High Performance Matrix Inversion on a Multi-core Platform with Several GPUs

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Matrix inversion of large-scale matrices

- Appears in a number of scientific applications like model reduction or optimal control
- Requires a high computational effort, 2n³ floating-point operations (flops)

Graphics processors (GPUs)

- Massively parallel architectures
- Good results on the acceleration of linear algebra operations

Motivation

Matrix inversion

- Implementations on a multi-core CPU and multiple CPUs
- Experimental analysis
- Concluding remarks

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Two different approaches

- Based on the Gaussian elimination (i.e., the LU factorization)
- Based on the Gauss-Jordan elimination (GJE)

Both approaches present similar computational cost but different properties

- PA = LU
- $\bigcirc U \to U^{-1}$
- Solve the system $XL = U^{-1}$ for X
- Undo the permutations $A^{-1} := XP$

Implementation

- The algorithm sweeps through the matrix four times.
- Presents a mild load imbalance, due to the work with triangular factors.

Algorithm implemented by LAPACK

Based on Gauss-Jordan elimination

- In essence, it is a reordering of the operations
- Same arithmetical cost

Implementation

- The algorithm sweeps through the matrix once
 - \rightarrow Less memory accesses
- Most of the computations are highly parallel
 - $\rightarrow \text{More parallelism}$

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At a given iteration:

A00	A01	A02
A10	A11	A12
A20	A21	A22

A00	A01	A02		
A10	A11	A12		
A20	A21	A22		
$\left[\begin{array}{c}A_{01}\\A_{11}\\A_{21}\end{array}\right]:$	$= GJE_{\rm U}$	$_{\rm NB} \left(\left[\begin{array}{c} \overline{A_{01}} \\ A_{11} \\ A_{21} \end{array} \right] \right)$		

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 A_{11} is $b \times b$

Matrix inversion via GJE

A00	A01	A02
A10	A11	A12
A20	A21	A22

 $A_{00} := A_{00} + A_{01}A_{10}$

 $A_{20} := A_{20} + A_{21}A_{10}$

 $A_{10} := A_{11}A_{10}$

A00	A01	A02
A10	A11	A12
A20	A21	A22

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 $A_{02} := A_{02} + A_{01}A_{12}$

 $A_{22} := A_{22} + A_{21}A_{12}$

$$A_{12} := A_{11}A_{12}$$

Move boundaries for the next iteration

A00	A01	A02
A10	A11	A12
A20	A21	A22

 A_{11} is $b \times b$

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Motivation

- 2 Matrix inversion
- Implementations on a multi-core CPU and multiple CPUs
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Implementations on a multi-core CPU and multiple GPUs

Implementation GJE_{mGPU}

- Executes every operation on the most convenient device:
 - GJE_{UNB} on the CPU
 - Matrix-matrix products on the GPUs

Data distribution

- Data is uniformly distributed among GPUs
- Each GPU performs the operations that involve their respective panel



Implementation GJE_{mGPU}

- All GPUs compute concurrently
- The update of current panel on the CPU is overlapped with some updates on the GPUs
- The active column panel is transferred to the CPU initially, and broadcasted to the GPUs after being updated



Implementation GJE_{LA}

- Based on GJE_{mGPU} but reordering the operations applying a look-ahead approach
- The first *b* columns of block [*A*₀₂; *A*₁₂; *A*₂₂] are updated and transferred to the CPU



Implementation GJE_{LA}

- The CPU updates [A₀₁; A₁₁; A₂₁] and the new received block (that is, blocks [A₀₁; A₁₁; A₂₁] of the next iteration)
- Concurrently, the GPUs update the rest of the matrix.



Implementation GJE_{ML}

- The optimal algorithmic block-size for CPU and GPU are significantly different
- The use of the same block-size in both architectures limits the performance of GJE_{LA}
- In this version, the CPU employs a blocked version of GJE instead of the unblocked one
- The CPU and GPUs employ block-sizes *b* and *b_c* respectively, allowing each architecture to optimize its performance

Implementation GJE_{CD}

- At any iteration, one of the GPUs require more time than the rest, leading to load imbalance
- We can partially overcome this problem by employing a cyclic distribution
- The matrix is partitioned in blocks of b columns, and the *i*th block of columns is stored and updated by the (*i mod k*)-th GPU



Implementation GJE_{Merge}

- All GPUs perform 3 operations per iteration
- Performing a minor change on our algorithm, we can reduce it to one operation per iteration with the following advantages:
 - Less overhead due to routines invokations
 - Avoid the matrix-matrix products that involve small blocks

Implementations on a multi-core CPU and multiple GPUs Implementation GJE_{Merze}

At a given iteration:

A00	A01	A02
A10	A11	A12
A20	A21	A22

A00	A01	A02
A10	A11	A12
A20	A21	A22

$$\begin{bmatrix} A_{01} \\ A_{11} \\ A_{21} \end{bmatrix} := GJE_{\text{BLK}} \left(\begin{bmatrix} A_{01} \\ A_{11} \\ A_{21} \end{bmatrix} \right)$$

 A_{11} is b imes b

Implementations on a multi-core CPU and multiple GPUs

Implementation GJE_{Merge}

A00	A01	A02
A10	A11	A12
A20	A21	A22

$$W_1 := A_{10}$$

 $A_{10} := 0$
 $W_2 := A_{12}$
 $A_{12} := 0$

$$\begin{bmatrix} A_{00}A_{02} \\ A_{10}A_{12} \\ A_{20}A_{22} \end{bmatrix} := \begin{bmatrix} A_{00}A_{02} \\ A_{10}A_{12} \\ A_{20}A_{22} \end{bmatrix} + \begin{bmatrix} A_{01} \\ A_{11} \\ A_{21} \end{bmatrix} [W_1W_2]$$

Implementations on a multi-core CPU and multiple GPUs

Implementation GJE_{Merge}

Move boundaries for the next iteration

A00	A01	A02
A10	A11	A12
A20	A21	A22

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

Implementation GJE_{Merge}

- An important improvement in performance can be obtained by merging the extra copies with the swap stage required by pivoting.
 - Thus, *W*₁ and *W*₂ will contain blocks *A*₁₀ and *A*₁₂ after the pivoting has been applied.
 - This considerably reduces the number of memory accesses and partially hides the overhead introduced by the copies of A_{10} and A_{12}

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Processors	# Cores	Frequency	L2 cache	Memory
			(MB)	(GB)
Intel Xeon QuadCore	8 (2×4)	2.27	8	48
NVIDIA TESLA c1060	960 (4×240)	1.3	-	16(4x4)

BLAS Implementations

- MKL 11.1
- NVIDIA CUBLAS 3.0

Results for matrices with $1000 \le n \le 64000$

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Experimental analysis (Martix inversion on 2 GPUs)



Experimental analysis (Martix inversion on 4 GPUs)



Experimental analysis (Variant GJE_{Merge} on 1, 2, 3 and 4 GPUs)



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- We have presented five implementations of matrix inversion based on the GJE method on multiple GPUs
- Those implementations are between 6 and 12 times faster than LAPACK using 4 GPUs and exhibit excellent scalability properties (with a nearly linear speed-up)
- The use of multiple GPUs
 - Reduce the computational time
 - Increments the amount of memory available, allowing the inversion of larger matrices

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- Evaluation of double precision arithmetic on the new NVIDIA Fermi architecture
- GJE_{Merge} implementation is clearly limited by the performance of CUBLAS routine for matrix-matrix products. Other GPU Kernels should be evaluated

Questions ?

Alfredo Remón (remon@icc.uji.es) High Performance Matrix Inversion with Several GPUs

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