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ULTRAFISH -- GENERALIZATION OF SUPERFISH TO $m \geq 1$*

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Summary

The present version of the SUPERFISH program computes fundamental and higher order resonant frequencies and corresponding fields of azimuthally symmetric TE and TM modes (m=0) in an electromagnetic cavity which is a figure of revolution about a longitudinal axis. We have developed the program ULTRAFISH which computes the resonant frequencies and fields in such a cavity for azimuthally asymmetric modes ($\cos m\phi$ with $m \geq 1$). These modes no longer can be characterized as TE and TM and lead to simultaneous equations involving two field components. These are taken for convenience to be $rE\phi$ and $rH\phi$, in terms of which all four other field components are expressed. Several different formulations for solving the equations are being investigated. The resulting matrix consists of tridiagonal blocks of twice the dimension of SUPERFISH, but the matrix inversion and root finding procedures are the same. Care must be taken to remove the spurious singularity at $\omega\sqrt{\mu\varepsilon}r = m$ which appears in the formulation. We have also generalized SUPERFISH to obtain resonant frequencies of two dimensional cavities of arbitrary cross section. In addition, we have generalized SUPERFISH and ULTRAFISH to include regions of different permeability and dielectric constant. The programs have been tested on cavity shapes with analytically obtainable resonant frequencies.

I. Introduction

With the advent of high speed computing, techniques were developed for solving partial differential equations numerically by approximating the equations by difference equations involving the values of the function at mesh points. Iteration schemes were then used to solve these difference equations by "relaxation." For the calculation of azimuthally symmetric modes in azimuthally symmetric electromagnetic cavities, various codes were developed and applied to the design of cavities for linear accelerator sections.[1]

The next major step in the numerical approach to the cavity mode problem is described in SUPERFISH[2]. Specifically, this program used the more versatile triangular mesh and directly inverted the matrix using the driving point and root finder technique described in Section D.

The present paper describes the extension of the SUPERFISH program in the following ways:

1) Two dimensional cavities of arbitrary cross section.
2) Regions of different permeability, μ, and permittivity, ε.
3) Azimuthally asymmetric modes in azimuthally symmetric cavities.

We have designated the new program as ULTRAFISH.

The first two modifications are relatively simple and will only be described briefly. The bulk of the paper addresses the generalization to azimuthally asymmetric modes.

II. Two Dimensions

The existing SUPERFISH program is easily extended to two dimensions by letting $r \to \infty$ in all relevant terms. In the operating program the result is the elimination of one of the two terms in each of the coefficients in the difference equations. The modified program has been tested in cavities in the shape of a 45°, 45° right triangle and found to agree with the known analytic results for the frequencies and fields.

III. Regions of Different Permeability and Permittivity

The existing SUPERFISH program is easily extended to include regions of different ε and μ. The mesh must be drawn so that the border between regions of different ε and μ coincides with mesh lines, in which case the coefficients can be identified as having terms from the individual triangles. Thus, the ε and μ can be introduced as factors in Maxwell's equations corresponding to their values in each triangle of the mesh. The modified program has been tested in cylindrical cavities with two different radial regions of ε and μ, and with two different axial regions of ε and μ. In each case the numerical results agreed with the known analytic results for the frequencies and fields.

IV. Azimuthally Asymmetric Modes

A. Field Components -- Maxwell's Equations

We shall assume that E_z, E_r, H_ϕ all contain the factor $\cos m\phi$ that H_z, H_r, E_ϕ all contain the factor $\sin m\phi$. We further assume that all electric field components have a factor $e^{i\omega t}$, and that all magnetic field components contain the factor $ie^{i\omega t}\sqrt{\varepsilon_o/\mu_o}$. As a result, Maxwell's equations for the cylindrical components can be written as

$$k_o\mu H_r + \frac{m}{r}E_z = -\frac{\partial E_\phi}{\partial z}, \quad k_o\varepsilon E_r - \frac{m}{r}H_z = -\frac{\partial H_\phi}{\partial z}$$
$$\frac{m}{r}H_r + k_o\varepsilon E_z = \frac{1}{r}\frac{\partial}{\partial r}(rH_\phi) - \frac{m}{r}E_r + k_o\mu H_z = \frac{1}{r}\frac{\partial}{\partial r}(rE_\phi) \qquad (1)$$

*Work supported in part by Los Alamos National Laboratory, AT Division.

[1] T. Edwards, MURA Report 622 (1961), unpublished (MESSYMESH); H. C. Hoyt, Rev. Sci. Instrum 37, 755 (1966) (LALA).

[2] K. Halbach and R. F. Holsinger, Particle Accelerators 7, 213 (1976) (SUPERFISH).

$$k_o \varepsilon E_\phi = \frac{\partial H_r}{\partial z} - \frac{\partial H_z}{\partial r} \qquad (2)$$

$$k_o \mu H_\phi = \frac{\partial E_r}{\partial z} - \frac{\partial E_z}{\partial r} \qquad (3)$$

where μ and ε are the ratio of the permeability and permittivity to that of free space. It is well known[3] that the TE,TM designation of wave guide or cavity solutions applies to very special geometries, and that with azimuthally asymmetric modes one finds it necessary to use a combination of TE and TM modes, that is all six cylindrical components at the same time. This leads to the requirement that two functions must be specified at all mesh points in order to determine all field components. For reasons of simplicity, we shall use the two functions

$$f(r,z) = r\,E_\phi\,(r,z) \qquad (4)$$

and

$$g(r,z) = r\,H_\phi\,(r,z) \qquad (5)$$

This choice of variables also guarantees $f = g = 0$ for $r = 0$, as is the case for the choice of E_ϕ, H_ϕ in SUPERFISH (m=0). These functions are continuous in the cavity, even if ε and μ vary with position. Moreover, they satisfy the boundary conditions

$f = 0,\ \frac{\partial g}{\partial n} = 0$ on a metallic (electric) boundary

$g = 0,\ \frac{\partial f}{\partial n} = 0$ on a "magnetic" boundary

We now can solve Equation (1) for all field components in terms of f and g (E_ϕ and H_ϕ). The result is

$$\left.\begin{aligned} E_z &= \frac{k_o \mu r \frac{\partial g}{\partial r} + m \frac{\partial f}{\partial z}}{k_o^2 r^2 \mu\varepsilon - m^2} \\ E_r &= \frac{m \frac{\partial f}{\partial r} - k_o \mu\, r \frac{\partial g}{\partial z}}{k_o^2 r^2 \mu\varepsilon - m^2} \end{aligned}\right\} \qquad (6)$$

$$\left.\begin{aligned} H_z &= \frac{k_o \varepsilon r \frac{\partial f}{\partial r} - m \frac{\partial g}{\partial z}}{k_o^2 r^2 \mu\varepsilon - m^2} \\ H_r &= \frac{-m \frac{\partial g}{\partial r} - k_o \varepsilon r \frac{\partial f}{\partial z}}{k_o^2 r^2 \mu\varepsilon - m^2} \end{aligned}\right\} \qquad (7)$$

where $k_o^2 = \omega^2 \mu_o \varepsilon_o$. It appears that we have found a singularity at $r^2 = \hat{r}^2 = m^2/k_o^2\mu\varepsilon$. However, since the fields are finite, the singularity must be spurious, and the numerators in (6) and (7) will vanish identically at $r = \hat{r}$. This poses a numerical obstacle however, since in our mesh calculation, the values of f and g are not exact, and the cancellation may not be precise. Various smoothing techniques must be used in the triangles close to $r = \hat{r}$.

B. Difference Equations

We shall obtain two difference equations for f and g by integrating Equations (2) and (3) over the dodecagon surrounding each point, as constructed from the triangular mesh in SUPERFISH. Specifically, there are six triangles surrounding each mesh point. The dodecagon connects the centroids of these six triangles alternately to the midpoints of the sides of the triangles which form the spokes of the hexagon, as shown in Figure 1.

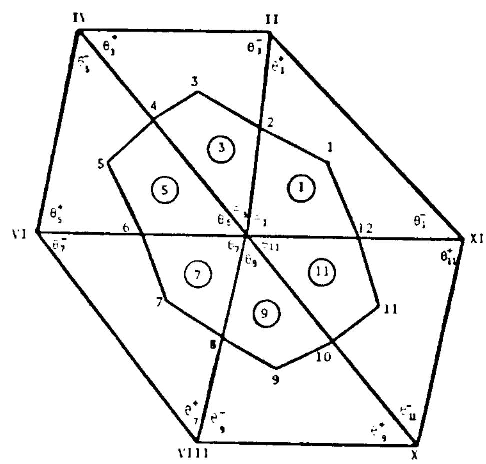

Fig. 1 Triangular mesh and corresponding dodecagon region of integration.

Using Stokes Law, we obtain

$$k_o \iint \frac{dr}{r}\, dz\, \varepsilon f = \oint (H_r dr + H_z dz) \qquad (8)$$

$$k_o \iint \frac{dr}{r}\, dz\, \mu g \quad \oint (E_r dr + E_z dz) \qquad (9)$$

where the left sides are integrals over the area of the dodecagon, and where the right sides are line integrals over the perimeter of the dodecagon. Using Equations (6) and (7), we write

$$k_o\, J_f = k_o\, L_f - m\, K_g \qquad (10)$$

$$k_o\, J_g = k_o\, L_g + m\, K_f \qquad (11)$$

where

$$J_f = \iint \frac{dr}{r}\, dz\, \varepsilon f \qquad (12)$$

$$J_g = \iint \frac{dr}{r}\, dz\, \mu g \qquad (13)$$

$$\left.\begin{aligned} L_f &= \oint \frac{r\varepsilon\left(\frac{\partial f}{\partial r} dz - \frac{\partial f}{\partial z} dr\right)}{k_o^2 r^2 \mu\varepsilon - m^2} \\ L_g &= \oint \frac{r\mu\left(\frac{\partial g}{\partial r} dz - \frac{\partial g}{\partial z} dr\right)}{k_o^2 r^2 \mu\varepsilon - m^2} \end{aligned}\right\} \qquad (14)$$

[3] cf. Stratton, Electromagnetic Theory, p. 526, McGraw Hill, 1941.

$$\left.\begin{aligned} K_f &= \oint \frac{\left(\frac{\partial f}{\partial r}\,dr + \frac{\partial f}{\partial z}\,dz\right)}{k_o^2 r^2 \mu\varepsilon - m^2} \\ K_g &= \oint \frac{\left(\frac{\partial g}{\partial r}\,dr + \frac{\partial g}{\partial z}\,dz\right)}{k_o^2 r^2 \mu\varepsilon - m^2} \end{aligned}\right\} \tag{15}$$

After extensive algebraic manipulation one obtains

$$\begin{aligned} 36J_f = \sum_{\substack{N=n\\ \text{even}}} & f_N [\varepsilon_{n+1} A_{n+1} (3a_n^{o,n+1} + 2a_{n+1}^{o,n} + 2a_{n+1}^{o,n+2}) \\ & + \varepsilon_{n-1} A_{n-1} (3a_n^{o,n-1} + 2a_{n-1}^{o,n} + 2a_{n-1}^{o,n-2})] \\ & + f_o \sum_{n\ \text{odd}} \varepsilon_n A_n (3a_{n-1}^{o,n} + 2a_n^{o,n-1} + 6a_o^{n-1,n} \\ & + 3a_{n+1}^{o,n} + 2a_n^{o,n+1} + 6a_o^{n,n+1}) \end{aligned} \tag{16}$$

where J_g is obtained by replacing f by g and ε by μ. Here A_n, ε_n are the area and permittivity of triangle n in Figure 1, f_N is the value of f at the vertex N (Roman numerals), and f_o is the value of f at the "hub" of the hexagon. The parameters $a_i^{j,k}$ are defined as

$$\begin{aligned} a_i^{j,k} = a_i^{k,j} &= \frac{r_i}{(r_i - r_j)(r_i - r_k)} + \frac{r_j^2\, \sigma_{ij}}{(r_i - r_j)(r_k - r_j)} \\ &+ \frac{r_k^2\, \sigma_{ik}}{(r_i - r_k)(r_j - r_k)} \end{aligned} \tag{17}$$

with

$$\sigma_{ij} = \sigma_{ji} = \frac{1}{r_j - r_i} \ln \frac{r_j}{r_i} \tag{18}$$

In these expressions r_i is the value of the radial coordinate at the dodecagon vertex, i, as shown in Figure 1. Clearly all running indices are modulus 12, that is

$$\begin{aligned} r_{13} &\equiv r_1,\ r_{14} = r_2,\ \text{etc.} \\ r_{-1} &\equiv r_{11},\ r_{-2} = r_{10},\ \text{etc.} \end{aligned} \tag{19}$$

The quantities K_f and K_g are given by

$$\begin{aligned} 6K_f = \sum_{\substack{N=n\\ \text{even}}} & f_N (Q^{n-1,n} + 2Q^{n-2,n-1} - Q^{n,n+1} - 2Q^{n+1,n+2}) \\ & + f_o \sum_{n\ \text{odd}} (Q^{n,n+1} - Q^{n-1,n}) \end{aligned} \tag{20}$$

where

$$Q^{i,j} = Q^{j,i} = \frac{1}{2mk}\, \frac{1}{(r_j - r_i)}\, \ln \frac{|kr_j - m|\,(kr_i + m)}{|kr_i - m|\,(kr_j + m)} \tag{21}$$

with

$$k^2 = k_o^2 \mu\varepsilon. \tag{22}$$

Once again K_g is obtained from K_f by replacing f by g.

The quantities L_f and L_g are given by

$$\begin{aligned} 6L_f = \sum_{\substack{N=n\\ \text{even}}} & f_N [\varepsilon_{n+1} (-P^{n,n+1} (2\cot\theta_{n+1}^{+} + \cot\theta_{n+1}) \\ & + P^{n+1,n+2} (\cot\theta_{n+1} - \cot\theta_{n+1}^{+})) \\ & + \varepsilon_{n-1} (P^{n-2,n-1} (\cot\theta_{n-1} - \cot\theta_{n-1}^{-}) \\ & - P^{n-1,n} (2\cot\theta_{n-1}^{-} + \cot\theta_{n-1}))] \\ & + f_o \sum_{n\ \text{odd}} \varepsilon_n (P^{n-1,n} (\cot\theta_n^{-} + 2\cot\theta_n^{+}) \\ & + P^{n,n+1} (\cot\theta_n^{+} + 2\cot\theta_n^{-})) \end{aligned} \tag{23}$$

where θ_n, θ_n^{+}, θ_n^{-} are the three angles of triangle (n) as shown in Figure 1, and where

$$P^{i,j} = P^{j,i} = \frac{1}{2k^2}\, \frac{1}{(r_j - r_i)}\, \ln \left| \frac{k^2 r_j^2 - m^2}{k^2 r_i^2 - m^2} \right| \tag{24}$$

Once again, L_g is obtained from L_f by replacing f by g and ε by μ.

Equations (10) and (11), supplemented by the expressions for J, K, L in Equations (16), (20) and (23), are then the coupled difference equations for f and g at the mesh points.

C. Boundary Conditions

The boundary conditions on a metallic (electric) surface are clearly that both tangential components of $\vec{E}$ must vanish. This clearly implies

$$f = 0 \quad , \text{"electric" boundary} \tag{25}$$

$$E_z dz + E_r dr = 0 \quad , \text{"electric" boundary} \tag{26}$$

where dz and dr are taken along the boundary. From Equation (6) one can immediately deduce that Equation (26) is equivalent to

$$\frac{\partial g}{\partial n} = 0 \quad , \text{"electric" boundary} \tag{27}$$

where the derivative is in a direction normal to the boundary in the r,z plane.

Equation (25) can be directly applied as a boundary condition for each mesh point along the boundary. However, as an alternate the Equation

(27), we shall use Equation (9) or (11) over that portion of the boundary dodecagon which lies within the active region. Operational this corresponds to setting $\varepsilon = 0$ and $f = 0$ in triangles outside the active region.

For "magnetic" boundaries, the corresponding boundary equations are obtained by interchanging ε, f and μ,g.

Both f and g are set equal to zero at the mesh points along the axis of rotation ($r = 0$).

D. Driving Point and Root Finder

As in all eigenvalue problems the solution of the homogeneous difference equations corresponding to Equations (10) and (11) requires obtaining the correct frequency. We shall proceed as in SUPERFISH to assume that either Equation (10) or (11) is driven by an external current element at one mesh point, and then search for the value of the frequency at which the left side of the corresponding difference equation at that point vanishes. In ULTRAFISH it is essential that we allow for such a driving point in either Equation (10) or (11). In this way we will be able to include modes which have either E_ϕ or H_ϕ identically zero through the cavity for some special geometries.

The root finder has also been taken from the successful experience in SUPERFISH. Specifically, we define

$$D(k_o^2) = -\frac{k_o g_o\, I_d\, \mu_d}{\iint \frac{drdz}{r}\, \mu[g^2+r^2H_z^2+r^2H_r^2]} \tag{28}$$

where I_d is the equivalent driving current at mesh point d, given by

$$I_d = -mK_g + k_o(L_f - J_f) \quad \text{(at mesh point d)} \tag{29}$$

It can be shown, using the method of SUPERFISH, that

$$\frac{d}{dk^2} D(k^2) = -1 \quad \text{at resonance.} \tag{30}$$

so that a rapidly convergent search method can be used to find the eigenfrequency.

Once again, it is necessary to use the expression corresponding to Equation (30) with g replaced by f, and μ by ε in order to handle special modes for which g may be identically zero.

E. Matrix Inversion

The matrix inversion process is similar to that used in SUPERFISH, except that the blocks now have twice as many columns and twice as many rows. And the initial matrix is still mostly sparse with the non-vanishing elements concentrated around the diagonals. Because of the increased matrix size the inversion time for a given mesh size is approximately 8 times that for SUPERFISH.

F. Spurious Singularly at $r = \hat{r}$

As mentioned in Section IVA, there is a spurious singularity in the expressions for E_z, E_r, H_z, H_r at $r = \hat{r}$. This makes its appearance in K_f, K_g, L_f, L_g where $Q^{i,j}$ and $P^{i,j}$ become singular in Equations (21) and (24) whenever

$$r_i = \frac{m}{k} \equiv \hat{r} \quad .$$

For this reason, the dodecagon vertices must avoid direct cancellation of r_i and $\hat{r}$, which may be difficult to guarantee as k changes in the eigenvalue search. We are presently exploring the best way of selecting the mesh points near $\hat{r}$ in order to minimize the effect of this singular behavior.

The spurious singularity also enters into the calculation of H_z, H_r in the normalization integral in the denominator of $D(\kappa^2)$ in Equation (28). Smoothing techniques are required in order to avoid the singular behavior at $r = \hat{r}$.

V. Test Cases

The program ULTRAFISH has been run on a cylindrical cavity in order to locate several of the TE and TM modes. We have chosen a cavity of radius 10cm and length 2.5πcm = 7.85398cm and have used a triangular lattice with approximately 600 mesh points. We have located the following modes

Mode	ULTRAFISH Freq.	Analytic Freq.	$\hat{r}/a$
TE_{111}	2102.1 MHz	2101.0 MHz	.23
TE_{211}	2409.1 MHz	2401.3 MHz	.20
TM_{122}	5105.9 MHz	5076.9 MHz	.19
TM_{010}	1147.49 MHz	1147.43 MHz	-

Plots of constant $f = rE_\phi$ and $g = rH_\phi$ are shown for the TE_{111}, TE_{211}, TM_{121} modes in Figures 2a, 2b, 2c respectively. These plots show no visible discontinuity near the spurious singularity at

$$\frac{\hat{r}}{a} = \frac{m}{ka} = \frac{mc}{2\pi fa} \; .$$

It should be noted that the program also works for the azimuthally symmetric modes such as TM_{010}. For comparison, SUPERFISH predicts a resonant frequency 1147.41 MHz.

The program has also been tested on a spherical cavity with about 500 mesh points in order to find the mode designated as TE_{111} (no radical electric field). In this case the frequency found by ULTRAFISH for a radius of 10cm is 2141.8 MHz while the correct frequency is 2144.0 MHz. The plots of f = const and g = const are shown in Figure 3 and have the expected behavior. Further tests are being pursued in order to determine the accuracy of the frequency and field determinations as a function of mesh size.

VI. Possible Program Improvements

Many persons have suggested possible improvements in the SUPERFISH and ULTRAFISH programs. Clearly, one can improve frequency and field accuracy by using more mesh points, but this can lead to unreasonable storage and time requirements for the computation. Recent interest in Finite Element Methods[4] also suggests using quadratic behavior in the triangular panels as a means of improving accuracy.[5] This of course leads to more complicated difference equations for the field values, but may be the most practical way to achieve greater accuracy.

Other possible improvements might be obtained by the following:

1) Modify the analysis and procedure in such a way that the spurious singularities are removed analytically. (Note: One can have several values of $\hat{r}$ if one has regions of different ε and μ.)

2) Use as the functions $r^m f$ and $r^m g$ for $m \geq 1$ in order to obtain greater accuracy for modes with high m.

3) Use r^2 and z as the variables in a radial plane. This simplifies some of the integrals in the coefficients J, K, L, and approximates more accurately the field dependence near r=0.

4) Multiply Equations (2) and (3) by a suitably selected weighting function before integration over the dodecagon. This technique is one of the options discussed in the Finite Element Method and may lead to more accurate fields and frequencies.

5) Use a variational formulation for the eigen-frequency and smooth the linear panel behavior <u>after</u> the matrix inversion but <u>before</u> the calculation of the eigen-frequency. This should lead to more accurate frequency determinations.

There are many other possibilities which have been raised and which also deserve further consideration.

VII. Conclusion

We have developed the program ULTRAFISH to calculate azimuthally asymmetric modes in an electromagnetic cavity which is a figure of revolution about a longitudinal axis. This represents a generalization of the program SUPERFISH for azimuthally symmetric modes, and requires determining the values of two field components (rE_ϕ and rH_ϕ) at mesh points from coupled difference equations and boundary conditions. The program has been successfully tested for various TE and TM modes in cylindrical and spherical cavities.

[4]See, for example, G. Strang and G.J. Fix, Analysis of the Finite Element Method, Prentice-Hall Series in Automatic Computation, 1973.
[5]See also S. Okumura, A Program Development of SUPERFISH, 1981, Linac Conference, Santa Fe, NM, Paper E19.

The program also permits including regions of different μ and ε. In addition, the program can be used for m=0, to solve the 2-D problem with an arbitrarily shaped boundary.

VIII. Acknowledgment

We would like to express our appreciation to Robert A. Jameson for encouragement, moral support, and patience.

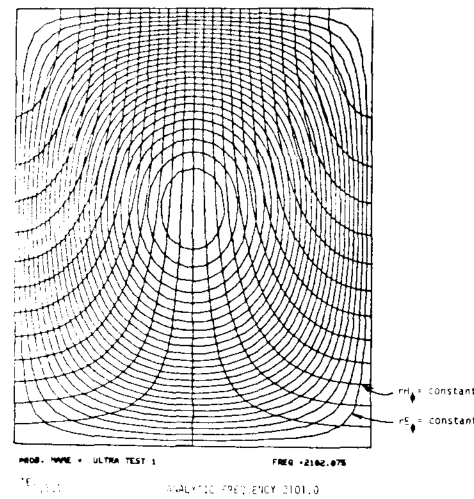

Fig. 2a Lines of constant f and g for a TE_{111} mode in a cylindrical cavity.

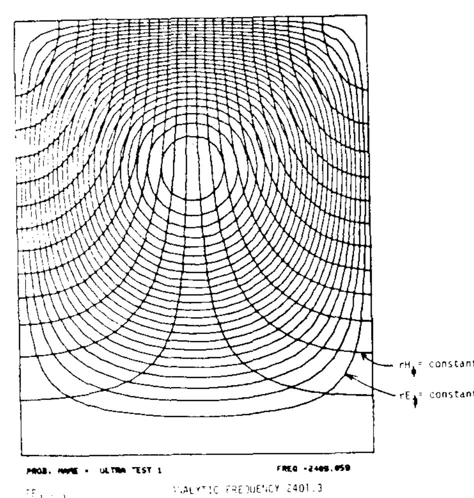

Fig. 2b Lines of constant f and g for a TE_{211} mode in a cylindrical cavity.

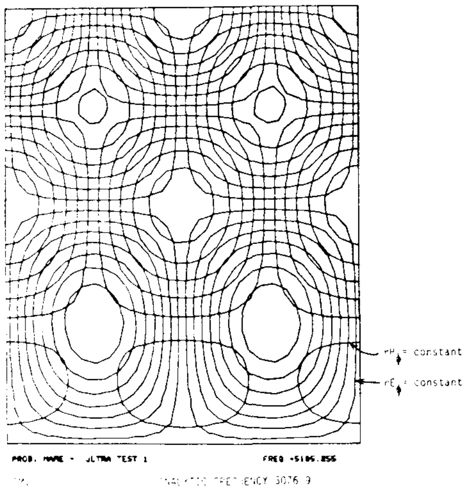

Fig. 2c Lines of constant f and g for a TM_{122} mode in a cylindrical cavity.

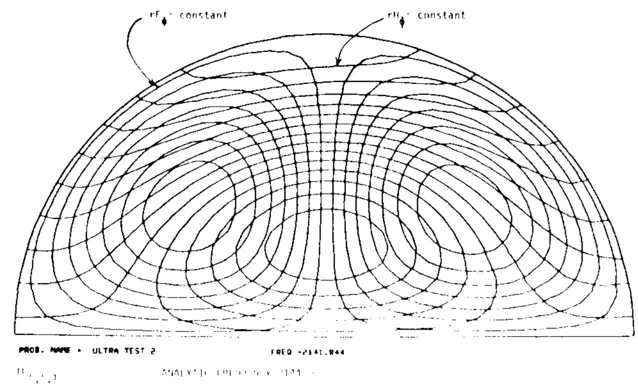

Fig. 3 Lines of constant f and g for a TE_{111} mode in a spherical cavity.

Discussion

The asymmetries seen in the present spherical test case will be studied further, for example by considering adaptive meshing. We could force symmetry by computing only a quarter of the sphere. Also, a production calculation would use many more mesh points than we used in the test case.

QUESTION: How were these calculations done in the good old days?

ANSWER: (Gluckstern): Well, if Lloyd Smith were here, he could probably comment more. I think actually he did most of those calculations in the MTA himself and I think he did most of them with a hand calculator; I'm not even sure it was electric. But it was a solution of the Bessel functions given boundary conditions and there were approximations made, but the big difference was that the people who were doing the calculating worked very closely with a whole host of people who were not programmers, but were modelers and who built copper models of the half cells that were calculated. They put in conductors in the places where there would be perturbations due to loops or to stems, or what have you, and made measurements and then corrected the calculations by an iterative process until there was a series of cells calculated for a linac and verified by a model. Then, they went ahead and built it.

(Livdahl): I can add a little bit to that. The method that was used for the first analytic calculations that I'm familiar with was developed by Walkinshaw and a number of others at Harwell. It corresponded to assuming a drift-tube geometry that was cylindrical, then matching the fields at the outer radius of the drift tube. In the gap, the first assumption was that you had a TM_{010} mode and in the outer region you also allowed for a sum of terms with different Z dependence. You matched the electric field at this boundary; that allowed you to express each of the terms in the outer region's sum in terms of a single parameter that is the electric field magnitude on the axis in the gap. Then you calculated the magnetic field and equated the average magnetic field in the gap at the boundary and that gave a single transcendental equation for the frequency that you could solve by hand computation. Christofolous also contributed to the progress in that field by starting to press for drift tubes of stranger shapes than just the usual with the rounded corners, because he was able to demonstrate that those would have a higher shunt impedance, and would be more efficient. I think that gave the impetus to the next generation of computer programs, which were the MESSYMESH iterative procedures that were developed at MURA, and the LALA iterative programs that were developed at Los Alamos.