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Author

Young, Jonathan D.

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Jonathan D. Young

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EIGENVALUES AND EIGENFUNCTIONS FOR LINEAR ACCELERATOR (ALVAREZ) CAVITIES BY THE MATRIX METHOD USING MODIFIED CUBIC SPLINE APPROXIMATION

Jonathan D. Young

Lawrence Berkeley Laboratory
University of California
Berkeley, California

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ABSTRACT

We approximate (lesser positive) eigenvalues and corresponding eigenfunctions for the partial differential equation and boundary conditions pertinent to the electromagnetic field for a linear accelerator cavity. We assume azimuthal independance. Symmetry requirements enable us to confine our computation to one-quarter of the cavity.[1]

We use a rectilinear grid on the domain of solution and along any grid line the eigenfunction is assumed (with certain exceptions) to be a cubic spline[2] in the pertinent variable with knots at the mesh-points. The requirement that this spline satisfy the differential equation at the mesh-points leads to a linear system in which the (unknown) eigenvalue appears. Finally, the differential eigenvalues are approximated by eigenvalues of a matrix derived from the linear system.[3] For any such real positive distinct eigenvalue, a corresponding approximate eigenfunction is obtained by finding a (non-zero) solution to the system.

Several eigenvalues (having least values) may be approximated and corresponding eigenfunctions obtained.

The advantages of the "matrix" method[3], described, over optimization techniques[1] (minimization of a Rayleigh quotient) are that:

1. Several lower value eigenvalues are obtained rather than just the least.

2. Extensive iteration is not required.

The advantages of using a cubic spline formulation rather than finite difference formulas are that:

1. The approximation to the eigenfunction is a (cubic spline) function rather than a set of approximate solution values at mesh-points.

2. Processes of differentiation (up to second order), integration and interpolation can be more easily applied.

INTRODUCTION

In connection with the electromagnetic field calculations for drift-tube loaded cavities of linear accelerators[1,5] we are required to consider:

1. A partial differential equation in two variables

$$\frac{\partial^2 u}{\partial r^2} - \frac{1}{r}\frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial z^2} + \lambda u = 0$$

2. A domain (see Figure 1)

$$D = (0,ZL)X(0,RH)U(0,ZG)X(RH,RB)U(0,ZL)X(RB,RC)$$

3. And boundary conditions

$$\frac{\partial u}{\partial n} = 0$$

$$u(z,0) = 0$$

We seek positive values for λ, (eigenvalues) for which a non-trivial solution u exists and solutions, u, (eigenfunctions) corresponding to such eigenvalues.

Computational procedures for finding the least positive value of λ and a corresponding solution, u, by use of finite difference formulas and iteration to minimize a Rayleigh-Ritz ratio are outlined in References 1 and 5.

If the domain, D, is a simple rectangle (ZG = ZL), the problem can be solved by the cubic spline formulation for the matrix method as is shown in Example 2 of Reference 4.

Essentially, we extend that method to the more general domain in question, but we limit our consideration to the partial differential equation and boundary conditions above. We are able, without extensive iteration, to approximate not only the least eigenvalue, but some of the successively higher ones. For such eigenvalues we construct an approximation for corresponding eigenfunctions.

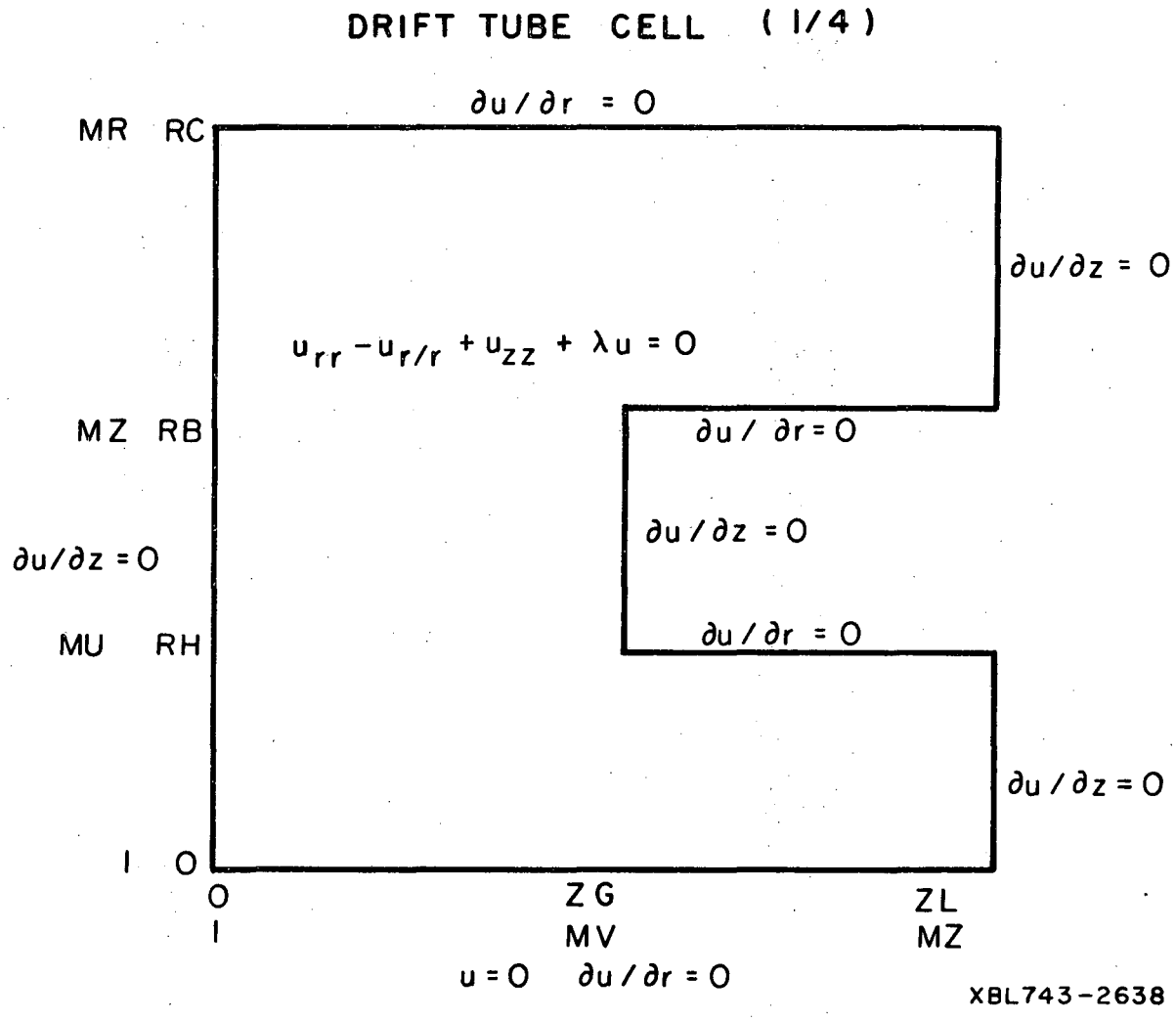
DRIFT TUBE CELL (1/4)
∂u/∂r = 0
MR RC
∂u/∂z = 0
$u_{rr} - u_{r/r} + u_{zz} + \lambda u = 0$
MZ RB
∂u/∂r = 0
∂u/∂z = 0
∂u/∂z = 0
MU RH
∂u/∂r = 0
∂u/∂z = 0
I O
0
I
ZG
MV
ZL
MZ
u = 0 ∂u/∂r = 0
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Fig. 1.

DISCRETIZATION

For some m greater than or equal to four we partition each of the intervals (see Figure 1)

(0,ZG), (ZG,ZL), (0,RH), (RH,RB), and (RB,RC)

into m-1 subintervals obtaining a rectilinear grid with gridpoints, (z_i, r_j) where

$z_1 = 0$, $z_m = ZG$, $Z_{2m-1} = ZL$ with $r_1 = 0$, $r_m = RH$ and with $r_{2m-1} = RB$, $r_{3m-2} = RC$

and $z_1 = 0$, $z_m = ZG$ otherwise,

for a total of $5m^2 - 4m$ gridpoints including all boundaries.

Since the singularity of the differential equation for $r = r_1$ (=0) is offset by the boundary condition that the solution be zero here, we confine our computation of an approximate solution to the remaining $5m^2 - 6m + 1$ gridpoints.

THE LINEAR SYSTEM

Upon the function approximating the (unknown) solution u we impose the requirements that it satisfy the boundary conditions at all boundary gridpoints and that it and its derivatives satisfy the partial differential equation at all gridpoints except those involving r_1. We shall show that by suitable choices of linear spaces in which the approximating function is sought and by convenient choices of bases (functions) for these spaces and by expressing the approximating function as a linear combination of these basic functions which must satisfy the partial differential equation we obtain a linear system of the form:

$$A\vec{u} + \lambda I\,\vec{u} = 0 \qquad (1)$$

where u is an (unknown) vector with $5m^2 - 6m + 1$ components consisting of values for the approximating function at the gridpoints (except those for $r = r_1$). Approximations for λ are obtained as the negatives

of the eigenvalues of the matrix, A. Zero, positive and multiple (if any) eigenvalues for A are discarded to obtain only distinct positive values for λ. For any approximation, λ^*, we obtain values for a corresponding solution by solving the homogeneous system

$$(A + \lambda^* I)\vec{u} = 0$$

SOLUTION SPACES AND BASES

For the gridline $r = r_j$ for $j = 2$ to $m-1$ or $j = 2m$ to $3m-2$ (see Figure 1) we shall seek our approximate solution as a cubic spline in z with knots at z_i for $i = 1$ to $2m-1$ and with zero first derivatives at z_1 and z_{2m-1}. The linear space of all such cubic splines[6] has dimension $2m-1$. A convenient basis for this space consists of the $2m-1$ cubic splines, s_i, all of which have zero first derivatives at z_1 and z_{2m-1} and such that

$$s_i(z_i) = 1$$

$$s_i(z_j) = 0 \quad j \neq i$$

For the gridlines $r = r_j$ for $j = m + 1$ to $2m - 2$ the approximate solution is sought as a cubic spline in z with knots at z_i for $i = 1$ to m and with zero first derivatives at z_1 and z_m. The linear space has dimension m. The basis used for this space consists of m cubic splines, p_i, with zero first derivatives at z_1 and z_m and such that

$$p_i(z_i) = 1$$

$$p_i(z_j) = 0 \quad j \neq i$$

The situation for $r = r_m$ and $r = r_{2m-1}$ is complicated by the fact that $\frac{\partial u}{\partial z}$ must vanish at (z_m, r_m) and (z_m, r_{2m-1}). The linear space and basis as described in the first paragraph of this section are modified to meet this added requirement. This is done by using a higher (than cubic) degree in the subintervals (z_{m-1}, z_m) and (z_m, z_{m+1}).

For the gridlines $z = z_i$ for $i = 1$ to $m-1$ the approximate solution space is a space of segmented polynomials with continuous

second derivatives, the functions having zero first derivatives at r_1, and r_{3m-2} and being cubics except on the interval $[r_1,r_2]$. For this first interval a special formulation is used reflecting the fact that u is an even function of r which vanishes at r=0. The space has dimension 3m-3. The convenient basis consists of functions, f_k,k=1, 3m-3 meeting the desired boundary conditions and such that

$$f_k(r_j)=1 \qquad j=k+1$$

$$f_k(r_j)=0 \qquad j\neq k+1$$

For the gridline $z=z_m$ the above linear space and basis are modified to accomodate the fact that $\partial u/\partial r$ must vanish at (z_m,r_m) and (z_m,r_{2m-1})

For the gridlines $z=z_i$ for i=m+1 to 2m-1 and for $r=r_j$,j=2 to m the space is similar to that for i=1 to m-1 except that it has dimension m and that the first derivatives vanish at r_m. However for $r=r_j$, j=2m-1 to 3m-2 the approximation is again sought in a linear space of cubic splines in r with knots at r_j for j=2m-1 to 3m-2 and with zero first derivatives at r_{2m-1} and r_{3m-2} the basis consists of m cubic splines, t_k for k=1 to m such that

$$t_k(r_j)=1 \qquad \text{for } j=k+2m-2$$

$$t_k(r_j)=0 \qquad \text{for } j\neq k+2m-2$$

with j=2n-1 to 3m-2

The convenience of the various bases appears in the fact that when the approximation is expressed as a linear combination of the pertinent bases the coefficients are in fact gridpoint values of the approximating function.

Definition of the Vector, $\vec{u}$, and Construction of the Matrix, A.

As stated earlier $\vec{u}$ is a vector of $5m^2-6m+1$ components consisting of values for the approximating function at gridpoints (excluding those for $r=r_1$, where u is zero). A sensible ordering of the components, u_n, for n=1 to $5m^2-6m+1$ in relation to the indices i

and j of z and r respectively is attained by

$$\begin{aligned} n &= i + (2m-1)\ (j-2) \text{ for } j=2 \text{ to } m \\ n &= 2m^2-2m+1+i+m(j-m-1) \text{ for } j=m+1 \text{ to } 2m-2 \\ n &= 3m^2-4m+1+i+(2m-1)\ (j-2m) \text{ for } j=2m-1 \text{ to } 3m-2 \end{aligned} \tag{2}$$

The component u_n then represents the approximate value of $u(z_i, r_j)$ for all points in the domain of computation (points (z_i, r_1) are not included). Thus the columns of the matrix A are coefficients for the unknown vector u in the component order described above.

The linear system (Equation (1)) is constructed by evaluating the partial differential equation successively at the gridpoints (in the order described above). In particular let us consider in detail how this is done at the first such gridpoint, (z_1, r_2). For the fixed argument $z = z_1$, our approximate solution is assumed to be a function in r from the linear space whose basis consists of a set of functions, f_k, described earlier. Thus for any r in approximation

$$u(z_1,r) = \sum_{k=1}^{3m-3} c_k f_k(r) \tag{3}$$

$$\frac{\partial u}{\partial r}(z_1,r) = \sum_{k=1}^{3m-3} c_k f_k'(r) \tag{4}$$

$$\frac{\partial^2 u}{\partial r^2}(z_1,r) = \sum_{k=1}^{3m-3} c_k f_k''(r) \tag{5}$$

where derivatives indicated are with respect to r.

Applying Equation (3) for r_j for j=2, 3m-2 we obtain

$$u(z_1,r_j) = \sum_{k=1}^{3m-3} c_k f_k(r_j) \tag{6}$$

and since $f_k(r_j)$ is 1 for j=k+1 and zero otherwise we have

$$c_k = u(z_1, r_{k+1}) \text{ for } k=1 \text{ to } 3m-3 \tag{7}$$

Using the above and applying Equations (4) and (5) at r_2 we have

$$\frac{\partial u}{\partial r}(z_1, r_2) = \sum_{k=1}^{3m-3} f_k'(r_2)\, u(z_1, r_{k+1}) \tag{8}$$

$$\frac{\partial^2 u}{\partial Z^2}(z_1, r_2) = \sum_{k=1}^{3m-3} f_k''(r_2)\, u(z_1, r_{k+1}) \tag{9}$$

A similar process applied to the basis, s_k for k=1 to 2m-1 for fixed $r=r_2$

$$\frac{\partial^2 u}{\partial Z^2}(z_1, r_2) = \sum_{k=1}^{2m-1} s_k''(z_\cdot)\, u(z_k, r_2) \tag{10}$$

The required simple derivatives for Equations (8), (9) and (10) are computed in the construction of the pertinent basis functions. Consequently we are able to write the first equation of our linear system by substituting from Equations (8), (9) and (10) into the partial differential equation, obtaining, in approximation:

$$\sum_{k=1}^{3m-3} \left[f_k''(r_2) - \frac{1}{r_2} f_k'(r_2)\right] u(z_1, r_{k+1}) + \sum_{k=1}^{2m-1} s_k''(z_1) u(z_k, r_2) + \lambda u(z_1, r_2) = 0 \tag{11}$$

Using the indexing rule for the components of the unknown vector, u, we have

$$\sum_{k=1}^{3m-3} \left[f_k''(r_2) - \frac{1}{r_2} f_k'(r_2)\right] u\,(z_1, r_{k+1}) + \sum_{k=1}^{2m-1} s_k''(z_1) u_k + \lambda u_1 = 0$$

From the above we are able to construct the first row of the

matrix, A and verify the first row of the identity matrix, I, in Equation (1).

A similar process applied at the remaining gridpoints in the order of n yields the entire matrix, A, and justifies completely the use of the identity matrix, I for Equation (1).

EIGENVALUES AND EIGENFUNCTIONS

Approximate differential eigenvalues can be obtained as follows:

$$\text{Let } \mu = -\lambda$$

then from Equation (1) we obtain

$$A\vec{u} - \mu I\vec{u} = 0 \tag{12}$$

and μ is seen to be an eigenvalue and u an eigenvector of the known matrix, A. Several algorithms are available for determining the eigenvalues of a real matrix. In the Examples solved later, we used the QR-algorithm[7]. By this method it is possible to obtain $5m^2 - 6m + 1$ eigenvalues. Strictly complex, multiple and non-negative values for are discarded. For the remaining values of we set $\lambda^* = -\mu$ and obtain distinct strictly positive approximations for differential eigenvalues. The set of λ^* is ordered in accordance with increasing magnitude. Usually we are interested in only a few (the lesser ones) of these approximations.

For any such λ^* we solve the homogeneous linear system

$$(A + \lambda^* I)\vec{u} = 0 \tag{13}$$

for a nontrivial solution vector, $\vec{u}$. This can be done by arbitrarily assigning the value one to some component of $\vec{u}$. In all cases tried we were successful in finding a solution when we assigned

$$u_{5m^2-6m+1} = 1$$

And replaced the last equation of the linear system by this equation. With this solution we have approximate values for u at all the gridpoints. Equations (8) and (9) and similar pertinent equations can be

used to compute the approximate partial derivatives, $\partial u/\partial r$, $\partial^2 u/\partial r^2$, $\partial u/\partial z$ and $\partial^2 u/\partial z^2$ at the gridpoints.

COMPUTER CODE

A computer code, DTCYC, has been written in FORTRAN for the CDC7600 to perform all the computation described above. The value, m=6, is used in obtaining a matrix 145x145. The computer subroutine, EIG5, written by B.N. Parlett and others with some change in dimensions was used to obtain 145 eigenvalues for the matrix. The code, DTCYC, discards strictly complex and non-negative eigenvalues and arranges those left in increasing order. Some number (specified in input) of the least of these are used to compute approximate eigenfunctions and partial derivatives at the gridpoints. These values are printed out.

A listing of this code, together with instructions for its use may be obtained from the author.

Numerical Examples

In all examples we find approximations for the five least eigenvalues for the differential equation and boundary conditions as given earlier. The domain is varied by specifying RH, RB, RC, ZG and ZL. The computer code with m=6, described in the previous section is used. Results are tabulated below.

Example	RH	RB	RC	ZG	ZL	Eigenvalues				
1	5.	10.	15.	5.	10.	0.0152	0.0925	0.1667	0.2810	0.3684
2	5.	10.	15.	4.	10.	0.0139	0.0855	0.1673	0.2761	0.3672
3	5.	10.	15.	6.	10.	0.0162	0.0978	0.1639	0.2806	0.3569
4	5.	10.	15.	5.	9.	0.0160	0.1090	0.1764	0.2894	0.3784
5	5.	10.	15.	5.	11.	0.0143	0.0787	0.1600	0.2728	0.3537
6	4.	10.	15.	5.	10.	0.0141	0.0934	0.1690	0.3483	0.4096
7	6.	10.	15.	5.	10.	0.0164	0.0904	0.1603	0.2303	0.3675
8	5.	9.	15.	5.	10.	0.0167	0.0967	0.1602	0.2810	0.3245
9	5.	11.	15.	5.	10.	0.0141	0.0873	0.1690	0.2794	0.3758
10	5.	10.	14.	5.	10.	0.0166	0.0932	0.1852	0.2887	0.4129
11	5.	10.	16.	5.	10.	0.0140	0.0917	0.1497	0.2681	0.3143
12	4.	8.	12.	4.	8.	0.0237	0.1446	0.2604	0.4390	0.5756

Conclusion

The technique described and the computer code to perform it provide a quick (in terms of computer time) and hence economical way to determine reasonable approximations for several (least) eigenvalues for a drift tube cell in a linear accelerator.

Methods of improving the approximations thus obtained are being studied.

Acknowledgement

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References

1. T. W. Edwards, "Proton Linear Accelerator Cavity Calculations", Midwestern University Research Association Report, MURA 622, June 1961.
2. J. Young, "Numerical Applications of Cubic Spline Functions", Logistics Review, 3 (1967).
3. J. Young and P. Luger, "Cubic Spline Formulation for Matrix Method for Second Ordinary Differential Eigenvalues", Lawrence Berkeley Laboratory Report, LBL 764, March 1972.
4. P. Luger, F. Valente and J. Young, "Bicubic Spline Solutions for Second Order Homogeneous Partial Differential Equations on a Rectangle", Lawrence Berkeley Laboratory Report, LBL 1516, November 1972.
5. T. W. Edwards, "Messymesh", Midwestern University Research Association Report, MURA 642, May 1962.
6. J. D. Young, "The Space of Cubic Splines with Specified Knots", Logistics Review, 7, 30, 3-8, (1971).
7. B.N. Parlett, "Applications of Laguerre's Method to Matrix Eigenvalue Problem," Mathematics of Computation, 18, 87, 464-485, (1964).

TECHNICAL INFORMATION DIVISION
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720