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T2SOLV: An Enhanced Package of Solvers for the TOUGH2 Family of Codes

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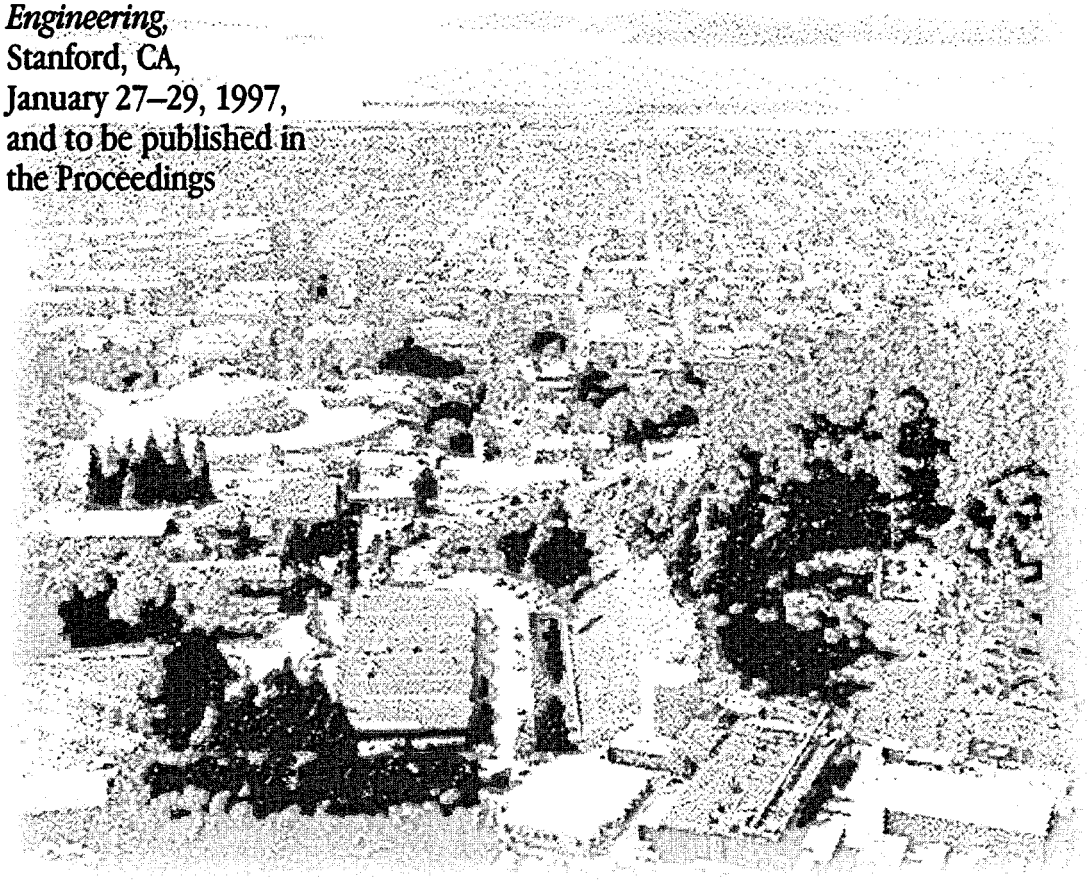

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T2SOLV: AN ENHANCED PACKAGE OF SOLVERS FOR THE TOUGH2 FAMILY OF CODES

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ABSTRACT

T2SOLV is an enhanced package of matrix solvers for the TOUGH2 family of codes. T2SOLV includes all the Preconditioned Conjugate Gradient (PCG) solvers used in T2CG1, the current solver package, as well as LUBAND, a new direct solver, and DLUSTB, a PCG solver based on the BiCGSTAB method. Additionally, T2SOLV includes the D4 grid numbering scheme and two sets of preprocessors. Results from test problems indicate that LUBAND is faster, more reliable and requires less storage than MA28, the BiCGSTAB solver is superior to the other PCG methods in T2SOLV, and that the preprocessors improve the performance of the PCG solvers and allow the solution of previously intractable problems.

INTRODUCTION

Most of the computational work in the numerical simulations of fluid and heat flow in permeable media arises from the solution of large systems of linear equations $\mathbf{Ax} = \mathbf{b}$, where $\mathbf{A}$ is a banded matrix of order N, $\mathbf{x}$ is the vector of the unknowns, and $\mathbf{b}$ the right-hand side. These are solved using either direct or iterative methods. The most reliable solvers are based on direct methods. The robustness of direct solvers comes at the expense of large storage requirements and execution times. Iterative techniques exhibit problem-specific performance and lack the generality, predictability and reliability of direct solvers. These disadvantages are outweighed by their low memory requirements and their speed especially in the solution of very large matrices.

In the TOUGH2 general-purpose reservoir simulator [*Pruess*, 1991] the matrix $\mathbf{A}$ is a Jacobian with a consistent structure. $\mathbf{A}$ has a known block structure with well defined sparsity patterns. Typically, $\mathbf{A}$ is non-symmetric, not positive definite, not diagonally dominant and ill-conditioned. Due to the fact that $\mathbf{A}$ is a Jacobian, the elements of $\mathbf{A}$ in a single row may vary by many orders of magnitude. TOUGH2 creates very challenging matrices with all the attributes that cause most iterative techniques to fail. In addition, the general-purpose nature of TOUGH2 means that different matrix characteristics may arise for different types of problems. This explains the past heavy reliance of TOUGH2 on the direct solver MA28 [*Duff*, 1977].

In the current TOUGH2 version, T2CG1, a package of preconditioned conjugate gradient solvers, complements the MA28 direct solver and significantly increases the size of tractable problems. T2CG1 includes three Preconditioned Conjugate Gradient (PCG) solvers: (a) DSLUBC, a routine based on the Bi-Conjugate Gradient (BiCG) method, (b) DSLUCS, a Conjugate Gradient Squared (CGS) routine, and (c) DSLUGM, a Generalized Minimum Residual (GMRES) routine. Tests of T2CG1 [*Moridis and Pruess*, 1995] on a variety of computing platforms and for problems with up to 30,000 equations have shown that the PCG routines in T2CG1 are significantly (and invariably) faster than MA28 and require far less memory.

T2CG1 is a reliable and fast solver package for most TOUGH2 simulations. In limited cases, however, the PCG solvers in T2CG1 are challenged by classes of certain very demanding numerical simulation problems, as well as by limitations in the underlying algorithms of the PCG (such as occasional oscillatory behavior as steady-state is approached). Moreover, MA28 has not well defined memory requirements and is limited to impractically small problems.

In this paper we discuss T2SOLV, an enhanced package of solvers for the TOUGH2 family of codes. It was developed as a replacement for T2CG1, the current solver package. T2SOLV includes all the PCG solvers used in T2CG1 as well as a new routine, DLUSTB, based on the Bi-Conjugate Gradient Stabilized (BiCGSTAB) method. T2SOLV also replaces the MA28 by LUBAND, a general banded-matrix direct solver. Additionally, it includes an option for using the D4 ordering scheme and two sets of matrix preprocessors to enhance the PCG performance.

THE LUBAND SOLVER

LUBAND is a direct solver which replaces the MA28 solver currently used in the TOUGH2 family of codes. It is derived from routines in the LAPACK [1993] package, which have been enhanced and extensively modified to conform to the TOUGH2 architecture and memory management approach. It is based on a LU decomposition with partial pivoting and row interchange, and allows the solution of systems with a large number of zeroes on the main diagonal. Unlike MA28 (which is a general solver), LUBAND is a banded matrix solver, and as such it capitalizes on the significantly lower and well defined memory requirements of this class of solvers.

LUBAND can be applied without any problem in the current TOUGH2 version and is fully backward compatible with all older input data files. The MESHMAKER routine was also enhanced to minimize the bandwidth of matrix A. Defining work W as the number of multiplications and divisions necessary to convert the full matrix to an upper triangular form and to perform back substitution, *Price and Coats* [1974] showed that for direct solvers $W = NM^2$ and the minimum storage $S = NB$, where N is the order of the matrix and M its half-bandwidth, the full bandwidth being $B = 2M+1$.

For a given problem size N, work and storage are minimized when M is minimized. If I, J, K are the number of subdivisions in the x-, y- and z-directions respectively, the shortest half-bandwidth is $M=JK$ when $I>J>K$. This is called *standard* ordering [*Aziz and Settari,* 1979], and the resulting matrices are banded. As W increases with the square of M, it is obvious that the penalty for non-optimization of the ordering of equations may be substantial.

THE DLUSTB SOLVER

DLUSTB was developed based on the BiCGSTAB(m) algorithm [*Sleijpen and Fokkema*, 1993], a recent extension of the more traditional BiCGSTAB algorithm of *van der Vorst* [1992] which is still an option in T2SOLV. It was developed to address the problem of irregular convergence behavior of the PCG solvers in situations where the iterations are started close to the solution (e.g. when approaching steady state). This is a weakness which afflicts most PCG solvers, and may lead to severe residual cancellation and errors. BiCGSTAB(m) alleviates the irregular (oscillatory) convergence common to the BiCG [*Fletcher*, 1976] and CGS [*Sonneveld*, 1989] methods, thus improving the speed of convergence. It also alleviates potential stagnation or even breakdown problems which may be encountered in traditional BiCGSTAB. According to *Sleijpen and Fokkema* [1993], BiCGSTAB(m) combines the speed of BiCG with the monotonic residual reduction in the Generalized Minimum Residual (GMRES) method, while being faster than both. Theoretical analysis indicates that the BiCGSTAB(m) algorithm is especially well-suited to the solution of very large (i.e. N>50,000) problems [*van der Vorst*, 1992].

DLUSTB uses the Boeing-Harwell matrix storage scheme of TOUGH2, and has the same architecture as the other routines in T2SOLV. As in all other PCG solvers in T2SOLV, it uses a modified LU decomposition for preconditioning. Its memory requirements increase linearly with the order m *of* the Minimal Residual polynomial. For $m = 4$, it requires twice the memory of BiCG or CGS. The optimum value of m is calculated internally in DLUSTB.

THE D4 SCHEME

The Alternating Diagonal Scheme (D4) for gridblock ordering was added as an option to T2SOLV. D4 is a matrix-banding technique, which derives its benefits from the numbering of the grid points. More details can be found in *Price and Coats* [1974].

D4 ordering partitions the matrix into four distinct entities. This structure allows forward elimination through the equations in the lower half of **A**, which zeroes all original entries in the lower left quadrant of **A** and transforms it into a null matrix, while creating non-zero entries in the submatrix $\mathbf{A}_{LU}$ in the lower right quadrant of **A**. The submatrix $\mathbf{A}_{LU}$ is of order $N/2$, and allows the calculation of the lower half of **x**, from which the upper half is obtained by simple substitution. The resulting reduced matrix $\mathbf{A}_{LU}$ can be solved using either direct (D4-direct) or iterative (D4-iterative) methods.

D4 numbering reduces the order of the matrix by 50% while not increasing the bandwidth. Depending on the grid geometry, D4 makes possible execution speed improvement by a factor ranging between 2 and 5.85 [*Price and Coats,* 1974] over standard ordering. Moreover, it reduces storage requirements by a factor of 2. Compared to iterative solvers, D4-direct is competitive in 2-D problems and slower in 3-D problems, while yielding a robust solution. D4 with LUBAND makes possible the robust direct solution of large multi-dimensional problems. However, D4 can only be used with regular grids.

THE Z-PREPROCESSORS

Some of the most numerically challenging matrices arising in TOUGH2 simulations involve a large number of zero entries on the main diagonal of the Jacobian. Such matrices are quite common in non-isothermal two-component systems (such as modeling of two-water geothermal systems using the EOS1

module) and result in at least $0.5N$ of non-zero entries on the main diagonal of the matrix.

Such matrices pose no problem for the LUBAND direct solver. The iterative solvers, however, are directly affected by the diagonal dominance of the matrix and the relative number of the zero entries on the main diagonals. Up to $0.1N$ zero elements have little discernible effect on the PCG solvers in T2SOLV. Matrices with as many as $0.3N$ (and occasionally up to $0.5N$) zero elements are tractable without any special treatment, but usually require a large number of iterations for convergence, i.e. exceeding $0.5N$.

The four Z-preprocessors implemented in T2SOLV enhance the performance of the PCG solvers in matrices with a large number of main-diagonal zeroes. These preprocessors are invoked only when (a) PCG solvers are used to solve (b) matrices with main diagonals populated with a large number of zeroes and (c) the number of the primary variables NEQ>1.

The first option, Z1, replaces the zeroes with a small number (typically 10^{-25}), and can substantially decrease the number of iterations for convergence in matrices with as many as $0.5N$ zero main-diagonal elements. The performance of the PCG solvers in Z1-processed matrices deteriorates rapidly when the main-diagonal zero elements exceed $0.5N$.

The second pre-processing option, Z2, is more computationally intensive and involves linear combinations of the flow equations in each gridblock. Z2 includes a search algorithm which identifies the appropriate equation to be added to the equation corresponding to the zero main-diagonal element. By adding the two equations, the corresponding elements in the Jacobian are replaced with the non-zero sum of the original elements. The Z2 option requires limited computational effort and significantly improves the performance of the PCG solvers.

While very effective, Z2-preprocessing can still suffer from poor conditioning because of persisting lack of diagonal dominance and large differences in the magnitude of the added elements. The problem can sometimes be alleviated by the Z3 option, which precedes the linear combination with normalization with respect to the largest element in the corresponding row. Addition of the normalized elements leads to an improved PCG performance because the relative magnitude of the elements and the corresponding roundoff error can be reduced. The Z3 option is more computationally intensive than Z2. The Z2 and Z3 preprocessors can easily handle up to $0.75N$ zero diagonal elements.

The Z4 option is somewhat more computationally intensive than Z3. It creates unit main-diagonal submatrices through multiplication by the inverse matrix A_M^{-1}, computed by the method of determinants. The PCG performance improvement delivered by Z4 can be affected by roundoff errors; under favorable conditions, it matches those of Z2 and Z3.

THE O-PREPROCESSORS

The O-preprocessors are applied to matrices with no zero entries on the main diagonal and aim to improve the PCG solver performance by improving the matrix conditioning. Four such preprocessors are available in T2SOLV. The first three options, O1 through O3, are in essence steps in the replacement of the A_M submatrix by the unit matrix through a central pivoting process, and involve increasing levels of computational effort.

The O1 option eliminates the lower half of the main-diagonal submatrix, and thus removes NEQ-1 subdiagonals from the global matrix. This reduces the computational effort by reducing the number of non-zero matrix entries and can improve the PCG performance. Execution times are burdened by the additional work for the elimination of the lower half of the matrix, but usually this is overcome by the savings in the PCG computations.

In the O2 option, in addition to O1 the upper half of the main-diagonal submatrix is eliminated, resulting in a diagonal submatrix and eliminating an additional NEQ-1 superdiagonals from the global matrix. Compared to the original, the O2-preprocessed matrix is significantly sparser and better-conditioned and the performance of the PCG solvers can be enhanced. The increased computational effort for the O2 preprocessing is usually compensated by the reduction in the PCG iterations.

The O3 option involves normalization of the O2 matrix, resulting in a unity main diagonal. O3 does not further increase matrix sparsity, but may improve the matrix conditioning. Finally, the O4 option is identical to the Z4 option discussed previously.

TEST PROBLEMS

The solvers were tested in four test problems. Performance results are presented in Figures 1 through 3 and Tables 1 through 4.

Test Problem 1

Test problem 1 involves a study of non-isothermal flow in a "two-water" system. Such systems are known to be the most challenging for the solvers in TOUGH2, as they routinely create matrices with $0.67N$ zeros on the main diagonal. The PCG routines in T2CG1 have in the past been unable to solve even the smallest of this class of problems. The problem discussed here involves injection of "water 2" at a temperature of 30 °C into a geothermal reser-

voir of "water 1" at 280 °C. The EOS1 module is used. The 3-D domain consists of 9×8×5 = 360 gridblocks in (x,y,z), with NK = 2 and NEQ = 3, resulting in a total of N = 1080 equations.

The fundamental weakness of MA28, i.e. its large (especially for 3-D problems) and not well defined memory requirement, was obvious in the problem. Despite memory allocation which sufficed for the LUBAND solution of 3-D problems 15 times larger on the same computer , MA28 could not complete the LU decomposition due to insufficient memory.

Table 1 and Figure 1 show that DLUSTB with and without the Z-preprocessors has the best performance. It is the fastest and requires the least number of PCG iterations to convergence. DLUSTB seems to be the only solver that can proceed without Z-preprocessing. Note that the use of the Z-preprocessors makes possible the solution of a previously-intractable problem by all the PCG solvers in T2SOLV. The Z2 preprocessor seems to offer the best overall performance.

Test Problem 2

Test problem 2 involves a laboratory convection cell experiment. A porous medium consisting of glass beads fills the annular region between the two vertical concentric cylinders. Application of heat generates a thermal buoyancy force, giving rise to the development of convection cells. This problem has been discussed in detail by *Moridis and Pruess* [1992]. The EOS1 module is used. The domain consists of 16×26 = 416 gridblocks in (r,z), with NK = 1 and NEQ = 2, resulting in a total of N = 832 equations.

Table 2 and Figures 2 and 3 show the performance of the various solvers in Problem 2, which does not pose any significant challenges to the T2SOLV routines. DLUSTB is the fastest routine and requires the least number of iterations to convergence.

In this 2D problem LUBAND appears as a competitive alternative. The effect of the O-preprocessors vary. With O1, it is pronounced in terms of PCG iterations and execution times in DSLUBC and DLUSTB, but seems to be limited in DSLUCS and DSLUGM. The evolution of residuals of DSLUCS and DSLUGM in the first Newtonian iteration of the first timestep is identical with and without O1 preprocessing (Figures 2 and 3), while the DSLUCS execution time with O1 increases. Conversely, the use of the O2 and O3 preprocessors seems to offer the greatest improvement in the performance of DSLUCS and DSLUGM.

Test Problem 3

Test problem 3 examines fluid and mass flow in a large three-dimensional model of a geothermal reservoir. The basic computational grid is composed of 15×15×20 = 4500 grid blocks in (x,y,z). Cold water is injected through 4 wells, while hot water is withdrawn from 5 wells. EOS1 is used with NK = 1, NEQ = 2, resulting in a total of N = 9000 equations.

This is a relatively large but well-behaved problem, the size of which precluded the use of a direct solver. The use of D4 allowed a direct solution by LUBAND, which is competitive with the PCG solutions. D4 with DLUSTB had a performance on a par with DLUSTB, the fastest PCG solver. In light of the overhaed needed to set up the D4 system, this result is very encouraging.
DLUSTB demonstrated its superiority by being the fastest and requiring the least number of PCG iterations to convergence. DSLUGM seems to be an inappropriate method for this type of problem. As expected, the benefits of O-preprocessing in this well-behaved system are not evident in the execution times, although the PCG iterations are often reduced. It is noteworthy, however, that despite the increased computational load, the execution times for the O-preprocessed solutions are practically identical to those without any preprocessing.

Test Problem 4

Test problem 4 describes a variation of the Thermal Enhanced Vapor Extraction System process, which is designed to extract solvents and chemicals contained in the Chemical Waste Landfill at Sandia National Laboratories. No NAPL is present in this system. In this process the ground is electrically heated, and boreholes at the center of the heated zone are maintained at a vacuum to draw air and vaporized contaminants into the borehole and to a subsequent treatment facility. The 3-D grid consists of 1300 gridblocks. EOS3 is used (NK = 2, NEQ = 3), and N = 3900 equations are solved. Additional information can be found in *Moridis and Pruess* [1995].

Without any preprocessing, the performance of DLUSTB in this rather well-behaved problem is practically identical to that of DSLUCS. These two are the fastest solvers, but DLUSTB requires the least number of PCG iterations. D4 with LUBAND appears as a competitive alternative. DLUSTB is the most responsive to O1 preprocessing, which results in the fastest solution with the least number of PCG iterations.

CONCLUSIONS AND SUMMARY

The following conclusions can be drawn:

(1) Without any matrix preprocessing, DLUSTB is shown to be a fast and efficient solver which outperforms the other PCG routines. It is the fastest and the most robust in T2SOLV and is shown to be practically free of stagnation, oscillation, and divergence problems.

(2) The use of the Z-preprocessors makes possible the solution of problems which were previously intractable to all the PCG solvers. The combination of the Z-preprocessors with the BiCGSTAB routine gives the best performance in such problems.

(3) In problems which are known to confound the other PCG solvers, DLUSTB converges smoothly but slowly to a solution without invoking the matrix-preprocessing facility.

(4) The O-preprocessors are shown to improve the robustness and decrease the number of iterations to convergence, but their effect depends on the PCG solver in T2SOLV. DLUSTB appears to be the solver most consistently responsive to the O-preprocessors. In well-behaved problems the effect of the O-preprocessors on the execution speed is not significant.

(5) LUBAND is shown to be consistently faster and more reliable than MA28, and can solve much larger problems.

(6) The gains in execution speed when the D4 scheme is used in regular grids are shown to be significant (especially compared to the direct solution). D4-direct seems to be competitive (in speed) to the PCG solvers in medium-sized problems.

In large problems (especially in 3-D systems) and when not limited by significant memory requirements, D4-direct will still offer a predictably large improvement in execution speed over the direct solution, but is expected to be consistently and significantly outperformed by the PCG solvers. The performance of the D4-iterative approach (in which the reduced matrix is solved by the PCG solvers) has not yet been fully assessed.

T2SOLV enables the user of the TOUGH2 family of codes to solve some of the most challenging numerical problems (previously tractable only with direct solvers) using the PCG routines. Its suite of PCG solvers includes all the T2CG1 routines, and is enhanced by the addition of DLUSTB (based on the BiCGSTAB(m) algorithm), which combines speed of convergence with monotonic residual reduction and alleviates the oscillatory behavior of solutions as steady-state is approached (a common problem to most PCG solvers). T2SOLV enhances the performance and robustness of the PCG solvers by introducing a set of matrix preprocessors. Additionally, it introduces LUBAND, a new direct solver capable of solving problems orders of magnitude larger than the MA28 routine in T2CG1. It also doubles the size of problems tractable with direct solvers by implementing a D4 Alternative Diagonal Numbering option.

Table 1. Solver Performance in Problem 1 (Macintosh PowerPC 9500/132)

SOLVER	PP	Δts	NI	Imx	Imn	IT	ET
MA28	Fails - insufficient memory						
LUBAND	-	8	25	-	-	-	63.9
DSLUBC	-	Fails					
	Z1	Fails					
	Z2	8	29	109	5	830	29.0
	Z3	8	28	109	7	877	29.6
DSLUCS	-	Fails					
	Z1	Fails					
	Z2	12	41	109	4	1002	38.6
	Z3	12	46	109	4	1253	46.5
DSLUGM	-	Fails					
	Z1	Fails					
	Z2	8	30	51	7	531	21.3
	Z3	8	28	27	2	496	19.3
DLUSTB	-	Fails					
	Z1	15	94	109	7	642	93.2
	Z2	8	25	20	4	289	16.9
	Z3	8	25	27	4	288	17.0

PP: Preprocessors
Δts: Number of timesteps
NI: Newtonian iterations
Imx: Maximum number of PCG iterations
Imn: Minimum number of PCG iterations
IT: Total PCG iterations
ET: Execution time (sec)

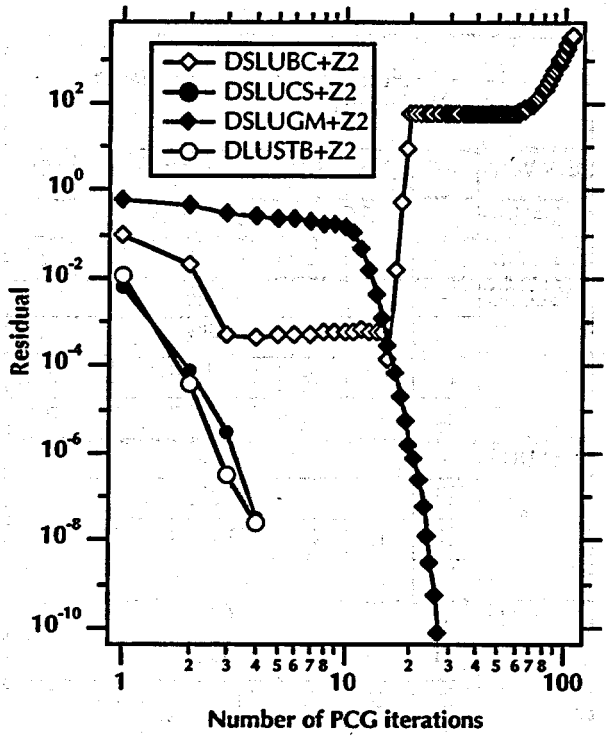

Fig. 1. PCG solvers with Z2 preprocessing in Test Problem 1 (1st NI of the 1st Δt).

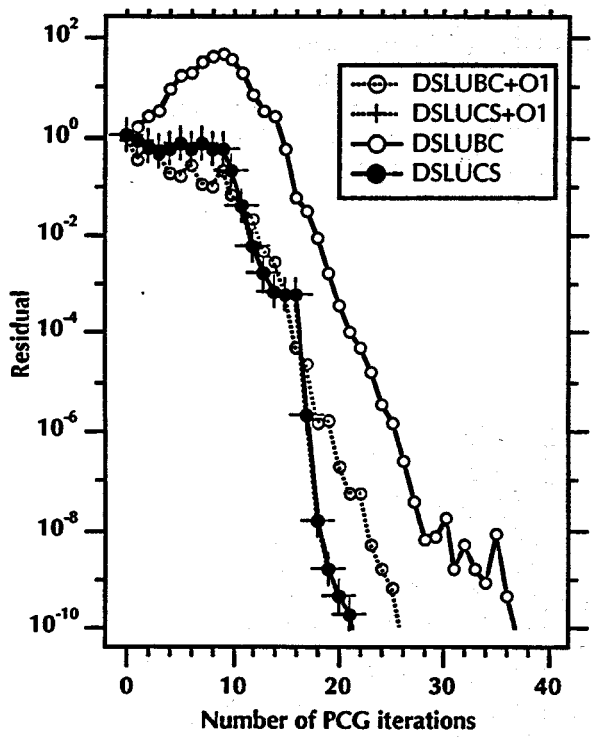

Fig. 2. DSLUBC and DSLUCS performance with and without O1 preprocessing in Test Problem 2 (1st NI of the 1st Δt).

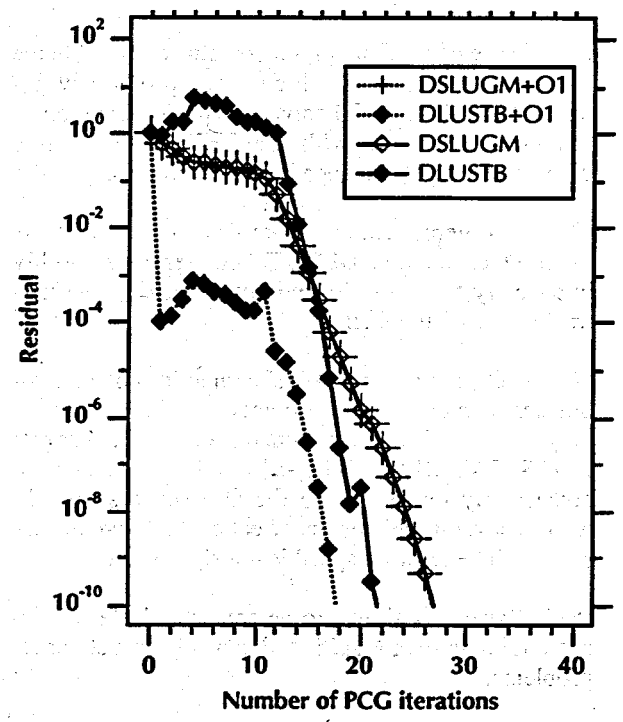

Fig. 3. DSLUGM and DLUSTB performance with and without O1 preprocessing in Test Problem 2 (1st NI of the 1st Δt).

Table 2. Solver Performance in Problem 2 (Macintosh PowerPC 9500/132)

SOLVER	PP	Δt	NI	Imx	Imn	IT	ET
MA28	-	26	108	-	-	-	78.1
LUBAND	-	27	111	-	-	-	55.8
DSLUBC	-	28	119	45	27	3275	56.2
	O1	26	105	41	23	2798	49.1
	O2	28	110	42	23	2868	50.9
	O3	26	106	53	21	2867	50.4
DSLUCS	-	26	112	37	18	2437	49.7
	O1	29	131	33	18	2851	59.0
	O2	28	111	35	18	2281	48.6
	O3	27	106	35	18	2187	46.9
DSLUGM	-	26	107	59	21	3644	50.3
	O1	26	105	58	21	3532	49.4
	O2	26	96	59	21	3021	44.0
	O3	26	98	59	21	3118	45.2
DLUSTB	-	26	106	37	1	1829	42.1
	O1	26	98	41	1	1685	38.9
	O2	26	102	39	1	1684	40.6
	O3	26	98	30	14	1728	39.7

Table 3. Solver Performance in Problem 3 (DEC AlphaStation 200/233)							
SOLVER	PP	Δt	NI	Imx	Imn	IT	ET
MA28	Insufficient Memory						
LUBAND	Insufficient Memory						
D4+ LUBAND	-	10	46	-	-	-	786
D4+ DLUSTB	-	10	46	57	43	1736	426
DSLUBC	-	10	46	106	63	2623	579
	O1	10	46	75	57	2477	565
	O2	10	46	75	52	2475	563
DSLUCS	-	10	46	95	50	2051	488
	O1	10	46	98	50	2034	485
	O2	10	46	94	50	2033	487
DSLUGM	-	10	46	930	95	14842	2087
	O1	10	46	930	95	14994	2178
	O2	10	46	930	95	15113	2189
DLUSTB	-	10	46	58	41	1736	423
	O1	10	46	60	37	1695	421
	O2	10	46	58	37	1719	429

Table 4. Solver Performance in Problem 4 (DEC AlphaStation 200/233)							
SOLVER	PP	Δt	NI	Imx	Imn	IT	ET
MA28	Insufficient Memory						
LUBAND	-	50	249	-	-	-	1227
D4+ LUBAND	-	50	249	-	-	-	678
DSLUBC	-	50	249	29	7	4756	712
	O1	50	250	28	7	4712	701
DSLUCS	-	50	249	29	4	3681	639
	O1	50	249	26	4	3669	649
DSLUGM	-	50	249	27	7	3986	506
	O1	50	249	26	7	3984	508
DLUSTB	-	50	249	15	4	2544	509
	O1	50	249	15	4	2232	484

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