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SOME NUMERICAL SCHEMES FOR NEUTRON DIFFUSION PROBLEMS

by

J. P. ROOS

1967

Joint Nuclear Research Center
Ispra Establishment - Italy

Scientific Data Processing Center - CETIS

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The mixed type scheme, suggested by FRIEDRICHS, seems very efficient in particular since it can easily deal with general interfaces.

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SUMMARY

In order to solve general elliptic equations we compare with respect to the convergence and accuracy three finite difference schemes, the five-point, the nine-point, and the mixed type formulas.

The mixed type scheme, suggested by FRIEDRICHS, seems very efficient in particular since it can easily deal with general interfaces.

Contents

Introduction (*)

In this study we solve numerically general elliptic partial differential equations. In order to solve them three types of finite difference formulas are derivedsystematically, using a variational principle established for these elliptic equations.

In particular, we derive

(i) the well known five-point formulas,
(ii) the nine-point formulas, as suggested by Nohel and Timlake [7],
(iii) the formulas of 'mixed' type.

As regards the formulas of mixed type, they have been suggested by Friedrichs [3] who used them, however, to prove the existence of the solution of the Neumann problem. In comparison with the scheme (ii) this type of formula has two advantages.

Firstly, it can be dealt with by the decomposition method, see [1], [8], [9]. This decomposition method gives a reduction of a factor two (roughly) in the number of meshpoints where the solution must be obtained iteratively.

Secondly, the mixed formulas can treat general interfaces.

In Chapter III some sufficient conditions are established in order that the coefficient matrices of these three difference schemes are M-matrices.

In Chapter IV we compare some of the numerical aspects of the three schemes. The conclusion of this research is that the scheme (iii) can efficiently be applied to the numerical solution of general elliptic operators.

(*) Manuscipt received on November 21, 1966

I. Statement of the Problem

1. The Differential Equations

In the diffusion approximation of the reactor calculation the following problem is typical.

Let D, A, and F be g×g matrices (D be a diagonal matrix), Φ be a g-dimensional vector and λ be a constant. R is a region with boundary $\Gamma = \Gamma_1 + \Gamma_2$, n denotes the external normal on the boundary.

$$\begin{aligned} - \nabla D \nabla \Phi + A\ \Phi &= \frac{1}{\lambda} F\ \Phi \quad &&\text{in } R\ , \\ \Phi &= 0 &&\text{on } \Gamma_1, \\ \frac{\partial \Phi}{\partial n} &= 0 &&\text{on } \Gamma_2, \end{aligned} \tag{1.1.1}$$

with the adjoint problem

$$\begin{aligned} - \nabla D \nabla \Phi^* + A^t\ \Phi^* &= \frac{1}{\lambda} F^t\ \Phi^* \quad &&\text{in } R\ , \\ \Phi^* &= 0 &&\text{on } \Gamma_1, \\ \frac{\partial \Phi^*}{\partial n} &= 0 &&\text{on } \Gamma_2. \end{aligned} \tag{1.1.2}$$

(* means the adjoint, t means the transposed).

The dominant eigenvalue and the corresponding eigenfunction are the most important quantities in this problem.

Under some conditions, to be imposed upon D, A, F, Φ, R and Γ ([4], [5]) this problem possesses a dominant, positive, simple eigenvalue with a corresponding non-negative eigenfunction Φ and a corresponding positive adjoint eigenfunction Φ^*.

For the sake of clarity we make some simplifying assumptions. We consider only a rectangular region R. About more general boundaries and interfaces see [2] and [3].

The interfaces are approximated by broken straight lines. We choose the axes along the sides (and the origin of the coordinate system in one of the angles).

Furthermore, we distinguish two classes of problems,

(i) problems with interfaces parallel to the axes,
(ii) problems with interfaces anyhow.

For the first class of problems the five- and nine-point formulas will be derived, while for the second class the mixed formulas will be derived. The derivation is sketched in chapter II.

2. The Variational Principle

For the functions Φ in a certain class $\{\Phi\}$ we wish to render a functional J stationary under condition H = constant (e.g., = 1), with

$$J = \iint_R (\nabla\Phi^* D\nabla\Phi + \Phi^* A\ \Phi)dR,$$

and (1.2.1)

$$H = \iint_R \Phi^* F\ \Phi\ dR\ .$$

See [4].

The solutions of this variational principle (if they exist) can be proved to be solutions of the problem (1.1.1) and (1.1.2). As is well known, we need to consider $I = J - \frac{1}{\lambda} H$.

In order to discretizise the problem a net must be set over the region R. The interfaces are assumed to be mesh links and the coefficients D, A and F are assumed to be constant in each cell of the net.

We consider two geometries:

(i) x-y-geometry (cartesian coordinates, Φ is independent of z),
(ii) r-z-geometry (cylindrical coordinates, Φ is independent of the polar angle ϑ).

Then, the element of area dR satisfies

$$dR = x^p \, dxdy ,$$

with
$$p = 0 \quad \text{in case (i)} ,$$
$$= 1 \quad \text{in case (ii)} .$$

II. Sketch of the Derivation of the Difference Equations for a Rectangular Region

1. The five- and nine-point formulas

A rectangular net will be set over the rectangular region R with mesh links parallel to the axes (sides of R). See figure 1.

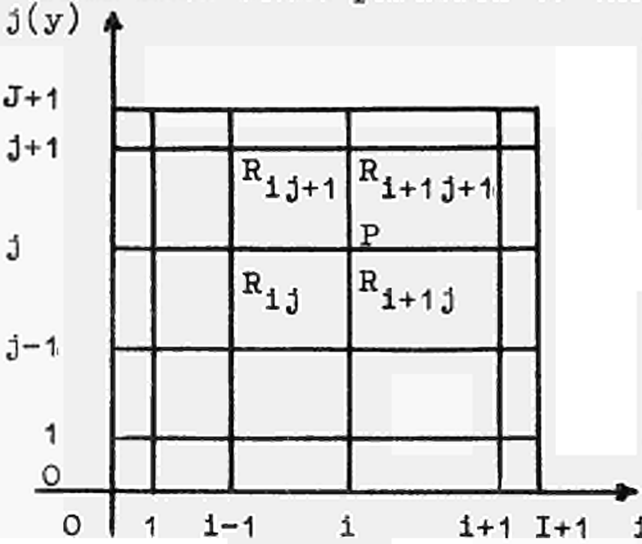


Figure 1

The functional I (see I.2) can be considered as the sum of functionals I_{ij} belonging to a cell R_{ij}.

$$I = \sum_{ij} I_{ij}$$

(summation over all the cells R_{ij}),

$$I_{ij} = \iint\limits_{R_{ij}} (\nabla\Phi^* D^{ij} \nabla\Phi + \Phi^* A^{ij} \Phi) dR . \qquad (2.1.1)$$

In each cell D, A and F are assumed to be constant; in cell R_{ij} they are D^{ij}, A^{ij} and F^{ij} resp. Moreover, we have written A^{ij} for $A^{ij} - \frac{1}{\lambda} F^{ij}$.

We have

$$I_{ij} = \sum_{n=1}^{g} D_n^{ij} \iint\limits_{R_{ij}} \nabla\Phi_n^* \nabla\Phi_n \, dR + \sum_{n,m=1}^{g} A_{nm}^{ij} \iint\limits_{R_{ij}} \Phi_n^* \Phi_m \, dR \qquad (2.1.2)$$

(products of vectors are to be understood as scalar products).

Now we approximate I_{ij} in a certain way such that $I = \Sigma I_{ij}$ is a linear function of $\Phi^*(P)$ and $\Phi(P)$ in all the interior nodes $P = (ij)$. In order that I is rendered stationary, it is necessary that

$$\frac{\partial I}{\partial \Phi_n^*(P)} = 0 \,, \qquad (2.1.3)$$

and $$\frac{\partial I}{\partial \Phi(P)} = 0 \,, \text{ for } n = 1,\ldots,g \text{ and all } P \,. \qquad (2.1.4)$$

We consider only (2.1.3) that gives us the difference equations for $\Phi(P)$, while (2.1.4) gives us those for $\Phi^*(P)$. In this approximation I_{ij} depends on $\Phi^*(P)$ if and only if P is an angle of R_{ij}, P = (ij) or

$$\frac{\partial I}{\partial \Phi_n^*(ij)} = \frac{\partial}{\partial \Phi_n^*(ij)} \left\{ I_{ij} + I_{i+ij} + I_{ij+1} + I_{i+1j+1} \right\} = 0 \,, \quad (2.1.5)$$

$n = 1,\ldots,g$.

The derivation of these formulas is given in more detail in the appendix A1. It may be remarked that the interfaces have to be meshlinks (parallel to the axes).

2. The mixed formulas

(See [3], [8])

In order to derive the mixed formulas we extend the rectangular net by adding in each cell one diagonal in the following way. We divide the nodes (interior and boundary) in two classes, (i) i+j is even and (ii) i+j is odd.

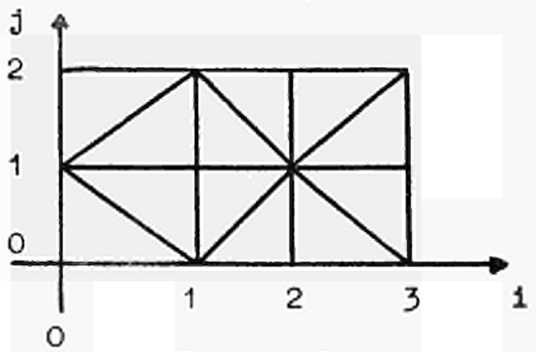


Figure 2

The points of one class are connected by cell diagonals (we choose the class i+j odd), see fig. 2.
In this way an extended net is generated.

Now we consider all the continuous functions which are linear in each triangle of this extended net. The variational principle will be applied to this class of functions. The interfaces are assumed to be mesh links of this extended net (either cell diagonals or mesh links of the first rectangular net).

Clearly, we have two kinds of mesh points (i) with a star Σ_5 (called "five-points") and (ii) with a star Σ_9 (called "nine-points"), figure 3. The points with a star Σ_5 give rise to five-point formulas and those with Σ_9 to nine-point formulas.
The coefficients D, A and F are assumed to be constant in each triangle. Quite similarly to 1., we now derive

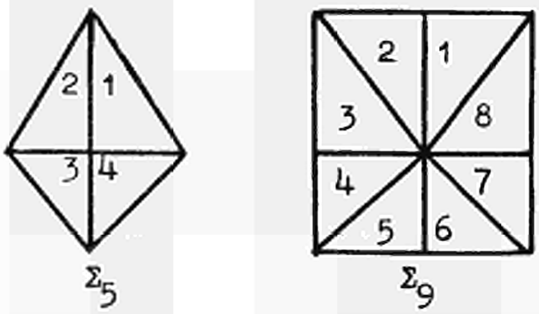


Figure 3

$$\text{for } \Sigma_5: \quad \frac{\partial I}{\partial \Phi_n^*(P)} = \frac{\partial}{\partial \Phi_n^*(P)} \sum_{k=1}^{4} I_k = 0 \, ,$$

and (2.2.1)

$$\text{for } \Sigma_9: \quad \frac{\partial I}{\partial \Phi_n^*(P)} = \frac{\partial}{\partial \Phi_n^*(P)} \sum_{k=1}^{8} I_k = 0 \, , \qquad \text{for } n=1,\ldots,g.$$

$$I_k = \sum_{n=1}^{g} D_n^k \iint_{T_k} \nabla\Phi_n^* \, \nabla\Phi_n \, dR + \sum_{n,m=1}^{g} A_{nm}^k \iint_{T_k} \Phi_n^* \, \Phi_m \, dR \qquad (2.2.2)$$

where T_k is any triangle.

The mixed formulas and their derivation are given in the appendix A2.

Remark The scheme described in II.2 is particularly efficient also for operators with the mixed derivatives (apart from the advantage of being able to treat arbitrary interfaces).

III. Treatment of the difference equations

1. Structure of the Equations

In the appendix A the equations have been derived. The boundary conditions (u or u_n equal zero) are very simple to deal with. See the appendix A3.

(i) The five-point formulas

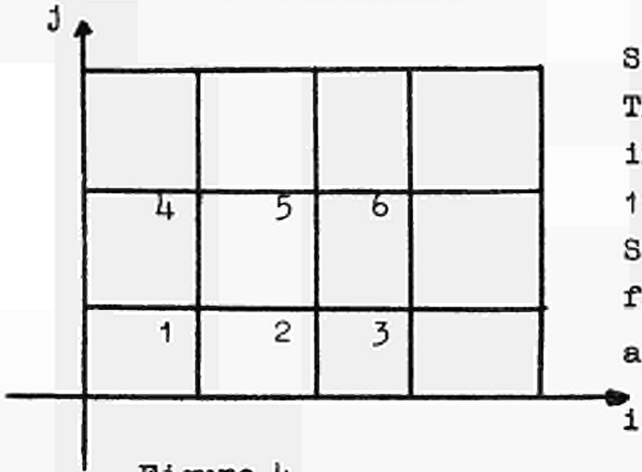


Figure 4

See appendix A.1(i) and figure 4. The (interior) nodes are ordered in the ordinary way, i.e., 11, 21..., I1, 12...,I2,...1J,...,IJ. Say N=I . J. It is clear that the five-point formulas can be written as

$$H_{(5)}\ \Phi = \frac{1}{\lambda} F_{(5)}\ \Phi\ , \qquad (3.1.1)$$

where $H_{(5)}$ is a N×N blocked, five-diagonal matrix (the entries are the coefficients in the formulas, each entry is a g×g matrix). A partitioning by lines gives $H_{(5)}$ the block-tridiagonal structure,

$F_{(5)}$ is a N×N block-diagonal matrix ,

and the transposed flux vector Φ^t is

$$\Phi^t = (\varphi_{11},\ldots,\varphi_{I1},\varphi_{12},\ldots\ \varphi_{I2},\ldots,\varphi_{1J},\ldots\ \varphi_{IJ})\quad ,$$

φ_{ij} is a g-vector $(\varphi_{ij}^{(1)},\ldots,\varphi_{ij}^{(g)})$, for all $i=1,\ldots,I$ and $j=1,\ldots,J$.

(ii) The nine-point formulas

In a way similar to (i), we can write (see appendix A.1(ii))

$$H_{(9)}\ \Phi = \frac{1}{\lambda} F_{(9)}\ \Phi \ , \qquad (3.1.2)$$

where $H_{(9)}$ and $F_{(9)}$ now are N×N block nine-diagonal matrices (by the partitioning by lines, they gain the block-tridiagonal structure).

(iii) The mixed formulas

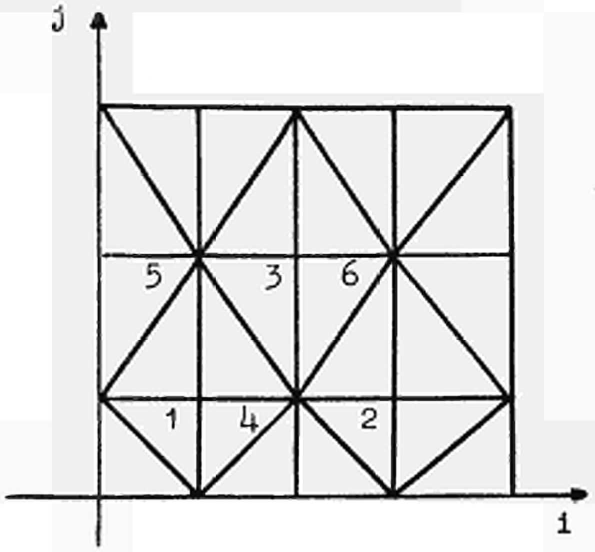


Figure 5

See appendix A.2 and figure 5. The total number of nodes be N=I J. The (interior) nodes are separated in two classes. The points in the class with i+j even are called the five-points, or points with star Σ_5, the other points are called nine-points.

The five-points are numbered from 1 to $N_o = \left[\frac{N+1}{2}\right]$, the nine-points from N_o+1 to N, both in the ordinary way. $N_1 = N-N_o$.

In this ordering : $\Phi^t = (\Phi_1^t,\ \Phi_2^t)$

$$\Phi_1^t = (\varphi_{11}, \varphi_{31}, \varphi_{51}, \dots, \varphi_{22}, \varphi_{42}, \varphi_{62}, \dots, \varphi_{13}, \varphi_{33} \dots)$$

$$\varphi_2^t = (\varphi_{21}, \varphi_{41}, \varphi_{61}, \dots, \varphi_{12}, \varphi_{32}, \varphi_{52}, \dots, \varphi_{23}, \varphi_{43} \dots)$$

Then we can write

$$H_{(59)}\ \Phi = \frac{1}{\lambda} F_{(59)}\ \Phi \ , \qquad (3.1.3)$$

where
$$H_{(59)} = \begin{vmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{vmatrix} , \qquad (3.1.4)$$

and $$F_{(59)} = \begin{vmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{vmatrix} , \qquad (3.1.5)$$

H_{11} and F_{11} are $N_o \times N_o$ block-diagonal matrices ,

H_{12} and F_{12} are $N_o \times N_1$ (i.e. N_o rows and N_1 columns) blocked, four-diagonal matrices) ,

H_{21} and F_{21} are $N_1 \times N_o$ blocked, four-diagonal matrices ,

H_{22} and F_{22} are $N_1 \times N_1$ blocked, five-diagonal matrices ,

The equation $H_{11}\ \Phi_1 + H_{12}\ \Phi_2 = \frac{1}{\lambda}\ (F_{11}\ \Phi_1 + F_{12}\ \Phi_2)$ represents the formulas for the five-points. The other equation in (3.1.3) similarly for the nine-points.

2. Iterative Methods

a) The five- and nine-point formulas

The equation to be solved is

$$H\Phi = \frac{1}{\lambda}\ F\Phi\ .$$

Write H = D+L+U, where D is the diagonal part of H (in this partitioning with respect to the g×g matrices), L is the lower triangular part and U the upper part.

(i) The power method

Start values $\Phi^{(0)}$ and $\lambda^{(0)}$ are assumed to be given.

Outer iteration : $H\Phi^{(n+1)} = \frac{1}{\lambda}\ F\Phi^{(n)}, \quad n = 0,1,\dots ,$ (3.2.1)

$$\lambda^{(n+1)} = \lambda^{(n)}\ \frac{\|F\Phi^{(n+1)}\|}{\|F\Phi^{(n)}\|} = \lambda^{(0)}\ \frac{\|F\Phi^{(n+1)}\|}{\|F\Phi^{(0)}\|}\ , \qquad (3.2.2)$$

until $$\left| \frac{\lambda^{(n+1)} - \lambda^{(n)}}{\lambda^{(n+1)}} \right| < \varepsilon\ . \qquad (3.2.3)$$

Inner iteration (to solve (3.2.2)) :

$$b = \frac{1}{\lambda^{(n)}} F\Phi^{(n)} ,$$

$$y^{(0)} = \Phi^{(n)} .$$

Solve $\quad (D+L)y^{(m)} = -Uy^{(m-1)}+b \quad m=1,2,\ldots ,$

until $\quad \max_i \left| \frac{y_i^{(m)} - y_i^{(m-1)}}{y_i^{(m)}} \right| < \eta \quad ; \qquad (3.2.4)$

the m for which the inner iteration stops be M,
then $\quad \Phi^{(n+1)} = y^{(M)}$ (being the last computed one).

(ii) <u>The method equipoise</u>

This method is similar to (i).

Here M=1 (only one inner iteration).
Moreover $\lambda^{(n)}$ is estimated by

$$\lambda^{(n)} = \frac{\| F\Phi^{(n)} \|}{\| H\Phi^{(n)} \|} \qquad n = 0,1,\ldots \qquad (3.2.5)$$

The proper method equipoise consists in taking $\|x\|_e = x \cdot e = \sum_i x_i$,
where e is the vector with each entry equal to the unity.

b) <u>The mixed formulas</u>

Here the decomposition method has been used

$$H\Phi = \frac{1}{\lambda} F\Phi ,$$

$$H = \begin{vmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{vmatrix} ,$$

with a block diagonal matrix H_{11} (see [1] , [8], [9]) .

If $\quad B = F\Phi$, and in this partitioning $B^t = (B_1, B_2)$,

and $\quad G = H_{22} - H_{21} H_{11}^{-1} H_{12}$ (see formulas A.2.3), then $$\Phi_1 = - H_{11}^{-1} H_{12} \Phi_2 + \frac{1}{\lambda} H_{11}^{-1} B_1 , \qquad (3.2.6)$$

$$G\Phi_2 = \frac{1}{\lambda} (B_2 - H_{21} H_{11}^{-1} B_1) \quad .$$

(i) The power method

Given the guesses $\Phi^{(0)}$ and $\lambda^{(0)}$ the iterative procedure is as follows.

Outer iteration: $B^{(n)} = F\Phi^{(n)}$, $n = 0,1,\dots,$

$$G\Phi_2^{(n+1)} = \frac{1}{\lambda^{(n)}} (B_2^{(n)} - H_{21} H_{11}^{-1} B_1^{(n)}), \qquad (3.2.7)$$

$$\Phi_1^{(n+1)} = - H_{11}^{-1} H_{12} \Phi_2^{(n+1)} + \frac{1}{\lambda^{(n)}} H_{11}^{-1} B_1^{(n)} ,$$

$$\lambda^{(n+1)} = \lambda^{(n)} \frac{\|F\Phi^{(n+1)}\|}{\|F\Phi^{(n)}\|} = \lambda^{(0)} \frac{\|F\Phi^{(n+1)}\|}{\|F\Phi^{(0)}\|} ,$$

with the criterion (3.2.3).
In the inner iteration, (3.2.7) is solved as follows. As usual, G is written as the sum of the diagonal, the lower and upper tridiagonal parts, G = D+L+U.

$$b = \frac{1}{\lambda^{(n)}} (B_2^{(n)} - H_{21} H_{11}^{-1} B_1^{(n)}) ,$$

$$y^{(0)} = \Phi^{(n)},$$

$$(D+L)y^{(m)} = -Uy^{(m-1)} + b , \quad m = 1,2,\dots ,$$

with the criterion (3.2.4) ,

$$\Phi^{(n+1)} = y^{(M)} \text{ (the last computed one).}$$

(ii) The method equipoise

As in a) (ii) this method means M=1 and the application of the eigenvalue estimation (3.2.5).

3. Some Matrix Properties

Whether the coefficient matrices are monotone [1], or not, is still an unsolved problem. In this section we shall establish some sufficient conditions in order that the matrices H (for the five- and nine-point formulas, see III.2a) and G (for the mixed formulas, see III.2b) are M-matrices. But under these conditions H for the mixed point formulas is certainly not an M-matrix.

We introduce some definitions.

Definition 1 : The matrix $A = (a_{ij})$ is said to have the M-structure if

$$a_{ii} > 0 \quad \text{for all } i \quad ,$$

and

$$a_{ij} \leqslant 0 \quad \text{for all } i \text{ and } j,\ j \neq i \ .$$

Remark 1 : Collatz calls this concept the 'sign distribution' [1, page 45].

Definition 2 : The matrix $A = (a_{ij})$ is said to be strongly diagonally dominant if

$$\left|a_{ii}\right| \geqslant \sum_{j \neq i} \left|a_{ij}\right| \quad ,$$

with strict inequality for at least one i.

Remark 2 : This concept is sometimes called the 'weak row-sum criterion' [1, page 46]. In [2, page 181] this property is simply called 'diagonal dominance'.

Remark 3 : An M-matrix may be defined as a monotone matrix [1] satisfying definition 1. If A is irreducible and satisfies definition 2, A is irreducibly diagonally dominant. If, moreover, A satisfies definition 1, A is an M-matrix [10].

Remark 4 : In the equation $H\Phi = \frac{1}{\lambda} F\Phi$ (see 3.1.1 , 3.1.2), H is irreducible by construction (R is a 'connected' region with a 'connected' mesh) and F is non-negative with positive diagonal entries. If we establish conditions such that H^{-1} is positive, $H^{-1}F$ is positive and irreducible. Then, $H^{-1}F$ has a positive, simple eigenvalue (equal to its spectralradius) with a corresponding positive eigenvector [10]. Moreover, if H is strongly diagonally dominant and irreducible, the Gauss-Seidel method applied in the inner iteration $H\Phi = b$ converges [1], [2].

(a) The five-point formulas

The five-point formulas are given in formula (A1.1). Since a^{ij} and b^{ij} are non-negative diagonal matrices and since c^{ij} has the M-structure, H has the M-structure too.

Theorem 1 : If A is strongly diagonally dominant, H is strongly diagonally dominant (by virtue of the introductory remarks H is then an M-matrix).

Proof : Let

$$f_k = \sum_{l=1}^{g} \left(c_{kl}^{ij} - a_{kl}^{ij} - b_{kl}^{ij} - b_{kl}^{ij+1} - a_{kl}^{i+1j}\right) =$$
$$= \sum_{l=1}^{g} \left\{\left(\gamma_{kl}^{ij} + \gamma_{kl}^{ij+1}\right)\tau_j^- + \left(\gamma_{kl}^{i+1j} + \gamma_{kl}^{i+1j+1}\right)\tau_i^+\right\} .$$

Since $\sum_{l=1}^{g} \gamma_{kl}^{ij} \geq 0$, with strict inequality for at least one k, H is strongly diagonally dominant.

(b) The nine-point formulas

These formulas are given in formula (A1.3).

Theorem 2 : Let

$$\mu_i = \frac{\rho_i}{\sigma_{i-1}^+} = \left(\frac{6x_i - 3h_i}{6x_i - 5h_i}\right)^p , 1 \leq \mu_i \leq 3 ,$$

$$\nu_{ij} = \min\left(3k_j^2 - h_i^2,\ \frac{3}{\mu_i} h_i^2 - k_j^2\right),$$

$$m_{ij} = \frac{h_i^2\ k_j^2}{12\ \nu_{ij}} .$$

If $\sqrt{\frac{\mu_i}{3}} < \frac{h_i}{k_j} < \sqrt{3}$, (3.3.1)

and $D_{11}^{ij} \geq m_{ij}\ A_{11}^{ij}$, for all i and j ,

H has the M-structure.

If, moreover, A^{ij} is strongly diagonally **dominant**, H is strongly diagonally dominant too.

<u>Proof</u> : The matrices a^{ij}, b^{ij}, and c^{ij} have non-negative off-diagonal entries.

If L = 1 (or, the left boundary condition is $\frac{\partial\Phi}{\partial n} = 0$, see the appendix A3), $\rho_1 = 0$ and we need not impose any condition. The conditions (3.3.1) are equivalent to

$$\alpha_{11}^{ij} + \beta_{11}^{ij} - \gamma_{11}^{ij} \geq 0 ,$$

$$3\alpha_{11}^{ij} - \beta_{11}^{ij} - \gamma_{11}^{ij} \geq 0 ,$$

$$3\beta_{11}^{ij}\ \sigma_i^- - (\alpha_{11}^{ij} + \gamma_{11}^{ij})\rho_i \geq 0 ,$$

$$3\beta_{11}^{ij}\ \sigma_{i-1}^+ - (\alpha_{11}^{ij} + \gamma_{11}^{ij})\rho_i \geq 0 , \text{ for all i and j.}$$

Hence a^{ij}, b^{ij}, and c^{ij} are non-negative matrices. Since e^{ij} has the M-structure, H has the M-structure too.

As regards the diagonal dominance,

$$f_k = \sum_{l=1}^{g} \left(e_{kl}^{ij} - a_{kl}^{ij} - b_{kl}^{ij} - b_{kl}^{ij+1} - a_{kl}^{i+1j} - c_{kl}^{ij} - c_{kl}^{i+1j} + \right.$$
$$\left. - c_{kl}^{ij+1} - c_{kl}^{i+1j+1}\right) =$$
$$= 4 \sum_{l=1}^{g} \left\{(\gamma_{kl}^{ij} + \gamma_{kl}^{ij+1})\rho_i + (\gamma_{kl}^{i+1j} + \gamma_{kl}^{i+1j+1})\rho_{i+1}\right\} ,$$

or $f_k \geq 0$, with strict inequality for at least one k. H is strongly diagonally dominant.

(c) The mixed formulas

See the formulas in appendix A2.

In theorem 3 we drop the cumbersome indices i,j (of the meshpoints and the squares), and +, - (of the triangles).

Since α, β and γ have the M-structure (α and β are diagonal matrices), the matrices d, $\bar{d}$, and e have the M-structure too.

Theorem 3 : If in each triangle (of the extended net)

$$\alpha_{ll} \geq \mu_1 \gamma_{ll} ,$$

and $\beta_{ll} \geq \mu_2 \gamma_{ll}$, for $l=1,\ldots,g$, (3.3.2)

the matrices a, b, and c are non-negative. It is sufficient to take

$$\mu_1 = 1.08 ,$$

and $\mu_2 = 1.8$,

but see appendix A3, remark.

Proof : The off-diagonal entries of a, b, and c are non-negative. By virtue of (3.3.2) a_{ll} and c_{ll} are non-negative. In fact,

$$\alpha_{ll} \rho^- \geq \gamma_{ll} \sigma^- ,$$

and $\alpha_{ll} \rho^+ \geq \gamma_{ll} \sigma^+$,

are satisfied in the whole region since

$$\max\left(\frac{\sigma^-}{\rho^-}, \frac{\sigma^+}{\rho^+}\right) \leq \mu_1 .$$

Similarly, b_{11} is non-negative.

<u>Remark</u> : (3.3.2) is equivalent to

$$m = \frac{1}{12} \max (\mu_1 h^2, \mu_2 k^2) ,$$

$$D_{11} \geq m A_{11} , l = 1,\ldots,g ,$$

in each triangle.

<u>Theorem 4</u> : If

(i) (3.3.2) is satisfied,
(ii) A^{ij} is strongly diagonally dominant for all i,j,
(iii) P^{ij}, Q^{ij}, R^{ij}, $S^{ij} \geq 0$,

G has the M-structure, and is strongly diagonally dominant (and hence an M-matrix).

<u>Remark</u> : Unfortunately we did not find sufficient conditions in order to satisfy (iii).

<u>Proof</u> : Since d^{ij} is non-singular and has the M-structure, the inverse δ^{ij} of d^{ij} is non-negative. By virtue of theorem 3 K^{ij}, L^{ij}, M^{ij}, and N^{ij} are non-negative too.

Moreover $T^{ij}_{lm} \leq 0$ for $m \neq l$.

As in the theorems 1 and 2 condition (ii) implies the strong diagonal dominance of the five- and nine-point formulas (here, in the mixed type). Hence,

$$c^{ij}_{lm} \leq \sum_{n=1}^{g} d^{ij}_{ln} , \qquad l = 1,\ldots,g ,$$

$$\text{or} \quad c^{ij} \leq d^{ij} . E , \qquad (3.3.3)$$

if E is the matrix with every entry equal to the unity. a^{ij} and b^{ij} can be estimated just as c^{ij} in (3.3.3). Then

$$T^{ij}_{11} = \bar{d}^{ij}_{11} - \Big(c^{i-1j}\,\delta^{i-1j}\,c^{i-1j} + b^{ij}\,\delta^{ij-1}\,b^{ij} +$$
$$+ b^{ij+1}\,\delta^{ij+1}\,b^{ij+1} + a^{i+1j}\,\delta^{i+1j}\,a^{i+1j}\Big)_{11} \geq$$
$$\geq \bar{d}^{ij}_{11} - \Big\{\Big(c^{i-1j} + b^{ij} + b^{ij+1} + a^{i+1j}\Big)E\Big\}_{11} > 0\,,$$

since the nine-point formulas are strongly diagonally dominant. By virtue of (iii) this means that T and hence G have the M-structure.

Let $\underline{1}$ be the vector with every entry equal to the unity; we consider now

$$T^{ij}.\underline{1} - \Big[K^{ij} + L^{ij} + M^{ij} + N^{ij} + Q^{ij} + R^{ij} + S^{ij}\Big].\,\underline{1} =$$
$$= - c^{i-1j}\,\delta^{i-1j}\Big[a^{i-1j} + b^{i-1j} + b^{i-1j+1} + c^{i-1j}\Big].\,\underline{1} +$$
$$- b^{ij}\,\delta^{ij-1}\Big[a^{ij-1} + b^{ij-1} + b^{ij} + c^{ij-1}\Big].\,\underline{1} +$$
$$- b^{ij+1}\,\delta^{ij+1}\Big[a^{ij+1} + b^{ij+1} + b^{ij+2} + c^{ij+1}\Big].\,\underline{1} +$$
$$- a^{i+1j}\,\delta^{i+1j}\Big[a^{i+1j} + b^{i+1j} + b^{i+1j+1} + c^{i+1j}\Big].\,\underline{1} +$$
$$+ \Big[\bar{d}^{ij} + e^{ij} + e^{ij+1} + e^{i+1j+1} + e^{i+1j}\Big].\,\underline{1} \geq$$
$$\geq \Big[- c^{i-1j} - b^{ij} - b^{ij+1} - a^{i+1j} + \bar{d}^{ij} + e^{ij} + e^{ij+1} +$$
$$+ e^{i+1j+1} + e^{i+1j}\Big].\,\underline{1} \geq 0\,,$$

with at least one strict inequality.
Hence G is strongly diagonally dominant.

IV Numerical Experiments

In order to compare the finite difference schemes (derived in chapter II and appendix A) programs were written and five examples, VAR1 through 5, were tested (these examples are described in appendix B).

In the iterative schemes (III.2) we have chosen $\varepsilon = 5.10^{-4}$, $\eta = 10^{-2}$, and the maximum of inner iteration (if present) 10.

Before applying the criterion (3.2.3) ten iterations were carried out (otherwise, one might find quite a wrong eigenvalue estimate).

In the iterative schemes a norm must be chosen. Let $x = (x_1, \ldots, x_n)$ an arbitrary vector, then

$$\begin{aligned} \|x\|_e &= \sum_{i=1}^{n} x_i \ , \\ \|x\|_1 &= \sum_{i=1}^{n} |x_i| \ , \\ \|x\|_2 &= \left(\sum_{i=1}^{n} x_i^2\right)^{1/2} , \\ \|x\|_\infty &= \max_{1 \leq i \leq n} |x_i| \ . \end{aligned} \qquad (4.1.1)$$

We call these norms the equipoise norm EQ, the absolute sum norm AB, the Euclidean norm EU, and the maximum element norm MA, respectively. These four norms are used in the equipoise method, while only the last three (AB, EU, and MA) are used in the power method.

As numerical estimates of the convergence rate and the truncation error, respectively, we introduce σ, the 'mean improvement factor' or the 'mean convergence rate', and α, the relative deviation between the eigenvalue estimate found and the 'exact' eigenvalue.

The sequences of the eigenvalue estimates here have generally a monotone character. We consider now that part of the sequence that is both monotone and 'rather accurate' (i.e. within a certain accuracy; we choose the first significant figure correct). Let this part of the sequence start with eigenvalue estimate λ_o, and end with the eigenvalue λ, and have the lenght m (either outer iterations only or outer and inner), then we define

$$\sigma = \sqrt[m]{\frac{\lambda}{\lambda_o}} \qquad \text{if } \lambda > \lambda_o$$

$$= \sqrt[m]{\frac{\lambda_o}{\lambda}} \qquad \text{if } \lambda < \lambda_o \, . \tag{4.1.2}$$

In table C2 we give τ, related to σ

$$\tau = (\sigma - 1)10^3 > 0 \, . \tag{4.1.3}$$

The second number α is defined by

$$\alpha = \left| \frac{\lambda - \lambda_e}{\lambda_e} \right| , \tag{4.1.4}$$

where λ = eigenvalue fond ,
λ_e = 'exact' eigenvalue, given in [4].

The results are given in the tables C 1,2,3, and 4.

V Conclusions

We study the various influences in the convergence.

1. Influence of the finite difference formulas

The application of the nine-point and mixed formulas can be recommended.

(i) About the convergence (here, the important criterion), we may conclude from table C2 that the mixed formulas have the best convergence rate σ while the five-point formulas have the worst rate σ.

(ii) About the truncation error, the truncation error is in the mixed formulas less than in the nine-point formulas but larger than in the five-point formulas. But a better insight in the truncation error will be obtained from a big number of meshpoints.

2. Influence of the norm choice

In some problems a certain norm is good (less iterations) and in another problem it is worse. But generally speaking, the norm AB is not to be recommended, while EQ and EU are good on the whole.

3. Influence of the inner iterations and the iterative method

From table C4 it is clear that the use of inner iterations has a very small influence in the power method.

Moreover we may conclude that the equipoise method seems very well suited to this class of problems.

Appendix A

1. Derivation of the Five- and Nine-Point Formulas for a Rectangle

As we already stated in II.1 the only contributions to the difference equations in P arise from the neighbouring cells (the cells which have P as an angle). Hence we consider figure 6. For the present we drop many cumbersome indices. To obtain the three other neighbouring cells h and k may have negative values.

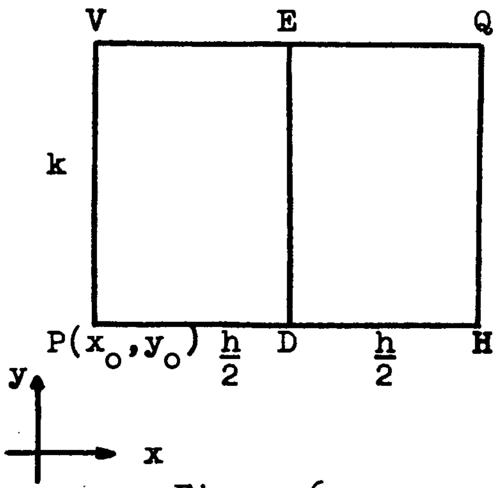


Figure 6

We need to approximate the next integrals

$$T_1 = \iint_R \Phi^*_x \, \Phi_x \, dR \, ,$$

$$T_2 = \iint_R \Phi^*_y \, \Phi_y \, dR \, ,$$

$$T_3 = \iint_R \Phi^* \, \Phi \, dR \, ,$$

where $dR = x^p \, dx \, dy$ (p=0 for the x-y-geometry and = 1 for the r-z-geometry). We always take Φ and Φ^* in the same class, i.e. every assumption about Φ is valid for Φ^* too, and conversely.

We intend to derive with the variational approach the same formulas as have been derived by Varga's method (using Green's theorem).

(i) The five-point formulas

We shall use for the x-y-geometry the approximations which have been given in [2]. For the r-z-geometry we split each square in two halves by DE (see figure 6).

The approximations we shall use are the next ones.

$$T_1 \simeq \frac{|hk|}{h^2}\left(x_o + \frac{h}{2}\right)^p \left[\left\{\Phi^*(H) - \Phi^*(P)\right\}\left\{\Phi(H) - \Phi(P)\right\} + \right.$$

$$\left. + \left\{\Phi^*(Q) - \Phi^*(V)\right\}\left\{\Phi(Q) - \Phi(V)\right\} \right] ,$$

$$T_2 \simeq \frac{|hk|}{k^2}\left[\left\{\Phi^*(V) - \Phi^*(P)\right\}\left\{\Phi(V) - \Phi(P)\right\}\left(x_o + \frac{h}{4}\right)^p + \right.$$

$$\left. + \left\{\Phi^*(Q) - \Phi^*(H)\right\}\left\{\Phi(Q) - \Phi(H)\right\}\left(x_o + \frac{3h}{4}\right)^p \right] ,$$

$$T_3 \simeq \frac{|hk|}{4}\left[\left\{\Phi^*(P)\ \Phi(P) + \Phi^*(V)\ \Phi(V)\right\}\left(x_o + \frac{h}{4}\right)^p + \right.$$

$$\left. + \left\{\Phi^*(Q)\ \Phi(Q) + \Phi^*(H)\ \Phi(H)\right\}\left(x_o + \frac{3h}{4}\right)^p \right] .$$

Proceeding in a way as has been given in [2] the next five-point formulas are derived.

$$- a^{ij}\ \Phi^{i-1j} - b^{ij}\ \Phi^{ij-1} - b^{ij+1}\ \Phi^{ij+1} - a^{i+1j}\ \Phi^{i+1j} + c^{ij}\ \Phi^{ij} =$$

$$= \frac{1}{\lambda}\, d^{ij}\ \Phi^{ij} , \qquad \text{(A1.1)}$$

$$a^{ij} = \left(\alpha^{ij} + \alpha^{ij+1}\right)\rho_i ,$$

$$b^{ij} = \beta^{ij}\ \tau_i^- + \beta^{i+1j}\ \tau_i^+ ,$$

$$c^{ij} = a^{ij} + b^{ij} + b^{ij+1} + a^{i+1j} + (\gamma^{ij}+\gamma^{ij+1})\tau_i^- + (\gamma^{i+1j}+\gamma^{i+1j+1})\tau_i^+ ,$$

$$d^{ij} = (\delta^{ij}+\delta^{ij+1})\tau_i^- + (\delta^{i+1j}+\delta^{i+1j+1})\tau_i^+ ,$$

$$\alpha^{ij} = \frac{k_j}{h_i} D^{ij} , \qquad \beta^{ij} = \frac{h_i}{k_j} D^{ij} ,$$

$$\gamma^{ij} = \frac{1}{2} h_i k_j\ A^{ij} , \qquad \delta^{ij} = \frac{1}{2} h_i k_j\ F^{ij} ,$$

$$\rho_i = \left(x_i - \frac{h_i}{2}\right)^p \quad ,$$

$$\tau_i^- = \left(x_i - \frac{h_i}{4}\right)^p \quad , \quad \tau_i^+ = \left(x_i + \frac{h_{i+1}}{4}\right)^p \quad ,$$

$p = 0$ for x-y-geometry ,
$\quad\;\; 1$ for r-z-geometry .

<u>Remark</u> : The formulas (A1.1) fully agree with those, which are derived by Varga's method. For the x-y-geometry they are given in [2] and [11], for the r-z-geometry in [6].

(ii) <u>The nine-point formulas</u>

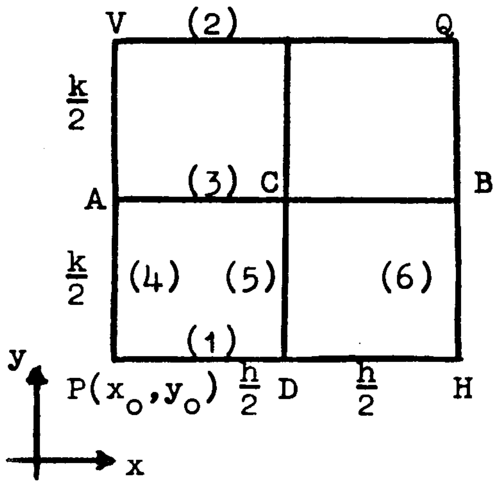


Figure 7

Following an assumption in [2], let Φ_x and Φ_x^* be independent of x. Then we may write

$$T_1 \approx \frac{hk}{4}\left(x_o + \frac{h}{2}\right)^p \left[\Phi_{x1}^* \; \Phi_{x1} + \right.$$

$$\left. + \; 2 \; \Phi_{x3}^* \; \Phi_{x3} + \Phi_{x2}^* \; \Phi_{x2}\right] \quad ,$$

where $\Phi_{x1} = \Phi_x$ along PH ,

$\Phi_{x3} = \Phi_x$ along AB etc.(see fig.)

Moreover

$$\Phi_{x3} \approx \frac{1}{2}\left(\Phi_{x1} + \Phi_{x2}\right) \quad ,$$

$$\Phi_{x1} \approx \frac{\Phi(H) - \Phi(P)}{h} \quad ,$$

$$\Phi_{x2} \approx \frac{\Phi(Q) - \Phi(V)}{h} \quad .$$

In this way we derive formula (A1.2^a). For T_2 we assume Φ_y and Φ_y^* to be independent of y. Then,

$$T_2 \simeq \frac{|hk|}{4} \left[x_o^p \, \Phi^*_{y4} \, \Phi_{y4} + 2\left(x_o + \frac{h}{2}\right)^p \Phi^*_{y5} \, \Phi_{y5} + \right.$$

$$\left. + \left(x_o + h\right)^p \Phi^*_{y6} \, \Phi_{y6} \right] ,$$

$$\Phi_{y5} \simeq \frac{1}{2} \left(\Phi_{y4} + \Phi_{y6} \right) ,$$

$$\Phi_{y4} \simeq \frac{\Phi(V) - \Phi(P)}{k} ,$$

$$\Phi_{y6} \simeq \frac{\Phi(Q) - \Phi(H)}{k} .$$

The result is formula (A1.2^b). T_3 is dealt with as follows,

$$T_3 \simeq hk \left(x_o + \frac{h}{2}\right)^p \Phi^*(c) \, \Phi(c) ,$$

$$\Phi(c) \simeq \frac{1}{4} \left[\Phi(P) + \Phi(V) + \Phi(Q) + \Phi(H) \right] .$$

The approximations are

$$T_1 \simeq \frac{|hk|}{4h^2} \left(x_o + \frac{h}{2}\right)^p \left[\left\{ \Phi^*(H) - \Phi^*(P) \right\} \left\{ \Phi(H) - \Phi(P) \right\} + \right.$$

$$+ \frac{1}{2} \left\{ \Phi^*(H) - \Phi^*(P) + \Phi^*(Q) - \Phi^*(V) \right\} \left\{ \Phi(H) - \Phi(P) + \Phi(Q) - \Phi(V) \right\} +$$

$$\left. + \left\{ \Phi^*(Q) - \Phi^*(V) \right\} \left\{ \Phi(Q) - \Phi(V) \right\} \right] , \qquad (A1.2^a)$$

$$T_2 \simeq \frac{|hk|}{4k^2} \left[x_o^p \left\{ \Phi^*(V) - \Phi^*(P) \right\} \left\{ \Phi(V) - \Phi(P) \right\} + \frac{1}{2} \left(x_o + \frac{h}{2}\right)^p \times \right.$$

$$\times \left\{ \Phi^*(V) - \Phi^*(P) + \Phi^*(Q) - \Phi^*(H) \right\} \left\{ \Phi(V) - \Phi(P) + \Phi(Q) - \Phi(H) \right\} +$$

$$\left. + (x_o + h)^p \left\{ \Phi^*(Q) - \Phi^*(H) \right\} \left\{ \Phi(Q) - \Phi(H) \right\} \right] , \qquad (A1.2^b)$$

$$T_3 \simeq \frac{|hk|}{16}\left(x_o + \frac{h}{2}\right)^p \left[\Phi^*(P) + \Phi^*(V) + \Phi^*(H) + \Phi^*(Q)\right] \times$$

$$\times \left[\Phi(P) + \Phi(V) + \Phi(H) + \Phi(Q)\right] \quad . \qquad (A1.2^c)$$

The next nine-point formulas are derived

$$- c^{ij}\,\Phi^{i-1j-1} - c^{ij+1}\,\Phi^{i-1j+1} - c^{i+1j}\,\Phi^{i+1j-1} - c^{i+1j+1}\,\Phi^{i+1j+1} +$$

$$- a^{ij}\,\Phi^{i-1j} - b^{ij}\,\Phi^{ij-1} - b^{ij+1}\,\Phi^{ij+1} - a^{i+1j}\,\Phi^{i+1j} + e^{ij}\,\Phi^{ij} =$$

$$= \frac{1}{\lambda}\Big(q^{ij}\,\Phi^{i-1j-1} + q^{ij+1}\,\Phi^{i-1j+1} + q^{i+1j}\,\Phi^{i+1j-1} + q^{i+1j+1}\Phi^{i+1j+1} +$$

$$+ r^{ij}\,\Phi^{i-1j} + s^{ij}\,\Phi^{ij-1} + s^{ij+1}\,\Phi^{ij+1} + r^{i+1j}\,\Phi^{i+1j} + t^{ij}\,\Phi^{ij}\Big) \quad , \qquad (A1.3)$$

$$c^{ij} = (\alpha^{ij} + \beta^{ij} - \gamma^{ij})\rho_i \quad ,$$

$$a^{ij} = 3(\alpha^{ij} + \alpha^{ij+1})\rho_i - (\beta^{ij} + \beta^{ij+1})\rho_i - (\gamma^{ij} + \gamma^{ij+1})\rho_i \quad ,$$

$$b^{ij} = -\alpha^{ij}\rho_i - \alpha^{i+1j}\rho_{i+1} + 3(\beta^{ij}\sigma_i^- + \beta^{i+1j}\sigma_i^+) - \gamma^{ij}\rho_i - \gamma^{i+1j}\rho_{i+1}$$

$$e^{ij} = 3(\alpha^{ij} + \alpha^{ij+1})\rho_i + 3(\alpha^{i+1j} + \alpha^{i+1j+1})\rho_{i+1} +$$

$$+ 3(\beta^{ij} + \beta^{ij+1})\sigma_i^- + 3(\beta^{i+1j} + \beta^{i+1j+1})\sigma_i^+ +$$

$$+ (\gamma^{ij} + \gamma^{ij+1})\rho_i + (\gamma^{i+1j} + \gamma^{i+1j+1})\rho_{i+1} \quad ,$$

$$q^{ij} = \delta^{ij}\,\rho_i \quad ,$$

$$r^{ij} = q^{ij} + q^{ij+1} \quad ,$$

$$s^{ij} = q^{ij} + q^{i+1j} \quad ,$$

$$t^{ij} = q^{ij} + q^{ij+1} + q^{i+1j} + q^{i+1j+1} \quad ,$$

$$\alpha^{ij} = \frac{k_j}{h_i} D^{ij} \quad , \quad \beta^{ij} = \frac{h_i}{k_j} D^{ij} \quad ,$$

$$\gamma^{ij} = \frac{1}{2} h_i k_j A^{ij} \quad , \quad \delta^{ij} = \frac{1}{2} h_i k_j F^{ij} ,$$

$$\rho_i = \left(x_i - \frac{h_i}{2}\right)^p \quad ,$$

$$\sigma_i^- = \left(x_i - \frac{h_i}{6}\right)^p \quad , \quad \sigma_i^+ = \left(x_i + \frac{h_{i+1}}{6}\right)^p \quad ,$$

$p =$ 0 for x-y-geometry,
1 for r-z-geometry.

Remark: Again these formulas fully agree with those which can be derived by Varga's method. For the x-y-geometry these formulas have been published in [7].

2. Derivation of the Mixed Formulas

From the observations we made in II.2 it is clear that we need to consider only those triangles which have P as an angle.

(i) Star Σ_5, fig. 8 , h and k may assume negative values. We introduce a coordinate transformation

$$x = x_o + \xi h ,$$

$$y = y_o + \eta k , \quad 0 \leq \xi, \eta \leq 1 .$$

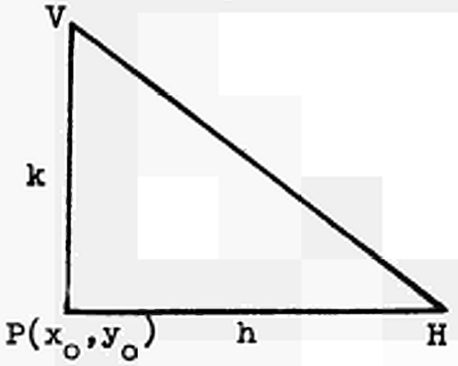


Figure 8

The triangle PHV is then mapped onto the unit triangle E (fig. 9).
In this triangle PHV the general admissible function (continuous and linear in each triangle) is

$$\Phi = \Phi(P) + \xi\left\{\Phi(H) - \Phi(P)\right\} + \eta\left\{\Phi(V) - \Phi(P)\right\} .$$

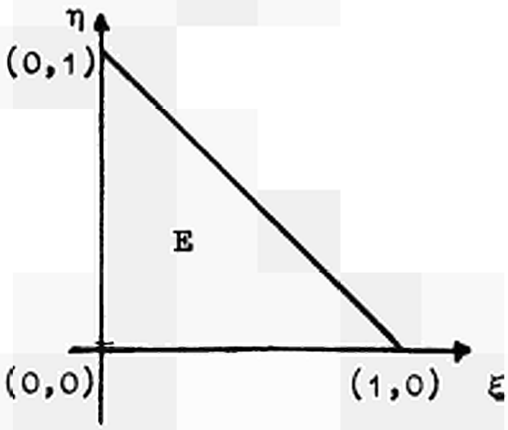


Figure 9

For the computations the next formula is useful

$$\iint_E \xi^m \, \eta^n \, d\xi d\eta = \frac{m! \, n!}{(m+n+2)!}$$

(m and n are natural numbers).
Formula (A2.1) can be derived now.

(ii) Star Σ_9 .

The procedure here is quite similar to above. We may introduce in triangle 1 (fig. 10)

$$x = x_o + \xi h ,$$

$$y = y_o + (1-\eta)k , \quad 0 \leq \xi, \eta \leq 1 ,$$

$$\Phi = \Phi(V) + \xi\left\{\Phi(Q) - \Phi(V)\right\} + \eta\left\{\Phi(P) - \Phi(V)\right\} ,$$

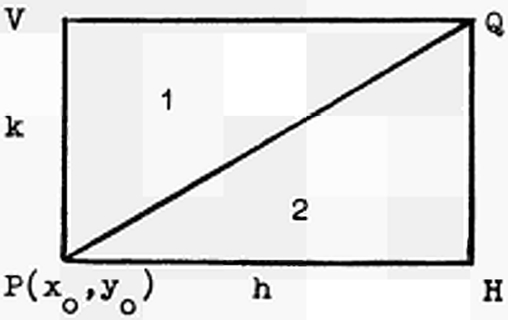


Figure 10

and in triangle 2

$$x = x_o + (1-\xi)h ,$$

$$y = y_o + \eta k , \quad 0 \leq \xi, \eta \leq 1 ,$$

$$\Phi = \Phi(H) + \xi\left\{\Phi(P) - \Phi(H)\right\} + \eta\left\{\Phi(Q) - \Phi(H)\right\} .$$

The computations finally lead to (A2.2).

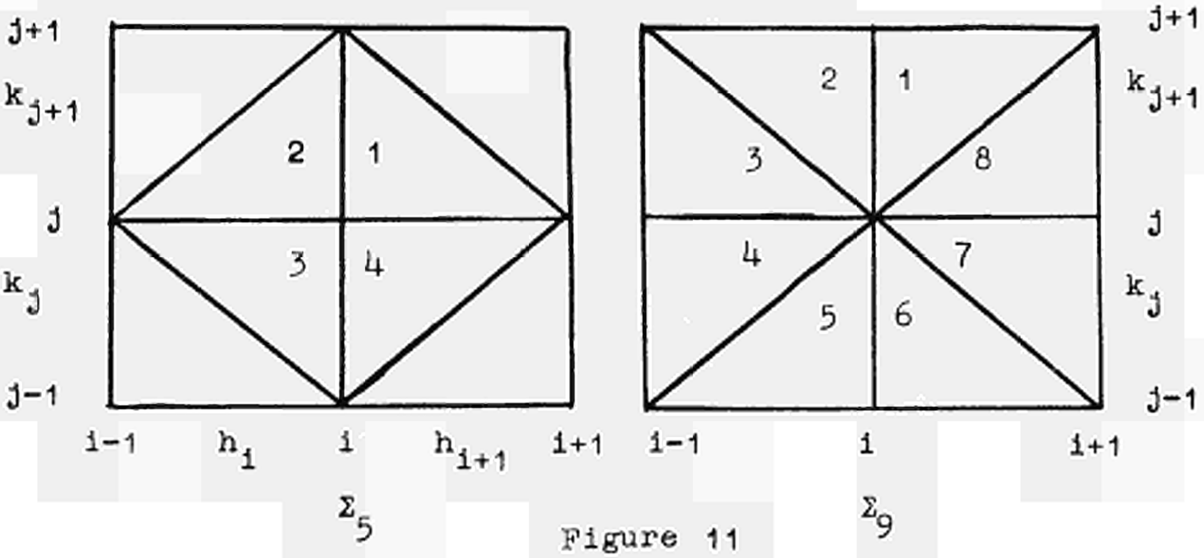


Figure 11

In each triangle the coefficients D, A and F are supposed to be constant. We now define D_+^{ij} (D_-^{ij}) as the coefficient D in the right (left, respectively) triangle of square R_{ij}, with the diagonal anyhow. $A_\pm^{ij}$ and $F_\pm^{ij}$ are defined in a similar way.

E.g., in Σ_9 , fig. 11 , $D_+^{i+1\,j+1} = D^8$, $D_-^{i+1\,j+1} = D^1$,

$$D_+^{i\,j+1} = D^2 , \quad D_-^{i\,j+1} = D^3 .$$

And, as usual, $\alpha_\pm^{ij} = \frac{k_j}{h_i} D_\pm^{ij}$, $\beta_\pm^{ij} = \frac{h_i}{k_j} D_\pm^{ij}$, $\gamma_\pm^{ij} = \frac{1}{12} h_i k_j A_\pm^{ij}$.

Σ_5 :

$$- a^{ij}\ \Phi^{i-1j} - b^{ij}\ \Phi^{ij-1} - b^{ij+1}\ \Phi^{ij+1} - c^{ij}\ \Phi^{i+ij} + d^{ij}\ \Phi^{ij} =$$

$$= \frac{1}{\lambda}\left[s^{ij}\ \Phi^{i-1j} + t^{ij}\ \Phi^{ij-1} + t^{ij+1}\ \Phi^{ij+1} + u^{ij}\ \Phi^{i+1j} + v^{ij}\ \Phi^{ij}\right] ,$$

(A2.1)

Σ_9 :

$$- c^{i-1j}\ \Phi^{i-1j} - b^{ij}\ \Phi^{ij-1} - b^{ij+1}\ \Phi^{ij+1} - a^{i+1j}\ \Phi^{i+1j} + \bar{d}^{ij}\ \Phi^{ij} +$$

$$+ e^{ij}\ \Phi^{i-1j-1} + e^{ij+1}\ \Phi^{i-1j+1} + e^{i+1j}\ \Phi^{i+1j-1} + e^{i+1j+1}\ \Phi^{i+1j+1} =$$

$$= \frac{1}{\lambda}\Big[u^{i-1j}\ \Phi^{i-1j} + t^{ij}\ \Phi^{ij-1} + t^{ij+1}\ \Phi^{ij+1} + s^{i+1j}\ \Phi^{i+1j} + \bar{v}^{ij}\ \Phi^{ij} +$$

$$+ w^{ij}\ \Phi^{i-1j-1} + w^{ij+1}\ \Phi^{i-1j+1} + w^{i+1j}\ \Phi^{i+1j-1} + w^{i+1j+1}\ \Phi^{i+1j+1}\Big] ,$$

(A2.2)

$$a^{ij} = (\alpha_+^{ij+1} + \alpha_+^{ij})\rho_i^- - (\gamma_+^{ij+1} + \gamma_+^{ij})\sigma_i^- ,$$

$$b^{ij} = \beta_+^{ij}\ \rho_i^- + \beta_-^{i+1j}\ \rho_i^+ - \gamma_+^{ij}\ \tau_i^- - \gamma_-^{i+1j}\ \tau_i^+ ,$$

$$c^{ij} = (\alpha_-^{i+1j+1} + \alpha_-^{i+1j})\rho_i^+ - (\gamma_-^{i+1j+1} + \gamma_-^{i+1j})\sigma_i^+ ,$$

$$d^{ij} = (\alpha_-^{i+1j+1} + \beta_-^{i+1j+1} + \alpha_-^{i+1j} + \beta_-^{i+1j})\rho_i^+ +$$

$$+ (\alpha_+^{ij+1} + \beta_+^{ij+1} + \alpha_+^{ij} + \beta_+^{ij})\rho_i^- +$$

$$+2(\gamma_-^{i+1j+1} + \gamma_-^{i+1j})\tau_i^+ + 2(\gamma_+^{ij+1} + \gamma_+^{ij})\tau_i^- ,$$

$$\bar{d}^{ij} = (\beta_-^{i+1j+1} + \beta_-^{i+1j})\rho_i^+ + (\beta_+^{ij+1} + \beta_+^{ij})\rho_i^- +$$

$$+ (\alpha_+^{i+1j+1} + \alpha_+^{i+1j})\rho_{i+1}^- + (\alpha_-^{ij+1} + \alpha_-^{ij})\rho_{i-1}^+ +$$

$$+2(\gamma_-^{i+1j+1} + \gamma_-^{i+1j})\tau_i^+ + 2(\gamma_+^{ij+1} + \gamma_+^{ij})\tau_i^- +$$

$$+2(\gamma_+^{i+1j+1} + \gamma_+^{i+1j})\sigma_i^+ + 2(\gamma_-^{ij+1} + \gamma_-^{ij})\sigma_i^- ,$$

$$e^{ij} = \gamma_-^{ij} \; \sigma_{i-1}^+ + \gamma_+^{ij} \; \sigma_i^- \quad ,$$

$$\rho_i^- = \left(x_i - \frac{1}{3} h_i\right)^p \quad , \quad \rho_i^+ = \left(x_i + \frac{1}{3} h_{i+1}\right)^p \quad ,$$

$$\sigma_i^- = \left(x_i - \frac{2}{5} h_i\right)^p \quad , \quad \sigma_i^+ = \left(x_i + \frac{2}{5} h_{i+1}\right)^p \quad ,$$

$$\tau_i^- = \left(x_i - \frac{1}{5} h_i\right)^p \quad , \quad \tau_i^+ = \left(x_i + \frac{1}{5} h_{i+1}\right)^p \quad ,$$

$p = 0$ for x-y-geometry, and $= 1$ for r-z-geometry.

The right-hand side coefficients s^{ij}, t^{ij}, u^{ij}, v^{ij}, $\bar{v}^{ij}$, and w^{ij} are obtained directly from $- a^{ij}$, $- b^{ij}$, $- c^{ij}$, d^{ij}, $\bar{d}^{ij}$, and e^{ij}, respectively, by replacing D^{ij} with the null matrix and A^{ij} with F^{ij}.

In the iterative procedure (III.2b) the right-hand sides of (A2.1) and (A2.2) are considered as known terms; we denote them by V_5^{ij} and V_9^{ij}, respectively.

Since d^{ij} is non-singular we can eliminate the fluxes Φ in the five-points from the left-hand side of (A2.2). Then we get a left-hand side merely consisting of nine-points, corresponding to the matrix G in III.2b and the formulas (3.2.6).

We obtain

$$- K^{ij} \; \Phi^{i-2j} - L^{ij} \; \Phi^{ij+2} - M^{ij} \; \Phi^{i+2j} - N^{ij} \; \Phi^{ij-2} + T^{ij} \; \Phi^{ij} +$$

$$- P^{ij} \; \Phi^{i-1j-1} - Q^{ij} \; \Phi^{i-1j+1} - R^{ij} \; \Phi^{i+1j+1} - S^{ij} \; \Phi^{i+1j-1} =$$

$$= \frac{1}{\lambda} \Big[V_9^{ij} + c^{i-1j} \; \delta^{i-1j} \; V_5^{i-1j} + b^{ij} \; \delta^{ij-1} \; V_5^{ij-1} + b^{ij+1} \; \delta^{ij+1} V_5^{ij+1}$$

$$+ a^{i+1j} \, \delta^{i+1j} \; V_5^{i+1j} \Big] \quad , \qquad \text{(A2.3)}$$

$$\delta^{ij} = (d^{ij})^{-1} \quad ,$$

$$K^{ij} = c^{i-1j} \; \delta^{i-1j} \; a^{i-1j} \quad ,$$

$$L^{ij} = b^{ij+1}\ \delta^{ij+1}\ b^{ij+2} \quad ,$$

$$M^{ij} = a^{i+1j}\ \delta^{i+1j}\ c^{i+1j} \quad ,$$

$$N^{ij} = b^{ij}\ \delta^{ij-1}\ b^{ij-1} \quad ,$$

$$P^{ij} = c^{i-1j}\ \delta^{i-1j}\ b^{i-1j} + b^{ij}\ \delta^{ij-1}\ a^{ij-1} - e^{ij} \quad ,$$

$$Q^{ij} = c^{i-1j}\ \delta^{i-1j}\ b^{i-1j+1} + b^{ij+1}\ \delta^{ij+1}\ a^{ij+1} - e^{ij+1} \quad ,$$

$$R^{ij} = b^{ij+1}\ \delta^{ij+1}\ c^{ij+1} + a^{i+1j}\ \delta^{i+1j}\ b^{i+1j+1} - e^{i+1j+1} \quad ,$$

$$S^{ij} = b^{ij}\ \delta^{ij-1}\ c^{ij-1} + a^{i+1j}\ \delta^{i+1j}\ b^{i+1j} - e^{i+1j} \quad ,$$

$$T^{ij} = \bar{d}^{ij} - c^{i-1j}\ \delta^{i-1j}\ c^{i-1j} - b^{ij}\ \delta^{ij-1}\ b^{ij} - b^{ij+1}\ \delta^{ij+1}\ b^{ij+1} -$$

$$- a^{i+1j}\ \delta^{i+1j}\ a^{i+1j} \quad .$$

3. Treatment of the elementary boundary conditions

In the examples VAR 1/5 (see appendix B) we always have either $\Phi = 0$ or $\frac{\partial\Phi}{\partial n} = 0$ on a side of R. Therefore we consider the side along the positive y-axis (see figure 1).

(i) $\Phi = 0$. We set $\Phi^{0j} = 0$ for $j = 0,1,\ldots,J+1$. Moreover, the coefficients of Φ^{0j} in the finite difference formulas are set equal to zero (by definition). This left boundary condition is characterized by $L = 0$.

(ii) $\frac{\partial\Phi}{\partial n} = 0$. See figure 12 . $AO = OE = h$. The condition $\frac{\partial\Phi}{\partial n} = 0$ is approximated by

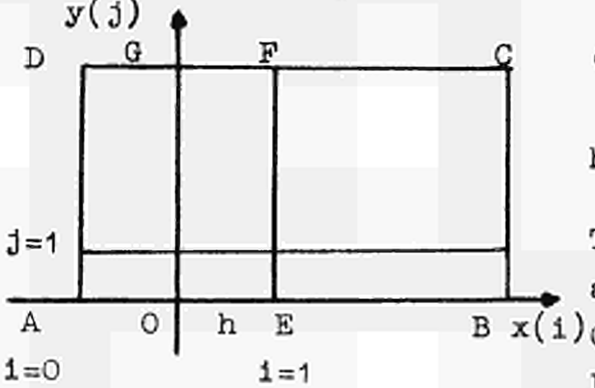


Figure 12

$$\Phi^{0j} = \Phi^{1j} \ , \ j = 0,1,\ldots,J+1,$$

$$h' = AE = 2h \ .$$

The coefficients of (1.1.1) in AOGD are assumed to be equal to those in OEFG. This case is characterized by $L = 1$.

Anyhow, in an expression like $a\Phi^{0j} + b\Phi^{1j}$ (in the finite difference formulas) b remains unchanged in case (i) and is changed in b+a in case (ii), while a is set equal to zero in both cases.

Remark : In theorem 3 we evaluate

$$\max_i \left(\frac{\sigma_i^-}{\rho_i^-}, \frac{\sigma_i^+}{\rho_i^+}\right) \text{and} \quad \max_i \left(\frac{\tau_i^-}{\rho_i^-}, \frac{\tau_i^+}{\rho_i^+}\right). \text{ We have}$$

$$\frac{h_i}{x_i} \leq 1 \quad \text{for all} \quad i = 2,3,\ldots, I$$

and

$$\frac{h_1}{x_1} = 1 + L \ .$$

Then $$\mu_1 = \max_i \left(\frac{\sigma_i^-}{\rho_i^-} \; , \; \frac{\sigma_i^+}{\rho_i^+} \right) = (1.05 + .03\ L)^p$$

and $$\mu_2 = \max_i \left(\frac{\tau_i^-}{\rho_i^-} \; , \; \frac{\tau_i^+}{\rho_i^+} \right) = (1.2 + .6\ L)^p \quad .$$

Appendix B

Description of the Test Examples

With reference to the problem description in chapter I we give for each example the next information.

(i) The region R with the kind of geometry (p = 0 or 1).

(ii) The boundary conditions.

L = 0 means the y-axis is a part of Γ_1,
= 1 means the y-axis is a part of Γ_2.

M = 0 means the x-axis belongs to Γ_1,
= 1 means the x-axis belongs to Γ_2.

The other sides belong to Γ_1 in each problem.

(iii) The number of sub regions where the coefficients are constant.

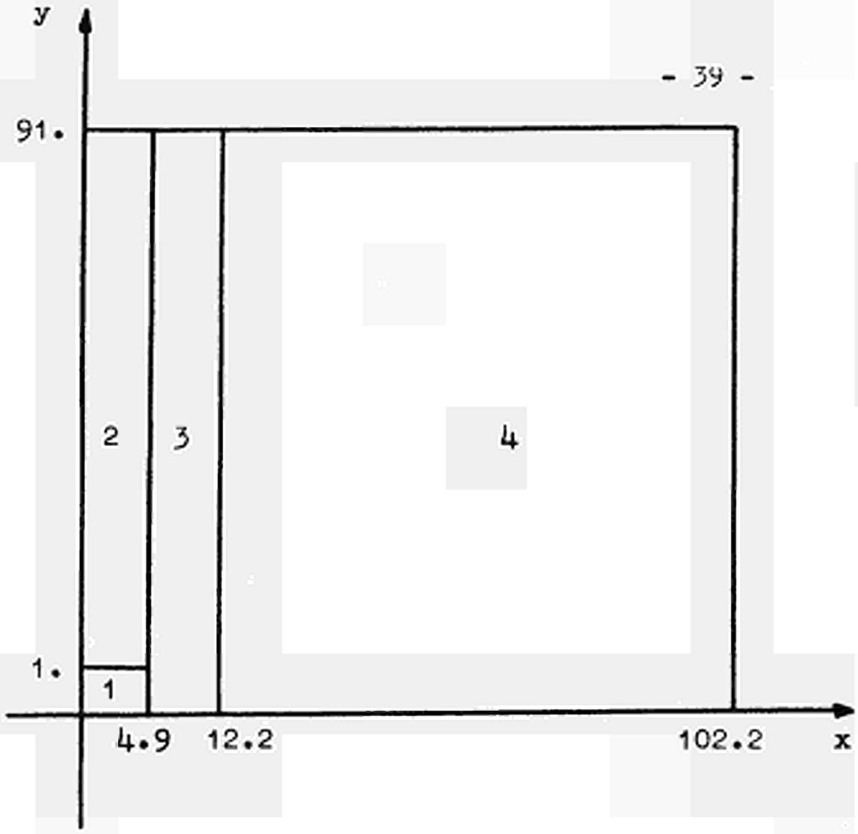
(iv) The eigenvalue found by Galligani [4].

(v) The mesh, i.e. the partitioning of the two axes.

E.g. y-axis (k_j) (0) .5 (2) 7.5 (14) means that the mesh length k_j = .5 from j = 0 to j = 2
and k_j = 7.5 from j = 2 to j = 14.

(vi) The coefficients D, A, and F, constant in each subregion.

VAR 1



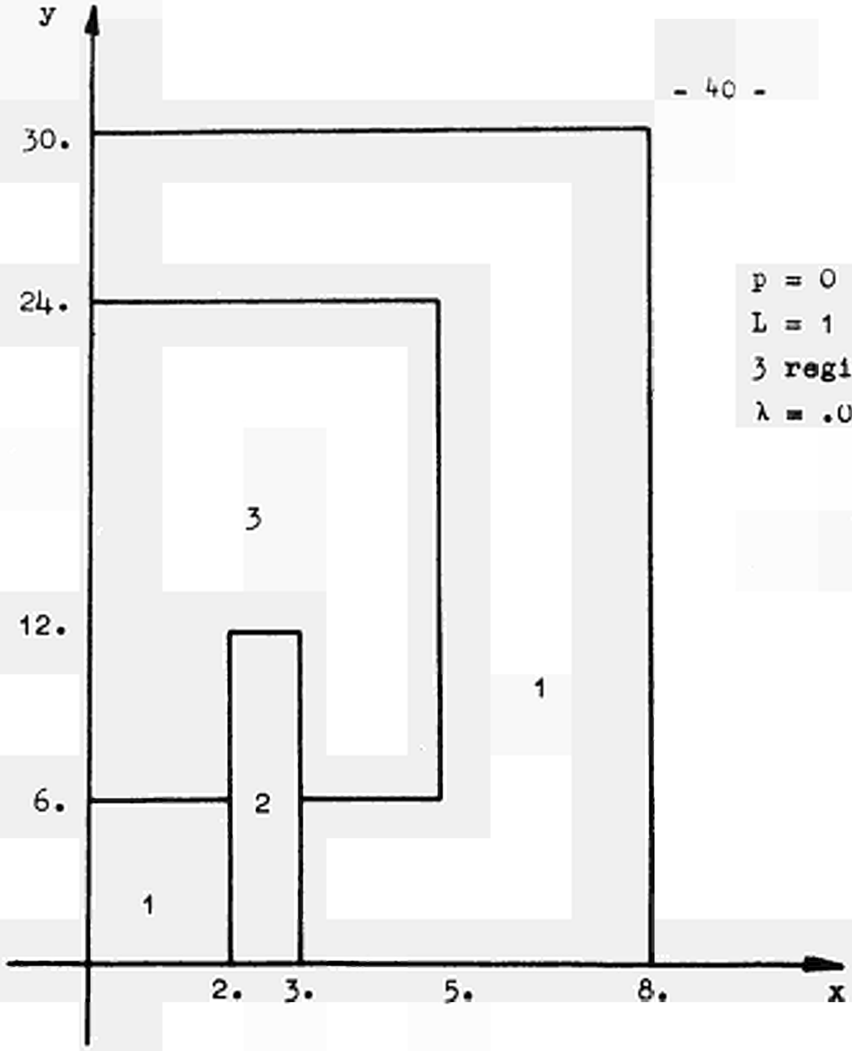
$p = 0$
$L = 0$, $M = 0$
4 regions
$\lambda = .5772$

Mesh
y-axis (k_j) (0) .5 (2) 7.5 (14)
x-axis (h_i) (0) 2.45 (2) 3.65 (4) 7.5 (16)

REGION	D_1	A_{11}	A_{12}	F_{11}	F_{12}
1	2.1744	.003672	.0	.0	.0
2	1.36515	.003214	.0	.0	.072019
3	1.274	.010317	.0	.0	.0
4	1.2847	.011045	.0	.0	.004629

REGION	D_2	A_{21}	A_{22}	F_{21}	F_{22}
1	1.0241	-.003455	.01048	.0	.0
2	.8061	-.000782	.0579	.0	.0
3	.8331	-.01019	.000153	.0	.0
4	.824605	-.009884	.003983	.0	.0

VAR 2



p = 0
L = 1 , M = 0
3 regions
λ = .02428

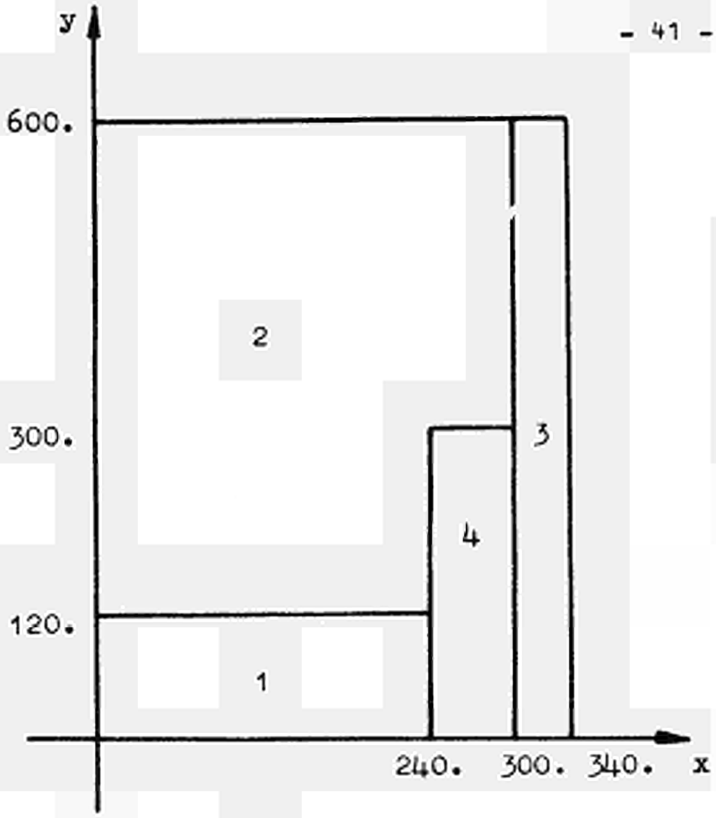
Mesh
y-axis (k_j) (0) 2. (15)
x-axis (h_i) (0) 1. (2) .5 (4) 1. (9)

Coefficients

REGION	D_1	A_{11}	A_{12}	F_{11}	F_{12}
1	1.52	.01186	-.0032	0.	0.
2	1.53	.01299	-.0041	.0041	.0042
3	1.50	.0107	.0	.0021	.0022

REGION	D_2	A_{21}	A_{22}	F_{21}	F_{22}
1	1.32	-.0052	.00804	0.	0.
2	1.33	-.0053	.00996	0.	0.
3	1.31	-.0053	.00382	0.	0.

VAR 3



p = 1
L = 1 , M = 0
4 regions
λ = 1.0465

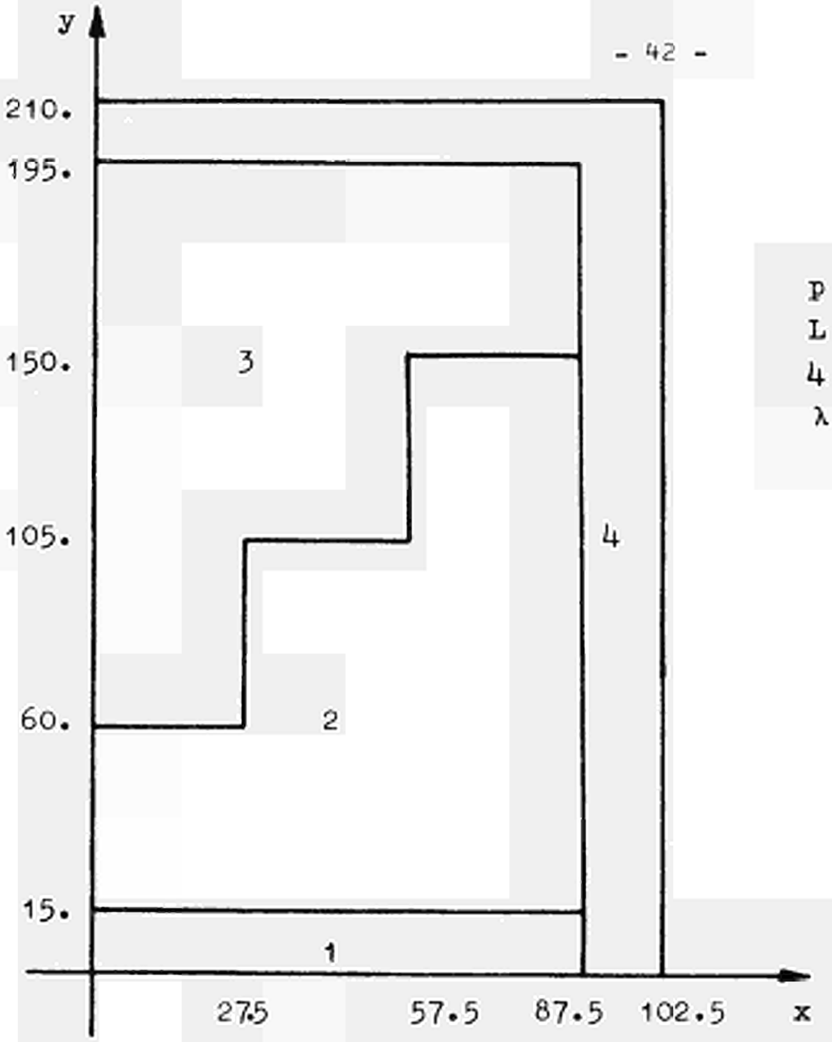
Mesh
y-axis (k_j) (0) 40. (3) 45. (7) 50. (13)
x-axis (h_i) (0) 30. (8) 20. (11) 10. (15)

Coefficients

REGION	D_1	A_{11}	A_{12}	F_{11}	F_{12}
1	1.27	.011978	.0	.0	.004938
2	1.27	.011978	.0	.0	.004938
3	1.29	.010570	.0	.0	.0
4	1.27	.011978	.0	.0	.004938

REGION	D_2	A_{21}	A_{22}	F_{21}	F_{22}
1	.836	-.0109	.004406	.0	.0
2	.836	-.0109	.004186	.0	.0
3	.842	-.01057	.000067	.0	.0
4	.836	-.0109	.004246	.0	.0

VAR 4



p = 1
L = 1 , M = 0
4 regions
λ = .9728

Mesh

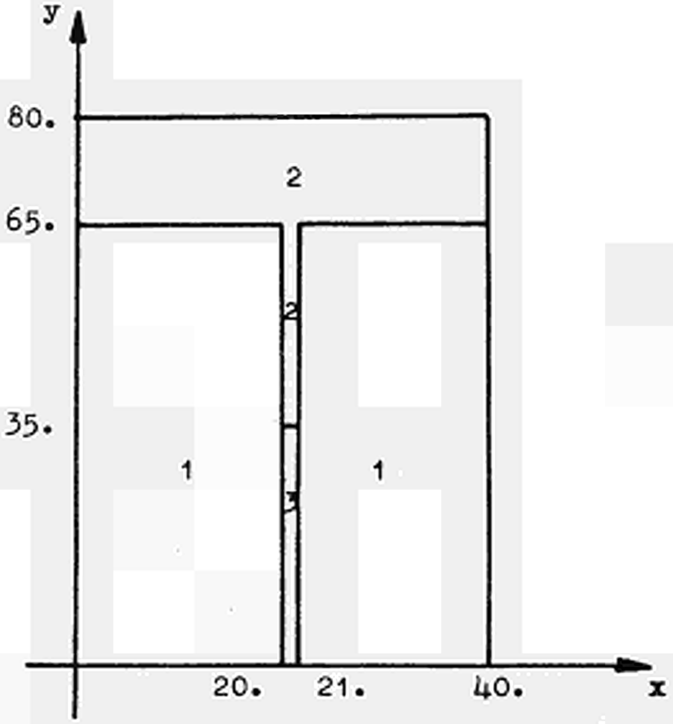
y-axis (k_j) (0) 7.5 (2) 15. (14) 7.5 (16)
x-axis (h_i) (0) 9.1667 (3) 10. (9) 7.5 (11)

Coefficients

REGION	D_1	A_{11}	A_{12}	F_{11}	F_{12}
1	1.75	.02118	.0	.0	.0
2	1.38	.02386	.0	.0	.113
3	1.38	.02386	.0	.0	.113
4	1.75	.02118	.0	.0	.0

REGION	D_2	A_{21}	A_{22}	F_{21}	F_{22}
1	.328	-.02118	.02008	.0	.0
2	.4717	-.0134	.07172	.0	.0
3	.4717	-.0134	.05972	.0	.0
4	.328	-.02118	.008083	.0	.0

VAR 5



p = 0
L = 1 , M = 0
3 regions
λ = 1.0124

Mesh

x-axis (k_1) (0) 5. (16)
x-axis (h_1) (0) 5. (4) .5 (6) 4.75 (10)

Coefficients

REGION	D_1	A_{11}	A_{12}	F_{11}	F_{12}
1	1.7	.016	.0	.0	.0832
2	1.7	.041	.0	.0	.0
3	.5	.1	.0	.0	.0

REGION	D_2	A_{21}	A_{22}	F_{21}	F_{22}
1	.42	-.016	.055	.0	.0
2	.23	-.041	.012	.0	.0
3	.1	-.0	1.5	.0	.0

TABLE C1

Eigenvalues and number of iterations in the equipoise and power methods

		Equipoise method						Power method with inner iterations					
		5		9		59		5		9		59	
Example	Norm	n	λ	n	λ	n	λ	n_{10}	λ	n_{10}	λ	n_{10}	λ
VAR1	EQ	31	.5795	23	.5734	24	.5731						
	AB	+100	.5423	+100	.5315	+88	.5513	54(19)	.5777	46(13)	.5708	44(15)	.5724
	EU	38	.5771	30	.5715	28	.5725	47(12)	.5779	41(7)	.5716	39(8)	.5730
	MA	37	.5759	26	.5697	17	.5762	63(25)	.5802	49(16)	.5737	50(16)	.5749
VAR2	EQ	46	.02426	37	.02418	29	.02420						
	AB	49	.02414	41	.02406	38	.02403	+120(50)	.02387	193(38)	.02448	148(24)	.02438
	EU	+100	.02476	85	.02450	66	.02439	+118(50)	.02384	197(39)	.02449	151(26)	.02442
	MA	+100	.02500	96	.02448	75	.02440	+112(50)	.02386	207(43)	.02451	164(33)	.02446
VAR3	EQ	26	1.024	22	1.026	21	1.027						
	AB	24	1.023	22	1.026	18	1.025	85(18)	1.027	76(17)	1.026	84(18)	1.027
	EU	11	1.025	8	1.026	13	1.026	78(15)	1.028	75(16)	1.028	69(14)	1.027
	MA	22	1.035	17	1.034	20	1.026	65(11)	1.032	61(11)	1.031	59(11)	1.031
VAR4	EQ	40	.9689	31	.9646	29	.9777						
	AB	41	.9690	31	.9646	28	.9658	149(26)	.9717	119(25)	.9654	116(26)	.9685
	EU	32	.9705	26	.9651	22	.9693	108(20)	.9728	94(19)	.9663	93(20)	.9694
	MA	28	.9735	17	.9664	22	.9707	51(8)	.9647	59(12)	.9704	51(11)	.9706
	EQ	38	1.020	32	1.021	25	1.027						
	AB	55	1.010	45	1.014	25	.9987	86(35)	1.010	67(20)	1.014	56(14)	1.018
	EU	24	1.017	22	1.018	16	1.018	80(29)	1.008	54(9)	1.015	52(7)	1.023
	MA	34	1.039	27	1.031	32	1.027	65(10)	1.015	63(14)	1.031	65(14)	1.028

In the second row, 5, 9, and 59 denote respectively the five-point, the nine-point, and the mixed formulas; n gives the number of iterations used in order to find λ (eigenvalue) in the equipoise method while n_{10} gives the total number of iterations with the number of outer iterations in brackets in the power method (10 is the maximum number of inner iterations). A plus sign means that the iterations reached a prescribed limit without converging.

TABLE C2

The 'mean improvement factor' σ, see (4.1.2); we give τ, see (4.1.3)

		Equipoise method						Power method with inner iterations					
		5		9		59		5		9		59	
Example	Norm	m	τ	m	τ	m	τ	m	τ	m	τ	m	τ
VAR1	EQ	1(11)	6.5	1(9)	7.6	1(8)	6.7						
	AB	1(52)	1.7	1(54)	1.3	1(40)	2.0	2(4)	5.2(3.3)	2(3)	12.1(4.6)	2(3)	9.8(4.9)
	EU	1(14)	5.9	1(12)	6.2	1(11)	7.5	2(4)	5.9(2.8)	2(3)	21.6(4.1)	2(3)	16.6(4.3)
	MA	2(12)	5.5	2(10)	6.4	2(8)	12.0	4(6)	1.5(1.4)	4(3)	2.5(1.6)	4(3)	3.0(1.8)
VAR2	EQ	1(10)	5.1	1(8)	5.9	1(6)	6.4						
	AB	1(10)	4.5	1(8)	4.9	1(8)	4.6	2(7)	3.1(2.2)	1(14)	6.1(2.3)	1(11)	9.3(2.5)
	EU	12(6)	2.2	9(5)	2.5	10(4)	2.4	2(7)	2.9(2.1)	1(14)	6.6(2.5)	1(11)	9.2(2.7)
	MA	10(41)	3.0	7(30)	3.0	9(18)	3.6	2(6)	3.0(2.2)	1(15)	5.4(2.3)	1(11)	8.4(2.9)
VAR3	EQ	1(8)	1.3	3(6)	1.5	3(6)	1.3						
	AB	1(8)	1.1	3(6)	1.1	1(4)	1.5	2(3)	1.5(0.3)	2(3)	1.6(0.4)	2(3)	1.5(0.3)
	EU	1(5)	2.0	1(3)	2.6	5(2)	0.8	2(2)	0.8(0.2)	1(1)	1.4(0.3)	1(1)	1.0(0.2)
	MA	7(3)	0.7	8(2)	1.3	4(2)	1.8	2(2)	1.2(0.2)	2(2)	1.3(0.3)	2(2)	1.4(0.3)
VAR4	EQ	3(8)	2.1	6(7)	2.5	4(5)	3.1						
	AB	3(8)	2.1	4(7)	2.8	6(7)	2.7	2(4)	3.4(0.6)	2(5)	3.2(0.7)	2(5)	3.1(0.7)
	EU	2(7)	2.8	4(6)	3.3	6(5)	3.6	2(4)	4.5(0.8)	2(5)	4.0(0.8)	2(4)	4.6(1.0)
	MA	8(3)	1.7	OSC	6.7	6(5)	3.2	OSC	8.7(1.2)	8(4)	0.8(0.1)	2(3)	4.5(0.9)
	EQ	2(23)	1.2	2(18)	1.3	2(13)	1.9						
	AB	2(40)	0.7	2(29)	0.9	2(14)	1.5	2(20)	0.6(0.6)	2(6)	1.0(0.7)	2(6)	1.2(0.8)
	EU	4(14)	1.7	2(12)	1.3	2(9)	1.7	1(16)	0.6(0.6)	2(5)	1.4(0.4)	2(4)	2.8(0.4)
	MA	11(9)	1.3	12(10)	0.8	7(5)	2.8	3(3)	0.9(0.2)	3(2)	5.9(1.5)	2(2)	5.5(1.6)

In the table, m gives both the iteration number where the monotony starts in the sequence of eigenvalue estimates, and, in brackets, the iteration number where the first significant figure in the estimate is correct. In the power method, τ gives two values, one being computed only for the outer iterations and another being computed for all the iterations (outer and inner).

Remark : OSC means the sequence was oscillating.

TABLE C3

Relative deviation α in ‰ between the estimate found here and the 'exact' eigenvalue (see 4.1.4)

		Equipoise method			Power method with inner iterations		
Example	Norm	5	9	59	5	9	59
VAR1	EQ	4	6.5	7			
	AB	< 60	< 79	< 45	1	11	8
	EU	0	10	8	1	10	7.5
	MA	2	13	2	6	5	4
VAR2	EQ	1	4	3			
	AB	6	9	10	< 2	1	.5
	EU	< 20	9	4.5	< 2	1	.5
	MA	< 30	8	5	< 2	2	.5
VAR3	EQ	21	19	18			
	AB	22	19	19	18	19	18
	EU	20	19	19	18	18	18
	MA	10.5	11	19	13	15	14
VAR4	EQ	4	8	5			
	AB	4	8	7	1	7.5	4.5
	EU	2	8	4	0	6.5	3.5
	MA	1	7	2	2	2.5	2
VAR5	EQ	8	9	15			
	AB	2	2	13	2	3	6
	EU	5	6	6	4	3	11
	MA	27	19	15	3	19	16

TABLE C4

Influence of the inner iterations. We present here a comparison for the power method between the application of inner iterations (with at most ten in each outer iteration) and the application of no inner iterations (or better, one inner iteration, coinciding with the outer iteration). We used the norm MA.

	Five-point formulas				Nine-point formulas				Mixed formulas			
Example	n_1	λ_1	n_{10}	λ_{10}	n_1	λ_1	n_{10}	λ_{10}	n_1	λ_1	n_{10}	λ_{10}
VAR1	49	.5773	63(25)	.5802	36	.5735	49(16)	.5737	35	.5747	50(16)	.5749
VAR2	+100	.02322	+112(50)	.02386	+100	.04763	207(43)	.02451	+100	.02966	164(33)	.02446
VAR3	13	1.031	65(11)	1.032	21	1.031	61(11)	1.031	17	1.031	59(11)	1.031
VAR4	27	.9743	51(8)	.9647	15	.9687	59(12)	.9704	21	.9750	51(11)	.9706
VAR5	92	1.007	65(10)	1.015	37	1.013	63(14)	1.031	19	1.017	65(14)	1.028

n_1 = number of iterations 'without' inner iterations,

λ_1 = corresponding eigenvalue,

n_{10}= total number of iterations (inner and outer), where the number of outer iterations is given between brackets

\+ means the iterations reached a prescribed limit without converging.

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Alfred Nobel

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