Recent Progress in General Sparse Direct Solvers

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Abstract. During the past few years, algorithmic improvements alone have shaved almost an order of magnitude off the time required for the direct solution of general sparse systems of linear equations. Combined with a similar increase in the performance to cost ratio due to hardware advances during this period, current sparse solver technology makes it possible to solve those problems quickly and easily that might have been considered impractically large until recently. In this paper, we compare the performance of some commonly used software packages for solving general sparse systems. In particular, we demonstrate the consistently high level of performance achieved by WSMP—the most recent of such solvers. We compare the various algorithmic components of these solvers and show that the choices made in WSMP enable it to run two to three times faster than the best amongst other similar solvers. As a result, WSMP can factor some of the largest sparse matrices available from real applications in a few seconds on 4-CPU workstation.

1 Introduction

Developing an efficient parallel, or even serial, direct solver for general sparse systems of linear equations is a challenging task that has been the subject of research for the past four decades. Several breakthroughs have been made during this time. As a result, a number of very competent software packages for solving such systems are available [2,4,6,8,17,23,26,25].

In this paper, we compare the performance of some commonly used software packages for solving general sparse systems and show that during the past few years, algorithmic improvements alone have shaved an order of magnitude off the time required to factor general sparse matrices. Combined with a similar increase in the performance to cost ratio due to hardware advances during this period, current sparse solver technology makes it possible to solve those problems quickly and easily that might have been considered impractically large until recently. We demonstrate the consistently high level of performance achieved by the Watson Sparse Matrix Package (WSMP) and show that it can factor some of the largest sparse matrices available from real applications in a few seconds on 4-CPU workstation. The WSMP project's original aim was to develop a scalable

parallel general sparse solver for a distributed-memory parallel computer like the IBM SP. However, after completing the serial version of the solver, we realized that we couldn't find enough large problems that would justify the use of an SP with several nodes. Therefore, we tailored the parallel version to use a few CPU's in a shared-memory environment. It is one of the objectives of this paper to make the user community aware of the robustness and speed of the current sparse direct solver technology and encourage scientists and engineers to develop bigger models with larger sparse systems so that the full potential of these solvers can be utilized.

2 Comparison of Serial Performance of Some General Sparse Solvers

In this section, we compare the performance of some of the most well-known software packages for solving sparse systems of linear equations on a single CPU of an IBM RS6000 S80. This is a 600 Mhz processor with a 64 KB level-1 cache and a peak theoretical speed of of 1.2 Gigafllops. 2 GB of memory was available to each solver. A more detailed comparison of the serial and the parallel versions of these solvers can be found in [19]. Table 1 lists all the test matrices, their dimensions, number of nonzeros, and application areas of their origin.

Table 2 lists the serial LU factorization time taken by UMFPACK [8], SuperLU [9], SPOOLES [4], SuperLU_{dist} [22,23], MUMPS [1,2], and WSMP [15,17]. This table also lists the year in which the latest version of each of these packages became available. The best factorization time for each matrix using any solver released before year 2000 is shown in *italics* and the overall best factorization time is shown in **boldface**.

The most striking observation in Table 2 is the range of times that different packages available before 1999 would take to factor the same matrix. It is not uncommon to notice the fastest solver being faster than the slowest one by one to two orders of magnitude. Additionally, none of them gave a consistent level of performance. For example, UMFPACK is 13 times faster than SPOOLES on *e40r5000* but 14 times slower on *fidap011*. MUMPS is clearly the fastest and the most robust amongst the solvers available before 2000. However, the latest solver WSMP appears to be about two and half times faster than MUMPS on this machine on an average. WSMP also has the most consistent performance. It has the smallest factorization time for all but two matrices and is the only solver that does not fail on any of the test matrices.

3 Algorithmic Features of the Solvers

In this section, we list the algorithms and strategies that these solvers use for the symbolic and numerical phases of the computation of the LU factors of a general sparse matrix. We then briefly discuss the role of these choices on the performance of the solvers. The description of all these algorithms is beyond

Table 1. Test matrices with their order (N), number of nonzeros (NNZ), and the application area of origin.

<i>Matrix</i>	<i>N</i>	<i>NNZ</i>	<i>Application</i>
af23560	23560	484256	Fluid dynamics
av41092	41092	1683902	F.E.M.
bayer01	57735	277774	Chemistry
bbmat	38744	1771722	Fluid dynamics
comp2c	16783	578665	Linear programming
e40r0000	17281	553956	Fluid dynamics
e40r5000	17281	553956	Fluid dynamics
ecl32	51993	380415	Electrical eng.
epb3	84617	463625	Thermodynamics
fidap011	16614	1091362	F.E.M.
fidapm11	22294	623554	F.E.M.
invextr1	30412	1793881	Fluid dynamics
lhr34c	35152	764014	Chemical eng.
lhr71c	70304	1528092	Chemical eng.
mil053	530238	3715330	F.E.M.
mixtank	29957	1995041	Fluid dynamics
nasasrb	54870	2677324	F.E.M.
onetone1	36057	341088	Circuit simulation
onetone2	36057	227628	Circuit simulation
pre2	659033	5959282	Circuit simulation
raefsky3	21200	1488768	Fluid dynamics
raefsky4	19779	1316789	Fluid dynamics
rma10	46835	2374001	Fluid dynamics
tib	18510	145149	Circuit simulation
twotone	120750	1224224	Circuit simulation
venkat50	62424	1717792	Fluid dynamics
wang3	26064	177168	Circuit simulation
wang4	26068	177196	Circuit simulation

the scope of this paper. The reader should be able to find them in the citations provided.

- 1. UMFPACK [8]
 - *Fill reducing ordering*: Approximate minimum degree [7] on unsymmetric structure, combined with suitable numerical pivot search during LU factorization.
 - *Task dependency graph*: Directed acyclic graph.
 - *Numerical factorization*: Unsymmetric-pattern multifrontal.
 - *Pivoting strategy*: Threshold pivoting implemented by row-exchanges.
- 2. SuperLU [9]
 - *Fill reducing ordering*: Multiple minimum degree (MMD) [13] on the symmetric structure of AA^T or $A+A^T$, where A is the original coefficient matrix.

Table 2. LU Factorization time on a single CPU (in seconds) for UMFPACK, SuperLU, SPOOLES, SuperLU_{dist}, MUMPS, and WSMP, respectively. The best pre-2000 time is shown in italics and the overall best time is shown in boldface.

Year →	1994	1997	1998	1999	1999	2000
Matrix	UMFPACK	SuperLU	SPOOLES	SuperLU _{dist}	MUMPS	WSMP
af23560	45.5	31.9	10.5	14.7	<i>8.93</i>	6.19
av41092	186.	772.	Fail	Fail	<i>30.6</i>	8.47
bayer01	<i>1.76</i>	2.40	Fail	3.23	2.26	1.33
bbmat	682.	214.	<i>97.7</i>	Fail	113.	36.7
comp2c	120.	3403	287.	42.0	<i>29.3</i>	4.08
e40r5000	29.7	43.9	395.	2.08	1.18	1.55
ec132	Fail	Fail	562.	Fail	<i>145.</i>	41.2
epb3	29.7	24.2	<i>5.00</i>	5.67	5.69	2.16
fidap011	168.	39.9	<i>12.2</i>	16.9	18.7	6.38
fidapm11	944.	88.9	<i>15.1</i>	Fail	25.3	11.2
lhr71c	<i>6.80</i>	12.5	Fail	23.0	11.7	3.05
nasasrb	81.8	102.	<i>25.0</i>	Fail	26.8	10.9
onetone1	12.2	184.	113.	10.7	<i>10.0</i>	7.25
onetone2	<i>1.79</i>	28.3	20.7	3.55	2.81	1.11
pre2	Fail	Fail	Fail	Fail	Fail	362.
raefsky3	39.0	146.	10.0	<i>6.86</i>	8.75	4.54
raefsky4	109.	1983	157.	28.1	<i>27.5</i>	7.78
rma10	15.7	Fail	10.7	<i>5.78</i>	9.62	3.76
tib	<i>0.52</i>	266.	1.75	1.47	0.62	0.31
twotone	30.0	Fail	724.	637.	124.	37.9
venkat50	16.2	Fail	11.6	<i>8.11</i>	19.4	4.40
wang3	106.	3226	62.7	36.9	<i>32.3</i>	13.4
wang4	97.3	318.	<i>16.2</i>	23.7	25.6	12.0

- *Task dependency graph:* Tree.
 - *Numerical factorization:* Supernodal Crout.
 - *Pivoting strategy:* Threshold pivoting implemented by row-exchanges.
3. SPOOLES [4]
- *Fill reducing ordering:* Generalized nested dissection/multisection [5] on the symmetric structure of $A + A^T$.
 - *Task dependency graph:* Tree.
 - *Numerical factorization:* Supernodal Crout.
 - *Pivoting strategy:* Threshold rook pivoting that may perform both row and column exchanges to control growth in both L and U .
4. SuperLU_{dist} [22,23]
- *Fill reducing ordering:* Multiple minimum degree [13] on the symmetric structure of $A + A^T$.
 - *Task dependency graph:* Directed acyclic graph.
 - *Numerical factorization:* Supernodal right-looking.

- *Pivoting strategy*: No numerical pivoting during factorization. Rows are preordered to maximize the magnitude of the product of the diagonal entries [11].

5. MUMPS [1,2]

- *Fill reducing ordering*: Approximate minimum degree [7] on the symmetric structure of $A + A^T$.
- *Task dependency graph*: Tree.
- *Numerical factorization*: Symmetric-pattern multifrontal.
- *Pivoting strategy*: Preordering rows to maximize the magnitude of the product of the diagonal entries [11], followed by unsymmetric row exchanges within supernodes and symmetric row and column exchanges between supernodes.

6. WSMP [15,17]

- *Fill reducing ordering*: Nested dissection [18,16] on the symmetric structure of $A + A^T$.
- *Task dependency graph*: Minimal directed acyclic graph [15].
- *Numerical factorization*: Unsymmetric-pattern multifrontal.
- *Pivoting strategy*: Preordering rows to maximize the magnitude of the product of the diagonal entries [11], followed by unsymmetric partial pivoting within supernodes and symmetric pivoting between supernodes. Rook pivoting (which attempts to contain growth in both L and U) is an option.

The multifrontal method [12,24] for the solving sparse systems of linear equations offers a significant performance advantage over more conventional factorization schemes by permitting efficient utilization of parallelism and memory hierarchy. Our detailed experiments in [19] show that all three multifrontal solvers—UMFPACK, MUMPS, and WSMP—run at a much higher Megaflop rate than their non-multifrontal counterparts. The original multifrontal algorithm proposed by Duff and Reid [12] uses the symmetric pattern of $A + A^T$ to generate an elimination tree to guide the numerical factorization, which works on symmetric frontal matrices. This symmetric-pattern multifrontal algorithm used in MUMPS can incur a substantial overhead for very unsymmetric matrices due to unnecessary dependencies in the elimination tree and extra zeros in the artificially symmetric frontal matrices. Davis and Duff [8] and Hadfield [21] introduced an unsymmetric-pattern multifrontal algorithm, which is used in UMFPACK and overcomes the shortcomings of the symmetric-pattern multifrontal algorithm. However, UMFPACK did not reveal the full potential of the unsymmetric-pattern multifrontal algorithm because of the choice of a fill-reducing ordering (AMD), which has now been shown to be less effective than nested dissection [3]. Moreover, the merging of the ordering and symbolic factorization within numerical factorization slowed down the latter and excluded the possibility of using a better ordering while retaining the factorization code. Other than WSMP, SPOOLES is the only solver that uses a graph-partitioning based ordering. However, it appears that the fill-in resulting from rook pivoting,

which involves both row and column exchanges in an attempt to limit pivot growth in both L and U , overshadows a good initial ordering. Simple threshold partial pivoting yields a sufficiently accurate factorization for most matrices, including all our test cases. Therefore, rook pivoting is an option in WSMP, but the default is a simple threshold pivoting.

WSMP achieves superior levels of performance by incorporating the best ideas of the previous solvers into one package, while avoiding their pitfalls and by introducing new techniques in both symbolic and numerical phases. The analysis or preprocessing phase of WSMP uses a reduction to a block-triangular form [10], a permutation of rows to maximize the magnitude of the product of the diagonal entries [11,20], a multilevel nested dissection ordering [16] for fill-in reduction, and an improved version [15] of the classical unsymmetric symbolic factorization algorithm [14] to determine the supernodal structure of factors and the minimal directed acyclic task- and data-dependency graphs to guide potentially multiple steps of numerical factorization with minimum overhead and maximum parallelism. The unsymmetric-pattern multifrontal LU factorization algorithm of WSMP [15] uses novel data-structures to efficiently handle any amount of pivoting and different pivot sequences without repeating the symbolic phase for each factorization.

4 Performance on a Shared-Memory Parallel Workstation

Having empirically established in Section 2 that MUMPS and WSMP are the fastest and the most robust among the currently available general sparse solvers, in Table 3, we give 1- and 4-CPU factorization times of these two solvers on an IBM RS6000 workstation with 375 Mhz Power 3 processors. These processors have a peak theoretical speed of 1.5 Gigafllops. They share a 4 MB level-2 cache and have a 64 KB level-1 cache each. 2 GB of memory was available to each single CPU run and the 4-CPU runs of WSMP. MUMPS, when run on 4 processors, had a total of 4 GB of memory available to it.

The relative performance of WSMP improves on the Power 3 as it is able to extract a higher Megaflop rate from this machine. The most noteworthy observation from Table 3 (last column) is that out of the 25 test cases, only 3 require more than 10 seconds on a mere workstation and all but one of the matrices can be factored in under 13 seconds. The factorization times reported in Table 3 use the default options of WSMP. Many of the large test matrices, such as *fidapm11*, *mil053*, *mixtank*, *nasasrb*, *raefsky3*, *raefsky4*, *rma10*, *venkat50*, *wang3*, and *wang4* have a symmetric structure and would need even less factorization time if the user switches off the optional pre-permutation of rows to maximize the diagonal magnitudes. This row permutation, which is on by default in WSMP, destroys the structural symmetry and increases the fill-in and operation count of factorization. Some of the matrices, such as *mil053*, *venkat50*, *wang3*, *wang4*, etc. do not require partial pivoting to yield an accurate factorization. Therefore, if the user familiar with the characteristics of the matrices, switches off the piv-

Table 3. Number of factor nonzeros, operation count, and LU factorization (with partial pivoting) times of MUMPS and WSMP on one and four 375 Mhz Power 3 processors.

Matrix	MUMPS				WSMP			
	NNZ _{LU} ×10 ⁶	Ops ×10 ⁹	1 CPU	4 CPU _s	NNZ _{LU} ×10 ⁶	Ops ×10 ⁹	1 CPU	4 CPU _s
af23560	8.34	2.56	7.75	3.82	11.1	3.27	4.17	2.13
av41092	14.1	8.42	19.8	10.7	9.28	2.02	4.71	2.90
bayer01	2.82	.125	2.23	1.26	1.75	.040	1.34	1.33
bbmat	46.0	41.4	76.3	32.2	36.6	20.1	23.7	8.68
comp2c	7.05	4.22	22.3	13.6	3.53	1.09	2.72	1.02
e40r0000	1.72	.172	1.70	1.20	2.32	.250	0.62	0.37
ecl32	42.9	64.6	82.6	41.0	30.3	21.0	23.9	8.71
epb3	6.90	1.17	5.10	2.49	5.64	.451	1.94	1.90
fidap011	12.5	7.01	14.5	11.8	10.2	3.20	4.22	2.01
fidapm11	14.0	9.67	18.2	10.2	14.9	5.21	6.77	2.73
invextr1	30.3	35.6	53.6	29.8	16.3	6.90	10.8	6.36
lhr34c	5.58	.641	5.30	2.43	3.47	.170	1.16	1.13
mil053	75.9	31.8	68.8	26.0	66.2	14.4	24.8	12.9
mixtank	38.5	64.4	80.0	38.4	27.0	19.5	22.9	9.34
nasasrb	24.2	9.45	23.0	16.4	21.7	5.41	7.22	3.86
onetone1	4.72	2.29	7.06	4.21	4.34	1.79	3.88	1.96
onetone2	2.26	.510	2.33	1.41	1.62	.206	0.90	0.94
pre2	358.	Fail	Fail	Fail	97.5	133.	189.	77.0
raefsky3	8.44	2.90	8.37	5.58	9.42	2.57	3.27	1.54
raefsky4	15.7	10.9	19.9	13.2	11.8	4.11	5.09	2.54
rma10	8.87	1.40	8.41	5.38	10.9	1.48	2.59	1.02
twotone	22.1	29.3	68.7	32.1	12.5	10.4	18.3	12.9
venkat50	12.0	2.31	9.75	5.27	12.9	1.75	3.01	1.24
wang3	13.8	13.8	20.1	8.34	11.9	5.91	6.92	3.31
wang4	11.6	10.5	16.6	7.67	12.2	6.09	7.06	3.51

oting for these matrices and, in general, tailors the various options [17] to her application, many of the test problems can be solved even faster.

5 Concluding Remarks

In this paper, we show that recent sparse solvers have improved the state of the art of the direct solution of general sparse systems by almost an order of magnitude. Coupled with the good scalability of these solvers [3] and the availability of relatively inexpensive high-performance parallel computers, it is now possible to solve very large sparse systems in only a small fraction of the time that these solutions would have required just a few years ago. Judging by the availability of real test cases, it appears that the applications that require the solution of such

systems have not kept pace with the improvements in the software and hardware available to solve these systems. We hope that the new sparse solvers will encourage scientists and engineers to develop bigger models with larger sparse systems so that the full potential of the new generation of parallel sparse general solvers can be exploited.

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