# Towards an Efficient Tile Matrix Inversion of Symmetric Positive Definite Matrices on Multicore Architectures

Emmanuel Agullo<sup>1</sup>, Henricus Bouwmeester<sup>2</sup>, Jack Dongarra<sup>1</sup>, Jakub Kurzak<sup>1</sup>, Julien Langou<sup>2</sup>, and Lee Rosenberg<sup>2</sup>

<sup>1</sup> Dpt of Electrical Engineering and Computer Science, University of Tennessee, 1122 Volunteer Blvd, Claxton Building, Knoxville, TN 37996-3450, USA

<sup>2</sup> Dpt of Mathematical and Statistical Sciences, University of Colorado Denver, Campus Box 170, P.O. Box 173364, Denver, Colorado 80217-3364, USA,

Research was supported by the National Science Foundation grant no. NSF CCF-811520.

**Abstract.** The algorithms in the current sequential numerical linear algebra libraries (*e.g.* LAPACK) do not parallelize well on multicore architectures. A new family of algorithms, the *tile algorithms*, has recently been introduced. Previous research has shown that it is possible to write efficient and scalable tile algorithms for performing a Cholesky factorization, a (pseudo) LU factorization, and a QR factorization. In this extended abstract, we attack the problem of the computation of the inverse of a symmetric positive definite matrix. We observe that, using a dynamic task scheduler, it is relatively painless to translate existing LAPACK code to obtain a ready-to-be-executed tile algorithm. However we demonstrate that non trivial compiler techniques (array renaming, loop reversal and pipelining) need then to be applied to further increase the parallelism of our application. We present preliminary experimental results.

#### 1 Introduction

The appropriate direct method to compute the solution of a symmetric positive definite system of linear equations consists of computing the Cholesky factorization of that matrix and then solving the underlying triangular systems. It is not recommended to use the inverse of the matrix in this case. However some applications need to explicitly form the inverse of the matrix. A canonical example is the computation of the variance-covariance matrix in statistics. Higham [12, p.260,§3] lists more such applications.

With their advent, multicore architectures [18] induce the need for algorithms and libraries that fully exploit their capacities. A class of such algorithms – called tile algorithms [8, 9] – has been developed for one-sided dense factorizations (Cholesky, LU and QR) and made available as part of the Parallel Linear Algebra Software for Multicore Architectures (PLASMA) library [2]. In this paper, we extend this class of algorithms to the case of the (symmetric positive definite) matrix inversion. Besides constituting an important functionality for a library such as PLASMA, the study of the matrix inversion on multicore architectures represents a challenging algorithmic problem. Indeed, first, contrary to standalone one-sided factorizations that have been studied so far, the matrix inversion exhibits many anti-dependences [4] (Write After Read). Those anti-dependences can be a bottleneck for parallel processing, which is critical on multicore architectures. It is thus essential to investigate (and adapt) well known techniques used in compilation such as using temporary copies of data to remove anti-dependences to enhance the degree of parallelism of the matrix inversion. This technique is known as *array renaming* [4] (or *array privatization* [11]). Second, *loop reversal* [4] is to be investigated. Third, the matrix inversion consists of three successive steps (first of which is the Cholesky decomposition). In terms of scheduling, it thus represents an opportunity to study the effects of *pipelining* [4] those steps on performance.

The current version of PLASMA (version 2.1) is scheduled statically. Initially developed for the IBM Cell processor [14], this static scheduling relies on POSIX threads and simple synchronization mechanisms. It has been designed to maximize data reuse and load balancing between cores, allowing for very high performance [3] on today's multicore architectures. However, in the case of the matrix inversion, the design of an ad-hoc static scheduling is a time consuming task and raises load balancing issues that are much more difficult to address than for a stand-alone Cholesky decomposition, in particular when dealing with the pipelining of multiple steps. Furthermore, the growth of the number of cores and the more complex memory hierarchies make executions less deterministic. In this paper, we rely on an experimental in-house dynamic scheduler [13]. This scheduler is based on the idea of expressing an algorithm through its sequential representation and unfolding it at runtime using data hazards (Read after Write, Write after Read, Write after Write) as constraints for parallel scheduling. The concept is rather old and has been validated by a few successful projects. We could have as well used schedulers from the Jade project from Stanford University [17] or from the SMPSs project from the Barcelona Supercomputer Center [15].

Our discussions are illustrated with experiments conducted on a dual-socket quad-core machine based on an Intel Xeon EMT64 processor operating at 2.26 GHz. The theoretical peak is equal to 9.0 Gflop/s per core or 72.3 Gflop/s for the whole machine, composed of 8 cores. The machine is running Mac OS X 10.6.2 and is shipped with the Apple vecLib v126.0 multithreaded BLAS [1] and LAPACK vendor library, as well as LAPACK [5] v3.2.1 and ScaLAPACK [7] v1.8.0 references.

The rest of the paper is organized as follows. In Section 2, we present a new algorithm for matrix inversion based on tile algorithms; we explain how we articulated it with our dynamic scheduler to take advantage of multicore architectures and we compare its performance against state-of-the-art libraries. In Section 3, we investigate the impact on parallelism and performance of different well known techniques used in compilation: loop reversal, array renaming and pipelining. We conclude and present future work directions in Section 4.

## 2 Tile in-place matrix inversion

Tile algorithms are a class of Linear Algebra algorithms that allow for fine granularity parallelism and asynchronous scheduling, enabling high performance on multicore architectures [3, 8, 9, 16]. The matrix of order n is split into  $t \times t$  square submatrices of order b ( $n = b \times t$ ). Such a submatrix is of small granularity (we fixed b = 200 in this paper) and is called a *tile*. So far, tile algorithms have been essentially used to implement one-sided factorizations [3, 8, 9, 16].

Algorithm 1 extends this class of algorithms to the case of the matrix inversion. As in state-of-the-art libraries (LAPACK, ScaLAPACK), the matrix inversion is performed *in-place*, *i.e.*, the data structure initially containing matrix A is directly updated as the algorithm is progressing, without using any significant temporary extra-storage; eventually,  $A^{-1}$  substitutes A. Algorithm 1 is composed of three steps. Step 1 is a Tile Cholesky Factorization computing the Cholesky factor L (lower triangular matrix satisfying  $A = LL^{T}$ ). This step was studied in [9]. Step 2 computes  $L^{-1}$  by inverting L. Step 3 finally computes the inverse matrix  $A^{-1} = L^{-1^T}L^{-1}$ . Each step is composed of multiple fine granularity tasks (since operating on tiles). These tasks are part of the BLAS (SYRK, GEMM, TRSM, TRMM) and LAPACK (POTRF, TRTRI, LAUUM) standards. A more detailed description is beyond the scope of this extended abstract and is not essential to the understanding of the rest of the paper. Indeed, from a high level point of view, an operation based on tile algorithms can be represented as a Directed Acyclic Graphs (DAG) [10] where nodes represent the fine granularity tasks in which the operation can be decomposed and the edges represent the dependences among them. For instance, Figure 1(a) represents the DAG of Step 3 of Algorithm 1.



**Fig. 1.** DAGs of Step 3 of the Tile Cholesky Inversion (t = 4).

**Algorithm 1**: Tile In-place Cholesky Inversion (lower format). Matrix *A* is the on-going updated matrix (in-place algorithm).

```
Input: A, Symmetric Positive Definite matrix in tile storage (t \times t \text{ tiles}).
Result: A^{-1}, stored in-place in A.
Step 1: Tile Cholesky Factorization (compute L such that A = LL^T);
for j = 0 to t - 1 do
     for k = 0 to j - 1 do
      A_{j,j} \leftarrow CHOL(A_{j,j}) (POTRF(j));
     for i = j + 1 to t - 1 do
     \begin{array}{c} \text{for } i = j + 1 \text{ to } i = 1 \text{ do} \\ \text{for } k = 0 \text{ to } j - 1 \text{ do} \\ \text{ } & \text{ } A_{i,j} \leftarrow A_{i,j} - A_{i,k} * A_{j,k}^T \text{ (GEMM(i,j,k)) }; \\ \text{for } i = j + 1 \text{ to } t - 1 \text{ do} \\ \text{ } & \text{ } A_{i,j} \leftarrow A_{i,j} / A_{j,j}^T \text{ (TRSM(i,j)) }; \end{array} 
Step 2: Tile Triangular Inversion of L (compute L^{-1});
for j = t - 1 to 0 do
     A_{j,j} \leftarrow TRINV(A_{j,j}) (TRTRI(j));
     for i = t - 1 to j + 1 do
        Step 3: Tile Product of Lower Triangular Matrices (compute A^{-1} = L^{-1T}L^{-1});
for i = 0 to t - 1 do
     for j = 0 to i - 1 do
       A_{i,j} \leftarrow A_{i,i}^T * A_{i,j} (\text{TRMM}(i,j)) ; 
     \begin{array}{l} A_{i,i} \leftarrow A_{i,i}^T \ast A_{i,i} \; (\text{LAUUM(i)}) \; ; \\ \textbf{for} \; j = 0 \; \textbf{to} \; i-1 \; \textbf{do} \end{array}
        \begin{bmatrix} \mathbf{for} \ k = i+1 \ \mathbf{to} \ t-1 \ \mathbf{do} \\ \\ A_{i,j} \leftarrow A_{i,j} + A_{k,i}^T * A_{k,j} \ (\text{GEMM}(\mathbf{i},\mathbf{j},\mathbf{k})) \ ; \end{bmatrix}
```

Algorithm 1 is based on the variants used in LAPACK 3.2.1. Bientinesi, Gunter and van de Geijn [6] discuss the merit of algorithmic variations in the case of the computation of the inverse of a symmetric positive definite matrix. Although of definite interest, this is not the focus of this extended abstract.

We have implemented Algorithm 1 using our dynamic scheduler introduced in Section 1. Figure 2 shows its performance against state-of-the-art libraries and the vendor library on the machine described in Section 1. For a matrix of small size, it is difficult to extract parallelism and have a full use of all the cores [3, 8, 9, 16]. We indeed observe a limited scalability (N = 1000, Figure 2(a)). However, tile algorithms (Algorithm 1) still benefit from a higher degree of parallelism than blocked algorithms [3, 8, 9, 16]. Therefore Algorithm 1 (in place) consistently achieves a significantly better performance than vecLib, ScaLAPACK and LAPACK libraries. A larger matrix size (N = 4000, Figure 2(b)) allows for a better use of parallelism. In this case, an optimized implementation of a blocked algorithm (vecLib) competes well against tile algorithms (in place) on few cores (left part of Figure 2(a)). However, only tile algorithms scale to a larger number of cores (rightmost part of Figure 2(b)) thanks to a higher degree of parallelism. In other words, the tile Cholesky inversion achieves a better strong scalability than the blocked versions, similarly to what had been observed for the factorization step [3, 8, 9, 16].



Fig. 2. Scalability of Algorithm 1 (in place) and its out-of-place variant introduced in Section 3, using our dynamic scheduler against vecLib, ScaLAPACK and LAPACK libraries.

#### 3 Algorithmic study

In the previous section, we compared the performance of the tile Cholesky inversion against state-the-art libraries. In this section, we focus on tile Cholesky

	In-place case	Out-of-place case
Step 1	3t-2	3t-2
Step 2	3t-3	2t - 1
Step 3	3t-2	t

Table 1. Length of the critical path as a function of the number of tiles t.

inversion and we discuss the impact of several variants of Algorithm 1 on performance.

Array renaming (removing anti-dependences). The dependence between SYRK(0,1) and TRMM(1,0) in the DAG of Step 3 of Algorithm 1 (Figure 1(a) represents the constraint that the SYRK operation (l. 28 of Algorithm 1) needs to read  $A_{k,i} = A_{1,0}$  before TRMM (l. 22) can overwrite  $A_{i,j} =$  $A_{1,0}$ . This anti-dependence (Write After Read) can be removed thanks to a temporary copy of  $A_{1,0}$ . Similarly, all the SYRK-TRMM anti-dependences, as well as TRMM-LAUMM and GEMM-TRMM anti-dependences can be removed. We have designed a variant of Algorithm 1 that removes all the anti-dependences thanks to the use of a large working array (this technique is called array renaming [4] in compilation [4]). The subsequent DAG (Figure 1(b)) is split in multiple pieces (Figure 1(b)), leading to a shorter critical path (Table 1). We implemented the out-of-place algorithm, based on our dynamic scheduler too. Figure 2(a)shows that our dynamic scheduler exploits its higher degree of parallelism to achieve a much higher strong scalability even on small matrices (N = 1000). For a larger matrix (Figure 2(b)), the in-place algorithm already achieved very good scalability. Therefore, using up to 7 cores, their performance are similar. However, there is not enough parallelism with a  $4000 \times 4000$  matrix to use efficiently all 8 cores with the in-place algorithm; thus the higher performance of the out-of-place version in this case (leftmost part of Figure 2(b)).

**Loop reversal (exploiting commutativity).** The most internal loop of each step of Algorithm 1 (l. 88, l. 17 and l. 26) consists in successive commutative GEMM operations. Therefore they can be performed in any order, among which increasing order and decreasing order of the loop index. Their ordering impacts the length of the critical path. Algorithm 1 orders those three loops in increasing (U) and decreasing (D) order, respectively. We had manually chosen these respective orders (UDU) because they minimize the critical path of each step (values reported in Table 1). A naive approach would have, for example, been comprised of consistently ordering the loops in increasing order (UUU). In this case (UUU), the critical path of TRTRI would have been equal to  $t^2 - 2t + 3$  (in-place) or  $(\frac{1}{2}t^2 - \frac{1}{2}t + 2)$  (out-of-place) instead of 3t - 3 (in-place) or 2t - 1 (out-of-place) for (UDU). Figure 3 shows how loop reversal impacts performance.

**Pipelining.** Pipelining the multiple steps of the inversion reduces the length of its critical path. For the in-place case, the critical path is reduced from 9t - 7 tasks (t is the number of tiles) to 9t - 9 tasks (negligible). For the out-of-place case, it is reduced from 6t - 3 to 5t - 2 tasks. We studied the effect of pipelining



Fig. 3. Impact of loop reversal on performance.

on the performance of the inversion on a  $8000 \times 8000$  matrix with an artificially large tile size (b = 2000 and t = 4). As expected, we observed almost no effect on performance of the in-place case (about 36.4 seconds with or without pipelining). For the out-of-place case, the elapsed time grows from 25.1 to 29.2 seconds (16 % overhead) when pipelining is prevented.

### 4 Conclusion and future work

We have proposed a new algorithm to compute the inverse of a symmetric positive definite matrix on multicore architectures. An experimental study has shown both an excellent scalability of our algorithm and a significant performance improvement compared to state-of-the-art libraries. Beyond extending the class of so-called tile algorithms, this study brought back to the fore well known issues in the domain of compilation. Indeed, we have shown the importance of loop reversal, array renaming and pipelining.

The use of a dynamic scheduler allowed an out-of-the-box pipeline of the different steps whereas loop reversal and array renaming required a manual change to the algorithm. The future work directions consist in enabling the scheduler to perform itself loop reversal and array renaming. We exploited the commutativity of GEMM operations to perform array renaming. Their associativity would furthermore allow to process them in parallel (following a binary tree); the subsequent impact on performance is to be studied. Array renaming requires extra-memory. It will be interesting to address the problem of the maximization of performance under memory constraint. This work aims to be incorporated into PLASMA.

#### References

- 1. BLAS: Basic linear algebra subprograms. http://www.netlib.org/blas/.
- E. Agullo, J. Dongarra, B. Hadri, J. Kurzak, J. Langou, J. Langou, and H. Ltaief. PLASMA Users' Guide. Technical report, ICL, UTK, 2009.
- E. Agullo, B. Hadri, H. Ltaief, and J. Dongarrra. Comparative study of one-sided factorizations with multiple software packages on multi-core hardware. In SC'09: Proceedings of the Conference on High Performance Computing Networking, Storage and Analysis, pages 1–12, New York, NY, USA, 2009. ACM.
- R. Allen and K. Kennedy. Optimizing Compilers for Modern Architectures: A Dependence-based Approach. Morgan Kaufmann, 2001.
- E. Anderson, Z. Bai, C. Bischof, L. S. Blackford, J. W. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen. *LA-PACK Users' Guide*. SIAM, 1992.
- P. Bientinesi, B. Gunter, and R. van de Geijn. Families of algorithms related to the inversion of a symmetric positive definite matrix. ACM Trans. Math. Softw., 35(1):1–22, 2008.
- L. S. Blackford, J. Choi, A. Cleary, E. D'Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet, K. Stanley, D. Walker, and R. C. Whaley. *ScaLAPACK Users' Guide.* SIAM, 1997.
- A. Buttari, J. Langou, J. Kurzak, and J. Dongarra. Parallel tiled QR factorization for multicore architectures. *Concurrency Computat.: Pract. Exper.*, 20(13):1573– 1590, 2008.
- A. Buttari, J. Langou, J. Kurzak, and J. Dongarra. A class of parallel tiled linear algebra algorithms for multicore architectures. *Parallel Computing*, 35(1):38–53, 2009.
- 10. N. Christofides. Graph Theory: An algorithmic Approach. 1975.
- 11. R. Eigenmann, J. Hoeflinger, and D. Padua. On the automatic parallelization of the perfect benchmarks. *IEEE Trans. Parallel Distrib. Syst.*, 9(1):5–23, 1998.
- 12. N. J. Higham. Accuracy and Stability of Numerical Algorithms. Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, second edition, 2002.
- J. Kurzak and J. Dongarra. Fully dynamic scheduler for numerical computing on multicore processors. University of Tennessee CS Tech. Report, UT-CS-09-643, 2009.
- J. Kurzak and J. Dongarra. QR factorization for the Cell Broadband Engine. Sci. Program., 17(1-2):31–42, 2009.
- J. M. Perez, P. Bellens, R. M. Badia, and J. Labarta. CellSs: Making it easier to program the Cell Broadband Engine processor. *IBM J. Res. & Dev.*, 51(5):593–604, 2007.
- G. Quintana-Ortí, E. S. Quintana-Ortí, R. A. van de Geijn, F. G. Van Zee, and Ernie Chan. Programming matrix algorithms-by-blocks for thread-level parallelism. ACM Transactions on Mathematical Software, 36(3).
- M. C. Rinard, D. J. Scales, and M. S. Lam. Jade: A high-level, machineindependent language for parallel programming. *Computer*, 6:28–38, 1993.
- H. Sutter. A fundamental turn toward concurrency in software. Dr. Dobb's Journal, 30(3), 2005.