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Application of Group Theory to the Method of Finite Elements for Solving Boundary Value Problems

ABHANDLUNG

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INTRODUCTION

The theory of groups has been applied in theoretical physics for a long time in order to exploit the symmetries of problems and to classify physical states accordingly. Examples of such fields are:

1. Quantum mechanics of atomic spectras (group of rotations, theory of the spin with the unitary group)

2. Spectra and oscillations of molecules (finite groups)

3. Solid state physics (discrete infinite groups)

In all these theories a dominant role is played by Schur's lemma and its extensions, due to the fact that it relates the eigenspace of an operator with the invariant subspaces of a group representation.

The aim of this work is to introduce the group theoretical approach as a tool for solving partial differential equations encountered within classical physics or in technical applications. A typical example is Poisson's partial differential equation

$$\Delta u(x_1,x_2) = f(x_1,x_2)$$

which has to be solved throughout a domain D for prescribed boundary values. It will be shown that the theory of groups is applicable, provided D permits a plane point group G. Neither $f(x_1,x_2)$ nor the boundary values of the Poisson problem need to present symmetries. A more general analysis shows that the method may still be applied if only a subdomain of D possesses symmetries.

The basic idea can be described as follows. By discretizing the problem (method of finite elements), we obtain a linear problem in a finite dimensional space R^n, in which a representation θ of G is induced. After having determined all the invariant subspaces R_k of θ, the problem can be split up into several linear subproblems.

This study will deal with all finite plane point groups as well as the octahedral group (other spatial groups, such as the tetrahedral group, have been investigated, but will not be included in this dissertation).

In each of these cases, the invariant subspaces of θ can be determined explicitly for arbitrarily high dimensions n of R^n. Synoptical tables on this matter are listed.

An example which yields a set of 169 linear equations is calculated in a final section. With the knowledge of all the invariant subspaces, it turns out to be possible to split the problem up into

23 systems of linear equations with 7 unknowns each

and 1 system of linear equations with 8 unknowns.

Several of these subsystems present the same matrix. By appropriate numbering, it is furthermore possible to generate band-type matrices. This also holds true in the general case.

This work also contains comments concerning eigenvalue problems, the condition of the resulting linear systems of equations and the computational effort of the group theoretical method.

Herewith I would like to express my deep gratitude to Prof. E. Stiefel for his constant encouragement and his useful suggestions for this work. I also wish to thank Prof. J. Hersch, J. Joss, J. Kriz and Dr. M. Vitins for very helpful discussions.

4. NUMERICAL EXAMPLES

4.1 Boundary Value Problems on a Circular Domain

Let us consider the following 2-dimensional problem on the unit disk D.

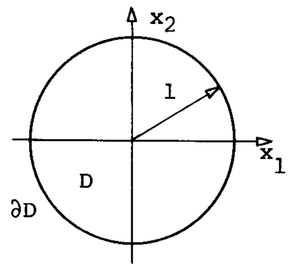


Fig. 15

$$\Delta\ u(x_1,x_2) = f(x_1,x_2) \quad \text{with the boundary condition} \quad u\big|_{\partial D} = \varphi(s) \tag{98}$$

where ∂D is the unit circle

In order to calculate a numerical solution by the method of finite elements, we construct a discretization net with the symmetry of the dihedral group D_{24}.

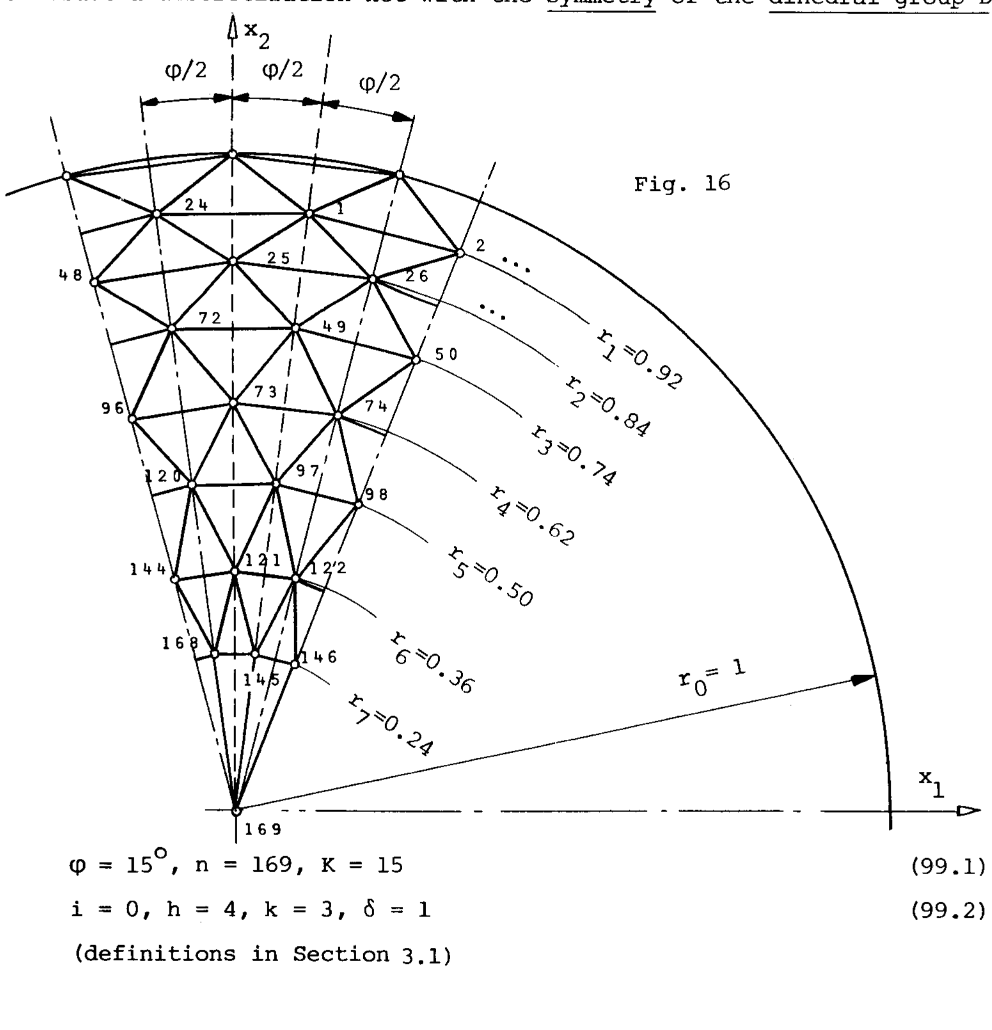


Fig. 16

$\varphi = 15^\circ$, $n = 169$, $K = 15$ (99.1)

$i = 0$, $h = 4$, $k = 3$, $\delta = 1$ (99.2)

(definitions in Section 3.1)

As an approximation of the solution we adopt a linear function $u(x_1,x_2) = c_1 + c_2x_1 + c_3x_2$ for each of the elements (cf. [7]).

4.11 The finite element matrix M

The discretization of the problem (98) then leads to a system of linear eqs.

$$M\ v = b \tag{100}$$

where M is a symmetric, positive definite 169x169 matrix.

In the fundamental domain of Fig. 16 we have eight points, which can be classified in three different topological configurations.

The 25-th equation of (100) for instance, has the structure

$$a\cdot x_{25} + r(x_1+x_{24}) + s(x_{26}+x_{48}) + t(x_{49}+x_{72}) = b_{25}$$

and corresponds to a star with six "arms".

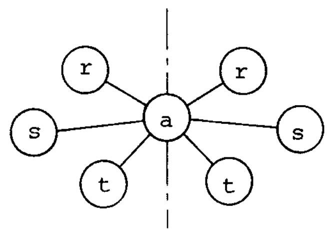


Fig. 17

The weights a,r,s,t appearing in the matrix M are the same for the points No. 25,26,27,...,48 in Fig. 16. There are five further "stars", namely for the points No. 1,49,73,97 and 121, with the same weight configuration as shown in Fig. 17 but with (in general) different numerical values of the weights.

The "star" corresponding to point No. 145 has five "arms" and therefore belongs to a second topological configuration. (Fig. 18)

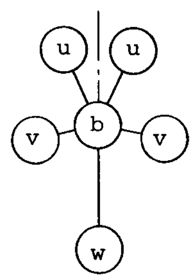


Fig. 18

Finally, for the center point No. 169, there are 24 "arms" with equal weights.

As a consequence of the symmetry just described, the storage of M requires only

$$\underbrace{6\cdot 4}_{6\text{ "arms"}} + \underbrace{1\cdot 4}_{5\text{ "arms"}} + \underbrace{2}_{\text{center point}} = 30 \text{ storage locations} \tag{101}$$

for the different weights.

4.12 The transformed problem

The transformation matrix S is orthogonal, provided the normed real basis vectors described in Section 3.1 are used as column vectors. Therefore the transformed problem of Eq.(100) has the form

$$\tilde{M}\,\tilde{v} = \tilde{b} \tag{102}$$

with

$$\tilde{M} = S^T M\, S \tag{103.1}$$

$$\tilde{b} = S^T b \tag{103.2}$$

$$v = S\,\tilde{v} \tag{103.3}$$

The substitution of the values (99.2) into Eqs.(63) leads to the statement, that

$$\tilde{M} \text{ splits up into } \begin{cases} \quad 1 \quad 8\text{x}8 \text{ matrix} \\ \quad 1 \quad 4\text{x}4 \text{ matrix} \\ \quad 1 \quad 3\text{x}3 \text{ matrix} \\ 11 \text{ pairs of } 7\text{x}7 \text{ matrices} \end{cases} \tag{104}$$

If we take advantage of the freedom to number the basis vectors within the different invariant subspaces of the matrix M in such a way that the vector attached with the corona of radius r_k (cf.Fig. 16) is chosen as No. k, then the submatrices $\tilde{M}_j$ of $\tilde{M}$ are t r i d i a g o n a l .
This follows from Subsection 4.11: The matrix M acting on a basis vector which belongs to a certain corona with radius r_k can not influence the coronas with radius r_j if $|j-k| > 1$: cf.Figs. 16, 17, 18.
The two matrices of the dimensions 4 and 3 are even diagonal because of the alternating components of the corresponding basis vectors (cf. columns No. 3 and 4 in Table (65)) and the symmetry axes of the different "stars".

In contrast to the example here, where there are interior net points in the fundamental domains, the submatrices can in general no longer be tri-diagonalized. However, by appropriate numbering it is still feasible to obtain a band matrix[18], independent of the point group G. The band width n_1 depends on the numbering of the net points in a fundamental domain. This is similar to the classical method, where numbering of all net points determines the band width n_2.

The proportion between n_1 and n_2 is roughly

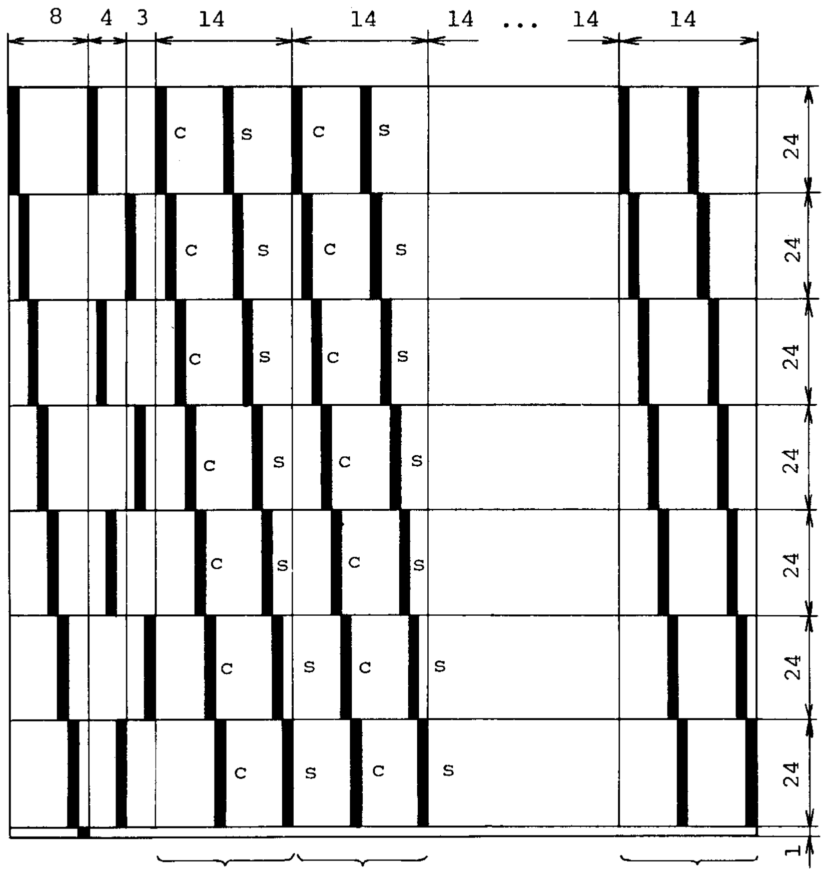
$$\frac{n_2}{n_1} \simeq |G| \tag{105}$$

where $|G|$ denotes the order of the point group G.

4.13 The transformation S

In (106) and (107) a complete description of the matrix S is offered.

S =



(106)

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18) A nxn matrix with elements a_{jk} is called a band matrix with the band width b, if there exists an integer b<n-1 such that the matrix elements $a_{jk}=0$ for $|j-k|>b$.

The vertical bars in the above matrix represent a section of a column vector, while the remaining part of the column vector consists of zero-elements. s and c stand for the sine and cosine functions (cf.(107)).
The matrix elements in the vertical bars have the following sequence from top to bottom (up to the normalizing factor $\sqrt{12}$):

Number of column	1 to 7	8	9 to 15	16,18 20,22	17,19,21	23,25 27,29	24,26,28	...
24 components	q	one non-vanishing element equal to $\sqrt{12}$	q	1	1	0	0	...
	q		-q	$\cos\ \varphi/2$	$\cos\ \varphi$	$\sin\ \varphi/2$	$\sin\ \varphi$	..
	q		q	$\cos\ 3\varphi/2$	$\cos\ 2\varphi$	$\sin\ 3\varphi/2$	$\sin\ 2\varphi$	..
	q		-q	$\cos\ 5\varphi/2$	$\cos\ 3\varphi$	$\sin\ 5\varphi/2$	$\sin\ 3\varphi$	...
	⋮		⋮	⋮	⋮	⋮	⋮	⋮
	q		-q	$\cos 23\varphi/2$	$\cos 23\varphi$	$\sin 23\varphi/2$	$\sin 23\varphi$	...

(107)

1-st block

where $q = 1/\sqrt{2}$, $\varphi = 15^{\circ}$.

The k-th block can be obtained by multiplying the arguments in the trigonometric functions of the 1-st block with k. The corresponding numbers of its columns are

$$j + (k-1)\cdot 14 \qquad \text{with } j = 16,17,\ldots,29$$

The final column in fact has the number

$$29 + 10\cdot 14 = 169$$

Please note:
The storage of the matrix elements of S, given in Table (107), is independent of the number n of the net points.

If one establishes an algorithm[19] based on trigonometrical identities, the computational effort reduces to the determination of $\cos\varphi/2$, $\sin\varphi/2$ and in $\left\{\begin{matrix}\text{two multiplications}\\ \text{one addition}\end{matrix}\right\}$ for each value $\cos k\varphi/2$ and $\sin k\varphi/2$.

19) cf. [12], page 22

4.14 Numerical results

In order to test the accuracy of a program using the transformation S, the solution was calculated on a CDC 6400 for several load functions $f(x_1,x_2)$ and boundary functions $\varphi(s)$.

For example
$$\left.\begin{aligned} f(x_1,x_2) &= 0 \\ \varphi(s) &= e^{x_1}\cdot\cos x_2 \text{ on the boundary } \partial D \end{aligned}\right\} \tag{108}$$

The exact solution on the unit-disk is

$$u(x_1,x_2) = e^{x_1}\cdot\cos x_2 \tag{109}$$

Hence its maximum value is equal to $e = 2.718...$

The absolute difference between the numerical values $v(x_1,x_2)$ and the analytical solution $u(x_1,x_2)$ turns out to be

$$|v(x_1,x_2) - u(x_1,x_2)| \leqq 0.006592 \tag{110}$$

4.2 Eigenvalue Problems

Let us consider the eigenvalue problem

$$\begin{aligned} &\Delta u(x_1,x_2) + \lambda u(x_1,x_2) = 0 \\ &\text{with the boundary-condition } u = 0 \end{aligned} \tag{111}$$

on a circular or on a concentric ring domain.

This enables us to choose a discretization with the symmetry of the dihedral group D_m. The number of symmetry axes m is supposed to be variable, depending on the total number n of the net points.

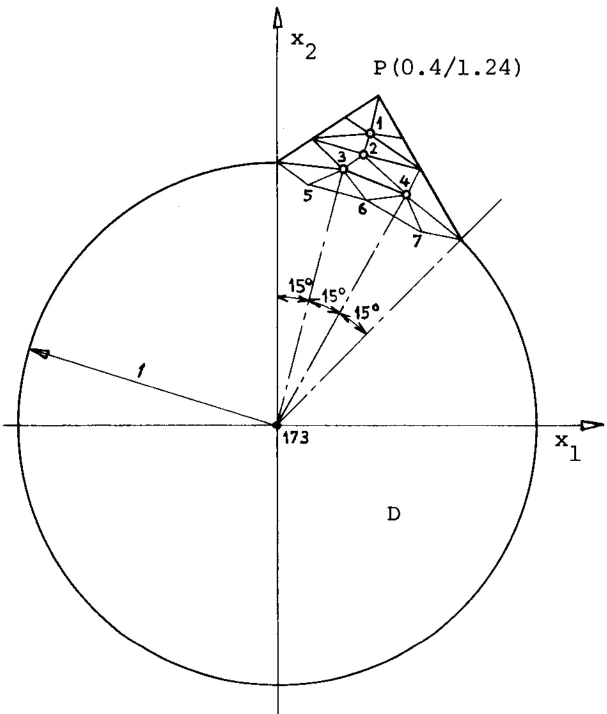
If there are no interior points, the problem again leads to tridiagonal submatrices independent of m and n (similar to Section 4.1).

Tridiagonal matrices are well adapted for calculating eigenvalues. This can be done for instance with the theory of Sturm's chain or with the QD-algorithm (cf. [7]).

But also in the general case, where we have an arbitrary point group G and possibly interior points in the fundamental domain,it is advantagous that the submatrices have a band structure. This is obvious, because the LR-transformation conserves the band structure, for instance when used for calculating eigenvalues (cf. [7], Satz 4.19, Seite 160).

4.3 An Asymmetrical Problem

Here again, we discuss the problem (98). In contrast to the previous case we now drop the condition of symmetry and consider a deformed boundary contour as depicted in Fig. 19.



The interior of the circle will be assumed to have the same discretization net as the symmetrical problem in Section 4.1, hence

$$n' = 169 + 4 = 173$$

The four new points are indicated by o in Fig. 19.

Fig. 19

The transformed 173x173 matrix $\tilde{\Lambda}$ (which is real symmetric and positive definite) of the finite element matrix Λ has the structure (34). For the tridiagonal submatrices along the diagonal, see (104). As a consequence of the finite element method, the rows No. 1 and 2 of the rectangular 4x169 matrix on the right hand side in (34) consists of zero-elements only.

At this stage, we can make the following general statement:
The proposed technique can be advantageous even if only a subset of the domain at hand displays symmetry.

Numerical results for the case (108),(109):

The absolute difference between the numerical values $v(x_1,x_2)$ and the analytical solution (109) on the domain D of Fig. 19 turns out to be

$$|v(x_1,x_2) - u(x_1,x_2)| \leqq 0.006655 \tag{112}$$

4.4 Computational Effort

Let us consider the symmetric problem in Section 4.1 again, whereby the domain D may also be a concentric ring.
To illustrate the merits of the group theoretical considerations, we are going to compare the total number of essential operations[20] (ess.op.) required by the proposed method on the one hand and by classical methods on the other hand.

The number n of unknowns is now supposed to vary as well as the number m of symmetry axes.

From the practical point of view we can assume that the different nets have no interior points, i.e.

$$i = 0 \tag{113}$$

From Eq.(62) and Eq.(113) it follows that

$$n = (h+k)\cdot m + \delta \text{ [21]} \tag{114}$$

For reasonable nets on a 2-dimensional domain, the following relation holds true

$$m \simeq \lambda \cdot \sqrt{n} \tag{115}$$

where the factor λ depends only on the shape of the domain.
In the case of the unit-disk, for instance, we have

$$\lambda \simeq \frac{24}{\sqrt{169}} \simeq 1.84 \tag{116}$$

4.41 Classical methods

Due to the optimal numbering of the unknowns in the ring domain or in the unit-disk, the positive definite and symmetrical matrix M of the finite element method is a band matrix with band width m (cf.Fig. 16).

Hence the solution needs the following number of essential operations for the Gaussian elimination or the Cholesky decomposition (cf.[2], p.131):

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20) essential operations are the multiplication and the division.

21) Definitions are given in Eqs.(57)

1^o) triangle decomposition of M	$\frac{1}{2}\cdot n\cdot m\cdot(m+1)$	ess.op.
2^o) forward- and backward substitution	$2\cdot n\cdot m$	ess.op.
total	$\tau \simeq \frac{1}{2}\,nm^2 + \frac{5}{2}\,nm$	ess.op. (117)

4.42 The group theoretical method

Using the transformation matrix S, one gets the following number of essential operations to solve the problem:

1^o) Construction of the transformation S[22] $\qquad \frac{m}{2}$ ess.op.

2^o) Calculation of $\tilde{M} = S^T M\, S$:

One tridiagonal submatrix with the dimension (h+k) needs $\leqq 5\cdot(h+k) \leqq 5\cdot\frac{n}{m}$ ess.op. (cf.Eq.(114))

Totally there are $\frac{m}{2}$ such submatrices (cf.Eqs.(63)), thus $\leqq \qquad \frac{5}{2}\,n$ ess.op.

3^o) triangular decomposition for the $\frac{m}{2}$ symmetrical tridiagonal submatrices needs $\frac{m}{2}\cdot(\frac{1}{2}\cdot\frac{n}{m}\cdot 1\cdot 2) = \qquad \frac{1}{2}\,n$ ess.op.

4^o) Calculation of $\tilde{b} = S^T b$ and $x = S\,\tilde{x}$ needs (cf.(106),(107)) $\quad \frac{1}{4}\cdot 2nm = \qquad \frac{1}{2}\,nm$ ess.op.

The factor $\frac{1}{4}$ is obtained by taking advantage of the elementary properties of the sine and cosine functions

total	$\tau' \simeq \frac{1}{2}\,nm + 3n$	ess.op. (118)

4.43 Comparison

With Eq.(115) follows

$$\frac{\tau}{\tau'} \simeq m \simeq \lambda\cdot\sqrt{n} \tag{119}$$

where m = number of symmetry axes.

For the example calculated in Section 4.1 we have

$$\frac{\tau}{\tau'} \simeq 24 \tag{120}$$

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22) cf. the remark at the end of Subsection 4.13.