Design of Scalable Dense Linear Algebra Libraries for Multicore Processors and Multi-GPU Platforms

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...

General Motivation

Who has a multicore processor on the desktop/laptop?

Who has a recent graphics card on the desktop/laptop?

General Motivation

Who has a multicore processor on the desktop/laptop?

Are you using more than 1 core?

Who has a recent graphics card on the desktop/laptop?

Are you using it for something else than games? ;-)

Outline

Part I: Multicore processors

Part II: GPUs

Motivation

New dense linear algebra libraries for multicore processors

- Scalability for manycore
- Data locality
- Heterogeneity?

Motivation

LAPACK (*Linear Algebra Package*)

- Fortran-77 codes
- One routine (algorithm) per operation in the library
- Storage in column major order

- Parallelism extracted from calls to multithreaded BLAS

- Extracting parallelism only from BLAS limits the amount of parallelism and, therefore, the scalability of the solution!
- Column major order does hurt data locality

Motivation

FLAME (*Formal Linear Algebra Methods Environment*)

- Libraries of algorithms, not codes
- Notation reflects the algorithm
- APIs to transform algorithms into codes
- Systematic derivation procedure (automated using MATHEMATICA)
- Storage and algorithm are independent

- Parallelism dictated by data dependencies, extracted at execution time
- Storage-by-blocks

Outline

Part I: Multicore processors

1. Motivation
2. Cholesky factorization (Overview of FLAME)
3. Parallelization
4. Other matrix factorizations: LU & QR
5. Experimental results
6. Concluding remarks

Part II: GPUs

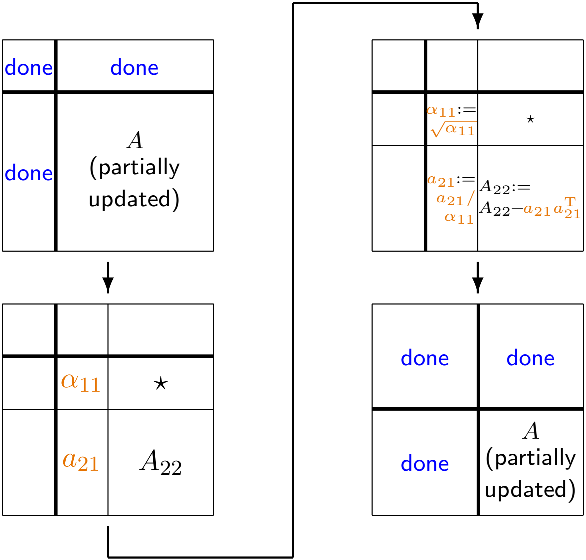
The Cholesky Factorization

Definition

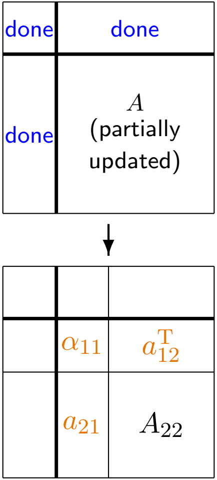
Given $A \rightarrow n \times n$ symmetric positive definite, compute

$$A = L \cdot L^T,$$

with $L \rightarrow n \times n$ lower triangular


done
done
done
A
(partially
updated)
α_{11}
$\star$
a_{21}
A_{22}
$\alpha_{11} := \sqrt{\alpha_{11}}$
$\star$
$a_{21} := a_{21} / \alpha_{11}$
$A_{22} := A_{22} - a_{21} a_{21}^T$
done
done
done
A
(partially
updated)

FLAME Notation



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 a scalar

FLAME Notation

Algorithm: $[A] := \text{CHOL\_UNB}(A)$

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 $n(A_{BR}) \neq 0$ **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 a scalar

$\alpha_{11} := \sqrt{\alpha_{11}}$

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

$A_{22} := A_{22} - a_{21} a_{21}^T$

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

FLAME/C Code

From algorithm to code...

FLAME notation

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 a scalar

FLAME/C code

```
FLA_Repart_2x2_to_3x3(
        ATL, /**/ ATR,       &A00,  /**/ &a01,     &A02,
     /* ************* */ /* ************************** */
                             &a10t, /**/ &alpha11, &a12t,
        ABL, /**/ ABR,       &A20,  /**/ &a21,     &A22,
        1, 1, FLA_BR );
```

(Unblocked) FLAME/C Code

```
int FLA_Cholesky_unb( FLA_Obj A )
{
  /* ... FLA_Part_2x2( ); ... */
  while ( FLA_Obj_width( ATL ) < FLA_Obj_width( A ) ){

    FLA_Repart_2x2_to_3x3(
            ATL, /**/ ATR,       &A00,  /**/ &a01,     &A02,
         /* ************* */   /* ************************** */
                                 &a10t, /**/ &alpha11, &a12t,
            ABL, /**/ ABR,       &A20,  /**/ &a21,     &A22,
            1, 1, FLA_BR );

    /*------------------------------------------------------------*/
    FLA_Sqrt( alpha11 );                /* a21 := sqrt( alpha11 )  */
    FLA_Inv_Scal( alpha11, a21 );       /* a21 := a21 / alpha11    */
    FLA_Syr     ( FLA_MINUS_ONE,
                  a21, A22 );           /* A22 := A22 - a21 * a21t */
    /*------------------------------------------------------------*/
    /* FLA_Cont_with_3x3_to_2x2( ); ... */
  }
}
```

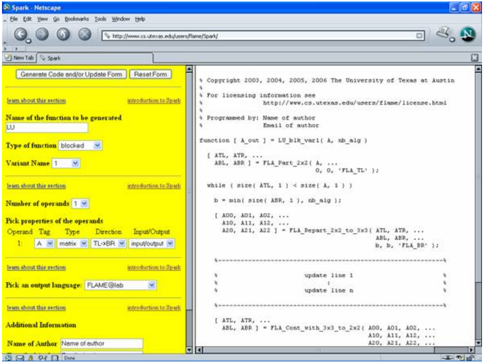
Blocked FLAME/C Code

```
int FLA_Cholesky_blk( FLA_Obj A, int nb_alg )
{
  /* ... FLA_Part_2x2( ); ... */
  while ( FLA_Obj_width( ATL ) < FLA_Obj_width( A ) ){
    b = min( FLA_Obj_length( ABR ), nb_alg );
    FLA_Repart_2x2_to_3x3(
            ATL, /**/ ATR,       &A00, /**/ &A01, &A02,
         /* ************* */   /* ******************** */
                                 &A10, /**/ &A11, &A12,
            ABL, /**/ ABR,       &A20, /**/ &A21, &A22,
            b, b, FLA_BR );

    /*---------------------------------------------------------------*/
    FLA_Cholesky_unb( A11 );            /* A21 := Cholesky( A11 )  */
    FLA_Trsm_rltn( FLA_ONE, A11,
                        A21 );      /* A21 := A21 * inv( A11 )'*/
    FLA_Syrk_ln ( FLA_MINUS_ONE, A21,
                             A22 );/* A22 := A22 - A21 * A21' */
    /*---------------------------------------------------------------*/
    /* FLA_Cont_with_3x3_to_2x2( ); ... */
  }
}
```

FLAME Code

Visit `http://www.cs.utexas.edu/users/flame/Spark/...`



- C code: FLAME/C
- M-script code for MATLAB: FLAME@lab
- Other APIs:
  - FLaTeX
  - Fortran-77
  - LabView
  - Message-passing parallel: PLAPACK
  - FLAG: GPUs

Outline

Parallelization on Multithreaded Architectures

LAPACK parallelization: kernels in multithread BLAS

$$\left(\begin{array}{c|c} A_{11} & \star \\ \hline A_{21} & A_{22} \end{array}\right), \quad A_{11} \text{ is } b \times b$$

- Advantage: Use legacy code
- Drawbacks:
  - Each call to BLAS is a synchronization point for threads
  - As the number of threads increases, serial operations with cost $O(nb^2)$ are no longer negligible compared with $O(n^2b)$

Parallelization on Multithreaded Architectures

FLAME parallelization: SuperMatrix

- Traditional (and pipelined) parallelizations are limited by the control dependencies dictated by the code
- The parallelism should be limited only by the data dependencies between operations!
- In dense linear algebra, imitate a superscalar processor: dynamic detection of data dependencies

FLAME Parallelization: SuperMatrix

```
int FLA_Cholesky_blk( FLA_Obj A, int nb_alg )
{
  /* ... FLA_Part_2x2( ); ... */
  while ( FLA_Obj_width( ATL ) < FLA_Obj_width( A ) ){
    b = min( FLA_Obj_length( ABR ), nb_alg );
    /* ... FLA_Repart_2x2_to_3x3( ); ... */

    /*------------------------------------------------------------*/
    FLA_Cholesky_unb( A11 );          /* A21 := Cholesky( A11 )  */
    FLA_Trsm_rltn( FLA_ONE, A11,
                            A21 );     /* A21 := A21 * inv( A11 )'*/
    FLA_Syrk_ln ( FLA_MINUS_ONE, A21,
                                 A22 );/* A22 := A22 - A21 * A21' */
    /*------------------------------------------------------------*/
    /* FLA_Cont_with_3x3_to_2x2( ); ... */
  }
}
```

The *FLAME runtime system* “pre-executes” the code:

- Whenever a routine is encountered, a pending task is annotated in a global task queue

FLAME Parallelization: SuperMatrix

$$\left(\begin{array}{c|c|c} A_{00} & \star & \star \\ \hline A_{10} & A_{11} & \star \\ \hline A_{20} & A_{21} & A_{22} \end{array}\right) \quad \overset{\text{Runtime}}{\longrightarrow}$$

1. FLA_Cholesky_unb(A_{00})
2. $A_{10} := A_{10}\ \text{TRIL}\,(A_{00})^{-T}$
3. $A_{20} := A_{20}\ \text{TRIL}\,(A_{00})^{-T}$
4. $A_{11} := A_{11} - A_{10} A_{10}^T$
5. ...

SuperMatrix

- Once all tasks are annotated, the real execution begins!
- Tasks with all input operands available are runnable; other tasks must wait in the global queue
- Upon termination of a task, the corresponding thread updates the list of pending tasks

FLAME Storage-by-Blocks: FLASH

- Algorithm and storage are independent
- Matrices stored by blocks are viewed as matrices of matrices
- No significative modification to the FLAME codes

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Part II: GPUs

LU factorization

- Pivoting for stability limits the amount of parallelism

$$\left(\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array}\right), \quad A_{11} \text{ is } b \times b$$

All operations on A_{22} must wait till $\left(\frac{A_{11}}{A_{21}}\right)$ is factorized

- Algorithms-by-blocks for the Cholesky factorization do not present this problem
- Is it possible to design an algorithm-by-blocks for the LU factorization while maintaining pivoting?

LU factorization with incremental pivoting

$$\left(\begin{array}{c|c|c|c} & & & \\ \hline & A_{11} & A_{12} & A_{13} \\ \hline & A_{21} & A_{22} & A_{23} \\ \hline & A_{31} & A_{32} & A_{33} \end{array}\right), \quad A_{ij} \text{ is } t \times t$$

1. Factorize $P_{11} A_{11} = L_{11} U_{11}$
2. Apply permutation P_{11} and factor L_{11}:

$$L_{11}^{-1} P_{11} A_{12} \;\Big|\; L_{11}^{-1} P_{11} A_{13}$$

3. Factorize $P_{21} \left(\dfrac{A_{11}}{A_{21}} \right) = L_{21} U_{21}$,
4. Apply permutation P_{21} and factor L_{21}:

$$L_{21}^{-1} P_{21} \left(\frac{A_{12}}{A_{22}} \right) \;\Bigg|\; L_{21}^{-1} P_{21} \left(\frac{A_{13}}{A_{23}} \right)$$

5. Repeat steps 2–4 with A_{31}

LU factorization with incremental pivoting

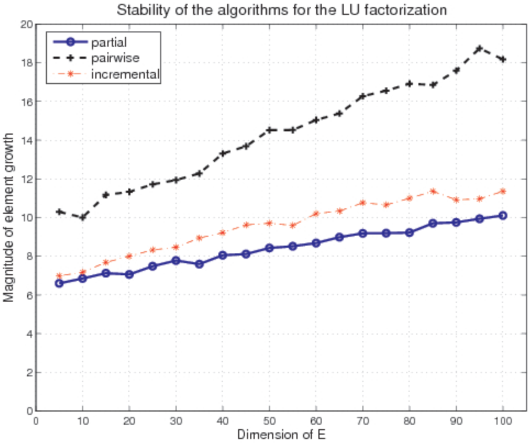
$$\left(\begin{array}{c|c|c|c}
 & & & \\ \hline
 & A_{11} & A_{12} & A_{13} \\ \hline
 & A_{21} & A_{22} & A_{23} \\ \hline
 & A_{31} & A_{32} & A_{33}
\end{array}\right), \quad A_{ij} \text{ is } t \times t$$

Different from LU factorization with column pivoting

- To preserve structure, permutations only applied to blocks on the right!
- To obtain high performance a blocked algorithm with block size $b \ll t$, is used in the factorization and application of factors
- To maintain the computational cost, the upper triangular structure of A_{11} is exploited during the factorization

LU factorization with incremental pivoting

Stability? Element growth with random matrices:



QR factorization

- Same problem as with LU: proceeding by blocks of columns limits the amount of parallelism

$$\left(\begin{array}{c|c|c} \hline & A_{11} & A_{12} \\ \hline & A_{21} & A_{22} \end{array}\right), \quad A_{11} \text{ is } b \times b$$

All operations on A_{22} must wait till $\left(\frac{A_{11}}{A_{21}}\right)$ is factorized

- Is it possible to design an algorithm-by-blocks for the QR factorization while maintaining pivoting?

QR factorization by blocks

$$\left(\begin{array}{c|c|c|c} & & & \\ \hline & A_{11} & A_{12} & A_{13} \\ \hline & A_{21} & A_{22} & A_{23} \\ \hline & A_{31} & A_{32} & A_{33} \end{array}\right), \quad A_{ij} \text{ is } t \times t$$

1. Factorize $Q_{11} A_{11} = R_{11}$
2. Apply factor Q_{11}:
$$Q_{11}^{\mathrm{T}} A_{12} \mid Q_{11}^{\mathrm{T}} A_{13}$$
3. Factorize $Q_{21} \left(\frac{A_{11}}{A_{21}}\right) = R_{21}$,
4. Apply factor Q_{21}:
$$Q_{21}^{\mathrm{T}} \left(\frac{A_{12}}{A_{22}}\right) \Bigg| \; Q_{21}^{\mathrm{T}} \left(\frac{A_{13}}{A_{23}}\right)$$
5. Repeat steps 2–4 with A_{31}

Outline

Experimental Results

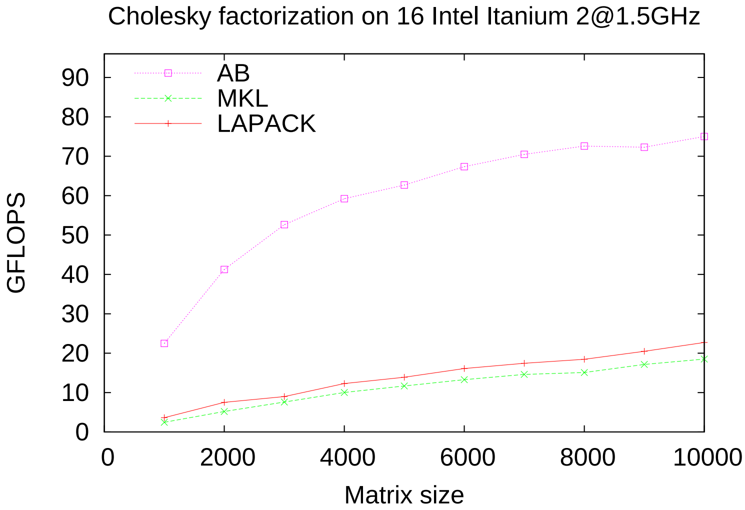
General

Platform	Specs.
SET	CC-NUMA with 16 Intel Itanium-2 processors
NEUMANN	SMP with 8 dual-core Intel Pentium4 processors

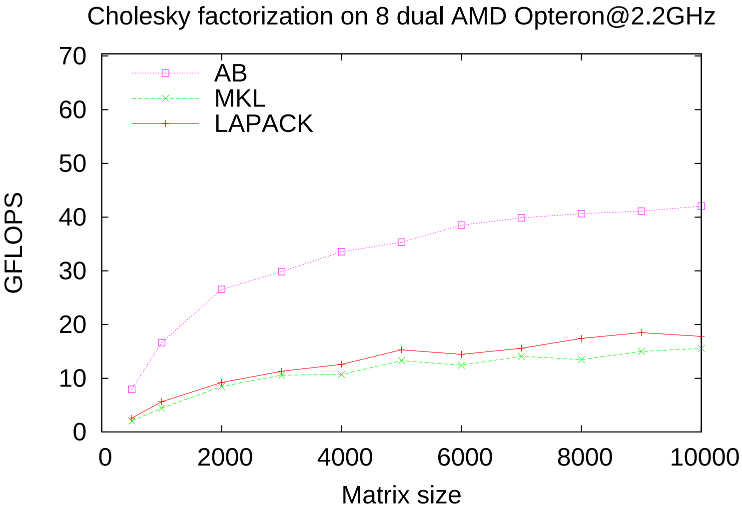
Implementations

- LAPACK 3.0 routine + multithreaded MKL
- Multithreaded routine in MKL
- AB + serial MKL
- AB + serial MKL + storage-by-blocks

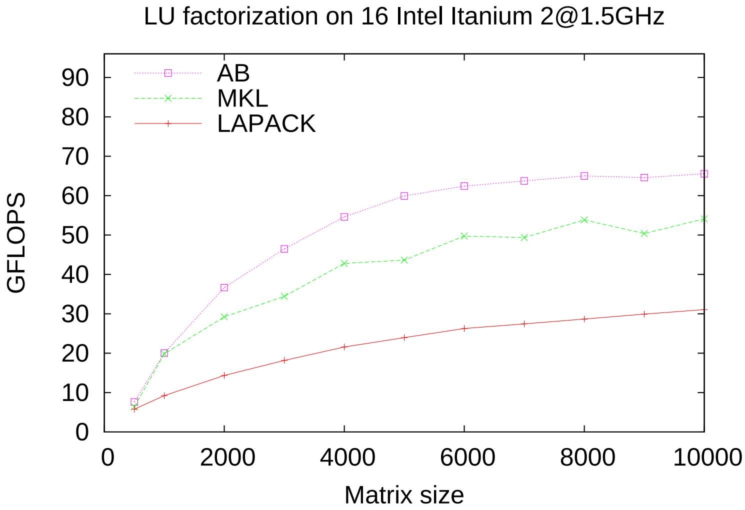
Experimental Results



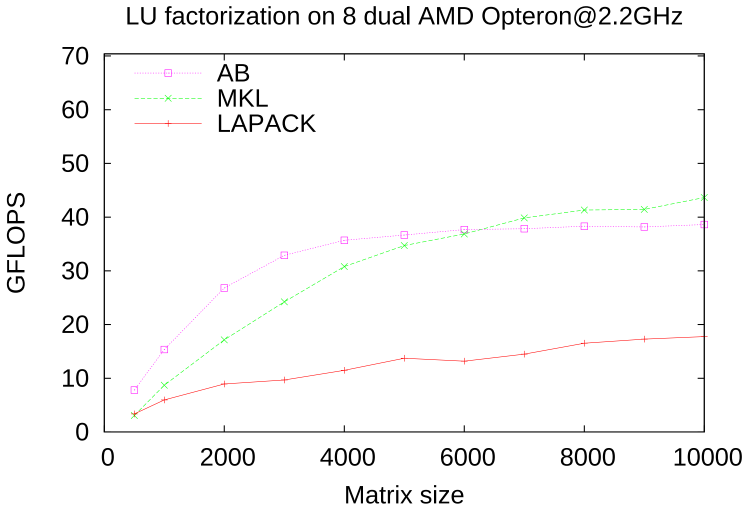
Experimental Results



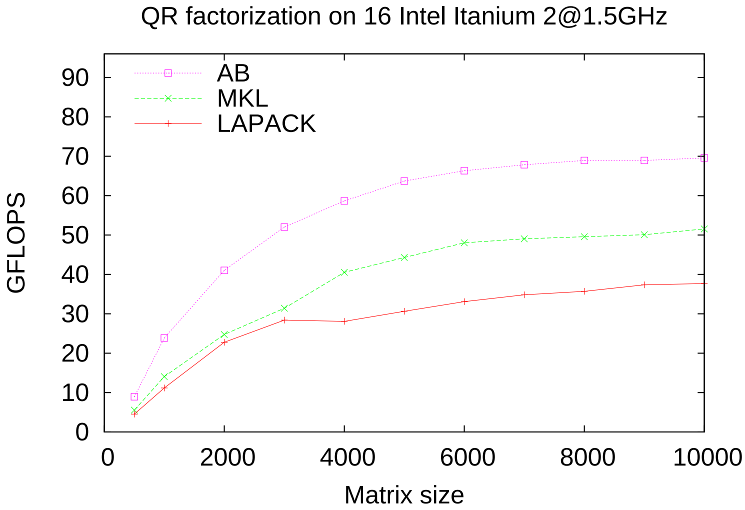
Experimental Results



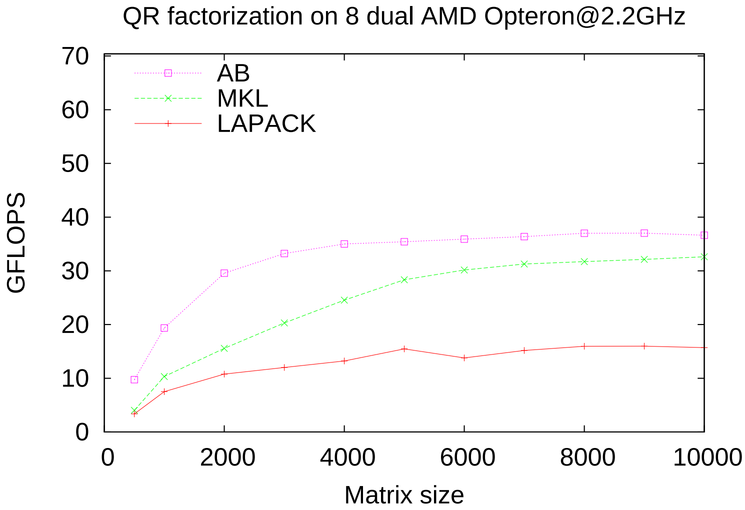
Experimental Results



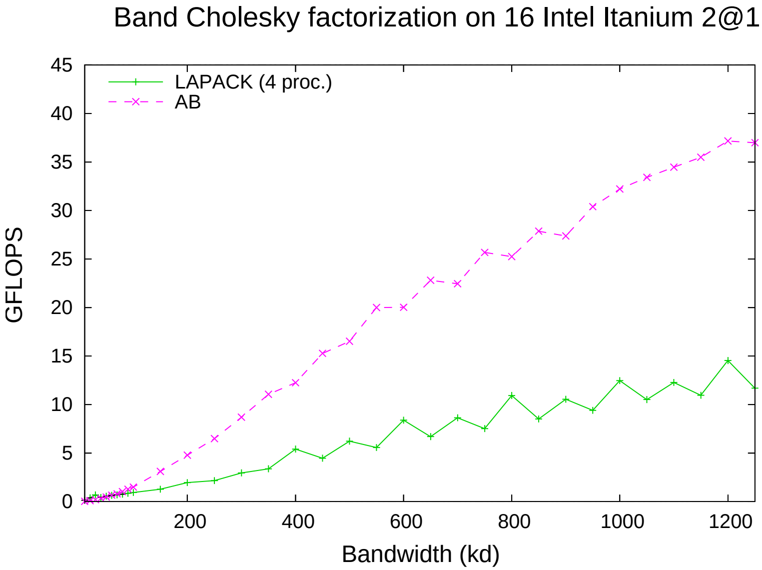
Experimental Results



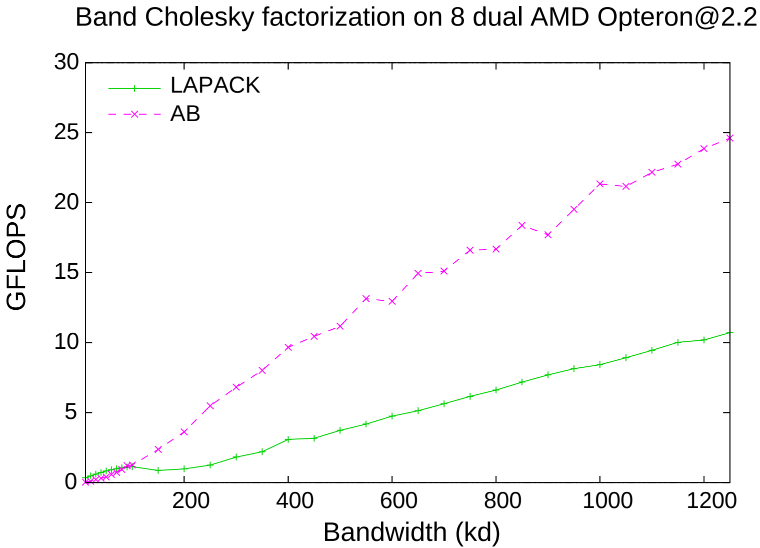
Experimental Results



Experimental Results



Experimental Results



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Part II: GPUs

Concluding Remarks

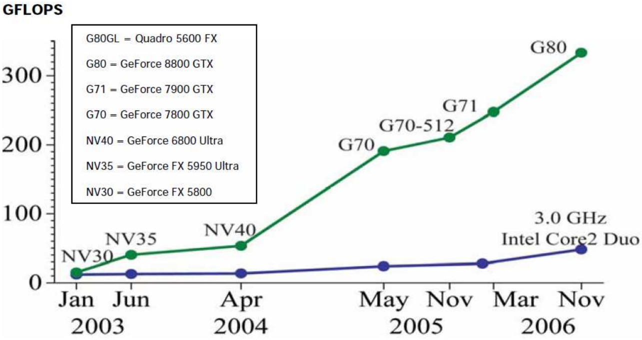
- More parallelism is needed to deal with the large number of cores of future architectures and data locality issued: traditional dense linear algebra libraries will have to be rewritten
- Some operations require new algorithms to better expose parallelism: LU with incremental pivoting, tiled QR,. . .
- The FLAME infrastructure (FLAME/C API, FLASH, and SuperMatrix) reduces the time to take an algorithm from whiteboard to high-performance parallel implementation

Outline

Part I: Multicore processors

Part II: GPUs

Motivation



The power and versatility of modern GPU have transformed them into the first widely extended HPC platform

Outline

Part I: Multicore processors

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Outline

Part I: Multicore processors

Part II: GPUs

1. Motivation
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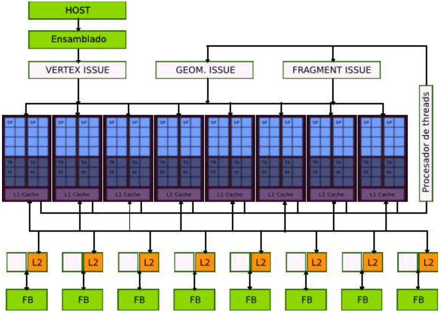
3. LAPACK on 1 GPU
4. LAPACK on multiple GPUs
5. FLAG@lab
6. Concluding remarks

CUDA Hardware

- A CUDA-enabled device is seen as a coprocessor to the CPU, capable of executing a very high number of threads in parallel
- Example: nVIDIA G80 as a set of SIMD Multiprocessors with On-Chip Shared Memory



- Up to 128 *Streaming Processors* (SP), grouped in clusters
- SP are SIMD processors
- Small and fast Shared Memory shared per SP cluster
- Local 32-bit registers per processor

CUDA Software

- The CUDA API provides a simple framework for writing C programs for execution on the GPU
- Consists of:
  - A minimal set of extensions to the C language
  - A runtime library of routines for controlling the transfers between video and main memory, run-time configuration, execution of device-specific functions, handling multiple GPUs,. . .

CUDA libraries

On top of CUDA, nVIDIA provides two optimized libraries: CUFFT and CUBLAS

CUBLAS Example

```
int main( void ){
  ...
  float* h_vector, * d_vector;

  h_vector = (float*)malloc(M*sizeof(float));

  ...
  cublasAlloc(M, sizeof(float),
              (void**) &d_vector);

  cublasSetVector(M, sizeof(float), h_vector,
                  d_vector, 1);
  cublasSscal(M, ALPHA, d_vector, 1);
  cublasGetVector(M, sizeof(float), d_vector,
                  h_vector, 1);

  cublasFree(d_vector);
  ...
}
```

A typical CUDA (and CUBLAS) program has 3 phases:

1. Allocation and transfer of data to GPU
2. Execution of the BLAS kernel
3. Transfer of results back to main memory

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Part II: GPUs

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Cholesky factorization. Blocked variants

Algorithm: $A := \text{CHOL\_BLK}(A)$

Partition ...
  where ...
while $m(A_{TL}) < m(A)$ **do**
  Determine block size b
  Repartition

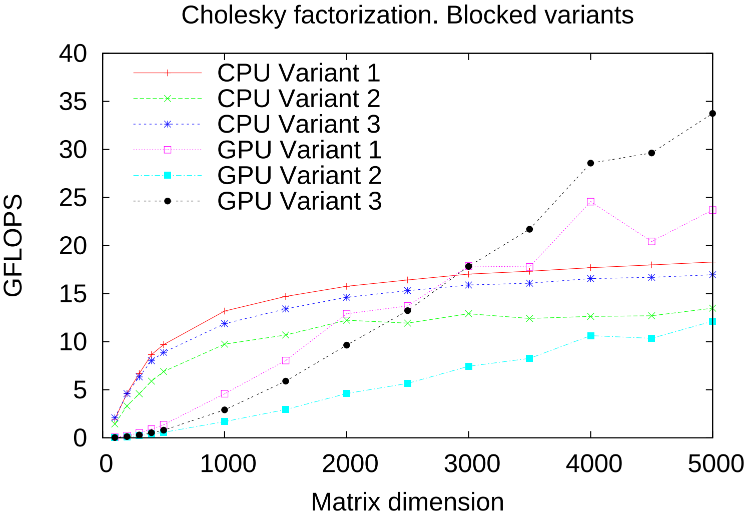
$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{array}\right)$$

  where A_{11} is $b \times b$

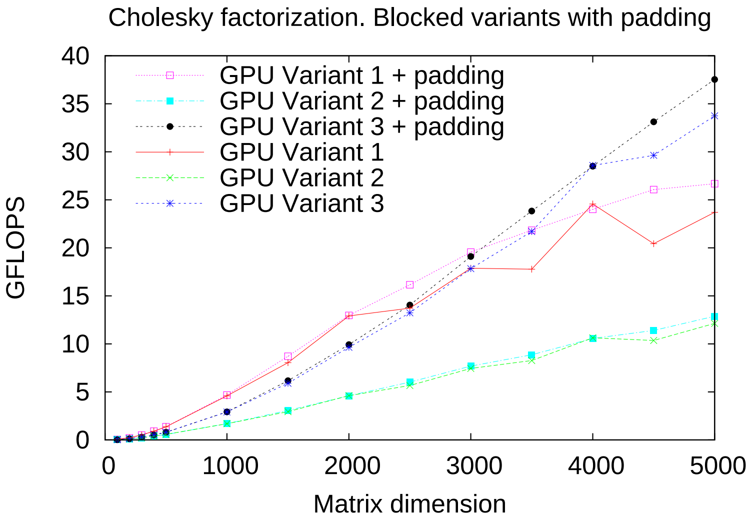
Variant 1:	Variant 2:	Variant 3:
$A_{11} := \text{CHOL\_UNB}(A_{11})$	$A_{10} := A_{10}\,\text{TRIL}\,(A_{00})^{-T}$	$A_{11} := A_{11} - A_{10}A_{10}^T$
$A_{21} := A_{21}\,\text{TRIL}\,(A_{11})^{-T}$	$A_{11} := A_{11} - A_{10}A_{10}^T$	$A_{11} := \text{CHOL\_UNB}(A_{11})$
$A_{22} := A_{22} - A_{21}A_{21}^T$	$A_{11} := \text{CHOL\_UNB}(A_{11})$	$A_{21} := A_{21} - A_{20}A_{10}^T$
		$A_{21} := A_{21}\,\text{TRIL}\,(A_{11})^{-T}$

  Continue with
   ...
endwhile

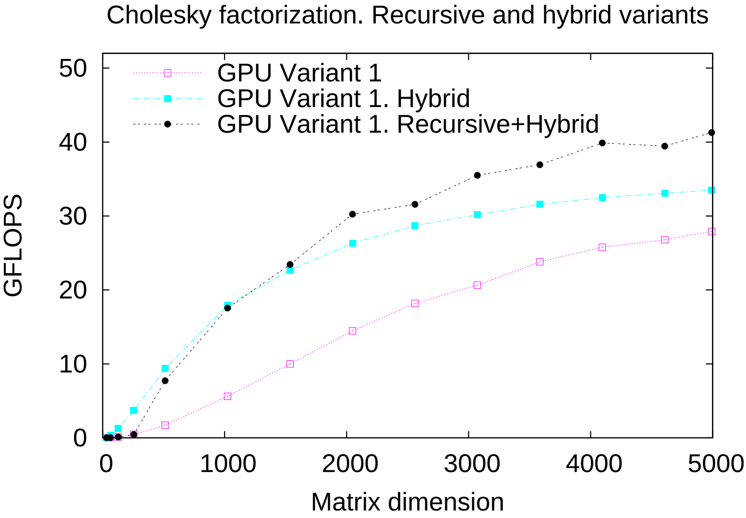
Cholesky factorization. Experimental results



Cholesky padding. Experimental results



Cholesky hybrid and recursive. Experimental results



Iterative refinement for extended precision

Compute the Cholesky factorization $A = LL^T$ and solve $(LL^T)x = b$ in the GPU

$\rightarrow$ 32 bits of accuracy!

$i \leftarrow 1$

repeat

$r^{(i)} \leftarrow b - A \cdot x^{(i)}$

$r^{(i)}_{(32)} \leftarrow r^{(i)}$

$z^{(i)}_{(32)} \leftarrow L^{-T}_{(32)}(L^{-1}_{(32)} r^{(i)}_{(32)})$

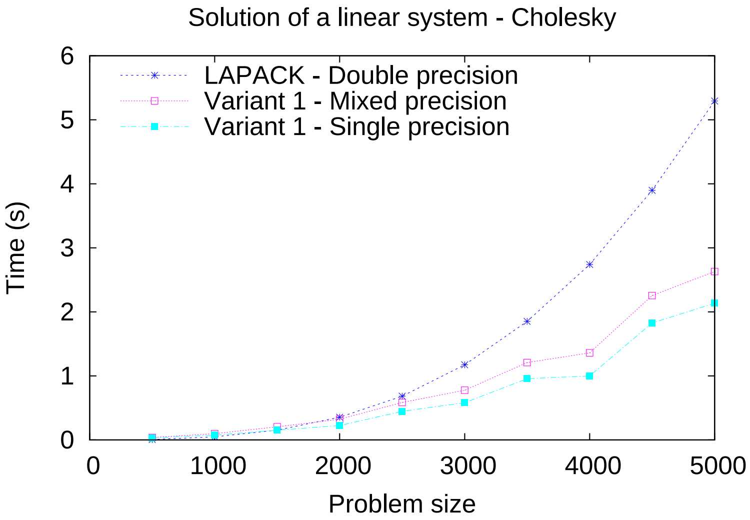
$z^{(i)} \leftarrow z^{(i)}_{(32)}$

$x^{(i+1)} \leftarrow x^{(i)} + z^{(i)}$

$i \leftarrow i + 1$

until $\|r^{(i)}\| < \sqrt{\varepsilon}\|x^{(i)}\|$

Iterative refinement. Experimental results



Outline

What if multiple GPUs are available?

Already here:

- Multiple ClearSpeed boards
- Multiple NVIDIA cards
- nVIDIA Tesla series

How are we going to program these?

What if multiple GPUs are available?

Already here:

- Multiple ClearSpeed boards
- Multiple NVIDIA cards
- nVIDIA Tesla series

How are we going to program these?

Porting SuperMatrix to multiple GPUs

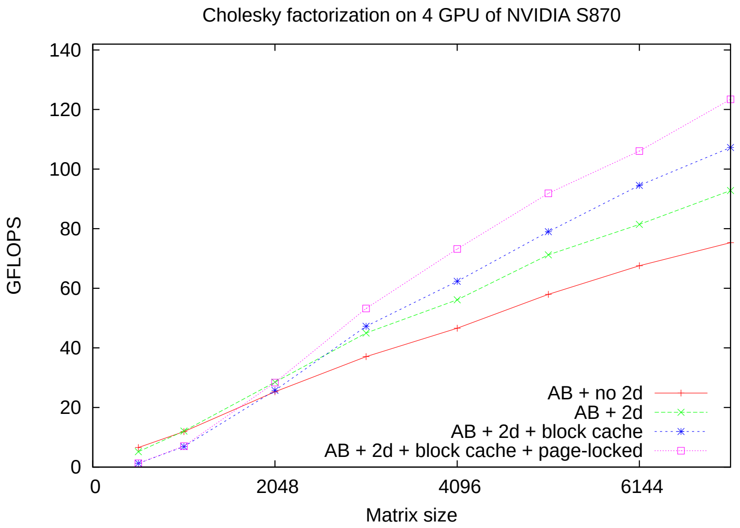
- Employ the equivalence: 1 core $\equiv$ 1 GPU
- Difference: Transference from RAM to video memory
- Run-time system (scheduling), storage, and code are independent
- No significative modification to the FLAME codes: Interfacing to CUBLAS

A software effort of two hours!

Experimental setup

	CPU	GPU
Processor	16 x Intel Itanium2	NVIDIA Tesla s870 (4 G80)
Clock frequency	1.5 GHz	575 MHz

Porting SuperMatrix. Experimental results

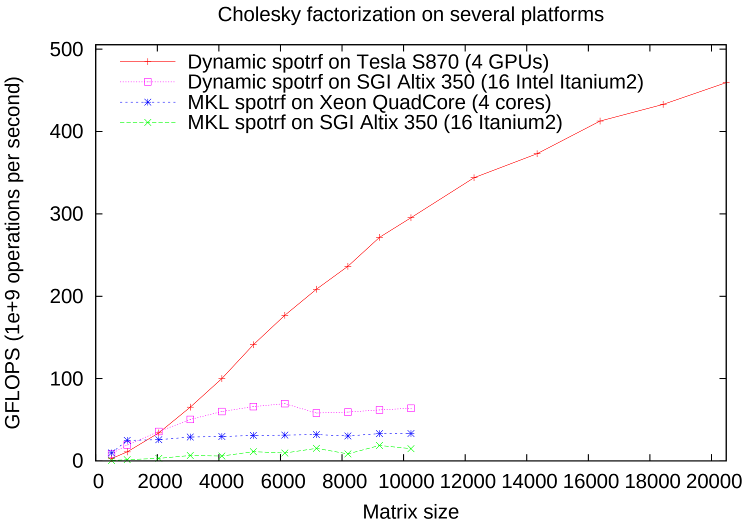


Porting SuperMatrix. Experimental results

A more elaborate port required for high-performance:

- 2-D work distribution
- Memory/cache coherence techniques to reduce transferences between RAM and video memory: write-back and write-invalidate

Porting SuperMatrix. Experimental results



Outline

FLAG@lab

Assorted flavours:

- FLAG: A M-script API for GPU computing from MATLAB/OCTAVE
- FLAGOOC: A M-script API for Out-of-Core GPU computing from MATLAB/OCTAVE

High-level APIs: FLAG

```
function [ A ] = FLAG_Chol( A )

  % [ ... ] = FLAG_Part_2x2( ... );

  while ( FLAG_Obj_length( ATL, 1 ) < FLAG_Obj_length( A, 1 ) )
    b = min( FLAG_Obj_length( ABR, 1 ), nb_alg );

    % [ ... ] = FLAG_Repart_2x2_to_3x3( ... );
    %------------------------------------------------------------%
    FLAG_Chol_unb( A11 );       % A11 = Chol( A11 )
    FLAG_Trsm_rltn( 1.0, A11,
                         A21 ); % A21 = A21 * tril( A11 )^-T
    FLAG_Syrk_ln( -1.0, A21,
                   1.0, A22 );  % A22 = A22 - A21 * A21';
    %------------------------------------------------------------%
    % [ ... ] = FLAG_Cont_with_3x3_to_2x2( ... );
  end
```

Just replace FLA_ in FLAME@lab by FLAG_!

Concluding Remarks

- Simple precision may not be enough. Double precision is coming, but at the expense of speed?
- Overlap transferences and computation is also needed (close?)
- Programming dense linear algebra using CUBLAS on NVIDIA hardware is easy
- Programming at CUDA level?

  I'll need to ask my student Francisco...

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Related Publications

- E. Chan, E.S. Quintana-Ortí, G. Quintana-Ortí, R. van de Geijn. SuperMatrix out-of-order scheduling of matrix operations for SMP and multicore architectures. *19th ACM Symp. on Parallelism in Algorithms and Architectures – SPAA'2007.*
- E. Chan, F. Van Zee, R. van de Geijn, E.S. Quintana-Ortí, G. Quintana-Ortí. Satisfying your dependencies with SuperMatrix. *IEEE Cluster 2007*.
- E. Chan, F.G. Van Zee, P. Bientinesi, E.S. Quintana-Ortí, G. Quintana-Ortí, R. van de Geijn. SuperMatrix: A multithreaded runtime scheduling system for algorithms-by-blocks. *Principles and Practices of Parallel Programming – PPoPP'2008.*
- E.S. Quintana-Ortí, R. van de Geijn. Updating an LU factorization with pivoting. *ACM Trans. on Mathematical Software, 2008.*

Related Publications

- S. Barrachina, M. Castillo, Francisco D. Igual, R. Mayo, E. S. Quintana-Ort´ i. Evaluation and tuning of the level 3 CUBLAS for graphics processors. *Workshop on Parallel and Distributed Scientific and Engineering Computing, – PDSEC'2008.*
- S. Barrachina, M. Castillo, F. Igual, R. Mayo, E. S. Quintana. Solving dense linear systems on graphics processors. *Euro-Par'2008.*
- M. Castillo, F. Igual, R. Mayo, R. Rubio, E. S. Quintana, G. Quintana, R. van de Geijn. Out-of-Core Solution of Linear Systems on Graphics Processors. *Parallel/High-Performance Object-Oriented Scientific Computing – POOSC'08 .*

Related Approaches

Cilk (MIT) and CellSs (Barcelona SuperComputing Center)

- General-purpose parallel programming
  - Cilk → irregular problems
  - CellSs → for the Cell B.E.
- High-level language based on OpenMP-like pramas + compiler + runtime system
- Moderate results for dense linear algebra

PLASMA (UTK – Jack Dongarra)

- Traditional style of implementing algorithms: Fortran-77
- Complicated coding
- Runtime system + ?

For more information...

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

Support...

- *National Science Foundation* awards CCF-0702714 and CCF-0540926 (ongoing till 2010)
- Spanish CICYT project TIN2005-09037-C02-02