Dense Linear Algebra Solvers for Multicore with GPU Accelerators

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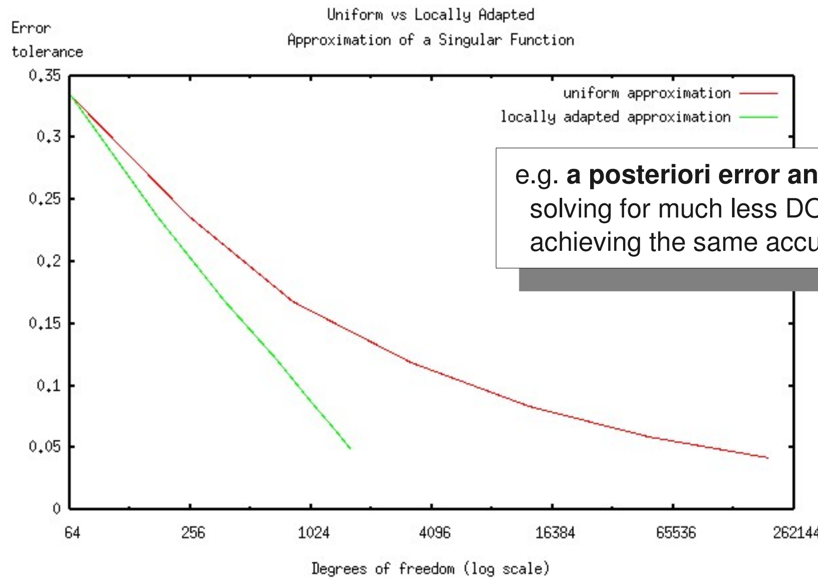
Outline

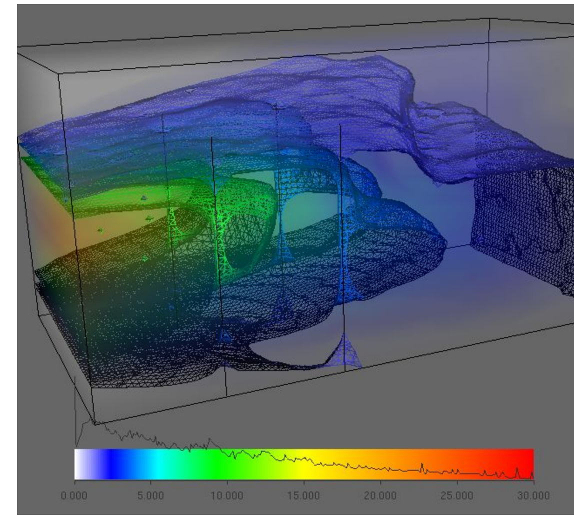
- **Introduction**
  - Hardware to Software Trends
- **The MAGMA library**
  - Challenges and approach
  - One-sided factorizations and solvers
  - Two-sided factorizations
- **Conclusions**

Speeding up Computer Simulations

Better numerical methods

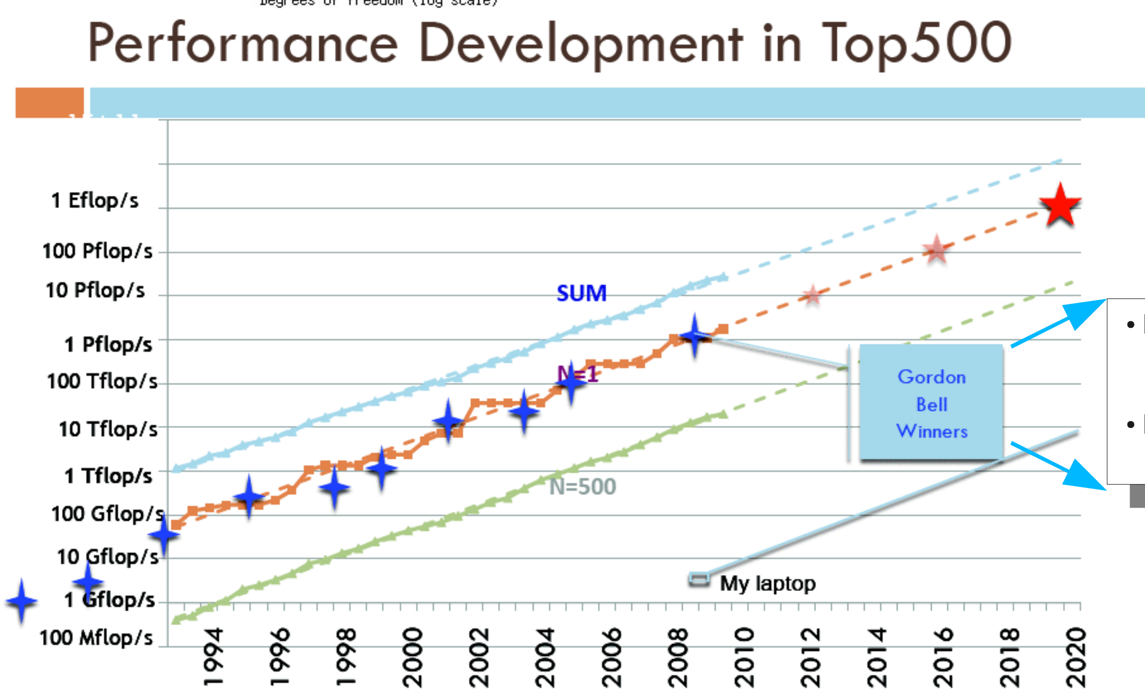


e.g. **a posteriori error analysis**: solving for much less DOF but achieving the same accuracy



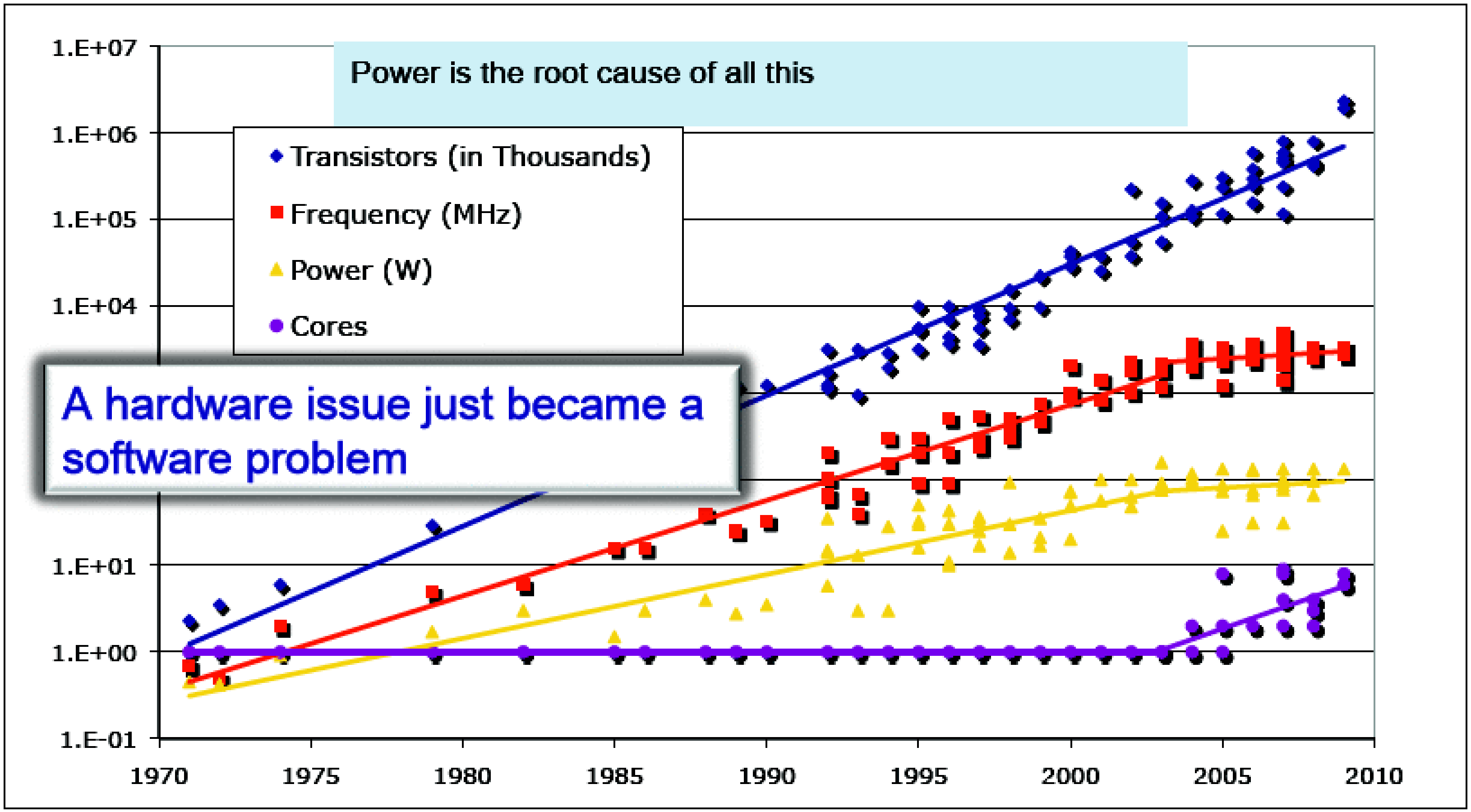
http://www.cs.utk.edu/~tomov/cflow/

Exploit advances in hardware



- Manage to use hardware efficiently for real-world HPC applications
- Match LU benchmark in performance !

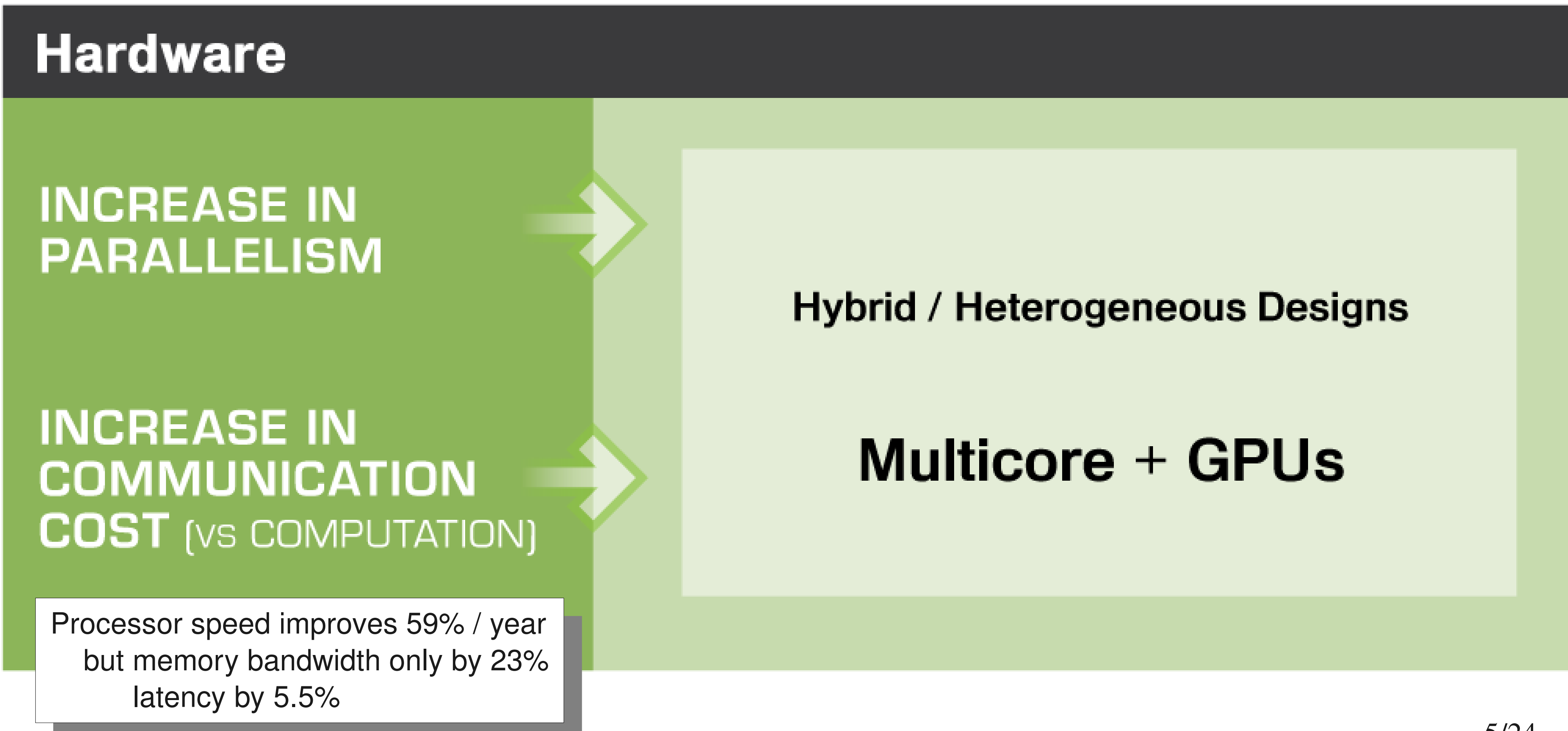
Clock Frequency Scaling Replaced by Scaling Cores/Chip



Data from Kunle Olukotun, Lance Hammond, Herb Sutter, Burton Smith, Chris Batten, and Krste Asanoviç
Slide from Kathy Yelick

Why GPU-based Computing ?

- Hardware Trends



Matrix **A**lgebra on **G**PU and **M**ulticore **A**rchitectures (**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**

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 (bi/tri-diagonalization developed)
- MAGMA BLAS
  - Routines critical for MAGMA (GEMM, SYRK, TRSM, GEMV, SYMV, etc.)

Challenges

- **Massive parallelism**

  Many GPU cores, serial kernel execution

  [e.g. 240 in the GTX280; up to 512 in ***Fermi*** – to have concurrent kernel execution]

- **Hybrid/heterogeneous architectures**

  Match algorithmic requirements to architectural strengths

  [e.g. small, non-parallelizable tasks to run on CPU, large and parallelizable on GPU]

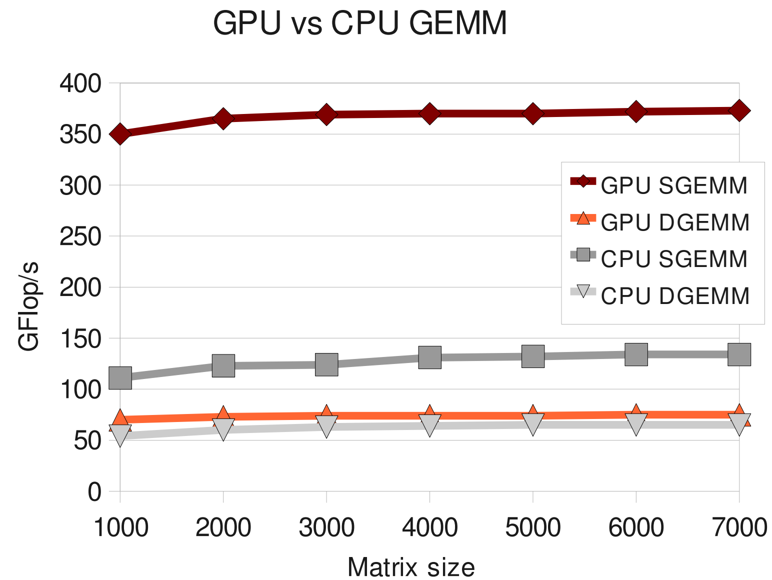
- **Compute *vs* communication gap**

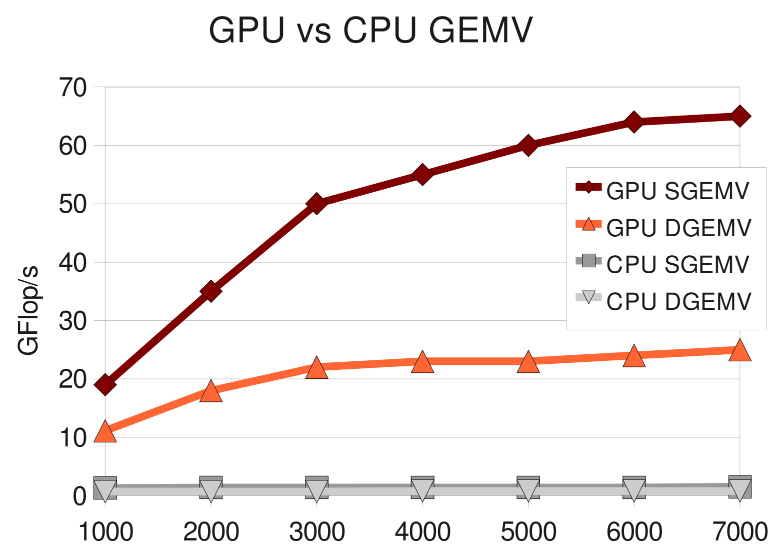
  Exponentially growing gap; persistent challenge

  [on all levels, e.g. a GPU Tesla C1070 (4 x C1060) has compute power of O(1,000) Gflop/s but GPUs communicate through the CPU using O(1) GB/s connection]

How to Code for GPUs?

- Complex question
  - Language, programming model, user productivity, etc
- Recommendations
  - **Use CUDA / OpenCL**
    [already demonstrated benefits in many areas;
    data-based parallelism; move to support task-based]
  - **Use GPU BLAS**
    [high level; available after introduction of **shared memory** –
    can do data reuse; leverage existing developments]
  - **Use Hybrid Algorithms**
    [currently GPUs – massive parallelism but serial kernel execution;
    hybrid approach – small non-parallelizable tasks on the CPU,
    large parallelizable tasks on the GPU]



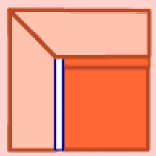
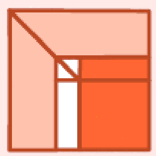
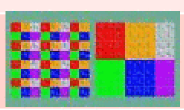
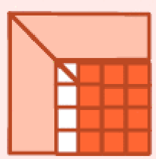


GPU: GTX280 (240 cores @ 1.30GHz, 141 GB/s)
CPU: 2 x 4 cores Intel Xeon @ 2.33GHz, 10.4 GB/s)

LAPACK to Multicore

A New Generation of Software:

Parallel Linear Algebra Software for **Multicore** Architectures (PLASMA)

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

Those new algorithms
- have a very low granularity, they scale very well (multicore, petascale computing, …)
- removes a lots of dependencies among the tasks, (multicore, distributed computing)
- avoid latency (distributed computing, out-of-core)
- rely on fast kernels

Those new algorithms need new kernels and rely on efficient scheduling algorithms.

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

Split BLAS into tasks and represent **algorithms as DAGs**; new algorithms where panel factorizations use **localized** (over tiles) elementary **transformations**

LAPACK to MAGMA

(multicore with GPU accelerators)

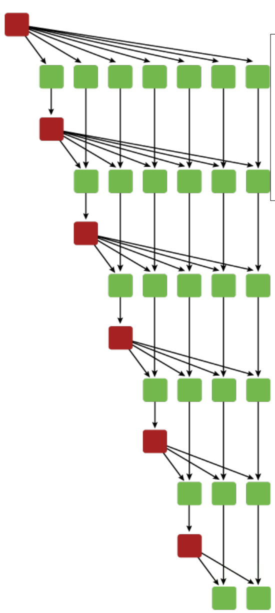
1) Development of **NEW LGORITHMS (parallelism, hybrid, optimized communication)**

2) **HYBRIDIZATION** of linear algebra algorithms

   - Represent the algorithms as a collection of **TASKS** and **DEPENDANCIES** among them
   - Properly **SCHEDULE** the tasks' execution over the multicore and the GPU

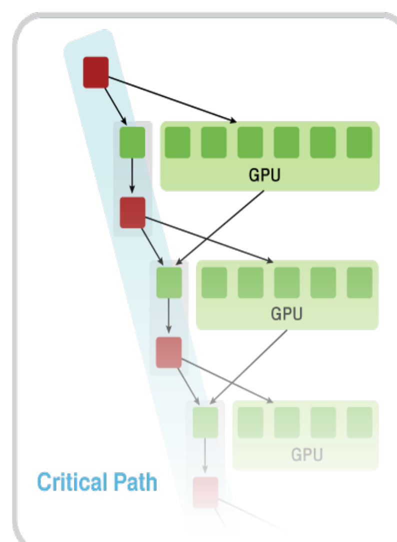
3) Development of GPU BLAS **KERNELS**

4) **AUTO-TUNED** implementations



Algorithms as DAGs

(small tasks/tiles for homogeneous **multicore**)

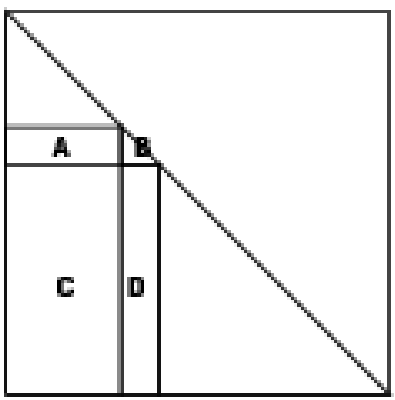


Hybrid CPU+GPU algorithms

(small tasks for multicores and large tasks for GPUs)

One-Sided Dense Matrix Factorizations (LU, QR, and Cholesky)

- Panels (Level 2 BLAS) are factored on CPU using LAPACK
- Trailing matrix updates (Level 3 BLAS) are done on the GPU using “look-ahead” (to overlap CPUs work on the critical path with the GPUs large updates)



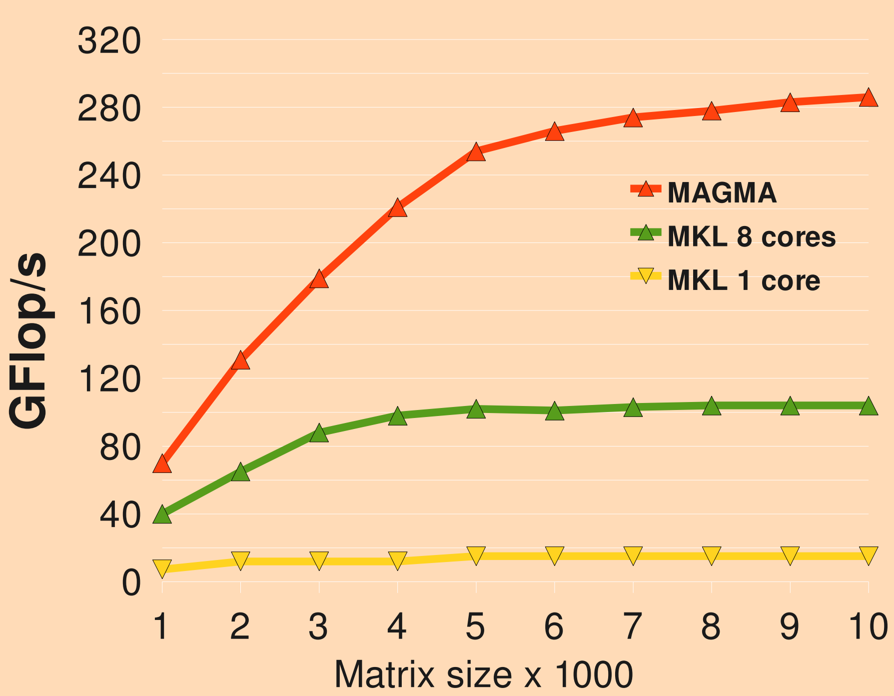
Example: Left-Looking Hybrid Cholesky factorization

MATLAB code	LAPACK code	Hybrid code
[1] B = B – A*A'	ssyrk_("L", "N", &nb, &j, &mone, hA[j,0], ...)	cublasSsyrk('L', 'N', nb, j. mone, dA[j,0], ...)
		cublasGetMatrix(nb, nb, 4, dA[j, j], *lda, hwork, nb)
[2] B = chol(B, 'lower')	spotrf_("L", &nb, hA[j, j], lda, info)	cublasSgemm('N', 'T', j, ...)
[3] D = D – C*A'	sgemm_("N", "T", &j, ...)	spotrf_("L", &nb, hwork, &nb, info)
		cublasSetMatrix(nb, nb, 4, hwork, nb, dA[j, j], *lda)
[4] D = D\B	strsm_("R", "L", "T", "N", &j, ...)	cublasStrsm('R', 'L', 'T', 'N', j, ...)

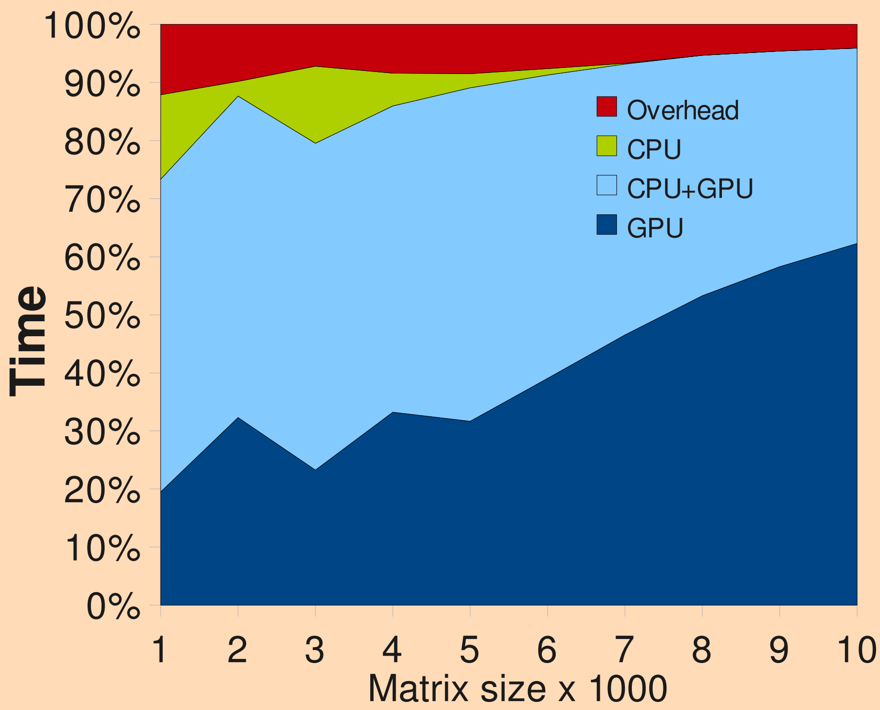
One-sided hybrid factorizations

QR factorization in single precision arithmetic, CPU interface

Performance of MAGMA *vs* MKL



MAGMA QR time breakdown

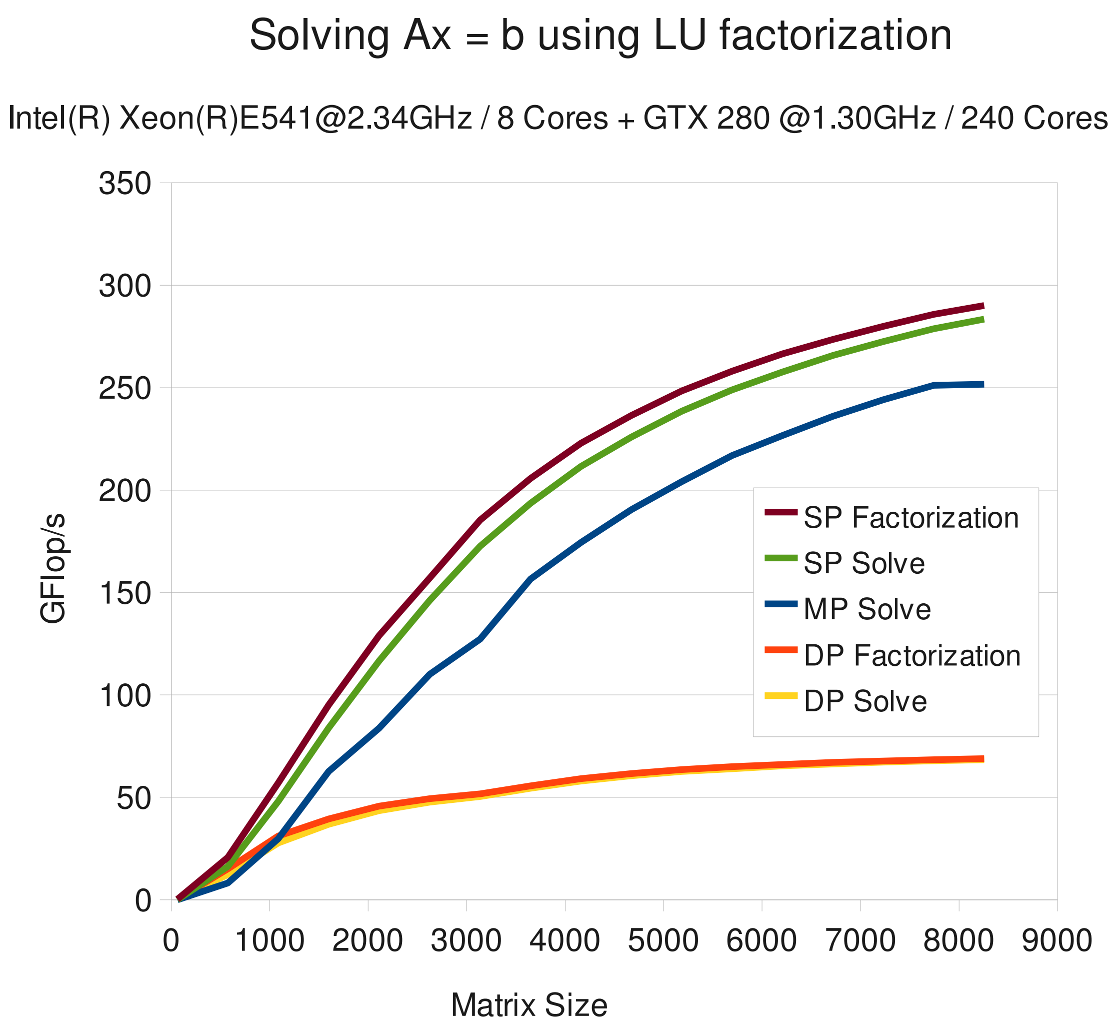


GPU : NVIDIA GeForce GTX 280 (240 cores @ 1.30GHz)
CPU : Intel Xeon dual socket quad-core (8 cores @2.33 GHz)

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

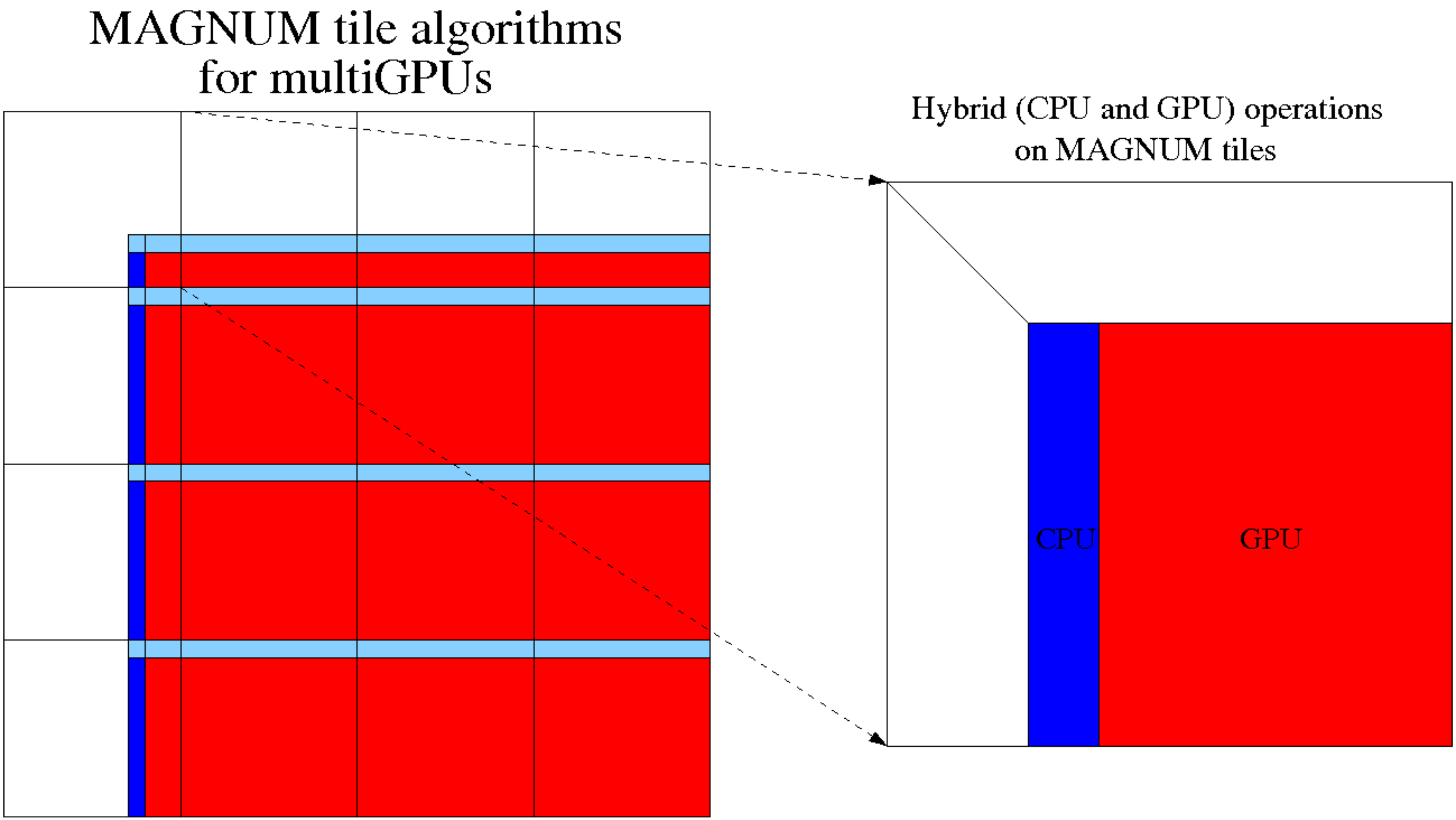
[for more performance data, see **http://icl.cs.utk.edu/magma**]

Linear Solvers



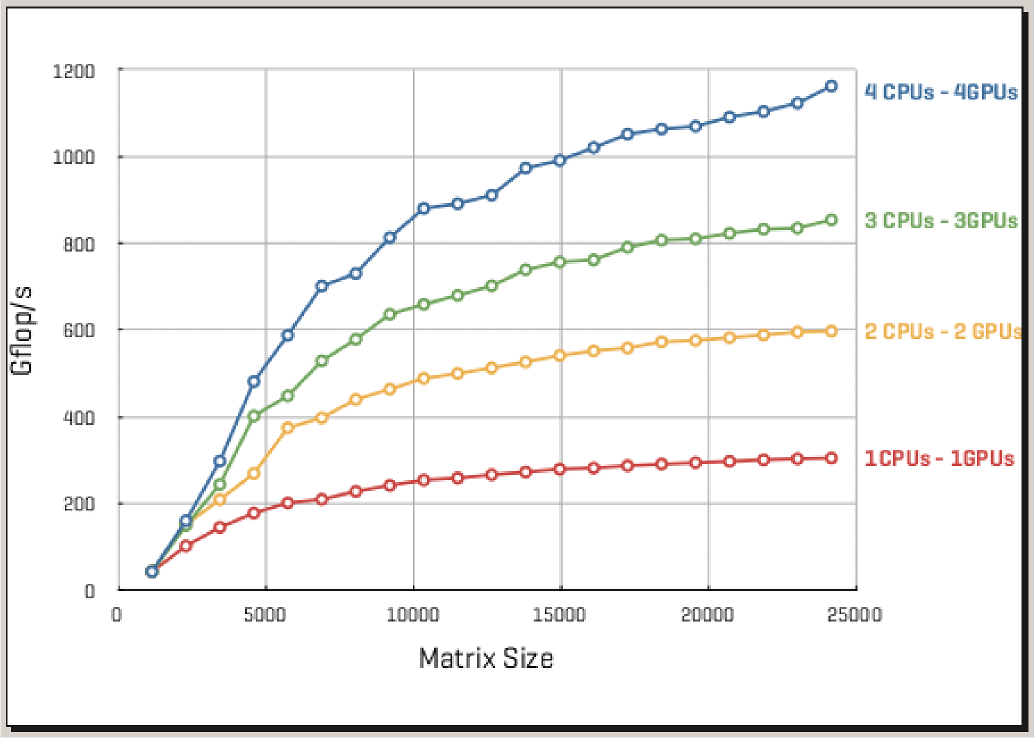
- Direct solvers
  - Factor and do triangular solves in the same, working precision
- Mixed Precision Iterative Refinement
  - Factor in single (i.e. the bulk of the computation in fast arithmetic) and use it as preconditioner in simple double precision iteration, e.g. $x_{i+1} = x_i + (LU_{SP})^{-1}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

Extension to Multicore and Multi GPUs



Performance using MultiGPUs

Cholesky factorization in SP
Strong Scalability



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

2 level nested parallelism
coarse: PLASMA tiled algorithm and static scheduling
fine : tasks/tiles are redefined for hybrid 1 core+GPU computing
- Defining a "***Magnum tiles approach***"

Two-sided matrix factorizations

- Two-sided factorizations

  $\boldsymbol{Q\ A\ Q' = H}$

  $\boldsymbol{H}$ – upper Hessenberg / bidiagonal / tridiagonal,
  $\boldsymbol{Q}$ – orthogonal similarity transformation

- **Importance**

One-sided factorizations - bases for linear solvers	**Two-sided factorizations** - bases for eigen-solvers

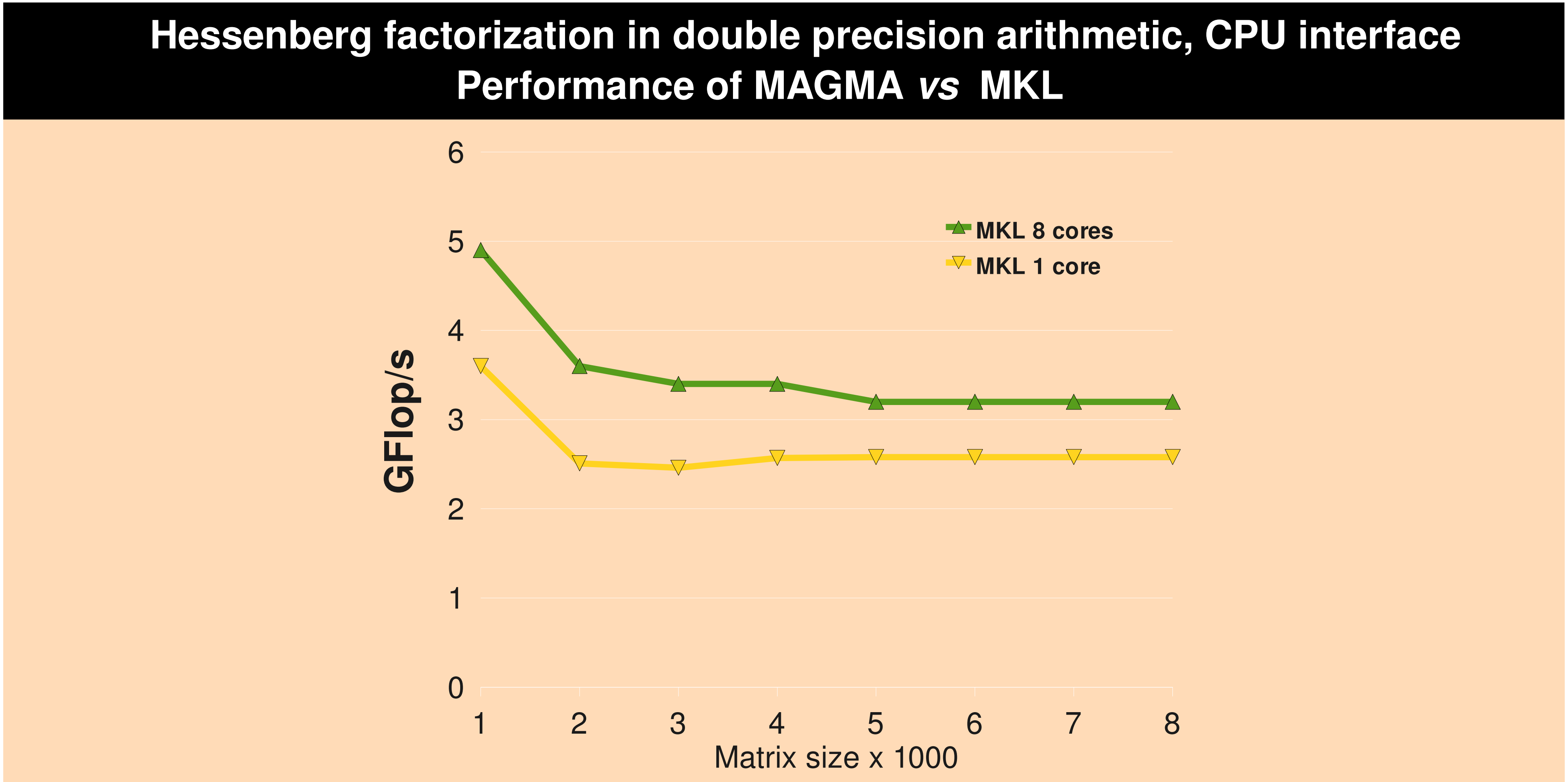
- Block algorithm

  $\boldsymbol{Q}$ – a product of n-1 elementary reflectors
  $\boldsymbol{Q = H_1\ H_2\ \ldots\ H_{n-1}}$, $\boldsymbol{H_i = I - \tau_i\, v_i\, v_i'}$
  $\boldsymbol{H_1\ \ldots\ H_{nb} = I - V\ T\ V'}$ (*WY transform*; the bases for delayed update or block algorithm)

- **Can we accelerate it ?**

  [similarly to the one-sided using hybrid GPU-based computing]
  [to see **much higher acceleration** due to a removed bottleneck]

Homogeneous multicore acceleration?

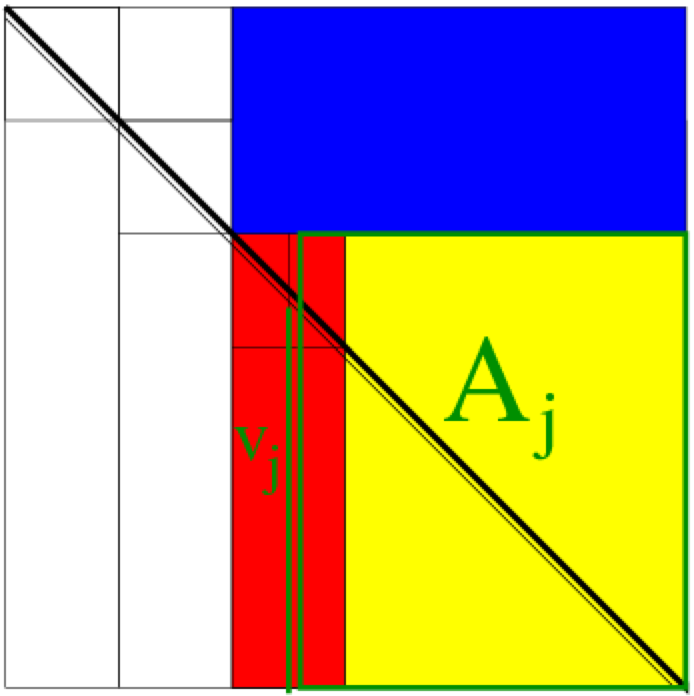


CPU : Intel Xeon dual socket quad-core (8 cores @2.33 GHz) **CPU BLAS** : MKL 10.0 , dgemm peak: 65 GFlop/s

- There have been difficulties in accelerating it on homogeneous multicores

The Bottleneck

Hessenberg factorization



Level 3 BLAS update
[80% flops; ~30% of the run time]

Level 2 BLAS update
[20% flops; ~70% of the run time]

$y_j = A_j \, v_j$

bidiagonalization & **tridiagonalization** have even more Level 2 BLAS (**50%**)

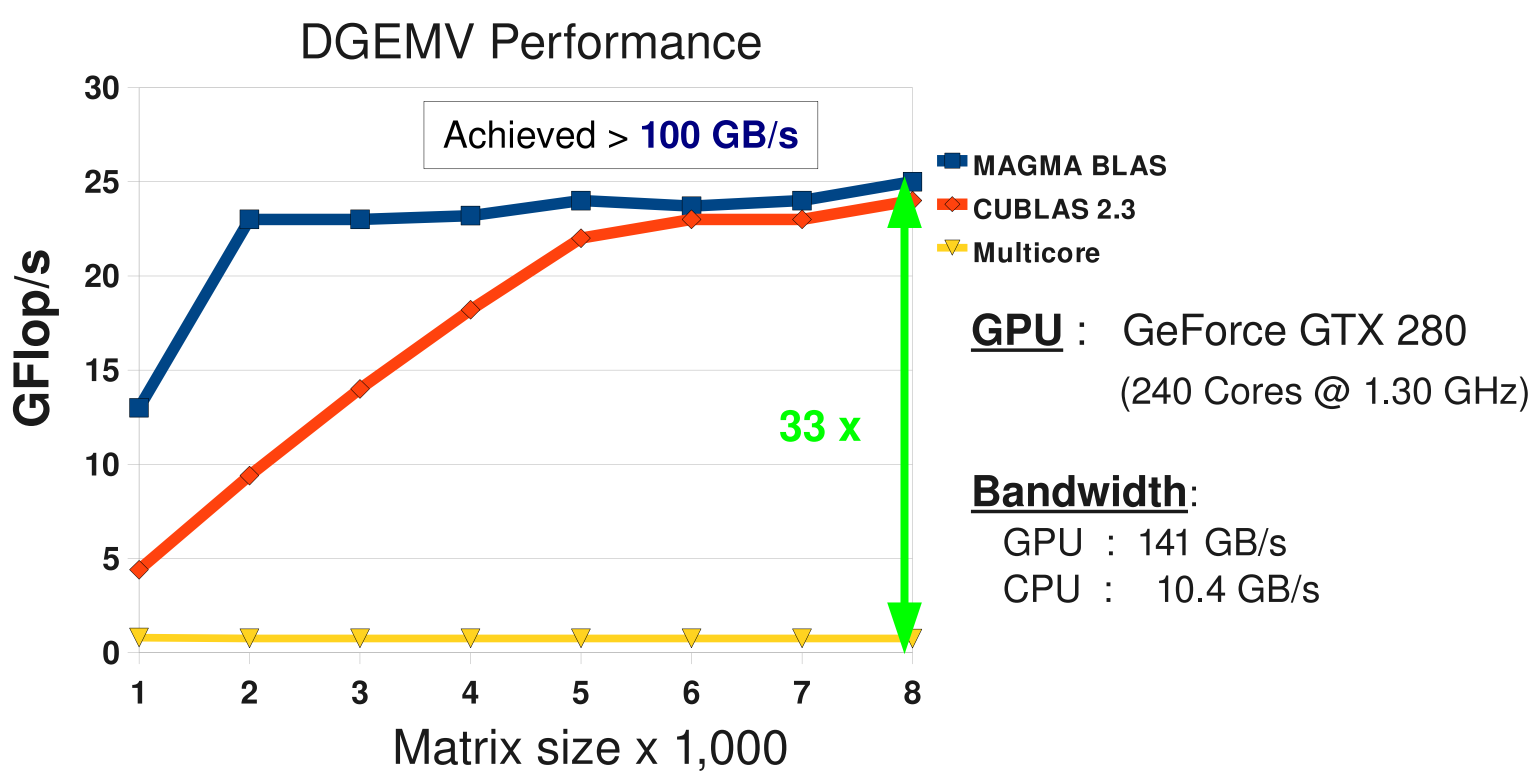
Reduction times in seconds for N = 4,000

# cores	**1**		**8**	1+GPU		8+GPU
Level 3 BLAS	**25** (30%)	/	**4**	**3.5** (60%)	/	**2.7**
Level 2 BLAS	**59** (70%)	/	**59**	**2.3** (40%)	/	**2.3**

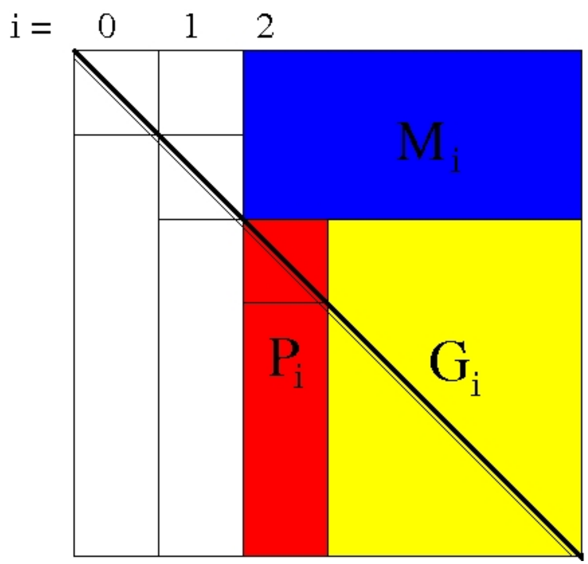
No improvement

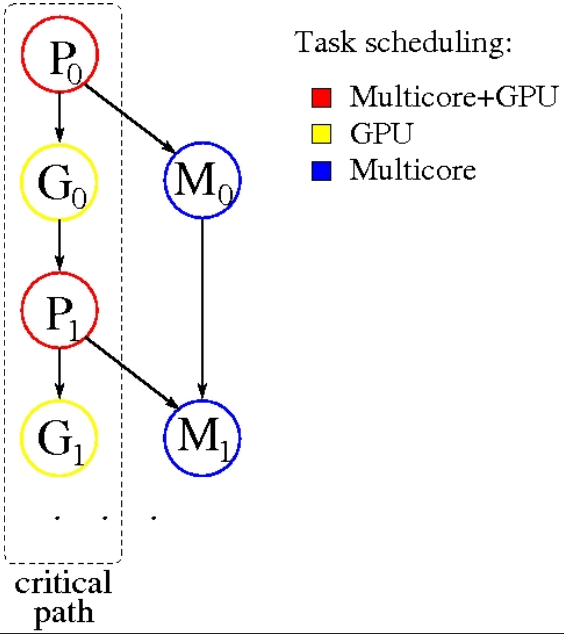
Hybrid computing acceleration?

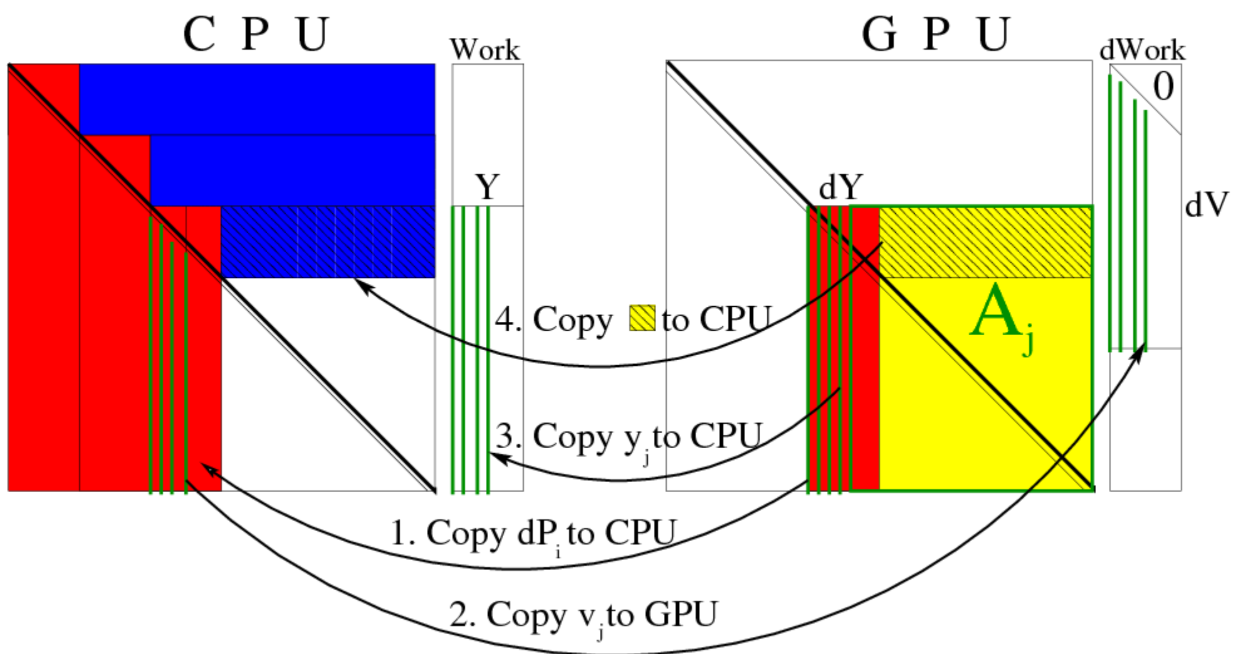
- Intuitively, yes, as matrix-vector product is fast on GPUs
  (e.g., sgemv up to 66 Gflop/s, ssymv up to 102 GFlop/s)
- How to organize a hybrid computation ?



Task **Splitting** & Task **Scheduling**

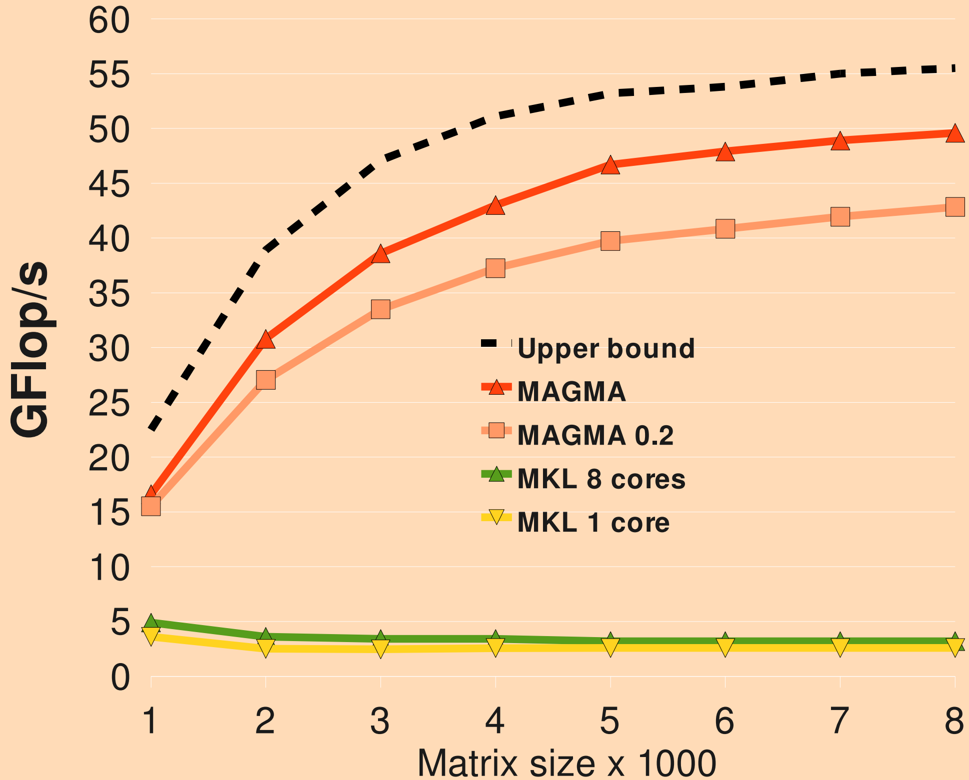






Performance

Hessenberg factorization in double precision arithmetic, CPU interface
Performance of MAGMA *vs* MKL



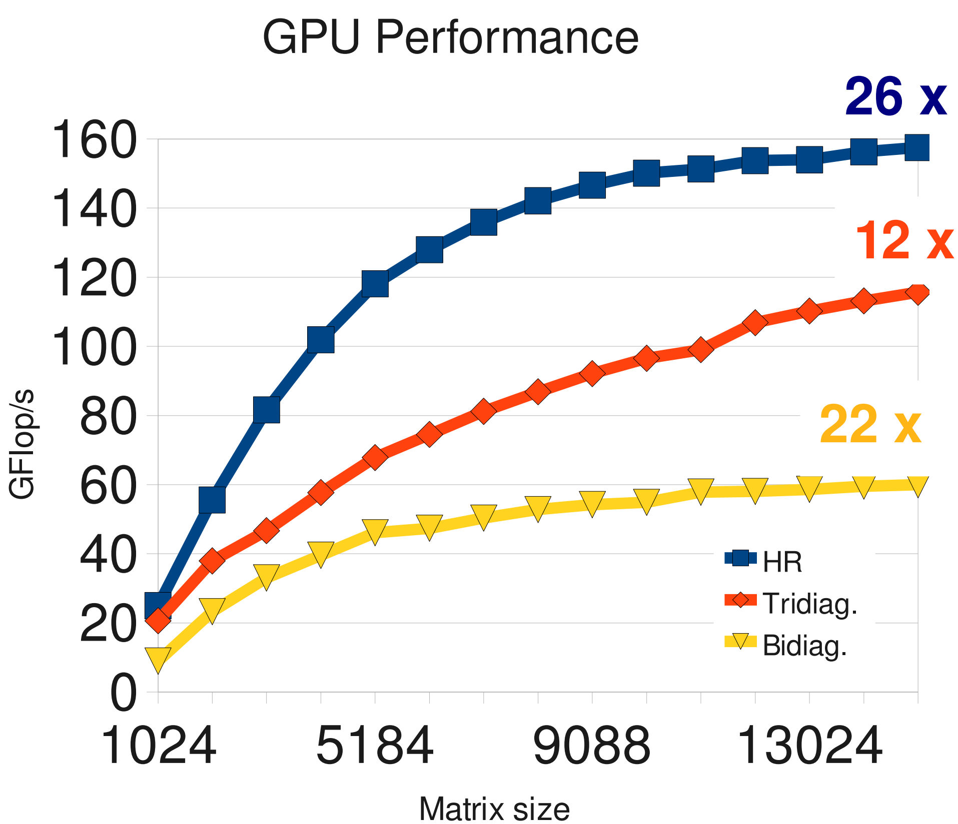
GPU : NVIDIA GeForce GTX 280 (240 cores @ 1.30GHz)
CPU : Intel Xeon dual socket quad-core (8 cores @2.33 GHz)

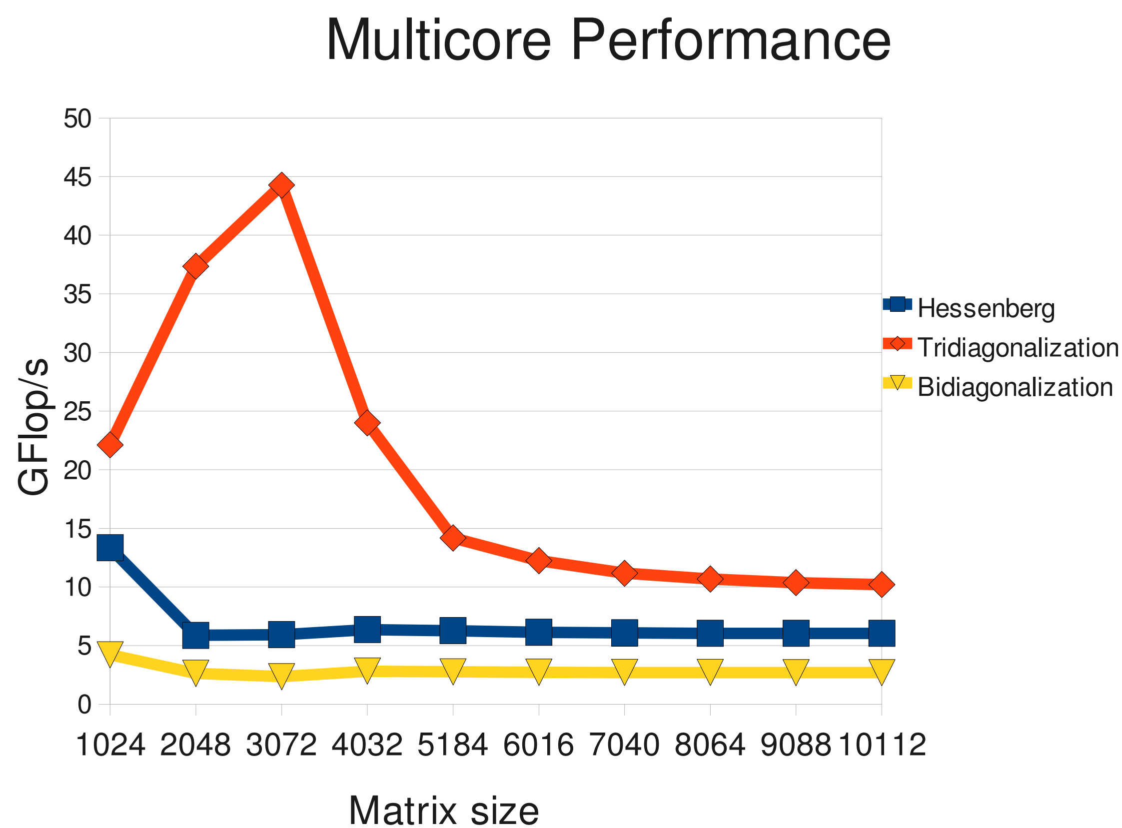
GPU BLAS : CUBLAS 2.3, dgemm peak: 75 GFlop/s
CPU BLAS : MKL 10.0 , dgemm peak: 65 GFlop/s

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

Two-sided factorizations

(performance in single precision arithmetic)





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

Conclusions

- **Linear algebra can be significantly accelerated using GPUs**
- **Described a hybridization methodology to achieve this acceleration**
  - **high level model**
  - **Leverage prior developments**
- **Hybridization can be used for a wide set of fundamental linear algebra algorithms**
  - **Linear and eigen/singular-value solvers**
  - **Incorporated in the MAGMA library http://icl.cs.utk.edu/magma/**