Future Computer Needs in the Dense Linear Algebra Domain

Enrique S. Quintana-Ortí

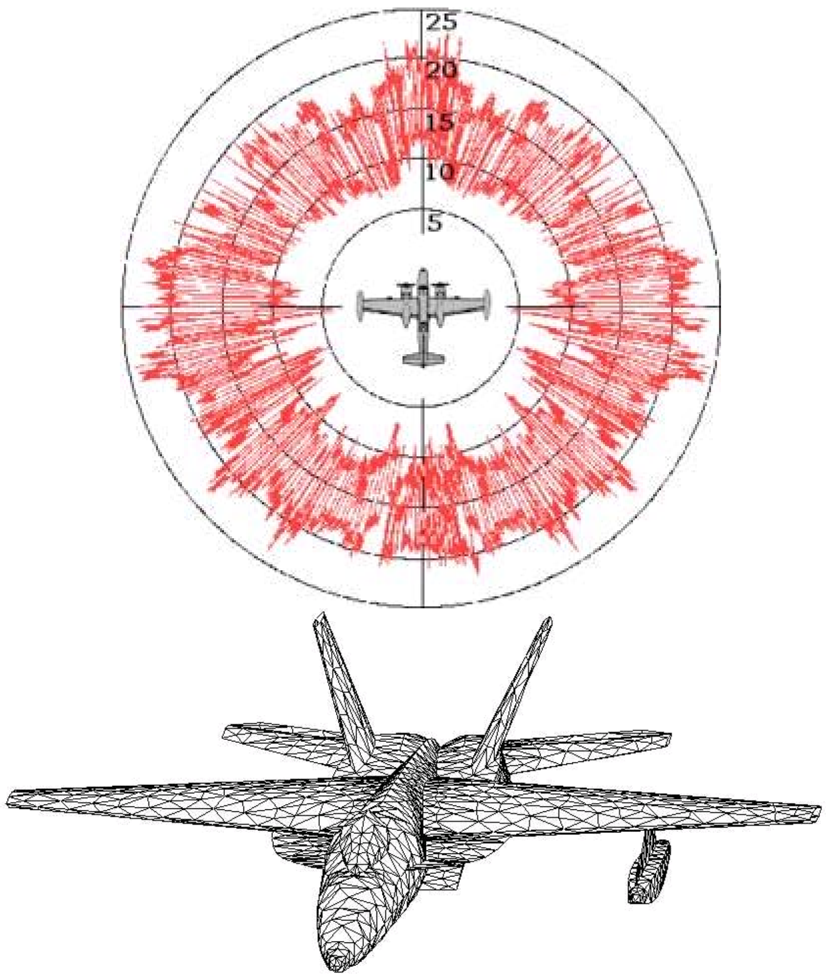
Universitat Jaume I

HPC&A

High Performance Computing and Architectures

Large-scale linear systems: Electromagnetism

- Radar cross-section problem (via BEM)



- Solve $A\,x = b$

  dense $A \rightarrow n \times n$

  n = hundreds of thousands of boundary points (or panels)

Large-scale LLS: Estimation of Earth's gravity field

- GRACE project

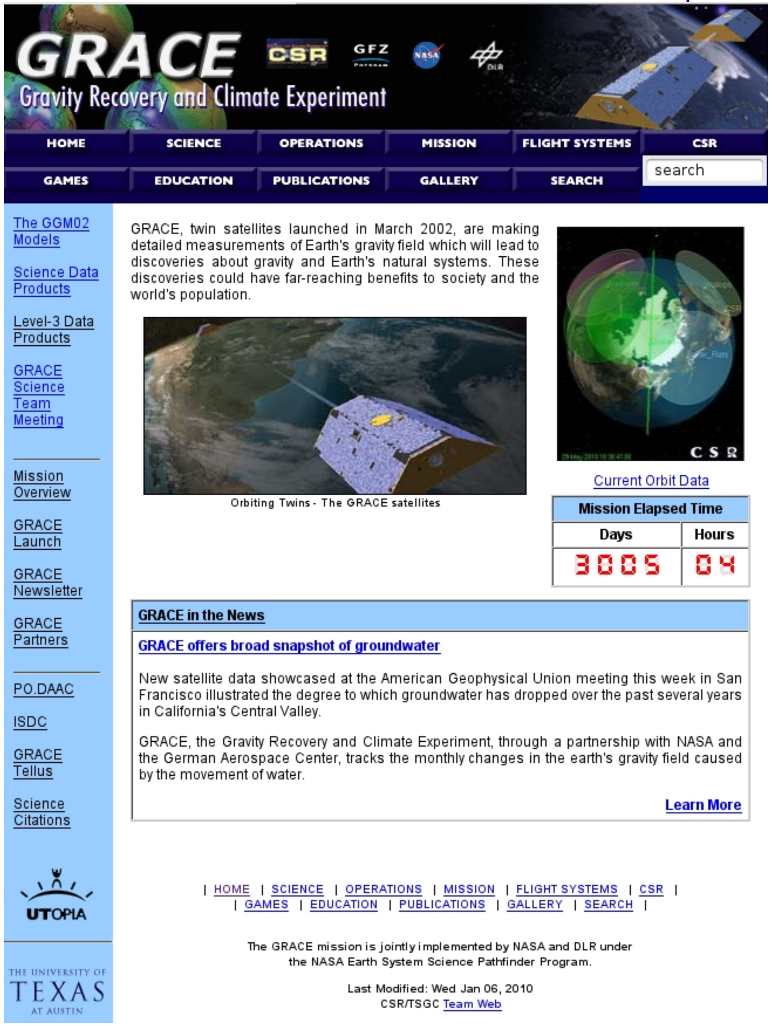
  www.csr.utexas.edu/grace

- Solve $y = H\, x_0 + \epsilon$,

  dense $H \rightarrow m \times n$

  m = 66.000 observations

  n = 26.000 parameters for a model of resolution 250km



Large-scale eigenvalue problems: Industrial processes

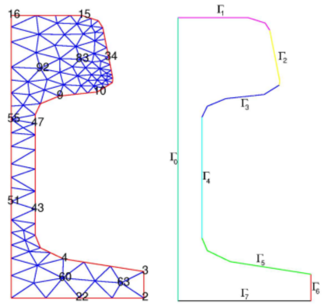
- Optimal cooling of steel profiles

- Solve

$$A^T X + X A - X S X + Q = 0,$$

dense $A \rightarrow n \times n$

$n = 5.177$ for a mesh width of $6.91 \cdot 10^{-3}$



Other applications

- Dense linear algebra is at the bottom of the “food chain” for many scientific and engineering apps.

- Molecular dynamics simulations
- Fast acoustic scattering problems
- Dielectric polarization of nanostructures
- Magneto-hydrodynamics
- Macro-economics

Challenges for dense linear algebra

- Future exascale platforms
  - Performance scalability
  - Architecture heterogeneity
  - Power consumption

- Impact on methods and libraries for dense linear algebra operations…

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Performance scalability

PFLOPS (10^{15} flops/sec.)

2010 JUGENE

- 10^9 core level

(3.4 GFLOPS)

- 10^1 node level

(Quad-Core)

- 10^5 cluster level

(73.728 nodes)

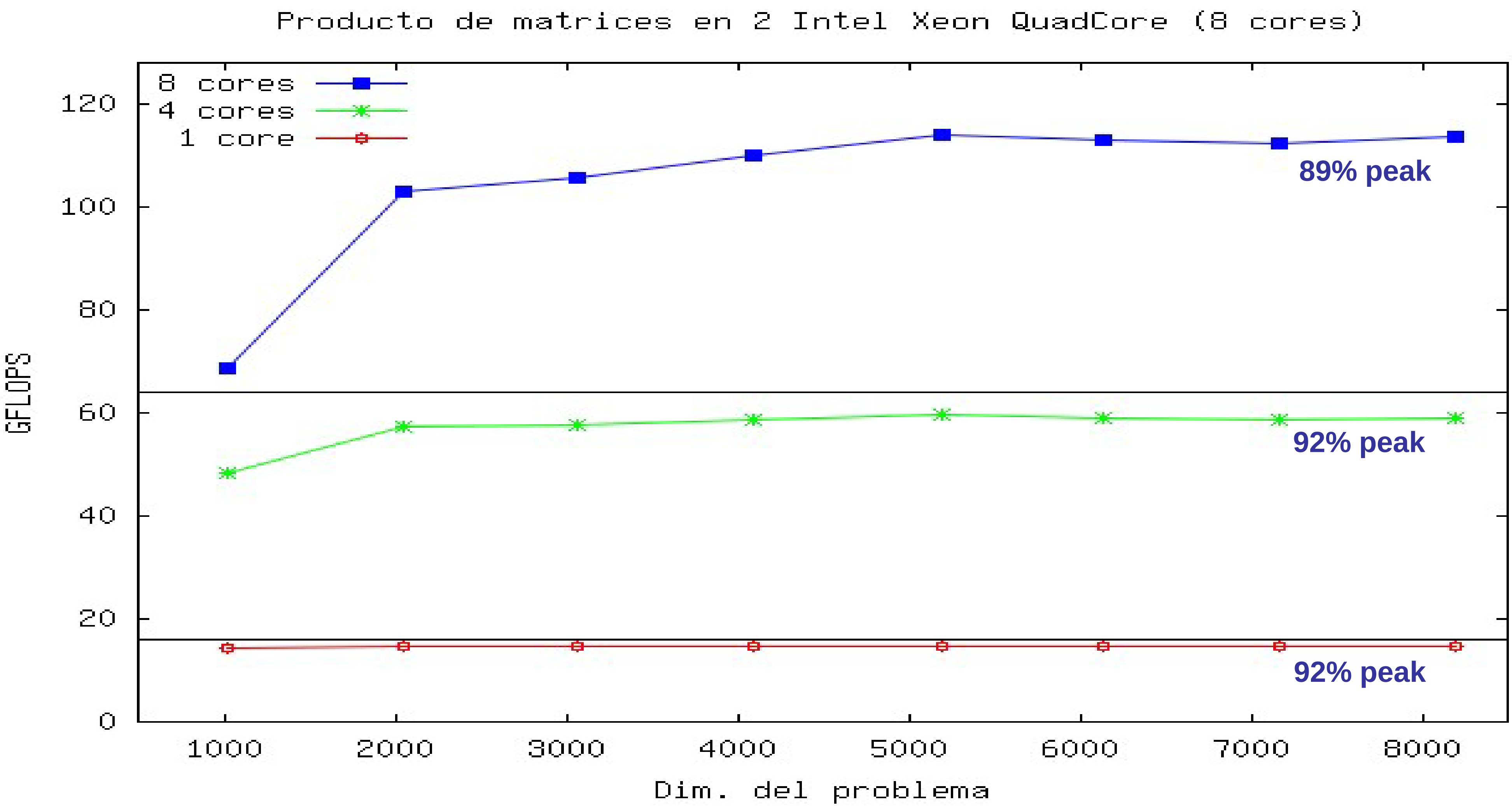
EFLOPS (10^{18} flops/sec.)

- $10^{9.5}$ core level
- 10^3 node level!
- $10^{5.5}$ cluster level

Performance scalability

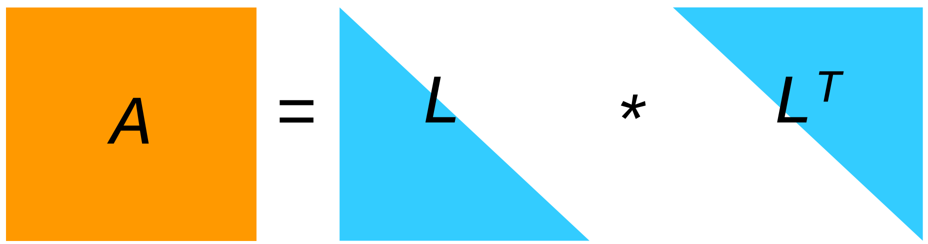
- Libraries for dense linear algebra:
  - BLAS
    - Multi-threaded (MT)
  - LAPACK
    - Use of MT BLAS: Excessive synchronization points
  - ScaLAPACK, PLAPACK:
    - 1 MPI process per core is not optimal: combine with MT-parallel approach

Performance scalability



Performance scalability
LAPACK

- Cholesky factorization



Key in the solution of s.p.d. linear systems

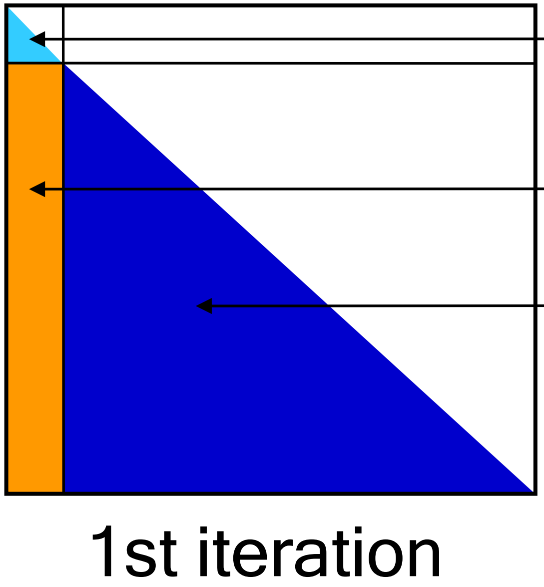
$$A\ x = b \equiv \quad (LL^T)x = b$$

$$L\ y = b \quad \Rightarrow \quad y$$

$$L^T x = y \quad \Rightarrow \quad x$$

Performance scalability LAPACK

- Cholesky factorization



F: $A_{11} = L_{11} * L_{11}^{T}$

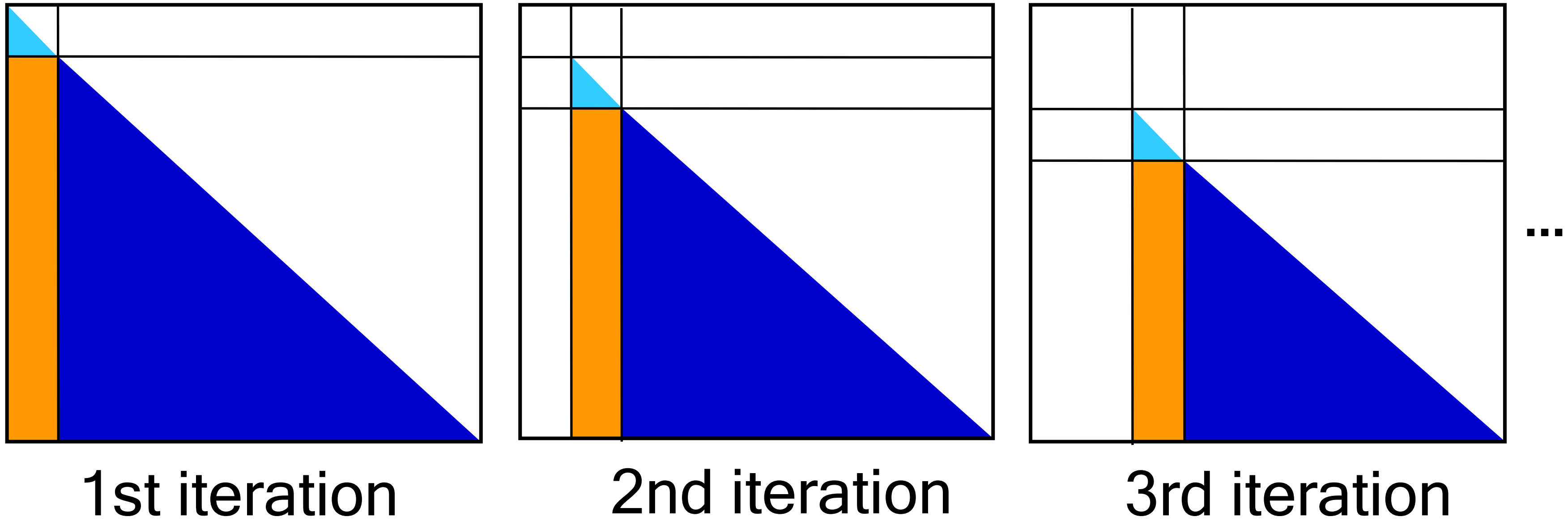
T: $L_{21} \leftarrow A_{21} * L_{11}^{-T}$

P: $A_{22} \leftarrow A_{22} - L_{21} * L_{21}^{T}$

MT processor: Employ a MT implementation of T and P

Performance scalability LAPACK

- Cholesky factorization



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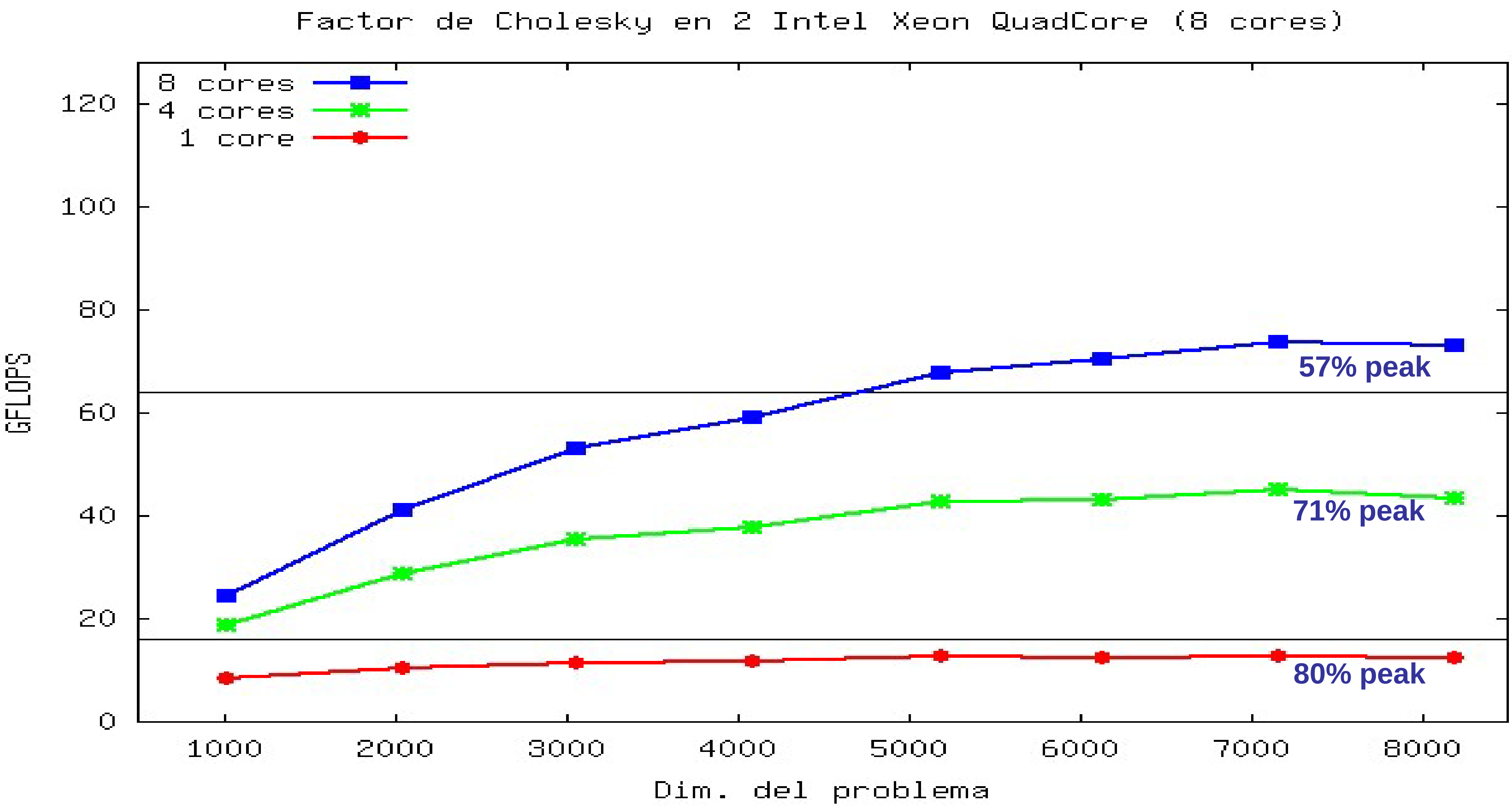
Performance scalability
LAPACK



Performance scalability
LAPACK

- Why?

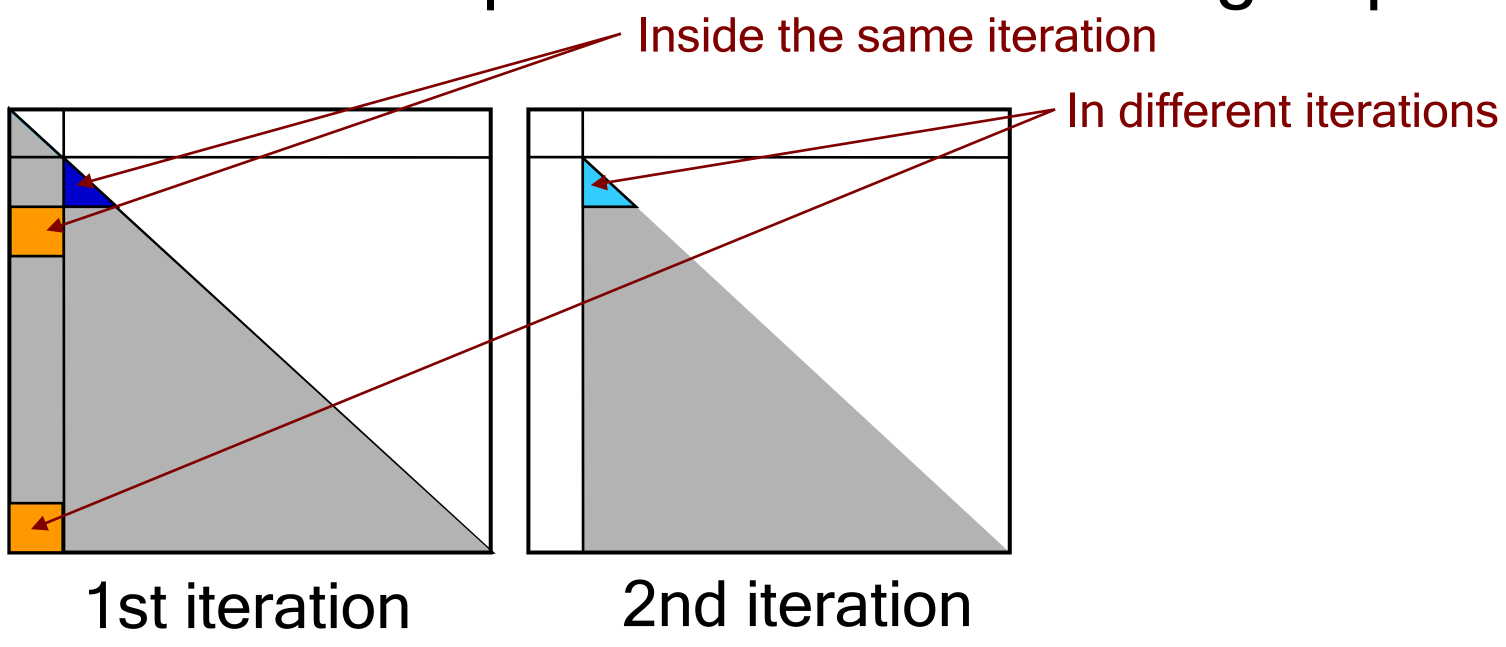
Excessive thread synchronization

```
for (k=0; k<nb; k++){
     Chol(A[k,k]);                  // A_kk     = L_kk * L_kk^T
  if (k<nb){
     Trsm(A[k,k], A[k+1,k]);        // L_k+1,k  = A_k+1,k * L_kk^-T
     Syrk(A[k+1,k], A[k+1,k+1]);    // A_k+1,k+1 = A_k+1,k+1
                                    //           - L_k+1,k * L_k+1,k^T
  }
}
```

Performance scalability LAPACK

- Why?

There is more parallelism than being exploited

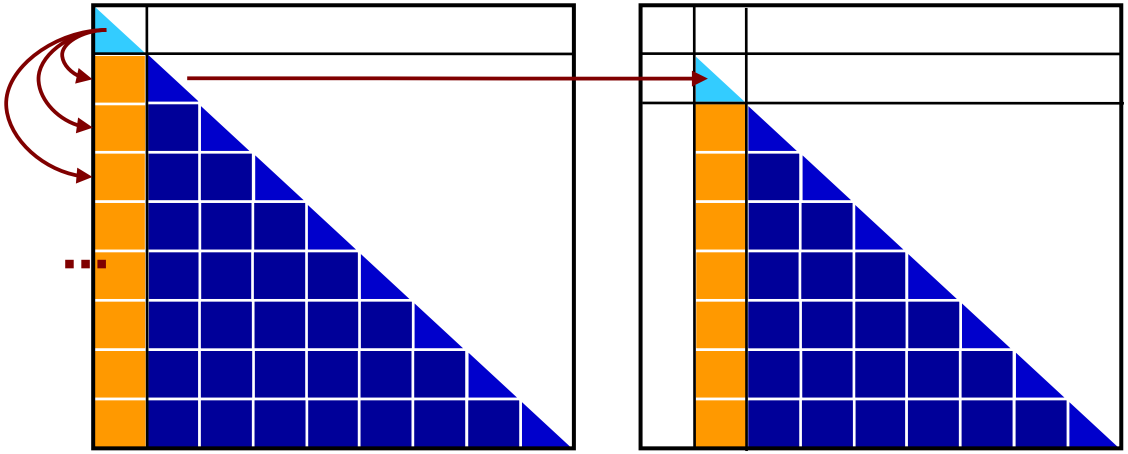


Performance scalability
LAPACK

- Exploit task-level parallelism dictated by data dep.

```
for (k=0; k<nb; k++){
      Chol(A[k,k]);
      for (i=k+1; i<nb; i++)
            Trsm(A[k,k], A[i,k]); …
```

Dependencies among tasks define a tree



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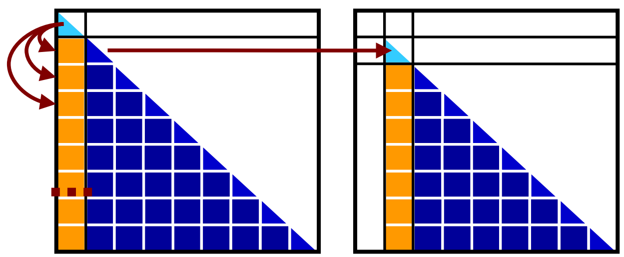
Performance scalability LAPACK

- Run-time:
  - Identifies/extracts TLP
  - Schedules tasks to execution
  - Maps tasks onto specific cores



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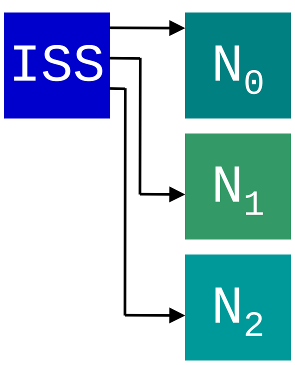
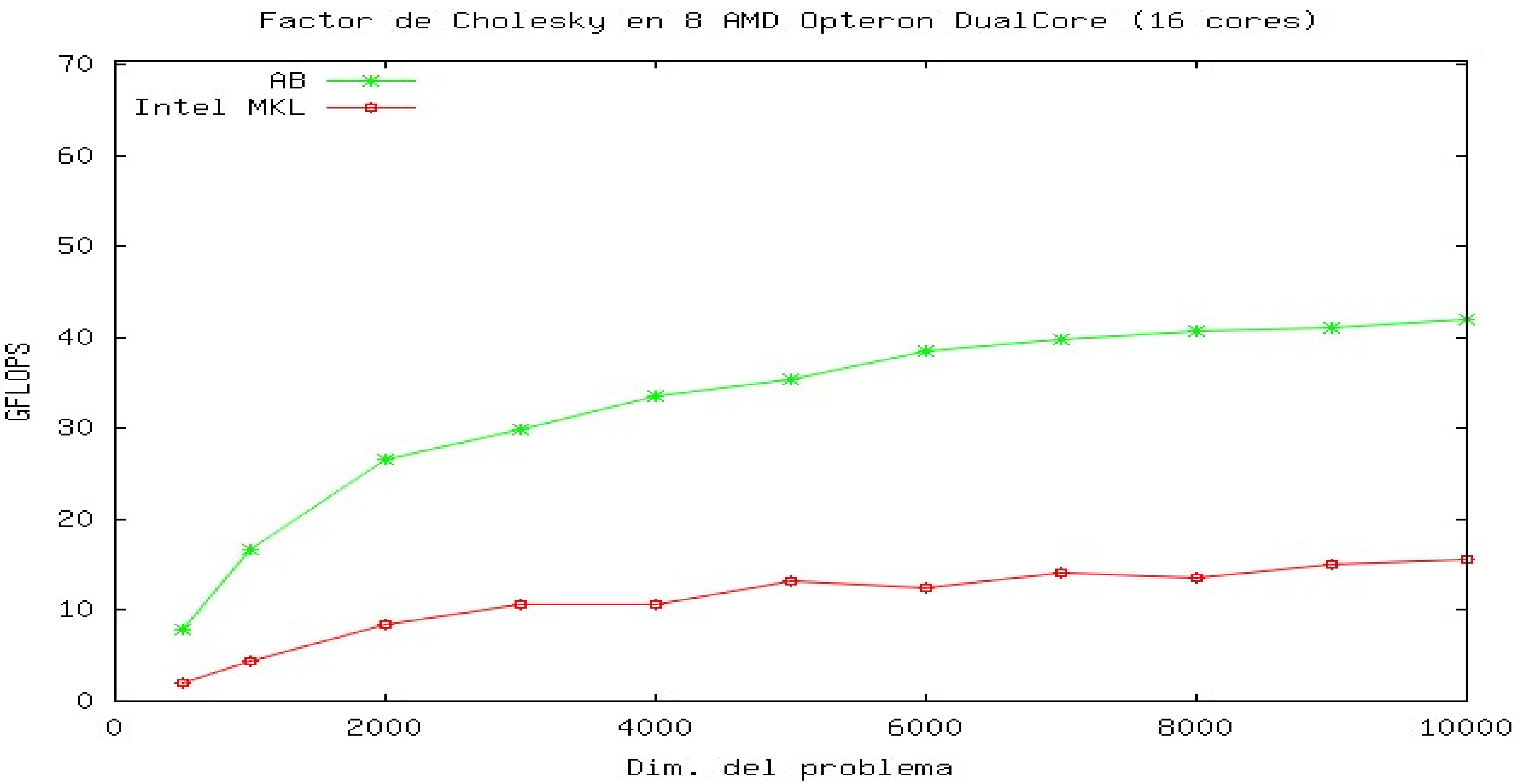


Performance scalability LAPACK



Challenges for dense linear algebra

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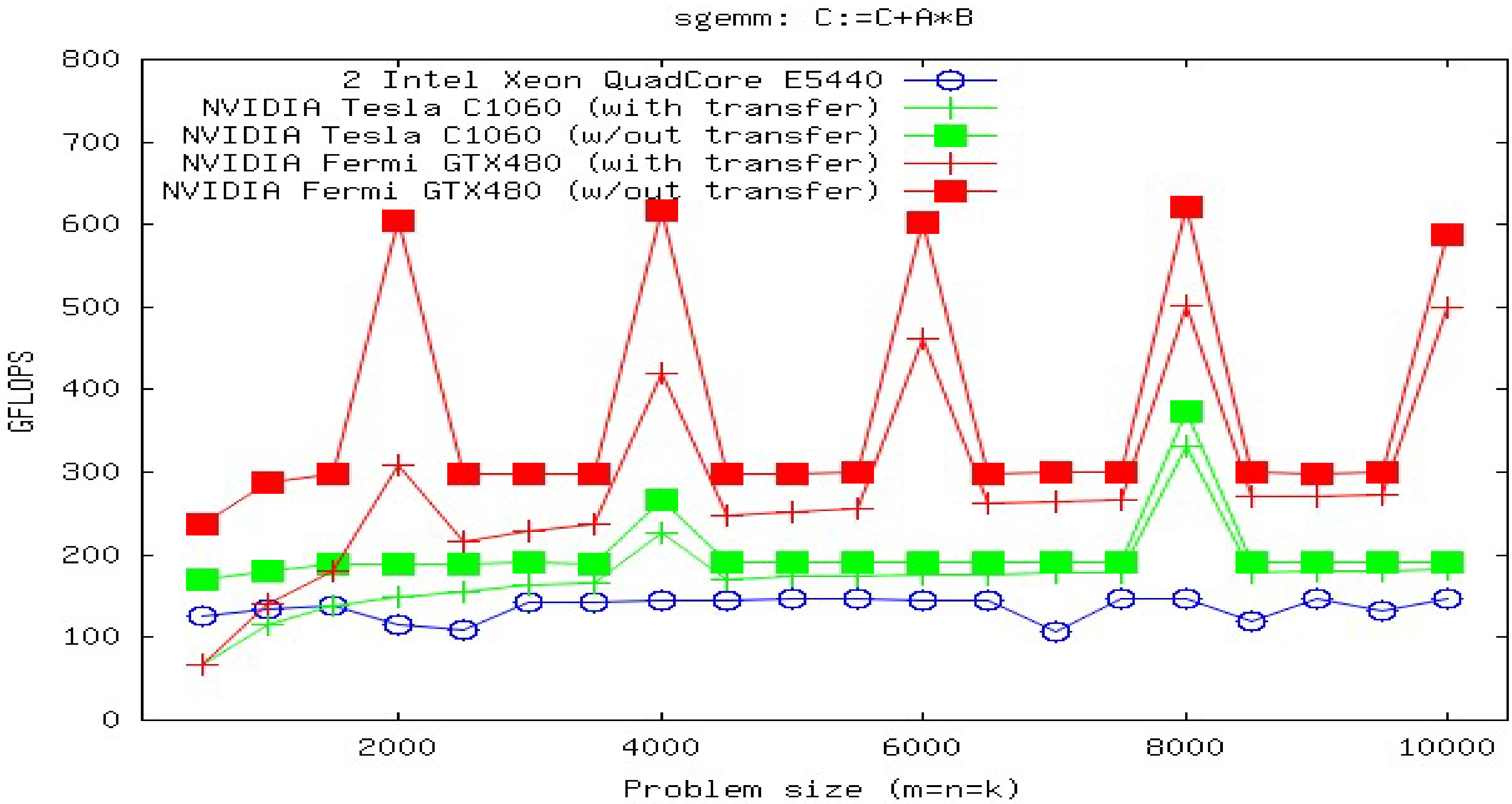
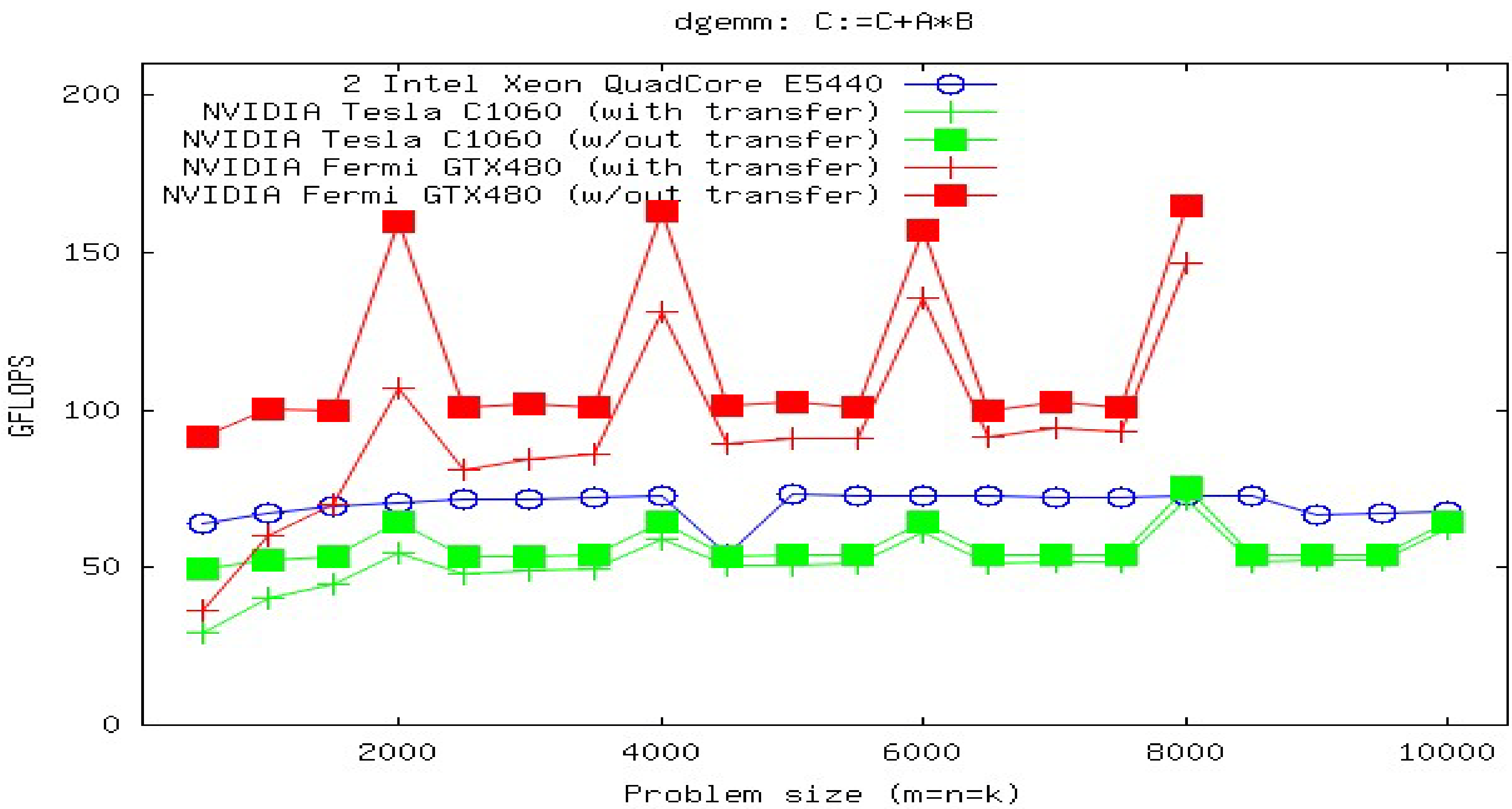
  - Architecture heterogeneity
  - Power consumption

- Impact on methods and libraries for dense linear algebra operations…

Architecture heterogeneity (CU)BLAS



Architecture heterogeneity (CU)BLAS



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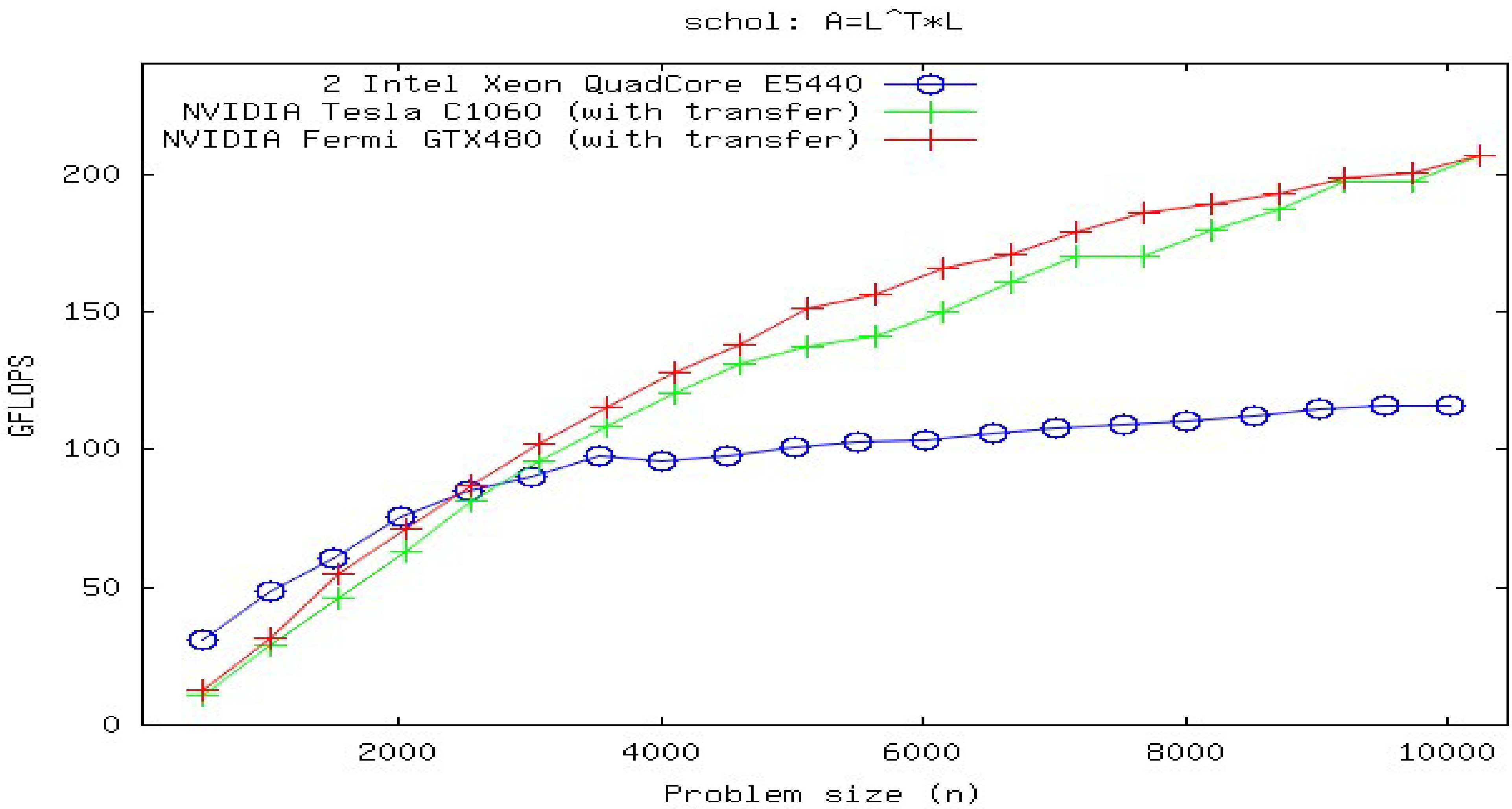
Architecture heterogeneity (CU)LAPACK



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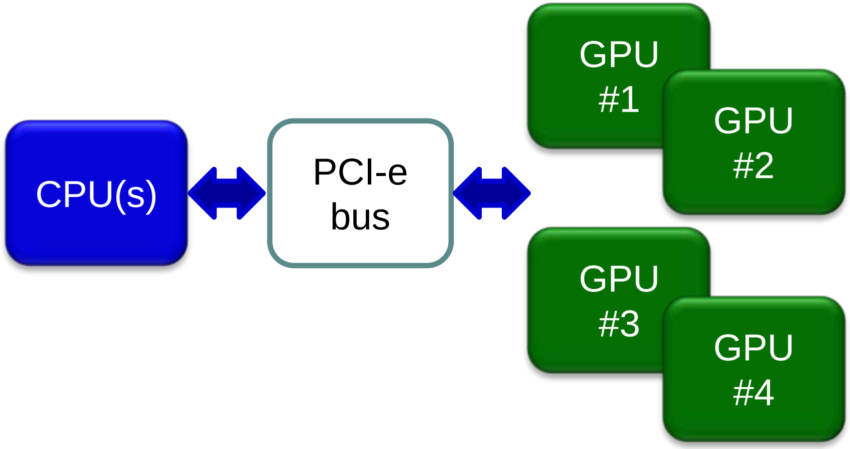
Architecture heterogeneity

- Libraries for dense linear algebra:
  - Multiple address spaces without hardware coherence (as difficult as message-passing)
  - Scheduling on heterogeneous resources (also much harder)
  - Possibly, more than one accelerator (per node)
  - Take advantage of single precision speed-up: iterative refinement

Architecture heterogeneity

- How do we program these?



View as a…

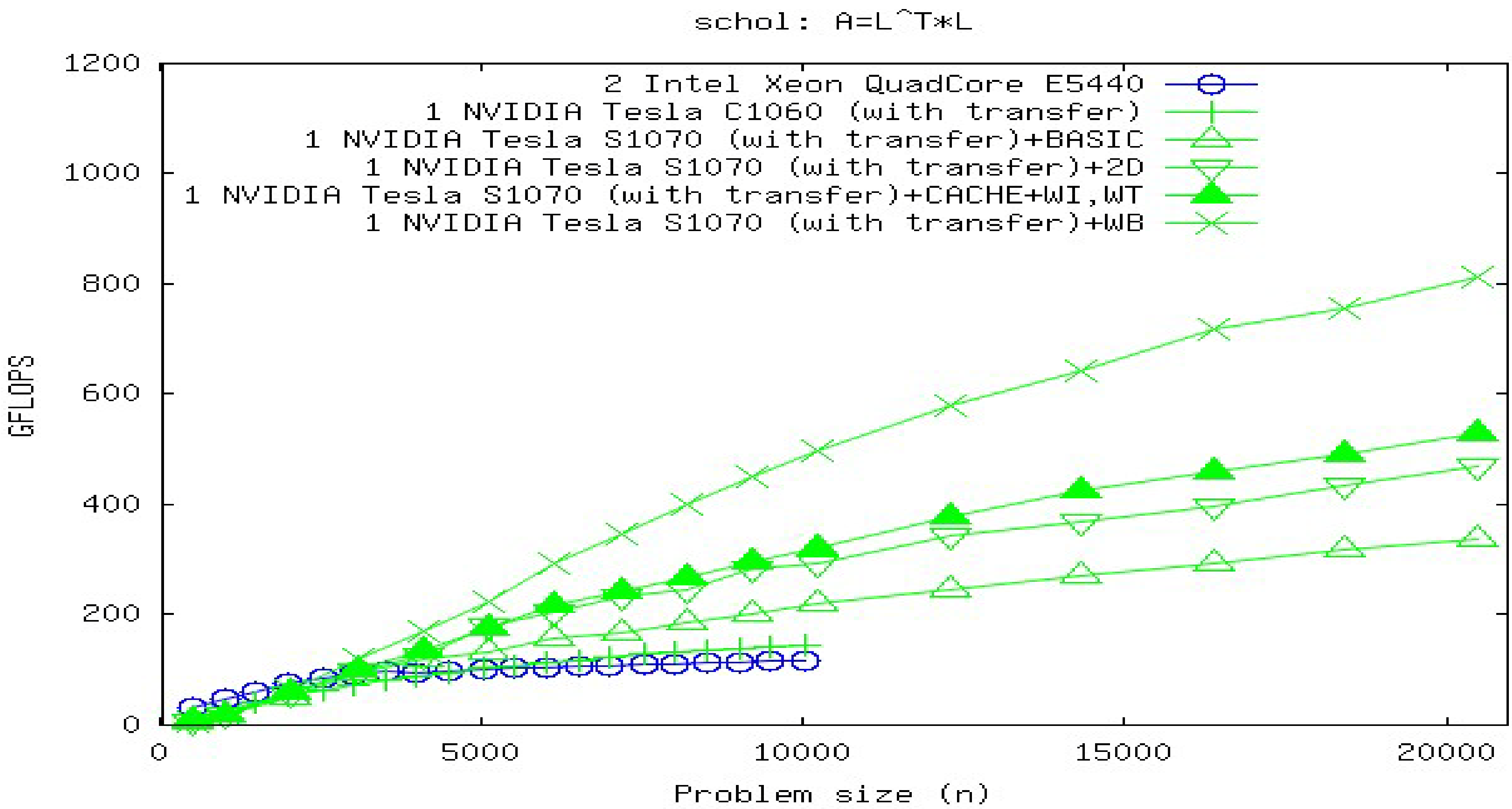
- Shared-memory multiprocessor + DSM

Architecture heterogeneity

- Software Distributed-Shared Memory (DSM)
  - Software: flexibility vs. efficiency
  - Underlying distributed memory hidden from the users
  - Reduce memory transfers using write-back, write-invalidate,…
  - Well-known approach, not too efficient as a middleware for general apps.

  - Regularity of dense linear algebra operations makes a difference!

Architecture heterogeneity
(CU)LAPACK for multi-GPU



Challenges for dense linear algebra

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Power consumption
Fuel efficiency

System	Top500	#cores	Rmax (TFLOPS)	Green500	Power (KW)	MFLOPS/ W	W to EFLOPS? (MW)
Jaguar	1	224,162	1,759.0	56	6,950.6	253.1	3,951
JUGENE	5	294,912	825.5	19	2,268.0	364.0	2,747
FZJ QPACE	131	4,608	44.5	1	253.1	773.0	1,293

Most powerful reactor under construction in France
Flamanville: 1,630 MWe

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Power consumption

- Future exascale platforms
  - Current approach of “few” (10.000-100.000) and “thick” nodes may not scale
  - “Many thin” nodes (MPI parallelism)?

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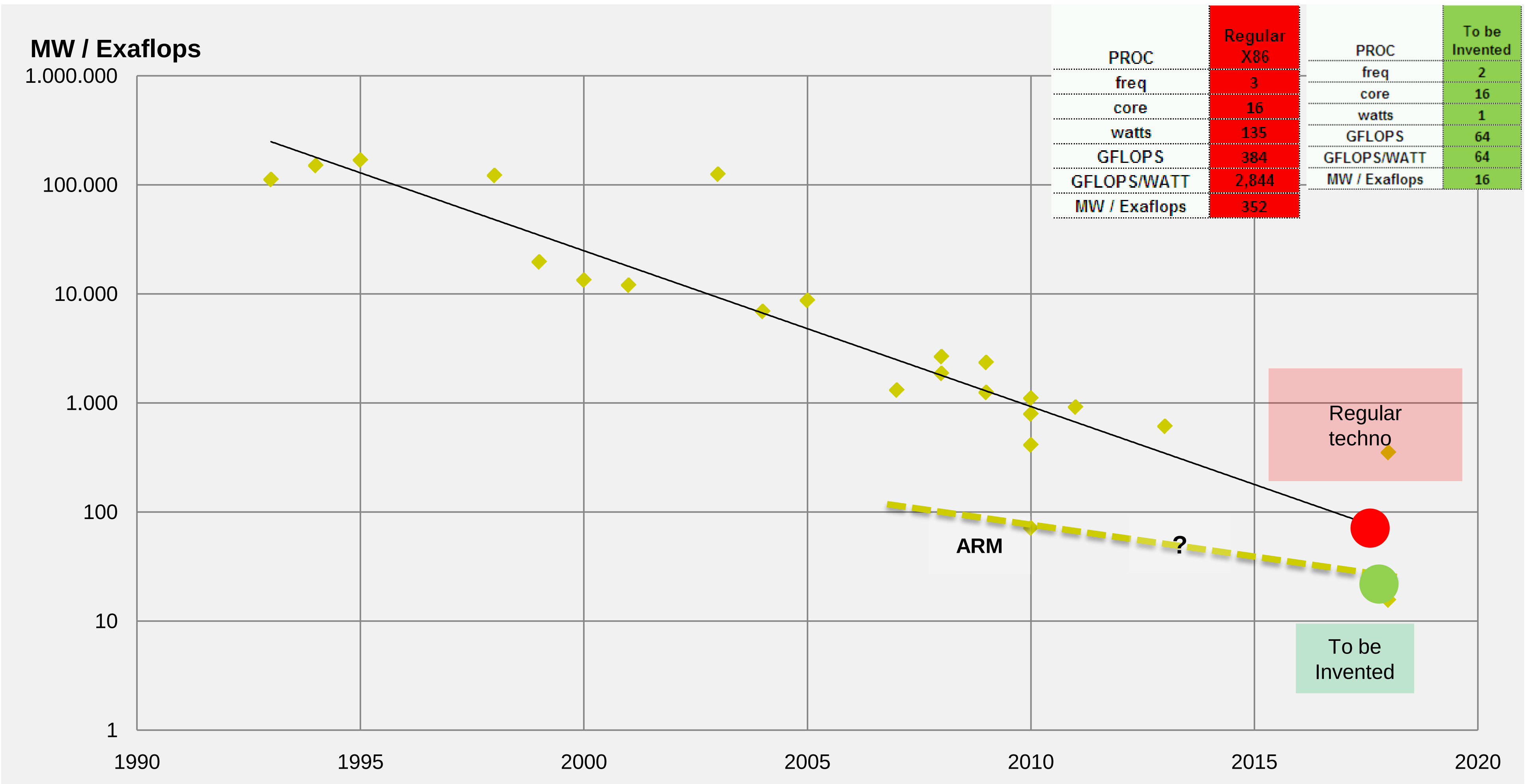
Power consumption



PROC	Regular X86
freq	3
core	16
watts	135
GFLOPS	384
GFLOPS/WATT	2,844
MW / Exaflops	352

PROC	To be Invented
freq	2
core	16
watts	1
GFLOPS	64
GFLOPS/WATT	64
MW / Exaflops	16

Power consumption
Dense linear algebra

- Need for energy-aware algorithms…

- Example*: solution of dense s.p.d. linear systems
  - Conjugate gradient (single precision) + iterative refinement
  - Cholesky factorization

*From “A new energy aware performance metric”; C. Bekas, A. Curioni; Comput. Sci. Res. Dev., 2010

Power consumption
Dense linear algebra

- Execution time in sec. (and percentage of peak performance) for a system with 32,768 unknowns on IBM BG/P, with 4 threads per node

Solver	32 nodes	64 nodes	128 nodes
CG	16.2 (4.6)	8.1 (4.5)	4.2 (4.1)
Cholesky	51.1 (48.0)	31.3 (43.0)	20.3 (33.1)

Power consumption
Dense linear algebra

- Power consumption in KJ for a system with 32,768 unknowns on 128 nodes of IBM BG/P, with 4 threads per node

Solver	Flops	Memory	Network	Total
CG	0.11	0.12	0.0	0.23
Cholesky	3.9	8.8	0.065	12.8

Challenges for dense linear algebra

- Future exascale platforms
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  - Architecture heterogeneity
  - Power consumption

- The “battle” will be played at the node level (TLP)
- Heterogeneity is great, but may greatly complicate programming
- Be power efficient or die…