Analysis and Comparison of Two General Sparse Solvers for Distributed Memory Computers

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This paper provides a comprehensive study and comparison of two state-of-the-art direct solvers for large sparse sets of linear equations on large-scale distributed-memory computers. One is a multifrontal solver called MUMPS, the other is a supernodal solver called SuperLU. We describe the main algorithmic features of the two solvers and compare their performance characteristics with respect to uniprocessor speed, interprocessor communication, and memory requirements. For both solvers, preorderings for numerical stability and sparsity play an important role in achieving high parallel efficiency. We analyse the results with various ordering algorithms. Our performance analysis is based on data obtained from runs on a 512-processor Cray T3E using a set of matrices from real applications. We also use regular 3D grid problems to study the scalability of the two solvers.

This work was supported by the France-Berkeley Fund and the National Energy Research Scientific Computing Center (NERSC) which is supported by the Director, Office of Advanced Scientific Computing Research, Division of Mathematical, Information, and Computational Sciences of the U.S. Department of Energy under contract number DE-AC03-76SF00098. Most of this work was done while P. R. Amestoy was visiting NERSC. The work of I. S. Duff was supported in part by the EPSRC Grant GR/M78502. The research of X. S. Li was supported in part by the National Science Foundation Cooperative Agreement No. ACI-9619020 and NSF Grant No. ACI-9813362.
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Categories and Subject Descriptors: G.1.3 [**Numerical Analysis**]: Numerical Linear Algebra—*Sparse, structured, and very large systems* (*direct and iterative methods*); G.4 [**Mathematics of Computing**]: Mathematical Software—*Parallel and vector implementations*

General Terms: Algorithms, Performance

Additional Key Words and Phrases: Sparse direct solvers, parallelism, distributed-memory computers, multifrontal and supernodal factorizations

1. INTRODUCTION

The direct solution of sparse linear systems using Gaussian elimination has a clear advantage over iterative methods in terms of numerical robustness and it remains the method-of-choice for many ill-conditioned systems. However, it is very challenging to implement such methods efficiently even on a single processor yet alone on multiprocessor machines. One of the main reasons is because of fill-in in the matrix factorization. Moreover, numerical pivoting involves dynamically tracking the fill-ins that are generated in a somewhat unpredictable way. Handling highly irregular data access and computation is further compounded by sophisticated computer architectures with several layers of memory hierarchy. Therefore, unlike many iterative algorithms that users can implement reasonably well and quickly by themselves, direct solvers require much more expertise and a longer time to develop. Indeed, users usually do not have the resources to develop such codes by themselves, but rather resort to off-the-shelf software. Despite the existence of a number of direct solvers (see Section 7), nonexpert users still find it difficult to choose the right code and find it even harder to anticipate the performance they will obtain, in terms of execution time, memory demand, and communication network demand. Therefore, a careful comparison of various direct solution codes gives useful and needed guidance to the user community. It is also valuable to the experts in the field because they get more insight into the various algorithms.

In this work, we restrict our attention to comparing codes for distributed memory computers where communication is by message passing, normally using `MPI`. In particular, we study in detail, two state-of-the-art solvers, `MUMPS` [Amestoy et al. 2000; Amestoy et al. 2001] and `SuperLU` [Li and Demmel 1999]. The reasons for choosing these are two-fold. First, the two codes use different algorithms that are representative of a far wider range of codes. `MUMPS` uses a multifrontal approach with dynamic pivoting for stability while `SuperLU` is based on a right-looking supernodal technique with static pivoting. Second, the two are among the best codes publicly available, and are widely used. Therefore, our conclusions in this paper, to a large extent, apply to a wider range of codes. We had originally planned a comparison with more of the sparse codes from Table XVII. However, our experience shows that such a comparison can be fraught with difficulties even when the authors of the codes are involved in the study. So we have shelved this more ambitious project for the moment.

There are many technical difficulties in achieving a truly fair comparison. The main reason is that there are usually many parameters in the codes that can be set by the user. Altering their values can result in a dramatic change in

performance. For example, some codes can use any sparsity ordering provided by the user, which is the case for both MUMPS and SuperLU; other codes can only use their own ordering algorithms which are sometimes buried deeply within the code. This will cause different amounts of fill-in; which difference is not intrinsic to the factorization algorithms. When we compared MUMPS and SuperLU, we spent a long time trying to understand the parameter space of the two codes, and made sure that the parameters were set properly so that the two codes performed the same preprocessing steps and sparsity ordering. We feel that the lessons we have learned in this present exercise are both invaluable to us in our future wider study and have given us some insight into the behaviour of sparse direct codes which is useful to share with a wider audience at this stage. In addition to valuable information on the comparative merits of multifrontal versus supernodal approaches, we examine the parameter space for such a comparison exercise and identify several key parameters that influence the two approaches to a differing degree.

The rest of the paper is organized as follows. Section 2 gives the characteristics of the test matrices and the parallel machines. In Section 3 we discuss the detailed algorithms used in the two codes. Two very important factors affecting the performance of both codes are the use of preprocessing to preorder the matrix so that the diagonal entries are large relative to the off-diagonals, and the strategy used to compute an ordering for the rows and columns of the matrix to preserve sparsity. We discuss these aspects in detail in Section 4. We compare the performance of the two codes in Section 5. Our performance metrics include execution time, memory usage, communication characteristics, scalability, numerical accuracy, as well as the preprocessing costs. In Section 6, problems with regular grids are used to further illustrate and analyse the relative performance of the two approaches. In Section 7, we summarize our general conclusions on the strength and weakness of each solver and list other potential solvers to evaluate in future work.

2. TEST ENVIRONMENT

Throughout this paper, we will use a set of test problems to evaluate the performance of our algorithms. Our test matrices come from the forthcoming Rutherford-Boeing Sparse Matrix Collection [Duff et al. 1997][1], the industrial partners of the PARASOL Project[2], Tim Davis' collection[3], SPARSEKIT2[4] and the EECS Department of UC Berkeley[5]. The PARASOL test matrices are available from Parallab, Bergen, Norway[6]. Two smaller matrices (GARON2 and LNSP3937) are included in our set of matrices but will be used only in Section 4.1 to illustrate differences in the numerical behaviour of the two solvers.

[1]Web page http://www.cse.clrc.ac.uk/Activity/SparseMatrices/
[2]EU ESPRIT IV LTR Project 20160
[3]Web page http://www.cise.ufl.edu/research/sparse/matrices
[4]Web page http://math.nist.gov/MatrixMarket/data/SPARSKIT/
[5]Matrix ECL32 is included in the Rutherford-Boeing Collection
[6]Web page http://www.parallab.uib.no/parasol/

Table I. Test Matrices

Real Unsymmetric Assembled (RUA)				
Matrix name	Order	No. of entries	StrSym(*)	Origin
BBMAT	38744	1771722	0.54	Rutherford-Boeing (CFD)
ECL32	51993	380415	0.93	EECS Department of UC Berkeley
FIDAPM11	22294	623554	1.00	SPARSKIT2 (CFD)
GARON2	13535	390607	1.00	Davis collection (CFD)
INVEXTR1	30412	1793881	0.97	PARASOL (Polyflow S.A.)
LHR71C	70304	1528092	0.00	Davis collection (Chem Eng)
LNSP3937	3937	25407	0.87	Rutherford-Boeing (CFD)
MIXTANK	29957	1995041	1.00	PARASOL (Polyflow S.A.)
RMA10	46835	2374001	1.00	Davis collection (CFD)
TWOTONE	120750	1224224	0.28	Rutherford-Boeing (circuit sim)
WANG4	26068	177196	1.00	Rutherford-Boeing (semiconductor)

(*) StrSym is the number of nonzeros matched by nonzeros in symmetric locations divided by the total number of entries (so that a structurally symmetric matrix has value 1.0).

Table II. Characteristics of the CRAY T3E-900 and the IBM SP2. The Factorization of Matrix WANG4 using MUMPS was used to Estimate the Effective Uniprocessor Performance of the Computers

Computer	CRAY T3E-900	IBM SP2
Frequency of the processor	450 MHertz	66 MHertz
Peak uniproc. performance	900 Mflops	264 Mflops
Effective uniproc. performance	340 Mflops	150 Mflops
Peak communication bandwidth	300 Mbytes/sec	36 Mbytes/sec
Latency	4 μsec	40 μsec
Bandwidth/Effective performance	0.88	0.24

Note that, for most of our experiments, we do not consider symmetric matrices in our test set because SuperLU cannot exploit the symmetry and is unable to produce an $\mathbf{LDL}^T$ factorization. However, since our test examples in Section 6 are symmetric, we do show a few results with both the symmetric and unsymmetric factorization versions of MUMPS. Matrices MIXTANK and INVEXTR1 have been modified because of underflow values in the matrix files. To keep the same sparsity pattern, we have replaced all entries with exponents smaller than -300 by numbers with the same mantissa but with exponents of -300. For each linear system, the right-hand side vector is generated so that the true solution is a vector of all ones.

All results presented in this paper have been obtained on the Cray T3E-900 (512 DEC EV-5 processors, 256 Mbytes of memory per processor, 900 peak Megaflop rate per processor) from NERSC at Lawrence Berkeley National Laboratory. We will also refer to experiments on a 35 processor IBM SP2 (66.5 MHertz processor with 128 Mbytes of physical memory and 512 Mbytes of virtual memory and 266 peak Megaflop rate per processor) at GMD in Bonn, Germany, used during the PARASOL Project. The performance characteristics of the two machines are listed in Table II.

Although in this paper we only provide a complete set of results on the T3E, it is important to look at machines with different characteristics because we have built parameters/options into the codes to balance the computation and

communication for different architectures. We used the SP2 to help understand tuning parameters (see Sections 3.1 and 3.2).

3. DESCRIPTION OF THE ALGORITHMS USED

In this section, we briefly describe the main characteristics of the algorithms used in the solvers and highlight the major differences between them. For a complete description of the algorithms, the reader should consult Amestoy et al. [2000]; Amestoy et al. [2001]; Li and Demmel [1998, 1999].

Both algorithms can be described by a directed acyclic graph [Gilbert and Liu 1993] whose nodes represent computations and whose edges represent transfer of data. This graph reduces to a tree in the case of the multifrontal method, MUMPS. In this case, some steps of Gaussian elimination are performed on a dense frontal matrix at each node and the Schur complement (or contribution block) that remains is passed for assembly at the parent node. In the case of the supernodal code, SuperLU, the distributed memory version uses a right-looking formulation which, having computed the factorization of a block of columns, then immediately sends the data to update the block columns in the trailing submatrix.

We would like to emphasize that our parallel codes are not both derived from their sequential and/or shared memory counterparts. On unsymmetric matrices, MUMPS is very similar to MA41 [Amestoy and Duff 1993] so that both the numerical behaviour and the uniprocessor performance of the two codes are very comparable. Parallel SuperLU is completely different from sequential SuperLU—the parallel code is right-looking and uses static pivoting, whereas the sequential one is left-looking and uses partial pivoting. These changes were made to enhance parallelism and scalability.

Both codes can accept any pivotal ordering and both have a built-in capability to generate an ordering based on an analysis of the pattern of $A+A^T$, where the summation is performed symbolically. However, for the present version of MUMPS, the symbolic factorization is markedly less efficient if an input ordering is given, since different logic is used in this case. The default ordering used by MUMPS is approximate minimum degree (AMD) [Amestoy et al. 1996] while the default for SuperLU is multiple minimum degree (MMD) [Liu 1985]. However, in our experiments using a minimum degree ordering, we consider only the AMD ordering since both codes can generate this using the subroutine MC47 from HSL [HSL 2000]. It is usually far quicker than MMD and produces a symbolic factorization close to that produced by MMD. We also use the nested dissection (ND) ordering from MeTiS [Karypis and Kumar 1998]. In addition, it is sometimes very beneficial to precede the ordering by performing an unsymmetric permutation to place large entries on the diagonal, and then scaling the matrix so that the diagonals are all of modulus one and the off-diagonals have modulus less than or equal to one. We use the MC64 code of HSL to perform this preordering and scaling [Duff and Koster 2001] and indicate clearly when this is done. The effect of using this preordering of the matrix is discussed in detail in Section 4.1. Finally, when MC64 is not used, our matrices are always row and column scaled (each row/column is divided by the maximum value in the row/column).

In both approaches, a pivot order is defined by the analysis and symbolic factorization stages. In MUMPS, the modulus of the prospective pivot is compared with the largest modulus of an entry in the row and is only accepted if this is greater than a threshold value, typically between 0.001 and 0.1 (our default value is 0.01). Note that, although MUMPS can choose pivots from off the diagonal, the largest entry in the column might be unavailable for pivoting at this stage if all entries in its row are not fully summed. This threshold pivoting strategy is common in sparse Gaussian elimination and helps to avoid excessive growth in the size of entries during the matrix factorization and so directly reduces a bound on the backward error. If a prospective pivot fails the test, all that happens is that it is kept in the Schur complement and is passed to the parent node. Eventually all rows with entries in the column will be available for pivoting, at the root if not before, so that a pivot can be chosen from the column. Thus the numerical factorization can respect the threshold criterion but at the cost of increasing the size of the frontal matrices and causing more work and fill-in than were forecast. For the SuperLU approach, a static pivoting strategy is used and we keep to the pivotal sequence chosen in the analysis. The magnitude of the potential pivot is tested against a threshold of $\epsilon^{1/2}\|A\|_1$, where ϵ is the machine precision and $\|A\|_1$ is the one-norm of A. If it is less than this value, it is immediately set to this value (with the same sign) and the modified entry is used as pivot. This corresponds to a half-precision perturbation to the original matrix entry. The result is that the factorization is not exact and iterative refinement may be needed. Note that, after iterative refinement, we obtained an accurate solution in all the cases that we tested. If problems were still to occur, then extended precision BLAS [Li et al. 2000] could be used.

3.1 MUMPS Main Parallel Features

The parallelism within MUMPS is at two levels. The first uses the structure of the assembly tree, exploiting the fact that computations at nodes that are not ancestors or descendants, are independent. The initial parallelism from this source (*tree parallelism*) is the number of leaf nodes but this reduces to one at the root. The second level is in the subdivision of the elimination operations through blocking of the frontal matrix. This blocking gives rise to *node parallelism* and is either by rows (referred to as *1D-node parallelism*) or by rows and columns (at the root and referred to as *2D-node parallelism*). Node parallelism depends on the size of the frontal matrix which, because of delayed pivots, is only known at factorization time. Therefore this is determined dynamically. Each tree node is assigned a processor *a priori*, but the subassignment of blocks of the frontal matrix is done dynamically.

Most of the machine dependent parameters in MUMPS that control the efficiency of the code are designed to take into account both the uniprocessor and multiprocessor characteristics of the computers. Because of the dynamic distributed scheduling approach, we do not need as precise a description of the performance characteristics of the computer as for codes such as PaStiX [Henon et al. 1999], that are based on static scheduling. Most of the machine dependent parameters in MUMPS are associated with the block sizes involved in the

parallel blocked factorization of the dense frontal matrices. Our main objective is to maintain a minimum granularity to efficiently exploit the potential of the processor, while providing sufficient tasks to exploit the available parallelism. Our target machines differ in several respects. The most important ones are illustrated in Table II. We found that smaller granularity tasks could be used on the CRAY T3E than on the IBM SP2 because of the relatively faster rate of communication to Megaflop rate on the CRAY T3E than on the IBM SP2. That is to say that the communication is relatively more efficient on the CRAY T3E.

Dynamic scheduling is a major and original feature of the approach used in MUMPS. A critical part of this algorithm is when a process associated with a tree node decides to reassign some of its work, corresponding to a partitioning of the rows, to a set of so-called *worker* processes. We call such a node a one-dimensional parallel node. In earlier versions of MUMPS, a fixed block size is used to partition the rows and work is distributed to processes starting with the least loaded process. (The load of a process is determined by the amount of work [number of operations] allocated to it and not yet processed, which can be determined very cheaply.) Since the block size is fixed, it is possible for a process in charge of a one-dimensional parallel node to give additional work to processes that are already more loaded than itself. This can happen near the leaf nodes of the tree where sparsity provides enough parallelism to keep all processes busy. On the other hand, insufficient tasks might be created to provide work to all idle processes. This situation is more likely to occur close to the root of the tree.

In the new algorithm (available since Version 4.1 of MUMPS), the block size for the one-dimensional partitioning can be dynamically adjusted by the process in charge of the node. Early in the processing of the tree (that is, near the leaves) this gives a relatively bigger block size, thereby reducing the number of worker processes; whereas close to the root of the tree the block size will be automatically reduced to compensate for the lack of parallelism in the assembly tree. We bound the block size for partitioning a one-dimensional parallel node, by an interval. The lower bound is needed to maintain a minimum task granularity, and to control the volume of messages. The upper bound of the interval is less critical (it is by default chosen to be about eight times the lower bound) but it is used in estimating the maximum size of the communication buffers and of the factors, and so should not be too large.

This "all dynamic" strategy of both partitioning and distributing work onto the processors could cause some trouble on a large number of processors (more than 128). In that case, it can be quite beneficial to take into account some "global" information to help the local decisions. For example, one could restrict the choice of worker processes to a set of candidate processors determined statically during the analysis phase. This notion, commonly used in the design of static scheduling algorithms such as Henon et al. [1999], could reduce the overhead of the dynamic scheduling algorithm, reduce the increase in the communication volume when increasing the number of processors, and improve the local decision. The tuning of the parameters controlling the block size for 1D partitioning would then be easier and the estimation of the memory required during factorization would be more accurate. This could be expected to improve

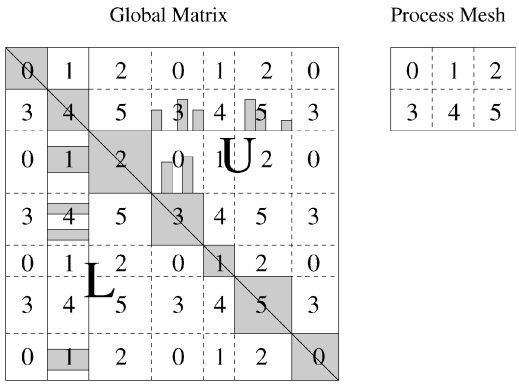


Fig. 1. The 2D block-cyclic layout used in SuperLU.

the performance, particularly on a large number of processors. This feature is not available in the current Version 4.1 of MUMPS but will be implemented in a future release and will address some of the current limitations of the MUMPS approach (see Section 5.2).

The solution phase is also performed in parallel and uses asynchronous communications both for the forward elimination and the back substitution. In the case of the forward elimination, the tree is processed from the leaves to the root, in a way similar to the factorization, while the back substitution requires a different algorithm that processes the tree from the root to the leaves. A pool of ready-to-be-activated tasks is used. We do not change the distribution of the factors as generated in the factorization phase. Hence, 1D-node and 2D-node parallelism are also used in the solution phase.

3.2 SuperLU Main Parallel Features

SuperLU also uses two levels of parallelism although more advantage is taken of the node parallelism through blocking of the supernodes. Because the pivotal order is fully determined at the analysis phase, the assignment of blocks to processors can be done statically, *a priori*, before the factorization commences. A *2D block-cyclic* layout is used and the execution can be pipelined, since the sequence is predetermined. The matrix partitioning is based on the notion of an *unsymmetric supernode* introduced in Demmel et al. [1999]. The supernode is defined over the matrix factor L. A supernode is a range $(r : s)$ of columns of L with the triangular block just below the diagonal, being full, and the same nonzero structure elsewhere (this is either full or zero). This supernode partition is used as the block partition in *both* row and column dimensions, that is, the diagonal blocks are square. If there are N supernodes in an n-by-n matrix, there will be N^2 blocks of non-uniform size. Figure 1 illustrates such a block partition. The off-diagonal blocks may be rectangular and need not be full. Furthermore, the columns in a block of U do not necessarily have the same row structure. We call a dense subvector in a block of U, a *segment*. The P processes are also arranged as a 2D mesh of dimension $P_r \times P_c = P$. By block-cyclic layout, we mean that block (I, J) (of L or U) is mapped onto the process at coordinate $((I-1) \bmod P_r, (J-1) \bmod P_c)$ of the process mesh. During the factorization,

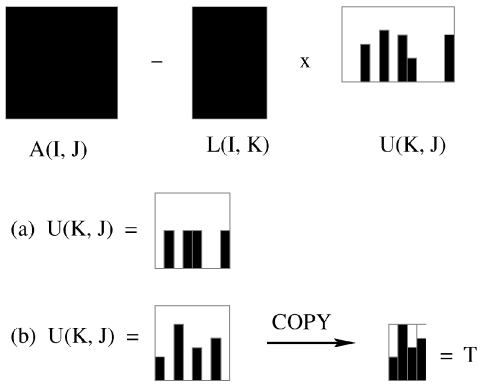


Fig. 2. Illustration of the numerical kernels used in SuperLU.

block $L(I, J)$ is only needed by the processes on the process row $((I - 1) \bmod P_r)$. Similarly, block $U(I, J)$ is only needed by the processes on the process column $((J - 1) \bmod P_c)$. This partitioning and mapping can be controlled by the user. First, the user can set the *maximum block size* parameter. The symbolic factorization algorithm identifies supernodes, and chops the large supernodes into smaller ones if their sizes exceed this parameter. The supernodes may be smaller than this parameter due to sparsity, and the blocks are then defined by the supernode boundaries. (That is, supernodes can be smaller than the maximum block size but never larger.) Our experience has shown that a good value for this parameter on the IBM SP2 is around 40, while on the Cray T3E, it is around 24. Second, the user can set the shape of the process grid, such as 2×3 or 3×2. Better performance is obtained when we keep the process row dimension slightly smaller than the process column dimension. This rule of thumb was used on the Cray T3E to define the grid shapes.

In this 2D mapping, each block column of L resides on more than one process, namely, a column of processes. For example in Figure 1, the second block column of L resides on the column of processes $\{1, 4\}$. Process 1 only owns two nonzero blocks, which are not contiguous in the global matrix.

The main numerical kernel involved during numerical factorization is a block update corresponding to the rank-k update to the Schur complement (see Figure 2):

$$A(I, J) \leftarrow A(I, J) - L(I, K) \times U(K, J),$$

In the earlier versions of SuperLU, this computation was based on Level 2.5 BLAS. That is, we call the Level 2 BLAS routine GEMV (matrix-vector product) but with multiple vectors (segments), and the matrix $L(I, K)$ is kept in cache across these multiple calls. This, to some extent, mimics the Level 3 BLAS GEMM (matrix-matrix product) performance. However, the difference between Level 2.5 and Level 3 is still quite large on many machines, for example the IBM SP2. This motivated us to modify the kernel in the following way, in order to use Level 3 BLAS. For best performance, we distinguish two cases corresponding to the two shapes of a $U(K, J)$ block.

—The segments in $U(K, J)$ are of same height, as shown in Figure 2 (a). Since the nonzero segments are stored contiguously in memory, we can call GEMM directly, without performing operations on any zeros.

—The segments in $U(K, J)$ are of different heights, as shown in Figure 2 (b). In this case, we first copy the segments into a temporary working array T, with some leading zeros padded if necessary. We then call GEMM using $L(I, K)$ and T (instead of $U(K, J)$). We perform some extra floating-point operations for those padding zeros. The copying itself does not incur a run time cost, because the data must be loaded in the cache anyway. The working storage T is bounded by the maximum block size, which is a tunable parameter. For example, we usually use 40×40 on the IBM SP2 and 24×24 on the Cray T3E.

Depending on the matrix, this Level 3 BLAS kernel improved the uniprocessor factorization time by about 20% to 40% on the IBM SP2. A performance gain was also observed on the Cray T3E. It is clear that the extra operations are well offset by the benefit of the more efficient Level 3 BLAS routines.

The current factorization algorithm has two limitations to parallelism. Here we explain, by examples, what the problems are, and speculate as to how the algorithm may be improved in the future. In the following matrix notation, the zero blocks are left blank. For each nonzero block we mark in **box** the process which owns the block.

—Parallelism from the sparsity.

Consider a matrix with 4-by-4 blocks mapped onto a 2-by-2 process mesh.

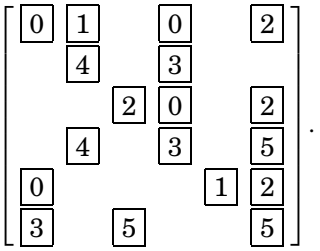
$$\begin{bmatrix} \boxed{0} & \boxed{1} & \boxed{0} & \boxed{1} \\ & \boxed{3} & \boxed{2} & \boxed{3} \\ \boxed{0} & \boxed{1} & \boxed{0} & \\ & \boxed{3} & & \boxed{3} \end{bmatrix}.$$

Although matrix column 2 depends on column 1, not all processes in column 2 depend on column 1. Only process 1 depends on the L block on process 0. Process 3 could start factorizing column 2 at the same time as process 0 is factorizing column 1, before process 1 starts factorizing column 2. But the current algorithm requires all the column processes to factorize the column synchronously, thereby introducing idle time for process 3. We can relax this constraint by allowing the diagonal process (3 in this case) to factorize the diagonal block and then send the factorized block down to the off-diagonal processes (using `mpi_isend`), even before the off-diagonal processes are ready for this column. This would eliminate some artificial interprocess dependencies and potentially reduce the length of the critical path.

Note that this kind of independence comes from not only the sparsity, but also the 2D process-to-matrix mapping. An even more interesting study would be to formalize these 2D task dependencies into a task graph, and perform some optimal scheduling on it.

—Parallelism from the directed acyclic elimination graphs [Gilbert and Liu 1993] (often referred to as *elimination dags* or *edags*).

Consider another matrix with 6-by-6 blocks mapped onto a 2-by-3 process mesh.



Columns 1 and 3 are independent in the elimination dags. The column process sets {0, 3} and {2, 5} could start factorizing columns 1 and 3 simultaneously. However, since process 2 is also involved in the update task of block $(5, 6)$ associated with Step 1 and our algorithm gives precedence to all the tasks in Step 1 over any task in Step 3, process 2 does not factorize column 3 immediately. We may change this task precedence by giving the factorization task of a later step higher priority than the update tasks of the previous steps, because the former is more likely to be on the critical path. This would better exploit the task independence coming from the elimination dags.

We expect the above improvements will have a large impact for very sparse and/or very unsymmetric matrices, and for the orderings that give wide and bushy elimination dags, such as nested dissection.

The triangular solution algorithm is also designed around the same distributed 2D data structure. The forward substitution proceeds from the bottom of the elimination dag to the root, whereas the back substitution proceeds from the root to the bottom. The algorithm is based on a sequential variant called "inner product" formulation. The execution of the program is completely *message-driven*. Each process is in a self-scheduling loop, performing appropriate local computation depending on the type of the message received. The entirely asynchronous approach enables a large overlap between communication and computation and helps to overcome the much higher communication to computation ratio, in this phase.

3.3 Comments on the Algorithmic Differences

Both approaches use Level 3 BLAS to perform the elimination operations. However, in MUMPS, the frontal matrices are always square. It is possible that there are zeros in the frontal matrix, especially if there are delayed pivots, or the matrix structure is markedly asymmetric, but the present implementation takes no advantage of this sparsity, and all the counts measured assume the frontal matrix is dense. It is shown in Amestoy and Puglisi [2000] that one can detect and exploit the structural asymmetry of the frontal matrices. With this new algorithm, significant gains can be obtained both in memory and in time to perform the factorization. For example, using MUMPS with the new algorithm, the number of operations to factorize matrices LHR71C and TWOTONE would be reduced by 30% and 37%, respectively. The approach, tested on the shared memory multifrontal

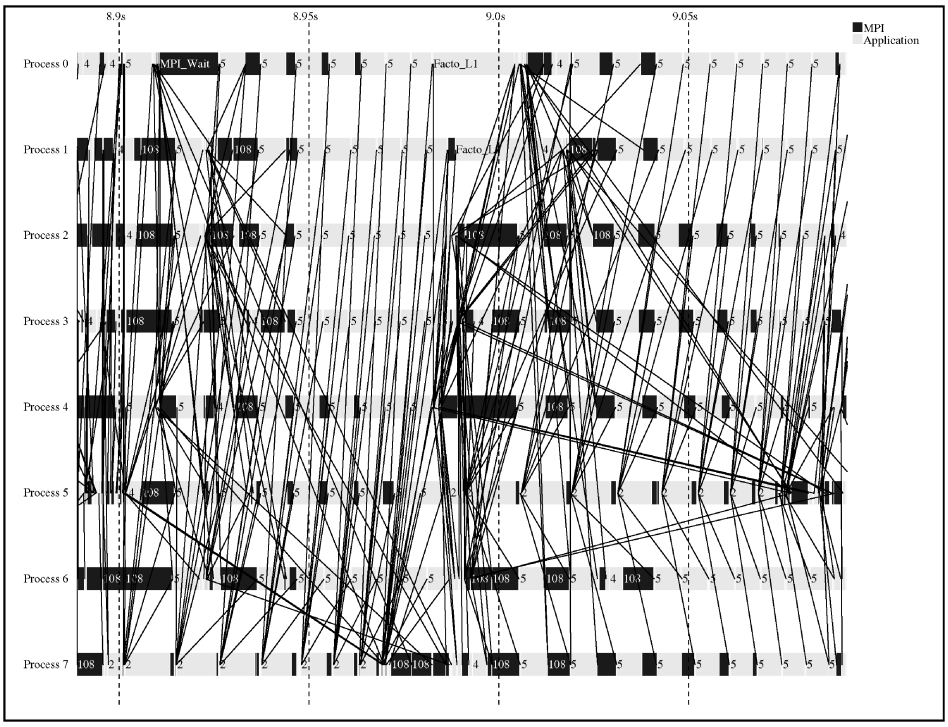


Fig. 3. Illustration of the asynchronous behaviour of the MUMPS factorization phase.

code MA41 [Amestoy and Duff 1993] from HSL [2000], is however not yet available in the current version of MUMPS. In SuperLU, advantage is taken of sparsity in the blocks, and usually the dense matrix blocks are smaller than those used in MUMPS. In addition, SuperLU uses a more sophisticated data structure to keep track of the irregularity in sparsity. Thus, the uniprocessor Megaflop rate of SuperLU is much worse than that of MUMPS. This performance penalty is to some extent alleviated by the reduction in floating-point operations because of the better exploitation of sparsity. As a rule of thumb, MUMPS will tend to perform particularly well when the matrix structure is close to symmetric, while SuperLU can better exploit asymmetry. We note that, even if the same ordering is input to the two codes, the computational graph generated in each case will be different. In the case of MUMPS, the assembly tree generated by MC47 is used to drive the MUMPS factorization phase, while, for SuperLU, the directed acyclic graphs (*dags*) are built implicitly.

In Figures 3 and 4, we use a vampir trace [Nagel et al. 1996] to illustrate the typical parallel behaviour of both approaches. These traces correspond to a zoom in the middle of the factorization phase of matrix BBMAT on 8 processors of the CRAY T3E. Black areas correspond to time spent in communications and related MPI calls. Each line between two processes corresponds to one message transfer. From the plots, we can see that SuperLU has distinct phases for local computation and interprocess communication, whereas for MUMPS, it is hard to distinguish when the process performs computation and when it

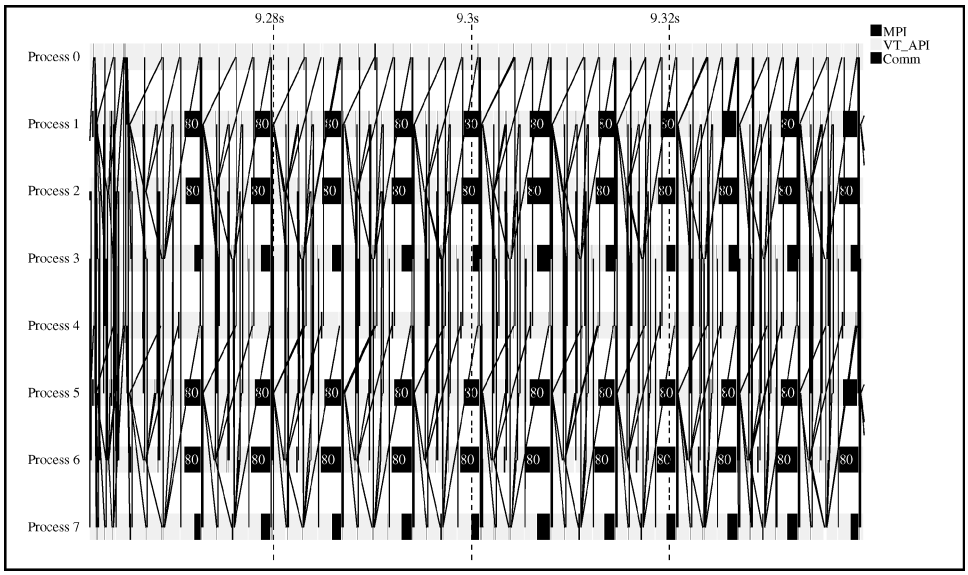


Fig. 4. Illustration of the relatively more synchronous behaviour of the SuperLU factorization phase.

transfers a message. This is due to the asynchronous scheduling algorithm used in MUMPS, which may have a better chance of overlapping communication with computation.

4. IMPACT OF PREPROCESSING AND NUMERICAL ISSUES

In this section, we first study the impact on both solvers of the preprocessing of the matrix. In this preprocessing, we first use row or column permutations to permute large entries onto the diagonal. In Section 4.1, we report and compare both the structural and the numerical impact of this preprocessing phase on the performance and accuracy of our solvers. After this phase, a symmetric ordering (minimum degree or nested dissection) is used, and we study the relative influence of these orderings on the performance of the solvers in Section 4.2. We also comment on the relative cost of the analysis phase of the two solvers.

4.1 Use of a Preordering to Place Large Entries onto the Diagonal and the Cost of the Analysis Phase

Duff and Koster developed several algorithms for permuting a sparse matrix so that the diagonal entries are large relative to the off-diagonal entries [Duff and Koster 2001]. They have also written a computer code, MC64 (available from HSL [2000]), to implement this algorithm. Here, we use option 5 of MC64 which maximizes the product of the modulus of the diagonal entries and then scales the permuted matrix so that it has diagonal entries of modulus one and all off-diagonals of modulus less than or equal to one.

The importance of this preordering and scaling is clear. For MUMPS, it should limit the amount of numerical pivoting (which increases the overall cost)

during the factorization. For SuperLU, we expect such a permutation to be even more crucial, reducing the number of small pivots that are modified and set to $\varepsilon^{\frac{1}{2}}\|A\|_1$. Li and Demmel [1998] gave a detailed analysis about the effect of this preordering on the backward error and accuracy using static pivoting, based on experiments with more than 60 unsymmetric matrices from real applications. Duff and Koster [1999] studied the benefits of using this preordering in iterative solvers and preconditioning. Benzi, Haws and Tůma [2000] conducted more extensive experiments on the effect of MC64 on preconditioning strategies.

The MC64 code of Duff and Koster [2001] is usually quite efficient and so should normally require little time relative to the matrix factorization, even if the latter is executed on many processors while MC64 runs on only one processor. Results in this section will show that although this is often true, there are cases when MC64 can be quite expensive so that it is of benefit to develop a strategy to use this preordering only when it will benefit the subsequent numerical factorization. Moreover, matrices which are unsymmetric but have a symmetric or nearly symmetric structure, are a very common problem class. The problem with these is that MC64 performs an unsymmetric permutation and will tend to destroy the symmetry of the pattern. Since both codes use a symmetrized pattern for the sparsity ordering (see Section 4.2) and MUMPS also uses one for the symbolic and numerical factorization, the overheads in having a markedly asymmetric pattern, can be high. Conversely, when the initial matrix is very asymmetric (as for example LHR71C), an unsymmetric permutation may actually help to increase structural symmetry, thus giving a second benefit to the subsequent matrix factorization.

We show the effects of using MC64 on some examples in Table III. In Table VII, we illustrate the relative cost of the main steps of the analysis phase when MC64 is used to preprocess the matrix.

We see in Table III that, for very unsymmetric matrices (LHR71C and TWOTONE), MC64 is really needed by MUMPS and SuperLU to factorize these matrices efficiently. Both matrices have zeros on the diagonal. Because of the static pivoting approach used by SuperLU, unless these zeros are made nonzero by fill-in and are then large enough, they will be perturbed during factorization and a factorization of a nearby matrix will be obtained. In the case of MUMPS, the dramatically higher fill-in obtained without MC64 makes it also necessary to use MC64. For MUMPS, the benefit from using MC64 is both structural (compare columns 3 and 5 of Table IV) and numerical (compare the differences between columns 2 and 3 with the differences between columns 4 and 5 of Table IV). The permuted matrix often has a larger structural symmetry (see column 4 of Table III) so that a symmetric permutation can be obtained on the permuted matrix, that is more efficient in preserving sparsity. SuperLU benefits in a similar way from symmetrization because the computation of the symmetric permutation is based on the same assumption, even if SuperLU preserves the asymmetric structure of the factors better, by performing a symbolic analysis on a directed acyclic graph and exploiting asymmetry in the factorization phase (compare, for example, results with MUMPS and SuperLU on matrices LHR71C, MIXTANK and TWOTONE).

The use of MC64 can also improve the quality of the factors and the numerical behaviour of the factorization phase, and can reduce the number of steps of

Table III. Impact of Permuting Large Entries onto the Diagonal (Using MC64) on the Size of the Factors and the Number of Operations. StrSym Denotes the Structural Symmetry after the Ordering

Matrix	Solver	Ordering	StrSym	Nonzeros in factors ($\times 10^6$)	Flops ($\times 10^9$)
BBMAT	MUMPS	AMD	0.54	46.1	41.5
	—	MC64+AMD	0.50	44.3	36.9
	SuperLU	AMD	0.54	41.2	34.0
	—	MC64+AMD	0.50	40.2	31.2
ECL32	MUMPS	AMD	0.93	42.9	64.6
	—	MC64+AMD	0.93	42.9	64.6
	SuperLU	AMD	0.93	42.4	68.3
	—	MC64+AMD	0.93	42.7	68.4
FIDAPM11	MUMPS	AMD	1.00	16.1	9.7
	—	MC64+AMD	0.46	28.5	29.4
	SuperLU	AMD	1.00	14.0	8.9
	—	MC64+AMD	0.46	24.8	22.0
GARON2	MUMPS	AMD	1.00	2.4	0.3
	—	MC64+AMD	0.83	2.7	0.4
	SuperLU	AMD	1.00	2.1	0.3
	—	MC64+AMD	0.83	2.5	0.4
INVEXTR1	MUMPS	AMD	0.97	31.2	35.8
	—	MC64+AMD	0.86	33.6	38.6
	SuperLU	AMD	0.97	24.8	22.6
	—	MC64+AMD	0.86	28.4	28.0
LHR71C	MUMPS	AMD(*)	0.00	285.8	1431.0
	—	MC64+AMD	0.21	11.8	1.4
	SuperLU	AMD(*)	0.00	222.5	†
	—	MC64+AMD	0.21	7.6	0.5
LNSP3937	MUMPS	AMD	0.87	0.3	0.02
	—	MC64+AMD	0.55	0.4	0.03
	SuperLU	AMD	0.87	0.2	0.02
	—	MC64+AMD	0.55	0.3	0.03
MIXTANK	MUMPS	AMD	1.00	39.1	64.4
	—	MC64+AMD	0.91	45.7	81.5
	SuperLU	AMD	1.00	38.4	64.1
	—	MC64+AMD	0.91	41.2	64.6
RMA10	MUMPS	AMD	1.00	8.9	1.4
	—	MC64+AMD	0.90	9.7	1.6
	SuperLU	AMD	1.00	8.9	1.5
	—	MC64+AMD	0.90	9.3	1.5
TWOTONE	MUMPS	AMD	0.28	235.0	1221.1
	—	MC64+AMD	0.43	22.1	29.3
	SuperLU	AMD	0.28	65.3	159.0
	—	MC64+AMD	0.43	11.9	8.0
WANG4	MUMPS	AMD	1.00	11.6	10.5
	—	MC64+AMD	1.00	11.6	10.5
	SuperLU	AMD	1.00	10.7	9.1
	—	MC64+AMD	1.00	10.7	9.1

(*)Estimation given by the analysis (not enough memory to perform factorization).
†The flop counts for SuperLU are calculated during factorization.

Table IV. Structural and Numerical Benefits of Preprocessing Based on MC64. Number of Operations (in Millions) during the Factorization Phase of MUMPS. Diag. Domin. Matrix: the Matrix to be Factorized is Made Diagonally Dominant (Done after MC64 Based Permutation when MC64 is Used)

	NO MC64		MC64	
	Original matrix	Diag. Domin. matrix	Original matrix	Diag. Domin. matrix
BBMAT	41.5	41.2	36.9	36.9
FIDAPM11	9.7	8.6	29.4	29.4
INVEXTR1	36.8	34.3	38.6	38.5
LHR71C	(*)	715.6	1.4	1.3
TWOTONE	1221.1	240.4	29.3	29.3

(*)Not enough memory to run the factorization phase.

Table V. Illustration of the Convergence of Iterative Refinement

		SuperLU		MUMPS	
Matrix	Iter.	No MC64	MC64	No MC64	MC64
BBMAT		Err = 2.1e−03	Err = 5.6e−01	Err = 1.3e−06	Err = 6.5e−08
	0	Berr = 4.0e−09	1.3e−05	Berr = 7.4e−11	1.2e−11
	1	Berr = 7.7e−16	4.6e−11	Berr = 3.2e−16	3.2e−16
	2	Berr = 5.2e−16	9.7e−15	Berr = 3.2e−16	2.7e−16
	3	Berr =	4.7e−16		
	4	Berr =	5.0e−16		
		Err = 2.5e−09	Err = 2.4e−09	Err = 3.0e−09	Err = 3.5e−09
LNSP3937		Err = 1.6e−01	Err = 2.7e−11	Err = 9.2e−07	Err = 3.6e−11
	0	Berr = 1.6e−07	3.5e−12	Berr = 4.3e−08	1.5e−12
	1	Berr = 1.5e−08	2.2e−16	Berr = 4.7e−16	2.4e−16
	2	Berr = 5.7e−10	2.5e−16	Berr = 2.1e−16	2.0e−16
	3	Berr = 1.6e−11			
	4	Berr = 4.2e−13			
	5	Berr = 1.1e−14			
	6	Berr = 3.2e−16			
	7	Berr = 3.2e−16			
		Err = 1.0e−11	Err = 2.2e−11	Err = 6.3e−12	Err = 6.4e−12
GARON2		Err = 9.2e−07	Err = 3.7e−12	Err = 1.7e−11	Err = 3.4e−12
	0	Berr = 2.5e−10	2.4e−15	Berr = 1.6e−15	2.1e−15
	1	Berr = 3.4e−16	3.8e−16	Berr = 2.2e−16	2.3e−16
	2	Berr = 3.4e−16	3.4e−16	Berr = 2.0e−16	1.8e−16
		Err = 2.9e−12	Err = 3.3e−12	Err = 1.6e−12	Err = 1.3e−12

iterative refinement required to reduce the backward error to machine precision. This is illustrated in Table V where we show the number of steps of iterative refinement required to reduce the componentwise relative backward error, $Berr = \max_i \frac{|r|_i}{(|A|\cdot|x|+|b|)_i}$ [Arioli et al. 1989], to machine precision ($\varepsilon \approx 2.2 \times 10^{-16}$ on the CRAY T3E). Iterative refinement will stop when either the required accuracy is reached, or the convergence rate is too slow (*Berr* does not decrease by at least a factor of two). The true error is reported as $Err = \frac{\|x_{true}-x\|}{\|x_{true}\|}$. This table illustrates the impact of the use of MC64 on the quality of the initial solution obtained with both solvers, prior to iterative refinement. In addition, it shows that, thanks to numerical threshold pivoting, the initial solution is almost always more accurate with MUMPS than with SuperLU, and is usually markedly

so. Note that parallel SuperLU uses static pivoting and has quite a different numerical behaviour from sequential SuperLU, where partial pivoting is used. These observations are further confirmed on a larger number of test matrices in Table VI. The same stopping criterion was applied for these runs as for the runs in Table V. In the case of MUMPS, MC64 can also result in a reduction in the number of off-diagonal pivots and in the number of delayed pivots. For example on the matrix INVEXTR1 the number of off-diagonal pivots drops from 1520 to 109 and the number of delayed pivots drops from 2555 to 42. One can also see in Table V (for example BBMAT) that MC64 does not always improve the numerical accuracy of the solution obtained with SuperLU.

As expected, we see that, for matrices with a fairly symmetric pattern (for example matrix FIDAPM11 in Table III), the use of MC64 leads to a significant decrease in symmetry which, for both solvers, results in a significant increase in the number of operations during factorization. Also, the time spent in MC64 can dominate the analysis time of either solver (see Table VII), even for matrices such as FIDAPM11 and INVEXTR1 for which it does not provide any gain for the subsequent steps. Thus, for both solvers, the default should be to not use MC64 on fairly symmetric matrices. In practice, the default option of the MUMPS package is such that MC64 is automatically invoked when the structural symmetry is found to be less than 0.5. For SuperLU, zeros on the diagonal and numerical issues must also be considered, so that an automatic decision during the analysis phase is more difficult.

We finally compare, in Figure 5, the time spent by the two solvers during the analysis phase, when reordering is based only on AMD (MC64 is not invoked). Since the time spent in AMD is very similar in both cases, this gives a good estimation of the cost difference of the analysis phase of the two solvers. Note that SuperLU is not currently tied to any specific ordering code and does not take advantage of all the information available from an ordering algorithm. A tighter coupling with an ordering, as is the case with MUMPS and AMD, should reduce the analysis time for SuperLU. However, during the analysis phase of SuperLU, all the asymmetric structures needed for the factorization are computed and the directed acyclic graph [Gilbert and Liu 1993] of the unsymmetric matrix must be built and mapped onto the processors. With MUMPS, the main data structure handled during analysis, is the assembly tree, which is produced directly as a by-product of the ordering phase. No further data structures are generated during this phase. Dynamic scheduling will be used during factorization so that only a simple massage of the tree and a partial mapping of the computational tasks onto the processors, are performed during analysis.

4.2 Use of Orderings to Preserve Sparsity

On matrices for which MC64 is not used we show, in Table VIII, the impact of the choice of the symmetric permutation on the fill-in and floating-point operations for the factorization. As was observed in Amestoy et al. [2001], the use of nested dissection can significantly improve the performance of MUMPS. We see here that SuperLU will also, although to a lesser extent, benefit from the use of a nested dissection ordering. We examine the influence of the ordering on

Table VI. Comparison of the Numerical Behaviour, Backward Error (Berr) and Forward Error (Err), of the Solvers. Nb Indicates the Number of Steps of Iterative Refinement

WITHOUT MC64						
		WITHOUT Iter. Ref.		WITH Iterative Refinement		
Matrix	Solver	Berr	Err	Nb	Berr	Err
BBMAT	MUMPS	7.4e−11	1.3e−06	2	3.2e−16	3.0e−09
	SuperLU	4.0e−09	2.1e−03	2	5.2e−16	2.5e−09
ECL32	MUMPS	3.6e−13	3.0e−11	2	3.1e−16	1.4e−11
	SuperLU	2.4e−14	2.6e−11	2	2.9e−16	7.0e−11
FIDAPM11	MUMPS	3.6e−11	1.7e−09	2	2.8e−16	1.2e−12
	SuperLU	1.7e−06	1.9e−04	4	3.1e−16	1.8e−12
GARON2	MUMPS	1.6e−15	1.7e−11	2	2.0e−16	1.6e−12
	SuperLU	2.5e−10	9.2e−07	2	3.4e−16	2.9e−12
INVEXTR1	MUMPS	4.4e−08	8.9e−01	2	8.3e−16	2.8e−05
	SuperLU	1.7e−07	1.0e−01	3	8.0e−16	1.3e−05
LHR71C	MUMPS	Not enough memory				
	SuperLU	Not enough memory				
LNSP3937	MUMPS	4.3e−08	9.2e−07	3	2.1e−16	6.3e−12
	SuperLU	1.6e−07	1.6e−01	7	3.2e−16	1.0e−11
MIXTANK	MUMPS	1.9e−12	4.8e−09	2	5.9e−16	1.4e−11
	SuperLU	3.6e−09	4.4e−04	3	4.8e−16	2.8e−11
RMA10	MUMPS	1.2e−13	8.3e−13	2	5.0e−16	1.2e−12
	SuperLU	2.2e−06	3.8e−05	3	4.2e−16	9.2e−13
TWOTONE	MUMPS	5.0e−07	1.3e−05	3	1.3e−15	2.1e−11
	SuperLU	1.0e+00	6.6e+126	1	1.0e+00	2.6e+220

WITH MC64						
		WITHOUT Iter. Ref.		WITH Iterative Refinement		
Matrix	Solver	Berr	Err	Nb	Berr	Err
BBMAT	MUMPS	1.2e−11	6.5e−08	2	2.7e−16	3.5e−09
	SuperLU	1.3e−05	5.6e−01	4	5.0e−16	2.4e−09
ECL32	MUMPS	5.6e−12	5.6e−10	2	3.0e−16	1.6e−11
	SuperLU	2.9e−14	1.3e−11	2	3.5e−16	1.7e−11
FIDAPM11	MUMPS	4.4e−12	2.3e−10	2	3.6e−16	6.8e−13
	SuperLU	1.3e−01	7.8e−01	12	3.5e−16	1.1e−12
GARON2	MUMPS	2.1e−15	3.4e−12	2	1.8e−16	1.3e−12
	SuperLU	2.4e−15	3.7e−12	2	3.4e−16	3.3e−12
INVEXTR1	MUMPS	6.7e−16	1.6e−05	2	6.3e−16	5.6e−06
	SuperLU	1.0e−05	9.8e−01	3	6.8e−16	1.2e−05
LHR71C	MUMPS	1.1e−05	9.9e+00	3	3.2e−13	1.0e+00
	SuperLU	7.1e−04	3.9e+06	2	8.9e−07	4.2e+07
LNSP3937	MUMPS	1.5e−12	3.6e−11	2	2.0e−16	6.4e−12
	SuperLU	3.5e−12	2.7e−11	2	2.5e−16	2.2e−11
MIXTANK	MUMPS	4.8e−12	2.3e−08	2	4.2e−16	4.0e−11
	SuperLU	8.2e−03	8.7e−01	5	5.1e−16	3.1e−11
RMA10	MUMPS	2.1e−12	3.4e−11	2	5.0e−16	1.0e−12
	SuperLU	1.3e−06	3.9e−05	3	4.9e−16	1.1e−12
TWOTONE	MUMPS	3.2e−13	1.6e−10	2	1.6e−15	2.3e−11
	SuperLU	1.0e−06	9.0e−03	4	6.1e−16	1.6e−11

Table VII. Influence of Permuting Large Entries onto the Diagonal (Using MC64) on the Time (in Seconds) for the Analysis Phase of MUMPS and SuperLU

Matrix	Solver	Preprocess.	Total	MC64	AMD
BBMAT	MUMPS	AMD	4.7	—	3.0
	—	MC64+AMD	7.2	2.1	3.1
	SuperLU	AMD	11.3	—	2.8
	—	MC64+AMD	11.8	2.0	2.9
ECL32	MUMPS	AMD	3.9	—	2.3
	—	MC64+AMD	4.5	0.5	2.3
	SuperLU	AMD	9.0	—	2.1
	—	MC64+AMD	14.1	0.6	2.1
FIDAPM11	MUMPS	AMD	1.7	—	0.6
	—	MC64+AMD	13.1	10.4	1.6
	SuperLU	AMD	2.7	—	0.5
	—	MC64+AMD	14.1	9.1	1.4
GARON2	MUMPS	AMD	0.4	—	0.1
	—	MC64+AMD	0.8	0.4	0.1
	SuperLU	AMD	0.8	—	0.1
	—	MC64+AMD	1.2	0.4	0.1
INVEXTR1	MUMPS	AMD	2.9	—	1.2
	—	MC64+AMD	47.2	42.6	1.5
	SuperLU	AMD	7.1	—	1.2
	—	MC64+AMD	45.8	36.8	1.5
LHR71C	MUMPS	AMD	47.5	—	39.4
	—	MC64+AMD	34.0	31.0	2.0
	SuperLU	AMD	120.6	—	35.0
	—	MC64+AMD	32.0	26.9	1.8
LNSP3937	MUMPS	AMD	0.1	—	0.1
	—	MC64+AMD	0.2	0.1	0.1
	SuperLU	AMD	0.1	—	0.1
	—	MC64+AMD	0.3	0.1	0.1
MIXTANK	MUMPS	AMD	3.2	—	0.8
	—	MC64+AMD	5.8	2.2	0.9
	SuperLU	AMD	8.4	—	0.8
	—	MC64+AMD	11.0	2.2	0.9
RMA10	MUMPS	AMD	2.3	—	0.4
	—	MC64+AMD	4.6	2.3	0.5
	SuperLU	AMD	3.6	—	0.5
	—	MC64+AMD	6.1	2.3	0.6
TWOTONE	MUMPS	AMD	12.7	—	8.7
	—	MC64+AMD	8.8	1.7	4.8
	SuperLU	AMD	21.4	—	7.9
	—	MC64+AMD	12.0	1.7	4.4
WANG4	MUMPS	AMD	1.7	—	0.8
	—	MC64+AMD	2.0	0.2	0.8
	SuperLU	AMD	2.4	—	0.7
	—	MC64+AMD	2.6	0.2	0.7

the performance further in Section 5. We also notice that, for both orderings, SuperLU exploits the asymmetry of the matrix somewhat better than MUMPS (see BBMAT with structural symmetry 0.53). We expect the asymmetry of the problem to be better exploited by MUMPS when the approach described in Amestoy and Puglisi [2000] is implemented.

Table VIII. Influence of the Symmetric Sparsity Orderings on the Fill-in and Floating-Point Operations on the Factorization of Unsymmetric Matrices. (MC64 is not Used)

Matrix	Ordering	Solver	NZ in **LU** $\times 10^6$	Flops $\times 10^9$
BBMAT	AMD	MUMPS	46.1	41.5
		SuperLU	41.2	34.0
	ND	MUMPS	35.8	25.7
		SuperLU	33.9	23.5
ECL32	AMD	MUMPS	42.9	64.6
		SuperLU	42.4	68.3
	ND	MUMPS	24.8	20.9
		SuperLU	24.3	20.7
INVEXTR1	AMD	MUMPS	31.2	35.9
		SuperLU	24.2	21.3
	ND	MUMPS	16.2	8.1
		SuperLU	13.3	5.9
MIXTANK	AMD	MUMPS	39.1	64.4
		SuperLU	38.2	64.4
	ND	MUMPS	19.6	13.2
		SuperLU	18.6	12.9

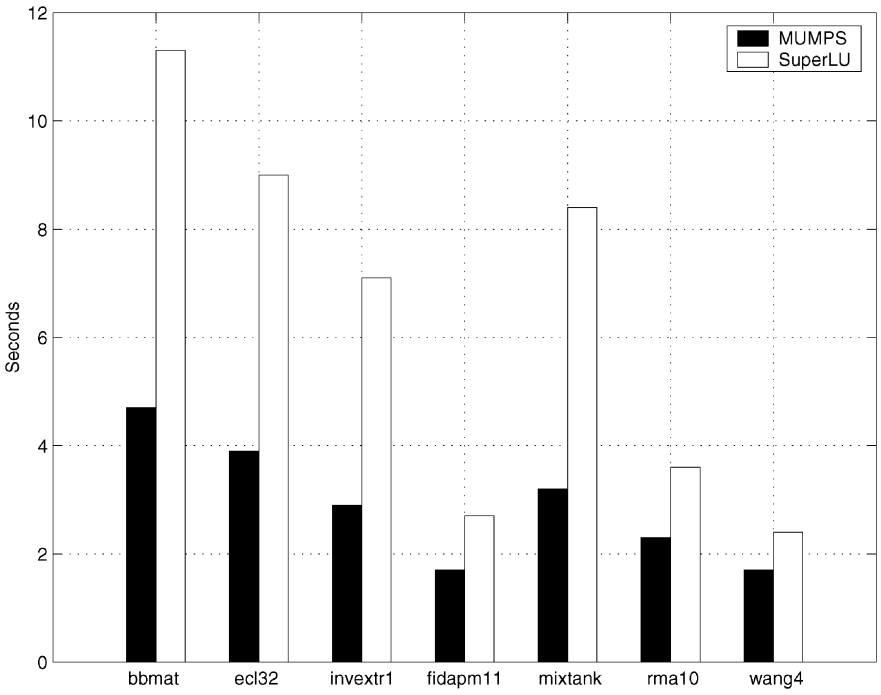


Fig. 5. Time comparison of the analysis phases of MUMPS and SuperLU. MC64 preprocessing is *not* used and AMD ordering *is* used.

Table IX. Factorization Time (in Seconds) of Large Test Matrices on the CRAY T3E

Matrix	Ordering	Solver	Number of processors								
			1	4	8	16	32	64	128	256	512
BBMAT	AMD	MUMPS	—	44.8	23.6	15.7	12.6	10.1	9.5	9.4	11.3
		SuperLU	—	64.7	36.6	21.3	12.8	9.2	7.2	6.7	6.8
	ND	MUMPS	—	32.1	10.8	12.3	10.4	9.1	7.8	8.9	9.7
		SuperLU	—	132.9	72.5	39.8	23.5	15.6	11.1	9.9	9.6
ECL32	AMD	MUMPS	—	53.1	31.3	20.7	14.7	13.5	12.9	14.0	14.1
		SuperLU	—	106.8	56.7	31.2	18.3	12.3	8.2	6.8	6.5
	ND	MUMPS	—	23.9	13.4	9.7	6.6	5.6	5.4	5.4	6.3
		SuperLU	—	48.5	26.6	15.7	9.6	7.6	5.6	5.7	6.1
INVEXTR1	ND	MUMPS	31.0	12.2	6.1	4.0	3.7	3.1	3.9	5.0	6.5
		SuperLU	68.2	21.3	12.8	8.2	5.6	4.9	3.7	3.5	3.8
MIXTANK	ND	MUMPS	40.8	12.4	7.5	5.3	3.8	3.3	3.2	3.6	4.8
		SuperLU	88.1	25.2	14.2	8.6	5.6	4.6	3.1	3.1	3.1
TWOTONE	MC64	MUMPS	—	40.3	21.8	17.5	12.6	12.9	11.4	11.0	11.7
	+AMD	SuperLU	—	103.8	57.8	32.8	19.5	13.3	9.7	7.6	9.0

"—" Indicates not enough memory.

5. PERFORMANCE ANALYSIS ON GENERAL MATRICES

5.1 Performance of the Numerical Phases

In this section, we compare the performance, and study the behaviour, of the numerical phases (factorization and solve) of the two solvers.

For the sake of clarity, we will only show results using the sparsity ordering giving the least factorization time for each approach. When the best ordering for one code is different from that for the other, results with both orderings will be given. This means that results with both nested dissection and minimum degree orderings are given, thus illustrating the different sensitivity of the codes to the choice of the ordering. We note that, even when the same ordering is given to each solver, they will usually not perform the same number of operations. In general, SuperLU performs fewer operations than MUMPS because it better exploits the asymmetry of the matrix, although the execution time is usually less for MUMPS because of the Level 3 BLAS effect (see Section 5.1.1 for a detailed discussion).

Although results are very often matrix dependent, we will try, as much as possible, to identify some general properties of the two solvers.

5.1.1 *Study of the Factorization Phase.* In Table IX we show the factorization time of both solvers. On the smaller matrices, we report in Table X only results with up to 64 processors.

We observe that MUMPS is usually faster than SuperLU, and is significantly so on a small number of processors. We believe there are two reasons. First, MUMPS handles symmetric and more regular data structures better than SuperLU because MUMPS uses Level 3 BLAS kernels on bigger blocks than those used within SuperLU. As a result, the Megaflop rate of MUMPS on one processor is on average about twice that of the SuperLU factorization. This is also evident in the results on the smaller test problems in Table X and from the results on 3-D grid

Table X. Factorization Time (in Seconds) of Small Test Matrices on the CRAY T3E

Matrix	Ordering	Solver	Number of processors					
			1	4	8	16	32	64
FIDAPM11	AMD	MUMPS	30.9	11.1	7.9	5.9	4.9	4.6
		SuperLU	58.4	16.2	10.2	6.1	4.2	3.4
LHR71C	MC64+AMD	MUMPS	12.7	4.1	2.7	1.6	1.4	1.4
		SuperLU	34.5	16.8	12.5	10.6	8.8	9.5
RMA10	AMD	MUMPS	7.6	2.8	2.1	2.0	1.9	1.8
		SuperLU	11.5	5.2	3.8	3.2	2.7	2.9
WANG4	AMD	MUMPS	29.9	10.8	6.3	4.7	3.5	3.3
		SuperLU	57.0	17.8	10.6	6.8	4.8	4.2

problems in Section 6. Note that, even on the matrix TWOTONE, for which SuperLU performs three times fewer operations than MUMPS, MUMPS is over 2.5 times faster than SuperLU on four processors. On a small number of processors, we also notice that SuperLU does not always fully benefit from the reduction in the number of operations due to the use of a nested dissection ordering (see BBMAT with SuperLU using 4 processors).

Furthermore, we can see that, with matrices that are structurally very asymmetric, SuperLU can be much less scalable than MUMPS. For example, on matrix LHR71C in Table X, speedups of 3.9 and 9.1 are obtained on 32 processors with SuperLU and MUMPS, respectively. This is due to the two parallel limitations of the current SuperLU algorithm described in Section 3.2. First, SuperLU does not fully exploit the parallelism of the elimination dags. Second, the pipelining mechanism does not fully benefit from the sparsity of the factors (a blocked column factorization should be implemented). This also explains why SuperLU does not fully benefit, as MUMPS does, from the better balanced graph generated by a nested dissection ordering.

We see that the ordering very significantly influences the performance of the codes (see results with matrices BBMAT and ECL32) and, in particular, MUMPS generally outperforms SuperLU when a nested dissection ordering is used. While this is not always true on the largest number of processors, the absolute best performance is often obtained by MUMPS on a fewer number of processors. On the other hand, if we use the minimum degree ordering, SuperLU can be faster than MUMPS on a large number of processors. We also see that, on most of our unsymmetric problems, neither solver provides enough parallelism to effectively benefit from using more than 256 processors. Our lack of other large unsymmetric systems gives us few data points in this regime but one might expect that, independently of the ordering, the 2D distribution used in SuperLU should provide better scalability (and hence eventually better performance) on a large number of processors, than the mixed 1D and 2D distribution used in MUMPS. To further analyse the scalability of our solvers, we consider three dimensional regular grid problems in Section 6.

To better understand the performance differences observed in Tables IX and X and to identify the main characteristics of our solvers we show, in Table XI, the average communication volume. The speed of communication can very much depend on the number and the size of the messages. We also

Table XI. Maximum Size of the Messages (Max in Mbytes), Average Volume of Communication (Vol in Mbytes) and Number of Messages Per Processor (#Mess) for Large Matrices during Factorization

			Number of processors								
			4			16			64		
Matrix	Ordering	Solver	Max	Vol	#Mess	Max	Vol	#Mess	Max	Vol	#Mess
BBMAT	AMD	MUMPS	4.9	44	3240	3.3	63	1700	2.9	20	2257
		SuperLU	0.18	81	23412	0.09	61	34176	0.05	35	35035
	ND	MUMPS	2.2	7	2214	2.8	43	1441	1.5	48	3228
		SuperLU	0.17	82	30698	0.09	62	45598	0.04	36	50925
ECL32	AMD	MUMPS	9.7	91	5451	3.7	117	2585	2.9	54	2743
		SuperLU	0.32	90	27437	0.16	67	37486	0.09	39	34981
	ND	MUMPS	8.5	37	3663	2.5	60	1981	1.5	29	2679
		SuperLU	0.25	56	28966	0.13	42	41172	0.07	24	41271
FIDAPM11	AMD	MUMPS	2.5	28	3000	2.4	22	1471	2.4	6	1323
		SuperLU	0.15	27	14768	0.08	20	19114	0.04	12	15621
INVEXTR1	ND	MUMPS	2.2	13	2320	1.1	18	1314	1.5	7	1550
		SuperLU	0.15	31	17774	0.08	23	25824	0.05	13	27123
LHR71C	MC64+AMD	MUMPS	1.0	1	96	1.1	1	342	1.1	1	377
		SuperLU	0.04	21	72932	0.03	15	95653	0.02	8	91640
MIXTANK	ND	MUMPS	3.5	30	3138	1.7	33	1650	1.2	11	1616
		SuperLU	0.19	40	13667	0.11	30	19635	0.05	18	19064
RMA10	AMD	MUMPS	0.7	3	114	0.7	2	302	0.7	1	337
		SuperLU	0.06	18	11346	0.03	13	14124	0.02	7	10883
TWOTONE	MC64	MUMPS	8.8	61	5076	2.9	139	4144	2.1	49	2762
	+AMD	SuperLU	0.26	27	120006	0.15	20	153995	0.05	11	104906
WANG4	AMD	MUMPS	3.9	16	3483	1.5	27	1682	1.5	8	1215
		SuperLU	0.19	24	27728	0.10	18	34495	0.05	10	27561

indicate the maximum size of the messages and the average number of messages. To overlap communication by computation, MUMPS uses fully asynchronous communications (during both sends and receives). The use of non-blocking sends during the more synchronous scheduled approach used by SuperLU also enables overlapping between communication and computation.

It is difficult to make any definitive comment on the average volume of communication, from the results in Table XI. Overall, it is broadly comparable, with either MUMPS or SuperLU sometimes having lower volume, occasionally by a significant amount. However, although the average volume of messages with 64 processors can be comparable with both solvers, there is between one and two orders of magnitude difference in the average number of messages and therefore in the average size of the messages. This is due to the much larger number of messages involved in a fan-out approach (SuperLU) compared to a multifrontal approach (MUMPS). Note that, with MUMPS, the number of messages includes the messages (one integer) required by the dynamic scheduling algorithm, to update the load on the processes.

The average volume of communication per processor, of each solver, depends very much on the number of processors. While, with SuperLU, increasing the number of processors will generally decrease the communication volume per processor, it is not always the case with MUMPS. Note that adding some global information to the local dynamic scheduling algorithm of MUMPS will help to

Table XII. Solve Time (in Seconds) for Large Matrices on the CRAY T3E. "+IR" Shows the Time Spent Improving the Initial Solution Using Iterative Refinement

Matrix	Ordering	Solver	Number of processors								
			1	4	8	16	32	64	128	256	512
BBMAT	AMD	MUMPS	—	0.52	0.37	0.29	0.28	0.28	0.31	0.33	0.38
		SuperLU	—	1.33	1.16	0.75	0.71	0.53	0.51	0.50	0.44
		SuperLU+IR	—	1.80	1.48	1.01	0.93	0.72	0.68	0.62	0.57
	ND	MUMPS	—	0.37	0.35	0.24	0.26	0.26	0.28	0.30	0.32
		SuperLU	—	1.99	1.60	1.07	0.93	0.76	0.65	0.59	0.44
		SuperLU+IR	—	2.43	1.95	1.34	1.16	0.96	0.86	0.78	0.62
ECL32	AMD	MUMPS	—	0.64	0.46	0.37	0.38	0.36	0.42	0.46	0.53
		SuperLU	—	1.72	1.60	1.09	1.13	0.75	0.79	0.66	0.56
	ND	MUMPS	—	0.47	0.32	0.28	0.26	0.24	0.28	0.31	0.36
		SuperLU	—	1.52	1.57	1.02	0.72	0.68	0.68	0.56	0.49
INVEXTR1	ND	MUMPS	0.57	0.30	0.18	0.14	0.14	0.13	0.16	0.18	0.21
		MUMPS+IR	1.50	0.16	0.11	0.27	0.26	0.24	0.23	0.31	0.39
		SuperLU	1.48	0.80	0.77	0.53	0.50	0.38	0.29	0.26	0.21
		SuperLU+IR	2.75	1.24	1.07	0.78	0.71	0.57	0.44	0.42	0.35
MIXTANK	ND	MUMPS	0.67	0.26	0.18	0.14	0.14	0.13	0.16	0.18	0.21
		SuperLU	1.47	0.73	0.68	0.45	0.43	0.31	0.23	0.21	0.17
TWOTONE	MC64	MUMPS	—	1.03	0.81	0.84	0.86	0.85	0.92	0.96	1.05
	+AMD	SuperLU	—	3.49	3.88	2.69	2.61	1.58	1.23	1.03	0.86
		SuperLU+IR	—	6.66	5.65	7.44	3.42	2.73	1.59	1.41	1.17

"—" Indicates not enough memory.

increase the granularity of the 1D-node subtasks without losing parallelism (see Section 3.1) and thus can result in a decrease in the average volume of communication on a large number of processors.

5.1.2 *Study of the Solve Phase.* In section 4.1 we discussed the difference in the numerical behaviour of the two solvers, showing that, in general, SuperLU will involve more steps of iterative refinement than MUMPS, to obtain the same accuracy in the solution.

In this section, we focus on the time spent to obtain the solution. We apply enough steps of iterative refinement to ensure that the componentwise relative backward error (*Berr*) is less than $\sqrt{\varepsilon} = 1.48 \times 10^{-8}$. Each step of iterative refinement involves not only a forward and a backward solve but also a matrix-vector product with the original matrix. With MUMPS, the user can provide the input matrix in a very general distributed format [Amestoy et al. 2001]. This functionality was used to parallelize the matrix-vector products. With SuperLU, the parallelization of the matrix-vector product was easier because the input matrix is duplicated on all the processors.

In Table XII, we report both the time to perform one solution step (using the factorized matrix to solve $\mathbf{A}x = b$) and, when necessary (*Berr* greater than $\sqrt{\varepsilon}$), the time to improve the solution using iterative refinement (lines with "+IR"). With SuperLU, except on ECL32 and MIXTANK which did not require any iterative refinement, one step of iterative refinement was required and was always enough to reduce the backward error to $\sqrt{\varepsilon}$. With MUMPS, iterative refinement was only required on the matrix INVEXTR1 and the backward error was already so close to $\sqrt{\varepsilon}$ (on one processor $Berr = 3.06 \times 10^{-8}$) that on 4 and 8 processors no step

Table XIII. Solve Time (in Seconds) for Small Matrices on the CRAY T3E

Matrix	Ordering	Solver	Number of processors					
			1	4	8	16	32	64
FIDAPM11	AMD	MUMPS	0.48	0.23	0.22	0.19	0.18	0.17
		SuperLU	1.22	0.55	0.51	0.33	0.33	0.23
LHR71C	MC64+AMD	MUMPS	0.90	0.53	0.29	0.21	0.20	0.22
		SuperLU	2.45	2.02	2.14	1.56	1.55	1.17
RMA10	AMD	MUMPS	0.44	0.21	0.22	0.20	0.21	0.21
		SuperLU	0.82	0.50	0.47	0.35	0.33	0.26
WANG4	AMD	MUMPS	0.57	0.27	0.19	0.17	0.15	0.15
		SuperLU	1.20	0.90	1.01	0.68	0.68	0.50

of iterative refinement was required (*Berr* for the initial solution was already equal to 1.17×10^{-8}). In this case, the time reported in the row "+IR" corresponds to the time to perform the computation of the backward error. We first observe (compare, for example, Tables IX and XII) that, on a small number of processors (less than 8), the solve phase is almost two orders of magnitude less costly than the factorization. On a large number of processors, because our solve phases are relatively less scalable than the factorization phases, the difference drops to one order of magnitude. On applications for which a large number of solves might be required per factorization, this could become critical for the performance and might have to be addressed in the future. We show solution times for our smaller matrices in Table XIII where we have not run iterative refinement.

The performance reported in Tables XII and XIII would appear to suggest that the regularity in the structure of the matrix factors, generated by the factorization phase of MUMPS, is responsible for a faster solve phase than that of SuperLU for up to 256 processors. On 512 processors, the solve phase of SuperLU is occasionally faster than that of MUMPS, although in all cases the fastest solve time is recorded by MUMPS usually on a fewer number of processors. The cost of iterative refinement can significantly increase the cost of obtaining a solution. With SuperLU, because of static pivoting, it is more likely that iterative refinement will be required to obtain an accurate solution on numerically difficult matrices (see BBMAT, INVEXTR1 and TWOTONE). With MUMPS, the use of threshold pivoting during the factorization will reduce the number of matrices for which iterative refinement is required. (In our set, only INVEXTR1 requires iterative refinement). For both solvers, the use of MC64 to preprocess the matrix can also reduce the number of steps of iterative refinement, and even avoid the need to use it in some cases (see Section 4.1).

5.2 Memory Usage

In this section, we study the memory used during factorization as a function of both the solver and the number of processors (see Table XIV).

We want to first point out that, because of the dynamic scheduling approach and the threshold pivoting used in MUMPS, the analysis phase cannot fully predict the space that will be required on each processor and an upper bound is therefore used for the memory allocation. With the static task mapping approach used in SuperLU, the memory used can be predicted during the analysis phase.

Table XIV. Memory Used during Factorization (in Megabytes, Per Processor)

Matrix	Ordering	Solver	Number of processors					
			4		16		64	
			Avg.	Max.	Avg.	Max.	Avg.	Max.
BBMAT	AMD	MUMPS	147	176	52	65	32	40
		SuperLU	113	114	50	51	33	34
	ND	MUMPS	114	118	44	53	28	35
		SuperLU	124	128	60	61	43	44
ECL32	AMD	MUMPS	190	212	55	64	32	41
		SuperLU	113	115	42	44	24	25
	ND	MUMPS	132	139	39	44	25	28
		SuperLU	79	81	33	34	21	22
FIDAPM11	AMD	MUMPS	65	67	25	30	16	19
		SuperLU	38	39	16	16	10	10
INVEXTR1	ND	MUMPS	65	85	23	28	17	22
		SuperLU	47	48	22	22	15	16
LHR71C	MC64	MUMPS	54	48	22	25	16	20
	+AMD	SuperLU	49	51	27	29	21	21
MIXTANK	ND	MUMPS	84	87	29	31	19	21
		SuperLU	55	56	23	23	14	15
RMA10	AMD	MUMPS	39	42	17	25	11	21
		SuperLU	32	33	15	16	10	11
TWOTONE	MC64	MUMPS	167	180	57	67	42	60
	+AMD	SuperLU	66	80	35	41	24	24
WANG4	AMD	MUMPS	69	82	22	23	15	20
		SuperLU	33	34	14	14	8	9

In this section, we only compare the memory actually used by the solvers during the factorization phase. This includes reals, integers and communication buffers. Storage for the initial matrix is, however, not included but we have seen, in Amestoy et al. [2001], that the input matrix can also be provided in a general distributed format and can be handled very efficiently by the solver. This option is available in MUMPS. In SuperLU, the initial matrix is currently duplicated on all processors.[7]

We notice, in Table XIV, a significant reduction in the memory required when increasing the number of processors. We also see that, in general, SuperLU requires less memory than MUMPS, although this is less apparent when many processors are used, thus showing the better memory scalability of MUMPS. One can observe that there is little difference between the average and maximum memory usage, showing that both algorithms are well balanced, with SuperLU the better of the two.

Note that memory scalability can be critical on globally addressable platforms where parallelism increases the total memory used. On purely distributed machines such as the T3E, the main factor remains the memory used per processor, which should allow large problems to be solved when enough processors are available.

[7]For MUMPS, note that the storage reported still includes another internal copy of the initial matrix in a distributed *arrowhead* form, which is necessary for the assembly operations during the multifrontal algorithm.

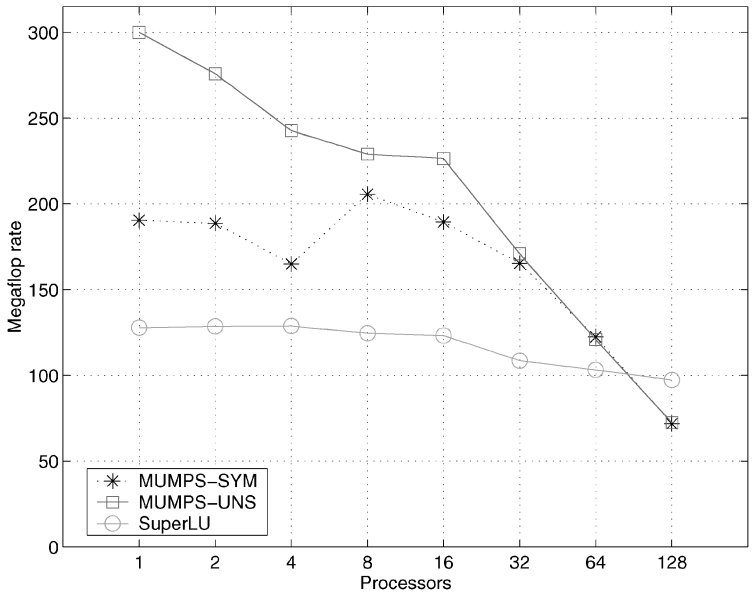


Fig. 6. Megaflop rate per processor (cubic grids, nested dissection).

6. PERFORMANCE ANALYSIS ON 3-D GRID PROBLEMS

To further analyse and understand the scalability of our solvers, we report, in this section, on results obtained for the 11-point discretization of the Laplacian operator on three-dimensional grid problems.

We consider a set of 3-D cubic (NX = NY = NZ) and rectangular (NX, NX/4, NX/8) grids on which a nested dissection ordering is used. The size of the grids used, the number of operations and the timings, are reported in Table XV. When increasing the number of processors, we have tried as much as possible to maintain a constant number of operations per processor, while keeping as much as possible, the same shape of grids. Not all of these constraints could be satisfied thus the number of operations per processor is not completely constant.

Since all of our test matrices are symmetric, we can use MUMPS to compute either an $\mathbf{LDL^T}$ factorization, referred to as MUMPS-SYM, or an **LU** factorization, referred to as MUMPS-UNS. SuperLU will compute an **LU** factorization. Note that, for a given matrix, the unsymmetric solvers (SuperLU and MUMPS-UNS) perform roughly twice as many operations as MUMPS-SYM.

To overcome the problem of the number of operations per processor being non-constant, we first report in Figures 6 and 7, the Megaflop rate per processor for our three approaches on cubic and rectangular grids, respectively. In our context, the Megaflop rate is meaningful because on those grid problems, the number of operations is almost identical for MUMPS-UNS and SuperLU (see Table XV), thus it corresponds to the absolute performance of the approach used for a given problem. We first notice that on up to 8 processors, and independent of the grid shape, MUMPS-UNS is about twice as fast as SuperLU, and also

Table XV. Factorization Time (in seconds) on Cray T3E. **LU** Factorization is Performed for `MUMPS-UNS` and `SuperLU`, $\mathbf{LDL}^T$ for `MUMPS-SYM`

				$\mathbf{LDL}^T$ factorization		**LU** factorization			
				`MUMPS-SYM`		`MUMPS-UNS`		`SuperLU`	
	Grid size			flops		flops		flops	
Processors	NX	NY	NZ	$\times 10^9$	time	$\times 10^9$	time	$\times 10^9$	time
Cubic grids (nested dissection)									
1		29		3.6	18.9	7.2	24.0	7.2	56.3
2		33		8.0	21.2	16.0	29.0	15.9	61.8
4		36		13.4	20.3	26.8	27.6	26.8	52.0
8		41		30.1	18.3	60.1	32.8	60.0	60.2
16		46		59.1	19.5	118.1	32.6	117.9	59.8
32		51		112.7	21.3	225.3	41.2	224.9	64.7
64		57		222.7	28.4	445.1	57.5	444.7	67.3
128		64		444.2	48.3	887.8	95.7	886.4	71.1
Rectangular grids (nested dissection)									
1	96	24	12	2.2	13.2	4.5	16.6	4.5	33.3
2	110	28	13	4.8	12.9	9.5	17.2	9.6	37.6
4	120	30	15	9.0	12.1	17.9	16.7	17.9	36.3
8	136	34	17	18.4	13.7	36.8	20.1	36.6	36.3
16	152	38	19	36.5	12.5	72.8	21.0	72.7	42.2
32	168	42	21	67.8	14.3	135.5	25.4	135.3	43.8
64	184	46	23	118.2	16.3	236.2	32.5	236.0	46.6
128	208	52	26	243.1	24.7	485.8	44.4	485.6	56.1

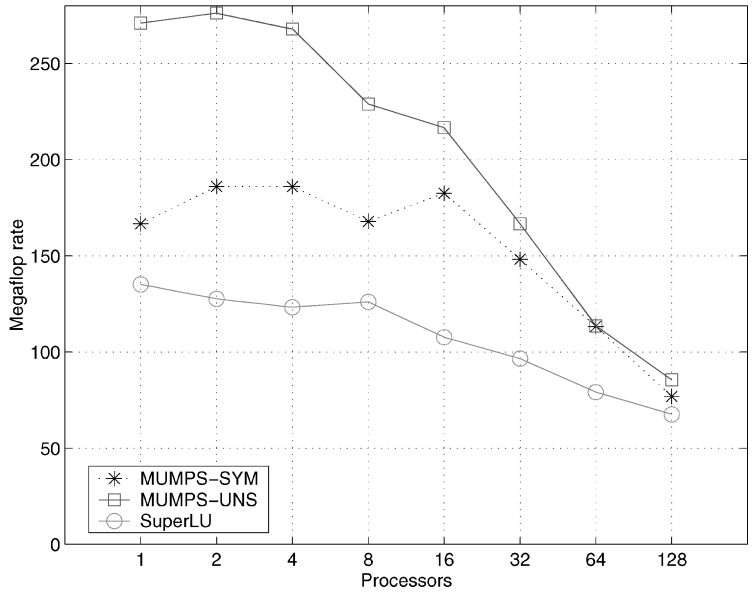


Fig. 7. Megaflop rate per processor (rectangular grids, nested dissection).

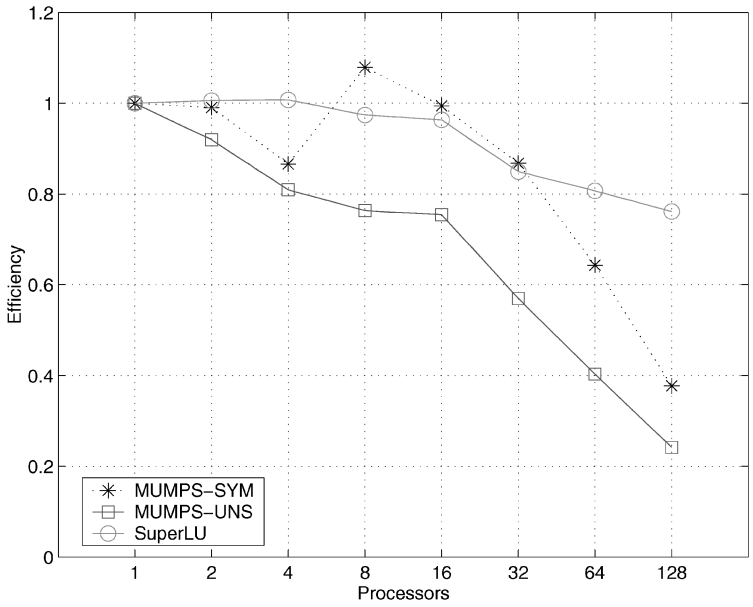


Fig. 8. Parallel efficiency (cubic grids, nested dissection).

has a much higher Megaflop rate than MUMPS-SYM. On 128 processors on both rectangular and cubic grids, all three solvers have similar Megaflop rates per processor.

In Figures 8 and 9, we show the parallel efficiency on cubic and rectangular grids respectively. The efficiency of a solver on p processors is computed as the ratio of its Megaflop rate per processor on p processors over its Megaflop rate on 1 processor.

SuperLU is generally more efficient on cubic grids than MUMPS-UNS even on a relatively small number of processors. MUMPS-SYM is relatively more efficient than MUMPS-UNS and the MUMPS-SYM efficiency is very comparable to that of SuperLU. On a large number of processors SuperLU is significantly more efficient than MUMPS-UNS. The peak ratio between the methods is reached on cubic grids (128 processors) for which SuperLU is about three and two times more efficient than MUMPS-UNS and MUMPS-SYM, respectively. On rectangular grids, the situation is different, with MUMPS-SYM showing comparable parallel efficiency to SuperLU.

Finally, we report in Table XVI a quantitative evaluation of the overhead due to parallelism on cubic grids, using the analysis tool vampir [Nagel et al. 1996]. In the rows "computation", we report the percentage of the time spent doing numerical factorization. MPI calls and idle time due to communications or synchronization are reported in rows "overhead" of the table.

Table XVI shows that SuperLU has less overhead than either version of MUMPS. We also observe a better parallel behaviour of MUMPS-SYM with respect to MUMPS-UNS, as analysed in Amestoy et al. [2000], which is mainly due to the fact

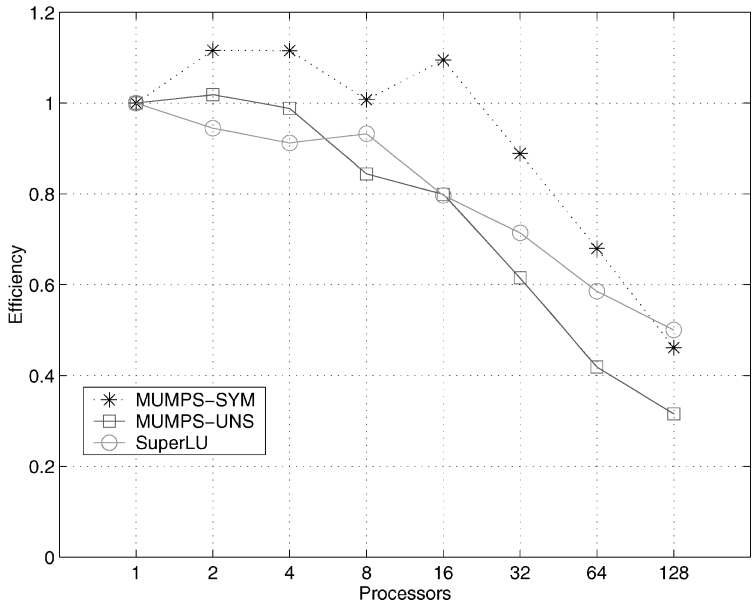


Fig. 9. Parallel efficiency (rectangular grids, nested dissection).

Table XVI. Percentage of the Factorization Time (Cubic Grids, NX = NY = NZ) Spent in Computation and in Overhead Due to Communication and Synchronization

Nprocs	Grid size	MUMPS-SYM	MUMPS-UNS	SuperLU
4	(NX = 36)			
	computation	69%	76%	87%
	overhead	31%	24%	13%
16	(NX = 46)			
	computation	67%	69%	75%
	overhead	33%	31%	25%
64	(NX = 57)			
	computation	50%	36%	56%
	overhead	50%	64%	44%

that node level parallelism provides relatively more parallelism in a symmetric context.

7. CONCLUDING REMARKS

In this paper, we have presented a detailed analysis and comparison of two state-of-the-art parallel sparse direct solvers—a multifrontal solver, MUMPS, and a supernodal solver, SuperLU. Our analysis is based on experiments using a massively parallel distributed-memory machine—the Cray T3E, and eleven matrices from different applications. Our analysis addresses many aspects of the efficiency of the solvers, including the role of preordering steps and their costs, the accuracy of the solution, sparsity preservation,

the total memory required, the amount of interprocessor communication, the times for factorization and triangular solves, and scalability. We found that both solvers have strengths and weaknesses. We summarize our observations as follows.

—Both solvers can benefit from a numerical preordering scheme implemented in MC64, although SuperLU benefits to a greater extent than MUMPS. For MUMPS, this helps reduce the number of off-diagonal pivots and the number of delayed pivots. For SuperLU, this may reduce the need for small diagonal perturbations and the number of iterative refinements. However, since this permutation is asymmetric, it may destroy the structural symmetry of the original matrix, and cause more fill-in and operations. This tends to introduce a greater performance penalty for MUMPS than for SuperLU although recent work by Amestoy and Puglisi [2000] might affect this conclusion. This is why by default MUMPS does not use MC64 on fairly symmetric matrices.

—MUMPS usually provides a better initial solution, due to the effect of dynamic versus static pivoting. With one step of iterative refinement, SuperLU usually obtains a solution with about the same level of accuracy.

—Both solvers can accept as input, any fill-in reducing ordering that is applied symmetrically to both the rows and columns. MUMPS performs better with nested dissection than minimum degree, because it can exploit the better tree parallelism provided by a nested dissection ordering, whereas SuperLU does not exploit this level of parallelism, and its parallel efficiency is less sensitive to different orderings.

—Given the same ordering, SuperLU better preserves the sparsity and the asymmetry of the L and U factors. SuperLU requires less memory than MUMPS, in general, and especially so with smaller numbers of processors. On 64 processors, MUMPS requires 25–30% more memory on average.

—Although the total volume of communication is comparable for both solvers. MUMPS requires many fewer messages, especially with large numbers of processors. The difference can be up to two orders of magnitude. This is partly intrinsic to the algorithms (multifrontal versus fan-out), and partly due to the 1D (MUMPS) versus 2D (SuperLU) matrix partitioning.

—MUMPS is usually faster in both factorization and solve phases. The speed penalty for SuperLU partly comes from the code complexity that is required to preserve the irregular sparsity pattern, and partly because of the greater number of communication messages. With more processors, SuperLU shows better scalability, because its 2D partitioning scheme does a better job in keeping all of the processors busy despite the fact that it introduces more messages.

As we said in the introduction, we started this exercise with the intention of comparing a wider range of sparse codes. However, as we have demonstrated in the preceding sections, the task of conducting such a comparison is very complex. We do feel though, that the experience we have gained in this task will be useful in extending the comparisons in the future.

Table XVII. Distributed Memory Codes

Code	Technique	Scope	Availability	Ref
CAPSS	Multifrontal	SPD	www.netlib.org/scalapack	[Heath and Raghavan 1997]
MUMPS	Multifrontal	SYM/UNS	www.enseeiht.fr/apo/MUMPS	[Amestoy et al. 2001]
PaStiX	Fan-in	SPD	see caption§	[Henon et al. 1999]
PSPASES	Multifrontal	SPD	www.cs.umn.edu/~mjoshi/pspases	[Gupta et al. 1997]
SPOOLES	Fan-in	SYM/UNS	www.netlib.org/linalg/spooles	[Ashcraft and Grimes 1999]
SuperLU	Fan-out	UNS	www.nersc.gov/~xiaoye/SuperLU	[Li and Demmel 1999]
S+	Fan-out†	UNS	www.cs.ucsb.edu/research/S+	[Fu et al. 1998]
WSMP‡	Multifrontal	SYM	IBM product	[Gupta 2000]

§dept-info.labri.u-bordeaux.fr/~ramet/pastix.
†Uses QR storage to statically accommodate any LU fill-in.
‡Only object code for IBM is available. No numerical pivoting performed.

Table XVIII. Shared Memory Codes

Code	Technique	Scope	Availability	Ref
GSPAR	Interpretative	UNS	Grund	[Borchardt et al. 1997]
MA41	Multifrontal	UNS	www.cse.clrc.ac.uk/Activity/HSL	[Amestoy and Duff 1993]
MA49	Multifrontal QR	RECT	www.cse.clrc.ac.uk/Activity/HSL	[Amestoy et al. 1996]
PanelLLT	Left-looking	SPD	Ng	[Ng and Peyton 1993]
PARDISO	Left-right looking	UNS	Schenk	[Schenk et al. 2000]
PSLDLT†	Left-looking	SPD	SGI product	[Rothberg 1994]
PSLDU†	Left-looking	UNS	SGI product	[Rothberg 1994]
SPOOLES	Fan-in	SYM/UNS	www.netlib.org/linalg/spooles	[Ashcraft and Grimes 1999]
SuperLU	Left-looking	UNS	www.nersc.gov/~xiaoye/SuperLU	[Demmel et al. 1999]
WSMP‡	Multifrontal	SYM/UNS	IBM product	[Gupta 2000]

†Only object code for SGI is available.
‡Only object code for IBM is available.

In Tables XVII and XVIII, we summarize the major characteristics of those parallel sparse direct codes of which we are aware. A clear description of the terms used in the tables is given by Heath et al. [1991].

ACKNOWLEDGMENTS

We want to thank James Demmel, Jacko Koster and Rich Vuduc for very helpful discussions. We are grateful to Chiara Puglisi for her comments on an early version of this article and her help with the presentation. We also want to thank John Reid for his comments on the first version of this paper and the anonymous referees for their helpful comments.

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Received December 2000; revised July 2001; accepted October 2001