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A NEW ORDERING SCHEME

FOR THE

HERMITE BICUBIC COLLOCATION EQUATIONS

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ABSTRACT

We present a new ordering scheme for the linear equations obtained from the Hermite bicubic collocation approximation to the solution of second order, linear, elliptic partial differential equations on rectangular domains. The resulting matrix has a non-zero diagonal and is a band matrix with band width $4(N_x-1)$ where N_x is the number of vertical grid lines. The matrix is block symmetric in that it consists of 4×4 blocks which if $B_{ij}\neq 0$ then $B_{ji}\neq 0$. There are at most 16 non-zero entries per row occurring in 4 blocks. All of the symmetric pairs of off-diagonal blocks can be stored in their natural order within one 4×4 block.

Keywords: elliptic partial differential equations, Hermite bicubic collocation, ordering scheme, non-zero diagonal

A New Ordering Scheme for the Hermite Bicubic Collocation Equations

Wayne R. Dyksen†

1. Introduction

Iterative techniques have been shown to be very effective for solving large, sparse systems of equations. Such systems are obtained from the Hermite bicubic collocation approximation to the solution of second order, linear, elliptic partial differential equations on rectangular domains. Thus, one would naturally like to solve the collocation equations by some type of iterative technique. In order to use an iterative technique, it is necessary that the system of equations has a non-zero diagonal. The usual ordering for the collocation matrix yields a system which has many zeros on the diagonal. With this motivation in mind, we present a new ordering scheme for the collocation matrix so that the resulting band matrix has a nice structure which includes a non-zero diagonal.

The ordering of the collocation points (equations, rows) is discussed in Section 2. The ordering of the Hermite bicubic basis functions (unknowns, columns) is discussed in Section 3. The reordering of the boundary basis functions is discussed in Section 4. An implementation within the ELLPACK system is discussed in Section 5. Appendix A contains a complete set of tables describing the boundary basis function reordering. Appendix B contains computer generated pictures of the structure of the collocation equations both using a standard finite element ordering and using the scheme described here.

Note: To insure a non-zero diagonal, we assume that the coefficient functions in the partial differential equation and the boundary conditions do not vanish. Also, the boundary condition on any side of the rectangular domain may include only values of the unknown function u and/or its normal derivative.

† This work supported in part by NSF grant MCS 76-20784.

2. The Ordering of the Collocation Points

In the usual way, a rectangular grid is imposed on the domain. The grid points (equations, rows) are then numbered in a natural way from west to east, south to north. The collocation points are associated with the nearest grid point and are numbered in groups of four in the order of their corresponding grid point. For example, with four vertical and four horizontal grid lines, there are 64 collocation points whose ordering is given in Figure 1.

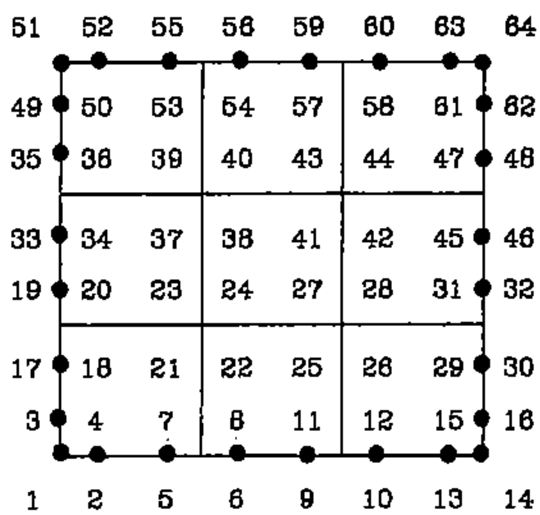


Figure 1: The Ordering of the Collocation Points
for a 4×4 Grid with 64 Unknowns

The important idea in the above ordering is that the grid points are first numbered in a natural way and then the collocation points are numbered in the order of their corresponding grid point. We could number the grid points south to north, west to east as long as we suitably modify the rest of the ordering scheme described in the following sections. Similarly, the four collocation points associated with any grid point may be locally ordered in any manner.

3. The Ordering of the Hermite Bicubic Basis Functions

To the $i^{th}[j^{th}]$ $x[y]$ grid coordinate there are associated two Hermite cubic functions: $f_i^x[f_j^y]$ which takes on function values and $d_i^x[d_j^y]$ which takes on derivative values. The Hermite bicubic basis functions (unknowns, columns) are then ordered corresponding to their support in a natural way from west to east, south to north. For example, with four vertical and four horizontal grid lines there are 64 bicubic basis functions whose ordering is given in Figure 2.

49 $f_1^x f_4^y$	53 $f_2^x f_4^y$	57 $f_3^x f_4^y$	61 $f_4^x f_4^y$
50 $f_1^x d_4^y$	54 $f_2^x d_4^y$	58 $f_3^x d_4^y$	62 $f_4^x d_4^y$
51 $d_1^x f_4^y$	55 $d_2^x f_4^y$	59 $d_3^x f_4^y$	63 $d_4^x f_4^y$
52 $d_1^x d_4^y$	56 $d_2^x d_4^y$	60 $d_3^x d_4^y$	64 $d_4^x d_4^y$
33 $f_1^x f_3^y$	37 $f_2^x f_3^y$	41 $f_3^x f_3^y$	45 $f_4^x f_3^y$
34 $f_1^x d_3^y$	38 $f_2^x d_3^y$	42 $f_3^x d_3^y$	46 $f_4^x d_3^y$
35 $d_1^x f_3^y$	39 $d_2^x f_3^y$	43 $d_3^x f_3^y$	47 $d_4^x f_3^y$
36 $d_1^x d_3^y$	40 $d_2^x d_3^y$	44 $d_3^x d_3^y$	48 $d_4^x d_3^y$
17 $f_1^x f_2^y$	21 $f_2^x f_2^y$	25 $f_3^x f_2^y$	29 $f_4^x f_2^y$
18 $f_1^x d_2^y$	22 $f_2^x d_2^y$	26 $f_3^x d_2^y$	30 $f_4^x d_2^y$
19 $d_1^x f_2^y$	23 $d_2^x f_2^y$	27 $d_3^x f_2^y$	31 $d_4^x f_2^y$
20 $d_1^x d_2^y$	24 $d_2^x d_2^y$	28 $d_3^x d_2^y$	32 $d_4^x d_2^y$
1 $f_1^x f_1^y$	5 $f_2^x f_1^y$	9 $f_3^x f_1^y$	13 $f_4^x f_1^y$
2 $f_1^x d_1^y$	6 $f_2^x d_1^y$	10 $f_3^x d_1^y$	14 $f_4^x d_1^y$
3 $d_1^x f_1^y$	7 $d_2^x f_1^y$	11 $d_3^x f_1^y$	15 $d_4^x f_1^y$
4 $d_1^x d_1^y$	8 $d_2^x d_1^y$	12 $d_3^x d_1^y$	16 $d_4^x d_1^y$

Figure 2: The Ordering of the Basis Functions
for a 4×4 Grid with 64 Unknowns

The ordering of the collocation points described in Section 2 combined with the ordering of the basis functions described in this section yield an intermediate collocation matrix which exhibits a nice structure. It is a band matrix with band width $4(N_x-1)$ where N_x is the number of vertical grid lines. The matrix is block symmetric in that it consists of 4×4 blocks which if $B_{ij} \neq 0$ then $B_{ji} \neq 0$.

There are at most 16 non-zero entries per row occurring in 4 blocks. All of the symmetric pairs of off-diagonal blocks can be stored in their natural order within one 4×4 block.

For example, in the case of a Poisson equation with Dirichlet boundary conditions and four grid lines in each direction, the structure of the collocation matrix is pictured below in Figure 3 where x="non-zero entry" and ·="zero".

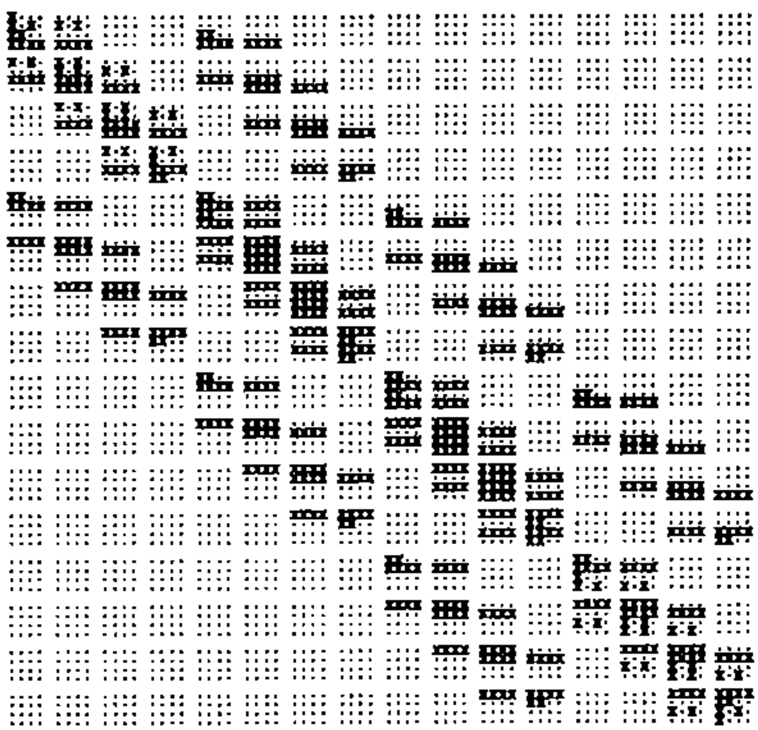


Figure 3: The Intermediate Collocation Matrix
for a 4×4 Grid with 64 Unknowns

We see from Figure 3 that the above matrix does not quite have a non-zero diagonal. However, unlike the usual collocation matrix structure (see Section 5), the intermediate collocation matrix resulting from the ordering discussed thus far is tri-banded with the center band going down the diagonal. This structure gives rise to the hope that perhaps by reordering some of columns of this matrix we can indeed obtain a non-zero diagonal. In the next section we discuss how to do just that.

4. The Reordering of the Boundary Basis Functions

The linear system resulting from the ordering discussed in Sections 2 and 3 consists of 4×4 blocks which can be identified with the grid points. Clearly, the non-zeros on the diagonal of the collocation matrix will occur only in the diagonal blocks corresponding to the boundary grid points. There are eight different types of boundary points which we label as follows:

North West	North	North East
West		East
South West	South	South East

Again we consider the case of a Poisson equation with Dirichlet boundary conditions and four grid lines in each direction. From Figure 3 we see that the 4×4 block in the upper left is associated with the south-west grid point and has the following format:

$$\begin{matrix} X & 0 & 0 & 0 \\ X & 0 & X & 0 \\ X & X & 0 & 0 \\ X & X & X & X \end{matrix}$$

We see that by permuting the second and third basis functions (columns 2 and 3), we obtain a non-zero diagonal in this block:

$$\begin{matrix} X & 0 & 0 & 0 \\ X & X & 0 & 0 \\ X & 0 & X & 0 \\ X & X & X & X \end{matrix}$$

By considering all nine possible boundary conditions which may occur at the south-west corner, one can show that it is aways possible to reorder the columns to obtain a non-zero diagonal in this diagonal block. The possible boundary conditions at the south-west corner with the corresponding permutations are given below in Table 1.

South West Corner				
Boundary Condition		Block Before	Column Permutation	Block After
West	South			
Dirichlet	Dirichlet	X000 X0X0 XX00 XXXX	$2 \rightarrow 3$ $3 \rightarrow 2$	X000 XX00 X0X0 XXXX
Neumamn	Dirichlet	X000 X0X0 00XX XXXX	$2 \rightarrow 4$ $3 \rightarrow 2$ $4 \rightarrow 3$	X000 XX00 0XX0 XXXX
Mixed	Dirichlet	X000 X0X0 XXXX XXXX	$2 \rightarrow 3$ $3 \rightarrow 2$	X000 XX00 XXXX XXXX
Dirichlet	Neumann	0X00 0X0X XX00 XXXX	$1 \rightarrow 3$ $2 \rightarrow 1$ $3 \rightarrow 4$ $4 \rightarrow 2$	X000 XX00 X0X0 XXXX
Neumann	Neumann	0X00 0X0X 00XX XXXX	$1 \rightarrow 4$ $2 \rightarrow 1$ $4 \rightarrow 2$	X000 XX00 0XX0 XXXX
Mixed	Neumann	0X00 0X0X XXXX XXXX	$1 \rightarrow 4$ $2 \rightarrow 1$ $4 \rightarrow 2$	X000 XX00 XXXX XXXX
Dirichlet	Mixed	XX00 XXXX XX00 XXXX	$2 \rightarrow 3$ $3 \rightarrow 2$	X0X0 XXXX X0X0 XXXX
Neumann	Mixed	XX00 XXXX 00XX XXXX	none	XX00 XXXX 00XX XXXX
Mixed	Mixed	XX00 XXXX XXXX XXXX	none	XX00 XXXX XXXX XXXX

Table 1: Column Permutations at the South-West Corner

By considering all possible boundary conditions at every type of boundary grid point, one can show that it is always possible to reorder the basis functions to obtain a non-zero diagonal in the corresponding diagonal block. A complete set of tables describing the reordering of the boundary basis functions is contained in Appendix A.

Recall that the ordering described in Sections 2-3 yields the intermediate collocation matrix given in Figure 3. After performing all of the boundary basis function permutations as described in the tables in Appendix B, the pattern of non-zero elements is as shown in Figure 4.

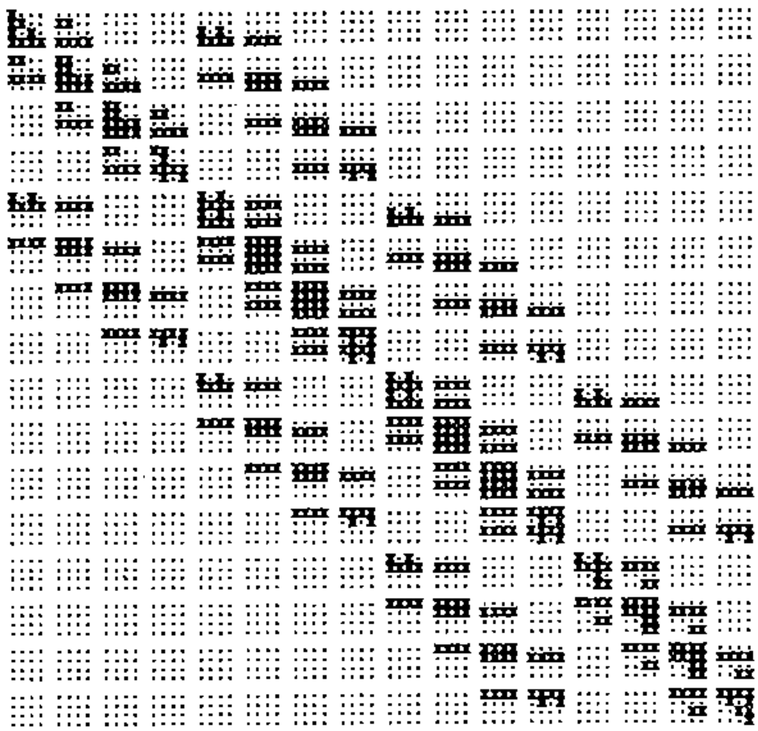


Figure 4: The Reordered Collocation Matrix
for a 4×4 Grid with 64 Unknowns

The matrix indeed has a non-zero diagonal.

5. Implementation

The ordering scheme described in Sections 2-4 has been implemented by the author as the indexing module, P3C1COLLORDER, within the ELLPACK system [Rice, 1977]. The ELLPACK module P3-C1 COLLOCATION generates the Hermite bicubic collocation linear system using a standard finite element ordering described in Appendix B. P3C1COLLORDER reorders the linear system generated by P3-C1 COLLOCATION so that the reordered system has a non-zero diagonal.

For example, in the case of a Poisson equation with Dirichlet boundary conditions and four grid lines in each direction, the structure of the P3-C1 COLLOCATION matrix is pictured in Figure 5.

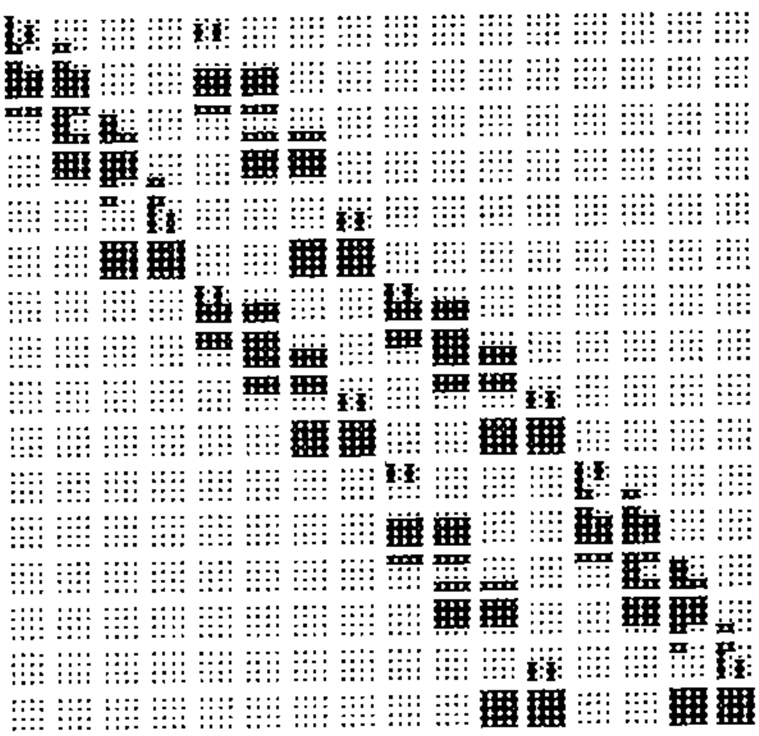


Figure 5: The P3-C1 COLLOCATION Matrix
for a 4×4 Grid with 64 Unknowns

The structure of the corresponding P3C1COLLORDER matrix is given in Figure 4. A complete set of computer generated pictures of the P3-C1 COLLOCATION and the P3C1COLLORDER matrices including all possible combinations of boundary conditions is given in Appendix B.

P3C1COLLORDER implements the cases of Appendices A and B. The program has 2023 lines of code, 544 of which are executable Fortran statements.

6. Conclusion

In the introduction we stated that the motivation for developing this ordering scheme for the collocation equations was the desire to use an iterative technique to solve the linear system. However, the collocation matrix resulting from this ordering is not symmetric, positive definite. In fact, we have seen computationally that it has complex eigenvalues some with rather large imaginary components. Hence, standard iterative techniques do not apply. The problem thus arises of developing an iterative technique which will solve the collocation equations in this form. Thus, we present this new ordering scheme as a first step towards the solution of this problem.

Acknowledgements

I thank Professor John R. Rice for suggesting the ordering described in Sections 2-3 and for encouraging me to continue this work to its present form.

REFERENCES

J. R. Rice, (1977), ELLPACK: A Research Tool for Elliptic Partial Differential Equations Software, in *Mathematical Software III* (J. Rice, ed.), Academic Press, pp. 319-342.

APPENDIX A

The tables in this appendix contain the basis function (unknown, column) permutations to be performed on the diagonal blocks which correspond to the boundary grid points. There are eight different types of boundary boundary points which we label as follows:

North West	North	North East
West		East
South West	South	South East

A table for each type of boundary grid point follows.

Note: The column permutations given in the tables are local in the sense that they refer to the column number within the diagonal block. Hence, switching columns 2 and 3 within a given diagonal block may actually involve switching columns 45 and 46 in the intermediate collocation matrix.

The boundary condition labels given in the tables have the following meanings:

Label	Boundary Condition
Dirichlet	$u = g$
Neumann	$\frac{\partial u}{\partial n} = g$
Mixed	$\alpha u + \beta \frac{\partial u}{\partial n} = g$

South West Corner				
Boundary Condition		Block Before	Column Permutation	Block After
West	South			
Dirichlet	Dirichlet	X000 X0X0 XX00 XXXX	2 → 3 3 → 2	X000 XX00 X0X0 XXXX
Neumann	Dirichlet	X000 X0X0 00XX XXXX	2 → 4 3 → 2 4 → 3	X000 XX00 0XX0 XXXX
Mixed	Dirichlet	X000 X0X0 XXXX XXXX	2 → 3 3 → 2	X000 XX00 XXXX XXXX
Dirichlet	Neumann	0X00 0X0X XX00 XXXX	1 → 3 2 → 1 3 → 4 4 → 2	X000 XX00 X0X0 XXXX
Neumann	Neumann	0X00 0X0X 00XX XXXX	1 → 4 2 → 1 4 → 2	X000 XX00 0XX0 XXXX
Mixed	Neumann	0X00 0X0X XXXX XXXX	1 → 4 2 → 1 4 → 2	X000 XX00 XXXX XXXX
Dirichlet	Mixed	XX00 XXXX XX00 XXXX	2 → 3 3 → 2	X0X0 XXXX X0X0 XXXX
Neumann	Mixed	XX00 XXXX 00XX XXXX	none	XX00 XXXX 00XX XXXX
Mixed	Mixed	XX00 XXXX XXXX XXXX	none	XX00 XXXX XXXX XXXX

Table A-1: Column Permutations at the South-West Corner

South East Corner				
Boundary Condition		Block Before	Column Permutation	Block After
South	East			
Dirichlet	Dirichlet	X0X0 X000 XXXX XX00	1 → 2 2 → 4 3 → 1 4 → 3	XX00 0X00 XXXX 0X0X
Dirichlet	Neumann	X0X0 X000 XXXX 00XX	1 → 2 2 → 3 3 → 1	XX00 0X00 XXXX X00X
Dirichlet	Mixed	X0X0 X000 XXXX XXXX	1 → 2 2 → 3 3 → 1	XX00 0X00 XXXX XXXX
Neumann	Dirichlet	0X0X 0X00 XXXX XX00	1 → 4 4 → 1	XX00 0X00 XXXX 0X0X
Neumann	Neumann	0X0X 0X00 XXXX 00XX	1 → 3 3 → 4 4 → 1	XX00 0X00 XXXX X00X
Neumann	Mixed	0X0X 0X00 XXXX XXXX	1 → 4 4 → 1	XX00 0X00 XXXX XXXX
Mixed	Dirichlet	XXXX XX00 XXXX XX00	1 → 4 4 → 1	XXXX 0X0X XXXX 0X0X
Mixed	Neumann	XXXX XX00 XXXX 00XX	none	XXXX XX00 XXXX 00XX
Mixed	Mixed	XXXX XX00 XXXX XXXX	none	XXXX XX00 XXXX XXXX

Table A-2: Column Permutations at the South-East Corner

North West Corner				
Boundary Condition		Block Before	Column Permutation	Block After
West	North			
Dirichlet	Dirichlet	XX00 XXXX X000 X0X0	1 → 3 2 → 1 3 → 4 4 → 2	X0X0 XXXX 00X0 00XX
Neumann	Dirichlet	00XX XXXX 00X0 X0X0	1 → 4 4 → 1	X0X0 XXXX 00X0 00XX
Mixed	Dirichlet	XXXX XXXX X0X0 X0X0	1 → 4 4 → 1	XXXX XXXX 00XX 00XX
Dirichlet	Neumann	XX00 XXXX X000 0X0X	1 → 3 2 → 1 3 → 2	X0X0 XXXX 00X0 X00X
Neumann	Neumann	00XX XXXX 00X0 0X0X	1 → 2 2 → 4 4 → 1	X0X0 XXXX 00X0 X00X
Mixed	Neumann	XXXX XXXX X0X0 0X0X	none	XXXX XXXX X0X0 0X0X
Dirichlet	Mixed	XX00 XXXX X000 XXXX	1 → 3 2 → 1 3 → 2	X0X0 XXXX 00X0 XXXX
Neumann	Mixed	00XX XXXX 00X0 XXXX	1 → 4 4 → 1	X0X0 XXXX 00X0 XXXX
Mixed	Mixed	XXXX XXXX X0X0 XXXX	none	XXXX XXXX X0X0 XXXX

Table A-3: Column Permutations at the North-West Corner

North East Corner				
Boundary Condition		Block Before	Column Permutation	Block After
North	East			
Dirichlet	Dirichlet	XXXX XX00 X0X0 X000	1 → 4 4 → 1	XXXX 0X0X 00XX 000X
Dirichlet	Neumann	XXXX 00XX X0X0 00X0	1 → 3 2 → 1 3 → 4 4 → 2	XXXX 0X0X 00XX 000X
Dirichlet	Mixed	XXXX XXXX X0X0 X0X0	1 → 4 4 → 1	XXXX XXXX 00XX 00XX
Neumann	Dirichlet	XXXX XX00 0X0X X000	1 → 4 3 → 1 4 → 3	XXXX 0X0X 0XX0 000X
Neumann	Neumann	XXXX 00XX 0X0X 00X0	2 → 3 3 → 4 4 → 2	XXXX 0X0X 0XX0 000X
Neumann	Mixed	XXXX XXXX 0X0X X0X0	3 → 4 4 → 3	XXXX XXXX 0XX0 X00X
Mixed	Dirichlet	XXXX XX00 XXXX X000	1 → 4 4 → 1	XXXX 0X0X XXXX 000X
Mixed	Neumann	XXXX 00XX XXXX 00X0	2 → 3 3 → 4 4 → 2	XXXX 0X0X XXXX 000X
Mixed	Mixed	XXXX XXXX XXXX X0X0	1 → 4 4 → 1	XXXX XXXX XXXX 00XX

Table A-4: Column Permutations at the North-East Corner

North Boundary			
Boundary Condition	Block Before	Column Switching	Block After
Dirichlet	XXXX XXXX X0X0 X0X0	1 → 4 4 → 1	XXXX XXXX 00XX 00XX
Neumann	XXXX XXXX 0X0X 0X0X	2 → 3 3 → 2	XXXX XXXX 00XX 00XX
Mixed	XXXX XXXX XXXX XXXX	none	XXXX XXXX XXXX XXXX

Table A-5: Column Permutations on the North Boundary

South Boundary			
Boundary Condition	Block Before	Column Switching	Block After
Dirichlet	X0X0 X0X0 XXXX XXXX	2 → 3 3 → 2	XX00 XX00 XXXX XXXX
Neumann	0X0X 0X0X XXXX XXXX	1 → 4 4 → 1	XX00 XX00 XXXX XXXX
Mixed	XXXX XXXX XXXX XXXX	none	XXXX XXXX XXXX XXXX

Table A-6: Column Permutations on the South Boundary

West Boundary			
Boundary Condition	Block Before	Column Switching	Block After
Dirichlet	XX00 XXXX XX00 XXXX	2 → 3 3 → 2	X0X0 XXXX X0X0 XXXX
Neumann	00XX XXXX 00XX XXXX	1 → 4 4 → 1	X0X0 XXXX X0X0 XXXX
Mixed	XXXX XXXX XXXX XXXX	none	XXXX XXXX XXXX XXXX

Table A-7: Column Permutations on the West Boundary

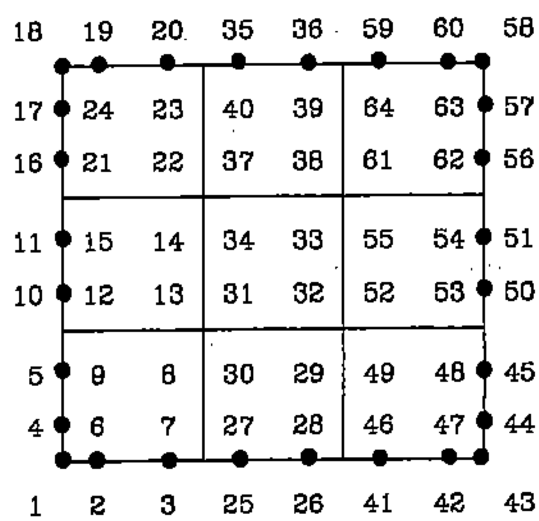
East Boundary			
Boundary Condition	Block Before	Column Switching	Block After
Dirichlet	XXXX XX00 XXXX XX00	1 → 4 4 → 1	XXXX 0X0X XXXX 0X0X
Neumann	XXXX 00XX XXXX 00XX	2 → 3 3 → 2	XXXX 0X0X XXXX 0X0X
Mixed	XXXX XXXX XXXX XXXX	none	XXXX XXXX XXXX XXXX

Table A-8: Column Permutations on the East Boundary

APPENDIX B

This appendix contains computer generated pictures of the structure of the matrices produced by the ELLPACK routines P3-C1 COLLOCATION and P3C1COLLORDER.

P3-C1 COLLOCATION numbers the grid rectangles from south to north, west to east. The collocation points are then numbered in a way corresponding to the ordering of the grid rectangles. For example, with four vertical and four horizontal grid lines there are 64 collocation points which P3-C1 COLLOCATION numbers as follows:

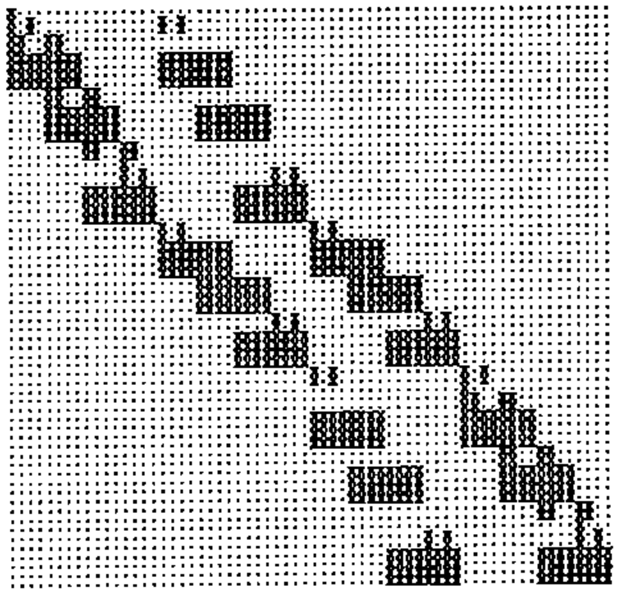


P3-C1 COLLOCATION orders the Hermite bicubic basis functions in a natural way from south to north, west to east similar to the ordering in Figure 2.

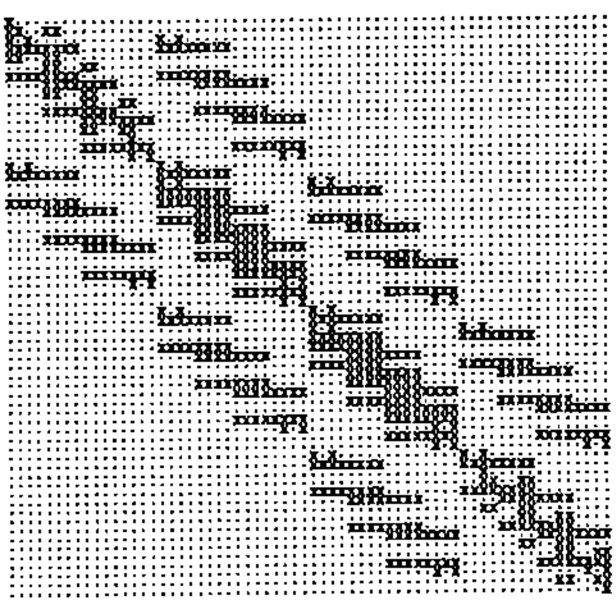
P3C1COLLORDER is an ELLPACK indexing module which reorders the linear system generated by P3-C1 COLLOCATION using the ordering scheme discussed in Sections 2-4.

The matrices pictured on the following pages were generated using the Laplace operator with four grid lines in each direction and with varied boundary conditions. The type of condition (see Appendix A) on each boundary is given at the top of each page in its respective location.

Dirichlet　　Dirichlet + Dirichlet　　Dirichlet

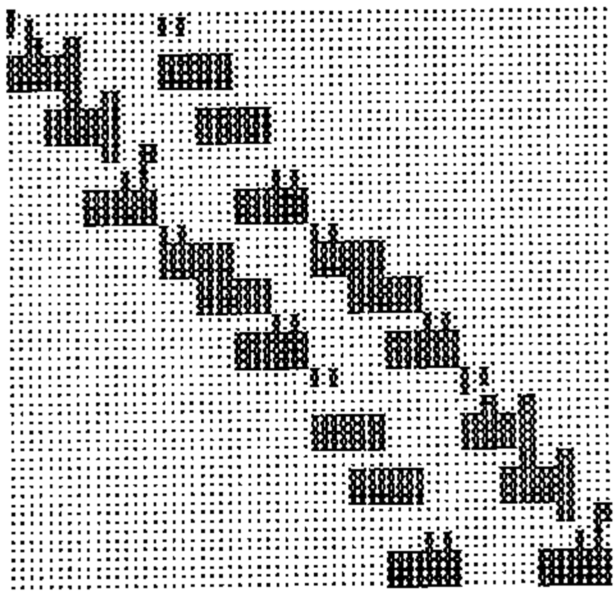


P3-C1 COLLOCATION matrix

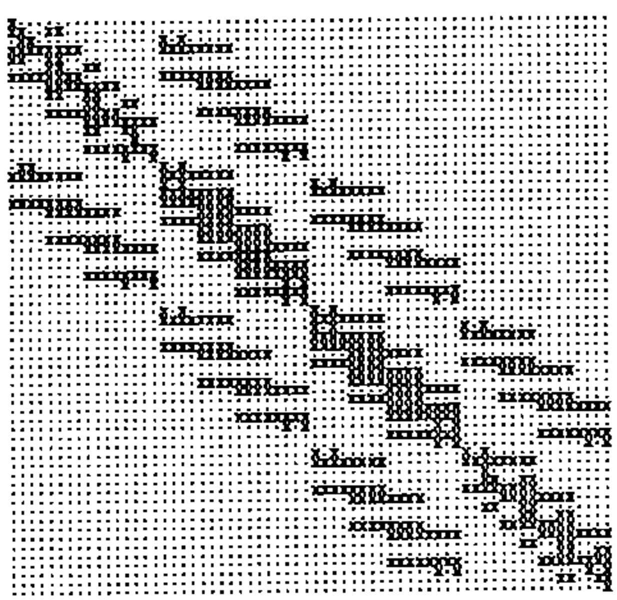


P3C1COLLORDER matrix

Neumann | Dirichlet + Dirichlet | Neumann

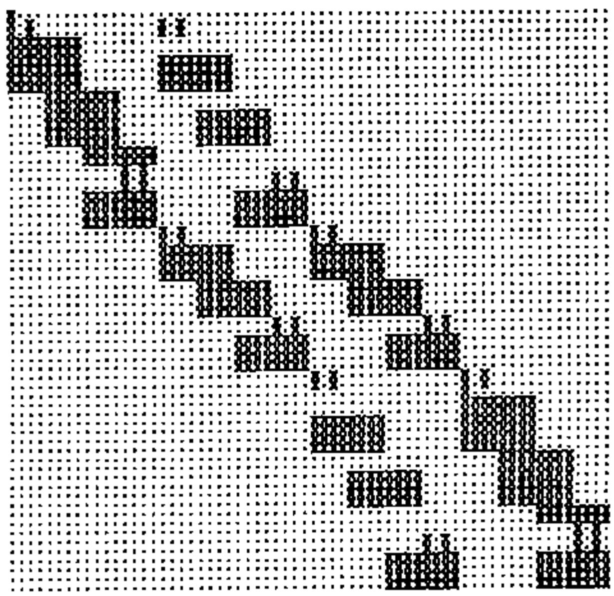


P3-C1 COLLOCATION matrix

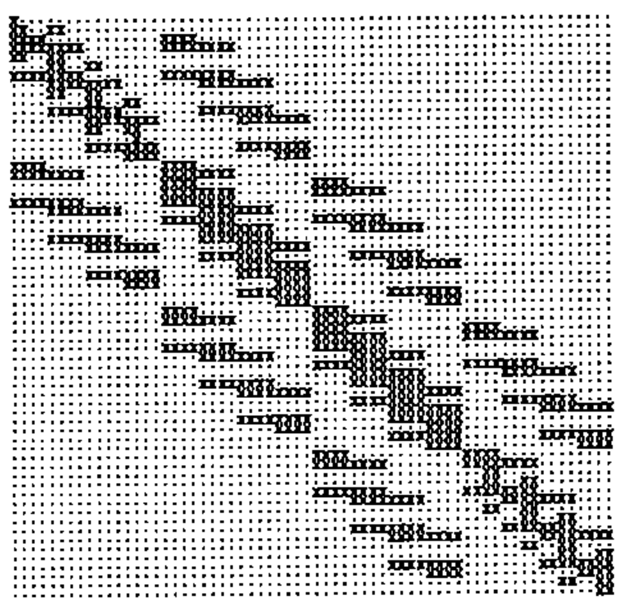


P3C1COLLORDER matrix

Mixed | Dirichlet + Dirichlet | Mixed

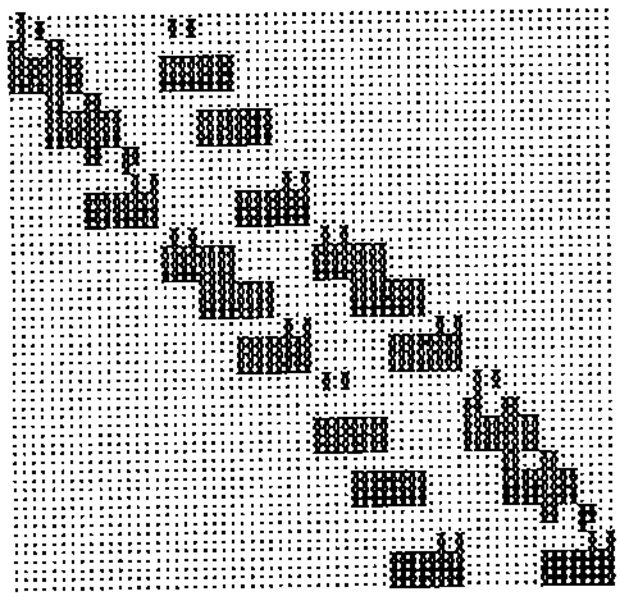


P3-C1 COLLOCATION matrix

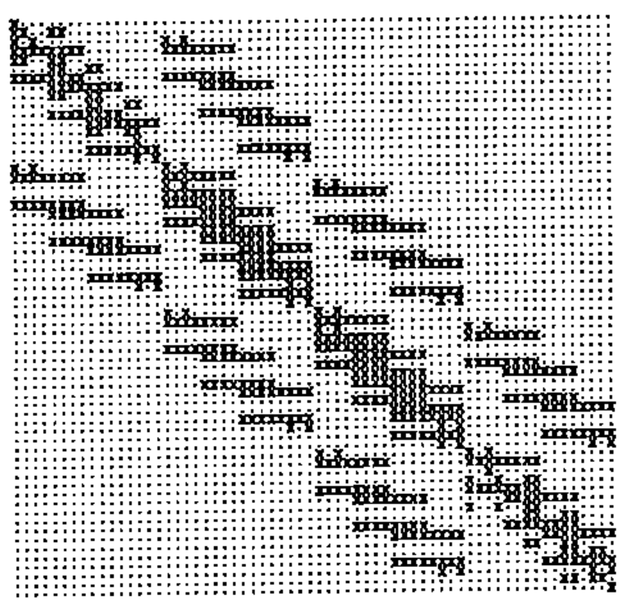


P3C1COLLORDER matrix

Dirichlet | Neumann + Neumann | Dirichlet

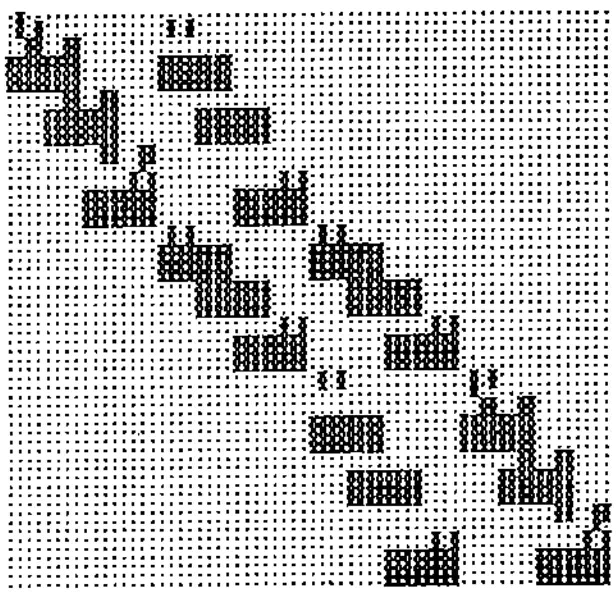


P3-C1 COLLOCATION matrix

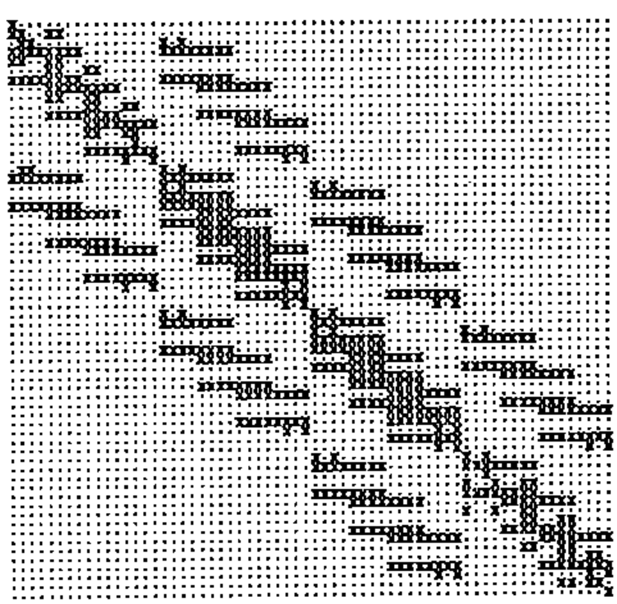


P3C1COLLORDER matrix

Neumann | Neumann + Neumann | Neumann

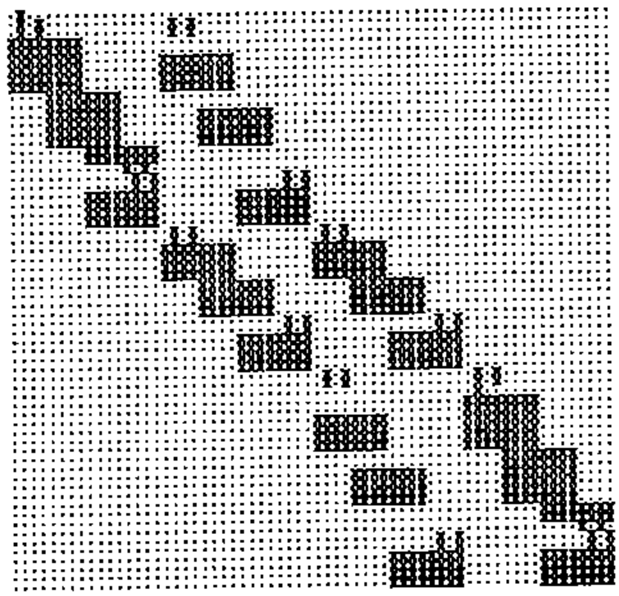


P3-C1 COLLOCATION matrix

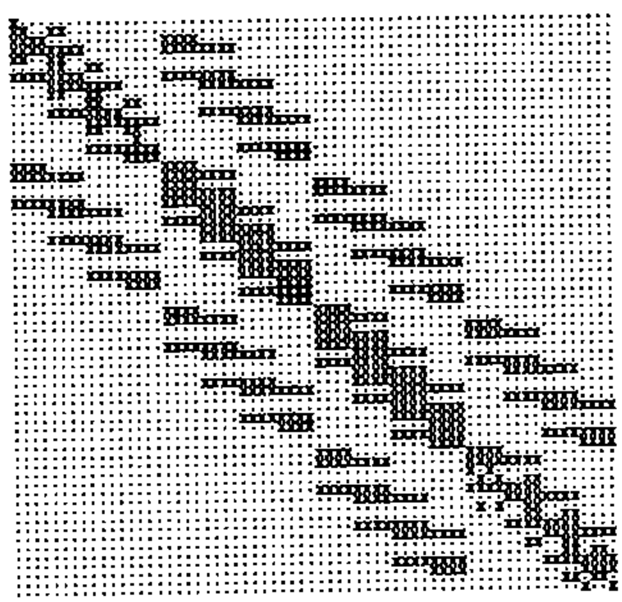


P3C1COLLORDER matrix

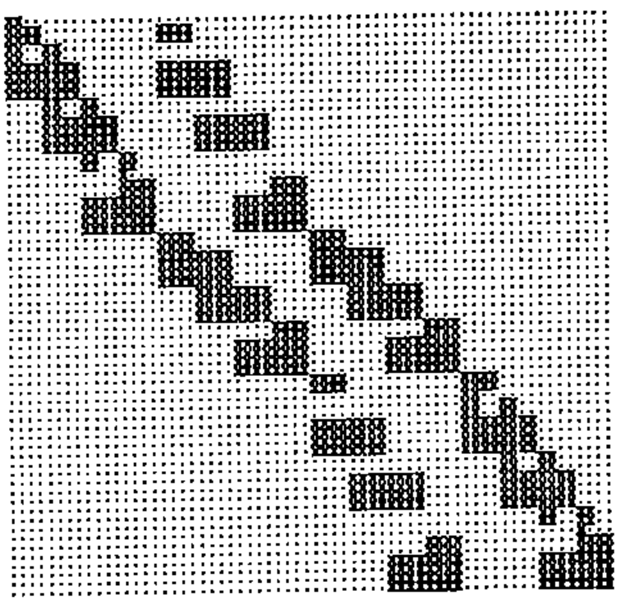
Neumann
Mixed + Mixed
Neumann



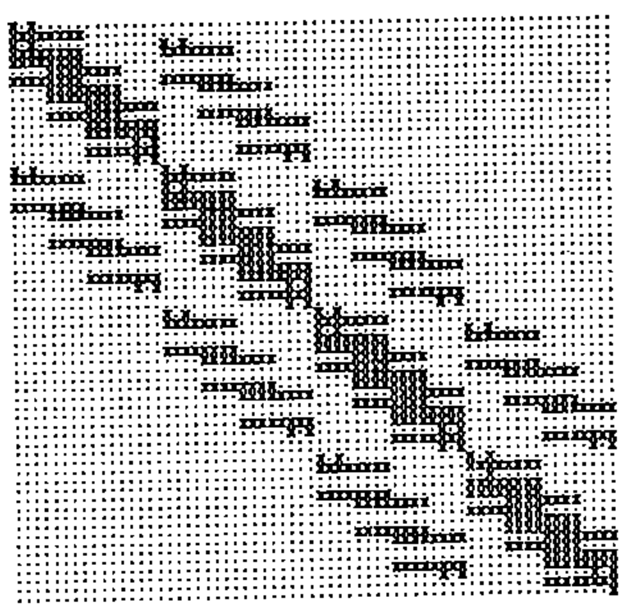
P3-C1 COLLOCATION matrix



P3C1COLLORDER matrix

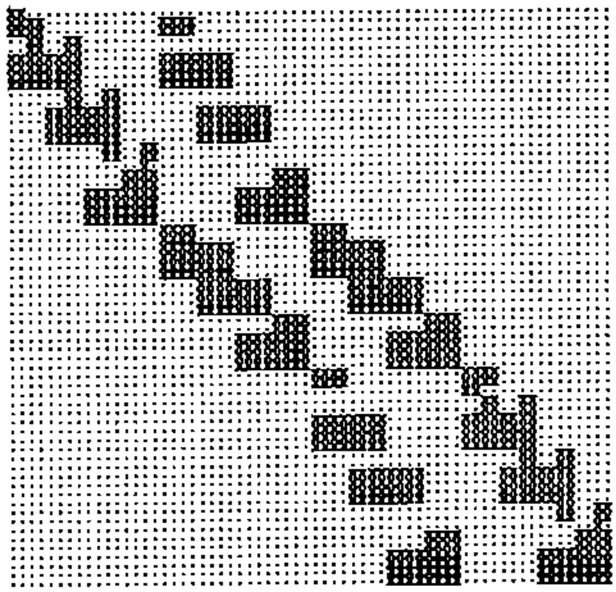


P3-C1 COLLOCATION matrix

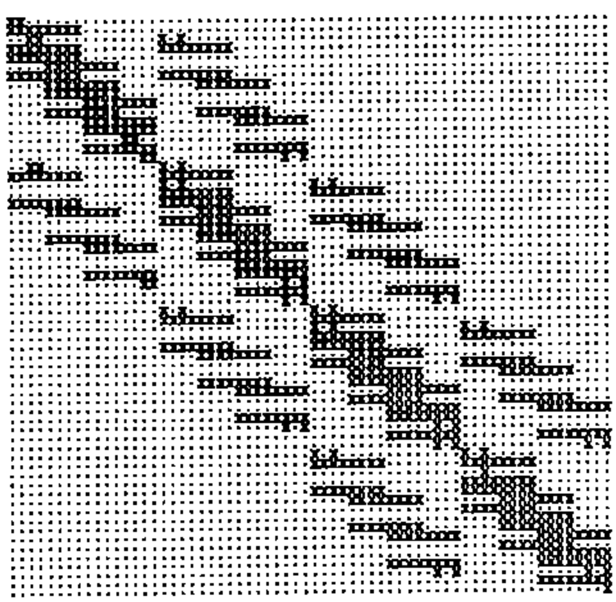


P3C1COLLORDER matrix

Mixed
Neumann + Neumann
Mixed



P3-C1 COLLOCATION matrix

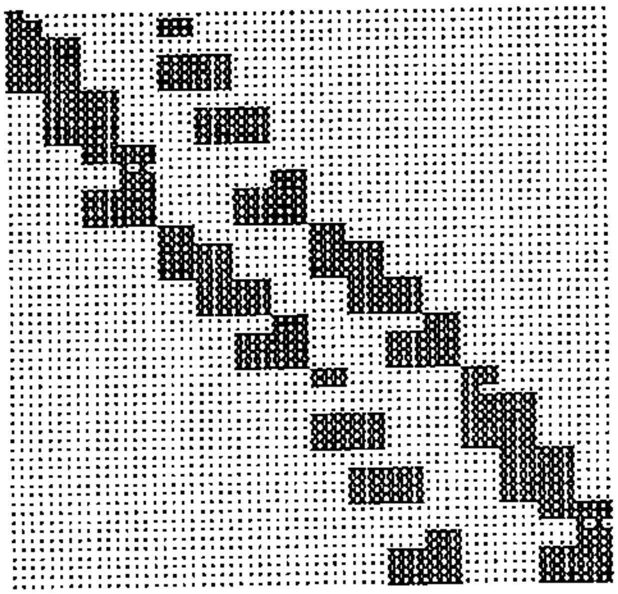


P3C1COLLORDER matrix

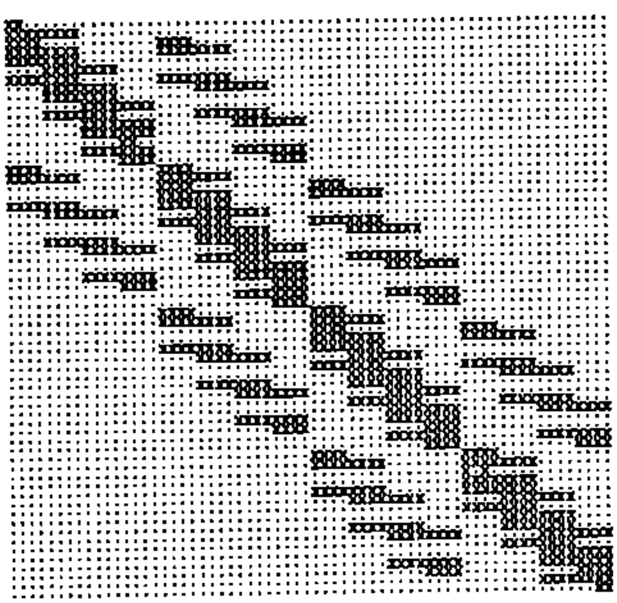
Mixed + Mixed

Mixed Mixed

Mixed



P3-C1 COLLOCATION matrix



P3C1COLLORDER matrix