SOME IMPLEMENTATIONS OF MULTIGRID LINEAR SYSTEM SOLVERS

P.W. Hemker and P.M. de Zeeuw

(Centre for Mathematics and Computer Science, The Netherlands)

ABSTRACT

In this paper portable and efficient FORTRAN implementations for the solution of linear systems by multigrid are described. They are based on ILU- or ILLU- relaxation. Scalar and vector versions are compared. Also a complete formal description of a more general multigrid algorithm is given in ALGOL 68.

1. INTRODUCTION

At the moment several implementations of multigrid methods are known for the solution of linear systems that arise from the discretization of more or less general elliptic partial differential equations (Dendy, (1982), Foerster and Witsch (1982), Hemker, Kettler, Wesseling and de Zeeuw (1983)). Also some experiences for computations on vector machines such as the CRAY 1 or the CYBER 205 have been reported (Barkai and Brandt (1983), Dendy (1983), Hemker, Wesseling and de Zeeuw (1983)). It appears that really efficient programs are now available. E.g. for the Poisson equation a code has been developed (Barkai and Brandt (1983)) for the CYBER 205, that solves the problem "up to truncation error" in 0.36 µsec per meshpoint. It will be clear that -even with the present day computer technology- such a high speed can be obtained only when the computer code is specially tuned for the one particular problem and for the one particular machine.

In this paper we discuss the implementation of multigrid methods, not for a particular machine or problem, but for general elliptic 7-point difference equations and in a machine independent programming language. We describe two FORTRAN codes of which the purpose is to provide the user with a program that efficiently solves a large class of difference equations. A first code of this type was introduced by Wesseling (1982a). The codes are autonomous, i.e. they solve the linear systems of equations just like any standard subroutine for the solution of linear systems. The user has to specify only the matrix and the right hand side. Two versions of the codes are available -both in portable FORTRAN- one for use on scalar- the other for vector- (=pipeline) computers.

In section 2 of this paper we describe the problems to be solved. In section 3 we give an outline of the MG-algorithms used. The structure of the FORTRAN implementation is given in section 4 and in section 5 some remarks are made about computing times. In the first appendix, we present an ALGOL 68 program that gives a complete formal description of the flexible algorithm as mentioned in section 3. In a second appendix we give the user interfaces of the FORTRAN codes.

2. THE DIFFERENCE PROBLEM

We consider the scalar linear second order elliptic PDE in two dimensions

$$a_{11}^{u}_{xx} + 2 a_{12}^{u}_{xy} + a_{22}^{u}_{yy} + a_{1}^{u}_{x} + a_{2}^{u}_{y} + a_{0} = f,$$
 (2.1a)

on a rectangle $\Omega \subset R^2,$ with variable coefficients $a_{\mbox{ij}},$ $a_{\mbox{i}}$ and with boundary conditions

$$\begin{cases} u_n + \alpha u_s + \beta u = \gamma & \text{on } \Gamma_{N'} \\ u = g & \text{on } \Gamma_{D'} \end{cases}$$
 (2.1b)

where Γ_N U Γ_D = $\delta\Omega.$ The subscripts n and s denote the derivates normal to and along the boundary. If the equation (2.1) is discretized on a regular triangulation of the rectangle as given in Fig. 1, then the discretization obtained by a simple finite element method (with piecewise linear trial— and test-functions on the triangulation) will be a linear system

$$A_h u_h = f_h, \qquad (2.2)$$

with a regular 7-diagonal structure. We consider codes for the solution of these linear systems. The 7-point discretization is the simplest one in which also cross-derivatives $\mathbf{u}_{\mathbf{x}\mathbf{y}}$ can be represented. It does not seem worthwhile to consider more complex difference molecules because the solution of higher order discretizations can be performed by means of defect correction iteration in which only systems of the above mentioned form have to be solved.

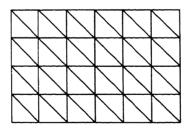


Fig. 1

On the rectangle Ω equidistant computational grids $\Omega^{k},$ k = 0,1,2,...,1, are defined by

$$\Omega^{k} = \{ (x_{1}, x_{2}) \mid x_{i} = m_{i} 2^{-k}, m_{i} = 0, 1, \dots, N_{i} 2^{k} \}.$$
 (2.3)

To obtain a solution u_h on Ω^h , for the codes we consider, the user has to define the matrix \mathbf{A}_h and the right hand side vector \mathbf{f}_h only for the discretization on the finest grid $\Omega^k := \Omega^h$.

The regular structure of the domain and the regular 7-point structure of the difference equations allows a simple structure of the data that are to be transferred to and from the programs. The solution and the right-hand-side can be stored in the most straightforward way in a 1-or 2- dimensional array. The coefficient matrix is stored similarly, by its diagonals.

There are many possible ways to solve the system (2.2) by multigrid. Based on previous work (Hemker, (1982), Hemker (1984), Hemker, Kettler, Wesseling and de Zeeuw (1983), Hemker, Wesseling and de Zeeuw (1983), Kettler (1982), Wesseling (1982a), Wesseling (1982b)), in this paper we select two particularly efficient strategies for which FORTRAN codes have been made available and we give the description of a more general multigrid algorithm. A detailed ALGOL 68 program which implements this more general algorithm is included in appendix 1. It can be used to experiment with the different possibilities.

3. THE MULTIGRID CYCLING ALGORITHM

The general multigrid algorithm for the solution of (2.2) is an iterative cycling procedure in which discretizations of (2.1) on all grids Ω^k , $k=0,1,\ldots,\ell$, are used. We denote these discretizations by A_k $u_k=f_k$, $k=0,1,\ldots,\ell$; k denotes the "level of discretization" and we take $A_k:=A_h$ and $f_k:=f_h$.

One multigrid iteration cycle on level k is defined by the subsequent execution of

- (1) p relaxation sweeps applied to the system $A_k u_k = f_k'$
- (2) the application of a "coarse grid correction", and
- (3) again q relaxation sweeps for $A_{k} u_{k} = f_{k}$.

The coarse grid correction consists of: (1) the computation of

$$f_{k-1} := R_{k-1,k} (f_k - A_k \tilde{u}_k),$$
 (3.1)

where $\tilde{\mathbf{u}}_k$ is the current approximation to the solution and $\mathbf{R}_{k-1,k}$ is a restriction operator which represents the current residual on the next coarser level; (2) the computation of $\tilde{\mathbf{u}}_{k-1}$, an approximation to the solution of the correction equation

$$A_{k-1} u_{k-1} = f_{k-1}. (3.2)$$

This approximation is obtained by application of s multigrid iteration cycles on level k-l, with a zero starting approximation; and (3) updating the current solution \tilde{u}_k by

$$\tilde{u}_{k} := \tilde{u}_{k} + P_{k,k-1} \tilde{u}_{k-1}$$
 (3.3)

where the prolongation operator $P_{k,k-1}$ denotes the interpolation from level k-1 to k.

On the coarsest level another method (at choice) can be used for the computation of $\tilde{\mathbf{u}}_{\text{O}}.$

In principle, the parameters p, q and s and the operators $R_{k-1,k'}$ A_{k-1} , $P_{k,k-1}$ are free to be chosen. Obvious restrictions are p+q>=1 and 1<=s<=3. A natural choice for combination with the finite element discretization (2.2) is the use of a piecewise linear interpolation over triangles in Ω^{k-1} for $P_{k,k-1}$. The corresponding restriction is the transposed operation $R_{k-1,k} = P_{k,k-1}^T$. This prolongation and restriction are exactly the 7-point prolongation and restriction as described in Wesseling (1982b). With these $P_{k,k-1}$ and $P_{k-1,k}$ the finite element discrete operators on coarser grids are easily derived from the fine grid finite element discretization by

$$A_{k-1} = R_{k-1,k} A_k P_{k,k-1}, k = \ell,\ell-1,\ell-2,...,1.$$
 (3.4)

Thus, the coarser grid discretizations are obtained by algebraic manipulation only.

An ALGOL 68 program, based on these choices for the operators is presented as a worked-out illustration in appendix 1. The multigrid cycling procedure is given in \underline{proc} MG. It is imbedded in a complete solution procedure \underline{proc} MGM, which also checks the consistency of the input data, which generates the coarse grid operators by (3.4) and which constructs an initial estimate by "full multigrid", i.e. first it finds an approximate solution on the coarser grid and interpolates this to the next finer ones. The parameters p, q, s, the relaxation procedure and the stopping strategy are still to be chosen. For a set of default parameters (that can be changed by the user) an autonomous procedure is given in \underline{proc} SOLVE SYS. This procedure requires as data only the matrix $\mathbf{A}_{\mathbf{h}}$, the right hand side vector $\mathbf{f}_{\mathbf{h}}$ and the number of levels ℓ . It delivers the solution $\mathbf{u}_{\mathbf{h}}$ without further interference by the user.

In the procedure MGM the user can select his own multigrid strategy (p,q,s) and he may select from different relaxation procedures: Point Gauss Seidel, Line Gauss Seidel or Incomplete Line LU-decomposition relaxation. V-cycles are obtained by s=1, W-cycles by s=2.

4. THE STRUCTURE OF THE FORTRAN IMPLEMENTATIONS

Less flexible but more efficient implementations have been written in FORTRAN. Here we consider two versions of the general MG-algorithm. Both use p= 0, s= q= 1 as the strategy. The first version (MGD1) uses Incomplete LU-decomposition (ILU-) relaxation as the relaxation procedure (Wesseling (1982a)), the other (MGD5) uses Incomplete Line LU-decomposition (ILLU-) relaxation (Kettler (1982)).

MGDl is particularly efficient because of the smoothing properties of the ILU-relaxation (Hemker (1982), Kettler (1982)) and the efficient residual computation. In this version on each level the 7-diagonal matrix $\mathbf{A}_{\mathbf{k}}$ is decomposed as

$$A_{k} = L_{k} U_{k} - C_{k},$$

where \mathbf{L}_k is a lower-triangular matrix (with unity on the main diagonal) and \mathbf{U}_k is an upper-triangular matrix. The requirement that \mathbf{L}_k and \mathbf{U}_k have non-zero diagonals only where \mathbf{A}_k has, determines \mathbf{L}_k and \mathbf{U}_k . The remainder matrix \mathbf{C}_k has only two non-zero diagonals of which the elements are easily derived from \mathbf{L}_k and \mathbf{U}_k .

One relaxation sweep of ILU-relaxation corresponds to the solution of the $\ensuremath{\mathsf{system}}$

$$L_k U_k u_k^{(i+1)} = f_k + C_k u_k^{(i)}$$
.

After such a relaxation sweep the residual is efficiently computed by

$$\mathbf{r}_{k}^{(\mathtt{i}+\mathtt{l})} := \mathbf{f}_{k} - \mathbf{A}_{k} \mathbf{u}_{k}^{(\mathtt{i}+\mathtt{l})} = \mathbf{C}_{k} (\mathbf{u}_{k}^{(\mathtt{i}+\mathtt{l})} - \mathbf{u}_{k}^{(\mathtt{i})}).$$

The other relaxation method, ILLU-relaxation, which is due to J.A. Meyerink, is described in Kettler (1982) and in more detail in Wesseling (these proceedings). A complete description in ALGOL 68 is found in the ALGOL 68 program in the appendix 1.

The global structure of both MGDl and MGD5 is the same. First, in a preparational phase, the sequence of coarse grid operators is constructed by a subroutine RAP, according to (3.4). Then the decomposition is performed (in DECOMP). Finally, in the cycling phase, at most MAXIT iterations of the cycling process are performed. On the basis of intermediate results -the detection of a small residual norm- the iteration can be stopped earlier. This necessitates the computation of this norm (in VL2NOR) in each cycle.

The following is an outline in quasi FORTRAN of the multigrid cycling process in MGDl. At all computational levels $k=1,2,\ldots,\ell,$ the matrix decomposition $\textbf{A}_k=\textbf{I}_k~\textbf{U}_k-\textbf{C}_k$ is available. At the beginning (or end) of each MG-iteration cycle, \textbf{u}_{ϱ} contains the current solution

and r_{ℓ} the corresponding residual. If no initial estimate is available we take u_{ℓ} Ξ O and r_{ℓ} Ξ f.

100 CONTINUE 200 CONTINUE

 $f_{0-1} = R_{0-1, \ell} r_{\ell}$ CALL RESTRI (F,R,L-1) DO 10 K=L-2, 1, -1 $f_k = R_{k,k+1} f_{k+1}$ CALL RESTRI(F,F,K) 10 CONTINUE $u_1 = (L_1 U_1)^{-1} f_1$ CALL SOLVE (U,F,1) DO 20 K=2.L-1 CALL PROLON (U, U, K) $u_k = P_{k,k-1} u_{k-1}'$ $v_k = C_k u_k + f_k$ CALL CTUPF (V, U, F, K) $u_{k} = (L_{k} U_{k})^{-1} V_{k},$ CALL SOLVE (U, V, K) 20 CONTINUE CALL PROLON (R,U,L) $r_{\ell} = P_{\ell_{-}\ell_{-}1} u_{\ell_{-}1}$ DO 30 J=1,NF $r_0 = r_0 + u_0$ R(J)=R(J)+U(J)30 CONTINUE $v_0 = C_0 r_0 + f_0$ CALL CTUPF(V,R,F,L) $u_{\varrho} = (L_{\varrho} U_{\varrho})^{-1} v_{\varrho},$ CALL SOLVE (U, V, L) $r_{g} = C_{g} (u_{g} - r_{g}),$ CALL CTUMV (U,R) RES = VL2NOR(R)||r,||2 IF (RES .LT. TOL) GOTO 200

In the actual implementation of MGDl, the matrix \mathbf{A}_k is not kept in storage, but it is overwritten by \mathbf{L}_k and \mathbf{U}_k . At minimal costs, the remainder matrix \mathbf{C}_k is recomputed each time from \mathbf{L}_k and \mathbf{U}_k (in the subroutines CTUMV and CTUPF).

The other program, MGD5, with ILLU-relaxation, is less efficient for problems like the Poisson equation, but it is more suitable for problems such as the convection-diffusion or the anisotropic diffusion equation, in which a small parameter multiplies the highest derivatives (Hemker (1984), Kettler (1982)).

The cycling process in MGD5 is similar to the one in MGD1. In this case, however, the matrices \mathbf{A}_k are not overwritten and the residual is computed in a straightforward way.

C THE MGD5 ITERATION PROCESS

DO 100 N=1, MAXIT

RES = VL2NOR(R)

100 CONTINUE 200 CONTINUE

IF(RES .LT. TOL) GOTO 200

CALL RESTRI (F,R,L-1) $f_{\ell-1} = R_{\ell-1,\ell} r_{\ell}$ DO 10 K=L-2, 2, -1 CALL RESTRI(F,F,K) $f_k = R_{k,k+1} f_{k+1}$ 10 CONTINUE $u_1 = R_{1,2} f_2$ CALL RESTRI(U,F,1) CALL SMOOTH (U,F,1) relax on level 1, DO 20 K=2,L-1 CALL PROLON(U,U,K) $u_k = P_{k,k-1} u_{k-1}'$ CALL SMOOTH (U.F.K) relax on level k, 20 CONTINUE CALL PROLON(R,U,L) $r_{\ell} = P_{\ell, \ell-1} u_{\ell-1}'$ DO 30 J=1,NF U(J)=U(J)+R(J) $u_0 = u_0 + r_0,$ 30 CONTINUE CALL SMOOTH (U,F,L) relax on level &, CALL RESIDU(R,F,U) $r_{\ell} = f_{\ell} - A_{\ell} u_{\ell},$

All subroutines in the iteration processes in MGDl or MGD5 have their own particular features that make them more or less feasible for vectorization. This will be shown in section 5.

Ir,II,

5. THE EFFICIENCY OF THE FORTRAN IMPLEMENTATIONS

Both algorithms MGDl and MGD5 have been coded in portable ANSI-FORTRAN. The codes pass the PFORT verifier, except that more complex subscript expressions appear than (I*M+N). (These expressions, where I is variable and M and N are constants, are the only ones that are allowed for subscripting by PFORT.) In this portable FORTRAN, optimized versions for scalar- and vector- architecture have been constructed. The corresponding codes are called MGDIS, MGDIV, MGD5S and MGD5V. They are all in the form of a FORTRAN subroutine. Their user-interface is given in appendix 2. The different versions run on several machines among which are the CYBER 205 and the CRAY 1.

If run on scalar architecture, after the preparational phase, the computing time for the programs is proportional to the number of iteration steps and to the number of points in the finest grid. The preparational work to generate the coarse grid operators and to form their decompositions is roughly equivalent to 3 iteration sweeps. The computing times for the scalar optimized versions on the CYBER 170 and the CYBER 205 (using scalar architecture) are given in table 5.1.

Table 5.1

Computing times for MGDl and MGD5 in scalar mode, in usec/(meshpoint.cycle).

	MGDLS	MGD5S
CYBER 170	15.4	24.9
CYBER 205	8.1	11.1

The relative time spent in the different subroutines (as defined in the previous section) is slightly different for the different machines (compilers). These times are given in table 5.2. We notice that the time to compute the prolongations, the restrictions and the norms is small compared to the relaxation or the residual computations. Further we see e.g. that the time spent in CTUMV is 3/4 of the time spent in CTUPF, as is expected (CTUPF runs over all points, whereas CTUMV only works on points on the finest grid).

Table 5.2

The time spent in the different subroutines in scalar mode, expressed in the time spent in a complete iteration cycle.

code machine	MGD1s CY 170	MGD1S CY 205	MGD5S CY 170	MGD5S CY 205
RAP DECOMP	2.32 0.86	1.50 1.40	1.40 0.76	1.10
PROLON RESTRI VL2NOR SOLVE CTUMV CTUPF	0.072 0.089 0.040 0.33 0.15 0.22	0.063 0.040 0.044 0.30 0.22 0.29	0.05 0.06 0.025	0.046 0.030 0.032
RESIDU SMOOTH			0.16 0.65	0.14 0.72

To run portable FORTRAN programs on a vector architecture we have to rely on the auto-vectorization capabilities of the available compilers. Both on the CRAY 1 and on the CYBER 205 we found it possible to vectorize all nonrecursive inner loops in this way. The length of the vectors in the experiments was $(2^{k+1}+1)^j$ with j=1 or j=2 and k=1,...,1, where 1 denotes the finest level of discretization. Most loops run over lines in the grid (j=1), but in a number of cases loops run over the entire net (j=2).

Some comparisons of the CRAY 1 and the CYBER 205 have been given in Hemker, Wesseling and de Zeeuw (1983) There it was shown that the essential difference between both machines in these computations is the

fact that the CYBER 205 is not very effective for loops with a stride unequal to 1. This is particularly important in the restriction and the prolongation, where frequently strides 2 occur. For the restriction the improvement of vector- over scalar- computing time was a factor $4.2-5.6~(\mbox{$\ell$=5,6$})$ for the CRAY 1 and $1.2-2.2~(\mbox{$\ell$=5,6$},7)$ for the CYBER 205.

Nevertheless, it was also shown that -although an essential part of the computation contains recursive loops- a reasonable gain of efficiency was obtained for MGDl using the CRAY l or CYBER 205 vector architecture.

Since the experiences reported in Hemker, Wesseling and de Zeeuw (1983), a new compiler for the CYBER 205 became available (FORTRAN 2.0). With this compiler it was possible to obtain in portable language a more efficient implementation of some recursive loops, whereas with the previous compiler reference had to be made to special "stacklib" routines.

With the portable FORTRAN program on the CYBER 205, an acceleration factor 3.3-4.6 is obtained for MGDl (acceleration of MGDlV in vector mode on a two-pipe CYBER 205 over MGDlS in scalar mode on the same CYBER). The program MGD5 is less amenable to vectorization. Its acceleration factor is only 2.1-2.3. Details of the performance of the different subroutines under vector-mode computation are given in table 5.3. In this table we see the CP-times that are spent in the different subroutines of MGDl and MGD5, when the vector version is run for one iteration cycle on the CYBER 205.

Table 5.3

The time (in m.sec.) for the different subroutines in the vector implementations MGD1V and MGD5V on the CYBER 205 (two pipes, FORTRAN 2.0 compiler). Between brackets the acceleration factor (compared with the scalar versions in scalar mode).

grid	65*65		129	129*129		257*257	
RAP	20	(2.8)	49	(4.2)	143	(5.6)	
DECOMP (MGD1)	12	(4.0)	43	(4.4)	161	(4.6)	
DECOMP (MGD5)	29	(3.1)	96	(3.7)	352	(4.0)	
CYCLE (MGD1)	1.1	(3.3)	3.3	(4.1)	11.6	(4.6)	
CYCLE (MGD5)	2.3	(2.1)	8.2	(2.3)	32.0	(2.3)	
PROLON	0.9	(2.4)	2.1	(4.1)	5.9	(5.7)	
RESTRI	1.2	(1.3)	3.0	(1.8)	9.5	(2.2)	
VL2NOR	0.1	(15)	0.4	(14.8)	1.6	(15.6)	
SOLVE	6.8	(1.6)	22.5	(1.8)	82.5	(1.9)	
CTUMV	0.3	(25)	1.3	(22.8)	5.8	(20.4)	
CTUPF	0.5	(20)	1.8	(21.6)	8.0	(19.4)	
RESIDU	0.7	(9)	3.1	(8.0)	13.2	(7.9)	
SMOOTH	19.3	(1.8)	72.3	(1.8)	287.5	(1.8)	

In table 5.4 we show the megaflop rates for the different subroutines. These rates are defined as the number of floating point operations per second divided by 1.0E+6. One can consider these numbers as a measure of how well the subroutines are suited for the hardware. For different

sizes of the finest grid, the rates for the vector- and scalar-version are given for the CYBER-205 (two pipes, with autovectorization via the FORTRAN 2.0 compiler). For the 65*65 grid also the rate for the CYBER 170-750 (with FORTRAN IV) is shown.

The CP-times used for the computation of the megaflop rate is the time spent in the subroutines on the finest and on all coarser grids. As can be expected for the vectormachine, the numbers are dependent on the vectorlengths (i.e. the number of points in the x-direction or the total number of gridpoints) and whether or not strides greater than one occur. If we compare the first column for the rates of the 129*129 grid with the first column for the rates of the 257*257 grid, we see both increases and decreases. The increases are explained by vectorlengths increasing from 129 to 257, the decreases are explained by vectorlengths increasing from 129*129 to 257*257 = 66049 which makes splitting of the long vectors necessary because of the restricted number of vectoraddresses (namely 65535) on the CYBER-205.

Table 5.4

Megaflop rates for the different subroutines. For each grid the rates for the efficient vector implementation (lst column) and the efficient scalar version (2nd column) on a two-pipe CYBER-205 (FORTRAN 2.0) are given. For the 65*65-grid also the rate for the CYBER 170-750 (FORTRAN IV) is shown (3rd column).

finest grid		65*65		129*129		257*257		
RAP	(MGD1,MGD5)	13.7	4.9	1.8	21.4	5.1	28.7	5.1
DECOMP	(MGD1)	8.6	2.1	1.8	9.4	2.1	9.9	2.1
DECOMP	(MGD5)	7.1	2.3	2.6	8.4	2.3	9.0	2.3
CYCLE	(MGD1)	15.5	4.7	2.6	20.3	4.9	23.0	5.0
CYCLE	(MGD5)	12.1	5.8	2.6	13.3	5.9	13.6	5.9
PROLON	(MGD1,MGD5)	11.5	4.7	2.2	19.0	4.7	26.5	4.6
RESTRI	(MGD1,MGD5)	8.7	6.9	1.6	13.1	7.4	16.3	7.5
VL2NOR	(MGD1,MGD5)	84.5	5.6	3.2	83.2	5.6	82.6	5.6
SOLVE	(MGD1)	11.8	7.5	3.7	13.9	7.7	15.0	7.7
CTUMV	(MGD1)	84.5	3.4	2.6	76.8	3.4	68.3	3.4
CTUPF	(MGD1)	68.5	3.4	2.4	74.5	3.4	66.3	3.4
RESIDU	(MGD5)	84.5	9.4	3.6	75.2	9.4	70.1	8.9
SMOOTH	(MGD5)	9.8	5.5	2.8	10.2	5.5	10.1	5.5

6. APPENDICES

6.1 Appendix 1

In this appendix the text is given of an ALGOL 68 program which implements a general multigrid algorithm. The solutions and the right hand sides are represented in nets, i.e. two-dimensional arrays corresponding to the grid Ω^k . The matrices in netmats, i.e. three-dimensional arrays; here the first 2 indices denote the equation (corresponding to a gridpoint), the 3rd index denotes the diagonal (for details, see the comments on page 98).

```
bristol algol68 text
```

```
PWH/15/12/83
```

```
# solution of a linear system by multigrid
   begin
                                       # a complete description
                                       # not an optimal efficient implementation
# mode declarations
                                             net = ref[,] real;
netmat = ref[,,] real;
                 mode
# elementary operators

      zero
      = ( ref / for i from lwb a to upb a do a [i]:= 0.0 od; a );

      zero
      = ( net / a ) net : ( for i from 1 lwb a to 1 upb a do zero a [i,] od; a );

      zero
      = ( netmat a ) netmat : ( for i from 1 lwb a to 1 upb a do zero a [i,] od; a );

      +:=
      = ( netmat a ) netmat : ( for i from 1 lwb a to 1 upb a do zero a [i,,] od; a );

      +:=
      = ( net / aa,bb ) net : ( int ll = 1 lwb aa, l2 = 2 lwb aa, u1 = 1 upb aa, u2 = 2 upb aa;

                 op
                 op
                 op +:=
                                                                                                                 u1 = 1 <u>upb</u> aa, u2 = 2 <u>upb</u> aa;
                                                                                                               i from 11 to u1 do

j from 12 to u2 do

aa[i,j]+:= bb[i,j] od od; aa);
                                                                                           for for
# prolongation: linear interpolation

        begin
        int
        11 = 1 lwb net, l2 = 2 lwb net; l2 look 
                                                                                                                                        upp= fine[2*11,02*12];
                                                                               jj:= 2*12; upp[jj]:= u4:= uip[12];
                                                                                  for jp from 12+1 to b2
do u3:= u4; u4:= uip[jp];
                                                                                                     upp[jj+:=1]:= (u3+u4)/2;
                                                                                                     upp[jj+:=1]:=
                                                                        ip from 11+1 to b1
ref [] real ui = net [ip-1 ,@ 12],
uip = net [ip ,@ 12],
umm = fine[2*ip-1,@2*12],
ine[2*ip ,@2*12];
                                                                            jj:= 2*12; u2:= ui[12]; u4:= uip[12];
                                                                          for jp from 12+1 to b2
do jj+:= 1; u2:= ui [jp];
u3:= u4; u4:= uip[jp];
                                                                                                 umm[jj] := (u2+u3)/2;
                                                                                                 upp[jj] := (u3+u4)/2;
                                                                                                  jj+:= 1;
                                                                                                  umm[jj] := (u2+u4)/2;
                                                                                                  upp[jj] :=
                                                      od ; fine
                   end ;
```

```
# interpolation: quadratic on finer grids
   odd (b1-l1) or odd (b2-l2)
then lin int pol (net)
   else int 111 = 2*11, 112 = 2*12;
          heap [111:2*b1,112:2*b2] real fine;
      int jj, jp;
real x1, x2, x3, y1, y2, y3, z1, z2, z3, yy2, yy3, zz2, zz3;
ref[] real ui= net[ 11,e12], fi= fine[l11,];
fi[112]:= x1:= ui[12]; jj:= 112+1;
      jj +:= 4; x1:= x3
      od;
      for ii from 11+1 by 2 to b1-1
do ref [] real uim= net[ii-1,@12], uii= net[ii ,@12],
                         uip= net[ii+1,@12];
           ref [,] real finei = fine[2*ii-1:2*ii+2,@112];
                       uim[12] /8;
           y3:= ( yy3:= uii[12] )/4;
z3:= ( zz3:= uip[12] )/8;
           finei[,112]:= (3*(x3+y3) - z3, yy3, 3*(y3+z3) - x3, zz3);
           for jj from 12+1 by 2 to b2-1

do jp:= jj+1; x1:= x3; y1:= y3; z1:= z3;
               z2:= ( zz2:= uip[jj] )/4; z3:= ( zz3:= uip[jp] )/8;
                 finei[,2*jj-1:2*jj+2]:=
                 ((2*(x2+y1)-z1+y2-x3,
                            2*(x2+y2)-x1+y1-z1,
                                        3*(x3+y2)-z1,
                                                  3*(x3+y3)-z3),
                  (2*(y1+y2)-x1+x2-x3,
                                         yy2,
                                        2*(y2+y3)-z1+z2-z3, yy3),
                  (3*(z1+y2)-x3,
                             2#(y2+z2)-x3+y3-z3,
                                        2*(z2+y3)-x3+y2-z1,
                                                  3*(z3+y3)-x3),
                  (3*(z1+z2)-z3, zz2, 3*(z3+z2)-z1,
     od
fine
            <u>od</u> ;
   fi;
```

```
# restriction: transposed linear interpolation #
   for i from 11 to u1-1
ti:= i+i; fco[i+1,12]:= 0;
        for k from 12 to u2-1
       <u>∞d</u>;
            fco[i+1,u2] := ffd:= ffi[ti+1,tkp ];
          ((fco[i ,u2]+:= ffd )*:=0.5)+:= ffi[ ti,2*u2]
        od;
        \underline{for} k \underline{from} 12 to u2-1 \underline{do} tk:= k+k; tkp:= tk+2;
            fco[u1,k+1]+:= ( ffb:= ffi[2*u1,tk+1] );
          ((fco[u1 ,k ]+:= ffb
                                  )*:=0.5)+:= ffi[2*u1, tk]
        od ; (fco[u1 ,u2]
                                    *:=0.5)+:= ffi[2*u1,2*u2];
            fco
    end ;
# residual evaluation
    # where the matrix does not define the netmat m, #
           # m should contain zeroes !
            ref [] real si = s[i,012], fi = f[i,012];
ref [,] real mi = m[i,012,0-3];
            int jm:= 12, jj, jp:= 12;
for j from 12 to u2
do ( jj:= jp; j=u2 ! skip ! jp+:= 1 );
                 ref [] real mij = mi[jj,@-3];
                si[jj]:= fi[jj] - (mij[-3]*uim[jj] + mij[-2]*uim[jp] +
mij[-1]*ui [jm] + mij[ 0]*ui [jj] + mij[ 1]*ui [jp] +
mij[ 2]*uip[jm] + mij[ 3]*uip[jj]);
                 jm := jj
            od ; uim:= ui
       od ;s
    end ;
```

bristol algol68 text

PWH/15/12/83

4

```
# coarse grid operator construction
```

orientation:

```
aco = coarse
  !
              fine
                       1
                              2
                                     3
  ! i-1
                1
                        a --
                              b ---
                                     c
                        1 / 1 / 1
                       d -- e -- f
! / ! / !
                2
  1
  ! i
                3
```

the slice [i,j,] corresponds to the coefficients in equation (i,j); the slice $[\ ,,k]$ corresponds to matrix diagonals as follows:

aco

end;

PWH/15/12/83

```
for i from 11 to u1-1
do ti:= i+i; tip:= ti+2;
tero aco[i+1,12,];
for k from 12 to u2-1
tk:= k+k; tkp:= tk+2;
      fine[1:3,1:3,]:= afi[ti:tip,tk:tkp,];
       ref[] real = aco[i, k, e-3], c = aco[i, k+1, e-3],
                            g = aco[i+1,k,\theta-3],
                            j = aco[i+1,k+1,e-3];
     \#aa\#((a[0]+:=(ab+ba+ad+da)*2+bb+dd+bd+db)*:=q)+:=aa;
    #adm (aL 0]#:= (ab+ba+ad+da)*z+ bb+dd+bd+db ]*:=q)*
#cd# c[ 0]+:= (ce+ec+cb+bc)*2+ ee+bb+be+eb+ef+fe;
#gg# g[ 0]+:= (ge+eg+gd+dg)*2+ ee+dd+de+ed+eh+he;
#jj# j[ 0] := fh+hf;
#ad# (a[ 1]+:= (ab+bc)*2 + bb+be+db+de)*:=q;
#-##( 1]
     \#ca\#(c[-1]+:=(ba+cb)\#2+bb+eb+bd+ed)\#:=q;
     #ag#( a[ 3]+:= (ad+dg)*2 + dd+bd+de+be)*:=q;
     #ga#( g[-3]+:= (da+gd)*2 + dd+db+ed+eb)*:=q;
     #gc#( g[-2] := (ge+ec)*2 + ee+he+de+hf+db+ef+eb)*:=q;
     #cg#( c[ 2] := (eg+ce)*2 + ee+eh+ed+fh+bd+fe+be)*:=q;
     #gj# g[ 1] := eh+hf+ef;
#jg# j[-1] := he+fh+fe;
     #cj# c[ 3] := eh+ef+fh;
     #jc# j[-3] := he+fe+hf
<u>∞d</u>;
     fine[1:3,1,]:= afi[ti:tip,tkp,];
      ref [] real a = aco[i ,u2,e-3],
g = aco[i+1,u2,e-3];
     \#aa\#((a[0]+:=(ad+da)*2+dd)*:=q)+:=aa;
     #gg# g[ 0]+:= (gd+dg)*2 + dd)*:=q;
#gg# (g[-3]+:= (gd+da)*2 + dd)*:=q;
#ag# (a[ 3]+:= (ad+dg)*2 + dd)*:=q;
              g[-2] := g[1] := 0.0
od ;
\frac{\text{for } k}{\text{do}} \quad \text{tk:=} \quad \frac{\text{from}}{\text{k+k}}; \quad \text{tkp:=} \quad \text{tk+2};
       fine[1,1:3,]:= afi[tip,tk:tkp,];
       <u>ref</u> [] <u>real</u> a = aco[u1,k ,e-3],
                          c = aco[u1,k+1,e-3];
     #aa#((a[ 0]+:= (ab+ba)*2 + bb)*:= q)+:=aa;
#cc# c[ 0]+:= (cb+bc)*2 + bb;
#ca#( c[-1]+:= (cb+ba)*2 + bb)*:=q;
     #ac#( a[ 1]+:= (ab+bc)*2 + bb)*:=q;
              c[ 2] := c[ 3]:= 0.0
      #aa#(aco[u1,u2,0]*:=q)+:=afi[2*u1,2*u2,0];
```

```
# point relaxation procedure
    proc pgs relax = ( ref netmat dec, netmat m, net u,f) void :
begin # point gauss seidel (pgs) #
       int 11:= 1 lwb u, u1:= 1 upb u, start1, step1, stop1,
            12:= 2 lwb u, u2:= 2 upb u, start2, step2, stop2;
       to (symmetric ! 2 ! 1)
       do ( backward ! start1:= u1; step1:= -1; stop1:= 11
            ! start1:= 11; step1:= 1; stop1:= u1 );
( reverse ! start2:= u2; step2:= -1; stop2:= 12
                       ! start2:= 12; step2:= 1; stop2:= u2 );
            ref [,] real mi= m[i,012,0-3];
for j from start2 by step2 to stop2
do int jm= (j>12!j-1!j), jp= (j<u2!j+1!j);
ref [] real mij = mi[j,0-3];
                       ui[j]:= ( mij[-3]*uim[j]+mij[-2]*uim[jp]+
mij[-1]*ui [jm] - fi[j]+mij[ 1]*ui [jp]+
mij[ 2]*uip[jm]+mij[ 3]*uip[j] )/ -mij[ 0]
                   od
             <u>∞d</u> ;
            ( symmetric! reverse:= not reverse; backward:= not backward)
       od
    end ;
# line relaxation procedure
    <u>int</u> st = ( zebra ! 2 ! 1 );
        int 11:= 1 1wb u, u1:= 1 upb u, start, step, stop;
        a=m[, 0], s=m[, 3], sw=m[, 2],
                               c= m[,-1];
               #not existing matrix elements: c[l]= b[k]= 0 !!#
             int l= lwb f, k= upb f; [1:k] real aa;
int i:=1; real g:= 0, p; aa[1]:= 1.0;
             ( j<k ! g -:=
u[ j]:= g; i:= j
                                                ne[j]*um[j+1] );
             od;

for j from k by -1 to 1

do u [j]:= g := ( u[j] - b[j]*g )/aa[j] od
```

```
        for
        k
        to
        ( symmetric
        or
        zebra ! 2 ! 1)

        do
        ( backward ! start := u1; step := -st; stop := l1

        ! start := l1; step := st; stop := u1 );

               zebra
           ! ( symmetric /= odd (k+start) ! start+:= sign step )
           # ( symmetric ! even-odd ! odd-even ) half step #);
            od;
           (symmetric ! backward:= not backward )
       od
    end;
# illu relaxation procedure
   ):
          rh:= residual(jac,u,f);
          soll(l1,rh);
           od ;
                soll(i,rh)
           od;
          du[u1,]:=rh[u1,];
           for i from u1-1 by -1 to 11

do for j from 12 to u2

do du[i,j] := jac[i,j, 3]*du[i+1,j ] +

( j>12 ! jac[i,j, 2]*du[i+1,j-1] ! 0.0 )
                 od :
                soll(i,du);
                 for j from 12 to u2
do du[i,j] := rh[i,j] - du[i,j] od
           <u>od</u>;
           <u>od</u>
                 <u>od</u>
    end;
```

PWH/15/12/83

```
# illu decomposition procedure
   int ip;
real dd,ll,ii,l dinv u;
        [12:u2,-1:+1] real d;
[12:u2,-2:+2] real dinv;
[12:u2,-1:+2] real 1 dinv;
         heap [11:u1,12:u2,-1:+1] real dec;
        d[12:u2,-1:+1]:= jac[11,12:u2,-1:+1];
        dd:= dec[11,12,0]:= 1.0/d[12,0];
         for j from 12 to u2-1
do dec[11,j +1]:= -d[j +1]*dd;
dec[11,j+1,-1]:= l1:=-d[j+1,-1]*dd;
            dec[11,j+1, 0]:= dd:= 1.0/(d[j+1, 0] + d[j,1]*]1)
         for i from 11 to u1-1 do ip:= i+1;
             dinv[u2,0]:= ii:= dec[i,u2,0];

for j from u2-1 by -1 to 12

do dinv[j,0]:= ii:= dec[i, j,0] +
                            ii * dec[i,j,1]*dec[i,j+1,-1]
             od;
             dinv[j-k, k]:= dinv[j-k+1,k-1]*dec[i,j-k,+1]
             <u>od</u>
             jac[ip,j,-2]*dinv[j+1,k-1]
             od ;
                 1 dinv[u2,k]:= jac[ip,u2,-3]*dinv[u2,k]
             (j+k<u2 !
                  l dinv u+:= l dinv[j,k+1]*jac[i,j+k+1,2]
                  d[j,k] := jac[ip,j,k] - 1 dinv u
             od od;
            dec[ip,j+1, 0]:= dd:= 1.0/(d[j+1, 0] + d[j,1]*11)
         od od;
        decomp:= dec
  end ;
```

PWH/15/12/83

```
15/12/83
```

```
# linear algebra solution procedure
     proc mgm = ( ref [] netmat lh, ref [] net uh,fh,
                         int itmax,p,q,s,t,
                         proc ( ref netmat , netmat , net , net ) void relax,
ref [] netmat decomp, ref int itused,
proc ( int , netmat , net , net ) bool goon mgm,
proc ( int , string ) void fail) void :

l= upb uh, r = s;
                  int l= upb uh, r = s;
ref [] netmat lhdec =
      begin
                                         ( decomp :=: ref [] netmat ( nil )
                                         ! loc [0:1] netmat ! decomp );
                proc mg = ( int 1) void :
# one multigrid cycle on level 1 #
                  if 1 = 0
then relax(lhdec[0],lh[0],uh[0],fh[0])
                  else # pre-relaxation #
                            to p do relax(lhdec[1],lh[1],uh[1],fh[1]) od;
                           # coarse grid correction #
                           fh[1-1]:= lin weight( residual (lh[1],uh[1],fh[1]) );
                           zero uh[1-1];

to (1=1!tls) do mg (1-1) od;

uh[1] +:= lin int pol (uh[1-1]);
                           # post-relaxation #
                            to q do relax(lhdec[1],lh[1],uh[1],fh[1]) od
                  fi;
                  int err =
                                                  # check consistency data

        lwb
        uh /= 0
        or
        lwb fh /= 0
        or
        lwb lh /= 0

        or
        upb fh /= 1
        or
        upb lh /= 1
        ! 1

                 !: netmat 11 = lh[1];
                       3 <u>lwb</u> 11 /=-3 <u>or</u> 3 <u>upb</u> 11 /= 3
                                                                                                  ! 2
                    3 | wb | 11 /=-3 | or | 3 | wpc | -- |

net | ff = fh[1];

int | 11 := 1 | wb | ff, | u1 := 1 | upb | ff, |

12 := 2 | wb | ff, | u2 := 2 | upb | ff; |

11 /= 1 | wb | 11 | or | u1 /= 1 | upb | 11 |

12 /= 2 | wb | 11 | or | u2 /= 2 | upb | 11
                                                                                                  ! 3
                 !: int tpl = 2**1;
                     11 mod tpl /=0 or u1 mod tpl/=0 or 12 mod tpl /=0 or u2 mod tpl/=0
                                                                                                  1 4
                 !: 11:= 11 over tpl; u1:= u1 over tpl; 
12:= 12 over tpl; u2:= u2 over tpl;
                      ( itused <= 0
                 ! 5
                                                                                                  ! 6
                 ( err>0 ! fail ( err, " mgm "));
                   if itused < 0
                                               # no coarse operators available #
                   then # create galerkin approximations #
                             for i from 1 by -1 to 1 do 1h[i-1]:= rap(lh[i]);
                                   fh[i-1]:= lin weight(fh[i])
                             od ; itused:= 0
                   fi;
```

bristol algol68 text

```
# apply full multigrid #
                  to t do mg(0) od;

for k to 1-1

do uh[k]:= sqr int pol (uh[k-1]);
                  to r do mg (k) od
od; uh[1]:= sqr int pol (uh[1-1]);
                 goon mgm (itused, lh[1], uh[1], fh[1])
           fi;
           to itmax
                               # multigrid iteration
           while mg (1); itused +:= 1;
goon mgm (itused, lh[1], uh[1], fh[1])
           do skip od
   end ;
# black box solution procedure
   ([0:1] netmat matrix; [0:1] net rhs, solution;
          matrix[1]:= lh; rhs[1]:= fh;
          mgm(matrix, solution, rhs, mgitmax, mgp, mgq, mgs, mgt, mgrelax,
          nil , loc int := -1, mgm goon, fail);
uh:= solution[1] );
# default global parameters
   mgrelax := illu relax;
    proc mgm goon:= ( int itnum, netmat lh, net uh,fh) bool:
                 true;
:= (int n,[] char text) void :
( print((newline,text,n,newline)); stop);
    proc fail
#example program #
    int 1:= 4;
    netmat matrix := loc [0:2**1,0:2**1,-3:3] real;
net solution, rhs := loc [0:2**1,0:2**1] real;
   read((matrix,rhs));
   solve sys (1,matrix,solution,rhs);
   print(solution)
 end
```

6.2 Appendix 2

BRISTOL FORTRAN COMMENTS

In this second appendix we give the user interfaces of the FORTRAN subroutines MGDlV (or MGDlS) and MGD5V (or MGD5S). We include also examples of a calling program. A tape with the complete programs can be obtained from the authors.

PWH/19/12/83

```
SUBROUTINE MGDlv(A,U,RHS,UB,US,TEMP,LEVELS,NXC,NYC,NXF,NYF,NF,NM,.ISTART,MAXIT,TOL,IOUT,RESNO)
COMMON /POI/ NGP(12),NGRIDX(12),NGRIDY(12)
COMMON /CPU/ CP(9)
        DIMENSION A (NM, 7), U (NM), UB (NF), RHS (NM), US (NM), TEMP (NXF), IOUT (5)
000000000000
        PURPOSE
        THIS PROGRAM SOLVES A USER PROVIDED 7-POINT DIFFERENCE
        EQUATION ON A RECTANGULAR GRID.
        MATHEMATICAL METHOD
        SAWTOOTH MULTIGRID CYCLING
        (I.E. ONE SMOOTHING-SWEEP AFTER EACH COARSE GRID CORRECTION)
        WITH SMOOTHING BY INCOMPLETE CROUT-DECOMPOSITION, 7-POINT PROLONGATION AND RESTRICTION,
               GALERKIN APPROXIMATION OF COARSE GRID MATRICES.
                           **** PARAMETERS ****
                           (INPUT DATA - SIZE OF PROBLEM)
NUMBER OF LEVELS IN MULTIGRID METHOD
SHOULD B.GE.2 AND .LE.12
NUMBER OF VERTICAL, HORIZONTAL GRID-LINES
        LEVELS
c
        NXC, NYC
                           ON COARSEST GRID
                           NUMBER OF VERTICAL, HORIZONTAL GRID-LINES
ON FINEST GRID
NUMBER OF GRID-POINTS OF FINEST GRID
NUMBER OF GRID-POINTS ON ALL GRIDS TOGETHER
        NXF, NYF
\circ
                           NOTE THAT THE FOLLOWING RELATIONS SHOULD HOLD,
                              NF=NXF*NYF
                              NXF = (NXC-1) * (2** (LEVELS-1))+1
                              NYF = (NYC-1) * (2**(LEVELS-1)) + 1
                           THE PROGRAM CHECKS THE CONSISTENCY OF THESE DATA
                           EXAMPLES
                                                                                6
3
                            LEVELS =
                                                                                          7
                                                                                          ŝ
                           NXC
NYC
                                             3
                                                            3
17
                                                                    3
                                                                                        129
                                                                               65
                            NYF
                                             5
                                                    9
                            NYF
                                                          289
404
                            NF
                                                                  1089
                                                                            4225
                                                                                     16641
                            NM
                           LEVELS =
NXC =
                           NXC
                            NXF
                                                                     65
                                                                             129
                                                                                        257
257
                            NYF
                                                            33
                                                                     65
                                                                              129
                            NF
                                          106
                                                         1484
                                                                  5709
                                                                           22350
                                                                                     88399
```

BRISTOL FORTRAN COMMENTS

2

```
ISTART
C
                 (TNPIIT)
                 =1 IF THE USER PROVIDES AN INITIAL ESTIMATE OF THE SOLUTION IN UB
c
C
C
                 =0 IF NO INITIAL ESTIMATE IS PROVIDED IN UB
С
С
      MAXIT
С
                 MAXIMUM NUMBER OF MULTIGRID ITERATIONS
С
      TOL
0000
                  (TNPIIT)
                 TOLERANCE DESIRED BY THE USER, TOL IS A BOUND OF THE
                 L2-NORM OF THE RESIDUAL REMARK IF EITHER MAXIT ITERATIONS OR THE TOLERANCE HAVE
C
                  ---- BEEN ACHIEVED, THEN MULTIGRID CYCLING IS STOPPED.
С
С
      IOUT
                 (INPUT)
С
                 INTEGER ARRAY DIMENSIONED AS IOUT (5) THAT CONTROLS
                 THE AMOUNT OF OUTPUT DESIRED BY THE USER.
SMALLER IOUT-VALUES MEAN LESS OUTPUT,
                 POSSIBLE VALUES ARE
                 IOUT(1)=1 CONFIRMATION OF INPUT DATA
                          Ø NONE
                 IOUT(2)=2 MATRICES AND RIGHT-HAND SIDES ON ALL LEVELS
                          1 MATRIX AND RIGHT-HAND SIDE ON HIGHEST LEVEL
                          Ø NONE
                 IOUT(3)=2 MATRIX-DECOMPOSITIONS ON ALL LEVELS
                          1 MATRIX-DECOMPOSITION ON HIGHEST LEVEL
                          Ø NONE
                  IOUT(4)=3 NORMS OF RESIDUALS, REDUCTION FACTORS,
                            FINAL RESIDUAL, FINAL SOLUTION
                          2 NORMS OF RESIDUALS, REDUCTION FACTORS,
                            FINAL RESIDUAL
                          1 NORMS OF RESIDUALS, REDUCTION FACTORS
                          Ø NONE
                  IOUT(5)=1 THE TIME SPENT IN VARIOUS SUBROUTINES
                          Ø NONE
                            REMARK CLOCK ROUTINES ARE NOT STANDARD
                                     FORTRAN. TO OBTAIN TIMINGS THE USER
                                     SHOULD ADAPT THE SUBROUTINE TIMING,
                            IT SHOULD DELIVER THE CPU-TIME ELAPSED.
С
                  (INPUT)
                  REAL ARRAY DIMENSIONED AS A (NM,7)
000000000000
                  THE USER HAS TO INITIALIZE A( 1,1),...,A( 1,7)
                                               A(K,1)
                                               A(NF,1),..,A(NF,7)
                 WITH THE MATRIX CORRESPONDING TO THE FINEST GRID. THE ORDERING OF THE POINTS IN THE GRID IS AS FOLLOWS
                  THE SUBSCRIPT K=(J-1)*NXF+I CORRESPONDS TO THE POINT
                  (X,Y) = (I*H, J*H)
                               Х
                                         I=1,...,NXF J=1,...,NYF
```

- 2 -

```
BRISTOL FORTRAN COMMENTS
                                                          PWH/19/12/83
                  THE 7-POINT DIFFERENCE MOLECULE AT THE POINT WITH
                  SUBSCRIPT K=(J-1)*NXF+I IS POSITIONED IN THE X.Y-PLANE
000000000000000000000000000
                  AS FOLLOWS
                           Y,J
                                 A(K,6)
                                           A(K,7)
                                 A(K,3)
                                            A(K,4)
                                                      A(K,5)
                                            A(K,1)
                                                      A(K,2)
                             O+ + + + + + + + + + + + + + + X, I
       IMPORTANT THE USER HAS TO PROVIDE THE MATRIX A ONLY ON THE FINEST
          ----- GRID.
       IMPORTANT THE USER HAS TO TAKE CARE THAT PARTS OF THE MOLECULES
       ----- OUTSIDE THE DOMAIN ARE INITIALIZED TO ZERO, OTHERWISE
                  WRONG RESULTS ARE PRODUCED.
       IMPORTANT THE COEFFICIENT MATRIX A IS OVERWRITTEN BY THE PROGRAM.
        ----- AFTER A CALL OF MGD1V (DECOMP), A CONTAINS THE INCOMPLETE
                  CROUT DECOMPOSITIONS.
0000000
       RHS
                   (INPUT)
                  REAL ARRAY DIMENSIONED AS RHS (NM)
                  THE USER HAS TO INITIALIZE RHS(1),..., RHS(NF) WITH
                  THE RIGHT-HAND SIDE OF THE EQUATION.
                  THE ORDERING IS THE SAME AS INDICATED FOR ARRAY A.
       IMPORTANT THE USER HAS TO PROVIDE THE RIGHT-HAND SIDE OF THE
C
            ---- DISCRETIZED EQUATION ONLY ON THE FINEST GRID
0000000
                   (OUTPUT)
                  REAL ARRAY DIMENSIONED AS U(NM)
                  CONTAINS THE (APPROXIMATE) NUMERICAL SOLUTION AFTER A
                  CALL OF MGDIV.
       UB
                   (WORKSPACE/INPUT)
000000
                  REAL ARRAY DIMENSIONED AS UB (NF)
                  IS USED AS A SCRATCH ARRAY. IF ISTART=1 THEN UB(1),...
..,UB(NF) SHOULD CONTAIN AN INITIAL ESTIMATE OF THE
                  SOLUTION PROVIDED BY THE USER.
AFTER A CALL OF MGDLV, UB CONTAINS THE RESIDUAL OF THE
                  THE NUMERICAL SOLUTION.
С
C
C
       US
                   (WORKSPACE)
                  REAL ARRAY DIMENSIONED AS US (NM)
IS USED AS A SCRATCH ARRAY
0000000
       TEMP
                   (WORKSPACE)
                  REAL ARRAY DIMENSIONED AS TEMP(NXF) IS USED AS A (SMALL) SCRATCH ARRAY.
                   IF THE SCALAR VERSION OF SUBROUTINE SOLVE (DENOTED BY
                   COMMENT CARDS BEGINNING WITH CSC) IS USED THEN IT IS
C
                   SUFFICIENT TO DIMENSION TEMP AS TEMP(1).
С
       RESNO
                   (OUTPUT)
                   THIS VARIABLE CONTAINS THE L2-NORM OF THE RESIDUAL AT
```

- 3 -

THE END OF EXECUTION OF MGDLV.

c

PWH/19/12/83

BRISTOL FORTRAN COMMENTS

```
THIS IS AN EXAMPLE OF A MAIN PROGRAM USING MGDLV
^{\circ}
C-----
C
С
      ACTUAL USER PROVIDED DIMENSION STATEMENTS,
С
      DIMENSION A(88399,7), RHS(88399), U(88399), US(88399), UB(66049),
     .TEMP(257), IOUT(5)
      USER DATA STATEMENTS,
C
C
      DATA NXC, NYC, NXF, NYF/5, 5, 257, 257/
      DATA LEVELS, NM, NF/7, 88399, 66049/
      DATA MAXIT, ISTART/10,0/
      DATA IOUT(1), IOUT(2), IOUT(3), IOUT(4), IOUT(5)/1,0,0,1,1/
С
С
      PROBLEM SET UP
С
      CALL MATRHS (A, RHS, NM, NXF, NYF)
C****
                                    ,
****************
С
     MATRHS IS A SUBROUTINE WHICH FILLS THE MATRIX AND THE RIGHT-HAND
С
     SIDE, IT DOES NOT BELONG TO THE PACKAGE AND IS ONLY AN EXAMPLE.
C*****
С
С
      SOLUTION OF THE LINEAR SYSTEM
č
      CALL MGDIV (A, U, RHS, UB, US, TEMP, LEVELS, NXC, NYC, NXF, NYF, NF, NM,
     .ISTART, MAXIT, Ø. Ø, IOUT, RESNO)
С
С
      POSSIBLE REFINEMENT OF THE SOLUTION, 5 MORE ITERATIONS
С
С
      CALL CYCLES (A, U, RHS, UB, US, TEMP, LEVELS, NXF, NF, NM, 1, 5, 0.0, IOUT,
Ċ
     . RESNO)
0000
      POSSIBLE REFINEMENT UNTIL RESIDUAL NORM .LT. 1.0E-12
      CALL CYCLES (A, U, RHS, UB, US, TEMP, LEVELS, NXF, NF, NM, 1, 30, 1.0E-12, IOUT,
С
С
      STOP
      END
```

```
BRISTOL FORTRAN COMMENTS
                                                     PWH/19/12/83
      SUBROUTINE MGD5V(A,V,RHS,VB,LDU,WORK,LEVELS,NXC,NYC,NXF,NYF,
      NF,NM,ISTART,MAXIT,TOL,IOUT,RESNO)
COMMON /POI/ NGP(12),NGRIDX(12),NGRIDY(12)
      COMMON /CPU/ CP(10)
      REAL LDU
      DIMENSION A(NM,7), V(NM), VB(NM), RHS(NM), LDU(NM,3),
               WORK (NXF,9), IOUT (5)
C
0000
      PURPOSE
      THIS PROGRAM SOLVES A USER PROVIDED 7-POINT DIFFERENCE
СС
      EQUATION ON A RECTANGULAR GRID.
С
     MATHEMATICAL METHOD
Ċ
CCC
      SAWTOOTH MULTIGRID CYCLING
      (I.E. ONE SMOOTHING-SWEEP AFTER EACH COARSE GRID CORRECTION)
      WITH SMOOTHING BY INCOMPLETE LINE LU-DECOMPOSITION,
           7-POINT PROLONGATION AND RESTRICTION.
           GALERKIN APPROXIMATION OF COARSE GRID MATRICES.
C*
C
                          PARAMETERS
С
                    ***
C*********************************
                    (INPUT DATA - SIZE OF PROBLEM)
c
                    NUMBER OF LEVELS IN MULTIGRID METHOD
      LEVELS
                    SHOULD BE .GE.3 AND .LE.12
NUMBER OF VERTICAL, HORIZONTAL GRID-LINES
CCCC
      NXC, NYC
                    ON COARSEST GRID, NXC SHOULD BE .GE.5
AND NYC SHOULD BE .GE.3
      NXF, NYF
                    NUMBER OF VERTICAL, HORIZONTAL GRID-LINES
00000
                    ON FINEST GRID
                    NUMBER OF GRID-POINTS OF FINEST GRID
      NM
                    NUMBER OF GRID-POINTS ON ALL GRIDS TOGETHER
C
                    SEE COMMENTS IN MGDIV FOR FURTHER DETAILS.
С
      ISTART
                 (INPUT)
      MAXIT
                 (INPUT)
      TOL
0000000
                 (INPUT)
      IOUT
                 (INPUT)
                 (INPUT)
      RHS
                 (INPUT)
                 THESE INPUT PARAMETERS HAVE THE SAME MEANING AS IN MGD1V
                 THE ONLY DIFFERENCE IS THAT THE ARRAY A WILL NEVER BE
                 OVERWRITTEN BY MGD5V.
С
      LDU
                 (OUTPUT)
                 REAL ARRAY DIMENSIONED AS LDU(NM, 3)
CCC
```

- 5 -

LDU CONTAINS DECOMPOSITIONS OF ALL TRIDIAGONAL BLOCKS D

POSSIBLE REFINEMENT OF THE SOLUTION, 5 MORE ITERATIONS

000000 CALL CYCLES (A, V, RHS, VB, LDU, WORK, LEVELS, NXF, NF, NM, 1,5,0.0, IOUT, RESNO)

POSSIBLE REFINEMENT UNTIL RESIDUAL NORM .LT. 1.0E-12

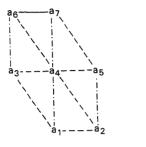
CALL CYCLES (A, V, RHS, VB, LDU, WORK, LEVELS, NXF, NF, NM, 1,30,1.0E-12, IOUT, RESNO)

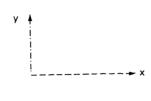
STOP END

С

6.3 Appendix 3

In this appendix we give a full description in FORTRAN of our implementation of the ILLU-decomposition. First we give a brief description of that decomposition and the corresponding relaxation sweep. Let the seven diagonal matrix A correspond with the following molecule:





Let the matrix A be decomposed in block tridiagonal form:

$$A = L + D + U = \begin{pmatrix} D_1 & U_1 & & & \\ L_2 & D_2 & U_2 & & \\ & L_3 & D_3 & U_3 & \\ & & \ddots & \ddots & \\ & & L_i & D_i & U_i \\ & & & L_n & D_n \end{pmatrix}$$

 L_i i = 2 (1) n corresponds with a_1 and a_2 , D_i i = 1 (1) n corresponds with a_3 , a_4 and a_5 , U_i i = 1 (1) n-1 corresponds with a_6 and a_7 .

Then the ILLU-decomposition is defined by L, \bar{D} , U, with

$$\bar{D}_{1} = D_{1},$$
 $\bar{D}_{j} = D_{j} - \text{tridiag } (L_{j} \bar{D}_{j-1} U_{j-1}),$
for $j = 2$ (1) n ,

The tridiagonal matrix \bar{D} is stored by means of its exact decomposition L, \mathcal{D} , \mathcal{U} . (L and \mathcal{U} are bidiagonal, \mathcal{D} is a main diagonal, the main diagonals of L and \mathcal{U} are equal to one.)

Let $u^{(i)}$ be an approximate solution of Au = f, then an ILLU-relaxation sweep reads:

Step 1: compute r:= f - A u (i);

Step 2: solve $(L+\overline{D})\overline{D}$ $(\overline{D}+U)$ v=r;

Step 3: $u^{(i+1)} := u^{(i)} + v$.

```
SUBROUTINE DECOMP (A1, A2, A3, A4, A5, A6, A7, N, M, NM)
      INCOMPLETE CROUT-DECOMPOSITION (ILU-DECOMPOSITION) OF THE SEVENDIA
      GONAL MATRIX A REPRESENTED BY A1, A2, A3, A4, A5, A6, A7.
C
      A IS OVERWRITTEN BY ITS DECOMPOSITION.
C
      THE MAIN DIAGONAL OF L IS ONE EVERYWHERE, THE OTHER DIAGONALS OF L
000
      ARE STORED IN A1, A2, A3.
THE DIAGONALS OF U ARE STORED IN A4, A5, A6, A7.
M IS THE NUMBER OF GRIDPOINTS IN THE X-DIRECTION,
С
С
      N IS THE NUMBER OF GRIDPOINTS IN THE Y-DIRECTION,
С
      NM=N*M.
С
      NOTE THE LOOPS 6, 10, 20, 30, 40, 50, 60, 400 ARE AUTOMATICALLY
С
             VECTORIZED.
č
             THE LOOPS 5 AND 55 ARE RECURSIVE AND WILL THEREFORE NOT BE
С
             VECTORIZED.
С
      DIMENSION A1 (NM), A2 (NM), A3 (NM), A4 (NM), A5 (NM), A6 (NM), A7 (NM)
      A4J = A4(1)
      DO 5 J=2,M
       A3(J) = A3(J) / A4J
       A4(J) = A4(J) - A3(J) * A5(J-1)
       A4J=A4(J)
     5 CONTINUE
      DO 6 J≈2,M
       A6(J) = A6(J) - A3(J) * A7(J-1)
     6 CONTINUE
      Ml=M-1
       JB=1
       JE=M
       DO 100 K=2,N
       JR=JR+M
       JE=JE+M
       DO 10 J=JB,JE
       A1(J) = A1(J) / A4(J-M)
   10 CONTINUE
       DO 20 J=JB,JE
       A2(J) = (A2(J) - A1(J) * A5(J-M)) / A4(J-M1)
   20 CONTINUE
       DO 30 J=JB,JE
       A3(J) = A3(J) - A1(J) * A6(J-M)
    30 CONTINUE
       DO 40 J=JB, JE
       A4(J) = A4(J) - A2(J) * A6(J-M1) - A1(J) * A7(J-M)
    40 CONTINUE
       DO 50 J=JB,JE
       A5(J) = A5(J) - A2(J) * A7(J-M1)
    50 CONTINUE
       A4J = A4(JB-1)
       DO 55 J=JB,JE
       A3(J) = A3(J) / A4J
       A4(J) = A4(J) - A3(J) * A5(J-1)
       A4J=A4(J)
    55 CONTINUE
       DO 60 J≃JB,JE
       A6(J) = A6(J) - A3(J) * A7(J-1)
    60 CONTINUE
   100 CONTINUE
 C----
       FOR ILU-RELAXATION THE RECIPROCAL OF A4 IS NEEDED, NOT A4 ITSELF.
 C----
        DO 400 JJ=1,NM,65535
        JJE=(JJ-1)+MIN0(65535,NM-(JJ-1))
        DO 400 J=JJ,JJE
       A4(J) = 1.0/A4(J)
   400 CONTINUE
        RETURN
        END
```

```
SGEROUTINE ILLUDC (A, DIMA, L, D, U, NX, NY, NXY, WORK)
C----
INCOMPLETE LINE LU (ILLU-DECOMPOSITION) OF THE SEVENDIAGONAL
       MATRIX A. A REMAINS INTACT, L D AND U ARE FILLED IN WITH THE
       DECOMPOSITIONS OF
                                    J = l(1)NY
       NX IS THE NUMBER OF GRIDPOINTS IN THE X-DIRECTION, NY IS THE NUMBER OF GRIDPOINTS IN THE Y-DIRECTION,
С
       NXY=NX*NY
Ċ
C-
C
       INTEGER DIMA
       DIMENSION A(DIMA, 7), L(NXY), D(NXY), U(NXY), WORK(NX, 9)
       CALL TRIDEC (A(1,3), A(1,4), A(1,5), L, D, U, NX)
       NPOLD=1
       DO 100 J=2,NY
       NPNEW=NPOLD+NX
       CALL BLOCKS (A (NPOLD, 1), A (NPNEW, 1), DIMA,
                     L(NPOLD),D(NPOLD),U(NPOLD),
L(NPNEW),D(NPNEW),U(NPNEW),NX,
                     WORK(1,1), WORK(1,2), WORK(1,3), WORK(1,4), WORK(1,5),
                     WORK(1,6))
       NPOLD=NPNEW
  100 CONTINUE
       RETURN
       END
       SUBROUTINE TRIDEC (DM, DZ, DP, LJ, DJ, UJ, NX)
C-----
       PERFORMS DECOMPOSITION OF A TRIDIAGONAL MATRIX REPRESENTED BY DM,
С
С
       DZ, DP.
С
       THE DECOMPOSITION CONSISTS OF A LOWER TRIANGULAR BIDIAGONAL MATRIX
        LJ, AN UPPER TRIANGULAR BIDIAGONAL MATRIX UJ AND AN ONE DIAGONAL
       MATRIX DJ, THE MAIN DIAGONALS OF LJ AND UJ EQUAL ONE.
       NX IS THE NUMBER OF POINTS IN THE X-DIRECTION.
C
       NOTE LOOP 20 IS AUTOMATICALLY VECTORIZED.
---- LOOP 10 IS RECURSIVE AND WILL THEREFORE NOT BE VECTORIZED.
С
        DIMENSION DM(NX), DZ(NX), DP(NX), LJ(NX), DJ(NX), UJ(NX)
        DJ(1) = 1.0/DZ(1)
        DJIM1=DJ(1)
        DO 10 I=2,NX
        LJ(I) = -DM(I) * DJIM1
        DJ(I) = 1.0/(DZ(I) + LJ(I) * DP(I-1))
        DJIM1=DJ(I)
    10 CONTINUE
        NX1=NX-1
        DO 20 I=1,NX1
        UJ(I) = -DP(I)*DJ(I)
    20 CONTINUE
        RETURN
        END
```

```
SUBROUTINE BLOCKS (AJM1, AJ, DIMA, LJM1, DJM1, UJM1, LJ, DJ, UJ, NX,
                       QM2,QM1,QZE,QP1,QP2, LD)
C-----
      INCOMPLETE LINE LU DECOMPOSITION (ILLU-DECOMPOSITION) OF J-TH ROW
С
      OF BLOCKS OF THE SEVENDIAGONAL MATRIX A.

AJ IS J TH ROW OF BLOCKS OF A,
С
С
С
      AJM1 IS (J-1) TH ROW OF BLOCKS OF A,
С
      LJM1, DJM1, UJM1 ARE (J-1) TH ROWS OF L, D, U WHICH REPRESENT
С
      BIDIAGONAL MATRICES (MAIN DIAGONALS EQUAL ONE) WHICH PRODUCT IS
С
č
          D
С
           (J-1)
      LJ, DJ, UJ BECOME THE J TH ROWS OF L, D, U AFTER A CALL OF BLOCKS. NX IS THE NUMBER OF GRIDPOINTS IN THE X-DIRECTION.
CCC
      QM2,QM1,QZE,QP1,QP2,LD ARE WORK ARRAYS.
С
¢
      NOTE THE LOOPS 10, 30, 40, 51, 52, 53, 54, 60, 70, 80 ARE AUTOMA-
ċ
            TICALLY VECTORIZED.
С
            LOOP 20 IS RECURSIVE AND WILL THEREFORE NOT BE VECTORIZED.
C
C-----
      INTEGER DIMA
      REAL LJM1,LJ,LD
      DIMENSION AJM1 (DIMA, 7), AJ (DIMA, 7), LJM1 (NX), DJM1 (NX), UJM1 (NX),
                LJ(NX), DJ(NX), UJ(NX),
                QM2(NX),QM1(NX),QZE(NX),QP1(NX),QP2(NX),
               LD(NX,4)
C-----
C
č
      FIRST STEP - COMPUTATION OF 5-DIAG( D
С
C
                   RESULTING DIAGONALS ARE QM2, QM1, QZE, QP1, QP2
C-----
      NX1=NX-1
      NX2=NX-2
      DO 10 I = 1.NX1
      QZE(I) = UJMl(I) * LJMl(I+1)
   10 CONTINUE
      QZE(NX)=DJM1(NX)
      QZEIP1=QZE(NX)
      DO 20 II=1,NX1
      I = NX - II
      QZE(I) = DJMl(I) + QZE(I) * QZEIPl
      QZEIP1=QZE(I)
   20 CONTINUE
       DO 30 I=2,NX1
       QMl(I) = LJMl(I) * QZE(I)
      QP1(I)=UJM1(I)*QZE(I+1)
   30 CONTINUE
      QP1(1)=UJM1(1)*QZE(2)
      QMl(NX) = LJMl(NX) * QZE(NX)
       DO 40 I=3,NX2
       QM2(I) = LJM1(I-1) *QM1(I)
       QP2(I)=UJMl(I)*QPl(I+1)
    40 CONTINUE
       QP2(1) = UJM1(1) * QP1(2)
       QP2(2) = UJM1(2) * QP1(3)
       QM2(NX1) = LJM1(NX2) *QM1(NX1)
```

QM2(NX) = LJM1(NX1) *OM1(NX)

```
С
      SECOND STEP - COMPUTATION OF 4 DIAGONALS OF L D
С
C-----
      QM1(1) = \emptyset.\emptyset
      QM2(2) = \emptyset.\emptyset
      QP2(NX1)=0.0
      OP1(NX) = \emptyset.\emptyset
      DO 51 I=1,NX1
      LD(I,1) = AJ(I,1) *QM1(I) + AJ(I,2) *QM2(I+1)
   51 CONTINUE
      DO 52 I=1,NX1
      LD(I,2) = AJ(I,1) *QZE(I) + AJ(I,2) *QM1(I+1)
   52 CONTINUE
      DO 53 I=1,NX1
      LD(I,3) = AJ(I,1) *QP1(I) + AJ(I,2) *QZE(I+1)
   53 CONTINUE
      DO 54 I=1,NX1
      LD(I,4) = AJ(I,1) *QP2(I) + AJ(I,2) *QP1(I+1)
   54 CONTINUE
      LD (NX,1) = AJ (NX,1) * QM1 (NX)
LD (NX,2) = AJ (NX,1) * QZE (NX)
C--
      THIRD AND FOURTH STEP - COMPUTATION OF D = D - 3-DIAG(LDU)
Ċ
С
č
č
      D IS REPRESENTED BY QM1, QZE, QP1
С
             ___________
      DO 60 I=2,NX
      QMl(I) = AJ(I,3) - LD(I,1) * AJMl(I-1,7) - LD(I,2) * AJMl(I,6)
   60 CONTINUE
      DO 70 I=1,NX1
      QZE(I) = AJ(I,4) - LD(I,2) * AJM1(I,7) - LD(I,3) * AJM1(I+1,6)
   70 CONTINUE
      DO 80 I=1,NX2
      QPl(I) = AJ(I,5) - LD(I,3) * AJMl(I+1,7) - LD(I,4) * AJMl(I+2,6)
   80 CONTINUE
      QZE(NX)=AJ(NX,4)-LD(NX,2)*AJM1(NX,7)
      QP1(NX1) = AJ(NX1,5) - LD(NX1,3) * AJM1(NX,7)
C-----
C
      FIFTH STEP - COMPUTATION OF DECOMPOSITION L ,D ,U OF D J J J \,
С
      CALL TRIDEC (QM1,QZE,QP1,LJ,DJ,UJ,NX)
      RETURN
      END
```

7. REFERENCES

- Barkai, D. and Brandt, A. (1983) Vectorized Multigrid Poisson Solver for the CDC CYBER 205, Appl. Math. Comp., 13, pp. 215-227.
- Dendy (Jr.), J.E. (1982) Black Box multigrid, J. Comp. Phys., 48, pp. 366-386.
- Dendy (Jr.), J.E. (1983) Black Box Multigrid for Non-symmetric Problems, Appl. Math. Comp., 13, pp. 261-283.
- Foerster, H. and Witsch, K. (1982) Multigrid software for the solution of elliptic problems on rectangular domains MGOO (Release 1), in Multigrid Methods, (W. Hackbusch and U. Trottenberg, eds.), Lecture Notes in Mathematics, 960, Springer Verlag, Berlin.
- Hemker, P.W. (1982) On the comparison of Line-Gauss Seidel and ILU relaxation in multigrid algorithms, in Computational and asymptotic methods for boundary and interior layers (J.J.H. Miller, ed.), Boole Press, Dublin, pp. 269-277.
- Hemker, P.W. (1984) Multigrid methods for problems with a small parameter, in Numerical Analysis (D.F. Griffiths, ed.), Proceedings of Dundee Conference 1983, Springer Lecture Series in Mathematics, Springer Verlag, Berlin.
- Hemker, P.W., Kettler, R., Wesseling, P. and de Zeeuw, P.M. (1983) Multigrid Methods: Development of Fast Solvers, Appl. Math. Comp., 13, pp. 311-326.
- Hemker, P.W., Wesseling, P. and de Zeeuw, P.M. (1983) A portable vector code for autonomous multigrid modules, in PDE Software: Modules, Interfaces and Systems (B. Engquist, ed.), Proceedings IFIP WG 2.5 Working Conference, (North Holland).
- Kettler, R. (1982) Analysis and comparison of relaxation schemes in robust multigrid and preconditioned conjugate gradient methods, in Multigrid Methods (W. Hackbusch and U. Trottenberg, eds.), Springer Lecture Series in Mathematics, 960, Springer Verlag, Berlin, pp. 502-534.
- Wesseling, P. (1982a) A robust and efficient multigrid method, in Multigrid Methods (W. Hackbusch and U. Trottenberg, eds.), Springer Lecture Series in Mathematics, 960, Springer Verlag, Berlin, pp. 614-630.
- Wesseling, P. (1982b) Theoretical and practical aspects of multigrid method, SIAM J. Sci. Stat. Comp., 3, pp. 387-407.