NVISION 08

THE WORLD OF VISUAL COMPUTING

Automatic Development of Linear Algebra Libraries for the Tesla Series

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Dense Linear Algebra

Major problems:	Source of large-scale cases:
• Linear systems $Ax = b$	• Aeronautics: BEM
• Eigenvalues $Ax = \lambda x$	• Computational chemistry
• Singular values $A = U\Sigma V^T$	• Data mining

Dense Linear Algebra

Major problems:	Algorithms:
• Linear systems $$Ax = b$$	• One-sided factorizations: LU, Cholesky, QR
• Eigenvalues $$Ax = \lambda x$$	• Two-sided factorizations: QR alg., Jacobi
• Singular values $$A = U\Sigma V^T$$	• Two-sided factorizations: SVD

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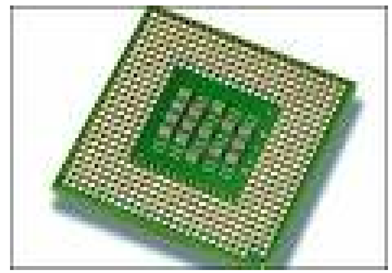
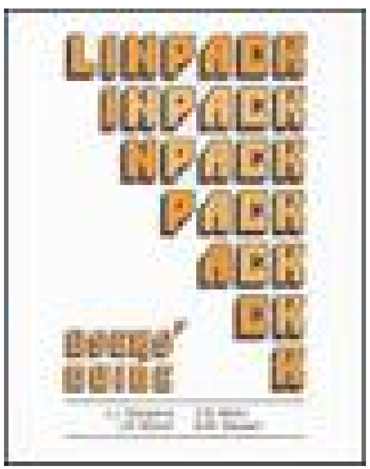
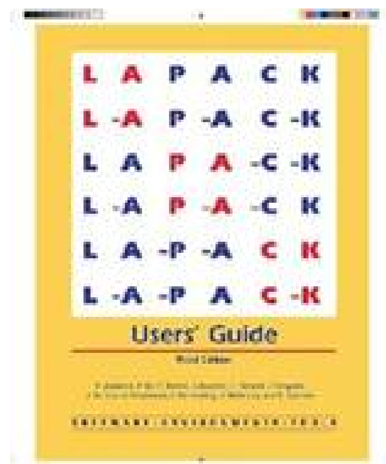
NVIDIA.

Dense Linear Algebra Libraries

Catching up with the current high-performance architecture...







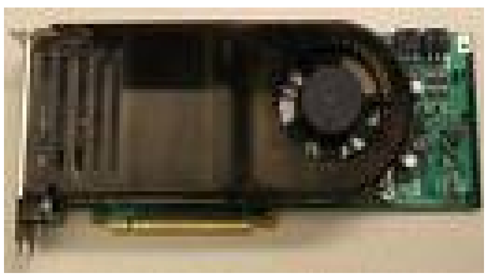
Vector instructions:
BLAS 1 and 2

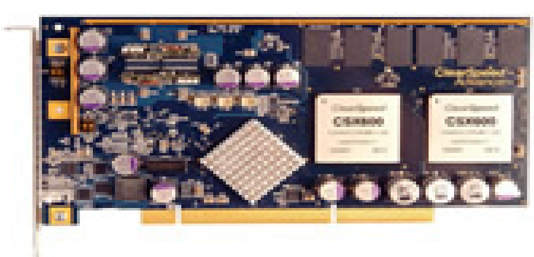
Cache memory:
BLAS 3

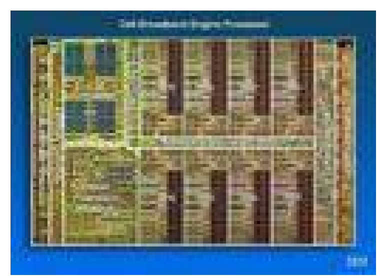
Distributed memory:
Message passing

Dense Linear Algebra Libraries

Catching up with the *current* high-performance architecture...







Dense Linear Algebra Libraries

Programmability is the key!

Application Programming Interfaces (APIs): Not that much of an evolution ;-(

- LAPACK and ScaLAPACK are written in F77 with C wrappers
- PLAPACK is C OO-like
- FLAME is more advanced...

Functionality:

- Libraries frequently updated with faster and/or more reliable algorithms developed by experts

Dense Linear Algebra Libraries

What if one had to design the *final* dense linear algebra library?

Compatible with unknown future…

New languages	Library independent from language
New functionality	Automatic development of new algorithms
New architectures	Library independent from architecture

Dense Linear Algebra Libraries

FLAME (Formal Linear Algebra Methods Environment)

http://www.cs.utexas.edu/users/flame

The University of Texas at Austin

Universidad Jaime I at Castellon (Spain)

Support from:

- NSF
- NEC Solutions, Inc.
- National Instruments

Support from:

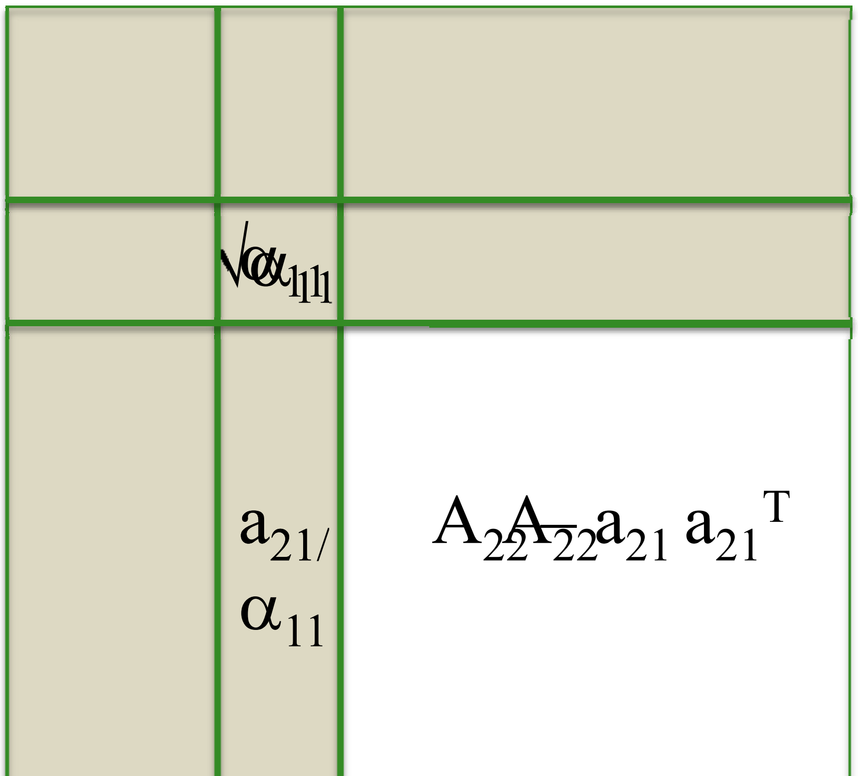
- Spanish Office of Science
- NVIDIA (2008 Professor Partner Grant)

Outline

- New languages:
  - object-oriented approach
  - XML code
  - Storage and algorithm are independent
- New functionality:
  - automatic development of (dense) linear algebra algorithms
- New architectures
  - NVIDIA G80
  - NVIDIA Tesla series

New Languages

FLAME notation: $A = LL^T$



Algorithm: $A := \text{CHOL\_L\_UNB\_VAR3}(A)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right)$

where A_{TL} is 0×0

while $m(A_{TL}) < m(A)$ **do**

Repartition

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array}\right)$$

where α_{11} is 1×1

$\alpha_{11} := \sqrt{\alpha_{11}}$
$a_{21} := a_{21}/\alpha_{11}$
$A_{22} := A_{22} - \text{TRIL}\left(a_{21}a_{21}^T\right)$

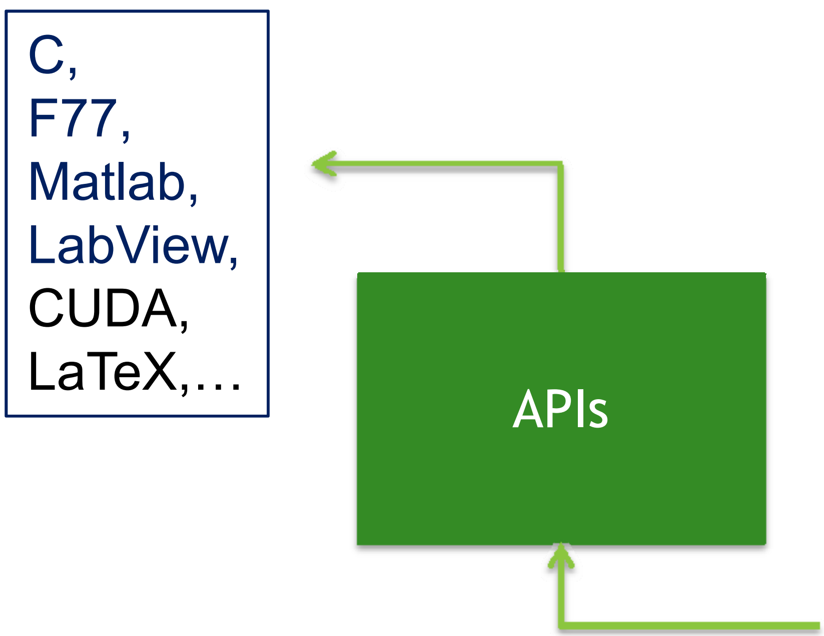
Continue with

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array}\right)$$

endwhile

New Languages

FLAME notation: $A = LL^T$



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  Continue with

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array}\right)$$

endwhile

Object-oriented, independence of language/ storage and algorithm

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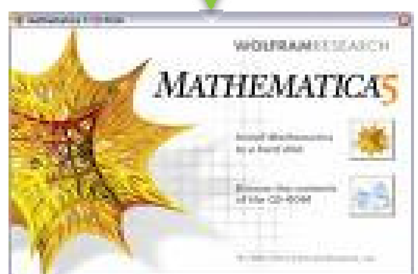
New Functionality

Automatic development from math. specification

$$A = LL^T$$

Mechanical procedure



Algorithm: $A := \text{CHOL\_L\_UNB\_VAR3}(A)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right)$

where A_{TL} is 0×0

while $m(A_{TL}) < m(A)$ **do**

Repartition

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array}\right)$$

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$a_{21} := a_{21} / \alpha_{11}$

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Continue with

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array}\right)$$

endwhile

New Architectures: NVIDIA G80

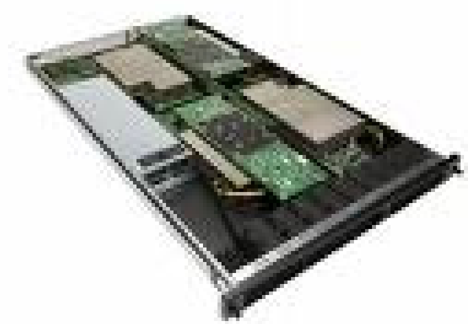
Algorithms:

- BLAS:
  MM, MV, TRSM
- One-sided factorizations:
  LU, Cholesky, QR
- Two-sided factorizations:
  QR alg., Jacobi, SVD

Some keys to high performance:

- CUBLAS
- Algorithms rich in matrix-matrix product
- Fast data transfer between RAM and GPU memory
- Reduce #data transfers
- Overlap communication and computation

Experimental Setup



- Two Intel QuadCore E5405 processors (8 cores) @ 2.0 GHz
- 8 Gbytes of DDR2 RAM
- Intel MKL 10.0.1

- NVIDIA Tesla S870 (4 NVIDIA G80 GPUs)
- 1.5 Gbytes of RAM per GPU (distributed-memory)
- CUBLAS 2.0

Two PCI-Express Gen2 interfaces (48 Gbits/sec.)
All experiments with real, single-precision
Performance measured in GFLOPS (10^9 flops/sec.)
Data and results in CPU RAM: transfer included in timings

Matrix-Matrix Product: $C = C + A \cdot B$

BLAS (Fortran-77):

```
CALL SGEMM( 'N', 'N',
            m, n, k,
            1.0, A, LDA,
                 B, LDB,
            1.0, C, LDC )
```

CUBLAS (C):

```
cublasSgemm( 'N',  'N',
             m, n, k,
             1.0, dA, LDA,
                  dB, LDB,
             1.0, dC, LDC );
```

Computation in GPU requires:

- Initialization of CUDA environment
- Allocation of data structures in GPU memory (handlers dA, dB, dC)
- Transfer of data (matrices A, B, C)
- Computation (cublasSgemm)
- Retrieve result (matrix C)
- Free data structures in GPU memory
- Termination of CUDA environment

Matrix-Matrix Product: $C = C + A \cdot B$

CUBLAS (C):

```
cublasSgemm( 'N',  'N',
             m, n, k,
             1.0, dA, LDA,
                  dB, LDB,
             1.0, dC, LDC );
```

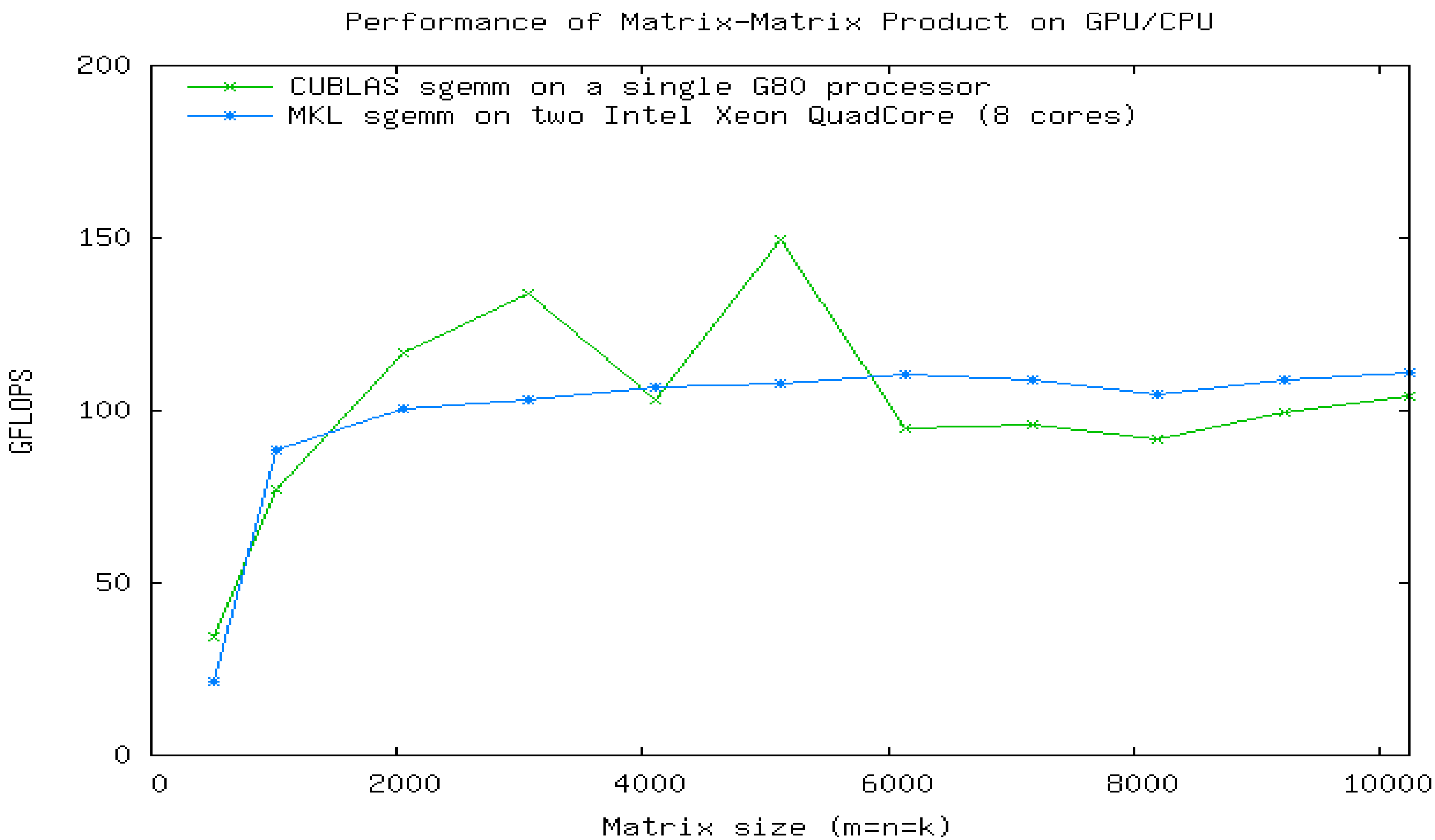
FLAME API to CUBLAS (C):

```
FLAG_Gemm( FLA_NO_TRANSPOSE,
           FLA_NO_TRANSPOSE,
           FLA_ONE, A,
                    B,
           FLA_ONE, C );
```

Computation with FLAME/GPU API:

- FLAG_Gemm is a wrapper to cublasSgemm
- Similar wrappers allow creation and free of data structures in the GPU, data transferences, etc.
- A, B, C are FLAME objects that contain information on the data type, dimension, and handler (dA, dB, dC)

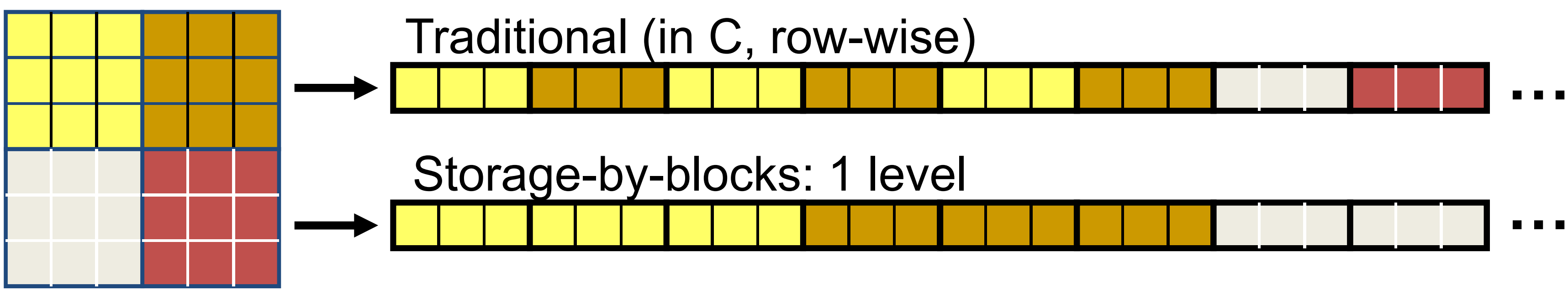
Matrix-Matrix Product: $C = C + A \cdot B$



- Timings of CUBLAS include data transfer (4 full matrices!)
- Observed peaks for 8 cores CPU/GPU are 110/160 GFLOPS
- Without data transfer CUBLAS delivers up to 200 GFLOPS

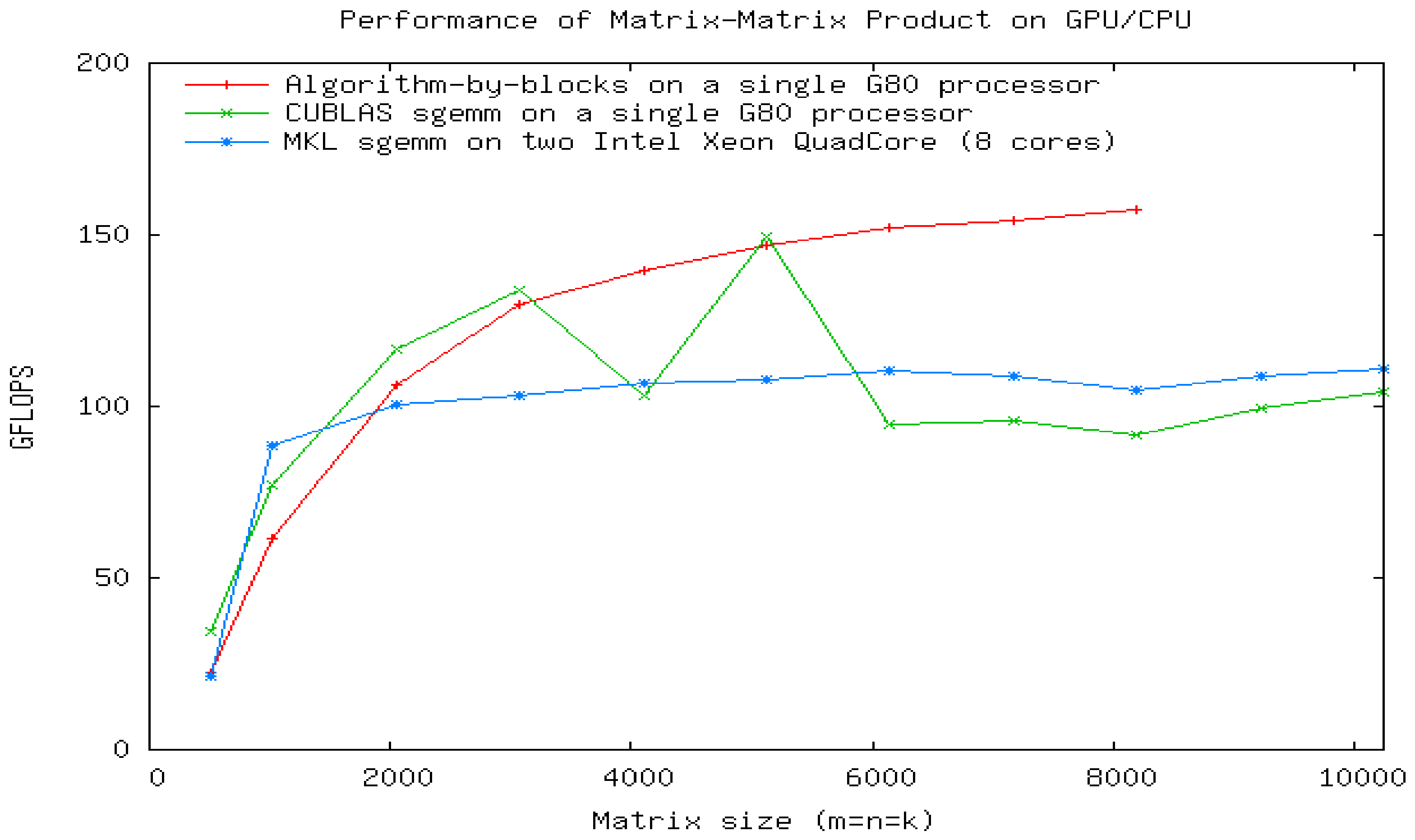
Matrix-Matrix Product: $C = C + A \cdot B$

- Impact of data transfer is important
  - Reduce by overlapping communication/computation (not possible on G80)
  - Store the matrices by blocks: contiguous access provides faster access to local data (in RAM and GPU memory) and also faster transfers

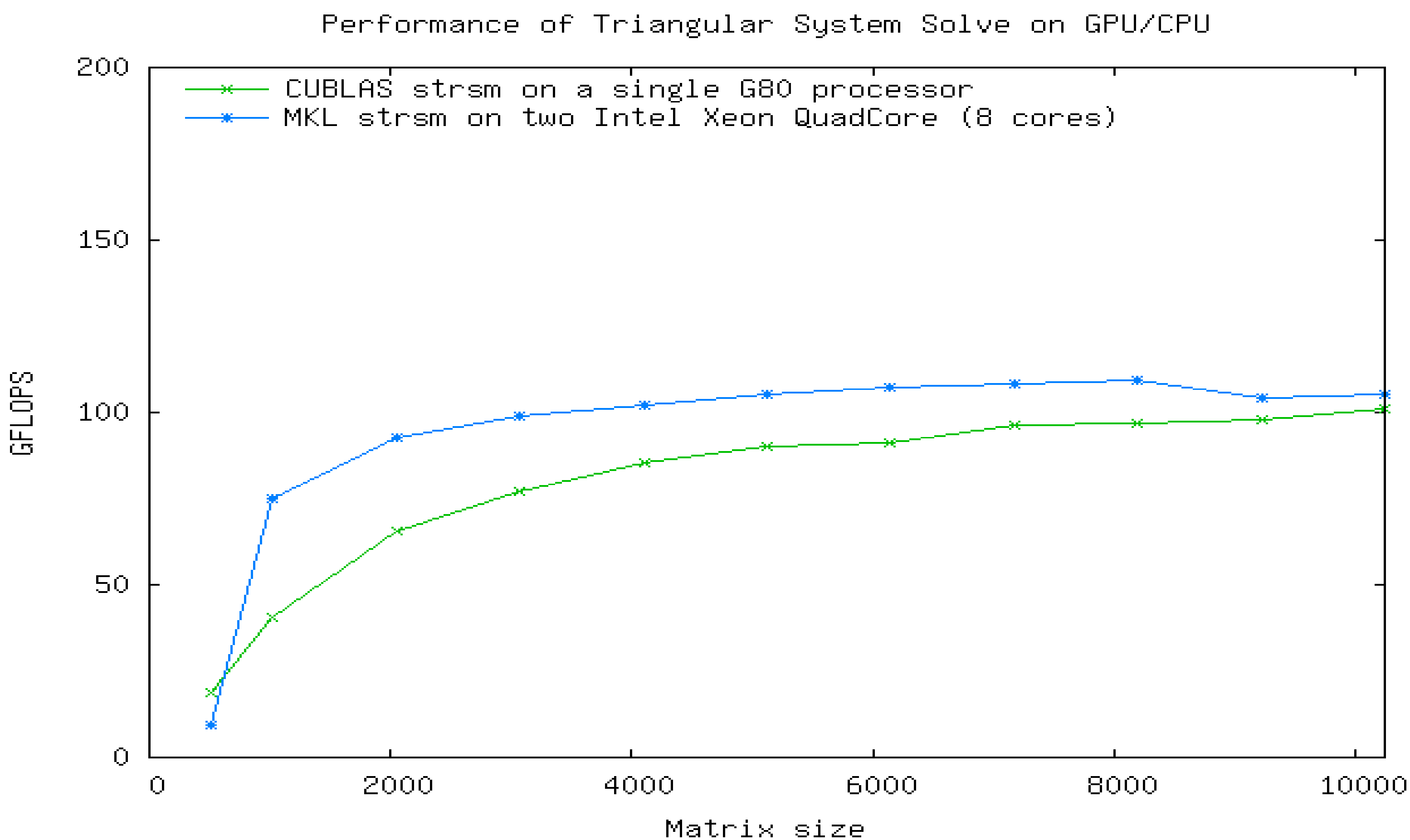


  - MKL internally employs a similar repacking

Matrix-Matrix Product: $C = C + A \cdot B$

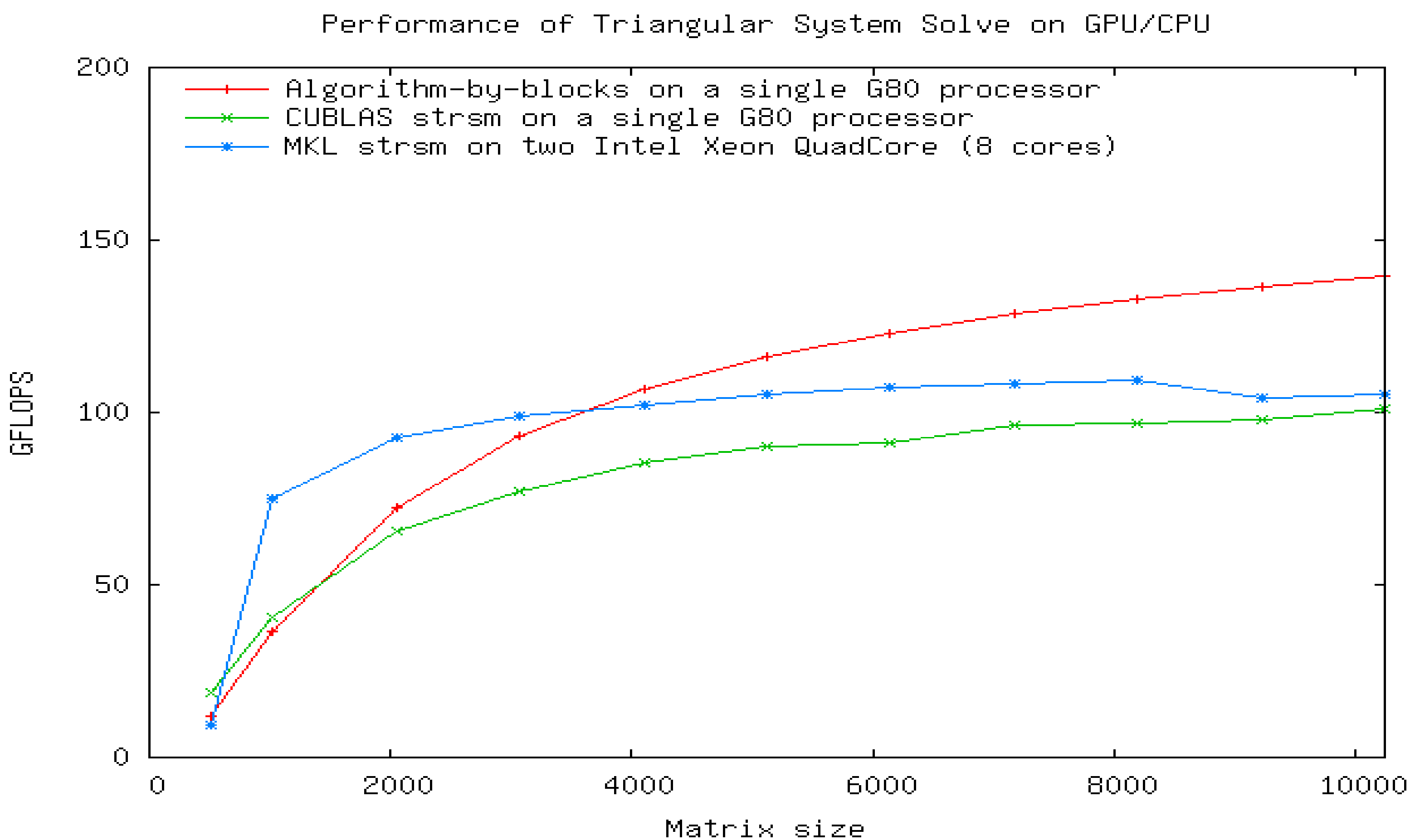


Triangular System Solve: A X = B



- Some kernels in CUBLAS can be further optimized
- Impact of data transfer is still important

Triangular System Solve: A X = B



- Observed peak performance for trsm is close to that of sgemm (160 GFLOPS)

Cholesky Factorization: $A = LL^T$

FLAME code for CPU:

```
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ) {
   ...
   /*-----------------------------------------------*/
   FLA_Chol_unb_var3(  A11 );
   FLA_Trsm(  FLA_RIGHT,     FLA_LOWER_TRIANGULAR,
              FLA_TRANSPOSE, FLA_NONUNIT_DIAG,
              FLA_ONE, A11, A21 );
   FLA_Syrk(  FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,
              FLA_MINUS_ONE, A21,
              FLA_ONE,       A22 );
   /*-----------------------------------------------*/
   ...  }
```

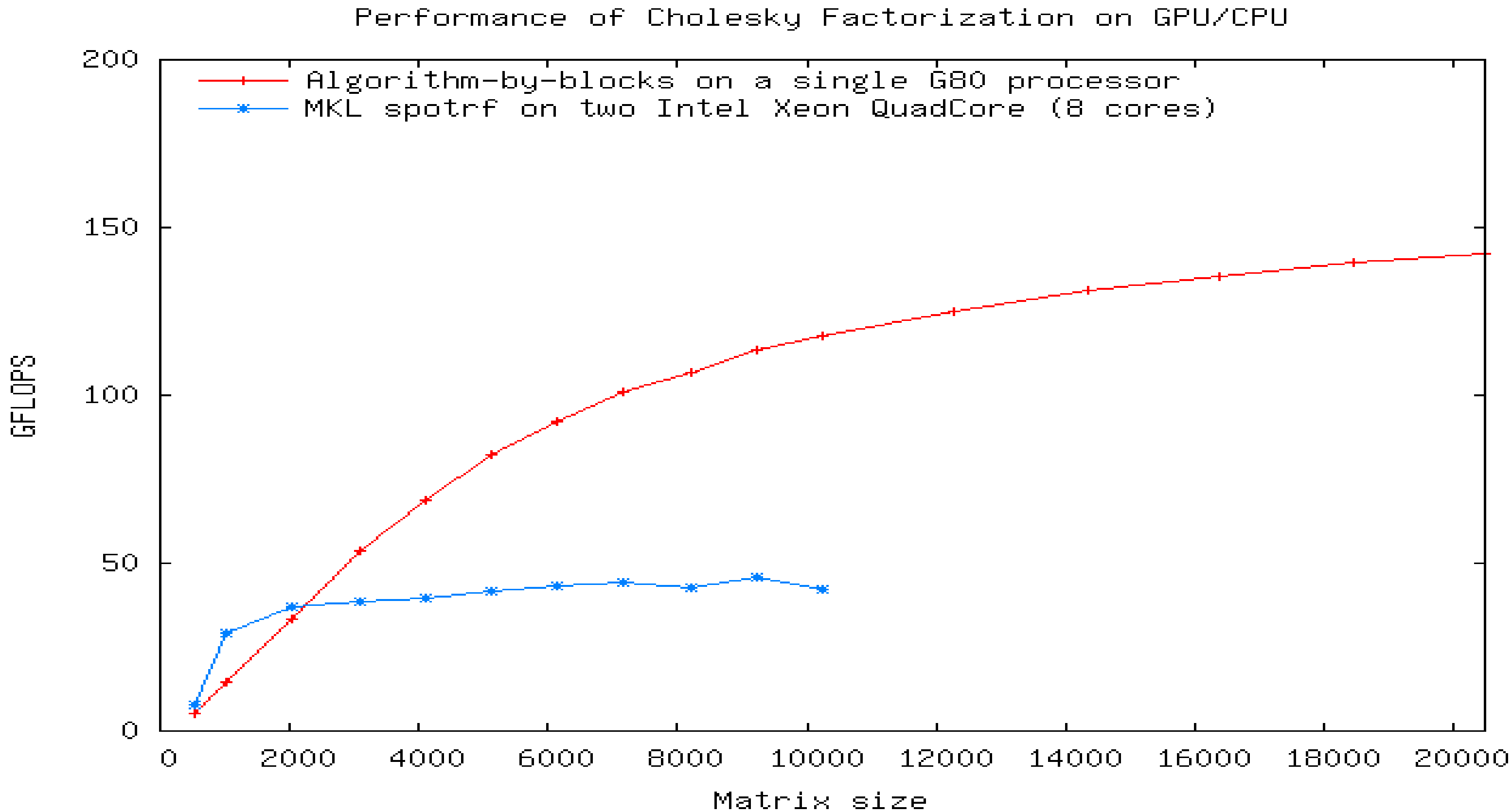
Cholesky Factorization: $A = LL^T$

FLAME code for GPU:

```
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ) {
   ...
   /*---------------------------------------------*/
   FLAG_Chol_unb_var3( A11 );
   FLAG_Trsm( FLA_RIGHT,     FLA_LOWER_TRIANGULAR,
              FLA_TRANSPOSE, FLA_NONUNIT_DIAG,
              FLA_ONE, A11, A21 );
   FLAG_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,
              FLA_MINUS_ONE, A21,
              FLA_ONE,       A22 );
   /*---------------------------------------------*/
   ...  }
```

Factorization of diagonal block on CPU!

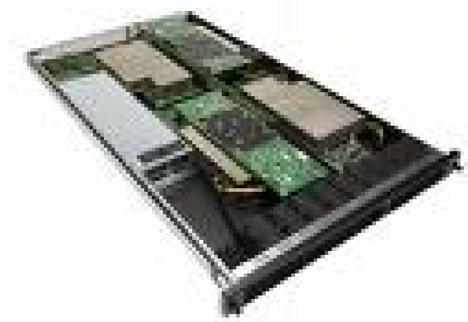
Cholesky Factorization: $A = LL^T$



- Observed peak performance for spotrf is close to that of sgemm (160 GFLOPS)

New Architectures: NVIDIA Tesla Series

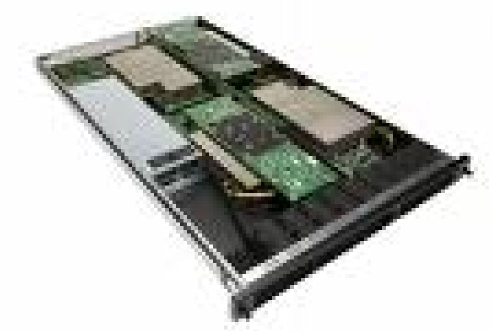
How do we deal with the multiple G80 processors in the Tesla?



- Akin distributed-memory:
  - GPU memory is distributed
  - No coherence mechanism
  - All transfer through CPU RAM
- Akin SMP:
  - GPU RAM is like cache of SMP processors
  - CPU RAM is like main memory in SMP

New Architectures: NVIDIA Tesla Series

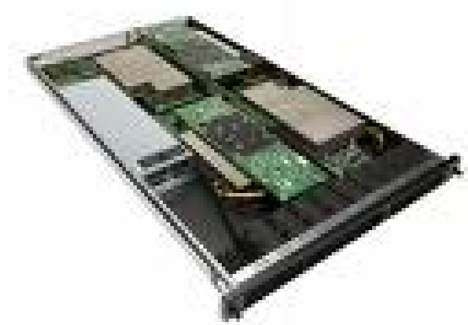
How do we deal with the multiple G80 processors in the Tesla?



- Possible solution:
  - Program as a cluster
  - Message-passing
  - Rewrite complete library: an effort similar to that of developing ScaLAPACK/PLAPACK

New Architectures: NVIDIA Tesla Series

How do we deal with the multiple G80 processors in the Tesla?



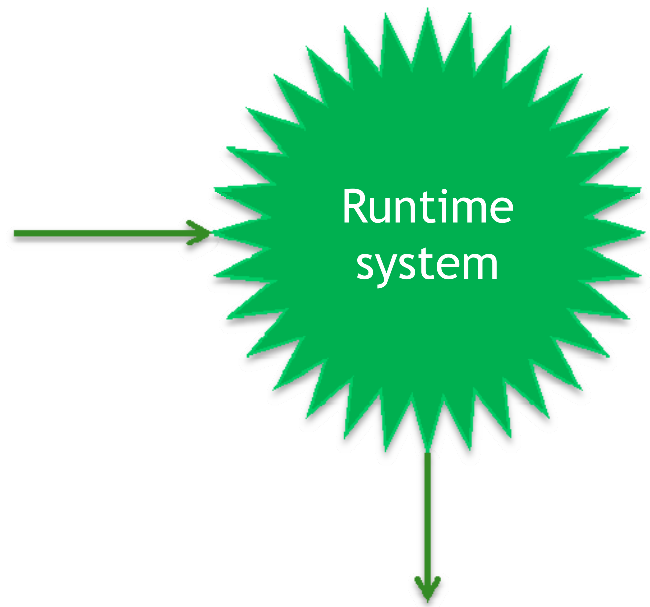
- FLAME solution:
  - Programmability is the key!
  - Algorithm (code) is independent from the architecture
  - Runtime system dynamically extracts the parallelism and handles data transfers

New Architectures: NVIDIA Tesla Series

First stage: symbolic execution of code by runtime

- Task decomposition
- Data depencencies identication

```
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ) {
    ...
    /*--------------------------------------------*/
    FLAG_Chol_unb_var3( A11 );
    FLAG_Trsm( FLA_RIGHT,     FLA_LOWER_TRIANGULAR,
               FLA_TRANSPOSE, FLA_NONUNIT_DIAG,
               FLA_ONE, A11, A21 );
    FLAG_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,
               FLA_MINUS_ONE, A21,
               FLA_ONE,       A22 );
    /*--------------------------------------------*/
    ...  }
```

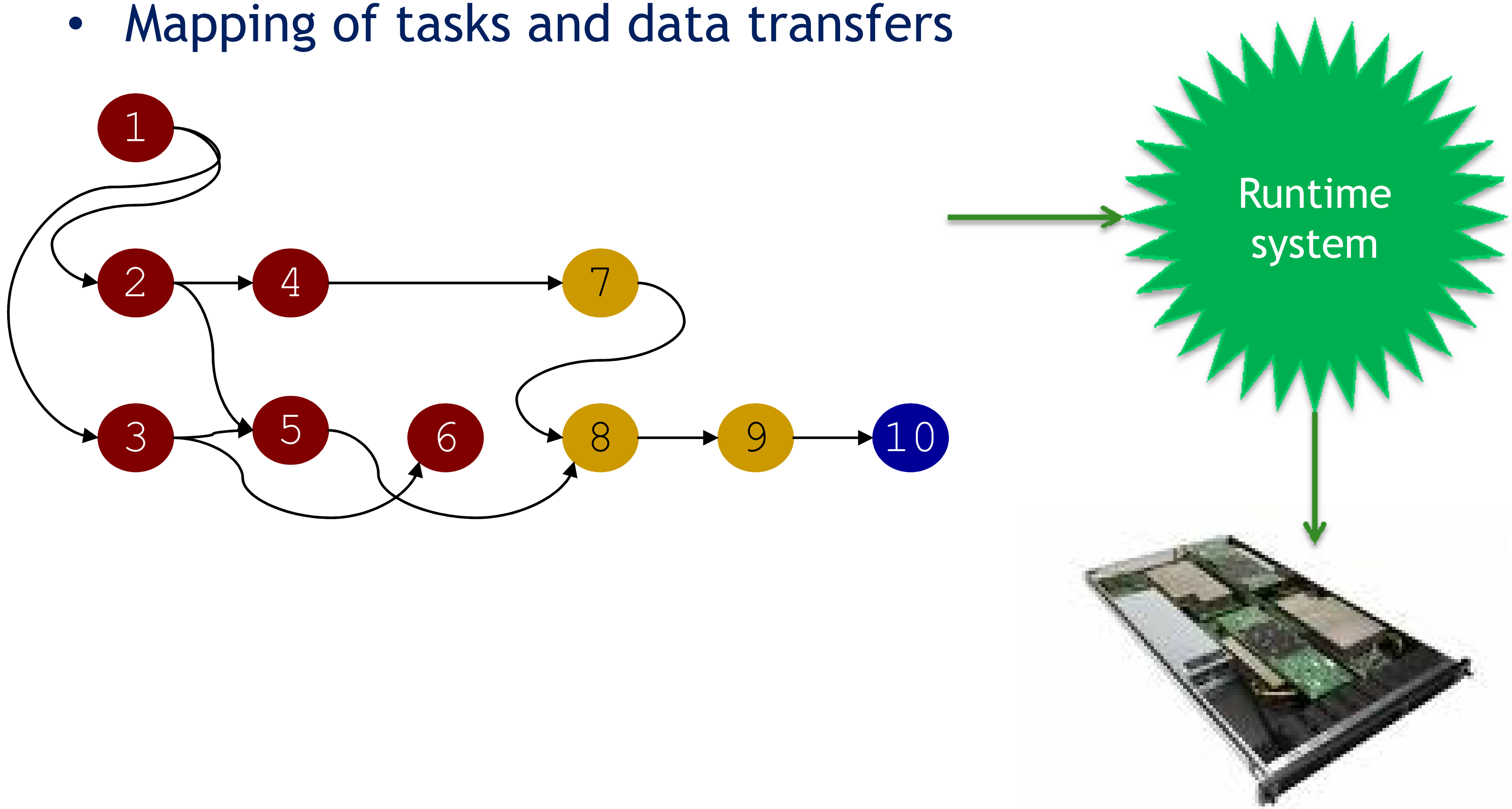


DAG of tasks

New Architectures: NVIDIA Tesla Series

Second stage: actual execution of code by runtime

- Scheduling of tasks
- Mapping of tasks and data transfers



New Architectures: NVIDIA Tesla Series

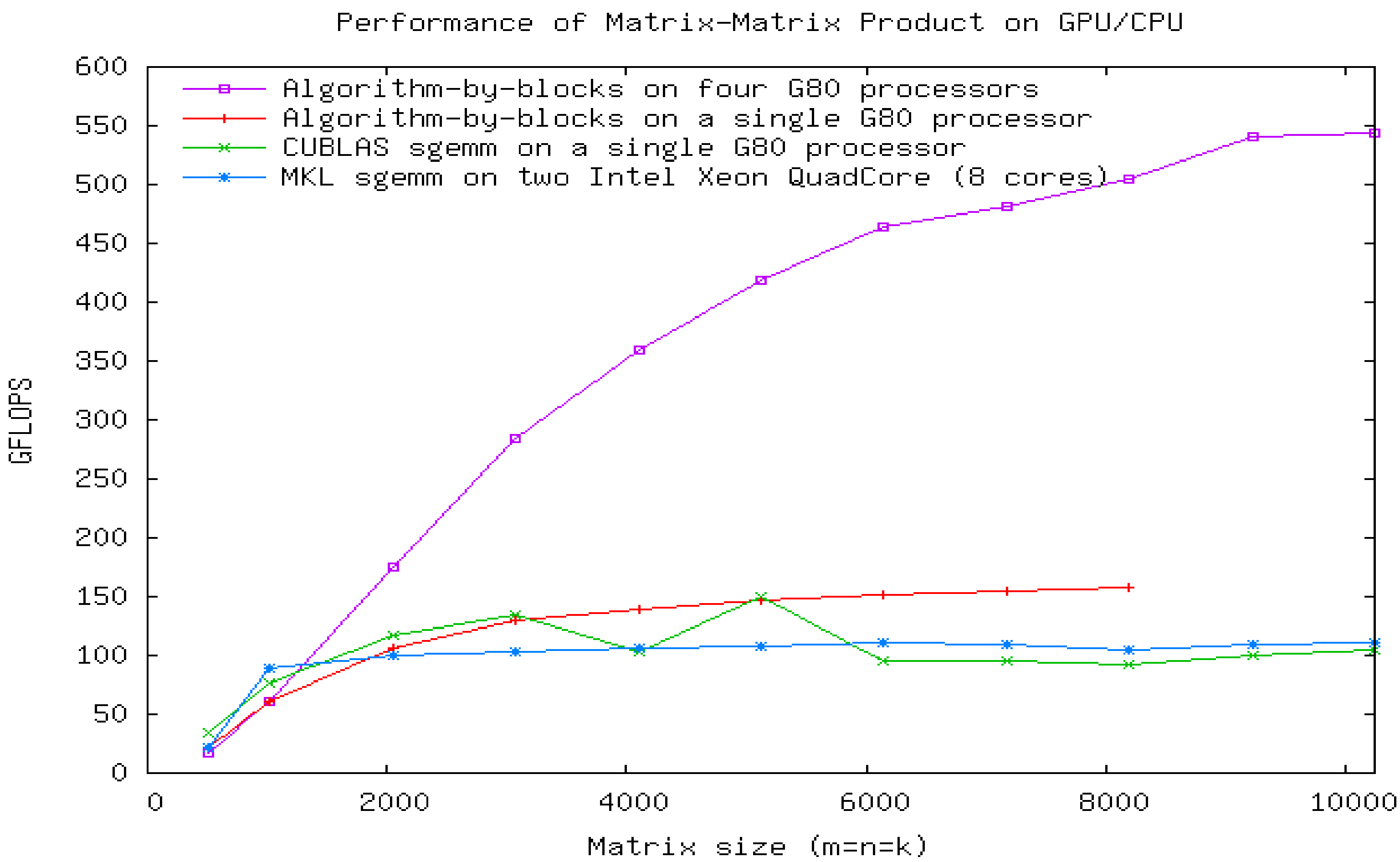
Architecture-aware runtime

- workload balance:
  - 2-D workload distribution
  - Owner-computes rule

Runtime system

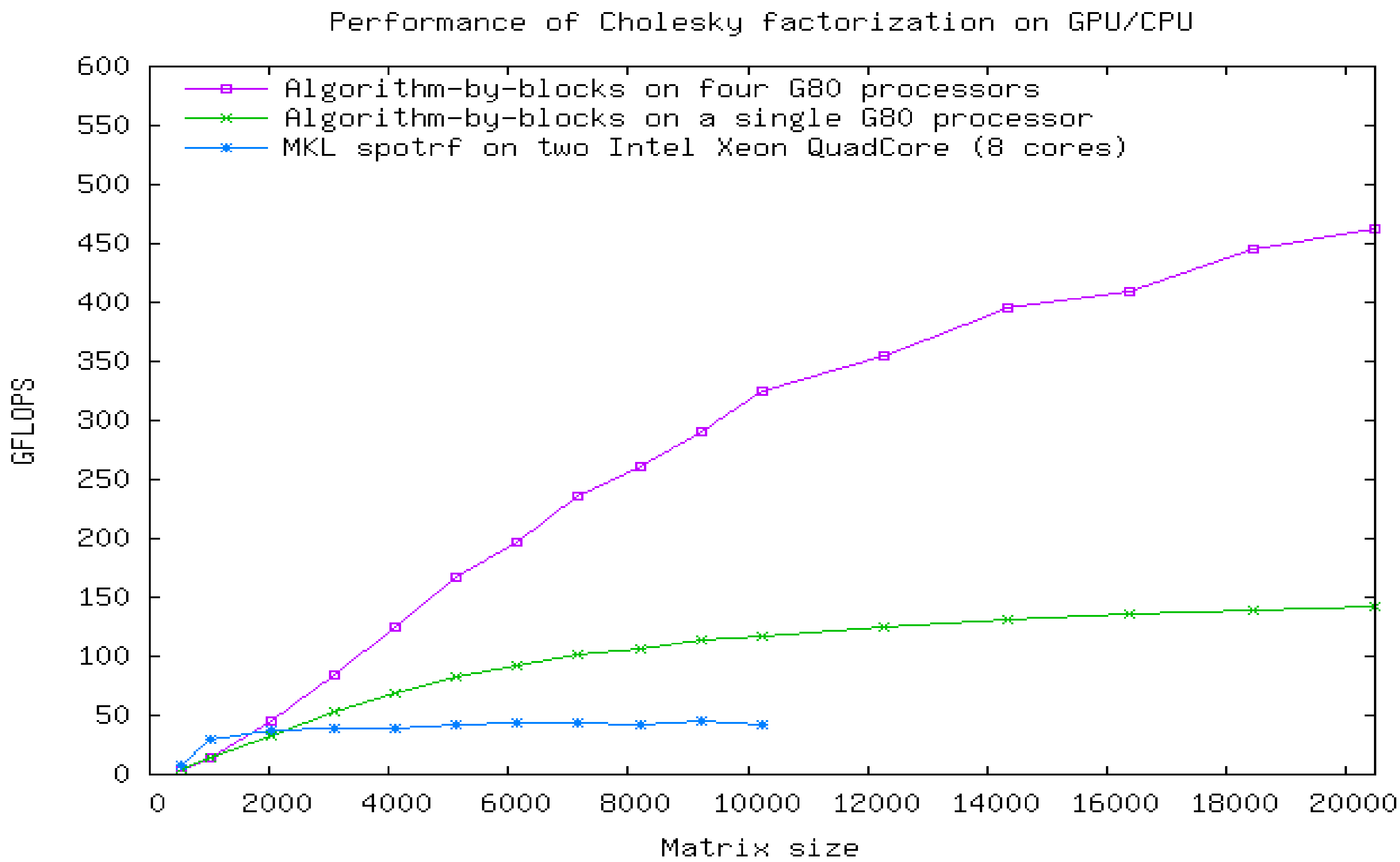
- Reduce communication: software coherence
  - write-back
  - write-invalidate
- Distributed Shared Memory (DSM) layer

Matrix-Matrix Product: $C = C + A \cdot B$



- For the largest problem size, speed-ups are 3.21/5.51 w.r.t. algorithm-by-blocks/CUBLAS on a single G80 processor

Cholesky Factorization: $A = LL^T$



- For the largest problem size, speed-up is 3.25 w.r.t. a single G80 processor

Concluding Remarks

- Programmability: algorithm, data storage, and architecture are independent. Let the runtime system deal with it!
- Similar techniques can also be applied to domains other than dense linear algebra
- However, DSM layer produces little overhead due to regularity of dense linear algebra codes

Concluding Remarks

- Performance of GPUs and multi-GPUs platforms can be improved by:
  - Tune all CUBLAS kernels
  - Employ storage-by-blocks
  - Provide hardware coherence
  - Implement direct communication among GPUs

Ongoing and Future Work

- Very large-scale problems
- Two-sided factorizations for eigenvalues and singular values
- Generic approach for numeric applications not necessarily dense linear algebra

Thanks for your attention!