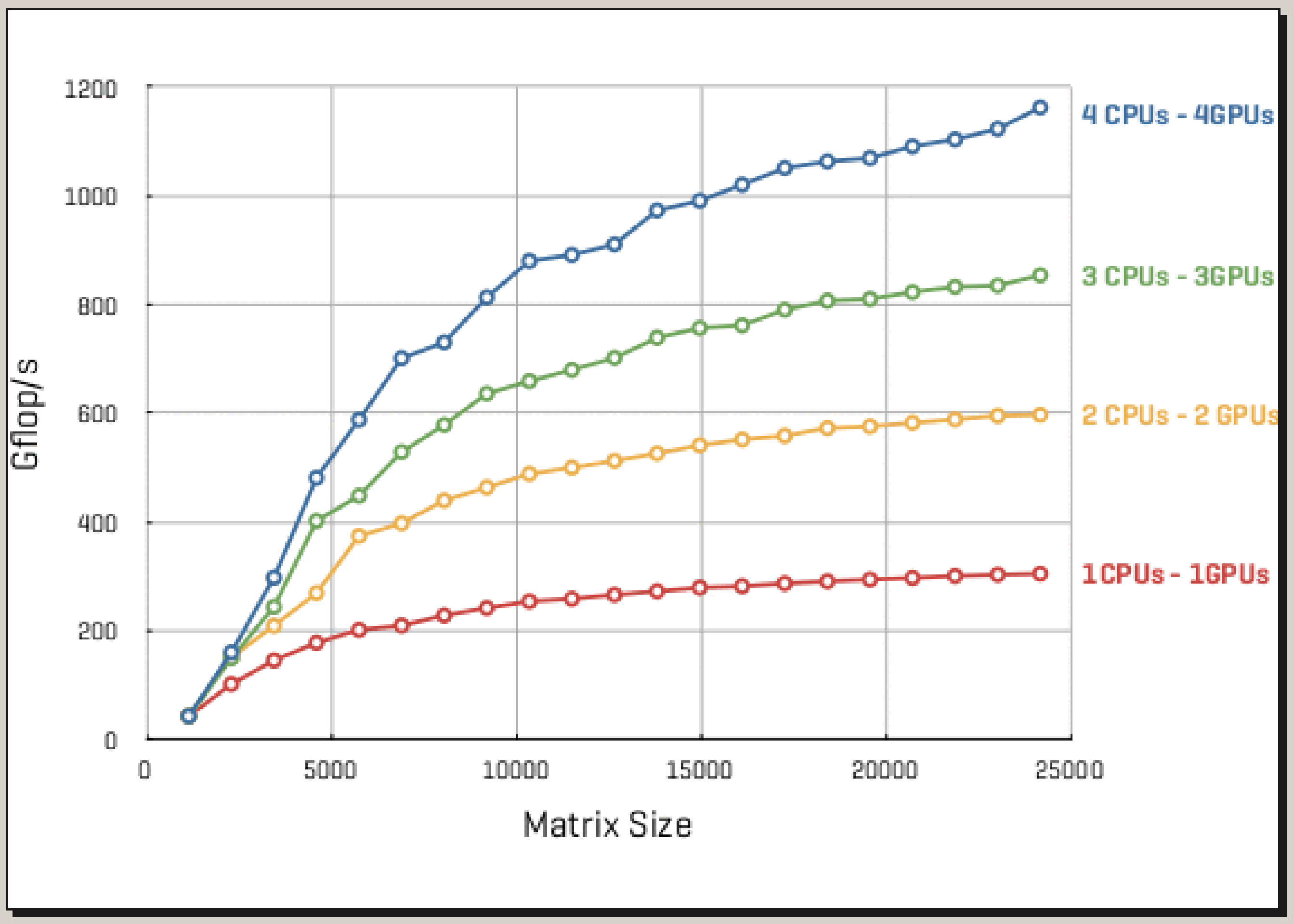
- Tiles of variable sizes to be used to account for the heterogeneity of the system
- To experiment with “communication-avoiding” algorithms

PLASMA tile algorithms

- A single GPU kernel processing multiple tile tasks in parallel
  [*vs* only one, but magnum tile, at a time]

Scheduling with PLASMA

Cholesky factorization in SP



HOST: 4x AMD Opteron core @1.8GHz
GPUs: 4x C1060 (240 cores each @1.44GHz)

Sparse Linear Algebra

Algorithm 1 GMRES for GPUs

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for $i = 0, 1, \ldots$ **do**
  $r = b - Ax_i$ (magma_sspmv)
  $\beta = h_{1,0} = ||r||_2$ (cublasSnrm2)
  check convergence and exit if done
  for $k = 1, \ldots, m$ **do**
    $v_k = r \; / \; h_{k,k-1}$ (magma_sscal)
    $r = A \; v_k$ (magma_sspmv)
    for j=1,...,k **do**
      $h_{j,k} = r^T v_j$ (cublasSdot)
      $r = r - h_{j,k} \; v_j$ (cublasSaxpy)
    end for
    $h_{k+1,k} = ||r||_2$ (cublasSnrm2)
  end for
  Define $V_k = [v_1, \ldots, v_k]$, $H_k = \{h_{i,j}\}$
  Find y_k that minimizes $||\beta e_1 - H_k \; y_k||_2$
  $x_{i+1} = x_i + V_k \; y_k$ (magma_sgemv)
end for

Algorithm 2 LOBPCG for GPUs

---

for $i = 0, 1, \ldots$ **do**
  $R = P(AX_i - \Lambda X_i)$ (magma_sspmv)
  check convergence and exit if done
  $[X_i, \Lambda]$ = Rayleigh-Ritz on
    span$\{X_i, \; X_{i-1}, \; R\}$ (hybrid)
end for

- The hybridization approach naturally works [e.g., Richardson iteration in mixed-precision iterative refinement solvers, Krylov space iterative solvers and eigen-solvers]
- Observed better accuracy (compared to CPU)
- Fast sparse matrix-vector product on Fermi does not have to use texture memory
- Explore ideas to reduce communication [e.g., mixed precision, reduced storage for integers for the indexing, etc.]
- Need high bandwidth

http://www.cs.utk.edu/~tomov/magma/sgmres.cpp

MAGMA Future Plans

- Experimentation with various schedulers (StarPU, PLASMA, DPLASMA) and improvements for multicore with multiGPUs
- “Communication avoiding” algorithms for systems of multicore CPUs and GPUs
- Kernels for FERMI (GEMM, SYRK, TRSM, SpMV)
- Auto-tuning framework
- Port [or facilitate the port] to Windows, Python and Matlab
- Krylov space iterative linear solvers and block eigensolvers

Collaborators / Support

- **MAGMA** Matrix Algebra on GPU and Multicore Architectures
  [**ICL team**: J. Dongarra, S. Tomov, R. Nath, H. Ltaief]
  http://icl.cs.utk.edu/magma/

- **PLASMA** Parallel Linear Algebra for Scalable Multicore Architectures
  http://icl.cs.utk.edu/plasma

- Collaborating partners

  University of Tennessee, Knoxville
  University of California, Berkeley
  University of Colorado, Denver

  University of Coimbra, Portugal
  INRIA Bordeaux Sud Ouest, France