A MESH-ITERATION PROGRAM FOR FIELD CALCULATIONS IN LINAC CAVITIES[*]

G. Parzen
Brookhaven National Laboratory
Upton, New York

I. Introduction

This paper summarizes some of the experiences met in applying the JESSY mesh-iteration program to the calculation of the fields and resonant frequency of cells in a 200-MeV proton linac.

Each tank of the linac consists of a large number of cells as shown in Fig. 1a. The number of cells varies from 57 in the first tank to 19 in the last or ninth tank. The length of the cells increases from about 6 cm for the first cell to about 84 cm for the last cell. Mesh-iteration programs cannot easily solve for the fields in the entire tank. Instead the mesh-iteration program treats the problem of the single cell whose end boundary conditions require the fields to be periodic with the period of the cell length. The cell is shown in Fig. 1b.

The lowest mode of the cell can be found by solving the differential equation

$$\frac{\partial^2 F}{\partial r^2} - \frac{1}{r}\frac{\partial F}{\partial r} + \frac{\partial^2 F}{\partial z^2} + k^2 F = 0 \quad , \qquad (1.1)$$

where $F = r\, H_\varphi$, and H_φ is the azimuthal component of the magnetic field. The lowest mode has only a H_φ component in the magnetic field because of the cylindrical symmetry. The function F is used because of its simple boundary conditions which are that $\partial F/\partial n = 0$ on all boundaries except the $r = 0$ boundary, where $F = 0$.

The electric field can be found from F according to the equations

$$E_z = \frac{i}{k}\frac{1}{r}\frac{\partial F}{\partial r} \quad , \qquad (1.2a)$$

$$E_r = -\frac{i}{k}\frac{1}{r}\frac{\partial F}{\partial z} \quad . \qquad (1.2b)$$

In addition, there exists a variational principle

$$k^2 \le \frac{\int \frac{1}{r}\left\{\left(\frac{\partial F}{\partial r}\right)^2 + \left(\frac{\partial F}{\partial z}\right)^2\right\}drdz}{\int \frac{1}{r} F^2 \, drdz} \quad , \qquad (1.3)$$

which can be used to find a more accurate result for the resonant frequency.

A number of mesh-iteration programs have been written to solve the above problems for the fields

and resonant frequency of the lowest mode, and they include programs written by Edwards and Christian,[1] Taylor and Kitching,[2] Hoyt, Simmonds and Rich,[3,4] Parzen,[5,6] Martini and Warner,[7] and Katz.

II. Iteration Procedure

The JESSY mesh-iteration program replaces the differential equation by a set of difference equations for each point on a rectangular mesh. For each interior mesh point one obtains a difference equation of the sort

$$\sum_{i=0}^{4} \alpha_i F_i + k^2 F_o = 0 \quad , \qquad (2.1)$$

where the four neighbors of each interior point are indicated by F_1 to F_4, and the interior point being considered is indicated by F_o. The α_i are found by standard methods.[1]

The iteration relation used by JESSY at each interior mesh point is given by

$$F_o^{(n+1)} = F_o^{(n)} - \alpha\, R^{(n)} \quad , \qquad (2.2a)$$

$$R^{(n)} = \alpha_1 F_1^{(n)} + \alpha_2 F_2^{(n)} + \alpha_3 F_3^{(n+1)} + \alpha_4 F_4^{(n+1)} + k^2 F_o^{(n)}. \qquad (2.2b)$$

In Eq. (2.2), n is the iteration number, and α is the over-relaxation parameter. α_1, α_3 refer to the right and left neighbors and α_2, α_4 refer to the above and below neighbors.

Before every iteration defined by Eq. (2.2), a new value of k^2 is computed to use in Eq. (2.2). In the JESSY program, the new k^2 is computed according to Eq. (2.1) by

$$k^2 = \frac{\sum FLF/R}{\sum FF/R} \quad , \qquad (2.3)$$

where the sum is over all interior mesh points, $LF = \sum \alpha_i F_i$ at each mesh point, and R is the distance of the mesh point from the z-axis.

Other programs[1,3] have used the actual variational principle, Eq. (1.3), to find a new value for k^2. One may note that the k^2 found from the variational principle, Eq. (2.1), is closer to the k^2 of the physical problem being solved, but this k^2 is not necessarily converging to the eigenvalue

of the set of difference equations, Eq. (2.1), that we are solving by iteration. The k^2 found from Eq. (2.3) is converging to the lowest eigenvalue of the difference equations and it may differ from the k^2 found from the variational principle by as much as 10% for the smaller cells. It is shown in Section III that either k^2 may be used in the iteration procedure.

The boundary condition $\partial F/\partial n = 0$ is also replaced by a difference equation which is used to iterate the boundary points. This difference equation has the form

$$\sum_{i=0}^{2} \beta_i F_i = 0 \quad , \qquad (2.4)$$

where the three mesh points used in Eq. (2.4) include the boundary point being considered and its two neighbors which lie closest to the normal. The β_i are found by standard methods.[8] This three-point algorithm is correct only to first order in the mesh size. An attempt was made in JESSY to use the second order relations for $\partial F/\partial n$ given in Ref. 8. However, the iteration process failed to converge when the second order relations were used for the geometry required by the linac cell.

III. Theory of the Iteration Procedure

The set of difference equations given by Eq. (2.1) may be written as a matrix equation,

$$AF = \lambda F \quad , \qquad (3.1)$$

where $\lambda = k^2$ is the eigenvalue, A is a matrix whose elements are the α_i of Eq. (2.1) and corresponds to the difference representation of the differential operat r, $-(\partial^2/\partial r^2 - (1/r)\ \partial/\partial r + \partial^2/\partial z^2)$, and F is a column vector whose elements are the values of rH_ϕ at the interior mesh points and on the boundary points.

In discussing the convergence of the iteration procedure we will at first limit ourselves to the case where over-relaxation is not used, and where in each step of the iteration only the values of F found from the previous iteration are used in finding the new values of F. In this case one may write the iteration equations as

$$F^{(n+1)} = F^{(n)} - R^{(n)} \quad , \qquad (3.2a)$$

$$R^{(n)} = D^{-1}\left[\ DF^{(n)} - LF^{(n)} - UF^{(n)} - \overline{\lambda}F^{(n)}\right]. (3.2b)$$

In Eq. (3.2), we have written A as $A = D - L - U$, where D is the diagonal, L is the lower triangle, and U is the upper triangle part of the A matrix. $\overline{\lambda}$ is the current guess for the eigenvalue λ which is used in the iteration.

Rewriting (3.2), one finds the iteration matrix C,

$$F^{(n+1)} = CF^{(n)} \quad , \qquad (3.3a)$$

$$C = D^{-1}\ (D + \overline{\lambda} - A) \quad . \qquad (3.3b)$$

We will further simplify the analysis by assuming that the diagonal matrix D has the same positive value for all of its diagonal elements, and which will be denoted by $\overline{\alpha}$. If we then expand F in the eigenfunctions, u_s, of the matrix A, with the eigenvalues λ_s, we see that each multiplication by the iteration matrix C reduces the component of F associated with u_s by the factor

$$f = 1 + \frac{\overline{\lambda} - \lambda_s}{\overline{\alpha}} \quad . \qquad (3.4)$$

Because of the diagonal dominance property of A, which is discussed below, one may show that the largest value of λ_s is limited by $\lambda_s < 2\overline{\alpha}$. Thus f ranges between

$$1 + (\overline{\lambda} - \lambda_o)/\overline{\alpha} \rightarrow -1 + \overline{\lambda}/\overline{\alpha} \quad . \qquad (3.5)$$

The factor f will have its largest value for $\lambda_s = \lambda_o$, if $\overline{\lambda}$, the guess for the eigenvalue, is very close to λ_o or somewhat larger than λ_o, and for this choice of $\overline{\lambda}$ the iteration process will converge to the eigenfunction with the lowest eigenvalue λ_o.

The two procedures for choosing $\overline{\lambda}$ mentioned in Section II will both lead to convergence because one choice which is based on the difference equations leads to a $\overline{\lambda}$ which converges to λ_o so that $\overline{\lambda}$ becomes very close to λ_o, and the other choice of λ, based on the variational principle, leads to a $\overline{\lambda}$ which is empirically known to be somewhat larger, at most about 10% larger, than λ_o.

The above discussion can be generalized to apply to the iteration process with over-relaxation, and where in each iteration values of F found from the current iteration as well as from the previous iteration are used in finding the new value of F. The procedure may be found in various textbooks,[9,10] and requires that the A matrix have the property of diagonal dominance and that the elements of A be non-zero only when they relate F at a mesh point to F at the four nearest neighbors.

The diagonal dominance property states that the elements of A satisfy

$$-\sum_{i=1}^{4} \alpha_i/\alpha_o \leq 1 \quad , \qquad (3.6)$$

where α_1 to α_4 all have the same sign, and the inequality holds for some mesh point.

IV. Convergence Acceleration Technique

Several techniques were applied in the JESSY program to accelerate the convergence:

The Mesh Interval Sequence

In the JESSY program, the mesh interval in the r and z directions may be unequal and are indicated by EL and H respectively. The convergence becomes slower when the mesh interval becomes small. The convergence may be accelerated by first doing the run with a large mesh interval, and then using the results for this run as the initial load for a second run, using a smaller mesh interval.

In the runs done on JESSY, EL was held constant in a sequence while H was decreased in each step by a factor of 2. Since the mesh with smaller H has more mesh points, it is necessary to interpolate to find F at the additional mesh points.

The Initial Load

The time required for the run is considerably affected by the correctness of the initial guess for F. By examining the solution found in several runs, an empirical result was found for the initial guess. This empirical result for F is

$$F = \frac{r^2}{(\overline{R}+d/2)^2} \frac{L/2}{\overline{R}} + \left(\frac{r}{R}\right)^2 \left[1 - 0.5 \left(\frac{r}{R}\right)^2\right] , \qquad (4.1a)$$

where

$$\overline{R} = \left[r^2 + (z - L/2)^2 \right]^{\frac{1}{2}} , \qquad (4.1b)$$

and the parameters R, d, L are defined in Fig. 1b.

The Over-Relaxation Scan

Over the wide range of cell dimensions which were run with the JESSY program, the choice of the over-relaxation parameter of $\alpha = 1.9$ would work quite well. In some cases, however, when the mesh size was large or when the boundary of the drift tube was close to mesh points, a smaller value of α was required for convergence and the convergence rate was slower.

An empirical method of choosing α was developed which scans a certain range of α and chooses the α with the fastest convergence rate. The scan covers three values spaced at ALFO - DALF, ALFO, ALFO + DALF. The program runs 20 iterations with each α and finds the α with the best convergence rate, ALFMX. The next scan is done for three values of α centered at ALFO = 0.5 (ALFO + ALFMX), and the DALF is reduced to DALF = 0.75 * DALF. The initial scan is done with ALFO = 1.8 and DALF = 0.1, so that the initial scan covers $\alpha = 1.7$, 1.8, 1.9.

There are several techniques included to keep the scan from going too far off. The choice of ALFMX after each scan is limited to be less than ALFLM, and ALFLM = 1.95. There is a recovery technique to keep the scan from narrowing down on an α with too low a convergence rate. After each

scan, the best convergence rate RTMX is compared with RTO, which is the lowest rate one will accept. If RTMX < RTO, the scan recovers or starts again with ALFO = 1.8 and DALF = 0.1. The value set for RTO is RTO = 0.001, where the rate is defined as the percentage change in the residual for each iteration.

Because of the large number of parameters in the α-scan, it is difficult to optimize the choice of these parameters. The choice given above may not be the best but it gives acceptable results. An α-scan using five values of α rather than three was attempted but did not give as good results. Runs with 10 iterations for each α seemed to do about as well as 20 iterations for each α.

Integerization

It sometimes happens that a boundary point is very close to a mesh point. This would give rise to very large weights in the iteration of the star point near the boundary point, which resulted in much lower convergence rates.

It was found advisable to integerize the boundary. If a boundary point was very close to a mesh point, it was moved onto the mesh point. The criterion for close that was used was a distance of 0.0005 cm.

V. Accuracy of the JESSY Program

The accuracy of mesh-iteration programs is difficult to estimate theoretically. A comparison of the program results with experimentally measured results provides a good estimate of the accuracy.

One criterion of the accuracy of the results which was found useful was to compare the average electric field along the axis, E_O, as computed by two different methods. One method of computing E_O is to simply integrate the electric field along the axis. The second method is to use the flux of the magnetic field across the r,z plane, which according to Maxwell's equations should also give E_O. The percentage disagreement in the result for E_O as found by these two methods was found to be a good measure of the error in the electromagnetic fields computed by the program.

The accuracy of the JESSY program, as found by comparison with the experimental measurements of MURA,[11] Brookhaven,[5] and the University of Tokyo,[12] may be summarized in the following statement: The error in the electromagnetic fields is of the order of a few percent, and the error in the resonant frequency is about 0.1% except possibly for the very low energy linac cells.

A more complete picture of the program accuracy is provided by Fig. 2, where the error in the frequency as determined by comparison with experimental measurements is plotted as a function of cell length for both the MESSYMESH and JESSY programs. The MESSYMESH program uses a mesh size of 0.25 by 0.25 cm. The JESSY program can go to the smaller mesh of 0.125 cm in the z-direction and

0.25 cm in the r-direction. The results from
Fig. 2 indicate an error of about 0.4% in the fre-
quency for the smaller L cells which can be reduced
by decreasing the mesh size.

Acknowledgments

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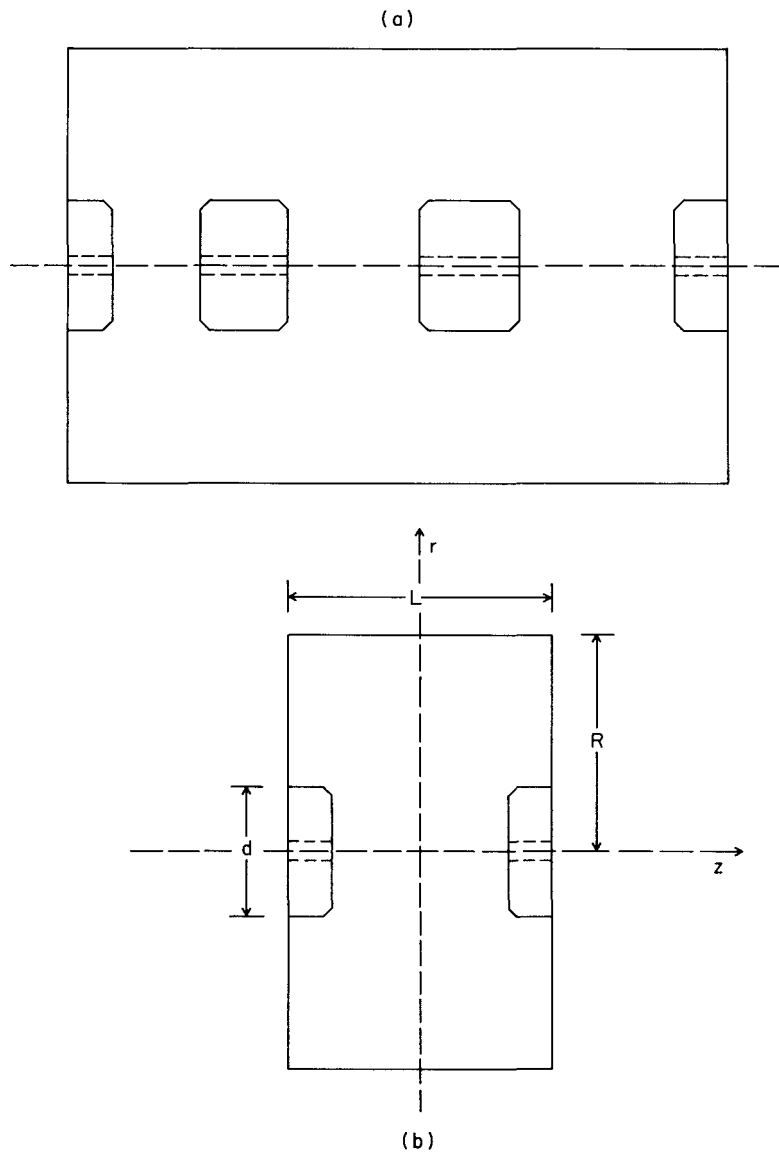   Report PS/INT/LINAC/68-1, January 1968.

(a)

(b)

Fig. 1.   The geometry of the linac cells.
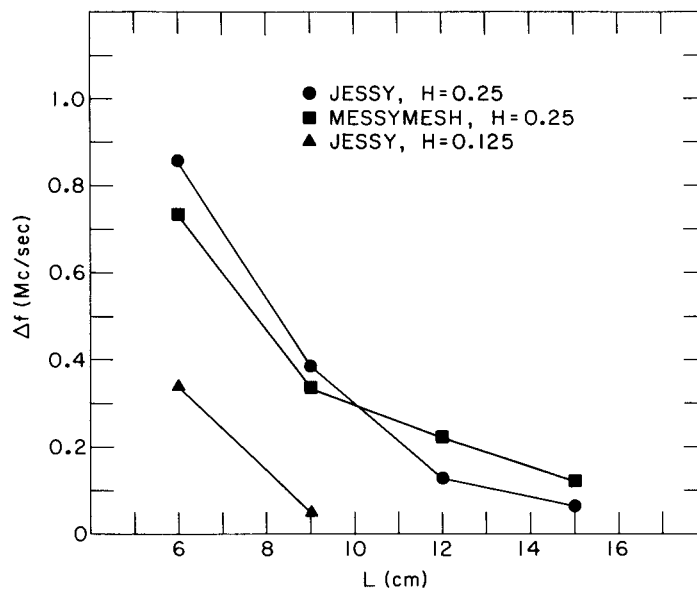
Fig. 2.   A plot of the error, Δf, in the results of mesh-iteration programs
           for the resonant frequency, as found by comparing computer results
           with experimental results. The experimental results used here were
           those of the University of Tokyo group.